

259th ACS National Meeting Philadelphia, PA March 22-26, 2020

Division of Environmental Chemistry Non-Technical Events, Technical Program, and Abstracts

ENVR Non-Technical Sponsored Events

Workshop: Getting A Sense Of Sensors

Location: Cannes, Hotel Sofitel Philadelphia **Date & Time:** Sunday, Mar 22, 1:00-4:00 PM This workshop aims to bring together researchers for a forum and information exchange on sensors in the water research community.

Industry Advisory Board Meeting

Location: Lyon, Hotel Sofitel Philadelphia Date & Time: Sunday, Mar 22, 1:00 PM

Program Planning Meeting

Location: Lyon, Hotel Sofitel Philadelphia **Date & Time:** Sunday, Mar 22, 2:00 PM

Long Range Planning Meeting

Location: Lyon, Hotel Sofitel Philadelphia Date & Time: Sunday, Mar 22, 3:00 PM

Executive Committee Meeting

Location: Nice, Hotel Sofitel Philadelphia Date & Time: Sunday, Mar 22, 7:00 PM

Division Reception -- Ticket required

Location: Ladder 15, 1528 Sansom St., Philadelphia **Date & Time:** Tuesday, Mar 24, 7:00 PM

WORKSHOP EXCHANGE:GETTING A SENSE OF SENSORS

JOIN US ON SUNDAY MARCH 22ND FOR A WORKSHOP EXCHANGE WITH THE SENSORS COMMUNITY!

SPONSORED BY ACS ENVR

For more information, please contact: rese David McCarthy: david.mccarthy@monash.edu Alandra Kahl: afk12@psu.edu Nathaniel Warner: nrw6@psu.edu

In this workshop exchange we aim to bring people together for a forum and information exchange on sensors in the water research community. Whether Arduino or Pi, stop by our session for conversations about successes, failures and everything in between. All users are welcome, from novice researchers to experienced hackers.



1:00 PM - 4:00 PM Sofitel Philadelphia at Rittenhouse Square: Cannes Division of Environmental Chemistry 259th ACS National Meeting Philadelphia, PA March 22-26, 2020

Technical Program

ENVR

DIVISION OF ENVIRONMENTAL CHEMISTRY

S. Obare, Program Chair

SUNDAY MORNING

Section A

Sofitel Philadelphia at Rittenhouse Square Strasbourg

Applications of Artificial Intelligence, Machine Learning & Data Analytics in Environmental Science & Engineering

Z. Cheng, Q. Li, X. Ma, Q. Ying, *Organizers* A. Z. Gu, H. Zhang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 1. BioManufacturing with Intelligent Adaptive Control (BioManIAC). **B.L. Marrone**, C. Iverson, G. Pilania

8:30 2. Machine learning kernel divergence-based *de novo* sampling size optimization for environmental applications: Cases study of single-cell Raman spectroscopic phenotyping of EBPR microbial communities. G. Li, C. Wu, D. Wang, D. Kaeli, J. Dy, **A.Z. Gu**

8:55 3. Identification of discriminatory ARGs and socio-economic factors in shaping resistome risk using machine learning algorithms. **S. Gupta**, G. Arango-Argoty, L. Zhang, A. Pruden, P.J. Vikesland

9:15 4. *In vitro* toxicogenomics-derived biodescriptors in *in silico* QSAR improve the phenotypic toxicity prediction accuracy. **S.M. Rahman**, J. Lan, N. Gou, A.Z. Gu

9:35 5. Endotoxin detection using liquid crystal droplets and machine learning. **S. Jiang**, J. Noh, A. Smith, N.L. Abbott, V. Zavala

9:55 Intermission.

10:10 6. Applications of artificial intelligence, machine learning, and data analytics in environmental science and engineering: Current status and future directions. **H. Zhang**

10:35 7. Structural features of ER α - and AR-mediated endocrine disrupting chemicals. **H. Tan**, X. Wang, W. Shi, Q. Chen, H. Yu

10:55 8. Deep neural network combined with molecular fingerprints (DNN-MF) to develop predictive models for hydroxyl radical rate constants of water contaminants. **S. Zhong**, J. Hu, X. Yu, H. Zhang

11:15 9. Machine learning approach for predicting defluorination of per- and polyfluoroalkyl Substances (PFAS) for their efficient treatment and removal. **B.M. Wong**, A. Raza, S. Bardhan, L. Xu, S.S. Yamijala, C. Lian, H. Kwon

11:35 10. Machine learning methods for the prediction of spectra and identification of opioids and their derivatives. C. Wang, D. Mashanova, A. Terracciano, A. Masunov, M. Xu, S. Vasu

11:55 Concluding Remarks.

Section B

Sofitel Philadelphia at Rittenhouse Square Nice

Advanced & Additive Manufacturing Materials & Technologies for Environmental Applications

N. Aich, W. Phillip, S. Rahaman, Organizers, Presiding

8:00 11. Comparison of two low-hazard organic solvents as individual and co-solvents for the fabrication of polysulfone membranes. X. Dong, T. Harris, **I.C. Escobar**

8:25 12. Engineering selective desalination membrane materials via polymer backbone rigidity and functional group position. H. Luo, K. Chang, K. Bahati, **G.M. Geise**

8:45 13. Facile grafting of Zwitterions onto the surface of ultrafiltration membranes to improve antifouling properties. **H. Lin**, N. Shahkaramipour

9:05 14. Trade-off in membrane distillation with monolithic omniphobic membranes. W. Wang, X. Du, H. Vahabi, S. Zhao, Y. Yin, A.K. Kota, **T. Tong**

9:25 15. Nutrient recovery from synthetic livestock wastewater effluent using electroactive membranes. **K.M. Kekre**, A. Ronen

9:45 Intermission.

9:55 16. Accelerating materials development via statistical learning methods for environmental engineering. **P. Nalam**

10:20 17. Dual-functional block copolymer brushes grafted reverse osmosis membranes with improved antifouling performance. **L. Yang**, W. Ma, T. Chen, Z. Ye, S. Rahaman

10:40 18. Permeate side-heated integrated solar thermal membrane distillation system. P. Yi, R. Tanvir

11:00 19. Biocatalytic membranes with self-contained radical polymer mediator for removal of persistent organic pollutants. F. Gao, J. Hodul, **Y. Wu**, B.W. Boudouris, W.A. Phillip, N. Wei

11:20 20. High-salinity membrane distillation: Impact of material properties on membrane performance. **A. McGaughey**, P. Karandikar, S.M. Iskander, A. Smith, M. Gupta, A. Childress

11:40 21. Performance enhancement and scaling mitigation of radio frequency induction heated membranes in vacuum membrane distillation. **A. Anvari**, A. Ronen

Section C

Sofitel Philadelphia at Rittenhouse Square Versailles

Biogeochemical Transformation in Underground Environments: Natural Processes & Engineered Implementations for Contaminant Abatement

Cosponsored by CEI and GEOC J. Ferry, K. Millerick, *Organizers* M. G. Siebecker, W. Yan, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 22. Reactive mineral phases from *in situ* biogeochemical processes: Key to abiotic natural attenuation? **P.G. Tratnyek**, K. Inoue, A. Pavitt, R.L. Johnson

8:35 23. Biodegradation of aniline and *p*-chloroaniline under different redox conditions at a contaminated chemical manufacturing site. **H.S. Almnehlawi**, J. Dallmeyer, J. Zhang, R.K. Dean, K.P. Dillon, F. Burns, L. Axe, D.E. Fennell

8:55 24. Contributions of iron and biological sulfate reduction to abiotic transformation of organic groundwater contaminants. **E. Berns**, R.A. Sanford, C. Schaefer, T.J. Strathmann, A.J. Valocchi, C.J. Werth

9:15 25. Quantifying 2,4-dinitroanisole transformation using compound specific isotope analysis after *in situ* chemical reduction of iron oxides. **M.J. Berens**, J. Bolotin, T.B. Hofstetter, W. Arnold

9:35 26. Reductive transformation of 3-nitro-1,2,4-triazol-5-one (NTO) by the hematite/Fe²⁺ redox couple and an iron-rich soil. **P. Cardenas**, K. Anderson, D.M. Ditoro, H.E. Allen, R.F. Carbonaro, P. Chiu

9:55 Intermission.

10:10 27. Anaerobic dechlorination of chlorinated dibenzo-*p*-dioxins in sediment cultures and clues from genetic sequencing. **R. Dean**, C.R. Schneider, H.S. Almnehlawi, **D.E. Fennell**

10:30 28. Withdrawn.

10:50 29. Withdrawn.

11:10 30. Removal of 1,4-dioxane during on-site wastewater treatment using nitrogen removing biofilters. **A. Venkatesan**, C. Lee, C. Asato, C. Gobler

11:30 31. Application of compound-specific isotope analysis combined with molecular modeling to evaluate abiotic and biotic degradation of DNAN and NTO. **C. Wang**, L. Heraty, A. Wallace, M. Fuller, P. Hatzinger, N.C. Sturchio

11:50 Closing Remarks.

Section D

Sofitel Philadelphia at Rittenhouse Square Montpellier

Applications & Implications of Nanomaterials in the Environment / Nanocomposite

S. Chakraborty, S. Kang, T. Phenrat, J. Stubbs, *Organizers* S. R. Kanel, M. Nadagouda, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 32. Environmental applications and risk assessment of cerium oxide nanoparticles. E. Andreescu

8:25 33. Sulfidized nanoscale zerovalent iron: Effect of sulfur content and speciation on reactivity, selectivity, and its ability to defluorinate organic groundwater contaminants. G. Lowry, **J. Xu**, A. Avellan, R. Kaegi

8:50 34. Parameterization and prediction of radius of influence of nanoscale zerovalent iron in field-scale subsurface application: Re-analyses using artificial neural network and regression. **T. Phenrat**, P. Babakhani

9:15 35. Controlling the self-assembly of supramolecular nanocontainers in solution: Green chemistry approach. **H. Kumari**

9:35 36. New approaches nanocomposites' imaging to facilitate development of safer and more robust consumer products. **A. Orlov**, Y. Zhao, K. Chen-Wiegart

10:00 Intermission.

10:15 37. Characterizing nanoparticle–protein coronas: Using analytical methods to detect and identify proteins adsorbed onto gold particle surfaces. C. Sayes, L. Steele, M. George

10:35 38. Withdrawn.

10:55 39. Do graphene oxide nanostructured coatings mitigate bacterial adhesion? S. Romero-Vargas Castrillon

11:15 40. Impact of Mn_2O_3 nanoparticles on nitrification under low and high dissolved oxygen conditions. **V. Kapoor**, D. Phan

11:35 41. Size dynamics control nanoparticle fate and transport in the environment: Toward an accurate and efficient model. **P. Babakhani**, T. Phenrat

11:55 Closing Remarks.

Section E

Sofitel Philadelphia at Rittenhouse Square Paris Ballroom

Impact of Engineered & Natural Nanomaterials on the Environment: A symposium in Honor of Dr. Michael F. Hochella / Properties of Nanomaterials

Cosponsored by GEOC D. D. Dionysiou, V. K. Sharma, Q. Wan, *Organizers* P. J. Vikesland, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 42. Biomineralization by attachment of nanoparticles during the last 550 million years. **P. Gilbert**, S. Porter, C. Sun, S. Xiao, B. Gibson, N. Shenkar, A. Knoll

8:30 43. Nucleation of mixed-cation amorphous carbonate precursors: Example of cadmium incorporation into calcite. **S.T. Mergelsberg**, T. Graham, S.L. Riechers, S.N. Kerisit

8:55 44. Facet-dependent aggregation of hematite nanoparticles. **X. Zhang**, Y. Wang, J. Zhou, M. Zong, Z. Wang, J.D. Yoreo, K. Rosso

9:20 45. *In situ* liquid cell transmission electron microscopy investigation on aggregation and dissolution of iron oxide nanoparticles. **J. Liu**

9:45 Intermission.

9:55 46. Coupling theory, spectroscopy, and electron microscopy to determine the bonding environments of metal impurities in Fe(III)-(oxyhydr)oxides. **E.S. Ilton**, E.J. Bylaska, S.N. Kerisit, S.T. Mergelsberg

10:20 47. Impact of water chemistry on metal adsorption to surface-functionalized iron oxide nanoparticles. **D. Giammar**, N. Sharma, A. Ghosh, Z. Pan, J. Fortner

10:45 48. Withdrawn.

11:10 49. Tailoring the (bio)activity of iron (hydr)oxide nanoparticles in abiotic and biotic environment. I. Chernyshova, S. Ponnurangam

11:35 50. Spectroscopy and redox reactions: Lessons learned from Mn and U nanomaterials. J.M. Cerrato

Sofitel Philadelphia at Rittenhouse Square Marseilles

Macromolecule Biosynthesis, Biodegradation, & Applications in Environmental Bioprocesses

S. Yi, Organizer X. Mao, Y. Men, C. M. Sales, W. Zhuang, Organizers, Presiding

8:15 Introductory Remarks.

8:20 51. Optimizing the methanotrophic production and types of polyhydroxyalkanoates (PHAs) by utilizing organic waste-derived methane and volatile fatty acids. K. Cheng, J. Myung, **W. Sun**

8:40 52. Robust soluble di-iron monooxygenases to tackle the commingled solvent-stabilizer contamination. F. Li, D. Deng, D.N. Pham, C. Wu, J.M. Antunes, **M. Li**

9:00 53. Identification of microorganisms responsible for reductive defluorination of PFASs in an enrichment culture. **Y. Yu**, K. Zhang, J. Liu, Y. Men

9:20 54. Biotransformation of sulfonamide antibiotics: Blind spots and emerging opportunities. **B. Li**, Y. Deng, L. Cao, T. Zhang

9:50 Intermission.

10:05 55. Improving wastewater treatment using free nitrous acid (FNA). S. Hu

10:35 56. Biological nitrogen removal through nitrite shunt and hydrogenotrophic denitrification in saline wastewaters. **Y. De Costa**, W. Zhuang

10:55 57. Global wastewater microbiome: Taxonomic and functional diversity. L. Wu, B. Zhang, D. Ning, Y. Yang, Q. He, T. Curtis, X. Wen, J. Zhou

11:15 58. Biorefineries using synthetic microbial consortia. Y. Men, S. Che

11:35 59. Metagenomics study of soil microcosms to evaluate the bioremediation of textile dyes in a contaminated ecosystem. **S. Patil**, M. Kurade, S.P. Govindwar, B.H. Jeon

11:55 Closing Remarks.

Sofitel Philadelphia at Rittenhouse Square Toulouse

Transformation of Organic Pollutants in Aquatic Systems: A Celebration of the Career of A. Lynn Roberts

Cosponsored by WCC W. Arnold, D. M. Cwiertny, M. L. Hladik, T. Kohn, *Organizers* Y. Chin, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 60. Choosing well among research topics, potential students, and collaborative opportunities. **J. Hering**

8:25 61. Kinetic isotope effects in the halogenation of dimethenamid. M. Rose, K. Reber

8:45 62. Influence of overlooked chlorinating agents on the halogenation kinetics of cyclic alkenes. **S. Lau**, K. Reber, A. Roberts

9:05 63. Esoteric electrophiles in chlorinated waters: When conventional kinetic models fall short. **J.D.** Sivey

9:25 64. Leachability, photodegradation, and potential ecotoxic impact of trifluralin-impregnated mulch. **K.J. Bisceglia**, M. Dharia, M. Kaur, F. Pavlovici

9:45 Intermission.

10:00 65. From solvents to steroids: Importance of accounting for chemical transformation pathways in achieving safe and sustainable water supplies. **D.M. Cwiertny**

10:20 66. Understanding and monitoring the decay of waterborne viruses during ozonation. C. Wolf, J. Torrey, U. Von Gunten, **T. Kohn**

10:40 67. Magnetite: Formation and reactivity. P.J. Vikesland

11:00 68. Building a more comprehensive understanding of offsite agrochemical runoff through the expansion of target analytes. **M.L. Hladik**, M. Gross, E. Woodward

11:20 69. Isomer specific reduction of hexabromocyclododecane by Fe(II) in iron oxide suspensions. U. Jans, X. Zhang, K. Roopnarine, E.G. Hohenstein

11:40 70. Abiotic reduction of RDX and NTO: Still investigating electron transfer, kinetics, and reaction pathways. Y. Tong, M.J. Berens, B. Ulrich, T.B. Hofstetter, **W. Arnold**

Frontiers in Environmental Chemistry

Sponsored by SOCED, Cosponsored by ENVR

Reactions on Surfaces in Liquid Media

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Multifunctional Surfaces for Cooperativity in Catalysis

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Activation of light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

SUNDAY AFTERNOON

Section A

Sofitel Philadelphia at Rittenhouse Square Strasbourg

Applications of Artificial Intelligence, Machine Learning & Data Analytics in Environmental Science & Engineering

Z. Cheng, A. Z. Gu, Q. Ying, Organizers Q. Li, X. Ma, H. Zhang, Organizers, Presiding

1:00 Introductory Remarks.

1:05 71. RAPID data-driven automated discovery of new organohalide perovskites. J. Schrier

1:30 72. Identifying the governing factors for plant uptake of engineered nanoparticles through machine learning. **X. Ma**, Z. Chen

1:55 73. Examining plant uptake and translocation of emerging contaminants using intelligent techniques. **M. Bagheri**, K. Al-Jabery, D. Wunsch, X. He, H. Shi, J.G. Burken

2:15 74. Predicting adsorption of organic contaminants on biochar, CNTs, GAC, and resins by artificial neural networks. **K. Zhang**, H. Zhang

2:35 75. Estimation of iron and manganese concentration in ground water using absorbance in UV-Vis spectrophotometer via artificial neural network. **J. Tasnim**, U.F. Piu, Z. Kaium, S.M. Rahman, D.A. Badruzzaman

2:55 Intermission.

3:10 76. Robots and AI for rapidly characterizing and remediating contaminated soils. **G. Lowry**, S. Wang, S. Hordern, C. Pavlov, J. Norby, A. Johnson

3:35 77. Topic modeling using natural language processing on facility source reduction comments submitted to the Toxics Release Inventory. **X. Xi**, L. Grogan-McCulloch, A.E. Tome

3:55 78. Data-driven innovations in water resource recovery facilities: Emerging era of sustainability intelligence. **X. Wang**

4:15 79. Novel physics-informed data-driven modeling to predict physiochemical state of water/wastewater system. **T. Wang**, C. Wang, Z. Xu, S. Matthew, B. Li

4:35 80. Quantification of uncertainty in drinking water lead levels for Southwest Pennsylvania. **S. Schwetschenau**, M.J. Small, J.M. Vanbriesen

4:55 Concluding Remarks.

Sofitel Philadelphia at Rittenhouse Square Nice

Advanced & Additive Manufacturing Materials & Technologies for Environmental Applications

N. Aich, W. Phillip, S. Rahaman, Organizers, Presiding

1:00 81. Toward single atom catalysis for environmental application. J. Kim

1:25 82. Advanced manufacturing of scalable easy-to-use sensors for field monitoring of water contamination. A. Finny, K. Kirk, F. Mustafa, **E. Andreescu**

1:45 83. Overcoming technical challenges in the synthesis and application of nanoscale adsorbents. **R. Tehrani**, K. Atmatzidis, F. Alimohammadi, A. Upadhyay, D.R. Strongin

2:05 84. Design of a 3D printed and energy efficient photostation to improve photocatalytic activity of carbon nitride composites. **D. Saha**, M. Desipio, T.J. Hoinkis

2:25 85. 3D printed structures for controlled analyte adsorption and desorption. M.R. Hartings

2:45 86. Methods of processing of thermoplastics and lignocellulosic biomass for 3D printing. **S. Bhagia**, A.J. Ragauskas

3:05 Intermission.

3:15 87. Environmental sustainability in advanced material manufacturing. D.L. Plata

3:40 88. VOC emissions influenced by polymer additives in 3D printing. **P. Potter**, S.R. Al-Abed, F. Hasan, S.M. Lomnicki

4:00 89. Taking it outside: Benefits and risks of additive manufacturing for environmental monitoring and remediation technologies. **A. Kennedy**, M. Ballentine, E. Alberts, M. Bortner

4:20 90. Potential health impacts of particle and volatile organic compound emissions from consumer level 3D printers. **Q. Zhang**, A. Davis, M. Black, R. Weber

4:40 91. Consideration of 3D-printed biofilm carriers for wastewater treatment. **B.G. Ovelheiro**, C. Butler, S. Gerasimidis

Sofitel Philadelphia at Rittenhouse Square Versailles

Biogeochemical Transformation in Underground Environments: Natural Processes & Engineered Implementations for Contaminant Abatement

Cosponsored by CEI and GEOC M. G. Siebecker, W. Yan, Organizers J. Ferry, K. Millerick, Organizers, Presiding

1:00 Introductory Remarks.

1:05 92. Quantifying and visualizing the spatial distribution of black carbon's electron storage capacity. D. Xin, **P. Chiu**

1:55 93. Impact of cobalt on mercury methylation in East Fork Poplar Creek, Oak Ridge, Tennessee. **E.D. Flynn**, G.E. Schwartz, S. Brooks, D. Giammar, J.G. Catalano

2:15 94. Redox properties of particulate organic matter from northern peatlands. **P. Joshi**, M.H. Schroth, M. Sander

2:35 95. Isotopic analysis of radionuclide association with aquifer solids in the Midwestern Cambrian-Ordovician aquifer system. **M. Mathews**, M. Gotkowitz, S. Scott, M.A. Ginder-Vogel

2:55 Intermission.

3:10 96. Arsenite complexation by dissolved organic matter and implications for uptake by microorganisms. L. Abu-Ali, H. Yoon, X. Zhang, **M.C. Reid**

3:30 97. Exploring factors governing metal uptake by wetland soils. **N. Sharma**, J. Yan, E.D. Flynn, J.G. Catalano, D. Giammar

3:50 98. Biotransformation of neonicotinoid insecticides and their metabolites on biologically activated carbon: Implications for human exposure, treatment, and biofilm transformation. **D. Webb**, G.H. LeFevre

4:10 99. Reductive transformation of 3-nitro-1,2,4-triazole-5-one (NTO) by black carbon. D. Xin, P. Chiu

4:30 Closing Remarks.

Sofitel Philadelphia at Rittenhouse Square Montpellier

Applications & Implications of Nanomaterials in the Environment / Nanocomposite/Membrane & Water Treatment

S. Chakraborty, T. Phenrat, J. Stubbs, *Organizers* S. R. Kanel, S. Kang, M. Nadagouda, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 100. Migration of quaternary ammonium cations from exfoliated clay/low density polyethylene nanocomposites into food simulants. J.E. Jablonski, L. Yu, S. Malik, A. Sharma, A. Bajaj, S. Lakshmi Balasubramaniam, R. Bleher, R.G. Weiner, **T.V. Duncan**

1:25 101. Application-focused study of metal hexacyanoferrates for the recycling of ammonium in various wastewaters. **D. Parajuli**, N. Zhang, H. Tanaka, A. Takahashi, T. Kawamoto

1:45 102. Nanoscale zerovalent iron particles for restoration of cadmium-contaminated paddy soil: Comparative evaluation of soil amendment vs. *in situ* magnet-assisted soil washing. **T. Phenrat**

2:05 103. Phosphate removal from synthetic urine matrices using nanoscale magnetite. **A. Rahman**, P.J. Vikesland

2:25 104. Stability of graphene oxide in water: Exploring the critical role of organic surface coatings. **C. Kim**, j. lee, J. Fortner

2:45 Intermission.

3:00 105. Withdrawn.

3:20 106. Improving the selective removal of a target organic compound from water using 3-D carbon nanomaterial aerogels. **R.E. Rogers**

3:45 107. Benign, renewable betaine-modified biochar-based nanocomposite containing zinc oxide for removal of phosphate from contaminated water. **A. Nakarmi**, S.E. Bourdo, S.R. Kanel, T. Viswanathan

4:05 108. Carbon nanotube immobilized membrane for ammonia separation via membrane distillation. **W. Intrchom**, S. Roy, S. Mitra

4:25 109. Ion-gated carbon molecular sieve membranes for enhanced gas separation that surpass the Robeson limit. **W. Guo**, S. Dai, S.M. Mahurin

4:45 Closing Remarks.

Sofitel Philadelphia at Rittenhouse Square Paris Ballroom

Impact of Engineered & Natural Nanomaterials on the Environment: A symposium in Honor of Dr. Michael F. Hochella

Properties of Nanomaterials

Cosponsored by GEOC D. D. Dionysiou, V. K. Sharma, P. J. Vikesland, Organizers Q. Wan, Organizer, Presiding

1:00 110. Macroscopic and spectroscopic characterization of the mechanisms of Ni(II) and Zn(II) sorption by green rust. **E. Elzinga**

1:25 111. Facet-selective adsorption of Fe(II) on hematite visualized by nanoscale secondary ion mass spectrometry. S. Taylor, L. Kovarik, J. Cliff, **K. Rosso**

1:50 112. Solution chemical and hydrodynamic factors control the formation of synthetic schwertmannite. **F. Michel**, H. King, M.F. Hochella

2:15 113. Mn(II)-promoted phase transformation of manganese oxides. M. Zhu, P. Yang

2:40 114. Transformation of metal and metal oxide nanoparticles via sulfidation. N. Kumar, V. Noel, J. Lezama Pacheco, C. Levard, M.F. Hochella, G.V. Lowry, **G.E. Brown**

3:05 Intermission.

3:20 115. Rate-limiting step of dissimilatory microbial iron oxide nanoparticle reduction. E.E. Roden

3:45 116. Growth of neutrophilic photosynthesis bacteria using metal sulfide nanoparticles as sole electron donors. **J. Xu**, H. Alarcon

4:10 117. Withdrawn.

4:35 118. Flatland in the energy landscape: Experimental theoretical condensed matter geochemistry of silica. **B. De Jong**, M. Ding

Section F

Sofitel Philadelphia at Rittenhouse Square Marseilles

Green Chemistry & the Environment

Cosponsored by CEI R. Luque, S. O. Obare, *Organizers, Presiding* 1:00 Introductory Remarks.

1:05 119. Green chemistry of nutrient recovery: From mechanochemistry to reduced nitrogen loss. M. Silva, **J. Baltrusaitis**

1:25 120. Green solvent for nano-enabled water treatment. N. Aich, N. Mehrabi

1:45 121. Benign-by-design nanomaterials for continuous flow tandem nanocatalysis. R. Luque

2:05 122. Synthesis of novel nanobiocomposite from kenaf fiber for heavy metal remediation and antibacterial activity. **S. Mandal**, S.B. Marpu, S.Q. Shi

2:25 123. Supercritical CO₂-induced alteration of polymer-metal matrix and selective extraction of valuable metals from electronic wastes. **P. Peng**, A. West, A.A. Park

2:45 Intermission.

3:00 124. Selective separation and enrichment of rare-earth elements from unconventional resources via co-precipitation and liquid-liquid extraction. **H.D. Huang**, Y. Gottesfeld, C. Zhou, Y. Park, A.A. Park

3:20 125. Diabetes as an environmental risk factor: Detailed mechanistic implications of chemistry and scavenging of methyl glyoxal by the formation of creatine's mono-and bis adducts. **B. Dayal**, A. Kulkarni, M.A. Lea

3:40 126. Plant-based polymers as effective treatment agents in removal of dissolved solids and ions in wastewater for reuse in plant irrigation. **R. Srinivasan**

4:00 127. Green coagulants for improved struvite recovery from agricultural waste. **M.A. Fleming**, Z. Oliver, O. Ndalamba, C. Portner, L.M. Blaney

4:20 128. Study of flame retardants in lounge chairs and electronics and their impact on emission, exposure, and flammability. **A. Davis**, M. Black, D. Harris

Section G

Sofitel Philadelphia at Rittenhouse Square Toulouse

Transformation of Organic Pollutants in Aquatic Systems: A Celebration of the Career of A. Lynn Roberts

Cosponsored by WCC Y. Chin, D. M. Cwiertny, M. L. Hladik, Organizers W. Arnold, T. Kohn, Organizers, Presiding

1:00 129. Aqueous organic chemicals: When speciation matters. A.T. Stone

1:20 130. Effects of ocean acidification on the organic complexation and bioavailability of trace metals. **F.** Morel

1:40 131. Enhanced degradation of β -lactam antibiotics: Roles of reactive copper species in the absence and presence of peroxydisulfate. **C. Huang**, J. Chen, P. Sun, X. Zhou, Y. Zhang

2:00 132. Impact of oxygen activation on substrate isotope effects of enzymatic oxygenations. **T.B. Hofstetter**, C. Bopp, S.G. Pati, H. Kohler

2:20 133. Identification and quantification of unsaturated C4-dicarbonyl ring cleavage products from chlorination of phenolic compounds: Structure-activity relationships. **Z. Zhang**, N. Pham, E. Golden, C. Prasse

2:40 Intermission.

2:55 134. Using mass spectrometry to identify chemical drivers of toxicity in drinking water. **S.D. Richardson**, J. Allen, M.J. Plewa, A. Jia, Y. Guo, A. Cuthbertson, H.K. Liberatore, T. Lee, R. Shirkhani, S.W. Krasner

3:15 135. Formation of organic electrophiles during water treatment with chemical oxidants: Precursors, mechanisms and implications for water quality assessment. **C. Prasse**, Z. Zhang, G. Zoumbouli, J. Wenk

3:35 136. Photochemical hydrolysis of aromatic trifluoromethyl groups. K.P. McNeill, A. Manfrin

3:55 137. Inhibitory effect of dissolved organic matter on the oxidation of aromatic amines induced by the sulfate and carbonate radicals. **S. Canonica**, U. Schönenberger

4:15 138. Geospatially resolved database of hydraulic fracturing wells for chemical transformation assessment. **D.L. Plata**, A.J. Sumner

Reactions on Surfaces in Liquid Media Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Multifunctional Surfaces for Cooperativity in Catalysis

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Activation of light (C1-C4) Hydrocarbons: Theory & Experiments Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Elucidation of Mechanisms & Kinetics on Surfaces Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

MONDAY MORNING

Section A

Sofitel Philadelphia at Rittenhouse Square Strasbourg

Applications of Artificial Intelligence, Machine Learning & Data Analytics in Environmental Science & Engineering

A. Z. Gu, Q. Li, X. Ma, Organizers Z. Cheng, Q. Ying, H. Zhang, Organizers, Presiding

8:25 Introductory Remarks.

8:30 139. Study on pollution characteristics of particulate matter in urban roads: High spatial and temporal resolution monitoring based on mobile sensors. **j. gao**

8:55 140. Estimating ground-level PM_{2.5} using micro-satellite images by a convolutional neural network and random forest approach. **T. ZHENG**, M. Bergin, S. Hu, D. Carlson

9:15 141. Assessing impact of particulate matter air pollution on solar energy production using a micro-satellite-based remote sensing approach. **T. ZHENG**, M. Bergin, J. Tapia, D. Carlson

9:35 142. Decadal changes in highway emissions: Comparison of six urban Ohio counties. **R. Kandiah**, K.V. Nedunuri

9:55 143. Development of a natural gas Wobbe Index prediction model. P. Roy, C. Ryu, C. Park

10:15 Intermission.

10:30 144. Machine learning assisted design of environmental responsive materials for healthy and energy efficient building environment. X. Yu

10:55 145. Evaluating links between drinking water violations and the incidence of waterborne disease. S. Schwetschenau, S.P. McElmurry, P.E. Kilgore, R.J. Smith

11:15 146. Practical application of econometrics for environmental management: Review of challenges and opportunities. R. Tehrani, N. Khajevand

11:35 147. Harnessing machine learning for predicting micropollutant removal during advanced oxidation processes in wastewater. **D. He**

11:55 Concluding Remarks.

Section B

Sofitel Philadelphia at Rittenhouse Square Nice

Current Status of Environmental Research on Water Contaminants

B. L. Loganathan, Organizer S. Ahuja, Organizer, Presiding

8:30 Introductory Remarks.

8:35 148. Assessing South American *Guadua chacoensis* bamboo biochar and Fe₃O₄ nanoparticle dispersed analogues for aqueous arsenic(V) remediation: Systematic study. **C. Navarathna**, J. Alchouron, A. Vega, T. Mlsna

8:55 149. Prediction of five-day biochemical oxygen demand (BOD₅) from some oxygen demand characteristics in surface water. **I.E. Uwidia**, **C.M. Ademoroti**

9:15 150. Novel oxone treated hydrochar for the removal of Pb(II) and methylene blue (MB) from aqueous solution. **S. Madduri**, I. Elsayed, E.M. Hassan

9:35 151. Natural plant pigments analysis applied to photodegradation of the pharmaceutical pollutants in water. **L. Jiang**, K. Patterson, K. Howlett, B. Wang

9:55 152. Treatment of kitchen wastewater using aerobic biological method and sand-bed filtration. **I.E. Uwidia**, **E. Michael**

10:15 Intermission.

10:30 153. Computational modeling vs. Adsorption isotherm experiments to gauge the capacity of cocoa shell biochars to remove stable and hydrolyzing pharmaceuticals from water. **M. Berger**, J.L. Goldfarb

10:50 154. Withdrawn.

11:10 155. Synthesis of cost-effective and sustainable pathways to wastewater treatment. **E. Aboagye**, M. Desai, C. Tran, K.M. Yenkie, F. Friedler

11:30 156. Adsorption of catechol/hydroquinone on TiO2 and iron(III) oxide. K. Abugazleh

11:50 Concluding Remarks.

Sofitel Philadelphia at Rittenhouse Square Versailles

Biogeochemical Transformation in Underground Environments: Natural Processes & Engineered Implementations for Contaminant Abatement

Cosponsored by CEI and GEOC J. Ferry, K. Millerick, *Organizers* M. G. Siebecker, W. Yan, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 157. Combined nano-bio technologies based on iron nanoparticles: Efficient tool for groundwater remediation. J. Filip, J. Semerad, O. Lhotsky

8:35 158. Ligand-controlled mobilization of tetravalent uranium. **K. Chardi**, D. Giammar, W. Schenkeveld, N. Kumar, S. Kraemer

8:55 159. Evolving reactivity and products of natural iron-bearing minerals toward sulfide. J. Daire, J. Voelz, K. Amen, R. Penn, N.W. Johnson, **C.L. Chun**

9:15 160. Impacts of cryogenic sampling processes on reactive iron mineral coatings in sediment. **H. Hua**, X. Yin, M.I. Renno, T.C. Sale, L.B. Axe

9:35 161. Arsenic fate under the shadow of sea-level rise. **F. Izaditame**, M.G. Siebecker, R. Tappero, P. Sricharoenvech, D.L. Sparks

9:55 162. Influence of surface-sulfidated iron particles on sulfate reducing microbial communities. A. Redwan, S. Islam, W. Yan, **K. Millerick**

10:15 Intermission.

10:30 163. Sulfide intrusion and distribution in the seagrass *Halodule wrightii*. **S. Rubiano Rincon**, P.D. Larkin

10:50 164. Sea level rise impacts on arsenic mobility in natural systems. **J. Sanchez**, J. Stuckey, R. Tappero, M.G. Siebecker, D.L. Sparks

11:10 165. Influence of phenolic structure on contaminant oxidation by manganese oxides in complex matrices. **E.L. Trainer**, M.A. Ginder-Vogel, C.K. Remucal

11:30 166. Saltwater intrusion affects peroxidase-mediated polymerization for remediation of coastal soils. F. Wang, S. Putnam, T.M. Makris, J.L. Ferry

11:50 Closing Remarks.

Section D

Sofitel Philadelphia at Rittenhouse Square Montpellier

Applications & Implications of Nanomaterials in the Environment / Membrane & Water Treatment

S. Chakraborty, S. R. Kanel, S. Kang, M. Nadagouda, T. Phenrat, J. Stubbs, Organizers

8:00 Introductory Remarks.

8:05 167. Enhanced removal of conventional and emerging pharmaceuticals and personal care products (PPCPs) from water by graphene-iron nanohybrid. **A. Masud**, N.G. Chavez Soria, D.S. Aga, N. Aich

8:25 168. Correlating material morphology and surface chemistry with the surface deposition process of graphene oxide. **Q. Zeng**, Y. Jiang, W. Li, C. Kim, J. Fortner

8:45 169. Withdrawn.

9:05 170. Environmentally friendly humic acid coated magnetic iron nanoparticles for removal of model styryl pyridinium type cationic dyes. **A. Esmaeilian**, K.E. O'Shea

9:25 171. Photocatalytic pathway toward degradation of various pharmaceutical molecules: Kinetics, mechanisms and toxicity assessment. **M. Ksibi**

9:45 Intermission.

10:00 172. Withdrawn.

10:20 173. Immobilization of enzymes on polymeric membranes: Quantum and molecular mechanics study. **S. Curcio**, F. Petrosino, S. Chakraborty, G. De Luca

10:40 174. Rhamnolipid impact on the biological activity of surface modified nanoparticles. **A. Ghosh**, J. Fortner

11:00 175. Comparing the fate of pristine and wastewater-aged gold nanoparticles in freshwater: Impacts of surface coating functionality. **M.C. Surette**, J.A. Nason

11:25 176. Rare earth elements doping enhanced surface oxygen effect in MnO₂ for toluene decomposition at low temperatures. **H. Zhang**, P. Zhang

11:45 Concluding Remarks.

Section E

Sofitel Philadelphia at Rittenhouse Square Paris Ballroom

Impact of Engineered & Natural Nanomaterials on the Environment: A symposium in Honor of Dr. Michael F. Hochella

Engineered Nanoparticles & Systems

Cosponsored by GEOC D. D. Dionysiou, V. K. Sharma, P. J. Vikesland, Q. Wan, *Organizers* V. Sharma, *Presiding*

8:00 177. Seasonal biogeochemical cycling of copper- and gold-based engineered nanomaterials in a freshwater wetland mesocosm. **G. Lowry**, A. Avellan, M. Simonin, H. Hsu-Kim, S. Laughton, M.F. Hochella, M. Wiesner

8:20 178. Incidental nanoparticles in the environment: identification and their implications. **Y. Yang**, M.F. Hochella

8:40 179. Role of nanoscale materials in environmental pollution and remediation. **C. Pearce**, S.E. Taylor, M. Flury, J. Liu, O. Qafoku, K. Rosso, M.F. Hochella

9:00 180. Palladium and platinum release from vehicle catalytic converter materials exposed to common environmental ligands. **D.M. Aruguete**, A.F. Wallace, M. Murayama, T. Blakney, R. Kerr, G. Gerber, J. Ferko, C. Winkler

9:20 181. Nano-mineralogical study on the weathering of gunshot residue in soils of a shooting range in Ontario, Canada. **M. Schindler**

9:40 Intermission.

9:55 182. Crumpling versus puncturing: Biomechanical threshold for the cellular toxicity of silver nanowires. **B. Gilbert**, S. Lehmann, D. Toybou, D. Arndt, A. Tagmount, A. Pradas del Real, M. Salomé, A. Pacureanu, P. Cloetens, S. Bohic, C. Celle, J.P. Simonato, C. Vulpe, L.L. Charlet

10:15 183. Plant interactions with engineered aluminum oxide nanoparticles. **B. Kim**, K.L. Hayes, J. Mui, E.S. Sani, S.W. Eisenman, J.B. Sheffield

10:35 184. High-throughput screening of engineered nanomaterials that enhance photosynthesis using mesophyll protoplasts. J.C. White, L. Zhao, R. Ji, J.L. Gardea-Torresdey

10:55 185. Developing nanocarriers for delivery of double stranded RNA as a biological pest control agent. **J.M. Unrine**, J. Laisney, S.S. Lichtenberg, Z. Elhaj Baddar, D. Gurusamy, S. Palli

11:15 186. Investigating nanoparticles for sustainable fashion. D. Berhanu, T. Schiros

11:35 187. Engineered K-fertilizer derived from hydrothermally altered K-feldspar. R. Hellmann, Y. Zhai

Section F

Sofitel Philadelphia at Rittenhouse Square Marseilles

Green Chemistry & the Environment

Cosponsored by CEI S. O. Obare, Organizer R. Luque, Organizer, Presiding

8:00 188. Diabetes as an environmental risk factor: Critical role of artificial intelligence (A.I.) as a screening tool in diabetic retinopathy. **B. Dayal**

8:20 189. Leaching of valuable metals from spent-lithium-ion batteries using organic aqua regia. L. Lin, W. Zhang

8:40 190. Characterization of hyperaccumulators for greener recovery of rare metals. **A. Upadhyay**, K. Atmatzidis, R. Tehrani

9:00 191. Creating more efficient, less hazardous syntheses of pharmaceutical using the 12 principles of green chemistry. L. Bastin

9:20 192. Withdrawn.

9:40 Intermission.

9:55 193. Techno-economic and life cycle analysis of biobased resin: Case study on acetoacetylated lignin resin. **R. Pandey**, D.C. Webster, G. Pourhashem

10:15 194. Paper-based fast and selective detection of lead in water. M.T. Islam

10:35 195. Enzymatic degradation of polyester plastics using a novel engineered biocatalyst. **B. Zhu**, N. Wei

10:55 196. Slow-release phosphate fertilizer using biochar. S. Bakshi, R. Smith, R.C. Brown

11:15 197. Microbial electrochemical treatment of biorefinery black liquor and resource recovery. X. Chen, X. Chen, M. Tucker, Z.J. Ren

11:35 198. Structural evaluation of humic acids and soil organic matter from integrated crop-livestock-forest systems. **A.M. Tadini**, L. Martin-Neto, D.M. Milori, A.C. Bernardi, V. Soares, L.A. Colnago, R. Garimella, P.G. Hatcher

11:55 Concluding Remarks.

Sofitel Philadelphia at Rittenhouse Square Toulouse

Transformation of Organic Pollutants in Aquatic Systems: A Celebration of the Career of A. Lynn Roberts

Cosponsored by WCC W. Arnold, Y. Chin, T. Kohn, *Organizers* D. M. Cwiertny, M. L. Hladik, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 199. Things I learned from Prof. A. Lynn Roberts during the early years of research on contaminant degradation by zerovalent metals. **P.G. Tratnyek**

8:25 200. Synergistic interaction between black carbon and sulfide in contaminant dehalogenation. K. Ding, X. Xu, J.D. Sivey, **W. Xu**

8:45 201. Reduction of N–O containing compounds (NOCs) by soluble and surface complexed Fe(II). **H.** Zhang

9:05 202. What a long, strange trip it's been: Zero valent iron retrospective. E. Carraway

9:25 Intermission.

9:40 203. Redox properties of iron-ligand complexes in dissolved organic matter. J. Hudson

10:00 204. Reductive degradation using Mg-based bimetal: Transformation and fate of 2,4-dinitroanisole (DNAN) and nitroguanidine (NQ) in wastewater. **A. Mai**, E. Hadnagy, C. Christodoulatos, A. Koutsospyros, B. Smolinski

10:20 205. Enhanced tribromoacetic acid (Br₃AA) degradation using pyrogenic carbonaceous matter (PCM). **P.V. Samonte**, Z. Li, S. Almassi, B.P. Chaplin, W. Xu

10:40 206. Abiotic reduction of the munitions compounds DNAN and NTO by carbonaceous reductants and carbon-rich soils. **J. Murillo Gelvez**, D.M. Ditoro, H.E. Allen, R.F. Carbonaro, P. Chiu

11:00 207. Modeling the reduction of nitroaromatics by humic acid using quantum chemically computed energies of reduction and oxidation half-reactions and quinone functional groups. **K. Hickey**, D.M. Ditoro

Perspectives on Climate Change Literacy & Education; Local to International Sponsored by CHED, Cosponsored by ENVR[‡]

Multifunctional Surfaces for Cooperativity in Catalysis

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Activation of light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Catalytic Conversion of Polymers: Upcycling to Useful Chemicals, Fuels & Materials Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC[‡], MPPG[‡] and POLY

Elucidation of Mechanisms & Kinetics on Surfaces

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MONDAY AFTERNOON

Sofitel Philadelphia at Rittenhouse Square Strasbourg

Micro- & Nano-Plastics in the Environment: Detection, Characterization, Fate & Impact

S. R. Al-Abed, M. J. Gallagher, P. Potter, Organizers, Presiding

1:00 208. Raman tweezers for small microplastics and nanoplastics identification in seawater. R. Gillibert, M. tardivel, O. Maragò, M. Lamy de La Chapelle, **F. Lagarde**, p. Gucciardi

1:20 209. Quantifying nanoplastic heterogeneity. K. Liao, A.C. Madison, A.L. Pintar, B.R. Ilic, C.R. Copeland, S. Stavis

1:40 210. Detection and analysis of microplastics using Raman spectroscopy. **S. Shidler**, T. Prusnick, R.W. Bormett

2:00 Intermission.

2:20 211. Methods to detect microplastics and nanoplastics in human tissue. **C. Rolsky**, **V. Kelkar**, D.F. Mastroeni, T.G. Beach, R.U. Halden

2:40 212. Metrological framework supporting the characterization of nanoplastics. **N. Farkas**, S. Papanu, J.A. Kramar

3:00 213. Novel approach to Infrared spectroscopy and imaging for the routine characterization of microplastics in environmental samples. **d. robey**

3:20 Intermission.

3:40 214. Transition size in polymer fragmentation processes may slow down nanoplastics production in the environment. F. Julienne, G. Balakrishnan, N. Errien, N. Delorme, T. Nicolai, C. Chassenieux, **F. Lagarde**

4:00 215. Extraction, concentration, and quantification of nanoplastics using functionalized magnetic nanoparticles. **M.C. Surette**, D.M. Mitrano, K.R. Rogers

4:20 216. Development of active sampling technique for the analysis of atmospheric microplastics. **N.C.** Eddingsaas, D. Mojica, O. Martin

Section B

Sofitel Philadelphia at Rittenhouse Square Nice

Current Status of Environmental Research on Water Contaminants

B. L. Loganathan, Organizer S. Ahuja, Organizer, Presiding

1:00 Introductory Remarks.

1:05 217. Withdrawn.

1:25 218. Withdrawn.

1:45 219. Pulsed electric field (PEF) device: Design, performance and deployment in an elderly home for tap water disinfection. **T.N. Dy**, J. Lopez Navas, J. Kwan, K. Yeung

2:05 220. Evaluation of persistent, bioaccumulative, toxic chemicals under the Frank R. Lautenberg Chemical Safety for the 21st Century Act. **J. Yan**

2:25 221. Mapping the antibiotic footprint in Minnesota. L. Frankson, W. Arnold

2:45 Intermission.

3:00 222. Synthetic dithiols and superparamagnetic nanoparticles: Purification of contaminated heavy metal water. **S.N. Bandara**, J. Walrod II, D.A. Atwood

3:20 223. Emerging environmental contaminants in water in Chennai, India: Comprehensive study on fate & occurrence. **T. Anumol**, A. Vijayanandan, L. Philip, S.A. Snyder

3:40 224. Analysis of dissolved organic matter and contaminants of emerging concern to detect leaking sewers in urban streams. **J.A. Batista Andrade**, E. Diaz, E.R. Hain, K. HE, L.M. Blaney

4:00 225. Modeling chromate removal using type 1 quaternary amine anion exchangers in drinking water applications. **F. Ghanem**, K.M. Yenkie

4:20 226. Withdrawn.

4:40 Concluding Remarks.

Sofitel Philadelphia at Rittenhouse Square Versailles

Performance of Stormwater Treatment Systems Under Changing Environments

Cosponsored by GEOC T. Dittrich, S. Ravi, *Organizers* S. K. Mohanty, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 227. Urban stormwater chemistry: Quality characterization and recommendation for synthetic stormwater. S. Pamuru, E. Forgione, K. Croft, B. Kjellerup, **A.P. Davis**

1:35 228. Raised versus inverted: Significance of bioretention underdrain configuration on denitrification in stormwater. **A.G. Donaghue**, E.R. McKenzie, S. Beganskas

1:55 229. Hydrologic and biogeochemical controls on seasonal soil nutrient dynamics in urban green spaces. **A. Parolari**, I. Horvath

2:15 230. Evaluating the efficacy of MnO_2 impregnated polypropylene fiber as a sorbent material to treat urban stormwater runoff. **C. Tummala**, T. Dittrich, M. Baskaran

2:35 Intermission.

2:50 231. Decision framework for biochar selection to remove PCBs, PAHs, Cu and Zn from stormwater. **D. Kaya**, S. Pamuru, K. Croft, Y. Chen, A.P. Davis, B. Kjellerup

3:10 232. Using rainfall measures to evaluate hydrologic performance of green infrastructure systems under climate change. L. Cook, **J.M. Vanbriesen**, C. Samaras

3:30 233. Elevated levels of pathogenic indicator bacteria and antibiotic resistance genes after hurricane Harvey's Flooding in Houston. **P. Yu**, P.J. Alvarez, L. Stadler

3:50 234. Development of a parsimonious model for nitrate removal in woodchip bioreactors under dynamic hydrologic and temperature conditions. **J. Israel**, P. McGuire, N. Butkevich, M. Reid

4:10 235. Bonechar as a potential sorbent for enhanced metal removal in green stormwater infrastucture. M. Dardona, R. Hakim, A. Alexandrova, C.M. Tummala, S. Mobasser, **T.M. Dittrich**

4:30 Discussion.

4:40 Concluding Remarks.

Section D

Sofitel Philadelphia at Rittenhouse Square Montpellier

Applications & Implications of Nanomaterials in the Environment / Environmental Application

S. Chakraborty, S. R. Kanel, S. Kang, M. Nadagouda, T. Phenrat, J. Stubbs, Organizers

1:00 Introductory Remarks.

1:05 236. Release of nanomaterial additives from automobile coatings and home siding during natural and artificial weathering. **R.S. Lankone**, E. Ruggiero, D.G. Goodwin, K. Vilsmeier, P. Mueller, S. Pulbere, K. Challis, Y. Bi, P.K. Westerhoff, J.F. Ranville, H. Fairbrother, L. Sung, W. Wohlleben

1:25 237. Evaluation of nanomaterials under the Frank R. Lautenberg Chemical Safety for the 21st Century Act. **A. Stanton**

1:45 238. Ameliorative role of antioxidant therapy against chronic arsenicosis in humans. **B. Mondal**, D. Chatterjee, M. Bhattacharyya

2:10 239. Ammonium as structure-inducing ions to synthesize ultrathin birnessite-type MnO₂ nanosheets with excellent catalytic activity of ozone. **R. Cao**, **P. Zhang**

2:35 Intermission.

2:50 240. Biocompatibility of two-dimensional transition metal carbides and nitrides (MXenes) and their potential in ophthalmic applications. **N. Noriega**, E. Ward, Y. Gogotsi, S. Sandeman

3:15 241. Construction of a bioinspired laccase-mimicking nanozyme for the degradation and detection of phenolic pollutants. **J. Wang**, R. Huang, W. Qi, R. Su, B. Binks

3:35 242. Release and transformation nanoparticle additives from surface coatings on pristine & weathered pressure treated lumber. **J.G. Clar**, S. Thornton, S. Boggins, D.M. Peloquin, T. Luxton

3:55 243. Ferrihydrite dissolution at the root zone of crops under semi-arid condition controls the plant uptake of uranium and arsenic. **A. Malakar**, M. Kaiser, D.D. Snow, C. Ray

4:15 244. Novel biomimetic system for the application of nanomaterials in water treatment: Implications and challenges. **K. Atmatzidis**, A. Upadhyay

4:35 245. Green engineering of gold nanoparticles. S. Sahi, S. Bhaskaran, N. Sharma

4:55 Closing Remarks.

Section E

Sofitel Philadelphia at Rittenhouse Square Paris Ballroom

Impact of Engineered & Natural Nanomaterials on the Environment: A symposium in Honor of Dr. Michael F. Hochella / Nanomaterials - General

Cosponsored by GEOC D. D. Dionysiou, V. K. Sharma, P. J. Vikesland, Q. Wan, *Organizers* F. Michel, *Presiding*

1:00 246. Myriad (nano)particulate phases emanating from hydrothermal vent and diffuse flow fluids fertilize the ocean. **G.W. Luther**, E.R. Estes, D. Berti, M.F. Hochella, N. Coffey, A.S. Wozniak, T.J. Shaw

1:25 247. Nanoparticle (and macroparticle) movement in the subsurface changes regolith chemistry. **S. Brantley**, X. Gu, H. Kim

1:45 248. Metal nanoparticle occurrence in nationwide municipal waters. L. Rand, N. Sharma, C. Zeng, P.K. Westerhoff

2:05 249. Mechanism of formation, stability, and toxicity of silver nanoparticles in aquatic environment. **V.K. Sharma**

2:25 250. Sequential determination of microplastics and nanoplastics in environmental waters. J. Liu

2:45 Intermission.

2:55 251. Atomic force microscope enabled systematic evaluation of nanomaterial transformations. **P.J.** Vikesland

3:20 252. Density functional theory modeling of nanoparticles. J.D. Kubicki

3:45 253. Nanophases in planetary processes. A. Navrotsky

4:10 254. Impact of Fe-oxide nanoparticles on biogeochemical cycling of elements in a changing environment. **D.L. Sparks**

4:35 255. From quantum confinement to global behavior: Overall state of nano-environmental and nanogeo research. **M.F. Hochella** Sofitel Philadelphia at Rittenhouse Square Marseilles

Industrial Applications of Environmental Chemistry

N. Lock, Organizer T. Anumol, S. C. Lingenfelter, Organizers, Presiding N. Lock, Presiding

1:00 Introductory Remarks.

1:05 256. Using microscopy techniques to quantitate biological systems for improving wastewater treatment plant performance. **G. Martin**, J. Betz, Y. Peng

1:25 257. Producing and optimizing extracellular lipase for remediation of refinery wastewater. **E.O. Nwaichi**, J.O. Osuoha, E.C. Egwim, B.W. Abbey

1:45 258. Treatment of textile sludge by coagulation and flocculation processes. I. Asia

2:05 259. Effects of reverse salt flux on the transport of disinfection byproducts in forward osmosis. **J. Xu**, T.N. Tran, H. Lin, N. Dai

2:25 Intermission.

2:40 260. Imagine a world without environmental chemistry: Let's not. **E. Denoyer**, J.L. Hedrick, R.A. Veeneman

3:00 261. Rare earth element recovery from coal fly ash: Hydrothermal extraction and ligand-associated media sorption. **T.M. Dittrich**, M. Dardona, J. Hovey, M.J. Allen, D. Kakaris Porter, S.K. Mohanty, H. Boukhalfa

3:20 262. Impacts of interfacial tension and critical micelle concentration on emulsion stability in bilgewater. J. Church, **M.R. Willner**, B.R. Renfro, Y. Chen, D. Diaz, W. Lee, C. Dutcher, J. Lundin, D.M. Paynter

3:40 263. Enhanced performance of carbon nanotube immobilized membrane for treatment of high salinity produced water via direct contact membrane distillation. **M.S. Humoud**, S. Mitra

4:00 264. Adsorptive removal of Cr(VI) by zwitterionic surfactant coated manganese ferrite (MnFe₂O₄) nanoparticle: Equilibrium and kinetic study. **S. Dan**, A. Chattree

4:20 789. Accurate quantitation of ethanolamines in oil and gas wastewaters. **G.D. de Vera**, G. Conte, L. Caldiero, D. Plata

4:40 Concluding Remarks.

Section G

Sofitel Philadelphia at Rittenhouse Square Toulouse

Transformation of Organic Pollutants in Aquatic Systems: A Celebration of the Career of A. Lynn Roberts

Cosponsored by WCC W. Arnold, D. M. Cwiertny, M. L. Hladik, T. Kohn, *Organizers* Y. Chin, *Organizer, Presiding*

1:00 265. Reactivity and *N*-nitrosodimethylamine formation potential of betrixaban with monochloramine, chlorine, and ozone. **T. Jasemi Zad, L.P. Padhye**

1:20 266. Insight into the interplay between graphitic carbon nitride aging and its photoreactivity. **M. LI**, D. Shuai

1:40 267. Microcystins degradation kinetics during chlorination: Role of water quality conditions. **K. Huang**, A.A. MacKay

2:00 268. Permanganate oxidation: From dissolved organic matter (DOM) to model compounds. J.R. Laszakovits, A.A. MacKay

2:20 269. Steric and electronic effects on reaction rates of substituted benzenes with often-overlooked brominating agents. **M.H. Schammel**, K. Martin-Culet, G.A. Taggart, J.D. Sivey

2:40 Intermission.

2:55 270. Environmental fate and transformation of herbicide safeners. **M. McFadden**, M.L. Hladik, J.D. Sivey, G.H. LeFevre, D.M. Cwiertny

3:15 271. Pharmaceuticals and personal care product accumulation in terminal lakes receiving reclaimed wastewater. **P. Sharma**, D. Hanigan

3:35 272. Sorption of organic cations to organic matter: Use of molecular docking simulations to understand binding interactions. **S. Scott**, C.M. Hadad, J. Fernandez, A.A. MacKay

3:55 273. Biotransformation of methoxylated polychlorinated biphenyls in whole poplar plants. **Y. Li**, J. Schnoor

4:15 274. Ecological and health risk assessment of organochlorine pesticides in an urbanized river network of Shanghai, China. **C. Chong**, L. Ma

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Meeting the Challenges of Heterogeneous Catalysis Controlled at Atomic Level Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Activation of light (C1-C4) Hydrocarbons: Theory & Experiments Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Catalytic Conversion of Polymers: Upcycling to Useful Chemicals, Fuels & Materials Sponsored by CATL, Cosponsored by ENFL, ENVR, I&EC[‡], MPPG[‡] and POLY

Elucidation of Mechanisms & Kinetics on Surfaces Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

MONDAY EVENING

Section A

Pennsylvania Convention Center Exhibit Hall A

Sci-Mix

S. O. Obare, Organizer

8:00 - 10:00

400, 402, 420, 423, 427, 430, 436, 440, 441, 442, 443, 444, 445, 447, 450, 451, 452, 454, 456, 459, 461, 463, 464, 466, 470, 473, 479, 483, 485, 486, 487, 489, 513, 514, 518, 519, 520, 522, 524, 527, 528, 531, 532, 533, 534, 537, 538, 539, 540, 542, 543, 544, 546, 547, 550, 551, 552, 554, 558, 559, 561, 562, 566, 567, 570, 571, 573, 577, 579, 580, 582, 586, 604, 605, 606, 607, 609, 612, 614, 618, 619, 621, 622, 623, 624, 625, 626, 627, 628, 631, 632, 634, 635, 636, 638. See Subsequent Listings.
TUESDAY MORNING

Sofitel Philadelphia at Rittenhouse Square Strasbourg

Micro- & Nano-Plastics in the Environment: Detection, Characterization, Fate & Impact

S. R. Al-Abed, M. J. Gallagher, P. Potter, Organizers, Presiding

8:00 Introductory Remarks.

8:20 275. Microplastics as a novel air pollutant: Successes and challenges. **S. Wright**, J. Levermore, F. Kelly

8:40 276. Organotin release from polyvinyl chloride (PVC) microplastics under photodegradation: Impacts from salinity, dissolved organic matter and light exposure. C. Chen, L. Chen, Y. Yao, F. Artigas, Q. Huang, **W. Zhang**

9:00 277. Fate of microplastics and microfibers in bioretention cells. K. Smyth, J. Drake, C. Rochman, E. Passeport

9:20 Intermission.

9:40 278. Limiting interactions between nano/microplastics and water filtration membranes using plasma surface treatment. M. Enfrin, **L.F. Dumee**, J. Lee

10:00 279. Physico-chemical properties of styrene oligomers as new pollutants in the environment. **B. Kwon**, K. Saido, S. Chung

10:20 280. Quantifying the weathering of aquatic plastic debris and the influence of weathering on pollutant sorption. **M.A. Maurer-Jones**, T. Hebner, F. Murphy, R. Trenary, R. Buckman

10:40 Intermission.

11:00 281. Effect of fabric type, washing conditions, and aquatic environment on the fate of microfibers released during home laundering. **M.C. Zambrano**, R.A. Venditti, J.J. Pawlak, J.J. cheng, C. Goller, J. daystar, M.A. Ankeny

11:20 282. Sorption behavior of antibiotics in water by virgin and aged micro-plastics. F. Yu, C. Yang

11:40 283. Characterization of the nanoplastics fate from soil to ocean: Coupling *in situ* measurement with experimental investigation. **J. Gigault**, B. Grassl

Section A

Section B

Sofitel Philadelphia at Rittenhouse Square Nice

Current Status of Environmental Research on Water Contaminants

B. L. Loganathan, Organizer S. Ahuja, Organizer, Presiding

8:15 Introductory Remarks.

8:20 284. Forgotten fungicide: Detection of strobin fungicides in minnesota waters. **M. O'Connor**, C. Weaver, D. Blumentritt, W. Varela, N. Mundahl, W. Arnold

8:40 285. Effect of pH on polyacrylamide degradation and methane production. **M. Akbar**, M. Khan, H. Wang

9:00 286. Chemically modified surfaces for the separation of non-polar organic contaminants from the water. **N. Baig**, T.A. Saleh

9:20 287. Sequential anaerobic and aerobic bioremediation of commingled contamination of trichloroethene and 1,4-dioxane. F. Li, D. Deng, L. Zeng, S. Abrams, **M. Li**

9:40 288. Detection of oxyhalides using ion chromatography system coupled with single quad mass spectrometry verus conductivity detection. B. Wang, J. Rohrer, **C. Shevlin**

10:00 Intermission.

10:15 289. Extraction of uranium from contaminated seawater using pistachio shells. **A. Younes**, J. Ali, M.T. Nur, A. Duda, J. Wang, L.C. Francesconi, S. Alexandratos, C.M. Drain

10:35 290. Estrogenicity and toxicity of environmentally relevant mixtures of endocrine active compounds. H. Yu, D.J. Caldwell, R. Suri

10:55 291. Understanding inhibition of anammox activity by nitrite, sulfide and recalcitrant carbonsat a functional gene level. **R. Goel, S. Hong**

11:15 292. Magnetized Douglas fir biochar for fast adsorptive removal of emerging contaminants in aqueous solutions. **A. Liyanage**, S. Canaday, T. Mlsna

11:35 293. Fast determination of haloacetic acids in drinking water. C. Shevlin, D. Jensen, P. Voelker

11:55 Concluding Remarks.

Sofitel Philadelphia at Rittenhouse Square Versailles

Performance of Stormwater Treatment Systems Under Changing Environments

Cosponsored by GEOC S. K. Mohanty, S. Ravi, *Organizers* T. Dittrich, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 294. Challenges and successes of green stormwater infrastructure in Detroit. A.R. Mathews, J. Parker

9:05 295. Quantifying heterogeneity of microbial community structure and the potential to remediate stormwater contaminants under varied biological and chemical conditions. **A.N. Fraser**, S.P. Preheim

9:25 296. Urban green roofs as new habitats for birds...and bacteria: Yearlong water quality assessment of storm water runoff of the Javits Center green roof. **J. He**, E. Owusu-Asumeng, J.R. Price, C. Zidar, J. Stolper, I. Lempitsky, F. Montalto, C. Sales

9:45 297. Biodegradation potential of PCBs in stormwater sediment. **K. Croft**, D. Kaya, Y. Chen, A.P. Davis, B. Kjellerup

10:05 298. Could fungi improve resilience of stormwater biofilters? **R. Valenca**, Y. Zu, Y. Miao, S. Mahendra, S.K. Mohanty

10:25 Intermission.

10:40 299. Applied mycology and integrated soil management in stormwater treatment. L. Olson

11:00 300. Presence of polycyclic aromatic hydrocarbons in stormwater sediment and bioretention cells. Y. Chen, D. Kaya, S. Pamuru, K. Croft, A.P. Davis, B. Kjellerup

11:20 301. Multi-tracer experiment in a bioretention cell to study the transport of trace organic stormwater contaminants. X. Gu, S. Spraakman, T. Rodgers, M.L. Diamond, J. Drake, **E. Passeport**

11:40 302. Effect of natural organic matter on urban stormwater trace organic compound and metal removal by polymer-clay composites. **J. Ray**, I. Shabtai, M. Teixido, Y. Mishael, D.L. Sedlak

12:00 303. Biofilter fingerprinting: Effluent suspended particles as indicator biofilter performance assessment. **S.K. Mohanty**, A. Borthakur, S. Mahendra, Y. Miao

12:20 Concluding Remarks.

Sofitel Philadelphia at Rittenhouse Square Montpellier

Innovative & Practical Approaches for the Treatment of Per- & Polyfluoroalkyl Substances (PFASs) / Reductive, Ultrasonic & Microwave Methods for PFAS Degradation

Y. Choi, S. Vyas, Y. Wang, Organizers J. Choe, J. Liu, Organizers, Presiding

8:00 Introductory Remarks.

8:05 304. Column and batch studies exemplifying the reductive decomposition of perfluoroalkyl substances by NiFe⁰ nanoparticles synthesized onto activated carbon. L.S. Lee, **M. Modiri Gharehveran**, J.E. Zenobio, Y. Choi

8:25 305. Influence of chemical structure on hydrodefluorination activity of poly- and perfluorocarbons by zeolite supported Rh catalysts. **S. An**, J. Choe

8:45 306. Reductive defluorination and removal of aqueous fluorinated pharmaceuticals using heterogeneous alumina supported bimetallic catalysts. **J. Park**, J. Choe

9:05 307. Degradation of perfluorooctane sulfonate by sub-bandgap irradiation of hydrogen terminated detonation nanodiamond. **W.A. Maza**, V.M. Breslin, T. Feygelson, P. DeSario, B.B. Pate, J. Owrutsky, A. Epshteyn

9:25 308. Degradation of main PFASs used as alternatives to PFOS/PFOA in China: Kinetics, intermediates and mechanism. **J. Huang**, Y. Bao

9:55 Intermission.

10:10 309. Elucidating structure-reactivity relationships for the redox degradation of major categories of PFAS pollutants in water. J. Liu, M.J. Bentel, M. Harake, W. Sui, Z. Liu

10:30 310. Effects of geochemistry on photo-reductive treatment of per- and polyfluoroalkyl substances (PFAS) by hydrated electrons in groundwaters impacted by aqueous film-forming foam (AFFF). **R. Tenorio**, G. McKay, A. Maizel, C. Schaefer, C.P. Higgins, T.J. Strathmann

10:50 311. Chemical destruction of PFAS sorbed on ion exchange resins: Solution to the PFAS pollution in water? **Y. Deng**

11:10 312. Degradation of short, medium and long-chain PFASs in water using high-frequency ultrasound and effect of process variables. G. Andaluri, T. Shende, R. Suri

11:30 313. Microwave-enhanced membrane filtration for degradation of PFASs. F. Liu

11:50 Closing Remarks.

Sofitel Philadelphia at Rittenhouse Square Paris Ballroom

Impact of Engineered & Natural Nanomaterials on the Environment: A symposium in Honor of Dr. Michael F. Hochella / Engineered and Incidental Nanoparticles

Cosponsored by GEOC V. K. Sharma, P. J. Vikesland, Q. Wan, *Organizers* D. D. Dionysiou, *Organizer, Presiding*

8:00 314. Atom probe tomography (APT) and its potential applications in nanogeosciences. **A. Perez-Huerta**

8:20 315. Illuminating the connections between the environmental nanosciences and the trace element biogeochemical sciences. **H. Hsu-Kim**

8:40 316. Lateritic nanophases: Witnesses of the fragility and promises of tropical soils. G. Calas

9:00 317. Influence of nanoparticle coatings on corona composition. J.A. Pedersen

9:20 318. Quantifying CeO₂-(nano)-particles from anthropogenic activities in sewage sludge samples. **R.** Kaegi, A. Gogos, J. Wielinski, A. Voegelin

9:40 319. Investigating toxicity of particulate emissions from combustion power plants. R. Giere

10:00 Intermission.

10:15 320. Nano-scale mineralogy of a rare earth element-rich Manchester coal lithotype, Clay County, Kentucky. **J. Hower**, D. Qian, N. Briot, M. Hood, C. Eble

10:35 321. Withdrawn.

10:55 322. Still plenty of room at the bottom: Nanoscience in geochemistry beyond nanoparticles. A.G. Stack, N. Rampal, H. Wang, A. Brady, L. Anovitz, K. Page, E. Mamontov

11:15 323. Reactive interfaces in engineered clay barriers. P. Wersin, U. Mäder, J. Hadi, A. Jenni

11:35 324. Development of heterogeneous advanced oxidation processes for the removal of contaminants of emerging concern in water and wastewater. B. Ren, A. Al-Anazi, W.H. Abdelraheem, Y. Huang, D.D. Dionysiou

Section F

Sofitel Philadelphia at Rittenhouse Square Marseilles

Great Achievements in ES&T: James J. Morgan Environmental Science & Technology Early Career Award Symposium

Cosponsored by PROF B. L. Loganathan, Organizer M. S. Mills, Organizer, Presiding B. Logan, Presiding

8:20 Introductory Remarks.

8:25 325. Curious incidences of PFASs at environmental interfaces impacted by aqueous film forming foams. T. Schwichtenberg, J. Zhang, C. Schaefer, D. Bogdan, C. Carignan, J.A. Field

8:50 326. Combating the spread of antibiotic resistance in water systems: Surveillance and risk. A. Pruden

9:15 327. Combating global expansion of toxic cyanobacterial blooms: Challenges posed by climate change. **H.W. Paerl**

9:40 Intermission.

10:00 328. Development of a three-dimensional electrochemical system using a blue TiO₂/SnO₂-Sb₂O₃ anode for treating low ionic strength wastewater. X. Meng, Z. Chen, c. wang, W. Zhang, K. Zhang, S. Zhou, J. Luo, N. Liu, D. Zhou, D. Li, **J.C. Crittenden**

10:25 329. Disrupting desalination: Temperature swing solvent extraction for hypersaline brines. **N. Yip**, C. Boo, H. Qi, R. Winton, I. Billinge, K. Conway, K. Shah

10:50 330. Electrocatalytic reduction of nitrate using Pd-based reactive electrochemical membranes. P. Gayen, J. Spataro, S. Avasarala, A. Ali, **J.M. Cerrato**, B.P. Chaplin

11:15 331. Roles of emerging reactive species in UV/chlor(am)ine and UV/permanganate processes. K. Guo, Z. Wu, C. Chen, **J. Fang**

11:40 332. Meet the editors of the ES&T family of journals. M.S. Mills

11:55 Concluding Remarks.

Sofitel Philadelphia at Rittenhouse Square Toulouse

Re-envisioning Chemistry's Role in Environmental Sustainability: Perspectives on Progress & Future Directions

Cosponsored by CEI[‡] and ENVR Financially supported by Cornell Institute of Politics and Global Affairs D. Kriner, E. Ryan, *Organizers* J. L. Goldfarb, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 333. Re-envisioning the American Chemical Society's role in environmental sustainability. **J.L. Goldfarb**

8:50 334. Sustainability metrics and environmental sustainability analytics for green chemistry from a life cycle perspective. **F. You**

9:15 335. Sustainable design for a circular economy: Bioenergy, bioproducts, and resource recovery systems. **J. Guest**

9:40 336. Sustainability in the chemical process industries through process intensification and modular manufacturing. **P. Yelvington**

10:05 Intermission.

10:20 337. Molecular farming, biomass valorization and platform chemicals: Sustainable and abundant materials from biosphere's molecular factories of renewable resources. **R.S. Varma**

10:45 338. Sustainability in the chemical enterprise: Renewable energy beyond the benchtop. E.B. Fox

11:10 339. Critical role of chemistry in efforts to achieve sustainability in agriculture on a global scale. **L.L. McConnell**

11:35 Panel Discussion.

11:55 Closing Remarks.

Bridging Surface Science to Catalysis

Sponsored by CATL, Cosponsored by COLL, ENFL and ENVR

Chemistry in Space: Novel Trends

Sponsored by YCC, Cosponsored by AGRO, BIOL, BMGT, COLL, ENVR, FLUO, GEOC, INOR, NUCL, PROF and RUBB

Meeting the Challenges of Heterogeneous Catalysis Controlled at Atomic Level

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Activation of light (C1-C4) Hydrocarbons: Theory & Experiments

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Re-envisioning Chemistry's Role in Environmental Sustainability: Perspectives on Progress & Future Directions

Cosponsored by CEI[‡] and ENVR

TUESDAY AFTERNOON

Section A

Sofitel Philadelphia at Rittenhouse Square Strasbourg

Aquatic Photochemistry

Cosponsored by CEI W. Arnold, K. P. McNeill, *Organizers* G. McKay, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 340. Photochemical reactivity of dissolved organic matter in the Adirondacks lakes. **J. Wasswa**, C.T. Driscoll, T. Zeng, R.C. Kevin, J. Stetler

1:25 341. On the quantification of hydroxyl radical and lower energy hydroxylator from dissolved organic matter photoirradiation. **F. Leresche**, K.D. Couch, J.A. Torres-Ruiz, G. McKay, F.L. Rosario

1:45 342. Photochemical formation and decay of superoxide radical in dissolved organic matter solutions. **W. Song**, J. Ma

2:05 343. Dissolved organic matter composition and electron-donating capacity determine photochemical reactivity of diverse waters. **C.K. Remucal**, S.M. Berg, J. Herrli, R. Winkels, K.H. Wammer

2:25 344. Comparing photoproduction rates of one-electron reductants and hydrogen peroxide in extracts and natural waters. **D. LeRoux**, N.V. Blough

2:45 Intermission.

3:00 345. Determining the importance of NOM type and water composition on the photochemical formation of VOCs at the air-water interface. **L.T. Stirchak**, L. Abis, C. George, D.J. Donaldson

3:20 346. Leveraging breakthroughs in light-emitting diode technology to probe the photochemical reactivity of arctic permafrost dissolved organic matter. **C.P. Ward**, J. Bowen, C.M. Sharpless, G. Kling, R. Cory

3:40 347. Aqueous aerosol processing in real time. S.H. Jones, D.J. Donaldson

4:00 348. Global model for depth-dependent carbonyl photochemical production rates in seawater. Y. Zhu, **D.J. Kieber**

Section B

Sofitel Philadelphia at Rittenhouse Square Nice

Current Status of Environmental Research on Water Contaminants

B. L. Loganathan, Organizer S. Ahuja, Organizer, Presiding

1:00 Introductory Remarks.

1:05 349. Disinfection byproducts (DBPs) in mixtures: Is cytotoxicity additive and what are the toxicity drivers? **S. Lau**, K. Hur, K. Bokenkamp, E. Wagner, M.J. Plewa, W. Mitch

1:25 350. Determination of low-level haloacetic acids, bromate, and dalapon in drinking water using IC-MS. **H. Yang**, J. Rohrer

1:45 351. Improving our understanding of point and non-point sources of contamination in a rural to urban watershed. **N.K. Marks**, P. Kremer, S. Goldsmith

2:05 352. Chemistry of surface waters in the agro-forested watersheds of Eastern Ohio experiencing unconventional natural gas exploration. **K.V. Nedunuri**, N. Zhang, R. Kandiah, X. Wei, H. Liu

2:25 Intermission.

2:40 353. Seawater augmented reuse: Study of upstream blending for potable reuse. **S.L. Plata**, D. McCurry, A. Childress

3:00 354. Evaluation for the fate and health impacts of trace organic chemicals in the reclaimed wastewater reused for agriculture. **A. Shahriar**, J. Tan, Y. Yang

3:20 355. Phosphate adsorption properties of ZSM-5 modified by metal cation exchange. A. Vij, C. Wang

3:40 356. Mineral precipitation for simultaneous toxic metal uptake from mining run-off and carbon dioxide fixation for reduction of greenhouse gases. **J.J. Kim**, C.A. Peters, S.C. Myneni

4:00 357. New insights to the degradation of 2,4-dichlorophenoxyacetic acid when applied to whole-lake treatments. **A. White**, C.K. Remucal, K. McMahon

4:20 Concluding Remarks.

Sofitel Philadelphia at Rittenhouse Square Versailles

Advancing Chemical Oxidation & Reduction for Addressing Emerging Environmental Issues

X. Guan, W. Song, H. Zhang, Organizers Y. Deng, Organizer, Presiding

1:00 Introductory Remarks.

1:05 358. Advances and challenges for using advanced oxidation processes to eliminate cyanotoxins. **D.D. Dionysiou**, M. Kong, X. Duan

1:35 359. Roles of reactive bromine radicals in the abatement of micropollutants by UV based AOPs in the presence of bromide. K. Guo, **J. Fang**

1:55 360. Light-driven degradation of Trace Organic Compounds (TOrC) by photosensitizing activity of Effluent Organic Matter (EfOM) for singlet oxygen production via indirect photolysis reactions. **V. Chichique Martinez**, N. Rojas Hosse, D. Lee, B. Barnett, K. Castella, C. Weiler, I. Márquez, A. Hussain, A.E. Saez, R. Arnold, D. Quanrud, M. Park

2:15 361. Template free mild hydrothermal synthesis of core-shell $Cu_2O(Cu)@CuO$ visible light photocatalysts for model pharmaceutical organics degradation. **K. Sekar**, K. Sasaki

2:35 362. Withdrawn.

2:55 Intermission.

3:10 363. Reactivity of aromatic organic compounds to radical species under cobalt/peracetic acid advanced oxidation process. **C. Huang**, J. Kim, P. Du, W. Liu, H. Zhao

3:40 364. Removal pathway of hydrogen peroxide induced by dissolved organic matters under solar irradiation. **J. Ma**, J. Nie, S. Yan, L. Lian, W. Song

4:00 365. Degradation mechanism of Benzophenone-3 during chlorination and UV/chlorination reactions. Y. Lee, G. Lee, M. Kim, **K. Zoh**

4:20 366. Enhanced degradation of 1,4-dioxane by photo-fenton reactive ceramic membrane. S. Xue

4:40 367. Degradation of tetracycline by medium pressure UV-activated peroxymonosulfate process: Influencing factors, degradation pathways, and toxicity evaluation. **X. Ao**, W. Sun

Sofitel Philadelphia at Rittenhouse Square Montpellier

Innovative & Practical Approaches for the Treatment of Per- & Polyfluoroalkyl Substances (PFASs) / Oxidative, Plasma, Hydrothermal, Photocatalytic & Electrochemical Methods for PFAS Degradation

J. Choe, Y. Wang, Organizers Y. Choi, J. Liu, S. Vyas, Organizers, Presiding

1:00 Introductory Remarks.

1:05 368. Density functional theory calculations on the reaction pathways for the transformation of 6:2 fluorotelomer sulfonate to perfluoroalkyl carboxylic acids initiated by hydroxyl radical in aqueous phase. **Y. Zhang**, A.H. Moores, J. Liu, S. Ghoshal

1:25 369. Investigating the Influence of pH on persulfate mediated oxidation of perfluoroalkyl carboxylates using DFT and transient absorption spectroscopy. **A. Carre-Burritt, S. Vyas**

1:45 370. Simple and Efficient Defluorination of PFAS in Wastewater by V₂C Nanosheets and H₂O₂. **Y. Ye**, J. Ray

2:05 371. Rapid removal of poly- and perfluorinated compounds from investigation derived waste (IDW) in a pilot-scale plasma reactor: laboratory and field demonstration studies. **S. Mededovic**, T.M. Holsen, R.K. Singh, N. Multari, C. Nau-Hix, R.H. Anderson, S. Richardson

2:35 372. Current use C6 aqueous film-forming foams (AFFF) containing per- and polyfluoroalkyl substances: Characterization and treatment options. **R. Singh**, S. Uwakweh, S. Woodard, S. Mededovic, T.M. Holsen

2:55 373. Regeneration of per- and polyfluoroalkyl substances (PFAS) contaminated granular activated carbon (GAC) using non-thermal plasma. **M. D'Souza**, A. Lewis, A. Rabinovich, G. Fridman, C. Bailey, A. Fridman, E.R. McKenzie, C. Sales

3:15 Intermission.

3:25 374. Efficient mineralization of fluoropolymers using subcritical water. H. Hori

3:55 375. PFAS degradation in UV/BOHP photocatalytic system: Mechanisms and pilot-scale studies. **M. Qanbarzadeh**, E.L. Cates

4:15 376. Treatment and removal of PFOA using an innovative technology of UV-vis/ Zn_xCu_{1-x}Fe₂O₄/oxalic acid. **E. Sahle Demessie**, M. Nadagouda, S. Verma, B. Mezgebe

4:35 377. Electrochemical mineralization of PFOA and PFOS. V.F. Pulikkal, M. Sun

4:55 Concluding Remarks.

Sofitel Philadelphia at Rittenhouse Square Paris Ballroom

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

Cosponsored by CEI T. Anumol, R. Marfil-Vega, T. M. Young, C. Zwiener, Organizers, Presiding

1:00 Introductory Remarks.

1:05 378. Role of sulfur functionality in the production of photogenerated water-soluble compounds from surrogate and MC252 crude oils. **S. Niles**, M.L. Chacon, R.P. Rodgers, A.G. Marshall

1:25 379. Using high-resolution mass spectrometry to identify transformation products of synthetic progestins in environmental matrices. **H. Zhao**, Z. Tian, K. Lam, K.T. Peter, E.P. Kolodziej

1:45 380. Application of HRMS in transformation of organic matters in the wastewater effluent. L. Lushi, S. Yan, H. Zhou, W. Song

2:05 381. Fate of agrochemicals during anaerobic digestion: Quantifying degradation and identifying transformation products using orbitrap mass spectrometry. **C.L. Brueck**, S. Nason, E.J. Bouwer, C. Prasse

2:25 382. Withdrawn.

2:45 Intermission.

3:00 383. Applications of high-resolution mass spectrometry in large-scale emerging contaminant monitoring: Per- and polyfluorinated alkyl substance testing network in North Carolina. **G.J. Getzinger**, N. DeStefano, D. Knappe, L. Ferguson

3:20 384. Investigating poly- and perfluoroalkyl substances (PFAS) degradation in non-equilibrium cold plasma technologies treatment using HRMS suspect screening. **E.R. McKenzie**, F. Ebrahimi, A. Lewis, M. D'souza, A. Rabinovich, G. Fridman, A. Fridman, M. Hadaya, I. Dragiev, T. Joyce, C. Sales

3:40 385. Development of a non-target workflow for the identification of industrial chemical contaminants. **T. Koeppe**, K. Jewell, C. Dietrich, A. Wick, T. Ternes

4:00 386. Using high resolution mass spectrometry to uncover advanced oxidation and disinfection byproducts in algal and wastewater-impacted drinking water. **D. Westerman**, M.L. Smith, S. Putnam, K.C. Cochran, W. Abdelraheem, Y. Huang, C.C. Montagner, J.L. Ferry, D. Dionysios, S.D. Richardson

4:20 Concluding Remarks.

Sofitel Philadelphia at Rittenhouse Square Marseilles

ACS Award for Creative Advances in Environmental Science & Technology / Chemicals at the Global Scale & Award Address

Cosponsored by PROF S. O. Obare, V. K. Sharma, *Organizers* S. J. Eisenreich, *Presiding*

1:00 Introductory Remarks.

1:05 387. Science and policy of POPs through passive air sampling. T. Harner

1:30 388. Importance of source inventories for our understanding of the global distribution of POPs. A. Sweetman, K. Breivik, K.C. Jones

1:55 389. Probing sources of persistent organic pollutants in the atmosphere of China and nexus. **G. Zhang**, S. Zhao, J. Li, X. Liu, K.C. Jones

2:20 390. From Lancaster to the poles: Chasing POPs in one ocean, one air. **R. Lohmann**, C. McDonough, L. Yeung, Y. Ma, E. Sunderland, D. Muir

2:45 391. Temporal trends of polycyclic aromatic hydrocarbons in the UK and the USA. R.A. Hites

3:10 392. Atmospheric deposition of polycyclic aromatic hydrocarbons and organohalogen compounds in high mountain areas of Europe. **J. Grimalt**, B.L. van Drooge, P. Fernandez

3:35 Intermission.

3:45 393. Award Address, ACS Award for Creative Advances in Environmental Science and Technology sponsored by the Aerodyne and the ACS Division of Environmental Chemistry. POPs: Story of global pollutants. K.C. Jones

4:30 Discussion.

4:45 Concluding Remarks.

Sofitel Philadelphia at Rittenhouse Square Toulouse

Re-envisioning Chemistry's Role in Environmental Sustainability: Perspectives on Progress & Future Directions

Cosponsored by CEI[‡] and ENVR Financially supported by Cornell Institute of Politics and Global Affairs J. L. Goldfarb, *Organizer* D. Kriner, E. Ryan, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 394. Environmental sustainability and routine organizational management. S. Cohen

1:30 395. Technological innovation and environmental regulation. R.L. Kleinberg

1:55 396. Strategic communication, social influence, and promoting sustainable behavior. B.W. Hardy

2:20 Panel Discussion.

2:40 Intermission.

2:45 397. Prospects for plastic material recycling by chemical and biological technology. J.A. Glaser

3:10 398. From assessing to scouting: Need for entropy indicators to identify plastics recycling opportunities. **P. Billen**

3:35 Panel Discussion.

3:55 399. Sustainability: Why chemistry will have many ways to engage. J.R. Ellis

4:15 Closing Remarks: Next Steps in ACS Sustainability.

Bridging Surface Science to Catalysis Sponsored by CATL, Cosponsored by COLL, ENFL and ENVR

Meeting the Challenges of Heterogeneous Catalysis Controlled at Atomic Level Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Activation of light (C1-C4) Hydrocarbons: Theory & Experiments Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Catalytic Conversion of Renewable & Waste Carbon Sources: Approaches to Improve Carbon Utilization

Sponsored by CATL, Cosponsored by ENFL and ENVR

Re-envisioning Chemistry's Role in Environmental Sustainability: Perspectives on Progress & Future Directions

Cosponsored by CEI[‡] and ENVR

TUESDAY EVENING

Section A

Pennsylvania Convention Center Exhibit Hall A

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

Cosponsored by CEI T. Anumol, R. Marfil-Vega, T. M. Young, C. Zwiener, *Organizers*

5:00 - 7:00

400. Comprehensive characterization of per- and polyfluoroalkyl substances (PFASs) in manufacturing wastewater. **P. Jacob**, D.E. Helbling

Section A

Pennsylvania Convention Center Exhibit Hall A

Advanced & Additive Manufacturing Materials & Technologies for Environmental Applications

N. Aich, W. Phillip, S. Rahaman, Organizers

5:00 - 7:00

401. New odor and corrosion control technologies for drainage system. M. Pamudji, K. Yeung, W. Han

402. Atomically precise membranes from molecular Legos. Y. Xie, J. Wiener, C.E. Schafmeister

403. Performance of a multifunctional odor control gel for H₂S abatement in drainage system. L. Luk, K. Yeung, W. Han

404. Enhancement of anaerobic digestion by direct interspecies electron transfer. **Z. Wang**, B. Si, J. Watson, T. Wang, Y. Zhang

405. Collection and speciation of gaseous and particulate nitrate for isotopic determination. **D. Blum**, W.W. Walters, M. Hastings

406. Withdrawn.

Pennsylvania Convention Center Exhibit Hall A

Advancing Chemical Oxidation & Reduction for Addressing Emerging Environmental Issues

X. Guan, W. Song, H. Zhang, Organizers Y. Deng, Organizer, Presiding

5:00 - 7:00

407. Roles of oxygen and Mn(IV) oxide in abiotic formation of humic substances by oxidative polymerization of polyphenol and amino acid. **J. Zuo**, J. Huang, D. Yue, H. Zhang

408. Accelerated degradation of micro-pollutant by permanganate: Comparison of organic and inorganic activations. **H. Dong**, Z. Qiang

409. Degradation of phenol by persulfate activated with zero-valent iron-biochar composites. T. Nguyen, **S. Oh**

410. Optimization of the landfill leachate treatment process using *Musa sp* flower extract in the process of coagulation, flocculation and sedimentation. D. Morais, A.S. Artur, B.P. Ribeiro, E.C. da Silva, D.H. Melo, K.A. Milagres, K.R. Xavier, **G. Lamas Samanamud**, C.C. Loures, L.L. Naves, F. Naves

411. Persulfate activation towards organic decomposition and Cr(VI) reduction achieved by a novel CQDs-TiO_{2-x}/rGO nanocomposite. **L. Xu**, P. Jin

412. Enhanced catalytic reduction of aqueous bromate by metal-organic framework Ni(HBTC)(4,4'-bipy) in the presence of NaBH₄. N.N. Nurlan, **W. Lee**

413. Effect of nitrite ion, chlorine dose, and pH on the ammonia chlorination reactions and speciation in clean water matrices. **S. Estahbanati**, **V. Diyamandoglu**

414. Role of carbonate radicals in the advanced oxidation process $(UV/H_2O_2 \text{ and } UV/K_2S_2O_8)$ for removing PPCPs. Z. Hao, J. Ma, **S. Yan**, L. Lian, W. Song

415. Arsenic(III) removal by the activated iron media system facilitated by O₂-initiated advanced oxidation reaction. Z. Yang, **Y. Huang**

416. Withdrawn.

417. Degradation kinetics and toxicity reduction during UV/persulfate reaction of benzophenon-3. Y. Lee, G. Lee, **K. Zoh**

418. Selective {012} facet exposure of CuFeO2 for efficient fenton-like degradation of antibiotic in water. **Y. Nie**, C. Dai, C. Yang

419. Enhanced transformation of emerging contaminants by permanganate in the presence of redox mediators. **J. Zhang**, Z. Shi, T.J. Strathmann

420. Destruction of tetrabromobisphenol-a (TBBPA) by UV advanced oxidation processes. **B. Taylor**, P.A. Ruiz-Haas

421. Rate constants and mechanisms of the reactions of Cl and Cl_2^- with trace organic contaminants. **Y.** Lei, X. Yang

422. Risk control of antibiotic-resistant bacteria, antibiotic-resistance genes and disinfection by-products during UV/chlorination process. **T. Zhang**

423. Simultaneous removal of ammonium and manganese from surface water in South China by manganese co-oxide film: Application effect. **X. Xing**

424. Manganese removal by iron–manganese co-oxide filter films under anaerobic condition in groundwater treatment. **Y. Cheng**, T. Huang

425. UV/TiO₂ photoelectrocatalysis as a novel alternative to degrade estrogens in food production systems. **J.L. Bennett**, Y. Gao, G. Gagnon

426. Kinetics of singlet oxygen indirect photolysis of trace organic compounds (TOrC) in wastewater effluent. **N. Rojas Hosse**, V. Chichique Martinez, D. Lee, B. Barnett, I. Márquez, K. Castella, A.E. Saez, R. Arnold, D. Quanrud, M. Park

427. Oxidized mercury compounds: Computational investigation. T. Asif, A. Asaduzzaman

428. Analysis of UV photodegradation of fluoroquinolone compound moxifloxacin. R. Shah, H. Santoke

429. Elucidation of imidazolium-based ionic liquid cations binding to iron porphyrin from a QM/MM framework. **J. Shah**, A. Banerjee

430. Removal of bisphenol F from water with UV/H_2O_2 advanced oxidation processes. **J. Balough**, P.A. Ruiz-Haas

Section A

Pennsylvania Convention Center Exhibit Hall A

Applications & Implications of Nanomaterials in the environment

S. Hussain, S. R. Kanel, S. Kang, B. A. Manning, M. Nadagouda, Organizers

5:00 - 7:00

431. Comparison of the phosphate adsorption capacity of MgAl- and MgAlZr-LDH. **T. Kim**, L. Lundehøj, U.G. Nielsen

432. Combining nanoparticles and foam transport in porous media for contaminated site remediation. Q. Li, **V. Prigiobbe**

433. Pressure drop and diffusion rate in 3D printed aerospace structure. S. Harger, **S.R. Kanel**, D. kim, R. Kemnitz

434. Unraveling nanostructures properties with potential environmental implications: *Ab-initio* study. **G. De Luca**, S. Chakraborty

435. Synthesis, characterization, morphological study, photocatalysis application of Ag doped ZnWO₄ nanoparticles. **A.A. Alothman**

436. Sub-nanocatalysis for efficient aqueous nitrate reduction: Effect of strong metal–support interaction. **J.** Li

437. Construction of g-C₃N₄/carbon ring/TiO₂ nanocomposite by improved heterojunction contact for enhanced photocatalytic performance. **C. Liu**, S. Dong, Y. Chen

438. Withdrawn.

439. Solar seawater evaporation based on hanging polyaniline-cotton photothermal fabrics. Z. Liu, Z. Chen

440. New magnetic nanoscavengers to clean water. **E. Santiago**, T. Liu, G.E. Pina-Luis, M.T. Oropeza-Guzmán

441. Controlled dissolution kinetics study of silver nanoparticles: Role of particle size. C. Liu

442. Electro-oxidation of trimethoprim using new electrode system based on graphite carbon paste modified with Au/Ag nanoparticles. **E. Tecuapa Flores**, P. Roquero Tejeda, T. Pandiyan

443. Application of copper nanomaterials to improve the resistance to root fungal disease in tomato (*Solanum lycopersicum*). **Y. Shen**, J.R. Borgatta, C. Ma, W. Elmer, J.C. White, R.J. Hamers

444. Phosphate recovery from wastewater by engineered green synthesized iron/bentonite nanocomposite. **E. Erdim**

445. Fluorescence microscopy of liposome-filled microwell arrays for studying interactions between laurdan-labeled liposomes and engineered nanoparticles. **L. Kesner**, C. Green, E. Laudadio, R.J. Hamers, Z. Rosenzweig

446. Shape-controlled dissolution of faceted nanomaterials by hybrid scanning electrochemical microscope-atomic force microscope (SECM-AFM). **Q. Ma**, X. Shi, W. Zhang

447. Mechanism of organosilanol compounds removal in water by adsorbent materials. **A. Aviles**, S. Uwakweh, P. Tarafa

448. Converting waste into worth: Fe_{1.72}Al_{0.28}O₃ nanoflakes harvesting from brown coal fly ash with crystal defects for enhanced water remediation. **B. Qian**, C. Liu, X. Hu, X. Zhang, L. Zhang

449. Withdrawn.

450. Enhanced anti-fouling performance in nitrogen removing MBRs using nanocellulose coated membrane. **S. Lotfikatouli**, P. Hadi, M. Yang, H. Walker, B.S. Hsiao, X. Mao

451. Voltammetric investigations of the sulfidation and dissolution of metal and metal oxide nanoparticles. **K.M. Mullaugh**, H. Lieb, B. Nguyen, E.R. Ramsayer

452. Fabrication of Cu(II)/TiO₂/GO ternary composite for photocatalytic degradation of tetracycline hydrochloride. **S. Pu**, S. Qian

453. Application of nanostructured bimetallic catalyst for oxyanion reduction. X. Min, Y. Wang

454. Selective adsorption and photocatalytic degradation of extracellular ARGs by partially molecular imprinted graphitic carbon nitride. **D. Zhang**

455. Withdrawn.

456. Utilization of magnetic nanomaterials for remediation of arsenic contaminated wastewater. **Y. Olaseni**, H. Huang, **L. Zhang**, S. Bashir, J.L. Liu

457. Graphene nanoplatelets in geopolymeric systems: New class of nanocomposites. **S. Candamano**, E. Sgambitterra, C. Lamuta, L. Pagnotta, F. Crea, S. Chakraborty

458. $Na_3V_2(PO_4)_3@C$ as faradaic electrodes in capacitive deionization for high performance desalination. **J. Ma**, F. Yu

459. Nanoplastic identification and quantification in aqueous media. O.K. Meyer, J. Hensler, D.G. Sykes

460. Photocatalytic degradation of pharmaceutical component a study with membrane reactor. **S. Chakraborty**, S. Curcio, D. Mukherjee, V. Calabro

461. Tannic acid-metal complex modified MXene membrane for water purification. **X. Tong**, S. Liu, H. Gao, Y. Chen, J.C. Crittenden

462. Passive sampling of various emerging contaminants in air and water using electrospun nanofiber mats. **M. Nagorzanski**, A. Martinez, J. Qian, R.F. Marek, D.M. Cwiertny

463. Patterned few-layer graphene (FLG) surfaces from plasma deposition. **E.B. Kennel**, C.L. Lake, P.D. Lake, P.J. Kauffmann, C.E. Richards, E.R. Prewitt

Pennsylvania Convention Center Exhibit Hall A

Aquatic Photochemistry

Cosponsored by CEI W. Arnold, G. McKay, K. P. McNeill, *Organizers*

5:00 - 7:00

464. Identifying phenolic photoproducts after exposure of crude oil over water to sunlight. **J. Zeron**, S. Patil, M.A. Tarr

465. Photoproduction and photolysis of acrylate in seawater. L. Xue, D.J. Kieber

466. Interfacial analysis of single aerosol particle. Y. Qian, G. Deng, Y. Rao

467. Photolysis of aqueous atmospheric aerosol mimics. M.M. Galloway, J. Sharp, S. Ma, J.L. Woo

468. Identification of highly fluorescent components of dissolved organic matter via size exclusion chromatography. **B. Hanson**

469. Combined effects of dissolved organic matter, pH, and divalent cations on UV-254 phototransformation of tetracycline antibiotics. **L. Harris**, M. Hopanna, L.M. Blaney

Section A

Pennsylvania Convention Center Exhibit Hall A

Biogeochemical Transformation in Underground Environments: Natural Processes & Engineered Implementations for Contaminant Abatement

Cosponsored by CEI and GEOC J. Ferry, K. Millerick, M. G. Siebecker, W. Yan, Organizers

5:00 - 7:00

470. Using fixed potential electrodes to quantify *in situ* iron redox in soils of the Susquehanna Shale Hills Critical Zone Observatory. **C. Hodges**, J.M. Regan, S.L. Brantley, J. Kaye

471. Identification of Sb(V) reducing bacteria and their potential metabolic traits by the combination of stable isotope probing and metagenomics analysis. **B. Li**, W. Sun, X. Sun, L. Lan

Pennsylvania Convention Center Exhibit Hall A

Current Status of Environmental Research on Water Contaminants

S. Ahuja, B. L. Loganathan, Organizers

5:00 - 7:00

472. Withdrawn.

473. Human are exposed to more than just water when inhalating aerosolized drinking water from ultrasonic humidifiers. **W. Yao**, R.M. DalPorto, D.L. Gallagher, A.M. Dietrich

474. Controls on the leaching of mercury from contaminated soils. **C. Miller**, D. Adekunle, J. McCurdy, S. Lukjan, A. Johs, B. Robertson

475. Revealing surface interactions between emerging pollutants and polymeric natural organic matter. **A. Stafford**, S. Schwenk, T. Amos, T.A. Williams, M. Subir

476. Withdrawn.

477. Withdrawn.

478. Toxicity of sunscreen active ingredients to Thalassiosira pseudonana. E.R. Hain, L.M. Blaney

479. High-performance degradation of bisphenol A by NaClO: Effect, dynamic process and mechanism. **Y. Tang**, M. Wu

480. Mountain Valley Pipeline's impact on the water chemistry of surrounding streams. **M. Bennington**, K. Bishop, K.R. Stefaniak

481. Effects of climate-induced increases in road salt contamination on dissolved organic matter in a northern Michigan wetland. **S. Perez**, T. Veverica

482. Contamination of grovnes peninsula in east Antarctica by persistent organic pollutants (POP's). L.K. Bhardwaj, T. Jindal

483. Quantification of nonylphenol and 4-tert-octylphenol in drinking water using UHPLC-MS/MS. **H. Zhao**, T. Anumol, J. Zweigenbaum

484. Detailing the mechanism of degradation of perfluoroalkyl substances by a cold atmospheric pressure plasma. **E. Juarez**, T. Contreras, A. Torres-Gonzalez, L. Her, P. Kelley, P. Bruggeman, U. Gangal

485. Determining the relationship between hydraulic fracturing activities and streamwater trace metal concentrations in North-Central Pennsylvania watersheds. **M. Borkoski**, J. Nguyen, N.B. Weston, S. Goldsmith

486. Phosphate removal from polluted waters by Iron hydroxide adsorption. **E. Flores**, A. Khodayari, L.M. Barge

487. Exploring the freshwater salinization syndrome along a gradient of suburban development. **A.F. Henderson**, **S. Goldsmith**

488. H₂O₂/UV-ceramic ultrafiltration membrane system for the mineralization of micropollutants: Role of V₂O₅-TiO₂ nanoparticles. H. Tak, Y. Chung, A. Jang, **S. Kang**

489. Partitioning of chlorpyrifos and tetrabromobisphenol A to sediments and dissolved organic matter in arctic lakes. L. O'Connor, J. Kerrigan, Y. Chin

490. Control of lead release from lead service lines with sodium silicate addition. **A. Mishrra**, D. Giammar, Z. Wang, V. Sidorkiewicz

Section A

Pennsylvania Convention Center Exhibit Hall A

General Posters

S. O. Obare, Organizer

5:00 - 7:00

491. Social history of U.S. kerosene standards in the late nineteenth century. **E.P. Venugopal**, **H.R. Cunningham**, M.A. Benvenuto

492. Effectiveness of raw versus activated coconut shells for removing arsenic and mercury from water. **I. Emahi**, P.O. Sakyi, P. Bruce-Vanderpuije, A. Issifu

493. Impact of fuel additives on oil-in-water emulsion stability. J. Church, G.C. Daniels, **M.R. Willner**, J. Lundin, D.M. Paynter

494. Monitoring water quality activity implemented in the ACS student chapter. L.I. Santiago

495. Preparation and reactivity of hydroxy-nitrate esters derived from atmospherically-relevant terpenes. **R.** LaLonde, E.A. McKnight, N. Kretekos, G.M. Bailey

496. Adaptive polyvalency in Klebsiella pneumonia NDM-1+ bacteriophage KL. R. Goel, E. Gilcrease

497. Ionic liquid-based air purification and disinfection systems. **W. Han**, X. Song, Y. Luo, J. Herrera Marin, V. Castillo Ramos, J. Kwan, K. Yeung

498. Intact carbonic acid is a strong reactive carboxilic acid affecting all aqueous environments. E. Pines

499. Investigation of personal care products for UV screening components and parabens, and their photolysis products. **C. Sargent**, Z.S. Davis

500. Withdrawn.

501. Withdrawn.

502. Wavelength dependence toxicity using various oils. I. Parker, L. Heidenreich, P.P. Benz, W. Jeffrey

503. Withdrawn.

504. Facile formation of ternary MgTiSi compounds from asbestos-chrysotile's abatement. **F.F. Bruno**, M. Bernabei, A. Chiappa, N. F. Farhadi, D. Ziegler

505. Development of engineered soil surrogates for predicting natural soil behavior. **G. Abdalla**, A. Pandey, B.J. Haywood, S.P. Smith, R.L. Cook, D. Spivak

506. Glyphosate as an underlying cause of increased dissolved reactive phosphorus loading in the Western Lake Erie basin. **C.E. Spiese**, K. Rossiter, A. Boise, M.N. Bowling, S. moeller, A. Pinkney, E. Richards, N. Schalitz, T. Street

507. High throughput methods for determining the formation parameters of struvite. J. Hostert, N. Kane

508. Assessing the potential of Markov state models in reducing the computational expense of estimating PMF, equilibrium constants and kinetics of reactions. **M. Saha**, J. Flora

509. Performance loss of activated carbon electrodes in capacitive deionization: Mechanisms and material property predictors. **X. Liu**, S. Shanbhag, S. Natesakhawat, J. Whitacre, M.S. Mauter

510. Unlocking potential of "green" aluminum batteries: Pulsed, amplified and proton boosted systems. **A.A. Gakh**

511. Acting through environmental chemistry and the sustainable global goals in an ACS local chapter. **F. Ocasio Idorwatt, L.I. Santiago**

512. Electrocatalytic and photocatalytic behavior of hybrid TiO₂ nanomaterials towards water removal of NSAIDS and selected dyes. **M. Cerro-Lopez**, L. Castro-Pastrana, J. Campos-Delgado, M.A. Mendez-Rojas, C. Martinez-Huitle

513. Creating awareness in undergraduate students and the community with environmental chemistry: Way of acting. **F. Ocasio Idorwatt, A.A. Ramírez Jiménez, L.I. Santiago**

514. Cave soil abiotic factors as an indicator of cave ecosystems. **D.M. Rosario Rojas, I.N. Serrano Rodríguez, K.A. Cartagena Rivera, R.N. Sanabria Dosal**, A.A. Acosta Colon

515. Characterization of pore structure of activated carbon manufactured from coffee waste. **O. Rogers**, **Q. Yang**, S. Youn

516. Optical properties and nanotoxicology of fluorescent CdS quantum dots. **E.A. Chaparro-Barriera**, S. Bailón-Ruiz

517. Effects of metal-containing SBA-15 materials on the aqueous photodegradation of acetaprimid. **R.** Liang, R. Manno, V. Sebastian, R. Luque

518. Fabrication of a composite nanostructured cellulose membrane for direct contact membrane distillation. **R. Joshi**, J. Zheng, T. Lindstrom, B.S. Hsiao

519. Exploring how to test the presence of bisphenol A (BPA) in various plastic water bottles through different analytical techniques. **S.M. Williams**, A. McGhee, J. Carvajal De Luna, R. Jawaid, H. Kouadio, E. Howard, L. Dean, D. Campos, A. Limones, M. Nelson, E. Thai, G. Scott, J. Siverand, N. Santos, M. Omary

520. Use of isothermal titration calorimetry and molecular docking to study cavity formation and desolvation effects in the binding of organic cations to organic matter. **S. Scott**, A.A. MacKay

521. Identification and bio-reactivity of chemical components of indoor dust and aerosol in palliative care clinic. K. Lui, **C. Suen**, K. Yeung

522. Ionic liquid - MOF composite materials for VOC capture from polluted air. V. Castillo Ramos, **W. Han**, H. Gao, X. Zhang, S. Zhang, K. Yeung

523. Quantification of trihalomethanes produced during chlorination of synthetic saline waters. **T.M. FitzGibbon**, J.D. Sivey

524. Selective adsorption and separation of dyes by dialdehyde cellulose and cationic dialdehyde cellulose. **X. Huang**, H. Zhuo, P. Hadi, B.S. Hsiao

525. Bromination of halosalicylates: Kinetics and product characterization. O.M. Driessen, J.D. Sivey

526. Stability of pharmaceuticals and personal care products in agricultural samples: Case study investigating effect of shipping and long-term storage on concentrations. **R. Dickman**, D.S. Aga

527. Investigation of functionalized metal-organic framework/polybenzimidazole mixed-matrix membrane for gas separation. **T. Chu**, B. Chang

528. Biofuels and slow release fertilizers for sustainable farm & food production waste management. **D. Mariuzza**, G. Lin, J.L. Goldfarb

529. Speciation, quantification, and release of arsenic bound to titanium dioxide (TiO₂, anatase) drinking water filter waste: Case study from the field to molecular scale. A. Zimmerman, **M.G. Siebecker**, D. Weindorf, V. Montero Campos, S. Deb, S. Ulate Chacón, G. Landrot

530. Carbon isotopic insights into processing of marine organic matter and transfer to sea spray aerosols. **D.R. Crocker**, R. Cao, J. Yin, M.H. Thiemens

531. Dominance of unintentionally-produced PCBs in the air of China. S. ZHAO, G. Zhang, K.C. Jones

532. Evaluating phenyltrimethylammonium as a probe compound for quantifying heterocyclic amine cation exchange to soils. **R. Rugama-Montenegro**, D. Vasudevan

533. Efficiency of polyhydroxyalkanoate (PHA) production from wastewater sludge. **B. DENG**, L. Rodriguez-Freire

534. Seasonal distribution of heavy metals in *Lemna minor* from a natural wetland. **T. Ulloa-Ponce**, **J. Rosa-Santiago**, **N. Cabán-González**, Y. Cortes Rosario, M.L. Ramos

535. Impact of surface oxidation on black carbon aerosols. **A. Wallace**, Q. Yao, A. Asa-Awuku, H. Fairbrother

536. Electrospinning of graphene and graphene oxide polymer composite membranes for water remediation. **S.G. Zetterholm**, J. Mattei-Sosa, J. Jefcoat, T.L. Thornell, C.S. Griggs

537. Quantification of estrogenic compounds by SPE-GC-MS in New Jersey natural and wastewater sources. **T.T. Handlovic**, J.D. Mizvesky, R. Wodzinski, J.D. Salierno, M.R. Elshaer

538. Absorption of estrogenic pollutants onto microfiltration membranes. S. Zhou, Y. Zuo

539. Strategies for the photoreduction of Tc-99 pertechnetate to low valent Tc by Keggin polyoxometalates. **I. Radivojevic Jovanovic, C.M. Gallagher, B.P. Burton-Pye, D.M. McGregor, W.W. Lukens, L.C. Francesconi**

540. Novel TA acid-metal complex coating layer for forward osmosis membrane with enhanced antifouling property. **S. Liu**, X. Tong, H. Gao, Y. Chen, J.C. Crittenden

541. Chlorine-free disinfection of water contaminated with *E.coli* by combination of electrolysis, ultrasonic and photochemical treatment: Role of hydroxyl radical formation and generation of singlet oxygen. **N. Barashkov**, T. Sakhno, I. Irgibaeva, A. Aldongarov

542. Dissolved organic matter percolated from periphyton in the Everglades: Characterization and interaction with mercury. **A. Anjuman**, Y. Cai

543. Coral's response to climate change: Characterization of coral's metabolome under varied pH conditions. **K. Gubsch**, J. Loewenstein, T. Schock

544. Phosphate removal by lanthanum-containing materials: Effect of alkalinity and pH on treatment effectiveness. **T. Stephen**, Y. Zhi, D.F. Call, D. Knappe

545. Use of gadolinium to track sewage effluent through the Poughkeepsie, New York water system. N. Fitzgerald, **M. Badia**, C. Bowser

546. Wildfires give rise to conditions encouraging disinfection byproduct formation. **P. Wilkerson**, Y. Yu, A. Retuta, H. Roth, F.L. Rosario, T. Borch

547. High performance of honeycomb-supported natural soda ash in the removal of hydrogen chloride gas. **N. Tsubouchi**, N. Matsuoka, K. Fukuyama, Y. Mochizuki

548. Determination of glyphosate, glufosinate and their metabolites concentrations in surface water along the Red River, northern Vietnam. C. Vu, P. Le, D. Chu, V. Bui, L. Phung Thi, J. Labanowski, L. Mondamert, M. Herrmann, P. Behra

549. Analysis of short, medium and long-chain PFAS in municipal wastewater effluents and environmental matrices. **G. Andaluri**, R.P. Suri

550. Developing software to connect aerodynamic and microscopic measurements on soot particles. **Y. Wu**, C. Hayes, B. Malouf, C. QIU

551. Aqueous bromate reduction by NZVI supported monometallic catalysts. E. Ramazanova, W. Lee

552. Solar induced emulsification of petroleum in neat films and films on water. **C. Brown**, C. Infante, A. Cluen-Brown, M. Giraudier, M.A. Tarr

553. Characterization of polar compounds released in urban runoff from three formulations of sealcoat. **A.E. Witter**

554. Pesticides concentrations in the atmosphere of an urban area in Brazil: Risk assessment for human health. **A.B. Yera**, S. Caumo, P.d. Vasconcellos

555. Characterization of soil carbon in native prairies and prairie restorations. J.D. Hill, E.O. Openiyi, **J.S. McConnell**

556. Simultaneous removal of radioactive Cs^+ and Sr^{2+} ions from wastewater by facile solid-state alkaliactivation of montmorillonite. **Y. Kim**, Y. Kim, D. Harbottle, J.W. Lee

557. Impact of shale gas extraction and other anthropogenic activities on surface water quality. **N.R. Mc Elroy**, A. Clark, A. Fagbuyi, B.W. Okey

558. Surface proclivity and interaction of emerging contaminants at the lipid monolayer membrane. **D. Deardorff**, G. Dalla Pozza, M. Subir

559. Poly(*N*-acryloylmorpholine)-grafted porous silica hybrid material for removal of organic dye from aqueous solution. **M. Islam**, M. Shahruzzaman, P. Haque, M. Rahman

560. Quantifying and imaging of membrane fouling using Raman chemical imaging. **S. Azizighannad**, W. Intrchom, S. Mitra

561. Characterization and photoreactivity of chromophoric marine-dissolved organic matter. **D. Gonzales**, M. Alves, D. Dang, K.A. Prather, V.H. Grassian

562. Determination of the equilibrium for 2-butanone with ice surfaces via static and dynamic experiments. **J. Huck**, R.R. Michelsen

563. Biodiesel production from waste cooked oil based on microwave irradiation and SrO catalyst. **R. Abu-Much**

564. Switchable hydrophilicity solvents: Single-droplet studies of CO₂-mediated solvent extraction in an intensified flow reactor. **S. Han**, K. Raghuvanshi, M. Abolhasani

565. Partitioning of 1-pentanol and ethanol to artificial snow surfaces. M. Askew, R.R. Michelsen

566. Bactericidal activity and mechanism of pulsed blue LED light. N. Zhan, W. Han, K. Yeung

567. New technology for controlling biofilm formation in water distribution system. **N. Zhan**, W. Han, Q. Wu, K. Yeung

568. Co-evolution of iron and phosphorous speciation during anaerobic digestion with inter-stage hydrothermal treatment of sewage sludge. **Q. Wang**, D. Patel, C. Zhang, P. Liu, H. Jung, B. Wan, S.G. Pavlostathis, Y. Tang

569. Electron-ionization gas chromatographic analysis of environmentally relevant chlorinated phenols. R.N. Leif, A.K. Vu, A. Alcaraz, **C.A. Valdez**

570. Enhanced reduction of doxycycline by sucrose modified NZVI. A. Akmanova, M. Babaa, W. Lee

571. Comparative laboratory studies of NO3 radical-initiated oxidation of monoterpenes. **A. Marsavin**, E. McLaughlin Sta. Maria, D. Draper, M. Dam, J. Smith, J.L. Fry

572. Interaction of small ketones with artificial snow surface. D. Teri, R.R. Michelsen

573. Investigating algae-derived reduced graphene oxide membranes for ionic and molecular nanofiltration. **D. Nde**, W. Zhao

574. Radiological and non-radiological leaching assessment of alkali-activated materials containing ground granulated blast furnace slag and phosphogypsum. **K. Gijbels**, S. Landsberger, P. Samyn, R. Iacobescu, Y. Pontikes, S. Schreurs, W. Schroeyers

575. Improved resolution of inorganic anions and oxyhalides in the presence of ethylenediamine. C. Shevlin, **P. Voelker**

576. Pefluorooctanesulfonate induces hepatomegaly and lipoatrophy in mice through phosphoenolpyruvate carboxykinase-mediated glyceroneogenesis inhibition. **Y. Liang**, **L. Wang**, H. Cao, Z. Zhou

577. Legacy phosphorus desorption from U.S. Mid-Atlantic agricultural soils. **M. Elavarthi**, K.D. Szerlag, D.L. Sparks

578. NMR-lipidomics measurement of Great Lakes mussels as an ecotoxicological assessment of areas of concern. **C. Welles**, K. Gubsch, E. Legrand`, W. Johnson, T. Schock

579. Photophysical characterization of phycocyanobilin to predict *in vivo* cyanobacteria health. **L.E. Dolmage**, D.C. Szlag, E.R. Trivedi

580. Controlling the pore sizes of graphene oxide nanostructures through hydrothermal reactions for efficient water purification. **M. Appiah-Kubi**, W. Zhao

581. Determining the pH of frozen and annealed acetic acid and sodium chloride solutions using infrared spectroscopy. **C. English**, R.R. Michelsen

582. Estimation of community drug use by detection and quantification of pharmaceuticals in wastewater using SPE and LC-MS/MS. **W. DeLafontaine**, L. Bartlett, T.H. Boles

583. Reduction rate of the hexavalent chromium in the presence of ascorbic acid: Kinetic study. **E. Pakas**, **C. Kim**

584. Mineralogical characterization of Fe(II)-oxidizing bacterial stalks. **R. Vigliaturo**, A. Marengo, E. Bitarello, I. Pérez-Rodríguez, G. Drazić, R. Gieré

585. Graphene oxide-MoS₂composite membranes for arsenic and lead polluted water purification. **K. Desai**, A. Basurrah, W. Zhao

586. Detection of toxins from harmful algae blooms: Identifying markers for Microsystin-LR. **I. Ledsky**, N.E. Olson, J. Shi, M. Cooke, J.A. Birbeck, S.J. Jacquemin, J. Westrick, D.G. Schmale, A.P. Ault

587. Exploring the relationship between the properties of biochar and heavy metal sorption. **a. lam**, T. Longbottom, O.R. Harvey

588. Melting point determination using a solar irradiation heat source. **B. Agee**

589. Industrial water corrosion control with nutrient free chemistries to minimize algal blooms and meet current and future discharge limits. **P.R. Frail**, J. Green, R. Hendel, C. Pierce

590. Role of inorganic chemistry in improving the sustainability of heterogeneous catalysts for oxyanion reduction. J. Liu, **J. Gao**, C. Ren

591. Is urban gardening safe in residential properties built prior to 1978? Field-assessment in the city neighborhoods of Rochester, NY. **D. Bolduc**, **M. Patton**, S. Zamule, P. Das

592. *In situ* synthesis of magnetic Fe₃O₄@plant polyphenol composite particles for *Chlorella vulgaris* harvesting. **X. Wang**, C. Liu, W. Zhang, W. Liang

593. Analysis of pesticide residues in strawberries: Multiresidue QuEChERS-LC-MS/MS method. **M. Li**, T. McManus

594. Properties analysis and quality comparative study of PET used plastic bricks. V. Retnaswamy

595. Promising FeOCl material for wastewater treatment: Controllable synthesis, modification and the investigation of H_2O_2 activation behavior. **J. Wang**

596. Brown carbon aerosol systems. J. Turley, D.O. Dehaan

597. Fate of nanoparticles in simulated gastric fluid studied using single particle-ICP-MS. **X. He**, H. Zhang, X. Shen, W. Liu, E. Sahle Demessie, H. Shi

598. Clean air: Critical review of benefits of the U.S. Clean Air Act Amendments of 1990 and worldwide implications. **S. Chitikela**

599. Water recovery from human urine by air gap membrane distillation (AG-MD). **Z. Hu**, **H. Yao**, W. Zhang

600. Antimicrobial air purification systems for effective improvement of indoor air quality in palliative care facility. **C. Suen**, K. Lui, T.N. Dy, Q. Chang, K. Yeung

601. Photophysical properties of coumarin-1 and coumarin-2 in water. **M. Khan**, J. Wu, C. Cheng, M. Akbar, B. Liu, C. Liu, J. Shen, Y. Xin, G. Mingming, L. Lu

602. Oil/water separation by using the photopolymerized porous hydrophobic and oleophilic materials. **N. Baig**, T.A. Saleh

Section A

Pennsylvania Convention Center Exhibit Hall A

Green Chemistry & the Environment

Cosponsored by CEI R. Luque, S. O. Obare, *Organizers*

5:00 - 7:00

603. CO₂ conversion by high-dose rate electron beam irradiation. **Y. Hosokawa**, S. Kajiya, A. Ohshima, N. Ishida, M. Washio, A. Usuki

604. Green approach for the synthesis of silica nanoparticles. H.A. Chauhan, A. Ahmad

605. Seasonal distribution of heavy metals in biotopes nearby the "Cavernas del Río Camuy" National Park. J. Torres Ayende, J.A. Velazquez Quintana, A. Santiago Cordero, L. Soto Ortiz, M.L. Ramos

606. Environmentally friendly clay filtration in the oil industry. A. Aranda, M.O. Montes

607. Bioaccumulation of heavy metals in West Texas. K. Driver

608. Fabrication of novel azo-linkage ion-exchange adsorbent based on green polymers for nitrate removal. **E. Tavakoli**, M. Browning, S. Kaviani, M. Bavarian, S. Nejati

609. Scalable and green synthesis of metal and metal alloy nanoparticles in a solid matrix. **M.T. Nguyen**, T. Yonezawa, K. Yu

610. Coenzyme vitamin B_{12} enhancing methane production during anaerobic digestion of food waste and mechanisms. **Y. Su**, Y. Chen

611. Investigation on methane production by threonine with L- and D-configurations. M. Wang, Y. Chen

612. Life cycle assessment and techno-economic analysis of epoxidized sucrose soyate: Novel biobased adhesive. **S. Ghasemi**, D.C. Webster, G. Pourhashem

613. Creation of a new fluorogenic estrogen-detecting sensor through computational modeling. **S. Watson**, S. Upadhyay, A. Dumi, D. Mulvey, C. Telmer

614. Investigating the enhanced solubility of carbon dioxide in nano-confined ionic liquids. **S. Kaviani**, T. Nguyen, A. Lopez, S. Nejati

Section A

Pennsylvania Convention Center Exhibit Hall A

Industrial Applications of Environmental Chemistry

T. Anumol, S. C. Lingenfelter, N. Lock, Organizers

5:00 - 7:00

615. Copper ferrocyanide functionalized with MIL-125 composites for Cs⁺ removal from aqueous solution. **J. Choi**, H. Kim, Y. Park, S. Cho, S. Choi

616. Morphology and adsorption removal of ^{110m}Ag in the radioactive waste liquid of the pressurized water reactor nuclear power plant. **Q. Zhao**

617. Assessing polyamide degradation kinetics by peracetic acid and chloramine using quartz crystal microbalance. **T.M. Mohona**, P. Nalam, N. Dai

Section A

Pennsylvania Convention Center Exhibit Hall A

Innovative & Practical Approaches for the Treatment of Per- & Polyfluoroalkyl Substances (PFASs)

J. Choe, Y. Choi, J. Liu, S. Vyas, Y. Wang, Organizers

5:00 - 7:00

618. Adsorption of zwitterionic and neutral per- and polyfluoroalkyl substances (PFASs) on differently charged cyclodextrin polymers. **C. Ching**, M. Klemes, W.R. Dichtel, D.E. Helbling

619. PFAAs identification and further classification through pKa analysis. M.C. Wedvik

620. Rapid and low energy degradation of PFAS in aqueous solutions by reverse vortex flow gliding arc plasma. **A. Lewis**, C. Sales

621. Bioelectrochemical treatment of per- ad Polyfluoroalkyl Substances (PFAS) using *Acidimicrobiaceae* sp. Strain A6. **W. Shuai**, M. Ruiz-Urigüen, S. Huang, P. Jaffe

622. Rational material design for rapid capture and detection of perfluoroalkyl species. **R. Khan**, A. Rehman, A. Othman, D. Andreescu, E. Andreescu

623. Design and application of a biological system for detection, sequestration, and degradation of polyand perfluorinated alkyl substances. **M. Mann**

624. Assessment of isotherm fittings on co-removal of trace concentration 14 per- and polyfluoroalkyl substance by various resins in groundwater matrix. **Y. Zhang**, R. Suri, M. Fuller, E.R. McKenzie

625. Assessment of endocrine disrupting effects of per- or polyfluoroalkyl substances on the H295R adrenocarcinoma cell line. **I. Running**, G. Atilla-Gokcumen, D.S. Aga

626. Application of electron beam for the degradation of short and long chain polyfluoroalkyl substances in drinking water. **K. Londhe**, C. Lee, S. Grdanovska, C. Cooper, T. Sullivan, D. Paquette, M. Mills, **A. Venkatesan**

627. Rapid removal of poly- and perfluorinated compounds from high conductivity water in a batch-scale plasma reactor. **R. Singh**, X. Su, R. Burlica, N. Multari, S. Mededovic, T.M. Holsen

628. Removal of per- and polyfluoroalkyl substances by anion-exchange fibers. **A. Feerick**, K. HE, L.M. Blaney

629. Determination of occurrence and levels of per- and polyfluoroalkyl substances (PFASs) in deer tissue. **S. Aponte**, M.E. Guardian, S. Travis, D.S. Aga

Section A

Pennsylvania Convention Center Exhibit Hall A

Macromolecule Biosynthesis, Biodegradation, & Applications in Environmental Bioprocesses

X. Mao, Y. Men, C. M. Sales, S. Yi, W. Zhuang, Organizers

5:00 - 7:00

630. Transformation of the neonicotinoid insecticides, thiamethoxam and imidacloprid, by select bacterial species. **C. Dupre**, **M. Mendola**, S. Zamule, P. Das

631. Photo-induced Fenton chemistry of naturally occurring ferritin. **J.N. Mason**, E.B. Cerkez, D.R. Strongin

632. Manganese loaded ferritin for hydrogen peroxide decomposition. **M. Gomez**, A. O'Brien, E.B. Cerkez, D.R. Strongin

Pennsylvania Convention Center Exhibit Hall A

Micro- & Nano-Plastics in the Environment: Detection, Characterization, Fate & Impact

S. R. Al-Abed, M. J. Gallagher, P. Potter, Organizers

5:00 - 7:00

633. Geospatial distribution and fate of microplastics in the Hudson-Raritan estuary. **K. Sipps**, K. Bailey, K. Walsh, R. Chant, G. Saba, N. Fahrenfeld, G.A. Arbuckle-Keil

634. Evaluation of microplastic load in a waste water treatment plant (WWTP). C. Ekechi, T.H. Boles

635. Investigating the fate and biological impacts of polystyrene nanoplastics on *Shewanella oneidensis* MR-1. **V. Fringer**, L. Fawcett, D.M. Mitrano, M.A. Maurer-Jones

636. Aqueous photochemistry of polyolefins. T. Mundhenke, M.A. Maurer-Jones

637. Release and transformation of organic additives from polymers in aqueous media. **C.L. Smith**, A. Wallace, Z. Zhang, C. Prasse, H. Fairbrother

Section A

Pennsylvania Convention Center Exhibit Hall A

Performance of Stormwater Treatment Systems Under Changing Environments

Cosponsored by GEOC T. Dittrich, S. K. Mohanty, S. Ravi, *Organizers*

5:00 - 7:00

638. Comparison of different filter media materials for metals removal from urban stormwater runoff using green stormwater infrastructure. **N. Esfandiar, R.P. Suri, E. McKenzie**

639. Fe-OM coprecipitation and its effects on bioavailability of Cu and OM to denitrifying organisms. R. Mendes, **T.M. Vadas**, A. Helton

640. Determination of optimum dosage of chemical coagulant/flocculants needed for sludge treatment. I. Asia

641. Metabolization of tire wear products in synthetic stormwater by three model white rot fungi. **E. Wiener**, G.H. LeFevre

WEDNESDAY MORNING

Section A

Sofitel Philadelphia at Rittenhouse Square Strasbourg

Aquatic Photochemistry

Cosponsored by CEI W. Arnold, G. McKay, *Organizers* K. P. McNeill, *Organizer, Presiding*

8:30 642. Dissolved organic matter as a photochemical source of reactive species: Current challenges and implications for the fate of aquatic contaminants. **S. Canonica**

8:50 643. Investigation of the phototransformation mechanisms of benzotriazole in surface waters using compound-specific isotope analysis. L. Wu, E. Passeport

9:10 644. Investigating the photodegradation of triclosan's photodegradation products: Chlorinated dibenzo-p-dioxins and hydroxylated biphenyls. **J. Apell**, K.P. McNeill

9:30 645. Fluorinated photoproduct formation from photolysis of pharmaceuticals and agrochemicals. **Q. Whiting**, W. Arnold, W.C. Pomerantz

9:50 646. Initial photochemical fate of dissolved amino acids in natural aquatic environment by coupling theoretical calculations and experiments. **D. Minakata**, B. Barrios, R. Kibler, P. Doskey

10:10 Intermission.

10:25 647. Interactions of light and chemical reactions in the aquatic environment: Kinetic and mechanistic aspects. **R.G. Zepp**

10:55 Discussion.

11:00 648. Photochemical production of dissolved inorganic carbon from terrestrial organic matter: Significance to the oceanic organic carbon cycle - then and now. **W.L. Miller**, K. Ma, L. Powers, J.A. Brandes

11:20 649. Coupling of multivariate statistics and advanced analytical techniques for understanding the composition of terrestrial organic matter and its changes during photo-irradiation. **A. Goranov**, A. Bryan, H. Chen, P. Hatcher

11:40 650. Sunlight converts polystyrene to carbon dioxide and dissolved organic carbon. **C. Reddy**, C. Armstrong, A.N. Walsh, J. Jackson, C.P. Ward

Sofitel Philadelphia at Rittenhouse Square Nice

Sensors & Biosensors for Widespread Environmental Monitoring

V. V. Rajasekharan, M. Romero-Gomez, W. Zhang, Organizers T. Li, P. L. Schorr, Organizers, Presiding

8:30 Introductory Remarks.

8:35 651. Nanoprobes for surface-enhanced Raman spectroscopy (SERS) based pH sensing in confined microenvironments. **H. Guo**, Q. Huang, L.C. Marr, P.J. Vikesland

8:55 652. Nanomaterial-based portable sensor for phosphate detection in eutrophic water. **F.M. Mustafa**, E. Andreescu

9:15 653. Chemical fingerprinting applied to environmentally relevant media. **M. Bonizzoni**, M.H. Ihde, Y. Xu

9:35 654. Sensitive detection and identification of antibiotic resistance genes (ARGs) enabled by surfaceenhanced Raman scattering (SERS) and multiclass support vector machine (MC-SVM). **S. KANG**, P.J. Vikesland

9:55 655. Genetically programmed optical biosensor for point-of-care pathogen detection. **Y. Wu**, C. Wang, N. Wei

10:15 Intermission.

10:30 656. Development of a colorimetric sensor for detection of PFOA and PFOS in water. M. Nayunigari, G. Andaluri, R.P. Suri

10:50 657. Characterize the chemical moiety and pH distribution at dynamic environmental interfaces with Raman spectroscopy. **Q. Huang**, P.J. Vikesland

11:10 658. Magnetic and electrically conductive polypyrrole nanoparticles as highly effective materials for heavy metal removal and sensing. **F. Hosseini Narouei**, D. Frascatore, E. Andreescu, D. Andreescu

11:30 659. Electrochemical determination of copper ions in water using polyacrylic-graphene-thiourea modified electrode. **N.B. Abdul Razak**, S.B. Hasbullah, L. Tan

11:50 Closing Remarks.
Sofitel Philadelphia at Rittenhouse Square Versailles

Advancing Chemical Oxidation & Reduction for Addressing Emerging Environmental Issues

Y. Deng, X. Guan, W. Song, Organizers H. Zhang, Organizer, Presiding

8:00 Introductory Remarks.

8:05 660. Chelating agents that offer insight into the speciation and reactivity of unusual oxidation states of manganese, iron, and copper. **A.T. Stone**

8:35 661. Enhancing water supply with ferrate(VI). Y. Deng

8:55 662. Assessment of activated ferrate oxidation for wastewater reuse. **J. Goodwill**, C. Spellman, C. Antolini, D. Hayes

9:15 663. Development of fluorescence surrogates to predict the iron(VI) oxidation of pharmaceuticals in wastewater effluents. **W. Song**

9:35 664. Withdrawn.

9:55 Intermission.

10:10 665. Redox reactions of iron and manganese oxides in complex systems. H. Zhang

10:40 666. Oxidation of H-phosphonate and other overlooked P(III)-containing oxyanions: Interconnections between speciation and reactivity. **W. Liao**, Y. Yuan, A.T. Stone

11:00 667. Formation of nitromethane during wastewater ozonation and implications for direct potable reuse. **D. McCurry**, J.L. Shi

11:20 668. Impact of dissolved organic matter composition on the formation of regulated and novel disinfection byproducts during chlorination. **R.P. Milstead**, C.K. Remucal

11:40 669. Application and prospects of UV-LED disinfection in drinking water treatment. B. Xu

Sofitel Philadelphia at Rittenhouse Square Montpellier

Innovative & Practical Approaches for the Treatment of Per- & Polyfluoroalkyl Substances (PFASs) / PFAS Detection & Biological Methods for PFAS Remediation

J. Choe, Y. Choi, J. Liu, Organizers S. Vyas, Y. Wang, Organizers, Presiding

8:00 Introductory Remarks.

8:05 670. Improved solid phase extraction of perfluoroalkyl substances using automation. J. Hu, C. Shevlin

8:25 671. Development of a rapid PFAS screening tool for drinking water. **G.F. Peaslee**, J.T. Wilkinson, S.R. McGuinness, M. Tighe, M. Lieberman

8:45 672. Volatile per- and polyfluoroalkyl substances released from aqueous film-forming foam. **I. Abusallout**, D. Hanigan

9:05 673. Application of COSMO-RS-derived octanol-water partition coefficients in characterizing emerging per- and polyfluoroalkyl substances. **S. Simpson**, M. Guardian, P. Vexelman, D.S. Aga

9:25 674. Per- and polyfluoroalkyl substances: Computational insight. Y. Eken, T. Lai, A.K. Wilson

9:45 Intermission.

10:00 675. Structural dependence of microbial reductive defluorination of per- and polyfluoroalkyl substances. Y. Men, Y. Yu, K. Zhang, Z. Li, C. Ren, J. Liu

10:30 676. Biotransformation and biodefluorination of FTCAs by actinomycetes. **C. Wu**, Q. Wang, H. Chen, M. Li

10:50 677. Sorption and desorption behavior of PFOS and PFOA onto a gram-positive and a gram-negative bacterial species. **M.L. Butzen**, J.T. Wilkinson, S.R. McGuinness, G.F. Peaslee, J. Fein

11:10 678. Interactions between Lemna minor (common duckweed) and PFAS intermediates: Perfluorooctanesulfonamide (PFOSA) and 6:2 fluorotelomer sulfonate (FTSA). **W. Zhang**, Y. Liang

11:30 679. PFAS distribution in contaminated soils and impact on rhizosphere and plant microbiota. **B. Wang**, L. Rodriguez-Freire

11:50 Closing Remarks.

Sofitel Philadelphia at Rittenhouse Square Paris Ballroom

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

Cosponsored by CEI T. Anumol, R. Marfil-Vega, T. M. Young, C. Zwiener, Organizers, Presiding

8:30 Introductory Remarks.

8:35 680. Efforts to determine best practices for using metabolomics for environmental monitoring. **S.R. Campagna**, A.L. May, S. Rosalina, Z. Tasnim, Y. Xie, F. Loeffler, D. Taggart

8:55 681. Impact of chlorinated compounds on natural organic matter analysis by ultrahigh resolution-mass spectrometry. **J.R. Laszakovits**, A. Somogyi, A.A. MacKay

9:15 682. Online gas chromatograph with thermal desorption preconcentrator and high-resolution time-of-flight mass spectrometric detection for measurement of volatile organic compounds. **M. Claflin**, J. Krechmer, M. Canagaratna, B.M. Lerner, J.T. Jayne, D.R. Worsnop

9:35 683. Analysis of persistent organic pollutants (POPs) by high-resolution GC/MS. S. Nieto, M. Curtis, **A. Andrianova**, P. Dumas

9:55 Intermission.

10:10 684. Benefits of sharing chemical structure data from commercial spectral databases for improved curation and chemical identification. A.J. Williams, C. Lowe, A. McEachran

10:30 685. Determination of pesticide occurrence in private wells by high-resolution mass spectrometry. N. Alexander, C. Ball, D. Knappe

10:50 686. Pesticide exposure in drinking water and biomarker detection in human urine using high-resolution orbital ion trap mass spectrometry. **C.L. Sweeney**, G. Gagnon, J. Kim, Y. Park, D. Shea, M. Ryan

11:10 687. Characterizing organic micropollutants in Onondaga Lake sediment traps using energized dispersive guided extraction coupled to liquid chromatography-high resolution mass spectrometry. **B.L. Murphy**, S. Wang, T. Zeng

11:30 Panel Discussion.

11:50 Closing Remarks.

Sofitel Philadelphia at Rittenhouse Square Marseilles

ACS Award for Creative Advances in Environmental Science & Technology

Chemical Processes, Exposures & Effects in the Environment

Cosponsored by PROF S. O. Obare, V. K. Sharma, *Organizers* S. J. Eisenreich, *Presiding*

8:15 Introductory Remarks.

8:20 688. PCB congeners in air and food of rural and urban communities in the United States midwest. **K.C. Hornbuckle**

8:45 689. Electronic waste recycling by the informal sector is a potential source for a cocktail of hazardous organic compounds in Indian cities: Atmospheric transport and risk assessment. **P. Chakraborty**, S. Sakthivel, B. Prithviraj, M. Mukhopadhyay, M. Nakamura, A. Cincinelli, H. Gadhavi

9:10 690. Towards integrated monitoring and holistic process understanding of pollutants. H. Zhang

9:35 691. Living the impossible dream: Measuring environmental mixture toxicity by combining equilibrium passive sampling and dosing. **K.E. Smith**, Y. Jeong, D. Kämpfer, H. Fuchte, A. Schäffer

10:00 Intermission.

10:15 692. Investigation of legacy and emerging organic contaminants in top predators and their prey to support chemicals management. **A. Cincinelli**, N. Alygizakis, R. Dekker, G. Duke, G. Gkotsis, N. Glowacka, B. Knopf, J. Koschorreck, T. Martellini, E. Carretti, D. Randazzo, S. Santini, P. Movalli, M. Nika, V. Nikolopoulou, M. Oswaldova, A. Badry, H. Rüdel, R. Shore, E. Chadwick, P. Jepson, M. Juergens, N.S. Thomaidis, g. treu, J. Slobodnik

10:40 693. Interactions between anthropogenic dissolved organic carbon and marine microorganisms: Implications at regional and global scales. **J. Dachs**, E. Cerro-Gálvez, A. Martínez-Varela, G. Casas, P. Casal, M. Fernández-Pinos, G. Belén, M. Vila-Costa

11:05 694. Trait driver ecological theory predicts complex responses of phytoplankton exposed to chemical stress. **L. Nizzetto**

11:30 Discussion.

11:45 Concluding Remarks.

Bridging Surface Science to Catalysis

Sponsored by CATL, Cosponsored by COLL, ENFL and ENVR

Meeting the Challenges of Heterogeneous Catalysis Controlled at Atomic Level

Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

Catalytic Conversion of Renewable & Waste Carbon Sources: Approaches to Improve Carbon Utilization

Sponsored by CATL, Cosponsored by ENFL and ENVR

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Materials & in Operando Methods / Metal Organic Frameworks & Composite Materials: Interaction with Threat Agents & Ambient Gases

Sponsored by CATL, Cosponsored by ENFL and ENVR

Recent Advances in Plasma-Enhanced Catalysis / **Fundamentals of Excited Processes at Surfaces** Sponsored by CATL, Cosponsored by ENFL, ENVR and PHYS

WEDNESDAY AFTERNOON

Section A

Sofitel Philadelphia at Rittenhouse Square Strasbourg

Aquatic Photochemistry

Cosponsored by CEI G. McKay, K. P. McNeill, *Organizers* W. Arnold, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 695. Reactive nitrogen species: Neglected radicals in the UV/monochloramine process. Z. Wu

1:25 696. Improved UV degradation of microcystin-LR by a novel KrCl excilamp. N. Hull, Z. Leciejewski

1:45 697. Development of quinine as a fluorescent probe compound for quantifying hydrated electron. **G. McKay**, D.J. Van Hoomissen, S. Vyas, T.J. Strathmann

2:05 698. Modeling the kinetics of UV/peracetic acid advanced oxidation process. T. Zhang, C. Huang

2:25 699. Wavelength dependence of E.coli photoreactivation in the presence of DOM. **M. Maghsoodi**, S. Snow, G. Lowry, I. Smith

2:45 Intermission.

3:00 700. Impact of sunlight on the fate of oil spilled in aquatic environments. M.A. Tarr

3:20 701. Photoaging of atmospheric particulate matter in the aqueous phase. **F. Leresche**, J. Salazar, D.J. Pfotenhauer, M.P. Hannigan, B.J. Majestic, F.L. Rosario

3:40 702. Impact of halogen radicals on dissolved organic matter transformation during chlorine photolysis. **C.K. Remucal**, D. Bulman

4:00 703. Photochemical transformation of Fe in the presence of natural organic matter (NOM): Implications to Fe availability and NOM transformation. **S. Garg**, T. Waite

4:20 704. Effects of sunlight on haloacetonitrile formation potential from wastewater effluents. **J. Xu**, Z.T. Kralles, C.H. Hart, N. Dai

Sofitel Philadelphia at Rittenhouse Square Nice

Sensors & Biosensors for Widespread Environmental Monitoring

T. Li, P. L. Schorr, Organizers V. V. Rajasekharan, M. Romero-Gomez, W. Zhang, Organizers, Presiding

1:00 Introductory Remarks.

1:05 705. Development of a poly(*N*-isopropylacrylamide)-based sensor for persistent per- and polyfluoroalkyl substances. **D. Savage**, J.Z. Hilt, T. Dziubla

1:25 706. Development of a simple analytical method for determination of Arsenate using FAM-labeled DNA and cerium oxide nanoparticles. **K. Matsunaga**, R. Hirano, H. Satoh

1:45 707. DNA-based tracers for hydrologic characterization. V. Kapoor, J. Green

2:05 708. Did we really use the intrinsic fluorescent properties of nitro-factualized metal-organic frameworks (MOFs) to realize H₂S detection in an aqueous system? **Z. ZHU**, **x. he**, **W. Wang**

2:25 709. Cross-linked UIO-66-NH₂/PIM-1 sensors for room temperature CH₄ detection. **T. Hong**, A. Sekizkardes, J. Culp, K. Kim, P. Ohodnicki

2:45 Intermission.

3:00 710. Bioenergetics by Lehninger coupled with "horizontal" nutrient transfer and "real time" spectrophotometric sensors offers an alternative explanation for algal blooms. **P.L. Schorr**

3:20 711. Self-immolative systems for the disclosure of reactive electrophilic alkylating agents. **F. Leroux**, W. Hayes, A.T. Russell, M. Sambrook

3:40 712. Use of airborne and ground-based physical and chemical sensors for monitoring tidal wetlands enhancement projects. M. Yepsen, **R.L. Lippincott**

4:00 713. Design and performance of a portable device for characterizing indoor and outdoor air. **H. Ravindran**, S. Sur, S. Dhaniyala

4:20 Closing Remarks.

Sofitel Philadelphia at Rittenhouse Square Versailles

Advancing Chemical Oxidation & Reduction for Addressing Emerging Environmental Issues

Y. Deng, W. Song, H. Zhang, Organizers X. Guan, Organizer, Presiding

1:00 Introductory Remarks.

1:05 714. Remediation with zerovalent metals more strongly reducing than iron. **P.G. Tratnyek**, G. Lee, J.Z. Bandstra

1:35 715. Degradation of triclosan by reduced nano-biochar. S. Lokesh

1:55 716. Highly efficient Au@3-D carbon nitride nanocomposites for ultrafast recyclable reduction of nitroarenes. T. Nguyen, **R. Doong**

2:15 717. Degradation efficiency of chlorinated hydrocarbons by a novel functionalized iron nanoparticle for improved remediation of contaminated sites. **Y. Zhang**, S. Ghoshal

2:35 718. Catalytic degradation of p-nitrophenol by nano zerovalent iron (nZVI) supported bimetallic catalyst. **G. Tokazhanov**, W. Lee

2:55 Intermission.

3:10 719. Continuous improvements on advanced reduction technologies for challenging oxyanions and fluorinated chemicals. J. Liu, C. Ren, J. Gao, T. Liu, M.J. Bentel

3:40 720. Potential application of metallic Mg milling scraps as a green and powerful contaminant reductant. **H. Ryu**, P.G. Tratnyek, G. Lee

4:00 721. Development of quantitative structure activity relationships (QSARs) for abiotic reduction of organic chemicals. **Y. Gao**, H. Zhang

4:20 722. UV/sodium percarbonate for the degradation of bisphenol A. J. Gao, X. Duan, D.D. Dionysiou

4:40 723. Efficient bromide removal from produced water by peroxymonosulfate for controlling disinfection byproduct formation in downstream water supplies. **K. Huang**, H. Zhang

Sofitel Philadelphia at Rittenhouse Square Montpellier

Innovative & Practical Approaches for the Treatment of Per- & Polyfluoroalkyl Substances (PFASs) / Materials & Models for PFAS Sorption & Ion-Exchange

J. Liu, S. Vyas, Organizers J. Choe, Y. Choi, Y. Wang, Organizers, Presiding

1:00 724. Electrosorption of perfluoroalkyl substances onto activated carbon. **D.F. Call**, S. Zhu, E. Hossen, Z. Hopkins, D. Knappe

1:20 725. Sorption behavior of perfluoroalkyl substances (PFASs) using on organic surface functionalized metal oxide nanoparticles. **J. Lee**, C. Kim, J. Fortner

1:40 726. Sorption of PFOA and PFOS on organic-modified Ca-montmorillonite: Effect of modifier structure. **Q. Dong**, Y. Wang

2:00 727. Anion-exchange membranes for passive sampling of per- and polyfluoroalkyl substances. **K. HE**, A. Feerick, L.M. Blaney

2:20 728. Ionic fluorogels as for PFAS remediation from water. F.A. Leibfarth

2:45 Intermission.

2:55 729. Determination of adsorbable organic fluorine as a surrogate to total PFASs in water samples. **Y. HAN**, M. Sun

3:15 730. Development of a predictive model for ion exchange treatment of mixtures of per- and polyfluoroalkyl substances (PFASs). **A. Ellis**, Y. Fang, C.P. Higgins, C. Schaefer, R.F. Carbonaro, T.H. Boyer, T.J. Strathmann

3:35 731. Evaluating the efficiency of various anion exchange resins for removing legacy and emerging per- and polyfluoroalkyl substances (PFAS). **Y. Liu**, M. Sun

3:55 732. Effective adsorption removal of short-chain polyfluoroalkyl and perfluoroalkyl substances (PFASs) using biochar. **N. Liu**, M. Li

4:15 733. Adsorption of PFAS by granular activated carbon: Scale-up of bench-scale data and factors controlling GAC use rates. **Z. Hopkins**, D. Knappe

4:35 734. Use of biochar from biosolid pyrolysis for PFAS management in landfills: Technical and economic feasibility. **N. Jesmani**, R. Tehrani, C. Curran

4:55 Closing Remarks.

Sofitel Philadelphia at Rittenhouse Square Paris Ballroom

General Papers in Environmental Chemistry / Environmental Processes

S. O. Obare, Organizer V. Dozortsev, Presiding

1:00 Introductory Remarks.

1:05 735. Design of porous MOF/polymer composites for selective and enhanced chemical separations in aqueous media. **D. Sun**

1:25 736. Speciation of legacy P in soils using multi-modal μ-XRF mapping and μ-XANES. **K.D. Szerlag**, F. Izaditame, P. Northrup, M.G. Siebecker, R. Tappero, D. Jaisi, D.L. Sparks

1:45 737. Understanding and application of genetically induced bacteriophage/nano-particle interactions in the environment. **R. Goel, E. Gilcrease**

2:05 738. Remediation of crude oil contaminated soil: Comparison of normal and microwave pyrolysis. U. Bassey, J. Robinson, C.E. Snape

2:25 739. Harnessing the power of stannous for trace metal remediation. V. Dozortsev

2:45 Intermission.

3:00 740. Role of solvent polarity and hydrogen bonding on nitrate radical reactivity. **M. Paradzinsky**, J. Tanko

3:20 741. Effects of affinity and aqueous speciation on uranium(VI) removal by ion exchange drinking water treatment processes. **M. Carolan**, T. Forbes, D.M. Cwiertny

3:40 742. Withdrawn.

4:00 743. Interfacial properties and crystalline transformations of doped MgO and MgCO₃ particles during nutrient (N and P) recovery from aqueous solutions. M. Silva, M. George, C. Sayes, **J. Baltrusaitis**

4:20 Closing Remarks.

Bridging Surface Science to Catalysis

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THURSDAY MORNING

Section A

Sofitel Philadelphia at Rittenhouse Square Strasbourg

Aquatic Photochemistry

Cosponsored by CEI W. Arnold, K. P. McNeill, *Organizers* G. McKay, *Organizer, Presiding*

8:30 744. Investigation of the production of hydroxylating species from DOM model sensitizers. **K.D. Couch**, F. Leresche, G. McKay, F.L. Rosario

8:50 745. Sunlight photodegradation of pharmaceuticals in land-applied biosolids: Case study of ibuprofen and naproxen. L. Su, N. Dai

9:10 746. Photochemical stability and degradation of carbon dots. **L.R. Sigmon**, B. Frank, A. Deline, B. Zhi, M.J. Gallagher, C.L. Haynes, H. Fairbrother

9:30 747. Photochemical fate of disinfection by-products formed during seawater desalination processes. L. **Powers**, P. Schmitt-Kopplin, M. Gonsior

9:50 748. Investigating effect of pH and ionic strength on surface adsorption of natural organic matters on TiO₂ nanoparticles. M. Maghsoodi, S. Snow

10:10 Intermission.

10:20 749. Photochemical fate of triphenyltin hydroxide in natural and engineered water systems: Reaction kinetics, transformation products, and residual toxicity. **M. Hopanna**, K. HE, C. Prasse, L.M. Blaney

10:40 750. Carbonate radical oxidation of cyanotoxins and its environmental application. Z. Hao, **S. Yan**, L. Lian, J. Ma, W. Song

11:00 751. Withdrawn.

11:20 752. Fundamental studies of the singlet oxygenation of Melanin model compounds: Product and mechanistic studies. **M. Jaramillo**, K.E. O'Shea

11:40 753. Withdrawn.

Sofitel Philadelphia at Rittenhouse Square Nice

General Papers in Environmental Chemistry / Environmental Remediation: Design Materials & Removal Strategies

S. O. Obare, Organizer W. Den, Presiding

8:00 Introductory Remarks.

8:05 754. Chitosan crosslinking into magnetic multi-walled carbon nanotubes beads for efficient Cr(VI) removal. A. Mohammed Islam, H. Kuo, **W. Den**

8:30 755. Hydroxyapatite is not an adsorbent: Shifting the paradigm on how HAP removes fluoride from water. **D. Mosiman**, B.J. Marinas

8:50 756. Rapid photocatalytic degradation of glyphosate by palladium-decorated *m*-BiVO₄/BiOBr nanosheets. S. Abaddi, N. Ensinger, **E.M. Zahran**

9:10 757. Developing best practices for combining fluorescence microscopy and water flux measurements to elucidate biofouling mechanisms. C. Widing, N.R. Ruffle-Deignan, **E.M. Stennett**

9:30 758. Removal of amoxicillin using activated carbon manufactured from coffee waste. **I. Kim**, **Y. Ha**, Q. Yang, **S. Youn**

9:50 Intermission.

10:05 759. Micromixers with bi-directional flow enhancing features to minimize scaling effects on reverse osmosis membranes. J. Walker

10:25 760. DPPC liposomes reveal their remarkable capacity to entrap an emerging class of environmental pollutants. A. Lozano, **M.D. Rieth**

10:45 761. Rational design of cerium-based metal-organic framework for the efficient uptake of phosphate from water. M.H. Hassan, R. Stanton, D.J. Trivedi, E. Andreescu

11:05 762. One-step tailoring surface roughness and surface chemistry to prepare superhydrophobic polyvinylidene fluoride (PVDF) membranes for enhanced membrane distillation performances. **W. Qing**, X. Shi, C.Y. Tang, W. Zhang

11:25 Closing Remarks.

Section C

Sofitel Philadelphia at Rittenhouse Square Versailles

General Papers in Environmental Chemistry / Environmental Processes

S. O. Obare, Organizer E. Marti, Presiding

8:00 Introductory Remarks.

8:05 763. Vertical profiles of therapeutic opioids and other pharmaceutical chemicals in sediment cores obtained from tidal marshes and river embayments in the Potomac River estuary, Virginia-Maryland, USA. **G.D. Foster**, A. Leahigh, W. Lominac, C. Hunter, E. Lang, T.B. Huff, R. McBride

8:25 764. Computational study of THz spectra of fentanyl and its analogs. **C. Wang**, A. Masunov, A. Terracciano, S. Vasu

8:45 765. Near real-time determination of the prevalence of illicit drugs, cannabinoids, cathinones, and synthetic opioids in four rural counties in Illinois using wastewater-based epidemiology. **C. O'Rourke**, B. Subedi

9:05 Intermission .

9:20 766. Development of an *in situ* self-template strategy for highly efficient PVDF/Cu-BTC composite ultrafiltration membrane. **Y. Luan**, X. Li

9:40 767. Nexus of natural and engineered nanomaterial: Biofilm eradication using magnetic phagenanocomposite conjugates. **P. Yu**, P.J. Alvarez

10:00 768. Withdrawn.

10:20 769. Alternative to analytical chemistry for assessing disinfection byproducts in potable water reuse. E. Marti, M. Attene-Ramos, **G. Kajjumba**

10:40 770. Low cost polyamine-modified graphene composites for effective mercury remediation in water. **P. Yap**, T. Tung, S. Kabiri, D. N.H. Tran, D. Losic

11:00 Closing Remarks.

Sofitel Philadelphia at Rittenhouse Square Montpellier

Advancing Chemical Oxidation & Reduction for Addressing Emerging Environmental Issues

Y. Deng, X. Guan, H. Zhang, Organizers W. Song, Organizer, Presiding

8:30 Introductory remarks.

8:35 771. Rapid transformation of H₁-antihistamines cetirizine (CET) and diphenhydramine (DPH) by peroxymonosulfate (PMS). X. He, **K.E. O'Shea**

9:05 772. Advancing heterogeneous catalytic ozonation for water treatment and reuse. W. Yang, X. Chen, M. Bunian, Y. Lei, **T. Wu**

9:25 773. Advanced oxidative destruction of cyanide by radicals generated from an activated iron media/O₂ system. C. Zhang, **Y. Huang**

9:45 774. Solar photoelectrochemical production of reactive oxidants as a sustainable method of water treatment. **W. Choi**, M. Koo, T. Jeon

10:15 775. Oxygen vacancy promoted heterogeneous fenton-like degradation of ofloxacin at pH 3.2-9.0 by Cu substituted magnetic $Fe_3O_4@$ FeOOH nanocomposite. **X. Tian**, H. Jin, Z. Zhou

10:35 Intermission.

10:40 776. Transformation of emerging contaminants during oxidation processes: Paying more attention to toxicity variation. **Z. Qiang**, H. Dong

11:10 777. Electrocatalytic degradation of short- and long-chain perfluoroalkyl substances (PFASs) at boron doped diamond (BDD) and Ti/RuO₂ electrodes: Effect of operational parameters and water matrix. R.P. Suri, **S. Barisci**

11:30 778. Withdrawn.

11:50 779. Effect and mechanism of NaClO-Fe(II) conditioning on the treatment of cyanobacteria-laden water and the dewatering performance of cyanobacteria-containing sludge. **M. Wu**, Y. Tang

12:10 780. Modulations of Bi_2MoO_6 for photocatalytic performance enhancement under visible light illumination. Q. Li

Section E

Sofitel Philadelphia at Rittenhouse Square Paris Ballroom

General Papers in Environmental Chemistry

S. O. Obare, Organizer, Presiding

8:00 Introductory Remarks.

8:05 781. Delivering an integrated data hub for opioid and cannabinoid chemicals via the US-EPA CompTox Chemicals Dashboard. **A.J. Williams**, C. Lowe

8:25 782. Coupled transformation of iron and phosphorous speciation during anaerobic digestion with hydrothermal pretreatment of sewage sludge. **Q. Wang**, C. Zhang, D. Patel, H. Jung, P. Liu, B. Wan, S.G. Pavlostathis, Y. Tang

8:45 783. U(IV) adsorption onto montmorillonite in an anoxic environment. **A. Satpathy**, J.G. Catalano, D. Giammar

9:05 784. Determining the growth capability of airborne methanotrophs. **K. Dillon**, V. Krumins, T. Han, G. Mainelis, L. Kerkhof, D.E. Fennell

9:25 Intermission.

9:40 785. Dibenzopyrenes and Benzo[c]fluorene as strong candidates for an extended list of priority pollutants. **J. Andersson**

10:00 786. Validation testing of disinfection and environmental parameters in ISO 30500: New international standard for chemistry-driven onsite sanitation systems. **C. Cid**, M.R. Hoffmann

10:20 787. Nutrient removal from blackwater using natural zeolites. L. Trotochaud, B.T. Hawkins, J.T. Glass, B.R. Stoner

10:40 788. Beyond Wood's metal: Low melting alloys made from it. S.P. Kosmas, S. Seagram, S. Plieth, S. Hedglin, **M.A. Benvenuto**

11:00 Discussion.

11:15 Closing Remarks.

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THURSDAY AFTERNOON

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Division of Environmental Chemistry 259th ACS National Meeting

Abstracts

Philadelphia, PA March 22-26, 2020

BioManufacturing with Intelligent Adaptive Control (BioManIAC)

Babetta L. Marrone¹, blm@lanl.gov, Carl Iverson², Ghanshyam Pilania³. (1) Bioscience, Los Alamos National Laboratory, Los Alamos, New Mexico, United States (2) Chemistry, Los Alamos National Laboratory, Los Alamos, New Mexico, United States (3) Materials Science & Technology, Los Alamos National Laboratory, Los Alamos, New Mexico, United States

Plastics made from petroleum are a mainstay in our daily lives, but the environmental problems they create are driving an urgent search for sustainable, bio-based alternatives. Ideally, we look to bio-based plastics to be sufficiently durable for specific applications, but more easily degradable in the environment. Bio-derived molecules have more diverse chemical functionalities than those of petroleum-based molecules and therefore offer a rich resource for discovering new monomers for synthesis of novel biopolymers for conversion into plastics materials with performance advantages. In the BioManIAC project, we are using polyhydroxyalkanoate (PHA)-based polymers synthesized naturally in cyanobacteria as a model system; and developing machine learning (ML) tools to optimize monomer-topolymer discovery and design. To develop new biopolymers with desired material properties, we need to gain a better understanding of what is possible to produce biosynthetically; and what biopolymer chemistries would be needed to achieve the desired biopolymer properties. Thus, we are developing adaptive ML approaches to understanding of both the enable chemical structure:property relationships of the PHA class of biopolymers (Chemistry Loop) and the biosynthetic routes that can be used or improved to biologically synthesize such polymers (Biology Loop). The Biology Loop uses DNA sequence, protein family, and metabolomics databases for comparison of metabolic diversity among target cyanobacterial strains. The Chemistry Loop uses a database of physical and mechanical characterization data for known PHA polymers taken from the literature. The Biology and Chemistry Loops will be supplemented with in-house experimental data on polymer biosynthesis, chemical synthesis, materials testing, and degradation studies. Our ML approach and workflow consists of domain-knowledge-based feature selection, feature engineering, machine learning model training, and validation and optimization routines for efficient polymer property predictions and design. We will then apply our adaptive-design-based ML approaches to integrate the Biology and Chemistry Loops with an aim to find common ground between the chemistry and biology to biosynthesize promising candidates with the desired functionality. Our work will provide a foundational knowledge base to advance the development of novel

1

biopolymers for the manufacture of bioplastics for a wide range of applications and optimal end-of-life degradation.

ENVR 2

Machine learning kernel divergence-based *de novo* sampling size optimization for environmental applications: Cases study of single-cell Raman spectroscopic phenotyping of EBPR microbial communities

*Guangyu Li*¹, *Chieh Wu*², *Dongqi Wang*³, *David Kaeli*², *Jennifer Dy*², *April Z. Gu*⁴, *aprilgu@cornell.edu*. (1) Civil and Environmental Engineering, Northeastern University, Boston, Massachusetts, United States (2) Electrical and Computer Engineering, Northeastern University, Boston, Massachusetts, United States (3) State Key Laboratory of Eco-hydraulics in Northwest Arid Region, Xi'an University of Technology, Xi'an, Shaanxi, China (4) School of Civil and Environmental Engineering, Cornell University, Ithaca, New York, United States

Raman Single-Cell spectroscopy (SCRS) is among the most promising technologies to characterize microbial ecology, which reveals single-cell level insights of microbial phenotypes in complementary to main-stream genotypic technologies. SCRS fingerprints chemical composition of un-cultured cells by measuring the spectra of photons that are scattered to a different frequency than the monochromatic incident laser. A major challenge in the application of single-cell technologies, such as SCRS, is the determination of sufficient sampling size in the balance between statistical power and the limitation on time, labor and resources. Current SCRS-based microbial ecology studies often assume a randomly chosen sample size, or determine the size based on prior knowledge without the ability to deduce true organism diversity in environmental samples. In this study, we proposed, tested and validated a computational sampling size planning protocol, taking advantage of a novel metric, kernel divergence, which compares dataset-wise distributional differences. The proposed method relies on no prior knowledge or extra human intervention. In addition, respective tests verified that its algorithm can appropriately handle datasets with both linear and nonlinear relationships. These advantages promise the proposed method to be a standardized approach for sampling size optimization, enabling more comparable and reproducible experiments and analysis. We validated this model with 8 SCRS phenotyping datasets each sampled from a different enhanced biological phosphorus removal (EBPR) microbial community located across North America. Results suggested that 40-60 spectra were likely sufficient for EBPR-like communities. Further experiments revealed that these communities had rather similar sample distributions, indicating that they share more common and intrinsic phenotypic characteristics despite the geological, operational and configuration differences of these wastewater treatment facilities.

Finally, though not tested, we expect that this technique can be easily generalized to other environmental applications and datasets as long as they contain only continuous features.

ENVR 3

Identification of discriminatory ARGs and socioeconomic factors in shaping resistome risk using machine learning algorithms

Suraj Gupta¹, surajg4@vt.edu, Gustavo Arango-Argoty², Liqing Zhang², Amy Pruden³, Peter J. Vikesland³. (1) Genetics, Bioinformatics and Computational Biology, Virginia Tech, Blacksburg, Virginia, United States (2) Department of Computer Science, Virginia Tech, Blacksburg, Virginia, United States (3) Via Department of Civil and Environmental Engineering, Virginia Tech, Blacksburg, Virginia, United States

The interconnectivities of built and natural environments can serve as conduits for the proliferation and dissemination of antibiotic resistance genes (ARGs), which in turn can result in human exposure and potential threats to public health. Several studies have compared the broad spectrum of ARGs (i.e., "resistomes") in various environmental compartments and the human gut, but there is a need to identify unique ARG occurrence "discriminatory ARGs") that are (i.e., patterns characteristic of each resistome. Such an approach will help identify factors influencing ARG proliferation, facilitate comparisons of the ARGs distinguishing various environments, and help pave the way towards ranking environments based on their likelihood of contributing to the spread of clinically relevant antibiotic resistance. Here we formulate and demonstrate an approach using an extremely randomized tree (ERT) algorithm combined with a Bayesian optimization technique to capture ARG variability in environmental samples and identify discriminatory ARGs. The approach was evaluated on both in silico metagenomic datasets and real metagenomic datasets. The approach was found to readily identify discriminatory ARGs in the in silico datasets. Analyses of real datasets further demonstrated that the ERT approach can effectively differentiate realworld samples and identify discriminatory ARGs based on pre-defined categorizing schemes. Furthermore, it is crucial to delineate the risk posed by resistomes on human health and link it with socio-economic risk factors. The analysis of sewage and human gut metagenomes from across the globe is underway. The objective is to build a machine learning model based on the World Bank's health, nutrition and population data to predict the risk of these resistomes and identify important contributing socioeconomic risk factors. The study provides insight into key markers and metrics for mitigating the spread of antibiotic resistance.

ENVR 4

In vitro toxicogenomics-derived biodescriptors in *in silico* QSAR improve the phenotypic toxicity prediction accuracy

Sheikh M. Rahman^{2,1}, rahman.sh@husky.neu.edu, Jiaqi Lan⁴, Na Gou², April Z. Gu³. (1) Department of Civil Engineering, Bangladesh University of Engineering and Technology, Dhaka, Bangladesh (2) Department of Civil and Environmental Engineering, Northeastern University, Boston, Massachusetts, United States (3) School of Civil and Environmental Engineering, Cornell University, Ithaca, New York, United States (4) Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing, China

Traditional in silico Quantitative Structure Activity Relationship (QSAR)-based toxicity prediction is susceptible to several limitations, including limited applicability domain with regards to chemical structures, possible inclusion of uninterpretable descriptors, and often lack in mechanistic interpretation of the model. Linking the abundant contemporary *in-vitro* high throughput screening (HTS) based toxicity assay data to the *in-vivo* toxicity endpoint, in line with the adverse outcome pathway, shows promises to overcome these limitations. In this study, we have explored the bioassay based Quantitative Biological Activity Relationship (QBAR) model, with in vitro HTS-based temporal transcriptomic and proteomic data of known stress response pathways as the biological descriptors, to predict in vivo toxicity. The study compares the predictive efficacy of the physical-chemical property-based QSAR model, bioassay-based QBAR model, and combined physical chemical property and bioassay-based Quantitative Structure and Biological Activity Relationship (QSBAR) model. Two separate case studies are conducted including cytotoxicity (E. coli EC₅₀) prediction from E. coli-based transcriptomic assay, and genotoxicity (in vivo carcinogenicity) prediction from yeast-based proteomic assay. For the cytotoxicity prediction, the bioassay assisted QBAR models perform better (higher R²) compared to the conventional physical-chemical based QSAR model or the QSBAR models with both physical-chemical and biological descriptors. Both QBAR and QSBAR models are constructed with biodescriptors derived and quantified at three biologically relevant levels - individual biomarker, specific pathway, and cellular level. Among the three levels, the QBAR model at the pathway level yields the best prediction with the highest R^2 (0.78), followed by the biomarker level model (R²=0.70). QBAR models also outperform the QSAR, and QSBAR models in predicting the in vivo carcinogenicity. The pathway level QBAR model produces the strongest model (accuracy=75%, sensitivity=77%, and specificity=71%) for the in vivo carcinogenicity prediction. The current study suggests that, bioassay-based QBAR model improves the predictive power of the in silico

toxicity prediction and facilitates effective chemical hazard identification and risk monitoring.

ENVR 5

Endotoxin detection using liquid crystal droplets and machine learning

Shengli Jiang¹, sjiang87@wisc.edu, JungHyun Noh², Alexander Smith¹, Nicholas L. Abbott², Victor Zavala¹. (1) University of Wisconsin, Madison, Madison, Wisconsin, United States (2) Cornell University, Ithaca, New York, United States

Endotoxins are lipopolysaccharides that are found in the outer membrane of gram-negative bacteria and that are accountable for many health hazards such as endotoxemia (a septic shock caused severe immune response). A number of methods have been proposed to detect the presence of endotoxins with a remarkably high sensitivity. However, available methods do not provide a quantitative estimation of concentration and/or are incapable of classifying endotoxin type. Liquid crystal (LC) droplets dispersed in water are sensitive to the presence of endotoxins and undergo ordering transitions when varying endotoxin species and concentrations. Specifically, LC shifts from a tangential orientation at the droplet surface (bipolar configuration) to orientating perpendicular to the droplet surface (radial configuration) under a higher concentration of endotoxins. Different internal configurations of LC droplets have distinct optical properties. As such, flow cytometry of LC droplets can be used to generate rich forward scattering/side scattering (FSC/SSC) data to characterize optical properties. Counting methods used in the analysis of FSC/SSC data can be used to predict endotoxin concentration. However, such counting methods are not robust (they are subject to significant variability). In this work, we demonstrate that machine learning techniques can be used to accurately predict endotoxin concentrations and species from FSC/SSC data. Our approach uses a convolutional neural network (CNN) to extract pattern information (features) from FSC/SSC density data. Our framework reveals that significant amounts of hidden information is available in FSC/SSC data. We also add prior knowledge of the counting method to the CNN by introducing a regularization term on trainable parameters and have achieved better results.

ENVR 6

Applications of artificial intelligence, machine learning, and data analytics in environmental science and engineering: Current status and future directions

Huichun Zhang, *hjz13*@*case.edu*. Civil Engineering, Case Western Reserve University, Cleveland, Ohio, United States

The past few years have witnessed the transformative impact of artificial intelligence (AI) and machine learning (ML) in many applications, such as speech and image recognition, consumer behavior prediction, and selfdriving cars, primarily driven by the tremendous growth in data collection and storage capabilities as well as in computing power. This talk will review the exciting opportunities in applying AI/ML and data analytics to solving environmental problems, and to identify research priorities our community should focus on in the near future. Examples of topics to be covered include developing quantitative structure-activity relationships for biotic/abiotic reactivity, adsorption, uptake, treatment, and toxicity of organic and inorganic compounds; big datainformed water/wastewater infrastructure management; characterize sources of pollution and model emissions of various contaminants in the air, water, soil and sediment; model and predict contaminant levels and conduct risk assessment in natural and engineered systems; predict and optimize treatment efficiencies in various treatment and remediation processes: and monitor and predict nutrients and contaminants levels in different environmental compartments.

ENVR 7

Structural features of ERα- and AR-mediated endocrine disrupting chemicals

Haoyue Tan, 417695798@qq.com, Xiaoxiang Wang, Wei Shi, Qinchang Chen, Hongxia Yu. Nanjing University, Nanjing, China

Endocrine disrupting chemicals (EDCs) can induce a large number of harmful effects on human's endocrine system by interacting with estrogen receptor α (ER α) and androgen receptor (AR). However, it is unknown (i) what structural features make chemicals active, (ii) what structural features determine the type of activity; (iii) and how these features exert their functions. In this study, a series of computational methods, including chemical informatics, hierarchy fragment method, molecular docking and molecular dynamics simulation, were combined with an experimental method of time-resolved fluorescence resonance energy transfer assay to resolve these questions. Primary fragments (20 for the ERα and 18 for the AR) and secondary fragments (38 for the ERa and 29 for the AR) were identified to distinguish active and inactive compounds. These fragments make active compounds forming hydrogen bond interaction with R394 and H524 of ERa LBD, N705 and T877 of AR LBD to induce activities. The types of disrupting activity of the compounds studied were found to be determined by 65 and 51 tertiary fragments for the ERa and the AR, respectively. This determination is explained by the interactions of tertiary fragments of ligands with location 1/2 of LBDs and the stability of H12, which are important for the formation of AF-2 surface and the process of coregulator recruitment. Our results are helpful for the in

silico screening of EDCs, and the design of compounds without endocrine disrupting activities, as well as promote our understanding about the behaviors of EDCs in other NRs.

ENVR 8

Deep neural network combined with molecular fingerprints (DNN-MF) to develop predictive models for hydroxyl radical rate constants of water contaminants

*Shifa Zhong*¹, *sxz535*@*case.edu, Jiajie Hu*¹, *Xiong Yu*¹, *Huichun Zhang*². (1) Case Western Reserve University, Cleveland, Ohio, United States (2) Civil Engineering, Case Western Reserve University, Cleveland, Ohio, United States

This work combined Deep Neural Network (DNN) with molecular fingerprints (MF) to develop models to predict the OH radical rate constants of 593 organic contaminants. Molecular descriptors, most often used in establishing quantitative structural-activity relationships (QSARs), were not used here because of their complicated generation processes that rely on advanced physicochemical and computational knowledge. Instead, we only fed the most basic information of the contaminant structures, i.e., MF encoding the types of atoms and how they are connected, to DNN and DNN then developed predictive models automatically. Here, a dataset containing 457 contaminants and their OH rate constants was first used to develop predictive models by DNN-MF. The hence developed models showed comparable accuracy with the traditional QSARs. The root mean square error (RMSE) values of the test sets were 0.358-0.384. The length of 2048 bits for the MF and 3 hidden layers (each with 1024 neurons) were found to be the optimal parameters for DNN. The model containing an additional 89 micropollutants in the training set was then successfully applied to predict the OH radical rate constants of 17 organophosphorus flame retardants and 29 additional micropollutants, with comparable accuracy to the reported molecular descriptors-based QSARs.

ENVR 9

Machine learning approach for predicting defluorination of per- and polyfluoroalkyl Substances (PFAS) for their efficient treatment and removal

Bryan M. Wong^{1,2}, usagi01@gmail.com, Akber Raza¹, Sharmistha Bardhan¹, Lihua Xu¹, Sharma S. Yamijala^{1,2}, Chao Lian^{1,2}, Hyuna Kwon¹. (1) Department of Chemical & Environmental Engineering, University of California, Riverside, Riverside, California, United States (2) Materials Science & Engineering Program, University of California, Riverside, Riverside, California, United States

We present the first application of machine learning on per- and polyfluoroalkyl substances (PFAS) for predicting and rationalizing carbon-fluorine (C-F) bond dissociation energies to aid in their efficient treatment and removal. Using a variety of machine learning algorithms (including Random Forest, Least Absolute Shrinkage and Selection Regression, and Feed-forward Operator Neural Networks), we were able to obtain extremely accurate predictions for C-F bond dissociation energies (with deviations less than 0.70 kcal/mol) that are within chemical accuracy of the PFAS reference data. In addition, we show that our machine learning approach is extremely efficient (requiring less than 10 minutes to train the data and less than a second to predict the C-F bond dissociation energy of a new compound) and only needs knowledge of the simple chemical connectivity in a PFAS structure to yield reliable results - without recourse to a computationally expensive quantum mechanical calculation or a three-dimensional structure. Finally, we present an unsupervised machine learning algorithm that can automatically classify and rationalize chemical trends in PFAS structures that would otherwise have been difficult to humanly visualize/process manually. Collectively, these studies (1) comprise the first application of machine learning techniques for PFAS structures to predict/rationalize C-F bond dissociation energies and (2) show immense promise for assisting experimentalists in the *targeted* defluorination of specific bonds in PFAS structures (or other unknown environmental contaminants) of increasing complexity.

ENVR 10

Machine learning methods for the prediction of spectra and identification of opioids and their derivatives

*Chun-Hung Wang*¹, Daria Mashanova^{1,2}, **Anthony Terracciano**¹, Anthony.Terracciano@ucf.edu, Artëm Masunov¹, Mengyu Xu¹, Subith Vasu¹. (1) University of Central Florida, Orlando, Florida, United States (2) Carnegie Mellon University, Pittsburgh, Pennsylvania, United States

Machine learning (ML) is applied broadly in chemical properties of single values such as ionization potential and electronic affinity. While the prediction of absorption spectrum by ML method is relatively few. In our study, accurate infrared (IR) and THz spectra of common organic molecules is determined by investigating the structure-property relationship. We choose multi-layer perceptron (MLP), recurrent neural network (RNN), and convolutional neural network (CNN) as the statistical classification algorithm, in accordance with molecular descriptors topological indices, MACCS fingerprint, adjacency matrix, or Coulomb matrix. All the 360 organic molecule IR spectra are from Pacific Northwestern National Lab (PNNL) database as the training set and are assessed. THz comparisons are made with recently calculated DFT specta of fentanyl and analogues. Current work will lead to intelligent detection schemes for future opiods and derivatives.

ENVR 11

Comparison of two low-hazard organic solvents as individual and co-solvents for the fabrication of polysulfone membranes

Xiaobo Dong¹, Tequila Harris², **Isabel C. Escobar**¹, isabel.escobar@utoledo.edu. (1) Chemical and Materials Engineering, Univ of Kentucky, Lexington, Kentucky, United States (2) Georgia Institute of Technology, Atlanta, Georgia, United States

Petroleum-derived solvents commonly used in membrane fabrication are often hazardous and toxic, so the investigation of safer alternatives is important. In this two low-hazard solvents, methyl study, 5-(dimethylamino)-2-methyl-5-oxopentanoate (Rhodiasolv® PolarClean) and gamma-valerolactone (GVL), were investigated as sole- and as co-solvents to cast polysulfone (PSf) membranes via non-solvent induced phase inversion. Normalized viscosity (NV) was introduced as an indicator of dope solution homogeneity and was used to compare the required time of mixing to achieve full dissolution of the polymer in the different solvents/solvent mixtures. All dope solutions made with low-hazard solvents were found to be more viscous than those made with traditional solvents, which meant additional mixing time was needed, and that fabricated membranes were morphologically different. With respect to operation, membranes cast from dope solutions containing equal amounts of PolarClean and GVL displayed the most similar flux curves and solute rejection to those made using the traditional solvent tested.

ENVR 12

Engineering selective desalination membrane materials via polymer backbone rigidity and functional group position

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Providing sustainable supplies of purified water and energy is a critical global challenge for the future, and polymer membranes will play a key role in addressing these clear and pressing global needs for water and energy. Polymer membrane-based processes dominate the desalination market because they are more energyefficient than thermal desalination processes, and polymer membranes are crucial components in several rapidly developing power generation and energy storage

applications that rely on membranes to control rates of water and/or ion transport. Much remains unknown about the influence of polymer structure on intrinsic water and ion transport properties, and these relationships must be developed to design next-generation polymer membrane For polymers that are of interest for materials. desalination, the water/salt selectivity is a critical property that describes the intrinsic ability of the polymer to transport water as opposed to salt. An observed tradeoff relationship between water/salt permeability selectivity and water permeability suggests that both sorption and diffusion phenomena contribute significantly to water/salt permeability selectivity. This presentation discusses an experimental investigation of the influence of polymer backbone rigidity and functional group position on water/salt selectivity properties of model hydrated polymers. The results suggest that increasing polymer backbone rigidity and distributing hydrophilic functional groups evenly throughout the polymer both drive increases in water/salt selectivity properties that are critical for effective desalination membranes.

ENVR 13

Facile grafting of Zwitterions onto the surface of ultrafiltration membranes to improve antifouling properties

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Superhydrophilic zwitterions have been extensively exploited for surface modification to improve antifouling properties. However, it remains challenging to form layers of < 20 nm with high zwitterion content on the surfaces with different degrees of hydrophilicity. We demonstrate that amine-functionalized sulfobetaine (SBAm) can be codeposited with dopamine on ultrafiltration (UF) membranes, leading to a thickness of 10 nm to 50 nm and an SBAm content of up to 31 mass% in the coating layers. The effect of coating and surface chemistry on the membrane properties (including molecular weight cut-off and water permeance) will be systematically investigated to derive the structure/property relationship. The covalently grafted SBAm is stable underwater and improves the antifouling properties, as evidenced by the lower trans-membrane pressure required to retain targeted water fluxes than that required for the pristine membranes. The SBAm is also more effective than conventionally used sulfobetaine methacrylate (SBMA) for the zwitterion grafting on the surface to improve antifouling properties.



ENVR 14

Trade-off in membrane distillation with monolithic omniphobic membranes

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Membrane distillation (MD) is a sustainable desalination technology suitable for the treatment of hypersaline wastewater, due to its high tolerance to salinity and the capability of leveraging low-grade thermal energy. However, MD suffers from membrane wetting when treating feedwaters containing low surface energy wastewater generated contaminants (i.e., from unconventional energy exploitation). Omniphobic membranes have been developed as functional materials to mitigate membrane wetting in MD because of their superior wetting resistance. However, a design framework for MD membranes remains incomplete, due to the complexity of omniphobic membrane fabrication and the lack of fundamental relationship between wetting resistance and water vapor permeability. Here we present a particle-free approach that enables rapid fabrication of monolithic omniphobic membranes for MD desalination. Our novel monolithic omniphobic membranes display excellent wetting resistance and water purification performance in MD desalination of hypersaline feedwater containing surfactants. We demonstrate that a trade-off exists between wetting resistance and water vapor permeability of our monolithic MD membranes. Utilizing membranes with tunable wetting resistance and permeability, we elucidate, for the first time, the underlying mechanism of such trade-off. We envision that our fabrication method as well as the mechanistic insight into the wetting resistance-vapor permeability trade-off will pave the way for smart design and manufacturing of MD membranes in diverse water purification applications.

ENVR 15

Nutrient recovery from synthetic livestock wastewater effluent using electroactive membranes

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Nitrogen (N) and phosphorus (P) are essential elements needed for agricultural crop fertilization. The production of both nitrogen and phosphorus fertilizers is energyintensive and their demand is expected to increase in the coming decades. Meanwhile, agricultural wastewater from livestock (LWW) farms contains high concentrations of nitrogen and phosphorus in addition to organic loads. Runoff of Livestock wastewater from farms to aquatic ecosystems leads to contamination and severe environmental problems. Currently. conventional wastewater treatment plants are unable to remove such concentrations, which require high complex anaerobic/anoxic treatment stages and reduce the efficiency of the treatment. An important strategy to mitigate phosphorus and nitrogen scarcity is to recycle them from waste streams back into agricultural We present a novel 'polishing' filtration production. process based on electroactive membranes to simultaneously produce a solid fertilizer and high-quality water from LWW effluents following anaerobic treatment, thereby closing resource cycles in agriculture. The suggested process uses low-voltage electrically-charged membranes to recover and separate Struvite, an ecofriendly fertilizer from LWW effluents. The recovery process is based on local hydrolysis and pH increase near the membrane surface and does not require chemical additives apart from magnesium. We evaluated permeate flux and change in pH of the permeate as a function of applied electrical potential, time, and solution's ionic strength. Results indicate rapid and continuous removal rates of Phosphorus and Nitrogen. In addition, membrane flux is easily restored to its initial value, and therefore, the recovery process can be repeated following the collection of the solid fertilizer.



Top Left : Microscopy imaging of recovered struvite Top Right : SEM images of recovered struvite Bottom : Schematic diagram of the recovery approach

ENVR 16

Accelerating materials development via statistical learning methods for environmental engineering

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Advancements in sustainable energy technologies for environmental engineering applications critically depend on the ability to design multiscale materials and establishing their structure-property correlations. Rapid discovery and synthesis of materials with optimum functional properties often involve the coupling of computational tools, experimental methods and more recently statistical learning methods. Two examples, one employing predictive Bayesian modeling to estimate the ease of shear between layers in two-dimensional (2D) materials to tune their aggregation behavior; and other employing an unsupervised learning method to extract and identify the topological features of porous, heterogeneous mycelium-based filtration membranes will be presented. Employing statistical learning approaches to accelerate the identification of material parameters that present efficient routes for membrane design will be discussed.

ENVR 17

Dual-functional block copolymer brushes grafted reverse osmosis membranes with improved antifouling performance

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In this study, dual-functional block copolymer brush with fouling resistant and antimicrobial properties is grafted on graphene oxide (GO) coated polyamide membranes to control biofouling. The block copolymer brush is constructed with a bacteria-"defending" zwitterionic poly (sulfobetaine methacrylate) (PSBMA) block and a bacteria-"attacking" biocidal poly (amino acid) (poly (methacryloyl-L-Lysine), PLysMA) block. Due to its abundant oxygen-containing functional groups, GO offers reaction sites for polymer brush grafting with minor compromise on membrane water flux. The activators regenerated by electron transfer-atom transfer radical polymerization (ARGET-ATRP) technique is utilized to controllably grow the block copolymer brush on the membrane with desired density, thickness and architecture. With the bacteria-"attacking" moiety on top, the fabricated membrane reduces biofouling caused by Gram-positive bacteria, B. subtilis, via the bacterial-"defending" and -"attacking" synergistic effect. The fabricated membrane exhibits a lower flux reduction (27%) associated with E. coli proliferation in comparison to that (80%) of the pristine polyamide (PA) membrane under the same operating condition. Nearly 100% flux recovery is observed on the fabricated membrane after two cycles of "fouling-cleaning", while only 94% recovery of flux is observed on the control polyamide membrane.

ENVR 18

Permeate side-heated integrated solar thermal membrane distillation system

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Globally, 844 million people live without even a basic drinking water service and thus urgently need economical off-grid water treatment devices. In this research, a permeate side-heated integrated solar thermal membrane distillation system has been developed to extract potable water from seawater, canal water, and municipal wastewater without using electrical devices. The system is mainly comprised of a feed water chamber, a hydrophobic membrane with a black permeate side, a distillate chamber, and a condensing channel. The permeate side of membrane absorbs solar thermal energy and heats the feed water in the pores and the near region of the membrane. The water vapor passes through the membrane and condenses into distilled water in the condensing channel. Experiments were conducted under both simulated and natural sunlight. Under the simulated sunlight, the distillate production rate during the initial four hours was 1.32-1.48 kg/(m²•h) at an irradiance of 900 W/m² (400–1100 nm wavelength), varying little regardless

of the type of feed water. Under natural sunlight, the distillate production rate was 8.56 kg/(m²•day) at a daily average irradiance of 614 W/m² (400-1100 nm wavelength), corresponding to an overall energy efficiency of 55%. The high energy efficiency probably results from the heat localization within the pores of membrane. The long-term performance of the system was assessed under simulated sunlight. The system worked for 41, 22, and 11 days when seawater, canal water, and municipal wastewater were used as the feed water, respectively. The distillate production rate from the respective feed water dropped by 18.18%, 11.03%, and 22% at the end of long-term experiments. The experiments were terminated when the feed water penetrated through the membranes, which may be due to the fouling of the membranes by the feed water. The distilled water had the turbidity of 0.1-0.2 NTU, the electrical conductivity of 3-451 µS/cm, the chemical oxygen demand of 1.9-7.8 mg/L, and the pH of 7.2-7.7, depending on the type of feed water and time length of operation. No bacteria or protozoa was found in the distilled water in spite of the type of feed water. Having a high production rate, good quality of distilled water, and operational simplicity, this device could be an affordable solution for providing drinking water in extremely poor areas and natural disaster situations. An international patent application has been filed for the invented system.

ENVR 19

Biocatalytic membranes with self-contained radical polymer mediator for removal of persistent organic pollutants

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Organic pollutants such as endocrine disruptors and pharmaceuticals have been widely detected in the environment as they tend to be persistent or partially removed by conventional wastewater treatment processes. These contaminants are biologically active and potentially harmful to human health and ecosystems. Thus, there is a critical need to develop advanced treatment processes in water reclamation. Enzymes biocatalysis, which uses biological enzymes to facilitate beneficial chemical transformations, demonstrates high catalytic efficiency, generates few toxic byproducts, and requires low energy consumption. Despite many merits of the enzyme biocatalysis, using free enzymes for contaminant removal faces challenges due to the low stability, non-reusability, and the high costs associated with a single use of these free enzymes. In this study, we developed a new type of biocatalytic membrane (BCM) by

immobilizing fungal laccase and radical polymer mediators in a crosslinked sodium alginate hydrogel that was cast on a porous support. The incorporation of the mediators, 2,2,6,6-tetramethyl-1radical polymer piperidinyloxy (TEMPO) or poly(2,2,6,6-tetramethylpiperidinyloxy methacrylate) (PTMA), enables the oxidation of recalcitrant compounds that are not directly oxidized by laccase alone. Results demonstrated the BCM had a higher enzyme activity than the control membrane that contained laccase alone. The stability of the BCM at room temperature and its reusability in repeated biocatalytic batch reactions were characterized and compared. The macromolecular radical mediator, PTMA, can be entangled within the crosslinked BCM while the small molecule mediator, TEMPO, tends to diffuse into the solution during treatment processes. Ongoing experiments are evaluating the effectiveness of the BCM in treating organic pollutants including tetracycline, bisphenol A and acetaminophen. Our results will provide insights into the factors affecting the efficacy and reusability of the radical mediator-contained BCMs. This study will provide a new route to develop highperformance biocatalytic membranes as an effective and renewable alternative for treating recalcitrant organic pollutants.

ENVR 20

High-salinity membrane distillation: Impact of material properties on membrane performance

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In membrane distillation (MD), a saline feed stream is distilled through a hydrophobic, vapor-filled membrane into a pure distillate stream. Unlike reverse osmosis, MD can theoretically treat high-salinity streams, even approaching zero liquid discharge of waste brine. However, salt precipitation (scaling) can facilitate wetting of membrane pores at high salinities. As a result, many researchers have sought to use advanced techniques to fabricate high-porosity, highly hydrophobic membranes. Superhydrophobic membranes are often fabricated via modifying high-porosity substrates (e.g., electrospun membranes) to increase surface roughness and reduce surface energy (e.g., by coating with functionalized nanoparticles). However, the relative importance of pore size, hydrophobicity, and surface/internal properties in preventing wetting are still not fully understood.

Previously, we observed that internal hydrophobicity (i.e., pore wall hydrophobicity) may be important, especially during long-term operation and/or under high-salinity conditions. In recent work, we utilized initiated chemical vapor deposition to deposit a hydrophobic copolymer (P(PFDA-co-EGDA)) on (1) a hydrophilic substrate, producing a superhydrophobic membrane with a high contact angle (157°) and average pore size (132 nm), and (2) a hydrophobic substrate, producing an asymmetric membrane with small feed-side porosity (3.5%) and average pore size (64 nm). While both membranes displayed similar wetting resistance with a surfactantcontaining feed solution, under scaling conditions, the asymmetric membrane displayed much higher wetting resistance than the superhydrophobic membrane. Results showed that surface pore size and porosity played a more important role than contact angle in preventing scaling-induced wetting. Currently, we are utilizing electrospinning to fabricate novel hydrophobic and hydrophobic-hydrophilic membranes with different thicknesses and pore sizes. We are testing these membranes under baseline and high-salinity conditions to determine the impact of thickness, pore size, and hydrophobicity on scaling-induced wetting for different feed solution compositions; results will be presented.

ENVR 21

Performance enhancement and scaling mitigation of radio frequency induction heated membranes in vacuum membrane distillation

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Recently, there is a growing interest in membrane distillation (MD) technology, a thermally driven membrane separation, to treat high salinity water or contaminated wastewater. However, MD commercialization is still limited by technical challenges such as temperature polarization (TP), scaling, and high-energy consumption, as the feed solution requires continuous heating to provide an efficient driving force. We suggest and assess the ability and efficiency of 'self-heating' thermally conducting membranes heated by radio frequency induction heating (RF-IH), to overcome distillation limitations. A composite membrane containing iron oxide coated carbon nanotubes (Fe-CNTs) (Fig.1 A) was spray coated on a PTFE membrane and heated by induction heating, using radio frequency (RF) altering magnetic fields (Fig.1 B). The performance of RF-MD system was evaluated in terms of distillate flux and specific heating energy consumption at optimized operating conditions and results were compared to a conventional MD system. In addition, the impact of RF heating on calcium sulfate (CaSO₄) scaling was addressed in terms of distillate flux and crystal formation. Results show the ability of heating water directly on the membrane surface in RF-MD

systems, leading to low TP, high distillate flux, and low specific heating energy compared to a conventional MD system (Fig.1 C). Scaling results showed the impact of RF magnetic field on salts crystallization, leading to smaller crystal size and overall less scaling. Following analysis of the RF-MD membrane surfaces, only sporadic small CaSO₄ crystals were detected, while high concentrations of small crystals were detected at the concentrate stream exiting the MD process. These results are promising as they show the RF-MD system has potential to improve MD processes, specifically for high salinity distillation where pressure-based applications cannot be used.



Figure 1. (A) TEM image of Fe-CNTs; (B) Illustration of the RF-MD process. Bottom layer: temperature profile in the feed; Middle layer: composite membrane; Top: vacuum chamber; (C) Permeate flux and specific heating energy of RF-MD and conventional MD.

ENVR 22

Reactive mineral phases from *in situ* biogeo-chemical processes: Key to abiotic natural attenuation?

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Many years of laboratory research on contaminant degradation by minerals has shown that freshly-formed (unaged) minerals generally are significantly more reactive than pre-formed (aged) minerals. However, the former are difficult to characterize and control, even in laboratory batch experiments, so the latter tend to dominate thinking about the role of mineral surfaces in contaminant fate and remediation. However, recent studies on the reactivity of pre-formed/aged minerals have shown that they may not be sufficient to explain the degree of contaminant degradation that is sometimes observed under (column or field) conditions that are favorable to abiotic natural attenuation (ANA). This inconsistency has led to renewed interest in the role of fresh-formed/unaged minerals in contaminant degradation under ANA conditions. It has been hypothesized that the phases most responsible for ANA reactivity are reactive mineral intermediates (RMIs) that are derived from the more familiar and stable iron/sulfur minerals such as magnetite, pyrite, etc. Evidence for the importance of RMI phases is mostly from laboratory studies, but these results have major implications for ANA, and in situ chemical reduction (ISCR) more generally. Several recent examples of this will be summarized, and new evidence will be presented from

our most recent work using nitro aromatic compounds (NACs) as model contaminants. The latter was performed by titration of suspended iron oxides with Fe(II) and measuring NAC reduction, dissolved Fe(II), and pH. The results show that even NACs—which are among the most easily reduced environmental contaminants—react much more rapidly under conditions where RMIs are formed.

ENVR 23

Biodegradation of aniline and *p*-chloroaniline under different redox conditions at a contaminated chemical manufacturing site

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Aniline and parachloroaniline (PCA) are used in manufacturing industries. Aniline and PCA are toxic and suspected carcinogenic pollutants. These compounds have entered the environment and are problematic groundwater pollutants. We are evaluating the potential for aniline and *p*-chloroaniline biodegradation by native aquifer microorganisms from a large, chemically and geologically complex industrial site historically contaminated with many different chemicals including aniline and chlorinated aniline. A 55-ft sediment core was recovered from the site along with groundwater from a multi-level sampler. The sediment core was divided into 2-inch slices. The ~300 sediment core slices were shared among multiple teams and characterized for in situ geochemistry and microbial community via next generation sequencing of 16S rRNA genes. We used this data to develop hypotheses for microbial activity and simulating in situ conditions. Sediments from a contaminated site were enriched with aniline and PCA as carbon sources. Two groups of microcosms, targeted and composited, were established. Aerobic, sulfate-, nitrate-, and iron-reducing microcosms were established and incubated in the dark at room temperature. Non-active microcosms were bioaugmented using pure isolate obtained from the site. Microcosms were ~15% sediment slurry in groundwater from a matching depth or in minimal medium. Autoclaved controls were also established. Experiments were performed under sterile conditions using triplicates. Microcosms were amended with aniline and PCA and monitored by HPLC. Active microcosms were plated (0.1 mL) on minimal media agar plates without carbon and nitrogen sources to isolate pure

cultures. Community analysis was done for the active aerobic microcosms. The targeted microcosms showed no substantial loss of aniline or *p*-aniline. The composited microcosms from the -9.2 to 10 ft depth showed a complete loss of aniline and some loss of p-aniline compared to the killed controls. Rhodococcus HA1 was isolated from the aerobic microcosms. HA1 uses aniline as a carbon and nitrogen source. Aniline was depleted in two weeks in non-active microcosms after bioaugmentation with pure isolates. Analysis of 16S rRNA genes showed a shift in the microbial community at the genus level in active microcosms in comparison to the original community. On-going work is focused on use of stable isotope probing (SIP) to determine which organisms are active in the microcosm bacterial community.

ENVR 24

Contributions of iron and biological sulfate reduction to abiotic transformation of organic groundwater contaminants

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Abiotic reactions with iron-sulfur minerals have shown potential for contaminant transformation. Previous studies have explored the influence of Fe:S ratios, pH, and ligand availability on iron sulfide reactivity for organic pollutant transformation in groundwater, but further research is necessary to understand the role of biogenic sulfide production and different iron sources on iron sulfide reactivity. This work explores the transformation of trichloroethylene (TCE) to acetylene in the presence of sulfate reducing bacteria (SRB) and iron, as either ferrihydrite or aqueous ferrous iron (Fe²⁺). In anaerobic, pH-controlled batch experiments, SRB were grown with lactate as the electron donor and sulfate as the electron acceptor, and iron was introduced as either ferrihydrite or Fe²⁺. TCE was added to batch experiments after aging, and acetylene production was measured over time using GC-FID. Aqueous iron and sulfur species were determined initially, after aging, and after reaction with TCE. After terminating experiments, the iron-sulfur solids were characterized using XRD, XPS, and SEM. This data was used to interpret the redox transformations of iron and sulfur during reaction from TCE to acetylene. Initial ferrihydrite experiments showed that increasing the Fe:S ratio from 2:1 to 20:1 results in more efficient acetylene

production, but an Fe:S ratio of 50:1 shows a decrease in acetylene production. The results of this work will contribute to the development of improved technologies focused on in situ transformation of organic contaminants as well as improved natural attenuation models. This research also lays the groundwork for future experiments focused on iron-sulfide precipitation and TCE transformation in diffusion-limited, heterogeneous environments.

ENVR 25

Quantifying 2,4-dinitroanisole transformation using compound specific isotope analysis after *in situ* chemical reduction of iron oxides

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Iron-bearing minerals are an important reductant for many anthropogenic pollutants during coupled biotic and abiotic processes. Despite an abundance of these minerals in the subsurface, pollutant transformation is often limited by competition for (bio)available Fe(II) and complex hydrogeologic conditions. In situ chemical reduction (ISCR) is one approach to circumvent many of these issues. Perturbations introduced to the subsurface by ISCR, however, present a challenge in quantifying pollutant concentrations and thus the extent of remediation. In this study, compound specific isotope analysis (CSIA) was used to characterize C and N isotope fractionation associated with the reduction of 2,4dinitroanisole (DNAN) by a suite of iron-bearing minerals and under various matrix conditions including systems representing ISCR. These data were used to generate models of DNAN transformation based on measurements of $\delta^{15}N$ and make quantitative estimates of DNAN removal. Not only was isotope fractionation unaffected in each set of conditions, but also the model was applied in a blind study to accurately predict the extent of DNAN transformation from $\delta^{15}N$ measurements. These observations illustrate the utility of CSIA as a robust analytical method to evaluate the success of in situ remediation techniques. These results are applicable to other nitroaromatic compounds in the subsurface and are important given the continuing need for assessment of the success of in situ remediation techniques.

ENVR 26

Reductive transformation of 3-nitro-1,2,4-triazol-5one (NTO) by the hematite/Fe²⁺ redox couple and an iron-rich soil

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Insensitive munitions compounds are commonly found in soils and groundwater at/near military training ranges and manufacturing sites across the U.S. Understanding how and how fast these compounds are transformed in soil and groundwater can provide insight into their fate in the subsurface and help to develop cost-effective site management strategies. We studied the reductive transformation of 3-nitro-1,2,4-triazol-5-one (NTO), a compound used in the IMX-101 and IMX-104 formulations, by the hematite/Fe²⁺ redox couple and an iron-rich (Aberdeen) soil reduced with dithionite, a reducing agent commonly used in field remediation. NTO was reduced predominantly to 3-amino-1,2,4-triazol-5one (ATO) in all experiments. Reduction of NTO followed pseudo-first order kinetics, and the rate constants (k_{SA}) increasing significantly with pH from 5.5 to 7.0, regardless of whether Fe²⁺ was externally added or produced in situ by dithionite. However, the k_{SA} values were about an order of magnitude lower for dithionite-generated Fe²⁺. The Aberdeen soil was inert toward NTO but showed increasing NTO reduction rate and capacity with increasing electron input via dithionite. ATO was also the primary reduction product in Aberdeen soil, but the mass recoveries were lower than with hematite/Fe²⁺. This work demonstrates the high reactivity and potentially important role of iron oxides in controlling the natural and enhanced attenuation of NTO in munitions constituent-impacted sites.

ENVR 27

Anaerobic dechlorination of chlorinated dibenzo-*p*dioxins in sediment cultures and clues from genetic sequencing

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Among the chlorinated compounds, dioxins are at the top of the list in terms of toxicity and persistence in the environment. The Passaic River in New Jersey is highly contaminated with 2,3,7,8-tetrachlorodibenzo-p-dioxin, the most toxic of the dioxin congeners. Despite fishing advisories, members of communities along the Passaic River continue to utilize it for sustenance fishing. We aimed to determine if dioxins are dechlorinated by bacteria native to the river sediments. We established anaerobic enrichment cultures inoculated with material from 1) original river sediment, 2) river sediment cultures previously enriched on trichloroethene, and 3) river sediment cultures previously enriched on dichlorobenzene. Microcosms were amended with three dioxin congeners: 2,7-dichlorodibenzo-p-dioxin (2,7-DiCDD); 1,2,3,4-tetrachlorodibenzo-*p*-dioxin (1,2,3,4-TeTCDD); 2,3,7,8-tetrachlorodibenzo-p-dioxin (2, 3, 7.8 and TeCDD). Select sets were also amended with trichloroethene or dichlorobenzene to test the additional effect of co-substrate during dioxin dechlorination. 16S rRNA gene amplicon sequencing was performed to assess differences in the community between active treatments. Whole-genome shotgun sequencing was also performed to learn about the breadth of functional genes in the entire microbial community of the 2,3,7,8-TeCDDdechlorinating culture. After 1.5 years, dechlorination was observed in at least one treatment of all tested dioxin congeners. Preliminary 16S rRNA gene sequencing indicates dominance of a Dehalococcoidia phylotype in the 2,3,7,8-TeCDD dechlorinating enrichment. By the time of presentation, we expect to have identified potential dehalogenases in the 2.3.7.8-TeCDDreductive dechlorinating culture from the sequenced metagenome. Further characterization of the bacteria involved in these processes can provide methods for monitoring dechlorination in contaminated sites and potentially lead to new in situ treatment technologies.

ENVR 28

Withdrawn

ENVR 29

Withdrawn

ENVR 30

Removal of 1,4-dioxane during on-site wastewater treatment using nitrogen removing biofilters

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1,4-Dioxane (1,4-D), a likely human carcinogen, is a widespread drinking water contaminant across the United

States. Though primarily used as an industrial solvent, commercial household products such as shampoos, body wash and laundry detergents have been shown to contain very high (parts-per-million) levels of 1,4-D. As a result, its presence and release from domestic wastewater serves as an important and ongoing source of environmental contamination. Due to its resistance to biodegradation, 1,4-D is not effectively removed (<30% removal) in conventional wastewater treatment systems (WTS) such as activated sludge treatment. In case of traditional on-site WTS (OWTS) such as septic tanks and cesspools, wastewater is directly discharged to the subsurface environment, increasing the risk of 1,4-D contamination in groundwaters. A combination of concentrated OWTS, sole-source aquifer (i.e. groundwater as the only source of drinking water), and elevated 1,4-D levels in groundwater, as observed in Long Island, NY, presents a unique challenge to prevent further contamination via wastewater discharges. In this study, we evaluated the performance of Nitrogen Removing Biofilters (NRBs) as OWTS, consisting of a top sand layer and a bottom woodchip + sand layer, to remove 1,4-D. NRBs have been demonstrated to reduce total nitrogen by >90% in residential wastewater and have the potential to remove other organic contaminants given that they take advantage of naturally occurring microorganisms and feature long hydraulic retention time (several days). We monitored 1,4-D removal in two NRB systems installed at residences on Long Island, NY. Monthly samples of tap water at the residence, influent, interface, and effluent of NRBs were analyzed from November 2018 to September 2019. During this period. the mean 1,4-D concentration was 2.0 µg/L (range: $0.2 \sim 8.4 \mu g/L$) in the influent and $0.6 \mu g/L$ (range: $0.1 \sim 2.6$ $\mu g/L$) in the effluent, and the overall removal efficiency was 64±17%. Tap water was not the primary source of 1,4-D in these systems, confirming that 1,4-D originated from the use of household products. The majority of 1,4-D removal (~80%) occurred in the top oxic layer (nitrifying sand layer) of the NRB systems, implying that the removal was likely driven by aerobic microbial degradation. The results thus far show that NRBs can consistently reduce 1.4-D to levels lower than the proposed NY State drinking water standard of 1 µg/L.

ENVR 31

Application of compound-specific isotope analysis combined with molecular modeling to evaluate abiotic and biotic degradation of DNAN and NTO

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Compound-specific isotope analysis (CSIA) can provide critical information on reaction mechanisms because the

breaking of a specific bond is typically associated with a characteristic kinetic isotope effect (KIE). The insensitive munitions compounds 2,4-dinitroanisole (DNAN) and 3nitro-1,2,4-triazol-5-one (NTO) are likely to exhibit substantial C, N, and O isotope effects during abiotic and biotic degradation. These KIEs can be derived from experiments designed to elucidate reaction mechanisms in the laboratory and to diagnose possible degradation pathways operating in field settings. We measured C, N, and O isotope fractionation during DNAN alkaline hydrolysis at 55 C and a range of pH values. The alkaline hydrolysis mechanism of DNAN was verified to be nucleophilic aromatic substitution by using contrasting 18-O labeled water and density functional theory (DFT) calculations. Furthermore, we measured C and N isotope effects during quinone reduction of DNAN which yielded KIE for both C and N that are similar to those obtained for a variety of nitroaromatic during reduction by ferrous minerals. The KIE for C and N measured during anaerobic and aerobic biodegradation with identical strain species indicated distinguishable degradation pathways. The ultimate goal of this work is to provide a substantial body of data on C, N, and O isotope effects that may be used to support remediation efforts in sites contaminated by use of new insensitive munitions formulations.

ENVR 32

Environmental applications and risk assessment of cerium oxide nanoparticles

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Cerium oxide nanoparticles (CeO₂) have shown promise as materials for sensors, catalytic convertors, chemical mechanical polishing and environmental decontamination applications. However, given their high reactivity, catalytic and adsorptive properties, the uses of CeO₂ NPs pose several challenges. These include: 1) potential toxicity and bioaccumulation in the aquatic ecosystem, 2) interaction with environmental contaminants with the NPs becoming carriers of contaminants, and 3) accumulation in water and soil with unknown long-term consequences potential cascading effects altering entire and communities. This presentation will provide an overview of the beneficial uses of CeO2 NPs for sensing and environmental remediation while highlighting the potential toxicity of these NPs in an aquatic model and their reactivity with environmental toxic constituents. An example of toxicity risk assessment of CeO2 NPs originating from chemical mechanical polishing waste will be provided. The observed physicochemical changes and interactions between the NPs and chemicals constituents in the waste will be discussed. These results can be used as a guideline to predict the impact of these materials in the environment and help make informed decisions to balance risks and reward associated with the use of these NPs in the environment.

ENVR 33

Sulfidized nanoscale zerovalent iron: Effect of sulfur content and speciation on reactivity, selectivity, and its ability to defluorinate organic groundwater contaminants

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Sulfidized nanoscale zerovalent iron (SNZVI) is a promising material for groundwater remediation. However, the sulfur speciation in the Fe⁰ matrix and its effects on SNZVI reactivity, especially it ability to defluorinate organic contaminants are unknown. Here, the effect of S content on the crystalline structure, hydrophobicity, S speciation, and electrochemical properties are determined for SNZVI with S/Fe molar ratios ranging from 0.010 to 0.130. These key material properties explain the reactivity and selectivity of SNZVI during reductive dehalogenation, including defluorination of groundwater contaminants. Sulfur incorporation extended the Fe⁰ BCC lattice parameter and reduced local vacancies in the structure. FeS and FeS₂ were the main sulfur species, and their relative amounts changed with the S/Fe ratio in the particles. The sulfur amount and speciation affected the SNZVI hydrophobicity and hence its reactivity. Impacts of sulfur incorporation on hydrophobicity were consistent with the measured water contact angle. While sulfur in the Fe⁰ matrix lowered the material's resistance to electron transfer, the concomitant increase in hydrophobicity inhibited the SNZVI reaction with water, giving it a high selectivity for hydrophobic groundwater contaminants. These findings can guide the rational design of robust SNZVI with properties tailored for specific application scenarios.

ENVR 34

Parameterization and prediction of radius of influence of nanoscale zerovalent iron in field-scale subsurface application: Re-analyses using artificial neural network and regression

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Over 20 years of nanoscale zerovalent iron (NZVI) research, development, and application, the number of contaminated sites treated by this remedial agent throughout the world are 77. Of these sites, twenty-five studies reported radius of influence (ROI) of NZVI treatment defined by either the extent of NZVI transport or the extent of contaminant removal. The ROI varies

substantially since particle condition, delivery condition, contamination condition, and subsurface condition vary greatly. No systematic parameterization and standardization of factors affecting ROI have been made. Thus, no model to predict ROI of NZVI for field-scale subsurface application is available. This current study applies artificial neural network (ANN) and regression analysis to the data sets of particle condition, delivery condition, contamination condition, and subsurface condition from the 25 previously published studies. Both ANN-based correlation and regression-based correlation are developed to predict the ROI as well as to understand the role of each parameter on the ROI. Despite being developed based on a "black-box" technique, both models are able to explain the effects of several theoretical parameters and can be used to preliminarily design NZVI injection or treatment under a particular subsurface and contamination conditions

ENVR 35

Controlling the self-assembly of supramolecular nanocontainers in solution: Green chemistry approach

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Self-assembly is a crucial step towards bottom-up fabrication of complex architectures. An articulate placement of fucntional groups on building blocks yeilds control over self-assembly of thermodynamic equilibrium state products which are often isolated in solid-state. Solid-state phenomeon are not necessarily mimicked in solution. Under non-equilibrium conditions or kinetic control, reaction mixtures can change to outcome of selfassembled products. Herein, we will discuss the solution effects in directing the self-assembly processes. Specifically, how greener methods can be employed to construct nanocontainers with unique applications in pharmacy and cosmetics.

ENVR 36

New approaches nanocomposites' imaging to facilitate development of safer and more robust consumer products

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Carbon nanotubes (CNTs), cylindrical molecules made of rolled-up graphene sheets, were first reported by lijima in 1991, and received emerging and exponentially growing interest and attention since then. CNTs possess a range of unique and superior properties including low density, high aspect ratios, large surface area, electrical

conductivity, thermal conductivity, and high strength. As a result, when CNTs are incorporated into polymers, they can significantly enhance mechanical, electrical and thermal properties of the polymer nanocomposites. It is important to mention that stability of polymer matrix and nanocomposites are of great importance, and have vital implications for their performance, usage, disposal and safety to the consumers. Achieving high degree of CNTs dispersion in the polymer matrices has been a significant challenge as imaging of CNTs distribution in the large volumes has been impossible so far. Without such imaging capability, the prepared composites have often exhibited а suboptimal performance, and, as demonstrated in our earlier work, posed significant risk to consumer. In our initial experiments at NSLS-II our group demonstrated for the first time a promise of X-ray nanotomography to detect the CNTs in polymers. This presentation discusses new capabilities of this technique.

ENVR 37

Characterizing nanoparticle–protein coronas: Using analytical methods to detect and identify proteins adsorbed onto gold particle surfaces

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The use of engineered nanomaterials in pharmaceutical research is of critical importance in drug discovery, targeted drug delivery, and personalized medicine. Drug products containing engineered nanomaterials provide unique therapeutic opportunities. However, because this field of research and development is rapidly changing, nanomaterial drug products present multiple pharmacological, toxicological, manufacturing, and regulatory challenges. This talk summarizes the evolving field of nanotheranostics by exploring the crucial factors that require a multidisciplinary strategy to reach nanoefficacy. Specifically, enabled drug safety and nanometer-sized materials have been proposed as drugcarriers and can deliver precise doses of specific drugs to targeted locations. Upon entering the blood stream, proteins readily adsorb onto and desorb from the surface of these products. This cloud of adsorbed proteins is known as the 'protein corona' and is postulated to critically alter either the drug product's therapeutic (positive) or toxicological (negative) effects. In order to understand the effects related to the protein corona, detection and identification of the associated proteins, as well as the changes in the nanoparticle's physical and chemical properties, are necessary. Data suggest control over protein corona formation is dependent on particle surface chemistry and may be predictable: the characterizationand-prediction process holds promise as an engineering technique to employ therapies. Lastly, with the safety of human health as a clear target, this talk will highlight manufacturing and analytical considerations that allow for constancy and control of novel drug products.

ENVR 38

Withdrawn

ENVR 39

Do graphene oxide nanostructured coatings mitigate bacterial adhesion?

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Despite the fact that surface functionalization with graphene oxide (GO) is effective in bacterial inactivation, the modification of interfacial properties due to the GO coating may in fact increase the bioadhesion (and biofouling) propensity of a substrate [1]. GO is biocidal; is it also anti-adhesive? This work addresses this question using AFM-based single-cell force spectroscopy, a technique that enables direct measurement of bacterial adhesion forces. We show that coatings displaying lowbioadhesion properties can be formed by binding GO nanosheets to a hydrophilic polymer brush [2]. Our work indicates that the underlying polymer layer enables a brush-like GO coating, which mitigates bacterial adhesion through steric repulsive forces. Conformational disorder (afforded by the polymer brush) is thus an important design variable for environmental interfaces (such as sorbents and membranes) seeking to exploit the antimicrobial properties of GO.

ENVR 40

Impact of Mn₂O₃ nanoparticles on nitrification under low and high dissolved oxygen conditions

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The use of Mn_2O_3 nanoparticles (NPs) is growing since they are known as environmentally friendly catalysts in removing carbon monoxide and nitrogen oxides from waste gases. Thus, the release of these materials into the environment as well as wastewater stream is evident. The entry of Mn_2O_3 NPs into the wastewater treatment plans (WWTPs) can affect nitrification performance. Nitrification is a key process for biological nitrogen removal in nitrogen cycle and WWTPs in which ammonia is converted to nitrite by ammonia oxidizing bacteria (AOB), and nitrite is converted to nitrate by nitrite oxidizing bacteria (NOB). Thus, the studies on impact of Mn_2O_3 NPs on nitrifying bacteria are crucial. To date, most batch studies on the impact of nanoparticles to nitrifying bacteria have been

employed without aeration (low DO) which can be seen as a model for several environmental conditions such as river or stream sedimentation. Herein, in accordance with traditional batch studies, we also set up a matrix of low DO batch tests along with aerated (high DO) batch tests with difference concentrations of Mn₂O₃ NPs exposed to nitrifying bacteria, which can be seen as a model for nitrification in WWTPs. Here, we investigate the physiological and transcriptional responses of the nitrifying bacteria due to the presence of Mn₂O₃ NPs based on the specific oxygen uptake rate (sOUR) tests and gene expression. The most sensitive step in nitrification is conversion of ammonia to nitrite by ammonia oxidizing bacteria (AOB). Two genes ammonia monooxygenase (amoA) and hydroxylamine oxidoreductase (hao) are linked to this biochemical step and they are considered as targets to study nitrification inhibition due to their sensitivity to environment. Thus, with the same sample for sOUR test, we examined the transcriptional response of these two genes. Our results showed that there was increase in nitrification inhibition as determined by sOUR with increasing dosages of Mn₂O₃ NPs for both cases- low DO and high DO. There was notable reduction in the transcript levels of amoA and Hao for increasing Mn₂O₃NPs dosage for the case of high DO and 3 h exposure, which corresponded well with sOUR. In addition, we observed gene expression stimulation after 3 h in low DO mode and 1h in high DO mode due to detoxification mechanism.

ENVR 41

Size dynamics control nanoparticle fate and transport in the environment: Toward an accurate and efficient model

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Nanoparticles (NP) offer special characteristics for various applications. includina environmental remediation, due to their fine sizes. Their size also controls their fate and transport behaviours in the environment. Once introduced into environmental media, the initial particle size distribution (PSD) changes spatiotemporally due mainly to NP aggregation and selective removal of certain size fractions. Considering the aggregation of NP in current fate and transport models is crucial whereas it is hindered by high computational expenses, mathematical complexity, and the variable used in current population balance models of aggregation, i.e., particle number concentration being different from that of fate and transport models, i.e., mass concentration. In this study an accurate population balance model, known as the fixed pivot technique, is combined with an accurate 3-D groundwater numerical model, MT3D-USGS, to investigate the impact of NP

aggregation on their transport behaviours in groundwater environments. Special attention is devoted to investigate concurrent occurrence of aggregation and size exclusion mechanism, which has long been known as being responsible for unexpectedly high mobility of colloidal particles in subsurface environments and carrying hazardous contaminants over long distances. Model simulations at a field-scale shows that aggregation increased NP mobility at regions close to the injection point and retains them at greater distances through alteration of their diffusivities, secondary interactionenergy minima, and settling behaviour. This results in a change of residual concentration profiles from exponential for non-aggregating dispersions to nonmonotonic for aggregating dispersions. High computation expenses encountered in these simulations led us to develop a new paradigm for modelling aggregation phenomenon in aquatic environment. This model which is based on a chain-reaction expression uses mass concentration, and is comparable or better than the current population balance model in terms of accuracy and efficiency; offering the potential for being combined with various NP fate, transport, and reaction models.

ENVR 42

Biomineralization by attachment of nanoparticles during the last 550 million years

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Diverse marine organisms form via the same two amorphous calcium carbonate (ACC) precursor phases, which then crystallize into calcite or aragonite in echinoderms or mollusk shell nacre and coral skeletons as revealed by difficult, lengthy, synchrotron spectromicroscopy experiments. Much simpler SEM experiments show that when the biominerals are formed via attachment of ACC nanoparticles, they also appear nanoparticulate after cryofracturing, with nanoparticle size in the 50-400 nm range. The latter is thus a proxy for the former. Having validated this proxy on well-known, modern biominerals, we can now use nanoparticulate texture as a proxy for crystallization by particle attachment (CPA) in many more modern and fossil samples. We find that CPA has evolved independently in diverse phyla. starting with the oldest know animal fossil, the Ediacaran Cloudina (550 Ma) and through the Cambrian explosion (~500 Ma), and in nacre from the Ordovician (450 Ma), the Cretaceous (100 Ma), the Miocene (13 Ma) and the modern (0 Ma).

ENVR 43

Nucleation of mixed-cation amorphous carbonate precursors: Example of cadmium incorporation into calcite

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Mineral nucleation and growth in natural environments often occur in mixed cation systems, where minor and trace elements either co-precipitate with or nucleate on abundant phases. As a result, particles of major mineral phases are coated by minor mineral phases - a phenomenon that significantly contributes to the complexity of geochemical systems. No current theoretical framework can reliably predict the outcomes of heterogeneous nucleation and growth reactions in complex geochemical systems. Recent work indicates heterogenous nucleation of otavite (CdCO3) on calcite (CaCO3) can proceed through non-classical pathways, whereby intermediate amorphous phases first form in solution before undergoing transformation to a heterogeneous crystalline product. This complimentary in situ study 1) establishes the thermodynamic landscape of physical and chemical mixtures of CaCO₃ and CdCO₃ structures and 2) quantifies the stability of metastable intermediates that form en route to crystalline polymorphs using Pair Distribution Fuction (PDF) analysis, Small-Angle X-ray Scattering (SAXS), and solution chemistry.

ENVR 44

Facet-dependent aggregation of hematite nanoparticles

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Nanomineral aggregation leading to hierarchical assemblies and even mineral growth is now recognized as a broadly important geochemical process. However, a major knowledge gap exists in fundamentally understanding the interactions between particles in situ during growth and the resulting response dynamics. Focusing on hematite as the model system, herein we describe additive-free synthesis protocols that yield diverse uniform hematite nanoparticles, such as bipyramids with twelve {111} facets and rhomboids with six {104} facets. Their growth, investigated in detail using

scanning electron microscopy (SEM) and scanning/ transmission electron microscopy (S/TEM), suggests a combination of particle mediated assembly and ion-by-ion coarsening leading to euhedral nanoparticles. We then report measurement of the anisotropic particle-particle forces between these hematite nanocrystals, as a function of their azimuthal orientation about the [001] axis via using atomic force microscopy (AFM)-based dynamic force spectroscopy (DFS). The collective findings help shed new light on hematite particle-based growth and the formation mechanism of hierarchical assemblies that define the physical characteristics of these nanomaterials. In addition to improving understanding of the occurrence, transformation, and fate of minerals in environmental and industrial settings, the results may help enable the development of novel materials for various catalytic applications.

ENVR 45

In situ liquid cell transmission electron microscopy investigation on aggregation and dissolution of iron oxide nanoparticles

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Lacking in situ techniques at sufficiently high spatial and temporal resolution is one of the main impediments to developing a better molecular-scale understanding of interface processes of mineral particles in an aqueous environment. The recent advent of liquid cell transmission electron microscopy (LCTEM) makes it possible to visualize the dynamic interfacial reactions of mineral nanoparticles in fluid with sufficiently high spatial and temporal resolution. Here, LCTEM was utilized to directly observe dissolution behavior of hematite particles in different particle sizes (10, 36, and 103 nm). The high spatial and temporal resolution of LCTEM enables us to differentiate the respective effect of primary particle size, crystal defects, and aggregation state on particle similar electron-beam irradiation dissolution. At parameters. the initial surface-area normalized dissolution rates (R_{SA.Int}) of isolated 10, 36, and 103 nm particles decreased with the increase of primary particle size, which agrees with the prediction of Ostwald-Freundlich equation. Interface free energy of the particles in different sizes were calculated from the measured R_{SA,Int}. Furthermore, the LCTEM images also presented that the dissolution of 10 nm, defect-free hematite nanoparticles occurs from particle surface without preferential sites, but the dissolution on 103 nm particles preferentially originates from structural defects, not from crystal surface. Aggregation behavior shows more significant impacts on the dissolution of 10 nm hematite particles than the others. The smallest nanoparticles tend to aggregate together, and dissolution occurs more rapidly on the particles that are more accessible to bulk solution than the others inside the aggregates. Moreover, as dissolution proceeds, the structure of aggregates show dynamic changes involving disaggregation, shrinkage, and re-aggregation. This study presented the different microscopic dissolution behavior of isolated and aggregated particles in different primary particle sizes, which may provide new insights into biogeochemical processes of mineral nanoparticles in aqueous environments.

ENVR 46

Coupling theory, spectroscopy, and electron microscopy to determine the bonding environments of metal impurities in Fe(III)-(oxyhydr)oxides

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Fe (oxyhydr)oxides are ubiquitous and exert a primary control on coupled redox cycles and the transport of minor but critical metals. In this regard, detailed information on the local coordination environment of impurities is necessary to understand host phase properties, biogeochemical cycling of micronutrients, the long-term stability of impurity/host phase associations, waste forms, and tailoring natural Fe oxides for industrial uses. Extended X-ray absorption fine structure (EXAFS) spectroscopy is the method of choice for determining the local coordination environment of impurities in a host phase. Nonetheless, and in particular for seemingly incompatible dopants, a lack of appropriate standard structures and a priori knowledge concerning thermal disorder, coordination numbers, and potential defect associations can render traditional shell by shell fitting unreliable. I will describe recent work that used ab initio molecular dynamics (AIMD) informed extended x-ray absorption fine structure (EXAFS) spectroscopy to detail the local coordination environment of U and Zn incorporated in hematite (α -Fe₂O₃) and goethite (α -FeOOH). Precise predictions concerning the distribution of Fe vacancies around U(VI) incorporated in hematite were confirmed by high resolution HAADF (high angle annular dark field) - STEM (scanning transmission electron microscopy). These examples demonstrate that AIMD-informed EXAFS can greatly increase our understanding of metal incorporation in Fe (oxyhydr)oxides.
Impact of water chemistry on metal adsorption to surface-functionalized iron oxide nanoparticles

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Surface-functionalized magnetic nanoparticles are promising adsorbents due to their large specific surface areas, tunable surface chemistries, and ease of separation after contaminant removal. We have quantified the equilibrium adsorption behavior and developed surface complexation models that can be used to interpret and predict metal adsorption as a function of the water chemistry. The first system explored is the adsorption of U(VI) to iron oxide nanoparticles with bilayer structures that have outward facing functional groups present in stearic acid, oleic acid and octadecylphosphonic acid. The second system studied extended the investigation of U(VI) adsorption to iron oxide nanoparticles with coatings composed of a natural rhamnolipid biosurfactants. The final set of experiments to be presented is an investigation of adsorption of Cr(VI), present as anionic CrO42 and HCrO4 species, to nanoparticles with a bilaver structure with the net positive (cationic) head group in trimethyloctadecylammonium bromide.

ENVR 48

Withdrawn

ENVR 49

Tailoring the (bio)activity of iron (hydr)oxide nanoparticles in abiotic and biotic environment

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Iron(III) (hydr)oxide nanoparticles are ubiquitous in the environment, where they exist in many forms and play important geochemical roles. Their physical and chemical properties have already found application in many areas including environmental remediation, water treatment, lubrication, heat transfer, (photo)catalysis, sensors, and energy storage/conversion. Biochemical and biological properties of iron(III) (hydr)oxides significantly contribute to microbially-mediated cycling and transport of elements

in the environment, as well as to iron homeostasis in all living organisms. Hence, it is important to have a general framework capable of predicting nanosize effects on chemical and biochemical properties of iron(III) (hydr)oxides. In my talk, I will summarize our research on the nanosize effect of hematite and ferrihydrite nanoparticles on their electronic, adsorption, catalytic, dispersion, and biochemical properties. We found that the nanosize-dependent crystallinity of the nanoparticles is behind the nanosize dependence of their electronic properties. This effect can explain the nanosizedependence of the adsorption, dispersion, catalytic, and biochemical properties of the iron(III) (hydr)oxides. We have assessed these properties in the studies of the adsorption of carbonate and fatty acids, catalytic oxygenation of Mn(II), and bioactivity of the nanoparticles with respect to bovine chondrocytes. The found correlation between the catalytic and biochemical properties of the nanoparticles implies that the bioactivity is directly related to the redox potential and the catalytic redox mechanism (including either the deactivation or generation of reactive oxygen species) of the metal oxide nanoparticles toward redox active constituents at the biointerface.

ENVR 50

Spectroscopy and redox reactions: Lessons learned from Mn and U nanomaterials

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This presentation will show how laboratory experiments, photoelectron spectroscopy (XPS), X-rav and synchrotron-based X-ray absorption spectroscopy (XAS) can be integrated for the investigation of Mn and U nanomaterials in the environment. The integration of XPS and XAS has been essential for the determination of oxidation states of Mn-oxide and U-bearing nanoparticles to better understand redox reactions affecting metal transport and remediation. Additionally, recent advances have facilitated understanding nanoparticle accumulation in plants and cell cultures which have important implication for toxicology, risk assessment, and risk reduction. This work pays tribute to the interdisciplinary spirit and scientific curiosity of Professor Michael Hochella who has illustriously mentored and inspired a new generation of scientists interested in nanotechnology for earth and environmental sciences and engineering.

Optimizing the methanotrophic production and types of polyhydroxyalkanoates (PHAs) by utilizing organic waste-derived methane and volatile fatty acids

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The use of petroleum-based plastics has caused serious economic and environmental problems. It is imperative to develop sustainable ways to produce valuable and environmentally friendly materials. Methanotrophic bacteria are known for assimilating methane while generating polyhydroxyalkanoates (PHAs) biopolymers, which are potential substitutes for conventional plastics. Additionally, biologically generated methane and volatile fatty acids (VFAs) are abundant and readily accessible through anaerobic digestion of organic wastes. Thus, optimizing the methanotrophic production and type of PHAs utilizing organic wastes derived substrates will bring significant economic and environmental benefits. In this study, a feast-famine based cultivation system was developed to produce PHAs using Methylocystis parvus OBBP, which was fed with methane with and without VFAs as co-substrates. Through 7 cycles of cultivations fed with methane alone, M. parvus OBBP started to produce the poly(3-hydroxybutyrate) (P3HB) consistently and achieved an average of 29.9 ± 2.7 wt%. By comparison, the P3HB production significantly increased up to 34.6 ± 3.6 wt% when acetic acid was added at an optimal concentration of 300 mg/L. Additionally, characterization of P3HB polymers (e.g. chemical composition and molecular weight) illustrated that the presence of VFAs facilitated the generation of different types of PHAs (e.g. P3HB and poly(3-hydroxybutyrateco-3-hydroxyvalerate) (P3HB-co-3HV)). Moreover, the production of biomethane and different types of VFAs was investigated through anaerobic digestion of organic wastes under different pHs. In neutral pH condition, biomethane and acetic acids were the dominant products, while both acidic and alkaline conditions inhibited the biomethane production but promoted the generation of various VFAs. Isobutyric acid predominantly accumulated in the acidic treatment, whereas butyric and isovaleric acids prevalently existed in the alkaline treatment. Furthermore, methanotrophic enrichment cultures were cultivated using various inocula from activated sludge and anaerobic digestion processes in wastewater treatment plants, which explored the feasibility and suitability for scaling up PHAs production in practices.

ENVR 52

Robust soluble di-iron monooxygenases to tackle the commingled solvent-stabilizer contamination

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Soluble di-iron monooxygenases (SDIMOs) are a family of multi-component non-heme bacterial enzymes that are of great interest to environmental scientists and engineers given their unique capability of catalyzing a wide array of emerging and legacy water pollutants, such as BTEX, chlorinated aliphatic hydrocarbons (CAHs), 1,4-dioxane (dioxane), methyl tertiary-butyl ether (MTBE), and N-Nitrosodimethylamine (NDMA). Based on the primary substrate range and evolutionary correlation, SDIMOs can be categorized into six groups. Here, we focused on group-6 SDIMOs given its unprecedented catalytic capability. First, a novel group-6 propane monooxygenase (PRM) has been identified in an archetypical dioxane metabolizer, Mycobacterium dioxanotrophicus PH-06, and characterized for its capability of initiating the oxidation of dioxane. Further, kinetic enzymatic tests in heterologous expression clones demonstrated a high affinity to dioxane (substrate) and a low susceptibility to co-existing inhibitors (e.g., TCE and 1,1-DCE). These results suggested group-6 SDIMOs may widely prevail and contribute significantly to dioxane attenuation in the field, necessitating the development of molecular tools for assessing and monitoring the intrinsic processes. Furthermore, PRM exhibits a highly versatile degradation capacity, which is not only responsible for the breakdown of cyclic molecules (e.g., dioxane, tetrahydrofuran, and cyclohexane), but also degrades a variety of short-chain alkanes/alkenes (e.g., ethane, propane, butane, isobutane, and ethene) and chlorinated and aromatic pollutants, including vinyl chloride, 1,2-dichloroethane, benzene, and toluene. This is the first to report the unique ability of group-6 PRM that synchronizes dioxane degradation and short-chain alkane/alkene assimilation, unraveling its essential role in aerobic biostimulation that utilizes propane, isobutane, or other alkane/alkene gases to select and fuel indigenous microorganisms for the costefficient remediation of the commingled contamination of dioxane and chlorinated compounds.

Identification of microorganisms responsible for reductive defluorination of PFASs in an enrichment culture

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We have recently discovered microbial reductive defluorination of two per- and polyfluoroalkyl substances (PFASs) by a dechlorinating enrichment culture. By examining the cell growth and activity, we found that the well-known dechlorinators (e.g., Dehalococcoides spp., Geobacter spp.) in the dechlorinating enrichment were not involved in the reductive defluorination, thus the responsible defluorinating microorganisms might be a minority member in the community. The goal of this study is to enrich and identify the microorganisms carrying out the defluorination of PFASs. We conducted enrichment experiments by providing PFAS and hydrogen as the sole electron acceptor and electron donor. We further conducted 16S rRNA gene amplicon sequencing and metagenomic sequencing to reveal the succession of community composition along the enrichment process. Results showed a significant shift of the community structure from the seed culture to the most recent enrichment culture caused by the community function changing from dechlorination to defluorination. More importantly, the phylogenetic groups have been significantly enriched as a response to the enhanced defluorination activity in the enrichment over several subcultures, suggesting their involvement in reductive defluorination. Genome reconstruction will reveal comprehensive metabolic properties of the plausible defluorinating microorganisms. Altogether, by identifying potential defluorinating microorganisms, this study brings significant insights into the development of cost-effective PFASs treatment technologies.

ENVR 54

Biotransformation of sulfonamide antibiotics: Blind spots and emerging opportunities

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The release of sulfonamide antibiotics into the environment is alarming because the existence of these antibiotics in the environment may promote resistance in clinically relevant microorganisms, which is a potential

threat to the effectiveness of antibiotic therapies. Controllable biodegradation processes are of particular significance for the inexpensive yet effective restoration of sulfonamide-contaminated environments. Cultivationbased techniques have already made great strides in successfully isolating bacteria with promising sulfonamide degradation abilities, but the implementation of these isolates in bioremediation has been limited by unknown microbial diversity, vast population responsiveness, and the impact of perturbations from open and complex environments. Advances in DNA seauencina technologies and metagenomic analyses are being used to complement the information derived from cultivationbased procedures. In this study, we provide an overview of the growing understanding of isolated sulfonamide degraders and introduce the genomic characterization, kinetics, and pathways of sulfonamide biodegradation by Paenarthrobacter spp.. The partnership of Arthrobacter and *Pimelobacter* in aerobic degradation of sulfadiazine is also deciphered by metagenomics analysis approach. In addition, we propose a technical paradigm that integrates experimental testing with metagenomic analysis to pave the way for improved understanding and exploitation of these ecologically important isolates. Overall, we aims to outline how metagenomic studies of isolated sulfonamide degraders are being applied for the bioremediation advancement of strategies for sulfonamide contamination.

ENVR 55

Improving wastewater treatment using free nitrous acid (FNA)

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Free nitrous acid (FNA), the protonated form of nitrite, was an unwanted substance in wastewater systems due to its inhibition on a wide range of microorganisms. However, in recent years, advanced understanding of FNA inhibitory and biocidal effects on microorganisms has led to the development of a series of FNA-based applications that improve wastewater management practices. FNA has been used in in wastewater treatment to achieve carbon and energy efficient nitrogen removal; in anaerobic digestion to improve the sludge reduction and energy recovery; and in aerobic digestion, sustained FNA accumulation can be achieved to increase sludge reduction and nitrogen removal. This paper aims to review the current status of FNA-based applications in improving wastewater managements. The underlying mechanisms of FNA inhibitory and biocidal effects will be reviewed. The experiences learned from operating FNA-based wastewater treatment system in both lab- and pilot-scales will be reviewed and discussed. Knowledge gaps and future opportunities of the FNA-based applications are identified. We conclude that the FNA-based technologies

have great potentials for enhancing the performance of wastewater treatment systems; however, further development and demonstration at larger scales are still required for their wider applications.



ENVR 56

Biological nitrogen removal through nitrite shunt and hydrogenotrophic denitrification in saline wastewaters

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Nitrite shunt is an economical nitrogen removal process that can reduce up to 25% in aeration costs and 40% in biomass production by minimizing the activities of nitrite oxidizing bacteria (NOB) in the nitrogen cycle. Furthermore, hydrogenotrophic denitrification has also proven its potential as a low-cost, effective method of denitrification with low sludge production. The aim of this study was to utilize the nitrite shunt bioprocess in combination with hydrogenotrophic denitrification for nitrogen removal in saline wastewaters. Adjacent nitrifying and hydrogenotrophic denitrifying reactors were maintained over time in saline conditions (4%) to enrich stable microbial consortiums. The nitrifying reactors achieved around 95% nitrite accumulation with peak ammonia oxidation rates of 50±5 mg NH4+-N L-1×d-1 revealing the successful suppression of NOB within the nitrifying reactors. The hydrogenotrophic denitrifying reactors achieved 92% denitrification (i.e. nitrate/nitrite removal), with peak removal of 135±5 mg NO₃-N L⁻¹×d⁻¹. Further analysis of the hydrogenotrophic microbial community found the abundant genus' of Thauera, Rhodobacterecaea and Hydrogenophaga all containing key enzymes required for PHA/PHB production. Highlighting the potential of obtaining added value products from the wasted sludge. It is envisioned that using the enriched microbial communities obtained in this study an efficient nitrogen removal treatment system can be designed to treat nitrogen containing pollutants in a sustainable manner. This system can be implemented in

common industries that produce saline wastewaters such as the dairy, seafood and tannery industries.

ENVR 57

Global wastewater microbiome: Taxonomic and functional diversity

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Microorganisms in wastewater treatment plants (WWTPs) play critical roles in sustaining ecosystem functioning, environments, human health and society, but the mechanisms controlling their diversity and biogeographic patterns remain elusive. Using a systematic globalsampling effort, we analyzed microbiomes from ~1,200 activated sludge samples taken from 269 WWTPs in 23 countries on 6 continents. These samples were characterized by 16S rRNA gene amplicon and part of them also by metagenomic sequencing. Our analysis revealed that the global AS microbial communities follow lognormal distribution with ~1 billion (10⁹) microbial species. Although the AS microbial communities are highly diverse with majority (~80%) of sequences not represented in the current databases at species level, there is a global core microbial community (0.05%) strongly linked to WWTP functions. In contrast to macroorganism studies, however, no latitudinal diversity gradient was observed. Mata-analysis with global datasets from various habitats indicated that AS microbiome is more closely related to freshwater microbiome. Further analysis revealed that spatial turnovers of the AS microbial communities are scaledependent and driven largely by stochastic (e.g. dispersal limitation, drifts) as well as deterministic (e.g. organic C, temperature) processes. We got 222 metagenomes with an average size of 14G. These metagenomes resulted in 3140 high-quality draft genomes with completeness > 70% and contamination < 5%, which represent a series of functionally important taxa in wastewater treatment.

ENVR 58

Biorefineries using synthetic microbial consortia

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Production of renewable energy has been the focus of our and lignocellulose, the most abundant society. macromolecule, appears to be an ideal feedstock due to its low cost and environmental impact. However, breaking down cellulose is the bottleneck of cellulose biorefinery. The cellulolytic isolates existing in nature have limited capacity to destruct the cellulose, and it is genetically difficult to engineer those strains. Synthetic microbial consortia are emerging as promising platforms for various engineering applications. The synthetic consortia hold promise for cellulose biodegradation, as more efficient nutrient cycle could be achieved by functional differentiation and metabolite exchange within the consortia. Enrichment of rumen fluid on cellulose showed robust degradation capacity of cellulose, and the metagenomic analysis revealed key species in cellulose degradation. Efforts have been made by researchers to use synthetic consortia to biodegrade lignocellulose together with production of valuable chemicals. Challenges exist in understanding the molecular mechanism of microbial interactions and rational design of consortia. The occurring revolution in systems biology and synthetic biology tools is likely to assist in optimizing the performance of synthetic microbial consortia for cellulose biorefineries.

ENVR 59

Metagenomics study of soil microcosms to evaluate the bioremediation of textile dyes in a contaminated ecosystem

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Textile dye contamination is a serious problem that reduces soil productivity by destabilizing microbial community structures. Here, we investigated the influence of bioaugmentation on the degradation of a mixture of dyes (MOD) and textile industry effluent (TIE) in soil microcosms using eight different dye-degrading bacteria. The biodegradation potential improved in the bioaugmented microcosms, especially in the initial phase. The bioaugmented MOD and TIE microcosms exhibited 98.33% and 94.19% decolorization and 96.92% and 95% chemical oxygen demand (COD) removal, respectively, at day 30. Several dye-catalyzing enzymes were examined, and the activities of lignin peroxidase, veratryl alcohol oxidase, tyrosinase, and azoreductase were found to be significantly induced (>three-fold increase) in bioaugmented microcosms due to the addition of textile dyes and bacteria. Changes in alpha diversity induced significant alterations in the microbial community structure of the microcosms because of continuous MOD and TIE flow. The Rheinheimera, Kocuria, Ruminococcaceae UCG-010, Ralstonia, and Pseudomonas bacterial assemblages were found to be dominant after exposure to MOD and TIE, indicating that these genera

are key in dye biodegradation. The bacteria used for augmentation, namely, Staphylococcus, Bacillus, Arthrobacter, and Pseudomonas, survived well in the soil microcosms and their relative populations increased, suggesting that they co-existed synergistically with the indigenous microflora. Functional annotation of metagenomes illustrated that xenobiotic pathways such benzoate. aminobenzoate. chloroalkane as and chloroalkene, etc. degradation may provide alternate pathways for MOD and TIE detoxification. Our results indicate that augmented dye degrading bacteria and soil microbiome have established a potentially mutualistic symbiotic relationship with increase in detoxification rate leading to sustainable approach for restoration of contaminated agricultural sites.

ENVR 60

Choosing well among research topics, potential students, and collaborative opportunities

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One of the great privileges of academic life is the freedom to choose. We are free to choose the topics of our research, the students we supervise, the courses we teach, the colleagues we collaborate with, and the service we provide for our scientific community and institutions. Of course, these freedoms are conditional - we have to find funding for our research topics, students have to be interested in working with us and taking our courses. colleagues have to share our interests and our scientific community and institutions have to value our service. Lynn Roberts' record - of projects she has conducted, students that she has mentored and taught, collaborations that she has contributed to, and service that she has provided - shows that she has exercised her freedom to choose thoughtfully, with consideration for others and with the highest professional standards. Lynn's professional choices set an example for all of us as her colleagues and friends.

ENVR 61

Kinetic isotope effects in the halogenation of dimethenamid

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Halogenation via electrophilic aromatic substitution (S_EAr) initiates formation of disinfection byproducts (DBPs). The S_EAr mechanism involves two steps: 1) electrophile (halogen) addition and 2) proton removal. Mechanistic

DBP formation models typically assume that halogen addition is the rate-determining step (RDS). Proton removal has been shown to be rate-determining in iodination, although this has never been examined under drinking water treatment conditions. Contributing to the uncertainty, iodination was recently proposed to undergo a concerted mechanism, rather than stepwise. lodinated DBPs tend to be more toxic than chlorinated and brominated analogues, which calls for better understanding of how iodination in disinfected water differs from bromination and chlorination. This study examines the RDS of halogenation in laboratorysimulated water disinfection using kinetic isotope effect (KIE) analysis. Dimethenamid (DM) was selected as an aromatic substrate because DM halogenation has been extensively characterized under water treatment conditions. Deuterated DM (DM-d) was synthesized with trifluoroacetic acid-d. DM and DM-d halogenation rates were measured in parallel reactors under identical conditions for each experiment. Chlorination and bromination did not exhibit KIEs ($k_H/k_D \approx 1$), consistent with halogen addition as the RDS. In contrast, primary KIEs (>1.4) were always observed in iodination, indicating involvement of proton removal in the RDS. Iodination rates increased as pH (5.2 – 8.9) and $[I^-]$ (10 – 100 μ M) decreased, although the magnitudes of KIEs did not vary substantially (1.47 (±0.08) to 2.06 (±0.40)). The influences of pH and [I-] suggest that iodine addition is also involved in the RDS. Adding 1 mM [CI-] enhanced iodination rates without affecting the KIE appreciably (1.71 (±0.08)), whereas [CI-] addition above 25 mM increased the KIE (2.9 - 3.4) but not the rates of iodination further. These results suggest that kinetic control shifts from iodine addition to proton removal with increasing [Cl-], consistent with the putative stepwise SEAr mechanism. rather than a concerted mechanism. Under typical drinking water conditions ($[CI^{-}] \le 7 \text{ mM}$), a kinetic model assuming iodine addition as the RDS performed well, even though the primary KIEs indicate that proton removal is part of the RDS. A model accounting for proton removal was required to capture the influence of $[C]^{-1} \ge 25$ mM on iodination (e.g., brine, seawater).

ENVR 62

Influence of overlooked chlorinating agents on the halogenation kinetics of cyclic alkenes

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 Cl_2 and Cl_2O , which are minor constituents of free available chlorine (FAC) under drinking water treatment

conditions, have been recognized as highly reactive chlorinating agents for some organic compounds. Nonetheless, robust rate constants for Cl₂ and Cl₂O remain scarce in the environmental literature. In this work, we explored the chlorination kinetics of three structurally related alkenes (α -ionone, β -ionone, and dehydro- β ionone), a class of compounds whose reactivities with Cl₂ and Cl₂O have not been previously investigated. Secondorder rate constants for Cl₂, Cl₂O, and HOCI were computed from experimental rate constants obtained at various pH values, [CI⁻], and [FAC]. Our results show that while HOCI is the predominant chlorinating agent for the most reactive alkene, Cl₂ and Cl₂O can dominate the chlorination kinetics of the less reactive alkenes at high [Cl⁻] and high [FAC], respectively. The tradeoff between overall reactivity with FAC and selectivity for Cl₂ and Cl₂O previously observed for aromatic compounds also applies to the alkenes examined. In laboratory experiments in which high [FAC] may be used, omission of Cl₂O in data modeling could yield second-order rate constants of dubious validity. In chlorinating real waters with elevated [Cl⁻], formation of Cl₂ may enhance the formation kinetics of chlorinated disinfection byproducts (DBPs).

ENVR 63

Esoteric electrophiles in chlorinated waters: When conventional kinetic models fall short

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A hallmark of Lynn Roberts's research group is the careful analysis of kinetic models associated with the transformation of organic compounds in natural and engineered systems. Particularly over the last decade, research from the Roberts Group has sparked a reexamination of traditional kinetic models associated with electrophilic substitution involving active halogenating agents. Such models generally assume that the most abundant halogenating agents present in chlorinated systems (e.g., HOCI and, if bromide is present, HOBr) are kinetically-relevant electrophiles. the These onlv traditional models often overlook the possibility that less abundant electrophiles (e.g., Cl₂, Cl₂O, Br₂, BrCl, and BrOCI) can influence (and in some instances control) overall halogenation rates of modestly nucleophilic organic compounds. This presentation will discuss the origins and more recent developments associated with the Roberts Group's scrutiny of conventional kinetic models by incorporating the effects of commonly overlooked electrophiles. Some of these electrophiles can, for example, account for the observed role of chloride catalysis on chlorination (Cl₂) and bromination (BrCl) of unsaturated organic compounds. Notina that anthropogenic activities such as road salting and hydraulic fracturing can increase chloride levels in potable waters, this presentation will also discuss how chloride

catalysis can influence the formation of toxic disinfection byproducts in chlorinated waters.

ENVR 64

Leachability, photodegradation, and potential ecotoxic impact of trifluralin-impregnated mulch

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The leachability, potential ecotoxicity, and photolysis of trifluralin-impregnated mulch, a popular retail consumer gardening product, were investigated under environmentally realistic conditions. Leachability of trifluralin from impregnated mulch was low (< 1% of total extractable compound) and in the range of reported values for agricultural soils. No trifluralin transformation products were detected in mulch leachate. Yeast-based estrogenicity and androgenicity screens indicated that aqueous trifluralin is not estrogenic but is moderately androgenic. Impregnated mulch leachate was not hormonally active, even at undiluted concentrations, but it did exert nonspecific toxicity at dilutions of ~1:10. Photolysis of trifluralin was investigated in acetonitrile and water and on mulch surfaces. Degradation on mulch surfaces was diffusion-limited; it was ~17 times slower than in aqueous solution, but faster than has been reported on kaolinite. An array of trifluralin transformation products was identified, but in no case did they exceed 10% of the parent compound.

ENVR 65

From solvents to steroids: Importance of accounting for chemical transformation pathways in achieving safe and sustainable water supplies

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Understanding chemical transformation pathways is integral to the management of impaired water supplies, optimization of new treatment technologies, and development of regulations for protecting ecosystem and human health. Inspired and shaped by the distinguished career of A. Lynn Roberts as researcher, educator, and mentor, this talk will discuss recent work focused on better predicting chemical transformation pathways in the environment and the implications of bioactive transformation products for safe and sustainable water supplies.

ENVR 66

Understanding and monitoring the decay of waterborne viruses during ozonation

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Ozone is rapidly becoming an integral part of many water and wastewater treatment trains, thanks to its high efficacy at inactivating pathogens and mitigating trace organic contaminants. Although ozone possesses potent antimicrobial activity, several barriers remain to fully exploit its potential as a disinfectant. First, the kinetics and mechanisms of ozone-inactivation of waterborne pathogens remain poorly understood. Second, the performance of ozone during water and wastewater treatment is difficult to monitor, due to a lack of real-time methods to assess pathogen infectivity. In this study, we investigated the fate of waterborne viruses during water treatment by ozone. We first developed an experimental system to accurately measure virus inactivation at very low ozone exposures. The inactivation rate constants were very high (~ 10⁶ M⁻¹s⁻¹) and within an order of magnitude for all viruses considered, independent of their composition or structure. Furthermore, the loss of infectivity coincided with loss of genome functionality, indicating that genome degradation is the main mechanism causing inactivation. Finally, we explored the use of proxies, which are easy to measure and correlate with virus inactivation, to circumvent the challenges associated with monitoring virus infectivity in real-time and assessing the ozone exposure in wastewaters. Proxies considered were the abatement of UV₂₅₄ and of carbamazepine ubiquitous (CBZ), а organic micropollutant with a similar abatement rate constant as human viruses. Both proxies were well-correlated with virus inactivation, and their applicability to virus inactivation monitoring was confirmed in a pilot-scale drinking water treatment setup. Overall, this study confirms that ozone has a high potential to mitigate waterborne viruses in water and wastewater, and provides tools to monitor ozone treatment performance.

ENVR 67

Magnetite: Formation and reactivity

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Magnetite (Fe₃O₄) is a ubiquitous environmental constituent found in weathered clays and soils, in atmospheric aerosols, and in recently deposited marine

and freshwater sediments. A mixed-valence Fe^{II}-Fe^{III} iron oxide, magnetite is produced when reduced iron corrodes. In this presentation, I will present work describing the formation of magnetite as a result of the oxidation of zero valent iron and will then discuss studies conducted to examine magnetite reactivity towards groundwater contaminants and dissolved oxygen and the potential application of magnetite as a sorbent for removing phosphate from urine.

ENVR 68

Building a more comprehensive understanding of offsite agrochemical runoff through the expansion of target analytes

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Agrochemicals, including pesticides and fertilizers, are essential to modern crop production. However, offsite transport of agrochemicals can be detrimental to ground and surface water quality. Analytical methods have been developed to include hundreds of pesticides from multiple classes to assess their offsite transport and persistence. The inclusion of pesticide metabolites, degradates and transformation products is limited by the availability of standards and suitable methods but is essential to better understand the fate of active ingredients. Recent work has been done to identify metabolites/degradates through both laboratory (dosed) studies and environmental samples (with an emphasis on the widely used neonicotinoid insecticides) to determine which are candidates to add to wider-scale monitoring methods. In addition to pesticides and metabolites, other agrochemicals are often applied to agricultural fields but are rarely measured; these include nitrification inhibitors (bactericides that are co-applied with fertilizers to limit the conversion of fertilizer ammonium to nitrate) and herbicide safeners (protect the crop from herbicide toxicity). The nitrification inhibitor nitrapyrin and the dichloroacetamide herbicide safeners were found to occur in waterways of the midwestern U.S. with peak concentrations co-occurring with peak herbicide concentrations (spring). Together these results can lead to a better understanding of what chemicals are being transported offsite, the potential toxicity single chemicals and complex mixtures pose to non-target organisms, and the potential changes to natural environmental cycles (e.g., the nitrogen cycle).

ENVR 69

Isomer specific reduction of hexabromocyclododecane by Fe(II) in iron oxide suspensions

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Hexabromocyclododecanes (HBCDDs) are a common brominated flame retardant known to accumulate in soil and sediments. The reaction of HBCDDs with iron oxides (i.e., magnetite, goethite, and hematite) in the presence of dissolved Fe(II) was investigated. The individual degradation rates of the three dominant isomers (α , β , and γ) of HBCDD with Fe(II)/iron oxides were investigated at room temperature. Kinetic experiments were performed at different pH with different concentration of Fe(II) and different iron oxide minerals to evaluate the influence of these environmental factors on the degradation of HBCDD. An isomer selective reaction was observed, and the observed reaction rates appear fast enough to be potentially relevant for the fate of HBCDD in soil and sediments.



Figure 1: Reaction of 1 mM HBCDD in the presence of 2.5 mg mL⁻¹ magnetite and an initial concentration of 6 mM Fe(II) at pH 7.17 and 27 °C

ENVR 70

Abiotic reduction of RDX and NTO: Still investigating electron transfer, kinetics, and reaction pathways

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The energetic compounds, hexahydro-1,3,5-trinitro-1,3,5triazine (RDX) and 3-nitro-1.2.4-triazole-5-one (NTO) have been extensively used in military operations. The potential toxicity, high solubility, and low volatility of these compounds have led to or have the potential to lead to widespread contamination in the subsurface. Monitored natural attenuation (MNA) is an important component of groundwater remediation strategies. Compound specific isotope analysis (CSIA) may be a powerful tool to address the needs of MNA for quantification of the extent and identification of the mechanism of contaminant degradation process. Iron-bearing minerals in soil and sediments are good electron donors, which may be important in the natural attenuation of energetic cyclic Nnitrosamines through abiotic reduction. In this study, abiotic reduction of RDX and NTO mediated by different mineral phases and buffer conditions was characterized to obtain rate constants and nitrogen (for RDX) and carbon (for NTO) isotope fractionation data. Besides experiments in simulated groundwater, real groundwater samples from an ammunition plant were measured using CSIA to estimate the extent of RDX degradation. The results show distinct reduction rates of RDX and NTO under different experimental conditions, while CSIA suggests a defined pattern of isotope fractionation for each compound regardless of the experimental conditions. Field data indicates abiotic reduction contributes to the decreasing concentration of RDX along a groundwater plume.

ENVR 71

RAPID data-driven automated discovery of new organohalide perovskites

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Organohalide perovskites are a promising new material for low-cost, high-performance photovoltaics, but existing compounds-such as methylammonium lead iodidesuffer from environmental instability and use potentially toxic elements. The tremendous structural diversity that can be achieved by modifying the organic and inorganic building units presents the possibility of developing new, stable, high performance materials, but presents the challenge of a tremendous chemical space that must be explored. Very little is known about the mechanistic details of the crystal formation, and the range of possibilities is too vast to explore by brute force methods. Can machine learning approaches help accelerate the discovery of new materials? To address this problem, we have developed the Robotic-Accelerated Perovskite Investigation and Discovery (RAPID) platform. This

consists of an open source software package-ESCALATE (Experiment Specification, Capture and Laboratory Automation Technology), for experiment description and data collection-combined with lab automation hardware. The first generation of RAPID uses inverse temperature crystallization (ITC) to grow halide perovskite single crystals for x-ray structure determination and bulk characterization using commercial liquid handling robots. Collected characterizations includes qualitative measurements of crystal quality (including photographic images of the samples), powder X-Ray diffraction, and spectroscopic measurements along with background laboratory conditions. The second generation of RAPID is extended to include antisolvent precipitation synthesis of perovskite single crystals and perovskite thin film synthesis and characterization including remote monitoring of long-term environmental stability. The comprehensive data of all experimental successes and failures is fed into an analysis pipeline that generate machine learning models relating reagent properties, composition, and reaction conditions to crystal formation, reports human-interpretable insights into the formation process, and creates recommendations for follow-up reactions. In addition to reporting on the chemical "successes", we will also describe work on benchmarking the effectiveness of different experiment recommendation algorithms for identifying new compounds.

ENVR 72

Identifying the governing factors for plant uptake of engineered nanoparticles through machine learning

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Engineered nanoparticles (ENPs) are now common ingredients in a wide variety of commercial products. significantly increasing the incidental or intentional release and buildup in the environment. A large fraction of these ENPs get into agricultural systems and their uptake and accumulation in food crops become a serious food safety concern. Even though numerous studies have been performed and some physiochemical properties of ENPs have been suspected to play more important roles than others in their uptake and accumulation, it remains uncertain which property is a dominant factor, and how the governing factor for plant uptake of ENPs may vary with different nanoparticle compositions and plant growing conditions. After compiling data from the past ten years of studies in the literature concerning the plant uptake and accumulation of ENPs. different machine learning tools were used to identify chief factors governing the extent of plant uptake of ENPs. Preliminary analysis with recursive feature elimination (RFE) algorithm indicated that nanoparticle size and surface charge are

two dominant parameters affecting plant uptake of ENPs in a hydroponic system. However, their relative significance varies with nanoparticle composition and the concerned plant tissues. For example, while the size of cerium oxide nanoparticles is the most dominant factor in their accumulation in plant roots, surface charge appears more important in their accumulation in plant shoots. For zinc oxide nanoparticles, the opposite becomes true that the surface charge is the most significant factor in plant root accumulation while the size is more critical in plant root accumulation. The presence of soil in the growth media has a substantial effect on plant uptake of some ENPs. In a soil growing condition, the total organic matter contents in soil becomes the primary factor controlling the uptake and accumulation of zinc oxide nanoparticles and copper oxide nanoparticles in plant shoots. These results generate significant insights into the extent of ENP uptake in different growing conditions and shed light on the sustainable manufacturing of engineered nanoparticles. The results also suggest that while hydroponic studies are important, they may not represent the full picture of plant uptake of ENPs in actual environment where soil is generally present.

ENVR 73

Examining plant uptake and translocation of emerging contaminants using intelligent techniques

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The multiple sources of emerging and fugitive contaminants (EFCs) have potential to impact vegetation and the quality of our food supply, particularly as a prominent part of the human expozome. Uptake of EFCs from the groundwater is one pathway of interest, and efforts have been made to relate root exposure to transloation throughout the plant. Mechanistic models desscribing uptake and translocation as function of chemical properties have been generated, but with limited applicability and acceptance. The current research was an effort to introduce artificial intelligence and machine learning techniques to investigate uptake and translocation of EFCs using physicochemical properties. Neural network (NN), fuzzy logic, and clustering algorithms, as intelligent techniques were used to predict transpiration stream concentration factor (TSCF), examine the interactions between compound properties. translocation of EFCs in plants. The NN models predicted uptake of EFCs with improved accuracy relative to mechanistic models. We found that log Kow, molecular weight, hydrogen bond donor, and rotatable bonds are the

most significant properties with different relative importance in transmembrane migration. Laboratory experiment screening 14 new compounds in rapid throughput analysis developed in this work providing data on emerging contaminants with unique physicochemical properties. We delivered new insight to compound properteis, the relationship between molecular weight and log Kow with TSCF was found to be both bell-shape and sigmoidal. Physiochemical property cutoffs obtain by fuzzy logic, i.e. restrictions, for compounds passing plant roots membrane were shown to be lower than the cutoffs for transmembrane transport in mammalian intestinal systems. This is important as the cutoffs for the compounds accumulating in the edible parts of the plants are more like the cutoffs for the compounds crossing the plant root membranes than the cutoffs for the compounds accumulating in the plant roots. Therefore, the human health impacts through consumption of contaminated crops should be considered.

ENVR 74

Predicting adsorption of organic contaminants on biochar, CNTs, GAC, and resins by artificial neural networks

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Artificial neural networks (ANN) coupled with ppLFERs (poly-parameter linear free energy relationships) provided an easy and powerful method for predicting aqueous adsorption on four most widely used adsorbents: biochar, CNTs, GAC, and resin. During the modeling process, two different data splitting approaches were compared and group-selection (rather than point-selection) was decided for the adsorption data splitting, which provided better consistency between the validation and test sets. Also, a cosine similarity approach, based on which only the data that shared high similarity with the test set were selected as the training set, was employed to further improve the accuracy of the prediction. Compared with the published results. ANN-ppLFERs could predict aqueous adsorption more accurately with the RMSE (root mean square error) values between 0.23 to 0.31 log unit, and the developed easy-to-use integrated GUI tool is user-friendly and can greatly enable non-modelers to conduct adsorption prediction. Overall, the well-improved results suggested a promising future of ANN-ppLFERs in aqueous adsorption prediction.

Estimation of iron and manganese concentration in ground water using absorbance in UV-Vis spectrophotometer via artificial neural network

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Groundwater is a key source of drinking water for 2 billion people around the world. Currently, groundwater is the major source of water for urban supply and for drinking in rural areas of Bangladesh. Despite the depletion in groundwater level due to high volume of extraction, groundwater is still preferable as drinking water source as surface water here is unhygienic. Recently, groundwater is being extracted from shallow wells to serve the Rohingya refugees at Cox's Bazar, Bangladesh, due to insufficient and unpalatable surface water. As Iron (Fe) and Manganese (Mn) concentration in most areas of Bangladesh exceed the standard limit for drinking purposes, it's important to monitor the quality of groundwater extracted for drinking. Both Fe and Mn occur through natural interactions of water and rock. They can pose health risk and lots of engineering and aesthetic problems if present at high concentration. Several methods such as Atomic Absorption Spectrophotometer (AAS), Inductively Coupled Plasma (ICP) and Colorimetric methods are used to measure Fe and Mn concentrations in water. These methods are often time consuming and require expensive devices, harmful chemical reagents and expert supervision. In this study, we used a quantitative approach, namely artificial neural networking (ANN), to estimate Fe and Mn in water using absorbance determined through UV-Vis spectrophotometer. UV-Vis Spectrophotometer is a relatively cheap, efficient, and portable device, which can provide absorbance of a spectrum instantly, requiring no additional chemical. We collected 52 groundwater samples, including both unfiltered and filtered ones, from Rohingya Camps. Absorbance of each sample in UV-Vis spectrophotometer were recorded for a spectrum covering wavelength of 200 nm to 1100 nm. Concentrations of Fe and Mn in these samples were determined using AAS method. An ANN model was developed to predict the Fe and Mn concentrations present in the samples from the measured absorbance values. From the model, we observed that the prediction models showed a strong correlation between Fe and absorbance values, reflected by the high R2-value for samples with relatively low concentrations of Fe (0.4 mg/L to 2 mg/L, R2 = 0.82) and Mn (0.008 mg/L to 0.3 mg/L, R2 = 0.91) than for samples with higher concentrations. Use of UV-Vis spectrophotometer coupled with application of artificial neural network may provide an efficient and cheap tool for groundwater quality monitoring for Fe and Mn.

ENVR 76

Robots and AI for rapidly characterizing and remediating contaminated soils

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Soil contamination often occurs over vast areas. The selection and cost of remediation alternatives requires a good understanding of the distribution and levels of contamination across the site. Current characterization practices require expensive and time-consuming measurements that often include large numbers of samples that are below detection, thereby providing minimal information. Autonomous vehicles (robots) equipped with appropriate on-board detectors and appropriate ML/AI algorithms to direct the robot to high value sampling locations can potentially provide rapid, cost-effective characterization of soil contamination. However, there are significant challenges with respect to mobility of the vehicles, sample collection, avoiding contamination between sampling events, and waste valorization that must be overcome to make these approaches robust. Similarly, there are challenges developing robust and accurate on-board detection methods capable of operating autonomously. Initial investigations have identified mobility platforms and detection systems capable of autonomously sampling for important soil contaminants including petroleum hydrocarbons and salt. These investigations have developed potential AI/ML algorithms to rapidly locate and characterize contamination hotspots. These findings are presented along with a forward-look at other opportunities for automation in environmental remediation.

ENVR 77

Topic modeling using natural language processing on facility source reduction comments submitted to the Toxics Release Inventory

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Industrial facilities reporting to EPA's Toxics Release Inventory (TRI) are required to report source reduction activities implemented during the year. Facilities may elaborate on pollution prevention (P2) activities they have

undertaken or any specific barriers to implementing P2 activities using an open text field (called 8.11 text). In recent years, there have been more than ten thousand comments submitted each year, which makes manual review extremely time consuming and difficult to interpret and extract useful information. As a result, the 8.11 text of the TRI program remains an under-explored yet large and potentially information-rich dataset. This presentation reviews efforts to conduct topic modeling on a selection of the TRI 8.11 text submissions for solvent chemicals from the chemical manufacturers' industry sector using machine learning algorithms such as latent Dirichlet allocation and bi-term topic modeling. The algorithms use various statistical modeling methods to group comments into an assigned number of topics based on their content. The algorithms can help identify latent topics within the large quantity of texts, creating a more objective and automated process to review the TRI 8.11 text. Initial results yielded topics such as solvent substitution, solvent recycling/reuse, and regulatory references.

ENVR 78

Data-driven innovations in water resource recovery facilities: Emerging era of sustainability intelligence

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Our changing planet presents a host of intertwined challenges that will affect the future of the environment and human well-being. Sustainability intelligence is the integration of environmental sustainability research with data science, artificial intelligence and cutting-edge digital approaches to provide the new and truly meaningful insight that is needed for individuals, industries and policy-makers to tackle these ever-severe challenges and mitigate the unwanted effects of environmental change. This presentation will provide a personal perspective of the increasingly widespread use of data and artificial intelligence technologies to address environmental changes. It describes the journey from how data-driven technologies can offer a promising foundation for dealing with the emerging issues and supporting transitions in water and sanitation systems to examples of alternative paradigms in current day. The accumulated evidence from the presenter's experience and literature shows that an emerging era of sustainability intelligence is already coming and allowing us to design and use innovative new methods to enhance the overall performance of existing water technologies, and to extend functionality of today's systems. Finally, the presentation also outlines avenues for future water and wastewater service protocols with sustainability intelligence.

ENVR 79

Novel physics-informed data-driven modeling to predict physiochemical state of water/wastewater system

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Existing machine learning and data-driven models are normally established upon big data without knowing physical of a given system properties (e.a. water/wastewater treatment unit). To conquer this problem of "Big data, Small Task", this study explored an innovative approach to obtain high spatiotemporalresolution data and equip models with physical meanings, through which prediction accuracy of data-driven models could be effectively enhanced as "Small Data, Big Task". Specifically, a novel physics-informed data-driven model was developed based on datasets obtained from flat millielectrode array (MEA) sensors (conductivity, pH and temperature) in a continuously-stirred tank reactor (CSTR) to predict system performance. Three of each type of MEA sensors were deployed along with the CSTR depth to real-time in situ profile heterogeneity (Fig.1a). Shock solution was individually injected into the CSTR using a syringe. For model development, the reactor was divided into four compartments (top, middle, low and mixing zone) (Fig.1b). Reduced-order multi-compartment models were established based on the transport mechanism of Na+ (conductivity), H+ (pH) and heat (Temperature). Rigorous deterministic global dynamic optimization algorithms were deployed to validate these data-driven models by solving the corresponding parameter estimation problems. This unique physicsinformed data-driven modeling effectively determined the best-possible predictive capability for mixing dynamics under shocks (Fig.1b), represented by excellent fitting to MEA sensor data without sacrificing physical meanings (Fig.1c). In contrast, machine learning Eurega® solely depended on data suffered from lack of physical meanings (Fig.1d) and could not be used for system prediction or control. By integrating two-fold physical-data properties, this powerful modeling could predict physicochemical state of water/wastewater systems, especially under transient shocks, and will ultimately enhance system resilience and enable energy-saving operation.



ENVR 80

Quantification of uncertainty in drinking water lead levels for Southwest Pennsylvania

learning data fitting without physical meaning under Top Conductivity Shock.

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Lead is a neurotoxin and detrimental to human health. Use of lead in piping and dissolution of that lead into drinking water remains a pervasive issue dating back to the early 20th century. Lead is most common in interior plumbing, solder and service lines that connect the house to the main water line. At locations where historical lead pipe is still in use, corrosive water conditions may cause dissolution of lead into drinking water conveyed by lead pipes. Water utilities typically manage historical lead materials and mitigate dissolution of lead through the use of corrosion control systems to chemically mitigate lead leaching and lead service line removal programs. The Lead and Copper Rule (LCR), promulgated in 1991, requires that the 90th percentile of regulatory samples collected have a lead level less than the action level (AL) of 15 ppb. If the AL is exceeded, additional sampling must be conducted, corrosion control systems must be adjusted or added, and a subset of residual lead service lines must be removed. For large drinking water systems (greater than 100,000 customers) the LCR action level and subsequent corrosion control modifications are assessed based on annual collection of 100 samples taken at customer taps. Due to the limited number of samples collected and the focus on the 90th percentile statistic, the LCR does not provide a water utility with sufficient information to understand the variability or uncertainty of lead levels across a large distribution system. With the LCR currently under review, there is a

need to evaluate how existing compliance data can be used in conjunction with new analytic methods to assess system wide lead release and improve corrosion control deployment. The present work seeks to evaluate LCR collected compliance data for Southwestern Pennsylvania (a region with existing lead concerns). Nonparametric imputation methods are used to estimate values for samples recorded as below the detection limit. Lognormal and empirical distributions are estimated and used to characterize the distribution of lead levels for a region in each year. Bootstrapping simulation methods are used to quantify the uncertainty associated with median and regulatory 90th percentile estimate. Results will be used to recommend new approaches for utilities to use to improve understanding of current and historical lead release.

ENVR 81

Toward single atom catalysis for environmental application

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Various noble metals have been employed as catalysts and co-catalysts to enhance the kinetics of reactions that are critical for environmental remediation. The need to maximize the available catalytic sites per unit mass, particularly due to noble metal scarcity and high cost, has driven the development of material architectures at the nanometer scale. Recent theoretical and experimental studies have explored noble metal catalysts on the subnanometer, atomic scale to maximize atomic efficiency. A single atom catalyst (SAC) is the theoretical limit in this endeavor, and previous studies have identified additional benefits such as low coordination state and strong interaction with the surrounding substrate resulting in enhanced selective catalysis. For past couple of years, our group has since been exploring various SACs (Pt, Pd, Ag, and Co) anchored on different substrates (SiC, C3N4, and TiO2) that exhibit unique catalytic properties. This talk summarizes our recent studies to advance the water treatment catalysts from the nano-scale toward the single atom scale such as (1) single-atom Pt anchored to SiC photocatalyst (Pt1/SiC) for selective defluorination of perfluorooctanoic acid (PFOA) and selective dehalogenation of various water pollutants and (2) spatial separation of two co-catalysts by coordinating single atom cobalt at the void center of C3N4 and anchoring anthraquinone at the edges of C3N4 platelets to significantly enhance the catalytic synthesis of H2O2, a precursor chemical for advanced oxidation.

ENVR 82

Advanced manufacturing of scalable easy-to-use sensors for field monitoring of water contamination

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Conventional methods for monitoring environmental contamination rely heavily on the use of laboratory-based spectroscopic methods that are sensitive and selective but require knowledge for operation, are expensive and cumbersome to use in the field. Simple on site detection is required for large-scale monitoring of contaminants. Easy to use analytical assays or sensors are needed for practical implementation. Recent advances in 2D and 3D printing have provided tremendous opportunities for designing methodologies to enable scalable production of point of use devices in large quantity and with suitable stability, selectivity and robustness. This presentation will design, fabrication, optimization describe and characterization of novel 2D and 3D printed analytical devices for monitoring water contaminants, including bisphenol A, copper and phosphate. Optimization of printing parameters such as ink formulation, viscosity and deposition layers and how this affect printing performance will be discussed. Side-by-side comparison on the fabricated sensors with conventional methods, method validation and examples of applications will be described. Considering their high portability, these sensors could be used for on-site detection and environmental monitoring in areas that require high throughput analysis of large number of samples.

ENVR 83

Overcoming technical challenges in the synthesis and application of nanoscale adsorbents

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Two dimensional, layered, and nano materials have been extensively explored in the past few decades, and consequently, the literature is flooded with nanomaterials research. Scientists have claimed nanomaterials are possibly the most promising alternative materials in developing the next generation of technologies, including water treatment and environmental remediation. However, the current literature subtly yet collectively agrees that the use of nanoscale adsorbents has major technical challenges such as aggregation, separation,

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instability, and release to the environment. This work presents the use of microwave-assisted synthesis of layered and nanomaterials as well as engineered solutions to tackle the mentioned technical challenges. One significance of this work is producing smaller nanomaterials that surprisingly tend to aggregate less in aquatic solutions. This technique requires less volume of chemicals and is executed much faster once compared to conventional methods. Additionally, to study the aggregation of layered and nanomaterials in natural environments, 3D printed microfluidics are being developed and tested. Lastly, a novel invention will be disclosed for the direct use of 2D, layered, and nanomaterials in waster treatment. This work introduces a holistic approach to overcome the challenges in the synthesis and application of nanoscale materials in environmental engineering.

ENVR 84

Design of a 3D printed and energy efficient photostation to improve photocatalytic activity of carbon nitride composites

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The degree of a photocatalytic reaction depends on the intensity of incoming light or number of photons. In many of traditional photostations, a major portion of light is not used as it does not reach the reaction zone thereby wasting a significant portion of light and energy, as well. In an effort to fabricate an energy efficient photostation, we have designed and 3D printed a photostation with parabolic reflective surface, so that all the incident light beams can reach the reaction zone. The photostation is fitted with two chips-on-board (COB) light emitting diodes (LEDs) reaching the total (visible) light intensity within the reaction zone over 290,000 lux (For comparison, it is commonly reported that the sun emits anywhere from 32,000 to 100,000 lux onto the Earth). Light simulation analysis confirmed that all incident light beams can reach the reaction zone of photostation. Graphitic carbon nitride (g-C₃N₄) is a relatively new organic photocatalyst, which is very inexpensive to synthesize, stable, non-hazardous and has a low bandgap energy of 2.7-2.8 eV suggesting that it can be activated under visible light. In order to test the performance of this photostation, we used two composites of graphitic carbon nitride, including (i) 0.5 to 2 wt.% iron oxide doped g-C₃N₄, and (ii) electrospun nanofiber of $g-C_3N_4$ composite with polyvinylidene fluoride (PVDF) as the fiber matrix. One organic pollutant (dicamba, (3.6-Dichloro-2-methoxybenzoic acid) and one inorganic pollutant (hexavalent chromium) were successfully oxidized and reduced, respectively, by the carbon nitride composites within the 3D printed photostation. It has been confirmed experimentally that the rate of degradation of the pollutants is directly

proportional to the light intensity and geometry of photostation thereby confirming the positive role of photostation design.

ENVR 85

3D printed structures for controlled analyte adsorption and desorption

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3D printing technologies are enabling in that they allow local users to generate complex three-dimensional objects from a range of materials. Our research has focused on expanding the bredth of available materials for 3D printing with a specific focus on materials that can adsorb environmentally relevant analytes. I will discuss my lab's work developing materials that adsorb molecules for environmental remediation (gases, heavy metals and organic pollutants), alternative energy (gases), and environmental monitoring (protons).

ENVR 86

Methods of processing of thermoplastics and lignocellulosic biomass for 3D printing

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Lignocellulosic biomass can be used as an additive in thermoplastics like polylactic acid (PLA) for making materials through the fused filament fabrication (FFF) 3D printing technology. Its use in 3D-printed materials opens a new path for utilization of low-value biomass or end-ofcycle waste that conforms to the idea of circular economy. However, biomass addition to plastics has a large impact on extrusion-based 3D printing filament production and 3D printing machine parameters which needed thorough investigation with the intent of developing good, reliable, reduced cost. environmental-friendly and consumerbased do-it-yourself methods. Here we present the findings from primarily using poplar hardwood at 20 wt.% with PLA using small-scale equipment to produce printed renewable materials. New methods of size reduction of plastics and poplar were developed that allowed superior and solvent-free filament production and consistent printing without clogging of the hot-end of a benchtop 3D printer. Size reduction by ultra-fine fibrillation technique was applied for the first time to see how fibrillated poplar affects printing processes in comparison to the conventionally used ball-milled poplar. A major finding was that the addition of poplar (and biomass in general) to PLA at 20% requires a higher printing temperature of 230 °C to achieve consistent flow. Several varieties of poplar were used to see how biomass structure affects the tensile properties of the composites. Overall, these findings show better methods for making 3D-printed materials that contain lignocellulosic biomass.



3D printed PLA + 20% poplar hardwood

ENVR 87

Environmental sustainability in advanced material manufacturing

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Advanced materials can unlock previously inaccessible performance parameter spaces and are poised to overcome long-standing challenges in environment, climate, and society. However, some of the intended benefits of the technologies could be offset by negative environmental impacts without careful evaluation of the manufacturing processes. This talk will focus on approaches to enhance early assessment of

environmental and technical performance to guide economically viable sustainable materials design, with emphasis on chemical environmental impacts and quantitative tools to enable simultaneous optimization strategies. While there are no one-size-fits-all design solutions, guiding principles and assessment tools will be presented. These include: The Principles of Green Engineering, life cycle considerations unique to additive manufacturing, and recent developments in materials sustainability databases for co-optimization of environmental and functional performance metrics (e.g., such as Ashby materials selection diagrams). Finally, efforts to delineate sustainable synthesis chemistries using machine learning tools and necessary systematization to achieve those goals will be described. Put into practice, these tools will help ensure that advanced materials achieve their noble goals of providing transformative, impactful technologies to advance the environment and society.

ENVR 88

VOC emissions influenced by polymer additives in 3D printing

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The increase in number of 3D printers found in households and workplaces has led to a growing concern over their hazardous emissions. One category of emissions from fused deposition modelling (FDM) printers consists of volatile organic compounds (VOCs). While VOC emissions from common pristine polymers have been investigated, these studies tend to focus on thermal degradation products that result directly from the polymer backbone. Many 3D printer filaments contain unreacted polymerization initiators or utilize additives to achieve various aesthetic and structural properties that may influence VOC emissions. Six filaments are highlighted in this work due to the advertised additives they contain or the discovery of an unadvertised additive during emissions analysis. The filaments include: а commercially-available, 3D printer nanocomposite filament of carbon nanotubes (CNTs) and acrylonitrilebutadiene-styrene (ABS), three metal-containing polylactic acid (PLA) filaments, a PLA filament that was found to contain siloxanes, and a polycarbonate (PC) filament that emitted chlorinated VOCs. VOC emissions were quantified and characterized under a variety of conditions to simulate the thermal degradation that takes place during FDM. In the ABS-CNT filament, increasing residence time and temperature resulted in significant increases in VOC emissions and oxygen content of the reaction gas influenced the VOC profile. The presence of CNTs in the filament influenced VOC yields and product ratios and suggests a reaction mechanism involving an adsorbed styrene species. The metal-containing PLA filaments emitted different VOC concentrations due to the type and amount of metal present in each. The PLA filament emitted six siloxane compounds under standard printing conditions, with some in higher concentration than any other common PLA VOC emission. The presence of unreacted phosgene in the PC filament led to the formation of chlorinated VOCs, most alarmingly, chlorobenzene. The present study has identified an increased risk associated with common additives used in 3D printing filaments, both advertised by the manufacturer and those not known to the user.

ENVR 89

Taking it outside: Benefits and risks of additive manufacturing for environmental monitoring and remediation technologies

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The recent affordability of desktop 3D printers has resulted in a surge of Additive Manufacturing (AM) research in interdisciplinary fields (toxicology, environmental chemistry). While mobile AM labs deploy 3D printers for parts-on-demand in remote locations, novel research expands mobile AM to deployment of 3D printed builds into environmental media. This paper summarizes our developing environmental applications research, including: (1) passive sampling for environmental contaminants; (2) remediation of waste streams; and (3) quantification of potential environmental implications of these technologies, including printer emissions and environmental degradation and hazard of polymers. The environmental life cycle of AM applications must be considered provided concerns with microplastics in the environment. First, we discuss passive sampling of polychlorinated biphenyls (PCBs) in water and sediment using low density polyethylene (LDPE). While LDPE has a proven track record for determining PCB concentrations in sediment porewater, the devices are simply cut sections of commercially available sheeting. Our research explores altering Fused Filament Fabrication (FFF) print parameters (nozzle size, speed, layer height) to determine if 3D printed LDPE devices can improve quality control and PCB uptake kinetics. Printed LDPE samplers were deployed in contaminated sediment and kinetically sampled to determine and optimize uptake efficiency and rates. We also investigated potential for highly filled thermoplastics to remediate contaminated waste

streams, including the feasibility of mixing rigid, particles (38-180 µm) into biocompatible polylactide (PLA) thermoplastic filaments to remove environmental contaminants from water. Our preliminary findings revealed that dual screw extrusion of PLA containing zeolite and activated carbon at 15 to 25% (by mass) produced printable filaments by FFF. High surface area prints from the PLA-zeolite filament resulted in deployable materials capable of reducing ammonia concentrations in water (50% in <24 hours). Finally, we characterized aerosolized emissions of filled PLA compared to neat PLA in confined space, using a fast mobility particle analyzer. Ultrafine particles emitted increased with extrusion temperatures and with fillers, although the increase was attributed to the thermoplastic binder. Simultaneous considerations of the applications and implications will foster responsible and sustainable AM technologies.

ENVR 90

Potential health impacts of particle and volatile organic compound emissions from consumer level 3D printers

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Consumer level fused filament fabrication (FFF) 3D printers are widely used in small-scale indoor environments and public spaces, where vulnerable populations like children may be exposed to the potentially hazardous emissions. Studies have found a mixture of particles and volatile organic compounds (VOCs) being emitted from operating those 3D printers, however the health impacts of the emissions are not well known. This study systematically characterized particle and VOC emissions from multiple 3D printers using various filament materials based on a standard test method and estimated the potential health impacts of emissions according to modelling and experimental assessment. The emission levels and characteristics of particles (ultrafine, fine and coarse) and numerous VOCs were investigated, as well as the operation parameters that affect the emission characteristics, such like print temperature, printer brand, filament material, brand and colour. Chemical composition of 3D printer emitted particles were analysed by different instrumentations and compared to the properties of the bulk filament material. Particle health impacts were assessed by in vivo exposure and *in vitro* cellular and chemical experimental methods, and exposure levels of VOCs were assessed by an indoor exposure model. The health-related results were discussed by relating to ambient particulate matter health related study and indoor air quality regulations and criteria. Overall, this study finds FFF 3D printing will emit high levels of particles and numerous VOCs, which are potentially hazardous to human health, indicating that exposure to 3D printing emissions should be controlled.

ENVR 91

Consideration of 3D-printed biofilm carriers for wastewater treatment

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Wastewater infrastructure is aging in the United States, and low-cost retrofits to existing infrastructure are needed for treatment facilities to maintain or improve treatment efficacy. Adding biofilm carriers to processes increases treatment capacity in physical space. However, limits in manufacturability of the biofilm carriers have limited growth of the field. Using additive manufacturing to 3Dprint novel geometries, we explore effects of geometry. unit cell density, and strut thicknesses on biofilm growth and bench-scale reactor performance. We used microscopy to measure biofilm growth on 50 different 3Dprinted biofilm support of varying architectures to detect trends in biofilm thickness. We found that more void space led to higher peak biofilm thickness the simple cube geometry (0.2 mm radius, Relative Density = 0.70%) grew to 0.59 +/- 0.13 mm, compared to denser geometries like the octet + simple cube geometry (0.2 mm radius, Relative Density = 3.26%) grew to a peak of 0.29 + - 0.06mm. The removal efficiency of COD and ammonium of the 3D-printed geometries and conventional carriers in continuous flow conditions with a long hydraulic retention time (1.3 days) were near complete in all cases. However, when the mature biofilm on optimized 3D-printed geometries and conventional carriers were subjected to batch conditions, the removal rates of COD and ammonium were much higher for the 3D-printed supports (e.g. 14.15 mg COD/L-hr max removal over 8 hours (B-4 geometry), 0.90 mg NH4-N/L-hr removal over 8 hours(O-6 geometry)) than the conventional carriers (1.1 mg COD/L-hr max removal over 8 hours, 0.35 mg NH4-N/Lhr max removal over 8 hours). The geometry of the biofilm support architecture particularly, void space, seem to play a role in biofilm formation, and on-going research is quantifying this role. Generally, we were successful in using additive manufacturing to improve biofilm carriers for aerobic processes associated with secondary wastewater treatment.

ENVR 92

Quantifying and visualizing the spatial distribution of black carbon's electron storage capacity

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The electron storage capacity (ESC) of black carbon (BC); i.e., the quantity of electrons BC can store and reversibly donate/accept, determines its capacity to mediate abiotic and microbial redox processes, many of which are relevant to biogeochemistry, greenhouse gas production, contaminant fate and remediation. Electrochemical and chemical analyses have shown the ESC of BC (such as plant-derived biochar) was on the order of a few mmol/g. However, it remains unknown where ESC is located. The spatial distribution of ESC is important because it controls the accessibility of ESC and the kinetics of redox reactions involving BC. In this study, we fully saturated the ESC of a model BC (a wood-derived biochar) and exposed it to silver ion (Ag⁺), a tagging agent that can diffuse into BC, react with the stored electrons, and be immobilized in situ as elemental silver nanoparticles (nAg). Up to 2.49 mmol Ag⁺ per gram BC was reduced to nAg, which served as an ESC marker and was visualized by electron microscopy. Abundant and dense nAg were observed on the BC surface. Furthermore, the cross-section images of a microtomed BC particle showed ubiquitous and well-dispersed nAg in the particle interior. The finding that a significant portion of the ESC resided in the interior of BC explains the partial (bio)accessibility of the ESC and the pore diffusioncontrolled nature of the electron exchange reactions in BC previously reported. These results further suggest the silver tagging method can be a new and useful tool for investigating ESC and elucidating how black carbon mediates biogeochemical redox reactions.

ENVR 93

Impact of cobalt on mercury methylation in East Fork Poplar Creek, Oak Ridge, Tennessee

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The formation and transport of methylmercury (MeHg), a neurotoxin, in aquatic environments is a global concern for human health as MeHg can bioaccumulate and biomagnify to high concentrations in aquatic food webs.

MeHg is formed by conversion from inorganic mercury through microbial mediated methylation. Sulfate-reducing bacteria have been identified as the primary organisms responsible for MeHg production. Pure-culture studies suggest that low availability of cobalt and copper may inhibit mercury methylation, but whether such limitations occur in the environment is unclear. In this study, mercury methylation in sediments from the East Fork Poplar Creek in Oak Ridge, Tennessee were incubated in the presence and absence of added dissolved cobalt. This section of the creek contains elevated mercury concentrations in the sediments due to industrial contamination and the rates and controls on methylation have been studied extensively. Two levels of cobalt addition to the sediment incubations were investigated to reach target dissolved concentrations within the range suggested to be ideal for MeHg production in pure culture studies. These concentrations were estimated from preliminary measurements of cobalt binding by the sediments. Sulfide was generated over the 72 hour incubation period indicating that sulfate-reducing bacteria were active. MeHg concentrations increased over the time period studied with no noticeable enhancement of methylation resulting from the addition of cobalt. Methylation and demethylation rates both decreased with increasing cobalt concentrations. Overall, cobalt appeared to either inhibit or have no effect on mercury methylation in the sediments. These initial results suggest that mercury methylation in natural systems may not be cobalt-limited but future work is needed to evaluate a broader range of cobalt additions, to more robustly assess cobalt bioavailability, and to explore longer incubation times.

ENVR 94

Redox properties of particulate organic matter from northern peatlands

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Northern peatlands play a significant role in the global carbon cycle, storing an estimated 15-30% of the global soil carbon in the form of peat organic matter, while contributing to 8-10% of global methane (CH₄) emissions. As methane has a high global warming potential, it is critical to understand the processes that control methane dynamics in these carbon-rich ecosystems. Methane is formed as the terminal step in the anaerobic microbial respiration but is suppressed in the presence of energetically more favourable terminal electron acceptors (TEAs). Based on field and laboratory studies of carbon dioxide (CO₂) and CH₄ emissions from peatlands, it has been hypothesized that peat particulate organic matter (POM) may act as a previously unrecognized TEA and that electron transfer to peat POM suppresses CH4 emissions from northern peatlands. A key gap in this hypothesis is the characterization of the redox properties

of peat POM, specifically the electron accepting capacity (EAC) of the peat POM and an assessment of electron transfer reversibility to and from peat POM. Here, we introduce a spectrophotometric method using the redoxcompound N,N'-bis(3- sulfonatopropyl)-4,4'active bipyridinium (ZiV) to quantify the EAC of POM. The oxidized species ZiV undergoes reversible one electron transfer to the reduced species ZiV., a reaction that results in pronounced changes in the UV-visible absorption spectra. We used the ZiV/ZiV-- couple to transfer electrons to the peat POM, and monitor the spectral changes resulting from ZiV* re-oxidation to ZiV to quantify the number of electrons transferred to peat POM. The EAC of dried peat POM was 0.38 (±0.04) mmol electrons per gram POM. This EAC was regenerated when reduced peat POM was exposed to O₂, suggesting that POM can act as a regenerable long-term electron acceptor for anaerobic microbial respiration at the oxicanoxic interface in northern peatlands. We complemented the laboratory measurements with field experiments in which we measured the redox state of peat POM in situ in ombrotrophic bogs in Värmland, Sweden, by monitoring the abiotic reduction of dissolved oxygen injected into the anoxic subsurface in push-pull tests. Combined with our previous calculations that POM comprises >90% of the organic matter in peatlands, this work strongly supports the hypothesis that POM is a significant TEA in northern peatlands and that electron transfer to POM can significantly lower CH₄ emissions from these systems.

ENVR 95

Isotopic analysis of radionuclide association with aquifer solids in the Midwestern Cambrian-Ordovician aquifer system

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The Midwestern Cambrian-Ordovician aquifer system (MCOAS) is known to contain radium (Ra) above the maximum contaminant level of 5 pCi/L for combined ²²⁶Ra and ²²⁸Ra. This aquifer system is used as a drinking water source by many municipalities; however, ingestion of Ra can result in an elevated risk of cancer. Parent isotopes (e.g., ²³⁸U and ²³²Th) located in the aquifer system undergo radioactive decay and emit ²²⁶Ra and ²²⁸Ra, respectively. We investigate the relationship between these radionuclides and Ra in the groundwater. Isotopic activities are used to determine whether Ra moves from the site of parent decay in the aquifer system, and examine geochemical implications for Ra association with bedrock stratigraphy. We ran a series of sequential extractions on MCOAS bedrock core and analyzed Ra isotopes by multi-collector inductively coupled plasma

mass spectrometry. For each stratigraphic unit, ²³⁸U and ²²⁶Ra activities resulted in a 1:1 ratio. This secular equilibrium between parent and daughter isotope determines that Ra is not mobilized to the groundwater flow system, and stays close to the site of parent decay. Ra associations with aquifer solids vary across stratigraphic units, indicating that aquifer geochemistry differs in impact on Ra mobility depending on stratigraphy. Due to the heterogeneous nature of the aquifer system, each stratigraphic unit will demonstrate potential Ra mobility due to the variation in distribution across geochemically sensitive associations. Local geochemical conditions at the site of parent decay impact the contribution of Ra to groundwater systems, influencing the availability of sorption sites and co-precipitated minerals.

ENVR 96

Arsenite complexation by dissolved organic matter and implications for uptake by microorganisms

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Changes in arsenic (As) speciation and toxicity in the environment are mediated by intracellular As metabolism enzymes (e.g., ArsM; ArsC), making cellular uptake a prerequisite for important arsenic biotransformation pathways. Cellular uptake of arsenate (As(V)) and arsenite (As(III)) is known to be mediated by phosphate and aquaglyceroporin (GlpF) transporters, respectively, but understanding of how solution chemistry impacts aqueous As bioavailability remains incomplete. In this contribution, we explore the influence of dissolved organic matter (DOM) quality on aqueous As speciation and bioavailability in anoxic systems and test the hypothesis that the density of thiol ligands in DOM controls As(III)-DOM complexation and, consequently, cellular uptake through GlpF transport channels. This investigation combines ligand exchange dialvsis equilibrium experiments, As K-edge X-ray absorption spectroscopy, fluorescence spectroscopy-based measurements of reactive thiol concentrations, and a whole-cell biosensor assay to probe interactions between As(III) and DOM samples with diverse chemical composition and assess the implications for As bioavailability. The study evaluates humic and fulvic acid reference samples as well as DOM samples extracted from sulfur-rich environments. Outcomes of this laboratory research will be discussed in the context of arsenic fate and transport in DOM-rich subsurface environments including wetlands and rice paddy soils.

Exploring factors governing metal uptake by wetland soils

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Wetland soils display vertical redox gradients that make them active sites for biogeochemical processes that include methanogenesis and denitrification. Recent laboratory studies have highlighted that low bioavailability of trace metals (Cu, Ni, Zn) may inhibit these processes, but the factors controlling this behavior in natural aquatic systems are not well understood. Trace metal bioavailability in aquatic systems, particularly wetlands, is controlled by iron and sulfur redox cycling and organic matter content. In this study, we quantified the uptake behavior of Cu, Ni and Zn on three different wetland soils and explored the causes of variation in uptake. Soils were collected from sites in Illinois, Tennessee, and South Carolina. New information on metal uptake will help us estimate environmental inputs of trace metal may bring bioavailable concentrations to optimal levels for methanogenesis and denitrification. The adsorption data, normalized to specific surface area, showed that there was significant variability in metal uptake among different metals and between different sites. The variability in uptake was examined with respect to soil organic carbon content, morphology, mineralogy, and sulfur content. Xray absorption spectroscopy probed the speciation of Cu and Ni taken up by these soils, finding that added metals form species that partially differ than those originally present in the soil. Copper forms CuS, increasing the fraction initially present in each system, but also metallic copper as well as Cu bound to thiol groups on organic matter. Complexation to organic matter and adsorption dominated Ni speciation in the Illinois and South Carolina sites, but an inorganic sulfide species formed when Ni was added to samples from the Tennessee site. These studies highlight that diverse mechanisms are responsible for trace metal uptake at each site.

ENVR 98

Biotransformation of neonicotinoid insecticides and their metabolites on biologically activated carbon: Implications for human exposure, treatment, and biofilm transformation

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Neonicotinoids are the most widely used insecticides in the world. The widespread application of neonicotinoids has led to their proliferation in waters across the U.S., including those used as drinking water sources. Although neonicotinoids exhibit relatively low toxicity towards mammals compared to some pesticides; however, formation of mammalian toxic metabolites is an exposure concern. Despite high solubility and polarity, our prior studies identified granular activated carbon (GAC) as a method for neonicotinoid and neonicotinoid metabolite removal from drinking water. Desorption tests of five-yearold used GAC (spent GAC) from the lowa City DWTP revealed that although imidacloprid was present on the GAC surface, no desnitro-imidacloprid was observed even though it is capable of adsorbing to GAC; these results suggest desnitro-imidacloprid degradation on the GAC surface. The objective of the present study was to determine if imidacloprid and its mammalian toxic metabolite desnitro-imidacloprid that is adsorbed to black carbon can be mineralized into less toxic products via biofilm-coated (bio-augmented) black carbon. Experiments with soil-microbe coated corn biochar and spent DWTP GAC probed possible imidacloprid and desnitro-imidacloprid degradation on bio-augmented black carbon. Batch experiments revealed that bioaugmented corn biochar readily transformed imidacloprid into desnitro-imidacloprid. In solutions containing spent GAC, imidacloprid was rapidly adsorbed to the spent GAC surface without any metabolites detected in solution. Nevertheless, in solutions containing GAC-associated microorganisms without GAC, imidacloprid was degraded into desnitro-imidacloprid suggesting the adsorbed neonicotinoid may be degraded on the black carbon surface. Sacrificial batch experiments are underway to determine the rates and possible mechanisms behind these biotransformation reactions. Further experiments are elucidating whether the mammalian toxic metabolite is a dead-end product or if the metabolite is further transformed by bio-augmented black carbon. This research may provide a promising method to remove neonicotinoids from water in natural and engineered systems by coupling GAC sorption to biofilm degradation.

ENVR 99

Reductive transformation of 3-nitro-1,2,4-triazole-5one (NTO) by black carbon

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Black carbon is ubiquitous in soils and sediments and can participate in a number of important biogeochemical processes. It has been shown recently that black carbon possesses a considerable electron storage capacity (ESC) and can serve as a reactive medium to support abiotic and biotic redox transformation. To understand how black carbon controls contaminant fate in subsurface environments and to evaluate its potential for remediation,

it is important that we determine the accessibility of ESC to contaminants, as well as the kinetics and mechanisms through which ESC promotes redox reactions. In this study, we investigated the reductive transformation of 3nitro-1,2,4-triazole-5-one (NTO) by a wood-derived black carbon (Soil Reef Biochar, or SRB). NTO is an insensitive munitions constituent in IMX-101 and IMX-104 formulations and has been detected in soil and groundwater near military sites across the U.S. due to its high solubility and mobility. NTO was chemically reduced to 3-amino-1,2,4-triazole-5-one (ATO) by reduced SRB. The amount of SRB's ESC that was accessible to and reactive toward NTO was constant over a range of pH and was a fraction of the total ESC measured using dithionite $(E_h = -0.43 \text{ V vs. SHE at pH 7})$ and dissolved O₂ (+0.80 V vs. SHE at pH 7, P_{02} = 0.21 atm). Similar to the reactions between SRB and redox agents in our recent study, the reduction of NTO by SRB appeared to be controlled by pore diffusion within black carbon particles. This study has important implications for the fate of NTO in contaminated groundwater, for the role of black carbon in the natural attenuation of NTO, and for the development of potential biochar-enhanced remediation strategies for military sites. In addition, the study offers insights into how black carbon ESC can influence contaminant fate in reducing environments.

ENVR 100

Migration of quaternary ammonium cations from exfoliated clay/low density polyethylene nanocomposites into food simulants

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Clav/polymer nanocomposites (CPNs) are polymers incorporating refined clay particles that are frequently functionalized with quaternary ammonium cations (QACs) as dispersion aids. There is interest in commercializing CPNs for food contact applications because they have improved strength and barrier properties, but there are few studies on the potential for QACs in CPNs to transfer to foods under conditions of intended use. In this study, we manufactured LDPE-based CPNs and assessed whether QACs can migrate into several food simulants under accelerated storage conditions. QACs were found to migrate to a fatty food simulant (ethanol) at levels of ~1 mg/mg CPN mass after 10 days at 40 degrees C, constituting about 4% total migration (proportion of the initial QAC content in the CPN that migrated to the simulant). QAC migration into ethanol was ~16x higher from LDPE containing approximately the same concentration of QACs but no clay, suggesting that most QACs in the CPN are tightly bound to clay particles and are immobile. Negligible QACs were found to migrate into aqueous, alcoholic, or acidic simulants from CPNs, and the amount of migrated QAC was also found to scale with the temperature and the initial clay concentration. The migration data were compared to a theoretical diffusion model and it was found that the diffusion constant for QACs in the CPN was several orders of magnitude slower than predicted, which we attributed to the potential for QACs to migrate as dimers or other aggregates rather than as individual ions. Nevertheless, use of the migration model resulted in a conservative estimate of QAC mass transfer from the CPN test specimens.

ENVR 101

Application-focused study of metal hexacyanoferrates for the recycling of ammonium in various wastewaters

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Eutrophication and PM2.5 being the largest visible issues due to the release of ammonia (NH₃ & NH₄⁺) into the environment, the energy consumed for the synthesis of ammonia is rather less concerned. In fact, for the production of ammonia from atmospheric nitrogen and for removing it from the environment, both consume a huge amount of energy. In this sense, draining ammonium into the water reservoirs and releasing the ammonia form into the atmosphere should not be the ultimate route of getting rid of these from various wastes. Draining of ammonium fertilizer along with the irrigation water is also causing energy loss globally. In this sense recycling the ammonia molecule can lead to a two-way energy saving: in the production as well as in the decontamination. It is now well known that the metal hexacyanoferrates, commonly known as the Prussian blue analogs (PBA), can adsorb both NH₃ & NH₄⁺ forms by two different mechanisms. So, we are studying the chemical and engineering aspects required for the utilization of these materials for the recycling of ammonia in various systems.

ENVR 102

Nanoscale zerovalent iron particles for restoration of cadmium-contaminated paddy soil: Comparative evaluation of soil amendment vs. *in situ* magnet-assisted soil washing

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Partly due to mining activity, paddy field in the northern part of Thailand has been contaminated with cadmium (Cd) (as high as 220 mg/kg of which half is in easily leached forms) for a decade. Institutional control via prohibiting farmers from cultivating rice has been used to decrease impact of the contamination on human health and food safety. As a result, even after a decade, no remediation takes place to restore the contaminated soil. The present study comparatively evaluated using nanoscale zerovalent iron (NZVI) as 1) a soil amendment agent to stabilize Cd in soil and as 2) an agent for in situ magnet-assisted soil washing to extract Cd from soil after the stabilization. NZVI was mixed with contaminated soil in situ for soil amendment but for in situ magnet-assisted soil washing, NZVI was also recovered, using a magnet separator, from soil. Diethylene triamine penta acetic acid (DTPA) was used as a leaching agent to evaluate the bioavailability of Cd after the two options of treatment. By adding NZVI in the Cd-contaminated paddy soil as soil amendment at the ratio of 1:10 (NZVI:soil), Cd leachability by DTPA was decreased by 43% and 16% in the paddy soil with and without water flooding, respectively. On the other hand, if the NZVI was allowed to mix with soil for 7 days prior to being removed from the paddy soil with the help of magnetic separation prior to doing the DTPA test, Cd leachability by DTPA was decreased by 71% and 43% in the paddy soil with and without water flooding, respectively. Presumably, DTPA is a powerful complexing agent which desorbes Cd from NZVI either by competitive desorption or by dissolution of NZVI sorption sites leading to poor remediation potential when using NZVI as a soil amendment without recovering Cd-sorbed NZVI back from soil. This suggests that using NZVI as a soil amendment followed by magnetic separation of Cdsorbed NZVI from soil is a promising restoration technique for Cd-contaminated paddy soil.

ENVR 103

Phosphate removal from synthetic urine matrices using nanoscale magnetite

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The potential for phosphate (PO_4^{3-}) recovery from synthetic urine matrices using PO_4^{3-} sorption to nanoscale magnetite was studied. Synthetic fresh and hydrolyzed urine were used to closely resemble the behavior of real urine. Nanoscale magnetite was synthesized by the coprecipitation of Fe (II) and Fe (III) salts. The BET (Brunauer-Emmett-Teller) surface area of as prepared 8-10 nm sized magnetite was measured as 192.5 m²/g. Adsorption isotherm experiments were conducted at pH 4, 6 and 8.5 using 0.5 to 2.5 g L⁻¹ magnetite dosage with 50 mg L⁻¹ initial PO_4^{3-} concentration in hydrolyzed urine. The adsorption data from the hydrolyzed urine matrices

were fitted using both Langmuir and Freundlich isotherms. Maximum adsorption capacity using the Langmuir isotherm model was calculated as 35.1 mg PO₄³⁻ as P/g magnetite at pH 4, 21.5 mg PO₄³⁻ as P/g magnetite at pH 6 and 10.9 mg PO₄³⁻ as P/g magnetite at pH 8.5. These results suggest that higher sorption capacity of the magnetite toward PO₄³⁻ at lower pH can be attributed to the favorable electrostatic attractions between positively charged magnetite and the negatively charged PO₄³⁻ species in solution. In experiments with fresh urine, using a 2 g L⁻¹ magnetite dosage with 50 mg L⁻¹ initial PO₄³⁻ concentration, up to 51% PO₄³⁻ as P removal was observed at pH 6 after 48h equilibrium. The results from this study contribute to an improved understanding of P and Fe chemistry in synthetic urine matrices, which is essential for developing efficient use of nanoscale iron oxide-based adsorbents towards P recovery.

ENVR 104

Stability of graphene oxide in water: Exploring the critical role of organic surface coatings

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In this presentation, I will describe the critical role of organic coatings with respect to the stability of graphene oxide (GO) in water. To systematically evaluate the role of organic coatings, we controlled the shape/dimension of GO with varied organic surface coatings. (propylamine, tert-octylamine, 1-adamantylamine, 3-amino-1-propanol, and 3-amino-1-adamantanol) With identical organic structures, hydrophilicity of coating was controlled by the presence of hydroxyl groups. Also, we synthesized GO with different C/O ratio and size (GO-dot). Quantitatively, we specified the role of surface organic coating by comparing critical coagulation concentration (CCC) in varied salt concentration (NaCl, MgCl₂, MgSO₄, and CaCl₂) with organic coated GO and pristine GO. Without coating (pristine GO), CCC was well matched with plateplate DLVO energy interaction relationships. The effects of divalent cations were significant in case of highly oxidized GO (HGO) and quantum dot. We observed that hydrophilically organic coated GO (phi-GO) was more colloidally stable than hydrophobically organic coated GO (pho-GO) when structure of coating was identical. Interestingly, effects of type of divalent cations were negligible for pho-GO. In addition, the strong steric/hydrophilic organic coatings provide excellent colloidal stability for GO. We also explored the critical role of organic coatings on GO with respect to the deposition and re-entrainment to determining transport behaviors of GO using a quartz crystal microbalance-based technique (QCM-D). Organic coating on GO hindered deposition of GO, and promoted the re-entrainment of GO.

ENVR 105

Withdrawn

ENVR 106

Improving the selective removal of a target organic compound from water using 3-D carbon nanomaterial aerogels

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In order to improve the remediation efforts of water sources, improved adsorbent media are required. Carbon nanomaterials have demonstrated enhanced uptake removal of organic, metallic, and biological compounds. To continue improving on the strengths of carbon nanomaterials, a focus on tailoring the adsorption towards select compounds is needed. In addition, taking advantage of high surface area per unit volume will provide greater efficiency in adsorption uptake. In this presentation, the use of a 3-D carbonaceous aerogel for selective adsorption of targeted organic compounds will be discussed. Working with a solution composed of natural organic matter (NOM) and a herbicide, the aerogel is functionalized to specifically go after the herbicide and not other organic material. Using computational tools, such as PARAFAC, as a verification technique, it will be shown that the aerogel is capable of achieving high uptake of the targeted compound. Regeneration capabilities of the aerogels will also be shared. In the end, the goal of this work will be to set the stage for advanced studies translating the findings from batch to continuous processes, which are more relevant.

ENVR 107

Benign, renewable betaine-modified biochar-based nanocomposite containing zinc oxide for removal of phosphate from contaminated water

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Biochar is one of the promising adsorbents for removal of phosphate as well as heavy metals present in contaminated water. It is a solid material, prepared from biomass, like wood waste, by low temperature pyrolysis under limited supply of oxygen. In this study, biochar was

used as the renewable resource material, which was impregnated with zinc oxide in the presence of glycine betaine. This nanocomposite was an excellent adsorbent for removal of phosphate and showed a high capacity and fast kinetics. The synthesis of this biochar-based nanocomposite is a simple and easy process which is eco-friendly and economically feasible. The nanocomposite was characterized using Scanning electron microscopy (SEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Brunner-Emmett-Teller (BET), and Fourier-transform infrared (FTIR) spectroscopy. Adsorption isotherms like Langmuir, Freundlich, Temkin, and Dubinin-Radushkevich (D-R) were performed to find out the adsorption capacity and mechanism. Lagergren pseudo-first and second order, Elovich, and Weber-Morris intra-particle diffusion studies were also performed. The maximum adsorption capacity was found to be 88.50 mg g⁻¹. The results showed the removal of phosphorus from contaminated water from 10,000 parts per billion to 10 parts per billion, which is below the EPA recommended maximum concentration limit

ENVR 108

Carbon nanotube immobilized membrane for ammonia separation via membrane distillation

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Enhanced ammonia separation via direct contact membrane distillation (DCMD) using carbon nanotube immobilized membranes (CNIMs) is presented. The CNIMs were prepared using raw carbon nanotubes (CNTs) as well as more polar carboxylated carbon nanotubes referred to as f-CNTs. The ammonia removal by both CNIMs were markedly superior to that of the original PTFE membrane, while functionalized CNIM (CNIM-f) showed the best performance in terms of flux, mass transfer coefficients and selectivity. The flux with f-CNTs was 63% higher than the PTFE membrane and 22% higher than raw CNTs. Similar trends were observed for ammonia removal efficiency and mass transfer coefficients that were also significantly higher for the f-CNTs. The ammonia selectivity with respect to water vapor decreased with temperature for the PTFE and CNIM with raw CNTs, but in the presence of f-CNTs the selectivity did not show any decrease with temperature. The enhancement in ammonia removal with f-CNTs is attributed to the favored chemisorption of ammonia on the f-CNTs which was evident from contact angle measurements that showed a dramatic decrease for aqueous ammonia in the presence of the carboxylic aroups.

lon-gated carbon molecular sieve membranes for enhanced gas separation that surpass the Robeson limit

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At present, the high energy consumption, high capital cost and potential environmental impact have limited the development of many carbon capture technologies. Membrane technology lies at the heart of many industrial gas separation processes and applications. Molecular sieving membranes that break the Robeson limit are desirable for energy-efficient gas separation. Herein, we report a facile strategy of directly integrating ionic liquids (ILs) into porous membranes. Particularly, the ILs form an ultra-thin layer on the carbon molecular sieve (CMS) membranes rather than penetrating into the pores, acting as a smart gate for gas entry to boost the selectivity. The hybrid membrane exhibits CO₂ permeability > 600 barrer and enhanced CO_2/N_2 selectivity > 50, which surpasses the Robeson limit and shows potential in CO₂/N₂ separation process. Molecular dynamics simulations confirm the gating effect of the IL layer of molecular thickness. This work demonstrates a universal strategy to improve CMS membrane performance by creating an ILmembrane interface and tuning the ion-pore interaction. We anticipate this methodology enlarges the possible strategies to improve CO₂ separation performance of various porous materials.

ENVR 110

Macroscopic and spectroscopic characterization of the mechanisms of Ni(II) and Zn(II) sorption by green rust

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Green rust (GR) minerals are mixed-valent iron (Fe) hydroxide minerals that are believed to be wide-spread at redox boundaries in natural and engineered environments. These Fe phases consist of brucitic $Fe^{II}(OH)_2$ sheets in which a portion of the ferrous (divalent) Fe cations have been replaced with ferric (trivalent) Fe. Because of their layered structure, nano-particulate size, and high Fe(II) content, GR minerals are well known to be effective reductants of a broad range of organic and inorganic compounds, and their redox reactivity has been studied in considerable detail. In contrast, little is known about the reactivity of GR minerals

towards redox-stable trace metals such as Ni(II) and Zn(II). The aim of the research presented here was to assess the mechanisms of Ni(II) and Zn(II) sorption onto GR in circumneutral anoxic solutes. The work involved a combination of macroscopic batch kinetic experiments and synchrotron-based X-ray absorption spectroscopic analyses to determine prevailing sorption mechanisms as a function of time. The results demonstrate that GR behaves quite differently as a sorbent of trace metal Ni(II) and Zn(II) than ferric-oxides such as goethite and hematite, as it induces the formation of secondary metal precipitate phases rather than surface complexes as the main mechanism of metal retention. This implies that GR acts as a dynamic sorbent of trace metals in suboxic systems, and suggests that precipitation rather than surface complexation reactions control the solubility of trace metals in Fe redox transitions zones

ENVR 111

Facet-selective adsorption of Fe(II) on hematite visualized by nanoscale secondary ion mass spectrometry

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Facet-specific reactivity of metal oxide particles is a wellknown but at times difficult to probe phenomenon. Here we exploit a mass-sensitive imaging approach to unveil the preferential binding of Fe(II) to various hematite surfaces. 56Fe-hematite microplatelets with various enclosing facets were reacted with aqueous 57Fe(II) at circumneutral pH, and the resulting 57Fe distribution was directly visualized using NanoSIMS. The results unambiguously show Fe(II) sorption is highly selective for the basal (001) surface, more than an order of magnitude larger than on (012) and (110) edges. Intergrowth defects exposing poorly-ordered surface structures show the least enrichment. These results resolving Fe(II)-Fe(III) reaction fronts across multi-facetted crystallites provide a clear correlation between uptake and surface structure. This new approach to understanding facet-specific ion uptake is generalizable to other interfacial processes such as electron transfer and heterogeneous catalysis, across a broad range of particle and thin-film systems. The work continues to expand the frontiers of nanogeoscience pioneered by Prof. Hochella many decades ago.

ENVR 112

Solution chemical and hydrodynamic factors control the formation of synthetic schwertmannite

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Schwertmannite is a ferric hydroxylsulfate nanomineral that controls metal and metalloid cycling in natural and contaminated systems. Recent investigations by highresolution transmission electron microscopy showed that freshly precipitated schwertmannite consists of sulfatepoor, goethite-like nanoparticles hosted in an amorphous ferric hydroxylsulfate matrix (French et al. 2012 & 2014). The observed chemical and physical heterogeneity has inspired new studies of schwertmannite nucleation and growth, which is difficult to reconcile using a classical model for crystallization by addition of monomeric species. We have investigated the multi-stage growth process of synthetic schwertmannite and goethite as a function of increasing solution sulfate concentration ([SO₄]/[Fe] at 1, 2, 3 and 5) and pH (2.4-5.6). In situ x-ray scattering experiments showed that the precursors to both schwertmannite (pH<4) and goethite (pH>4) had a structural coherence and particle size of <1.5 nm, and short-range order similar to goethite. At low pH, these precursors clusters were stable for up to 40 h as long as the solution was kept turbulent but would transform to poorly crystalline schwertmannite during particle aggregation and settling at static conditions. Synthesis at higher pH resulted in goethite formation with no apparent effect of solution hydrodynamics. We attribute the different pathways leading to schwertmannite or goethite to pH-induced differences in the surface composition of the goethite-like precursor clusters. At low pH the clusters have a strong affinity for SO₄²⁻ due to many positively charged Fe(OH)2+ surface groups. Adsorbed sulfate limits the amount of crystallization in schwertmannite and results in a large proportion of amorphous solid with relatively high SO₄ contents. At higher pH, goethite formation is favored and kinetically fast because more neutrally charged surface sites weaken the interaction with sulfate. We hypothesize that the unusual effect of solution turbulence at low pH is related either to shear forces between adjacent sulfate-capped particles that prevent permanent (i.e., Fe-O-Fe) bond formation or to changes in particle number density with aggregation. The model developed from these systematic in situ experiments helps explain the competing effects of solution chemistry and hydrodynamic factors on the formation of ferric nanominerals.

ENVR 113

Mn(II)-promoted phase transformation of manganese oxides

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Manganese (Mn) oxides possess extraordinary metal sorption and oxidation properties and thus affect environmental fate and transport of toxic metals and organic pollutants. There are more than 30 different types of Mn oxides that can be grouped into layered (LMOs), tunneled (TMOs), and low-valence (LVMOs) Mn oxides. The Mn in LMOs and TMOs is mainly Mn(IV) with some species containing Mn(III), while Mn exists as Mn(II), Mn(III) or both in LVMOs. It has been challenging to understand the formation of such a high diversity of phases in the environment. Studies showed that Mn(II) can promote transformation of LMOs to TMOs and LVMOs at room temperature, and the transformation products are controlled by the Mn(II)/LMO ratio and solution pH. The Mn(II)-Mn(IV) redox reaction drives the transformation, in which Mn(II) acts as either a catalyst or a reactant. In this presentation, I will review the controlling factors and mechanisms of the transformation.





ENVR 114

Transformation of metal and metal oxide nanoparticles via sulfidation

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Physical, chemical, and biological transformation of nanoparticles in natural environments can affect their surface properties, and thus their reactivity/toxicity and geochemical cycling. One such transformation is the

sulfidation of nanoparticles, both engineered (e.g., Ag) and natural (e.g., Fe(III)-(oxyhydr)oxides). We will discuss our studies of the sulfidation of synthetic Ag, CuO, ZnO, and Fe(III)-(oxyhydr)oxide (ferrihydrite, goethite, and hematite) nanoparticles. Nanoparticles were reacted with Na-sulfide aqueous solution at various sulfide/metal ratios and were characterized before and after sulfidation by Xray absorption spectroscopy, X-ray diffraction, and transmission electron microscopy, resultina in identification of metal-S species and intermediate sulfur species and an improved understanding of the mechanism(s) of sulfidation. For sulfidated Fe(III)-(oxyhydr)oxide nanoparticles, we investigated the impact of organic matter on Fe-S species at different pH values. An environmental consequence of the sulfidation of these nanoparticles is the release of sorbed contaminants and a reduction in toxicity of the transformed nanoparticles to organisms.

ENVR 115

Rate-limiting step of dissimilatory microbial iron oxide nanoparticle reduction

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Experiments were conducted with synthetic iron oxide nanoparticles to gain insight into the rate-limiting step during the initial stages of dissimilatory microbial iron oxide reduction (DIR) in the presence of excess electron donor for microbial respiration. Ten iron oxide phases with a range of surface areas and thermodynamic properties were reduced by Geobacter sulfurreducens under nongrowth conditions with excess H_2 as an energy source. Analogous experiments were conducted in the presence of 100 µM of the soluble electron shuttling compound AQDS. Other experiments examined the short-term kinetics of abiotic iron oxide reduction by excess (10 mM) AH₂DS. Longer term abiotic reduction experiments with 10 mM AH₂DS were used to estimate the reduction potential (Eh⁰) of the different oxide phases. There was a significant correlation between oxide Eh⁰ and short-term surface-area normalized rates of abiotic reduction by AH₂DS. In contrast, there was no correlation between oxide Eh⁰ and initial surface area-normalized DIR rates, either the presence or absence of AQDS. Separate experiments with amorphous hydrous ferric oxide showed that 1 µM AQDS was sufficient to saturate rates of DIR. Thus, the concentration of AQDS did not limit DIR in the reaction systems with 1 µM AQDS. These results, together with other data sets, suggest that the rate of electron flow from cytoplasmic metabolism to redox active components (i.e. multiheme cytochromes) in the outer membrane limits the rate of DIR in both the absence and presence of soluble electron shuttles. This conclusion is supported by the documented rapid electron transfer kinetics between isolated outer membrane multiheme cytochrome systems (e.g. mtrCAB in *Shewanella oneidensis*) and iron oxide nanoparticles. The analysis highlights the previously demonstrated (or inferred) importance of particle surface properties – as opposed to bulk thermodynamic properties – on the kinetics of biological electron transport to iron oxide surfaces.

ENVR 116

Growth of neutrophilic photosynthesis bacteria using metal sulfide nanoparticles as sole electron donors

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Nanoscale minerals, with diverse and unusual physicochemical properties, are being recognized as intrinsic components of most natural systems. Latest field evidence has attested to their abundances in critical zones, groundwater aguifers, thawing permafrost, hot springs, and lacustrine, riverine, and marine waters and sediments. As such, elucidating these tiny phases' relationships with other biogeochemical components in the same environment becomes a logical next step. The current study is focused on illuminating how the formation and presence of naturally occurring nanoparticles may enable the growth and modify the metabolic behavior of associated microorganisms, which remains largely an understudied theme. We have chosen model strains of neutrophilic photosynthetic bacteria and studied their growth using metal sulfide nanoparticles as the sole electron-donor source. The major questions we intend to address are if the bacteria can grow using metal sulfide nanoparticles as electron donors and what mechanisms are involved in the metal sulfide-driven bacterial growth.

ENVR 117

Withdrawn

ENVR 118

Flatland in the energy landscape: Experimental theoretical condensed matter geochemistry of silica

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Le Chatelier comments in his La silice et les silicates (de Jong, B.H.W.S. and G.E. Brown, 1980) on the number of silica polymorphs and their large difference in thermal expansion. To address these issues, we have revisited our 1980 molecular orbital calculations on the $H_6Si_2O_7$ molecule reaffirming its conclusions for SiO₂. Thus: the calculated absence of a rotational barrier results in

innumerable identical energy configurations (the flatland) for a given Si-O-Si angle accounting for glass and gel formation but not for the puzzling small number of observed silica polymorphs vis a vis those feasible. The slight thermal expansion of silica glass is due its Si-O-Si angular variation inferred from ²⁹Si NMR. It involves lengthening of Si-O bonds at small and shortening at large Si-O-Si angle regressing to the minimum at 142 degrees as a result of the O-O repulsion minimum and net Si-Si attraction.

ENVR 119

Green chemistry of nutrient recovery: From mechanochemistry to reduced nitrogen loss

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Population growth is necessitating a significant increase in crop production while regulations are requiring less use of nitrogen (N) fertilizer, such as urea, to minimize environmental influx. A large fraction of applied N is currently lost with significant negative environmental effects. The work presented will focus on engineering organophosphorus-free urea cocrystals using a solventfree sustainable mechanochemical synthesis and quantifying the resulting N gas emissions, N partitioning into soil (longevity/stability therein) and plants. Traditional methods of producing N-P-K fertilizers that use NH3 as a reactant, typically produce 1.4-2.6 kg of CO₂ equivalent per kg of N fixed in energy consumed. On the other hand, a typical industrial ball-mill requires ~0.01 kWh/kg of solid (monoammonium phosphate, MAP) milled, which translates to 0.005 kg of CO2 equivalent per kg of solid milled. The main purpose of this work is hence to quantify and compare differences in N-loss between urea and urea cocrystals to yield the same amount of biomass as significant savings are expected due to improved Nefficiency.

ENVR 120

Green solvent for nano-enabled water treatment

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Deep eutectic solvents (DESs) have emerged as a new class of solvents with low cost and enhanced biodegradability. The most common class of DES refers to a mixture of a quaternary ammonium or phosphonium salt and a hydrogen bond donor (e.g., carboxylic acid) with melting point lower than that of individual components. DESs have recently shown promise for surface modification of graphene oxide (GO) with different

functional groups. We will discuss two studies - (i) use of DES for synthesizing new graphene-metal nanohybrids for adsorption based pollutant removal; and (ii) use of DES for nano-functionalized nanofiltration membranes for high water flux and high selective dye desalination. For the first project, we conjugated Fe₃O₄ nanoparticles and GO nanosheets using DES as coupling agent to prepare magnetic nanohybrids. Physicochemical characterization not only confirmed the ability of DES to successfully prepare DES/GO-Fe₃O₄ nanohybrids, but also evidenced the influence of DES on the homogeneity and size distribution of Fe₃O₄ nanoparticles in these nanohybrids. DES/GO-Fe₃O₄ nanohybrids can perform better than both GO and Fe₃O₄ as adsorbents for organic dyes (methylene blue, MB) and heavy metals (Lead (II)). However, depending on the contaminant type, the contaminant removal performance varied differently for DES/GO-Fe₃O₄ nanohybrids with different ratios. For the second project, we modified ultrafiltration membrane by DESfunctionalized GO. The effect of functionalization time on the water flux, dve and salt rejections, and physical and chemical properties of the obtained membranes were studied. Results indicated that the functionalized GO membranes (F-GO) could provide very high water flux, about 4-6 times of the GO nanofiltration membrane, while keeping high dye rejection (~99% for Congo Red, Direct Red, and Evan Blue). Furthermore, F-GO membrane showed lower rejection towards Na₂SO₄ salts indicating the successful engineering of the channel size achieved by the functionalization to provide a membrane with high water flux, high dye rejection and low salt rejection that is the best for achieving satisfactory dye recovery.

ENVR 121

Benign-by-design nanomaterials for continuous flow tandem nanocatalysis

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The design of benign and environmentally sound methodologies has been the driving force of scientists in recent years. Attractive and innovative protocols that nowadays are even part of industrial ventures including porous carbonaceous materials, biomass-derived designer nanomaterials for (photo)catalytic applications and catalytic strategies for biomass/waste conversion into useful materials, chemicals and fuels have been recently developed in our group in recent years. These topics have extensively covered the preparation and design of (nano)materials and their utilisation in heterogeneously (photo)catalysed processes, flow chemistry as well as in biomass and waste valorisation practises. This contribution aims to provide an overview of recent efforts from our group in the design of nanomaterials for catalytic applications, particularly focused on continuous flow (tandem) nanocatalytic processes. Examples on the use

of scrap catalytic converters, waste feedstocks and MOFs-based materials will be provided.

ENVR 122

Synthesis of novel nanobiocomposite from kenaf fiber for heavy metal remediation and antibacterial activity

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Ensuring reliable access to clean and affordable water is one of the greatest global challenges of the twenty-first century. Contaminants in water bodies are usually organic, inorganic and microbes which cause a potential threat to humans as well as to the environment. A hybrid material consisting of inorganic nanomaterials and sustainable cellulose can be used for the removal of heavy metals as well as pathogens from the wastewater. The objective of the study is to prepare a new nanobiocomposite from plant-based activated carbon followed by in situ impregnations of antibacterial nanosilver that can capture heavy metals like lead and copper and deactivate bacteria from water matrices. The optical and chemical properties of nanobiocomposite will be characterized extensively using UV Vis and Fourier Transform Infrared (FTIR) Spectroscopy. Dynamic Light Scattering (DLS) and scanning electron microscope (SEM) will be helpful for understanding the size distribution of nanosilver. The antimicrobial efficacy and heavy metal remediation of nanobiocomposite will be explored in comparison to commercial activated carbon. Adsorption studies for divalent copper and lead will be carried out and quantified using atomic absorption spectroscopy (AAS). Operating parameters like contact time, adsorbent dosage and agitation speed on adsorption will be also be investigated.

ENVR 123

Supercritical CO₂-induced alteration of polymer-metal matrix and selective extraction of valuable metals from electronic wastes

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Waste electrical and electronic equipment (WEEE), one of the fastest-growing waste segments, has become one of the most difficult challenges faced by humanity. Despite increasing efforts in recycling and reuse, a large fraction of WEEEs, such as waste printed circuit boards (PCBs),

are being disposed into the environment. Even worse, the amount of WEEEs being transferred/exchanged between states and countries (particularly to developing countries) significant social and economic are causing complications. The current PCB recycling procedures include physical separation, followed by metal extraction via pyro/hydro metallurgical pathways. The intensive physical separation of PCBs introduces environmental concerns including toxic gas emissions, and energy deficiency. Pyrometallurgy is also environmentally hazardous due to the formation of toxic gas, slag, and other industrial wastes. Hydrometallurgy involves a series of acid or caustic leaches of e-waste followed by metal recovery techniques. Although hydrometallurgy is more controllable, solvents that are economical and less corrosive (e.g. sulfuric acid) cannot be used to extract gold, which is the most valuable metal within most PCBs. The use of concentrated, or highly reactive acids to extract gold is costly and generates gaseous and liquid pollutants. In this research, we aim to develop a greener, and more selective way to extract both precious (e.g., gold) and common metals (e.g., copper) in waste PCBs utilizing supercritical CO₂ (scCO₂). The use of supercritical CO₂ has resulted in the reduction of the use of concentrated acids. The mechanisms of how scCO₂ interacts with various components in the PCBs are studied and it has been found that the CO₂ interaction with the polymeric portion of PCBs has significantly influenced the subsequent leaching behaviors of metals. Once leached, a wide range of separation options including precipitation and electrowinning are considered to selectively recover different metals.

ENVR 124

Selective separation and enrichment of rare-earth elements from unconventional resources via coprecipitation and liquid-liquid extraction

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The availability of resources is one of the key foundations of the rapid development of our modern society. Unfortunately, high grade ores have been depleted and the environmental concerns have placed restrictions on our ability to use the natural resources. Thus, it is important to find sustainable pathways to obtain resources with reduced environmental footprints. In light of this challenge, closing the material cycle and extracting the useful materials from the end of life of products have

a great potential to reduce both the supply risk and landfill pressure. In particular, rare-earth elements (REE) has a hiah economic incentive in recovering from unconventional resources such as industrial wastes due to their high market demand. Iron slag and steel slag are alkaline silicate wastes that are produced during steelmaking processes. Those wastes are environmentally hazardous when landfilled but do contain a large amount of valuable materials including calcium, aluminum, and magnesium as well as silica and REEs depending on the geographic regions of their feedstock origins. In our study, we have developed a REE enrichment scheme from slag that involves hydrometallurgical treatment, selective dissolution, and co-precipitation of iron and REE. Depending on the concentration ratio of Fe and REEs, the grade of recovered REEs can vary significantly. Thus, a step-wise separation of precipitated Fe-oxides and Feoxide/REEs is needed. Solvent extraction is another option to selectively separate REEs from the leachate containing high concentrations of different metal ions. In this study, different pH conditions and chemical additives for the co-precipitation of REEs are experimented and the possibility of integrating a liquid-liquid extraction process that is using greener solvents such as ionic liquids to extract high purity REEs are investigated.

ENVR 125

Diabetes as an environmental risk factor: Detailed mechanistic implications of chemistry and scavenging of methyl glyoxal by the formation of creatine's mono-and bis adducts

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Diabetes is an environmental risk factor and is caused by the accumulation of advanced glycation end products (AGEs). Metabolic inhibitors such as 2-amino quanidine. metformin and phenformin are all nucleophilic hydrazino compounds which block the formation of fluorescent AGEs. Efficacy of biguanides metformin and phenformin have also been demonstrated very recently in preventing pancreatic ductal adeno carcinoma (PDAC) and specifically phenformin was five times better drug than metformin: http://clincancerres.aacrjournals.org/ April 25, 2018. Studies by Brownlee et al. (Science 1986) elucidated that glycosylation products in diabetes patients are toxic mediators of macro-and microvascular complications and a monoquanide. 2- aminoquanidine prevented diabetes-induced arterial wall protein crosslinking. Protein cross-links are also formed spontaneously not only in diabetes individuals but also are formed in aging populations. Our recent studies elucidated the anti

glycosylation effect of well established drugs, 2aminoguanidine, metformin, and phenformin were comparable with the flavonoids present in Okra Seed Extracts (OSE) (ACS Book Chapter 2012, ACS 255). The inhibition and anti-glycosylation activity of methylglyoxalinduced modification of human serum albumin and lysozyme by stereo-chemically well-defined OSE was illustrated by SDS-PAGE, fluorescence spectroscopy and changes in protein concentrations via Nano-drop spectrophotometry (2016). Present studies will describe mechanistic implications of the scavenging effects of an amino acid creatine. An extremely facile microwaveinduced organic synthesis of creatine-MGO adducts was achieved and characterized by LC-MS/MS. Our results demonstrated that mono-and bis-adducts of creatinemethyl glyoxal adducts were inhibited successfully.

ENVR 126

Plant-based polymers as effective treatment agents in removal of dissolved solids and ions in wastewater for reuse in plant irrigation

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Reports on Dockum aguifer show that this aguifer can be an important source of groundwater for irrigation, public supply, oil field activity, livestock and manufacturing. Dockum aquifer is high in total dissolved solids and hardness. The solution to this problem would be to reduce the contaminant levels in the water to standard accepted values. It was proposed to use the plant-derived ecofriendly polysaccharides as adsorbents/ flocculants to reduce the contaminant levels. Food drade polysaccharides were extracted from fenugreek seeds and psyllium husk using standard methods. Tamarind polysaccharide is commercially available and was used as it is. The polysaccharides were characterized using FTIR. Water samples from different wells from Dockum aquifer were collected and brought to our lab and were characterized for suspended solids (SS), Total dissolved solids (TDS), nitrates, phosphates, chlorides, pH, sulfates, sodium, potassium, magnesium and calcium. Lab scale adsorption experiments were done to study efficiency of the polymers in removal of above mentioned contaminants. The contaminants concentrations were measured before and after treatment to determine the efficiency of the polysaccharides as treatment agents. Gravimetric and Ion chromatographic methods were used to detect contaminant concentrations. The concentrations of the polymers were varied from 0.5g/L to 2g/L. The contact time of the polymers with water were varied from immediately to 2 hours to determine the best contact time for maximum removal of contaminants using different polymer doses. Irrigation experiments were conducted in the green house using three different types of plants. These plants were chosen based upon their salt tolerant

capacity. These plants were irrigated with treated untreated and tap water for 10 weeks. It was found that the green polymers used are capable of removing the suspended solids, total dissolved solids, cations and anions. Results showed that treated water can be reused for irrigation purposes.

ENVR 127

Green coagulants for improved struvite recovery from agricultural waste

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Agricultural runoff significantly contributes to eutrophication events around the world. In the Chesapeake Bay watershed, poultry litter serves as a major source of nutrients. To address this problem, we have developed technologies to extract phosphate from poultry litter. Farmers can apply the nutrient-deficient poultry litter to their fields without contributing to nutrient loads. At the same time, the extracted phosphate can be recovered in the form of struvite, a slow-release fertilizer. The objective of this work was to investigate the addition of green coagulants, such as bentonite, chitosan, potato starch, and sodium alginate, to generate flocs of struvite particles that quickly settle. These natural coagulants are more cost-effective than conventional options, such as alum and ferric chloride. In addition, phosphate strongly interacts with aluminum and iron oxyhydroxides, decreasing the agricultural value of particles recovered with conventional coagulants. We hypothesized that natural coagulants would also provide better control of phosphate release, allowing generation of fertilizers with moderately customized time-release. The optimum dose of the individual natural coagulants, and select mixtures, was determined using jar tests conducted with extracts from 20 g/L poultry litter slurries. For example, the size of suspended particles was reduced from 33.9 µm (no coagulant addition) to 8.5 µm with addition of 500 mg/L of chitosan and 100 mg/L of bentonite. This change in particle size distribution caused the optical density to decrease by 57%, indicating better settling and recovery of struvite. The volume concentration of recovered particles increased with bentonite addition up to 100 Scanning electron microscopy with energy ma/L. dispersive x-ray spectroscopy was applied to confirm the impacts of individual and mixed coagulant use on the morphology and composition of recovered struvite particles. Overall, the use of green coagulants improved phosphorus recovery from agricultural waste.

ENVR 128

Study of flame retardants in lounge chairs and electronics and their impact on emission, exposure, and flammability

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Chemical flame retardants (FRs) have been added in consumer products including furniture in order to meet flammability requirements. Due to recent changes in state-level regulations and/or other cases, FR usage is being reduced through elimination or replacement with more benign alternatives. Exposure to some FRs have been found to lead to health concerns such as cancer, thyroid disruption, delayed mental and physical development, advanced puberty, and reduced fertlity. This study examined chemical exposure levels from daily usage of residential chairs and electronics. All lounge chairs were constructed exactly the same except for the four different FR technologies applied: no FR; application of a textile fire barrier; use of polyurethane foam with an added organophosphorus FR: and use of polyurethane foam manufactured with a reactive FR. The studied electronics were a 55" TV and a 15" laptop. The chairs and the electronics were first measured for volatile organic compound (VOC) and semi-volatile organic compound (SVOC) emissions using an environmentally controlled chamber for inhalation, ingestion, and dermal exposure levels. Following chemical studies, the test products were burned in a controlled fire laboratory to measure flammability parameters and VOC/SVOC emissions from the burn. Results show differences in chemical exposure and flammability performance among the different products and chair types. Added FRs were detected in some of the environmental samples during the environmental chamber exposure measurements. The fire barrier technology had the greatest impact on suppressing furniture combustion. With the amount of FRs added to the constructed chairs, the chemical FRs did not show a measurable fire suppression advantage over chairs without any FRs. The study also shows the presence of other chemicals that should be considered in evaluating chemical exposure risks during daily use and during ignition. This study provides scientific data to assess chemical exposure risks and flammability from furniture and electronics.

Aqueous organic chemicals: When speciation matters

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Hydrophobic, refractory organic compounds that bioaccumulate have received a great deal of attention. There are applications and circumstances, however, where we're forced to consider organic chemicals with very different properties, i.e. those that protonate, coordinate metal ions, and adsorb onto mineral surfaces. Those that hydrate (e.g. carbonyls becoming gem-diols) and tautomerize. Those that have only a transitory existence yet sit at reaction pathway branch points. In such instances our task is to link speciation and reactivity. Making small, systematic changes in functional groups and structure is a good approach. Exploration of medium effects helps too, i.e. changes in pH, major ion concentrations, and additions of organic co-solvents. Often concepts tied most strongly to inorganic chemistry (e.g. the thermodynamic concept "basicity") and those tied to organic chemistry (e.g. the kinetic concept "nucleophilicity") share foundations and can be profitably merged. There are aspects of inorganic chemistry that make most sense when view from the perspective of H-phosphonate/phosphite organic chemistrv (e.g. tautomerization) and vice versa. Connecting aqueous speciation to reactivity in a holistic way will of course aid environmental chemistry. It will also enable the development of greener, water-based synthesis and manufacturing.

ENVR 130

Effects of ocean acidification on the organic complexation and bioavailability of trace metals

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The CO₂ released into the atmosphere by fossil fuel burning dissolves in the surface ocean, simultaneously increasing its CO₂ concentration and decreasing its pH. The potential direct and indirect biological effects of these changes in seawater chemistry, collectively called "ocean acidification," are extremely active research topics. Particular foci include potential effects on key biological processes such as photosynthesis, calcification and nitrogen fixation. A more subtle potential effect of ocean acidification concerns the changes in the chemical speciation and bioavailability of trace metals such as Fe, Cu and Zn that play a key role in the productivity of marine ecosystems. As demonstrated through electrochemical analyses, most biologically active trace metals in seawater are complexed to a mixture of mostly uncharacterized organic compounds. Acidification increases or decreases the bioavailability (and electrochemical reactivity) of metals depending on the relative acidities of the weak and strong ligands to which they are complexed.

ENVR 131

Enhanced degradation of β -lactam antibiotics: Roles of reactive copper species in the absence and presence of peroxydisulfate

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The β-lactam antibiotics such as penicillins and cephalosporins are among the most widely used antibiotics and frequently detected in the environment. Owing to the O- and N-containing functional groups of their structures, β-lactam antibiotics complex favorably with transition metal ions such as copper. This metal complexation tendency not only influences the environmental fate of β -lactam antibiotics but also can be harnessed in treatment technologies to promote their removal. Our recent in-depth studies have identified two new reaction mechanisms that were previously overlooked for *β*-lactam antibiotics and copper under environmentally relevant conditions. First, while Cu(II) ions are known to promote hydrolysis of β-lactams, we discovered that Cu(II) ions can promote hydrolysis and/or oxidation of β-lactam antibiotics, depending on β-lactams' structural characteristics and solution pH. Most significantly, β -lactam antibiotics that contain a phenylglycine primary amine group on the side chain can undergo oxidation by Cu(II) via this functional group, and this transformation involves cycling of Cu(II)/Cu(I). Second, while free Cu(II) ion is known to be ineffective to activate peroxydisulfate (PDS) for advanced oxidation, we discovered that Cu(II) complexed with β-lactam antibiotics are effective activators for PDS which generates Cu(III) and radicals. The generated Cu(III) (major contributor) and radicals in turn can guickly degrade the β-lactam antibiotics, resulting in cycling of Cu(II)/Cu(III) in this system. Further studies show that this novel activation mechanism of PDS is much less influenced by water matrix components and is common with a wide range of contaminants and ligands, with Ncontaining functional groups (i.e. amines) identified to be critical ligand characteristics. Overall, these new findings mark important contributions to a more accurate mechanistic understanding of the reactions between βlactam antibiotics and copper species, as well as activation of PDS by copper.

ENVR 132

Impact of oxygen activation on substrate isotope effects of enzymatic oxygenations

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Enzyme-catalyzed oxygenations are among the most important biodegradation and detoxification reactions of organic pollutants in contaminated soil and water. Because such processes typically take place over timescales of decades and lead to products that are difficult to detect, it is very challenging to quantify the extent of oxidative biodegradation. These issues can be circumvented with compound-specific isotope analysis (CSIA), where the extent of transformation is inferred from the isotope fractionation measured in the remaining pollutant and a priori knowledge of isotope effects pertinent to enzymatic oxygenations. However, the kinetics of such reactions may be governed by enzymatic activation of molecular O2 which do not involve a transformation of the organic pollutant and thus compromise the application of CSIA. Little is known to date about the relative contributions of O₂ activation to the rate of oxidative pollutant removal from contaminated environments. Here, we elucidated the catalytic mechanism of Rieske non-heme iron dioxygenases (RDOs), a class of oxygenases that is responsible for the hydroxylation of several classes of aromatic pollutants by microorganisms. In model systems for nitroarene dioxygenases, we observed a correlation of substrate 13C kinetic isotope effects for various nitroaromatic compounds with the extent of uncoupling of O₂ activation and formation of reactive oxygen species. Our results suggest that O₂ uncoupling allows the detection of substrate isotope effects after the rate-determining O₂ activation by the release of the unreacted substrate from activated enzyme-substrate complex. Our findings provide new insights into the catalytic mechanism of RDOs and the application of CSIA to monitor biodegradation reactions initiated through oxygenation reactions.

ENVR 133

Identification and quantification of unsaturated C4dicarbonyl ring cleavage products from chlorination of phenolic compounds: Structure-activity relationships

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Despite decades of research on the formation of disinfection by-products (DBPs) during chlorination of phenols, there is still considerable uncertainty about the relevance and nature of ring cleavage products. To address this knowledge gap, we investigated the reaction of hypochlorous acid (HOCI) with a variety of phenolic compounds, including commonly used personal care product ingredients, plasticizers and pharmaceuticals as well as naturally occurring phenols. Formation of DBPs was investigated using liquid chromatography-high resolution mass spectrometry using both positive and negative electrospray ionization. In addition, a novel amino acid reactivity assay that utilizes the nucleophilic amino acid N-alpha-acetvl-lvsine (NAL) was used to detect electrophilic DBPs. As expected, the reaction of HOCI with phenolic compounds initially led to the formation of chlorophenols which is attributable to electrophilic aromatic substitution. This was followed by the formation of ring cleavage products such as chlorinated carboxylic acids. In addition, results from the amino acid reactivity assay further revealed the formation of several electrophilic ring cleavage products, including 2-butene-1,4-dial (BDA), its chlorinated analogue chloro-2-butene-1,4-dial (CI-BDA) as well as several other alpha.beta-unsaturated dialdehvde compounds. For BDA we were able to demonstrate that the formation and yields are strongly dependent on the ring substituents, in particular of those in para-position to the phenolic hydroxyl group. Furthermore, the formation of BDA and other ring cleavage products was also impacted by the composition of the aqueous media including the buffer that was used to maintain a stable pH during the chlorination experiments. The application of in-silico toxicity prediction models indicated the formation of several DBPs that are of toxicological concern.

ENVR 134

Using mass spectrometry to identify chemical drivers of toxicity in drinking water

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This project seeks to identify drivers of in vitro toxicity as a metric of human health risk for disinfection by-products (DBPs), which are formed from the reaction of disinfectant and natural organic matter (NOM), in drinking water across the United States. While it is known that individual bromine- and iodine-containing DBPs are more toxic than their chlorine-containing analogues, the correlation of total organic chlorine (TOCI), total organic bromine (TOBr), and total organic iodine (TOI) with a wide range of individual DBPs has not been well studied. Newly developed methods to quantify nearly 60 priority, unregulated DBPs using GC-MS, along with these chemical surrogates, hold great potential for accounting for risk associated with drinking water, both from known and unknown DBPs. Priority, unregulated DBPs were quantified by liquid-liquid extraction and analyzed by GC-MS and GC-MS/MS. Regulated trihalomethanes (THMs) and all bromo-chloro-haloacetic acids (HAAs) were measured using EPA Method 551.1 and 552.2, respectively. To comprehensively identify known and potentially unknown DBPs, 20 or 40 L of water were extracted using XAD resins and analyzed by low and high resolution GC-MS; a portion of this extract was also used for cyto- and genotoxicity assays. Total organic halogen measurements were carried out using a combustion-ion chromatography system. Overall, more unregulated DBPs form in water disinfected with chloramine. than sites that disinfect with chlorine. Further, plants using chloramine disinfection and where a "chlorine burn" event occurred (to remove nitrifying bacteria), generally exhibited higher toxicity in finished water than those using Cl₂ or pre-ozonation followed by Cl₂. Plants that employ activated carbon pretreatment generally have lower overall DBP formation. However, more brominated and iodinated DBPs form; this is due to the fact that activated carbon does not remove halides effectively, thus increasing the halide to organic matter ratio. Although more brominated and iodinated DBPs can form, GAC is effective at limiting overall DBP formation and can thus still lower toxicity. More toxic iodinated DBPs, as well as higher measured TOI, were also found in areas with higher iodide in source waters: the resulting cytotoxicity is generally seen to be higher with increased TOI, and this may be a good indicator for predicting toxicity of drinking water.

ENVR 135

Formation of organic electrophiles during water treatment with chemical oxidants: Precursors, mechanisms and implications for water quality assessment

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Oxidative treatment technologies that utilize oxidants such as hydroxyl radicals, ozone and chlorine are now widespread in a variety of water treatment applications, including wastewater, water reuse and drinking water. While these technologies are highly effective in removing organic contaminants, there is increasing evidence that their degradation can lead to the formation of transformation products that are of toxicological concern. However, the identification of transformation products, especially those with low molecular weights, is frequently hampered by their high polarity and lack of ionizable groups which makes them difficult to detect by conventional analytical techniques. To address this issue. we developed a novel analytical approach that uses nucleophilic amino acids such as N-alpha-acetyl lysine as derivatization agents. Applying this approach to the degradation of phenolic compounds by HOCI or hydroxyl radicals allowed us to identify a,b-unsaturated aldehydes as important electrophilic transformation products. In order to investigate the formation of organic electrophiles more widely, we have now extended our investigations to other compound classes. This talk will discuss our findings, including the relevant reaction mechanisms leading to the formation of electrophiles and resulting implications for the quality assessment of treated waters.

ENVR 136

Photochemical hydrolysis of aromatic trifluoromethyl groups

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Trifluoromethyl-substituted benzene rings are a common feature in the structure of modern pharmaceuticals and pesticides. Some of these compounds, such as flufenamic acid, have been reported to undergo rapid photochemical hydrolysis, converting the trifluoromethyl group into a carboxylic acid. Other trifluoromethylsubstituted benzene-containing compounds are photostable. The critical difference lies in the other ring substituents. Here we report the results of a structurefunction study involving 60 trifluoromethyl-substituted benzene compounds. The substituent effects on photohydrolysis of the trifluromethyl group will be reported, with the key findings being the effects on the absorbance properties of the compounds and on the quantum yields.

ENVR 137

Inhibitory effect of dissolved organic matter on the oxidation of aromatic amines induced by the sulfate and carbonate radicals

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Dissolved organic matter (DOM) is known to slow down the transformation of aromatic amines that is initiated by excited triplet states as one-electron oxidants. This inhibitory effect was attributed to the reduction of oxidation intermediates of the amines by antioxidant mojeties of DOM. leading to the reformation of the parent compounds. In this contribution we present the results of recent detailed investigations of an analogous inhibitory effect of DOM occurring for the oxidation of anilines and sulfonamide antibiotics induced by the sulfate and carbonate radicals. For both radicals, which are relevant in various engineered and natural aquatic systems, a significant inhibitory effect was observed in most cases at concentrations of 1 mgc L⁻¹ DOM. The DOM of the second-order dependence concentration transformation rate constants for a selected subset of the studied compounds was qualitatively similar for both radicals. It consisted of a first phase at low DOM concentrations, in which the rate constant significantly decreased with increasing DOM concentration, and a second phase with small further decrease or even an increase with DOM concentration. This behavior was interpreted in terms of the inhibitory effect and an additional transformation pathway of the aromatic amines induced by secondary radicals produced from oxidation of DOM by the sulfate and carbonate radicals. The quantification of both effects is important to assess the abatement of aromatic amines in aquatic systems in which the sulfate radical or the carbonate radical play a significant role.

ENVR 138

Geospatially resolved database of hydraulic fracturing wells for chemical transformation assessment

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Hydraulically fractured wells with horizontal drilling (HDHF), accounted for 69% of all oil and gas wells drilled and 670,000 of the 977,000 producing wells in 2016. However, only 238 flowback and produced water samples have been analyzed to date. To aid the development of predictive tools, we constructed a database combining additive disclosure reports and physicochemical conditions at respective well sites with the goal of making synthesized analyses accessible. As proof-of-concept, we used this database to evaluate transformation pathways through two case studies: (1) a filter-based approach for flagging high-likelihood cinnamaldehyde halogenation sites according to experimental criteria and (2) a regionally comparative trihalomethane formation model using a predictive empirical equation, the latter of which could not have been possible without the work contributed by the prolific careers of Prof. A. Lynn Roberts and her students. Study (1) highlighted 173 wells with high cinnamaldehyde halogenation likelihood based on combined criteria related to subsurface conditions and oxidant additive usage. Study (2) found that trihalomethane formation in certain wells within five specific basins may exceed regulatory limits for drinking water based on reaction-favorable subsurface conditions, but variability in conditions and limitations in empirical modelling led to wide uncertainty. While experimentation improves our understanding of subsurface reaction pathways, this database has immediate applications for informing environmental monitors and engineers about potential transformation products in residual fluids, guiding well operators decisions to avoid unwanted transformations and highlighting regions for necessary follow-up measurement and/or treatment. With future discoveries and developments that build on the work of the Roberts group and others, we envision more robust components incorporating transformation, transport, toxicity, and other physicochemical parameters to fully predict subsurface interactions and flowback composition.

ENVR 139

Study on pollution characteristics of particulate matter in urban roads: High spatial and temporal resolution monitoring based on mobile sensors

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In order to analyze the change characteristics of particle pollution in urban road environment in real time, this study took taxi as the carrier of PM sensor, and built a mobile monitoring platform with 300 taxis equipped with sensors. At the same time, the evaluation, calibration and application of mobile sensors were discussed in combination with a wireless sensor network(WSN)

consisting of 1700 fixed sensors and 30 standard air quality monitoring stations. In this study, the intercomparison between fixed and mobile methods was analyzed. By analyzing the influence of relative humidity(RH) and particle size distribution on the PM sensor, a two-step calibration model was established to calibrate the mobile sensor. Based on the monitoring data of high spatial and temporal resolution, the Jinan city road network system was divided into 1021 sections, and highresolution pollution maps were drawn to analyze the spatial distribution of road pollution. The diurnal variation of PM concentration in urban road environment and the influence of morning and evening peaks were studied. At the same time, the background baseline of the urban road was extracted from the big data of the mobile sensor by statistical method to quantify the PM emission level of the urban road.

ENVR 140

Estimating ground-level $PM_{2.5}$ using micro-satellite images by a convolutional neural network and random forest approach

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PM_{2.5} poses a serious threat to public health, yet it is poorly managed due to low spatial coverage of regulatory air quality monitoring (AQM) stations. This motivates novel low-cost methods to infer ground-level PM2.5 at a finer spatial resolution to better quantify PM_{2.5} exposure in epidemiological research. Most existing modeling approaches exploit aerosol optical depth (AOD) satellite information that is subject to large uncertainties, require extensive land-use variables as inputs, and predict PM_{2.5} at a coarse 1 km resolution. These limitations have motivated us to devise an algorithm for inferring groundlevel PM_{2.5} by directly processing global-coverage, daily, real-time, 3 m resolution, 3-band micro-satellite imagery of sizes smaller than 1 km×1 km. In this study, we used a deep convolutional neural network (CNN) to process the imagery by extracting image features that characterize the dynamic changes in the built environment and the image colors reflecting AOD, and a random forest (RF) to predict PM_{2.5} from the extracted image features along with meteorological conditions. We validated our model on 35 AQM stations in Beijing from 2017 to 2019. We trained our CNN-RF model on 10,400 daily images of the stations labeled with the ground-truth PM2.5 and evaluated the model on 2,622 holdout images. Our model predicts PM2.5 accurately at a 200 m resolution with a mean absolute error (MAE) and a root mean squared error (RMSE) as low as 10.1 µg m⁻³ (23.7% error) and 17.6 µg m⁻³ (41.2% error), respectively, and an R^2 up to 0.83. Compared to current state-of-the-art approaches, our model's errors are comparable at a much finer spatial resolution and are much simpler to implement as it only requires satellite imagery and meteorological inputs. Our results highlight the potential of augmenting limited spatial predictors of PM_{2.5} with satellite imagery to enhance spatial resolution that is useful for a wide range of applications.



Example satellite image for each of the 35 AQM stations in Beijing. The stations are located at the center of the images.

ENVR 141

Assessing impact of particulate matter air pollution on solar energy production using a micro-satellitebased remote sensing approach

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Atmospheric particulate matter (PM) can diminish solar energy production through both ambient PM and PM deposited on solar photovoltaics (PVs). The global solar energy loss due to PM pollution is equivalent to tens of billions of US dollars annually. Regions such as northern India and eastern central China with the most expanding solar PV energy production are also having the highest PM pollution. Solar energy loss was estimated to be an enormous ~25-35% in these regions with almost equal contributions from ambient and deposited PM. Even though the importance of both types of PM pollution on solar PV energy production has been soaring given a projected 4-fold increase of global solar power capacity over the next 20 years, to date few studies have quantified their respective and combined impacts at a granular level on individual solar farms in a cost-effective way. In this study, we combined global-coverage, daily, 3 m resolution, 3-band (RGB) micro-satellite imagery with energy production data at a solar farm in Pune, India to predict solar energy loss due to PM. We measured the probability distribution difference in pixel values between each solar farm's solar panel image and background image by computing the Kullback-Leibler (KL)-

divergences in all RGB channels. We show that a random forest using RGB KL-divergences and several ancillary variables as features can on average over a period of 2.5 years predict the solar farm's daily solar energy production and as a result the total solar energy loss from both sources within 5.5%. We assessed the total loss in non-monsoon seasons from both sources to be ~11-17% over the sampling period. We further used both standard and ambient PM-corrected satellite images to estimate the contributions from ambient and deposited PM and obtained an average of ~30-40% contribution from deposited PM. Our approach can inform solar companies about the breakdown of their daily solar energy production loss due to PM and help them determine the optimal solar panel cleaning strategies.



The KL-divergences between a solar farm's solar panel image and its background image's pixel values in RGB channels on a clear and a hazy day

ENVR 142

Decadal changes in highway emissions: Comparison of six urban Ohio counties

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A considerable amount of pollution to the air in the forms of criteria pollutants and greenhouse gases comes from the on-road mobile sources. In the USA, since the Clean Air Act of 1970, there is a significant improvement in curbing transportation-related air pollutant emissions on roads through better technology, alternative fuels, planning, and implementation strategies. However, there are also more vehicles on roads than they were in the 1970s. Hence, it is important to assess the changes in the contribution of various parts of the highways to air pollutant emissions in a period of time. This study focuses on studying the changes in the emissions of four criteria pollutants (CO, NO_x, SO₂, and PM) and three greenhouse gases (CH₄, N₂O, and CO₂) on three types of highways in six Ohio urban counties in the period of 2008-2018. For the study purposes, on-road vehicles are considered as gasoline-run passenger cars and diesel-run trucks. Traffic data is obtained from Ohio Department of Transportation in the form of Annual Average Daily Traffic (AADT). Individual air pollutant emission is estimated with the EPA's MOtor Vehicle Emission Simulator (MOVES). The classification of the roads based on the emissions is done using Self Organizing Maps in the beginning years and the ending years of the study period, and comparison analysis is performed based on the SOM maps.

ENVR 143

Development of a natural gas Wobbe Index prediction model

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Wobbe Index (WI) is the ratio of the fuel's calorific value to the square root of its specific gravity or relative density. WI is a critical factor in evaluating the interchangeability of fuel gases, such as natural gas and liquefied petroleum gas (LPG), by comparing the combustion energy output between the different compositions of fuel gases. Natural gas quality (WI) in the United States varies regionally and seasonally in between 47 and 57 MJ/Nm³. WI is used in a wide variety of equipment and processes that require a specific NG combustion energy output. However, WI is typically measured using bulky and expensive analyzers. These devices measure the energy value of the fuel via direct calorimetry followed by a separate measurement of density using an optical method. The complexity of the existing WI measurement systems prevents its off-site application. A machine learning-based predictive model is proposed for accurate estimation of WI of the gaseous fuel mixture. The model uses thermal conductivity, sound velocity at different temperatures and pressure for estimation of WI. The results can enable the technology needed to develop an intelligent sensor that can estimate the WI of natural gas online and in real-time, economically and reliably, overall increasing fuel efficiency and emission performance.

ENVR 144

Machine learning assisted design of environmental responsive materials for healthy and energy efficient building environment

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Most people spend over 70% of times indoor. Therefore, the building environment has significant impacts on the quality of life and health of residents. Conventional building materials are designed primarily considering the structural, thermal, and aesthetic functions. The ability to modulate the environment is not typically considered unless for specific types of space (such as clinic surgery room). This presentation will focus on design of building materials that actively modulate the building environment by utilizing the ambient energy. To complement conventional engineering design principles and analyses, machine learning and artificial intelligent are used to assist the material design to achieve the function of environmental improvements with high efficiency. The performance and economic benefits of new building materials are analyzed with standard software.

ENVR 145

Evaluating links between drinking water violations and the incidence of waterborne disease

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Drinking water quality is closely related to public health. The lack of access to clean water for sanitation purposes can lead to illness and even death. Municipal drinking water systems are responsible for major improvements in public health. Ensuring optimal performance of drinking water systems is critical for reducing exposure to waterborne pathogens and the spread of communicable diseases. Due to this close association between clean water and health, the US EPA has set stringent drinking water standards to safeguard the public. Violations of these drinking water standards are assumed to be associated with increased disease risk. Rather than monitoring human health indicators, violations are determined based on chemical and biological samples collected from within the drinking water system. Relevant acute health related water tests include disinfectant residual concentration and total coliforms in the distribution system, among others. Beyond reporting violations, there are other water system events that may impact public health and require issuance of boil water advisories. In this study, we evaluate if drinking water violations and advisories are related to the incidence of disease. For selected study region, including Michigan and North Carolina, reports of drinking water system violations, health related public notices, and reports of waterborne diseases from 2011-2019 are evaluated. Statistical methods, such as spatial autocorrelation, kriging and classification and regression tree (CART) techniques, will be applied to water system violations data and other water quality samples (e.g., disinfectant residual, total coliforms and other water quality samples

underpinning health based violations) to show how water system violations are related to disease outbreaks and cluster geographically.

ENVR 146

Practical application of econometrics for environmental management: Review of challenges and opportunities

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Environmental econometrics is the application of economic analysis to support decision making in natural resources and environmental management. Despite its proven track record of success in various scientific fields, econometrics has not been exploited to its fullest for environmental engineering applications, such as the prediction of municipal solid waste generation. Traditionally, environmental econometrics heavily relied on regression methods such as Ordinary Least Squares (OLS). While these methods are popular due to their easy implementation and simple mathematical analysis, they have fundamental limitations. Typically, these methods perform poorly when dealing with outliers, non-linearities, a large number of variables, or when a subset of independent input variables is highly correlated to each other. Despite their limitations, these methods can still provide robust estimations that could assist environmental policy-makers. Over the past few years, there has been a growing interest in the use of Artificial Intelligence (AI) in general and Machine Learning (ML) in particular for waste management. ML algorithms address some of the limitations associated with classical methods, but they also present new challenges. A brief review of the traditional methods, as well as the ML algorithms, is presented, and the pros and cons of each are discussed. Lastly, specific practical cases in waste management are discussed.

ENVR 147

Harnessing machine learning for predicting micropollutant removal during advanced oxidation processes in wastewater

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Micropollutants, also known as emerging contaminants, are increasingly seen as a threat to aquatic environment over the last few decades. A major pathway for the micropollutants entering surface water is the discharge from wastewater effluent. While many of these

contaminants are only partially removed by conventional wastewater treatment processes, advanced oxidation processes (AOPs), such as ozonation, ultraviolet/ hydrogen peroxide (UV/H2O2) and Fenton processes, can serve as promising techniques to minimize the input of micropollutants to water resources. Micropollutants are eliminated by direct reactions with ozone or with hydroxyl radical (•OH) generated during various AOP processes. However, the efficiency of these AOPs to remove micropollutants is strongly influenced by the variation of wastewater matrices. Matrix components such as effluent organic matter (EfOM) and the inorganic salts vary considerably in wastewater and the interaction among micropollutants, matrix components and •OH is inherently complicated and poorly understood. Therefore, it is difficult to predict micropollutant removal and to generalize the results across different wastewater matrices by common mechanistic models and simple regression models. Using a variety of machine learning algorithms including Random Forest, Decision Tree and Neural Networks, we were able to accurately predict micropollutant removal during various AOPs in different without considering the underlying wastewater mechanism. Water quality parameters like dissolved organic carbon (DOC), UVA₂₅₄, and inorganic concentrations and AOP parameters like ozone dose, UV fluence and micropollutant reactivity with •OH were selected as input variables, while percent removal of target micropollutants by certain AOP process can be predicted by model as output. Using machine learning to predict micropollutant removal by AOPs can provide a useful tool for utilities to decide the most efficient AOPs based on target pollutants and local wastewater quality.

ENVR 148

Assessing South American *Guadua chacoensis* bamboo biochar and Fe₃O₄ nanoparticle dispersed analogues for aqueous arsenic(V) remediation: Systematic study

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Arsenic concentrations up to 200 fold ($2000 \mu g/L$) of WHO limit 10 $\mu g/L$ has been reported in Latin American (LA) drinking waters. This situation is often neglected, and millions of people are still affected. Providing safe drinking water is a major challenge. In this work, biochar (BC) was developed from a single and taxonomically identified woody bamboo species, *Guadua chacoensis*, unlike mixtures of culm fragments from unidentified species or a pool of species which can't be repetitively duplicated. The discarded, locally available, and silica-rich culms enable a total productive use of *G. chacoensis* clumps by

transforming this valueless waste into biochar adsorbents and iron oxide dispersants for As(V) removal from water. Two biochars were compared; raw biochar (BC) which was produced using slow pyrolysis at 700 °C for 1 h, and its chemically co-precipitated iron-nano particle dispersed analogue (BC-Fe). The surface morphology of the adsorbents was examined by SEM, PZC and BET. Fixedbed column sorption was carried out at different pH's (5, 7 and 9), and breakthrough curves were used to describe its performance. Breakthrough capacities spanned in the range 7.5-8.2 mg/g. The regeneration of the beds was evaluated by employing 1M solutions of ammonium sulfate, sodium hydroxide, and potassium phosphate. The effect of competing ions on As (V) adsorption onto BC and BC-Fe was tested in the presence of ten different ions (sulfate, phosphate, nitrate, acetate, chromate, molybdate, selenate, carbonate, fluoride and chloride) at three different concentrations (0.01, 0.1 and 1 M). The adsorption capacity and the ability of BC and BC-Fe to provide safe arsenic (V) water was finally evaluated in a natural contaminated water from Latin American in both batch and fixed-bed column studies. Adsorbents and their As-laden analogues were characterized using a comprehensive XPS study. This bamboo biochar can be considered as an environmentally friendly and costeffective adsorbent candidate to provide arsenic (V) free water.



ENVR 149

Prediction of five-day biochemical oxygen demand (BOD₅) from some oxygen demand characteristics in surface water

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The five-day biochemical oxygen demand test is an empirical test used in standard laboratories to measure organic load and thus pollution strength in effluents and polluted waters. This study investigated the functional relationship between BOD₅ and some quality parameters of surface water such as Chemical Oxygen Demand (COD) and Permanganate Value (PV) obtained from Omadino River in Warri, Delta State, Nigeria. The aim

was to provide a quick evaluation of BOD₅ for effluent monitoring. The linear regression equations and correlation established were: BOD₅ = 1.20 PV + 0.25; r = 0.708 and COD = 9.38 BOD₅ + 18.76; r = 0.900 respectively. Confidence intervals were: 0.77 \leq a \leq 1.64 at 95%; 0.56 \leq a \leq 1.84 at 99% for BOD₅/PV and 9.23 \leq a \leq 9.53 at 95%; 9.16 \leq a \leq 9.60 at 99% for COD/BOD₅. Results established strong relationship which will be useful for BOD₅ prediction.

ENVR 150

Novel oxone treated hydrochar for the removal of Pb(II) and methylene blue (MB) from aqueous solution

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This study focuses on, developing a novel adsorbent for the efficient removal of different contaminants from wastewater. Pine wood hydrochar (PWC) was prepared by hydrothermal treatment at 300 °C and oxidized with Oxone to produce oxidized pine wood hydrochar (OPWC). The OPWC adsorbents were characterized using SEM, FT-IR, TGA, Elemental analysis, and BET. Conductometric titration of OPWC showed a significant increase in the content of carboxylic groups on the surface of the hydrochar to (600 L/g). The OPWC sorption performance was assessed by using lead Pb(II) and methylene blue (MB) as two models of contaminants. Sorption benchmarks were performed by varying the contaminant initial concentration, time, and temperatures. Sorption kinetic data were fitted well to 2nd order kinetic model giving high correlation coefficients (R2)>0.99 and isothermal data were fitted with Langmuir model. The highest sorption capacities for Pb(II) and methylene blue were 45 mg/g and 80 mg/g, respectively. This study proves that Oxone treatment could be a potential sustainable oxidation method to tune the hydrochar surface to increase selectivity towards heavy metal ions and dye sorption

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Natural plant pigments analysis applied to photodegradation of the pharmaceutical pollutants in water

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Photocatalysis has shown great potential as a low-cost and sustainable technology in water treatment. However, low efficiency in solar energy harvesting is one of the major challenges in its application, and discovering natural dyes using analytical chemistry tools such as HPLC/MS and NMR would be a significant contribution in improving the solar energy harvesting efficiency. In this study, a group of 22 different tropical natural plants with intense colors (leaves or flowers) were screened for the potential applications on dve-sensitized TiO₂ in Ibuprofen treatment. As a result, Begonia 'Martin's Mystery' was discovered to be the best candidate for further study. Moreover, the promising discovery of *Begonia* application in Ibuprofen treatment has been successfully applied to Warfarin and Famotidine treatment. Similar results were also observed in many other species of Begonia with even better results for some pollutants which indicate that Begonia extracts could be excellent potential sensitizers for TiO₂ based photodegradation of pharmaceutical pollutants. Our results also suggested that the total intensity of both UV-vis and visible light screening process might be an easy and efficient way to narrow down dye sensitizer species for natural pigment discovery in tropical plants. The screening process may potentially open a brand-new way for future TiO₂ photodegradation studies before the complex and time-consuming detailed mechanism studies. Analytical flatforms such as HPLC/MS/MS and NMR are currently applied to the Begonia species and combined with multivariate model data analysis to analyze the best natural pigment compounds and combinations for photocatalysis.

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Treatment of kitchen wastewater using aerobic biological method and sand-bed filtration

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Lack of sufficient fresh water supply is a serious issue that affects at least one-fifth of the world's population. Majority of the population far exceed the quantity available for human sustenance. Wastewater recycling processes are necessary and capable of producing large volumes of water for reuse. In this study, kitchen wastewater was characterized and treated using aerobic biological treatment and sand bed filtration. Results obtained revealed the following: pH 7.4, turbidity, 6.9NTU, conductivity (EC) 365 µS/cm, hardness 16.0mg/L, total dissolved solids (TDS) 141mg/L, total suspended solids (TSS) 5mg/L, total solids (TS) 146mg/L, biochemical oxygen demand (BOD) 5.5mg/L, chemical oxygen demand (COD) 36mg/L, alkalinity 6.3mg/L, chloride 0.18mg/L, nitrate 1.5mg/L sulphate 0.12mg/L and total colony forming unit (CFU) was 381 x 10⁻⁴ respectively for the raw wastewater. Also the biologically treated grey water revealed pH 7.9, turbidity, 6.0NTU, conductivity (EC) 311 µS/cm, hardness 15.0mg/L, total dissolved solids (TDS) 121mg/L, total suspended solids (TSS)

2mg/L, total solids (TS) 123mg/L, biochemical oxygen demand (BOD) 1.82mg/L, chemical oxygen demand (COD) 32mg/L, alkalinity 7.3mg/L, chloride 0.35mg/L, nitrate 2.0mg/L sulphate 0.15mg/L and CFU too numerous to count (TNC). Results obtained were compared with water quality standards. Biological treatment and sand-bed filtration were effective and rendered the wastewater useful for secondary re-use.

ENVR 153

Computational modeling vs. Adsorption isotherm experiments to gauge the capacity of cocoa shell biochars to remove stable and hydrolyzing pharmaceuticals from water

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Pharmaceuticals and personal care products are often discarded into freshwater supplies due to improper disposal and human/veterinary waste, posing the potential to contaminate nearby ecosystems and drinking water supplies. Activated carbons are often used to adsorb water pollutants. To increase the sustainability of such water treatment options, we must identify renewable sources such as biomass wastes to replace traditional fossil-based adsorbents. In this study, cocoa shells were obtained from Lindt Chocolate in Stratham, NH following removal of the cocoa nib. Samples were dried overnight in a laboratory oven at 110°C and mechanically ground and sieved to three particle size fractions: <125mm, 250-300mm, 600mm-2mm. Samples were pyrolyzed at 550°C under N₂for 30 minutes to generate a biochar. Biochars were physically activated for 30 minutes at 650°C under CO₂and chemically activated using а 1:2:14 biomass:water:KOH ratio at room temperature, then heated under CO2at 650°C for 30 minutes. The small and medium particles had high mesoporosity; the chemically activated samples showed overall surface areas above 800 m²/g, with mesoporous surface area of the small samples of 770 m²/g, and medium samples of 600 m²/g. Using adsorption isotherm experiments, we explored the relationships between particle size, surface area and diffusion limitations for oxytetracycline removal. While CO₂physical activation did not increase adsorption capacities, KOH chemical activation increased the capacity threefold to 40 mg/g for the smallest particles. The removal of oxytetracycline and sulfamethoxazole was characterized using traditional analytical techniques via best fit for pseudo first or second order kinetics as well as with computational modelling using Stella®software. In general, the traditional analysis overestimates the adsorption capacity by conflating hydrolysis and adsorption, while the computational analysis reveals a simultaneous removal process where hydrolysis leads to smaller overall reported adsorption capacities.

ENVR 154

Prediction on hydrolysis mechanisms and kinetics of environmental chemicals

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Hydrolysis is an important degradation pathway that determines fate and persistence of chemicals with hydrolytic functional groups. Nevertheless, hydrolysis mechanisms and kinetics of for hydrolizable chemicals are largely unknown. Experimental data on hydrolysis kinetics are lacking, which limits the development of models and tools for predicting hydrolysis kinetics of chemicals. Experimental determination of hydrolysis kinetics and pathways for chemicals encounters various difficulties. Herein, prediction methods or models on hydrolysis kinetics of organic chemicals were investigated by density functional theory (DFT) calculation and quantitative structure-activity relationships (QSAR) modeling. Cephradine and phthalate esters (PAEs) were selected as model compounds. Hydrolysis pathways, mechanisms and kinetics of cephradine and PAEs were investigated. By combining experimental and DFT calculated data, QSAR models for predicting basecatalyzed hydrolysis kinetics of PAEs were developed. The combination of DFT calculation and QSAR modeling successfully pave a promising way for predicting hydrolysis kinetics and pathways of chemicals.

ENVR 155

Synthesis of cost-effective and sustainable pathways to wastewater treatment

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Water is one of the most essential resources to sustain all forms of life. The upsurge in global demand at a rate of about 1% per year is due to the rise in population growth, economic development, climate change, among other factors. Unlike energy, water has no ancillary alternatives. There is, therefore, the need to treat and re-use wastewater to meet this increasing global demand. There are various treatment technologies that have been developed over the years – like, sedimentation, filtration, advanced oxidation processes, ultrasonic, among others. One of the main problems associated with the treatment

process is that there are different combinations of technologies that inadvertently give rise to different pathways. Furthermore, the cost of treatment is always a major deciding factor in choosing a particular pathway. It is, therefore, imperative to develop wastewater treatment pathways that are capable of meeting the standards for a specific kind of task with a lower cost association. In order to meet these demands, we formulated an optimization problem to find the different pathways that satisfy our functional models, and as well, give the cost of each pathway in a ranking order, from the least to the greatest. These problems were formulated as a mixed integer programming (MIP) optimization problem. They were solved using the integer programming solver, advanced branch-and-bound (ABB) in P-Graph software. A life cycle analysis was carried out for each ranked order using the SPI index methodology.

ENVR 156

Adsorption of catechol/hydroquinone on TiO_2 and iron(III) oxide

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Water pollution has a profound effect on water resources. Harmful chemicals entering the water cycle have been found in industrial and household wastewater. The most common chemicals are personal care products (PCPs) that are found in shampoos and detergents. In this research, Iron (III) oxide (Fe₂O₃) and Titanium oxide (TiO₂) was used to investigate the adsorption of PCPs like Catechol and Hydroquinone using Fourier Transform Infrared - Attenuated Total Reflection (FTIR-ATR) spectroscopy. Adsorption isotherms, kinetics and pH effects were also tested to identify optimum adsorption conditions. From the results of the experiments, it was found that TiO₂ is a good adsorbent for Hydroquinone while Iron oxide was a better adsorbent for Catechol and maximum adsorption occurred near the point of zero charge (pzc) of the oxides. Future implications of this research could help us find a cost effective naturally available adsorbent compared to other toxic adsorbents that are currently in use.

ENVR 157

Combined nano-bio technologies based on iron nanoparticles: Efficient tool for groundwater remediation

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Over the past two decades, nanoscale zero-valent iron (nZVI) particles turned out to be a promising tool for degradation of various organic compounds (mainly chlorinated solvents represented most typically by TCE) and immobilization of broad range of inorganic compounds (metals, metalloids, etc.; most typical example is the reduction of hexavalent chromium). The advantage of nZVI particles lies mainly in their (i) small particle size allowing their migration in groundwater, (ii) high specific surface area providing them the key property of high reactivity (i.e., significant effect on solution redox conditions leading to the decrease of oxidation reduction potential typically below -400 mV), as well as high sorption capacity, and (iii) possibility of their easy modification (surface or bulk chemical treatment, deposition on various substrates, etc.) for targeted application. Although the degradation/removal of organic/inorganic compounds by nZVI is typically successful and highly efficient in laboratory-scale conditions, the nZVI-based technologies face many problems in real contaminated sites. They include mainly the large-extent of contamination, its inhomogeneous distribution in subsurface, complex geology/lithology and variable hydrogeological conditions. Therefore, the strong reduction power of nZVI particles must be further enhanced by other (and mostly cheap) complementary processes - biotic and/or abiotic - in real groundwatertreatment technologies. The efficiency of such nano-bio combined technology was successfully demonstrated at numerous field-scale applications of such technology. In this contribution, we will present the basic properties of nZVI particles and derived Fe-based materials, their optimization for higher reactivity with the strong accent to their utilization for removal of emerging persistent/ halogenated organic compounds. The major part will be focused on the combination of nZVI with biotic and/or abiotic sources of electrons, both in laboratory-scale and filed-scale tests. Moreover, the effect of nZVI on microbial communities typical for groundwater, as well as toxicity of nZVI, will be covered in the presentation. Generally, the nZVI-based nano-bio technologies turn out to be one of the highly promising and cheap ways to significantly enhance nZVI performance for groundwater treatment.

ENVR 158

Ligand-controlled mobilization of tetravalent uranium

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The recent discovery of non-crystalline U(IV) species in the environment, and the mounting evidence of their larger lability compared to crystalline U(IV) minerals (e.g. uraninite), has necessitated a deeper understanding of how aquatic biogeochemistry affects different U(IV) species disproportionately. Furthermore, it has been shown that organic ligands may increase U(IV) solubility and mobilization rates. Therefore, we tested the hypothesis that uraninite and non-crystalline U(IV) are mobilized by organic ligands at different rates. Experiments were done on various U(IV) species (uraninite, non-crystalline U(IV), and field-collected sediments) to elucidate mechanisms and rates of U(IV) mobilization by ligands (low-molecular-weight organic acids, synthetic chelators, siderophores). Continuousflow stirred-tank reactor, batch, and flow-through column experiments were conducted with a variety of organic ligands. The results from these experiments provide valuable insights in regard to the propensity of U(IV) for mobilization in bioremediation scenarios that may be the basis for costly future decisions.

ENVR 159

Evolving reactivity and products of natural ironbearing minerals toward sulfide

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Iron minerals play dynamic roles on sulfur cycle in natural and engineered environments. Sulfate enters surface waters through oxidation of sulfur-bearing minerals like pyrite or wastewater effluents and diffuses into sediments. In anoxic environment, sulfate-reducing bacteria produce hydrogen sulfide that reacts with Fe(II) and iron (oxyhydr)oxides to produce iron sulfide minerals along with elemental sulfur and other species. Due to the importance, reactivity of pure or synthesized iron minerals have been widely studied with sulfur species but knowledge on heterogeneous nature of iron-bearing materials on their reactivity with sulfur is limited. This work has elucidated reaction capacities, products, and kinetics of two natural iron-bearing minerals derived from taconite towards aqueous sulfide using batch and column reactors. Siderite (SR)- and iron oxide (IO)-rich were selected based on iron mineralogical characteristics and quantity. Generally, the siderite rich SR reacted with more

hydrogen sulfide per gram (Δ HS) over the iron oxide rich IO. SR produced more solid phase sulfur, liberated by HCI and chromic acid, where IO produced more elemental sulfur and thiosulfate. Sulfate as an oxidation product was minimal for both materials in batch and column reactors. Reaction kinetics were dependent on the molar ratio of the amount of sequestered sulfide to initial sulfide concentration (Δ HS/HS_{inital}). Initial reaction rate increased with increasing Δ HS/HS_{inital}, or as iron becomes the dominant reactant. SR maintained an appreciable reaction rate with each sequential spike, while reactivity of IO decreased with sequential sulfide spikes. Their reactivity and products in the column reactors were comparable with those observed in the batch reactors. A reactive-transport model was developed using batch reactor kinetic results to establish reaction rate and dependence on Δ HS/HS_{inital} to describe sulfide reactivity evolution through a column. In summary, the selected materials generally reacted predictably with sulfide with respect to their iron mineralogy and, with predictable sulfur reaction kinetics and capacities. These results represent an important step toward elucidating the reactivity of heterogeneous iron-bearing materials at the interfacial processes with the cycles of iron and sulfur and developing applications of natural iron-bearing material for sulfur treatment system.

ENVR 160

Impacts of cryogenic sampling processes on reactive iron mineral coatings in sediment

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This study focused on comparing reactive mineral coatings found in sediment from a cryogenic (Cryo Core) core versus an anaerobic core. To characterize reactive mineral coatings in oxidation reduction (redox) transition zones of sediments, the Cryo Core was collected using liquid nitrogen at 77K at a historically-contaminated site. After being thawed in an oxygen-free glovebox, a suite of sediment analyses was applied that included pH, redox potential, X-ray fluorescence (XRF), X-ray diffraction (XRD), and field-emission scanning electron microscopy (FESEM) with energy dispersive X-ray analyzer (EDX). Among the identified reactive iron minerals found. crystalline pyrite was found to a greater degree in the Cyro Core than in the Anaerobic Core that was collected under oxygen-free conditions and at room temperature. Moreover, mackinawite and greigite which are ubiquitous

in the Anaerobic Core were not observed in Cryo Core samples. To better understand why the metastable minerals were not present, the freeze/thaw process was simulated on Anaerobic Core samples using a liquidnitrogen quench with surface coatings characterized by FESEM/EDX. In quenched samples, mackinawite was no longer observed, and in its place was pyrite. In addition, both greigite and pyrite were found to be unique morphologically after quenching. The dissolutionprecipitation process for the iron sulfide coatings may explain the change in geochemistry of pore water during the freeze/thaw process through two main mechanisms of freeze-concentration and freezing potential.



XRD identification and semi-quantification results.



FESEM/EDX results. A and C: framboidal pyrite (highlighted) and granular pyrite coatings on the bulk mineral surface; B and E: well-developed crystalline pyrite; D: spherical framboidal pyrite.

ENVR 161

Arsenic fate under the shadow of sea-level rise

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Climate change is hitting home as a global menace and a serious challenge for the 21st century. Sea-level rise (SLR), as an indicator and an outcome of climate change, has a vital influence on coastal hydrogeological systems, biogeochemical processes, and thus, the fate of toxic metal(loid)s. High levels of toxic metals are found along many coasts in the US, particularly along the Mid-Atlantic coast, where SLR rates are higher than elsewhere in the world. Coastal sediments are subject to episodes of resuspension due to a combination of SLR-induced flooding, waves, and currents that can disturb sediments and mobilize pollutants into overlying water. However, the mechanisms of mobilization and impacts on water quality are yet to be fully understood. In this study, sediments collected from an As-contaminated industrial site in Wilmington, DE, USA, which is projected to be inundated by 1 m of SLR-induced flooding by 2100, were used to quantify the release of heavy metals due to sediment resuspension. A range of shear stresses typically encountered in coastal environments ($\tau = 0.028$ N m⁻²) was imposed at the sediment-water interface using a laboratory-based erosion chamber. The concentrations and speciation of metal(loid)s in the overlying water, and resuspended sediment were further quantified. In general, the results indicated that As concentration in solution and solid phases, its distribution in the sediment profile after flooding, and its aqueous speciation were significantly impacted by the imposed shear stress levels. However, the speciation of As in the solid phase does not considerably vary with different flooding scenarios. Sediment characteristics and the amount of As in the sediment were found to be the key parameters governing the solid phase concentrations and the magnitude of the release. With climate change as a factor contributing to sediment disturbances, and due to the current legislative limitations restricting pollutant discharge to the environment, the relative importance of sediment resuspension as a source of dissolved metals is expected to expand.

ENVR 162

Influence of surface-sulfidated iron particles on sulfate reducing microbial communities

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Sulfate-reducing bacteria (SRB) may be used to biologically sufidate reactive zero valent iron surfaces, which may lead to improvements in the rates of the surface-mediated dechlorination of trichloroethene (TCE) and tetrachloroethene (PCE). This work examines the

influence of reactive iron particles upon the sulfate reducing bacteria used during sulfidation. Previous work has shown that nanoscale zero valent iron (nZVI) particles may inhibit SRB, but the influence of surface-sulfidated iron, nanoscale or otherwise, on indigenous SRB is unknown. To address this knowledge gap, batch experiments were setup to compare the impact of sulfidated and non-sulfidated ZVI (as nanoparticles or macroscale iron granules) on a sulfate reducing culture enriched from contaminated sediments. Results with nZVI show significant enrichment of methanogens when enrichment cultures are exposed to non-sulfidated nZVI particles, presumably due to H₂ production from nZVI. In contrast, microbial communities exposed to sulfidated nZVI showed loss of diversity and richness but suppressed methanogenic growth. Systems containing sulfidated macroscale ZVI also showed suppression of methanogens but maintained overall richness and diversity. These preliminary data show that biological sulfur amendments, in addition to promoting abiotic dechlorination activity, may shift microbial communities populations towards that promote biological dechlorination.

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Sulfide intrusion and distribution in the seagrass *Halodule wrightii*

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Sulfides are known environmental stressors to marine angiosperms. Reduction of sulfate to sulfides by sediment bacteria results in their accumulation in anoxic environments. Gaseous sulfide (H₂S) is able to enter marine plants through their roots and rhizomes. We used stable sulfur isotopes to assess sulfide intrusion into the seagrass *Halodule wrightii* and determine its distribution throughout the plant. We found a gradient in δ^{34} S values (-5.58± 0.54 ‰ to +13.58 ± 0.30 ‰), from roots to leaves, suggesting that H₂S enters through underground tissues and is then distributed throughout the plant. The presence of sulfide-derived sulfur in varying proportions (14%-76%) among the leaf, rhizome and root tissues indicates they are able to assimilate it into non-toxic, metabolic forms.

ENVR 164

Sea level rise impacts on arsenic mobility in natural systems

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Sea level rise (SLR) as a result of climate change is affecting the world's coastlines, especially in the mid-Atlantic region of the US. Impending SLR will change coastal hydrologic regimes and cause an increase in salinity and flooding, which can lead to major variations in current metal/metalloid cycling. Arsenic (As) is a ubiquitous element that can accumulate in dangerous concentrations in coastal soils due to anthropogenic or natural processes. Arsenic is of particular interest due to its carcinogenic nature as well as its sensitivity to changes in redox potential, which generally cause it to become more mobile as redox conditions reduce. Currently, there are limited data on the geochemical controls governing As cycling in variable saline and brackish water environments. To help address this knowledge gap, arsenate was sorbed to goethite in artificial river water (ARW) and artificial seawater (ASW) in variable pH systems to simulate the effects of encroaching seawater in a model system. Additionally, to further simulate the effects SLR and redox potential, model systems of an iron(III) oxide and As(V) co-precipitate were reacted in microcosm vessels over redox and salinity (ARW to ASW) gradients. Aqueous samples were analyzed via inductively coupled plasma mass spectrometry and solid phase samples were analyzed via arsenic and iron Kedge EXAFS spectroscopy to determine local bonding environments. Sorption experiments reveal an inverse relationship between increasing pH and As sorption; as pH increases. As sorption to goethite decreases in ARW. However, in ASW, As sorption was greater at pH>8 compared to ARW. Solid phase analysis of the microcosm studies indicate as redox potential decreases, mineral transformation from iron(III) oxide to a mixed valence iron(II/III) oxide and As(V) co-precipitate occurred in both ARW and ASW, however, mineral transformation was more apparent in ARW. Results from this study will help improve the current understanding of As mobility and contribute to management strategies and remediation plans in SLR impacted coastal soils throughout the world.

ENVR 165

Influence of phenolic structure on contaminant oxidation by manganese oxides in complex matrices

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Manganese oxides are considered to be one of the strongest naturally occurring oxidants in near surface environments. These minerals can oxidize several classes of inorganic and organic contaminants, including those with phenolic functional groups. As a result, manganese oxides such as MnO2 influence contaminant fate in natural soils and may be a key driver of reactivity and contaminant fate in natural waters interfacing Mnenriched soils. Furthermore, manganese oxides have also been proposed for the passive, in situ treatment of pollutants in stormwater, landfill leachate, and other contaminated surface waters. These water and soil interfaces are complex matrices containing a variety of organic contaminants, inorganic ions, and dissolved organic matter (DOM), which may interact with manganese oxides through sorption, redox reactions, complexation, and other mechanisms. This study evaluates the ability of synthetic birnessite and reclaimed Mn oxides to oxidize a series of phenolic compounds by both sorption-limited and electron transfer-limited reaction pathways. These compounds range from simple model phenols to complex environmental contaminants including antimicrobial agents (4-cresol, triclosan), endocrine disruptors (bisphenol A, estrone, 17βestradiol), and surfactants (4-n-nonylphenol, 4-tertoctylphenol). The rates and rate-limiting steps of phenolic contaminant oxidation are used as a metric to mechanistically investigate the interactions between organic carbon and Mn oxide materials. The role of contaminant substituents, manganese characteristics, and water composition are investigated. The results of this study suggest that complexities in near surface environments mechanistically impact contaminant degradation by manganese oxides.

ENVR 166

Saltwater intrusion affects peroxidase-mediated polymerization for remediation of coastal soils

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Coastal groundwaters can be affected by saline intrusion caused by fresh groundwater withdrawal from aquifers or surface level salt addition from king tides, sea level rise, and storm surges. The increased background of halides relative to initial conditions results in changes in the apparent ability of native peroxidase enzymes to catalyze the polymerization of humic materials and anthropogenic contaminants in soils. Halophenols were observed to polymerize internally and also copolymerize with natural organic matter, with polymerization driven by the natural abundance of hydrogen peroxide and peroxidase found in saturated coastal soils. Halophenols and other probes were also removed from the aqueous phase by sorption

onto the freshly formed polymeric particulates in this system. Chloride, bromide, and iodide salts were added to determine the effect of saline intrusion on this process, testing the hypothesis that oxidative equivalents would be diverted from polymerization to the production of hypohalites. Three different peroxidases; horseradish peroxidase, Lyngbya (marine spp) peroxidase, and a newly discovered freshwater Lyngbya peroxidase were tested for their ability to affect contaminant removal. Polymerization under freshwater conditions resulted in formation of polymers with molecular weights corresponding to \sim n=10 for condensation. These precipitated from solution and acted as adsorbents for other non-polar contaminants 14% the activity of a corresponding mass of activated carbon. Simulated seawater intrusion caused partial consumption of enzymatically derived reactive oxygen species by dissolved halides, reducing the overall stoichiometric effectiveness of the process for removing organics.

ENVR 167

Enhanced removal of conventional and emerging pharmaceuticals and personal care products (PPCPs) from water by graphene-iron nanohybrid

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The increasing presence of pharmaceutical and personal care products (PPCPs) in aquatic environment poses serious health concern due to their pharmacological active properties. Especially selective serotonin reuptake inhibitors (SSRIs), one of the most prescribed antidepressants, have been positively correlated with adverse health effect and has recently been found as an emerging pollutant in fresh water systems and fish. Engineered nanomaterials with high surface area, tunable adsorption sites, and unique redox behavior, offer greater prospect for removing PPCPs through adsorption and advanced oxidation respectively in comparison to bulk materials. In this study, we utilized reduced graphene oxide (rGO) to support nanoscale zero-valent iron (nZVI) resulting in rGO-nZVI nanohybrid for the removal of a mixture of 12 conventional PPCPs and emerging SSRIs from water at environmentally relevant sub-ppm level concentration (200 ppb). The rGO-nZVI hybridization provides a synergistic improvement in PPCP/SSRI removal through adsorption on rGO surface and simultaneous catalytic oxidation by nZVI in the presence of H_2O_2 . The rGO-nZVI nanohybrid, with or without H_2O_2 , removed more than 95% of all the PPCPs/SSRIs within 30 minutes, which was significantly higher than the removal performance of parent nanomaterials (rGO or nZVI) or their mixtures. However, with H₂O₂, the removal kinetics was much faster.

Correlating material morphology and surface chemistry with the surface deposition process of graphene oxide

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In this study, we correlated the deposition behavior of graphene oxide (GO) materials with their morphology and surface chemistry. GO materials with various crumpling extents (flat, wrinkled, and crumpled) and different surface chemistries (surface reduction extents) were produced using an aerosol-based method. In a furnace aerosol reactor (FuAR), flat 2D GO nanosheets were transformed into 3D wrinkled and crumpled structures via the capillary force caused by water evaporation. For all the synthesized materials, the aggregation and deposition kinetics were investigated over a wide range of monovalent and divalent cation concentrations by employing time-resolved dynamic light scattering (DLS) and a real-time quartz crystal microbalance with dissipation monitoring (QCM-D), respectively. Critical coagulation concentrations (CCC) and critical deposition concentrations (CDC) were determined for NaCl and CaCl₂ electrolytes. Flat GO first turned into wrinkled and then into crumpled GO (CGO), and the corresponding CCC increased by 89% and CDC increased by 46%. indicating a weakened interaction between nanoparticles or with the microbalance sensor surfaces, caused by the crumpled morphology. In addition, for the same crumpled morphology, CCC decreased by 31% and CDC decreased by 23% with a higher degree of reduction. Based on simulations. CGO nanoparticles fit better with the DLVO model for classic 3D colloids, while the flat GO nanosheet deviated from predictions due to its ultrathin 2D structure. The release of GO was highly dependent on material properties and salt types, with the flat GO in the initial CaCl₂ suspension forming the most stable layer on the silica sensor surface, due to its effective contact with the smooth shape and the bridging effect of Ca²⁺. Based on these aggregation, deposition, and release kinetics studies, both material morphology and surface chemistry can have significant influences on GO's fate and transport in the environment.

ENVR 169

Withdrawn

ENVR 170

Environmentally friendly humic acid coated magnetic iron nanoparticles for removal of model styryl pyridinium type cationic dyes

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The removal of cationic dyes from industrial wastewaters is critical prior to their discharge into the environment. Iron based humic acid coated magnetic nanoparticles (HA-MNP) were evaluated for the potential remediation of polluted wastewaters using 2-[4-(Dimethylamino)styryl]-1-methylpyridinium iodide (2-ASP) as a model to cationic styryl pyridinium dyes. HA-MNPs were prepared by coprecipitation from a mixture of ferrous chloride tetrahydrate (FeCl₂:4H₂O) and ferric chloride hexahydrate (FeCl⁶H₂O). The HA-MNPs were characterized by FTIR, SEM and BET. The adsorption of 2-ASP, measured by fluorescence, demonstrates HA-MNPs are efficient for the removal of 2-ASP with a maximum adsorption capacity of 8 mg/g. Detailed kinetic studies showed the adsorption process is most accurately modeled by a pseudo 2nd order process. The adsorption also follows Langmuir type adsorption and is relatively fast with ~ 70 % of the adsorption complete within 30 min. The overall removal increases from 40 % at pH = 3 to 66 % at pH = 7.5. The observed increase with increasing pH can be assigned to an enhanced electrostatic attraction between the positively charged 2-ASP and the increase in the negative charge on the HA-MNP surface as a function of increasing solution pH. The increase in adsorption of a function of solution pH is not linear and may be related to specific pKa values of different functional groups present at the surface, for example carboxylates and phenols. The measurement of the temperature effects on the adsorption yields ΔG° = -2.48 (kJ mol⁻¹) at 318.15 °K indicating a spontaneous adsorption process. The positive value of ΔH° =7.696 (kJ mol⁻¹) shows the endothermic nature of the HA-MNP-2-ASP system. The sorption study of model dye, 2-ASP indicate that HA-MNP has potential as a powerful sorbent for the removal of cationic dyes.

ENVR 171

Photocatalytic pathway toward degradation of various pharmaceutical molecules: Kinetics, mechanisms and toxicity assessment

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Pharmaceutical residues have been found in municipal wastewater and have raised concerns about the potential risks they pose to both humans and our ecosystems. Among the different AOPs, heterogeneous TiO₂ photocatalysis is reported to be a promising technology for the degradation of such toxicants. The aim of this paper is to examine the degradation of various pharmaceutical compounds (Paracetamol, Naproxen and Ibuprofen) by the heterogeneous photocatalysis processes TiO₂ / UV, UV-LED and solar irradiations. The operating parameters, namely, pH, catalyst load and light intensity (number of LEDs) were optimized. The main parameter of degradation as a function of pH was the adsorption of the molecules studied on the TiO₂ entities. Thus, the rate of degradation increases as a function of the catalyst load, but the excess of catalyst load decreases the rate of degradation by opacity effect. The mineralization of the treated solutions was followed by the chemical oxidation demand (COD) measurement and/or the dissolved organic carbon (DOC). Significant mineralization was observed, however, no complete mineralization was observed in our study. Using different chromatographic techniques (HPLC) and ultra-highperformance liquid chromatography coupled to tandem mass spectrometry (UHPLC-MS/MS), an attempt was made to identify some reaction intermediates formed during the degradation of our molecules studied. Reaction mechanisms have been established according to the results obtained in order to try to understand the degradation of the compounds studied and their mineralization. The effect of the matrix on the degradation was examined and the effect of the present ions was studied. In photocatalysis TiO₂ / solar, a study of the reusability of the supported TiO₂ film was carried out and the film maintained a stable catalytic activity after five reuses. The toxicity of the molecules studied and of the reaction intermediates was monitored by the avoidance test on Eisenia andrei earthworms and by the Microtox test on Vibrio Fischeri bacteria. The results showed that photocatalysis reduced the toxicity of the molecules studied.

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Withdrawn

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Immobilization of enzymes on polymeric membranes: Quantum and molecular mechanics study

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Adsorption of phosphotriesterase enzymes on polysulfone membrane surface was investigated through a double-scale computational approach. Surface charges of enzyme as well as membrane were calculated at subnanoscopic and nanoscopic scales, whilest protein adsorption was simulated at a bigger scale. Adsorption energies were calculated as a function of the enzymesurface distance and, for each distance, several protein rotations were tested in order to find the most stable orientations of the macromolecule. The results of this model were useful to obtain information about adhesion of the enzyme and to give indications on the orientations of its binding site. Adsorption energies agreed with the literature data. Furthermore the binding site of the immobilized phosphotriesterase was less accessible with respect to native enzyme due to the steric hindrance of the polymer surface; thus, a reduction of its efficiency is expected. The proposed methodology made use of fundamental quantities, calculated without resorting to adjustable or empirical parameters, providing basic outputs useful for ascertaining enzymatic catalysis rate.

ENVR 174

Rhamnolipid impact on the biological activity of surface modified nanoparticles

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Increased use of engineered nanomaterial in commercial products warrants better understanding of nanoparticle fate, transport, and ultimate impact in environmental systems. Understanding nanoparticle release in the environment will be confounded by surface modification via a number of biotic and abiotic actors. In particular, biosurfactants, produced extracellularly by bacteria, fungi and yeast, among others, are hypothesized to be impactful. One of the most extensively studied class of biosurfactants is rhamnolipid(s), for which *Pseudomonas* aeruginosa can excrete in relatively large quantities. In this presentation, I will describe the synthesis of highly monodisperse iron oxide (Fe₃O₄) nanoparticles (8 nm) with different surface functional groups and then discuss the influence of surface charge on the behavior and ultimately the toxicity of the nanoparticles using quartz crystal microbalance (QCM-d) and supported lipid bilayer(SLB) as model cell membranes. Interfacial behaviors of rhamnolipid(s) and nanoparticles will be described and compared with model bacterial systems (e.g. *E. coli*).

ENVR 175

Comparing the fate of pristine and wastewater-aged gold nanoparticles in freshwater: Impacts of surface coating functionality

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When synthesizing engineered nanomaterials (ENMs), surface coatings are applied to prevent their aggregation and impart specific functionality (e.g., targeted drug delivery). These surface coating also influence the fate of ENMs in aquatic environments by mediating the adsorption of natural organic matter and altering interactions with suspended particulate matter. To investigate this phenomenon, researchers typically use 'pristine' ENMs that are representative of their 'asproduced' form. However, it is unlikely that ENMs released to the environment will resemble their 'pristine' state. Instead, the physiochemical properties of ENMs will be altered through a variety of processes during their lifecycle. Engineered systems, such as sewers and wastewater treatment plants, represent one such lifecycle stage where ENM properties can be transformed (termed 'aging') prior to their incidental discharge to the environment. The aim of this study was to compare the aggregation behavior of 'pristine' and 'aged' ENMs in samples of raw and filtered river water. Gold nanoparticles (AuNPs) coated with polyethylene glycol lipoic acid (COOH) (PEG), and branched polvethylenimine (bPEI) were selected as model ENMs. Using a previously reported technique, the AuNPs were aged in filtered primary wastewater. During this aging process, the physiochemical properties of the AuNPs were altered via aggregation and the acquisition of an organic matter corona. When added to river water, only two AuNP types in their pristine form were removed to a significant extent via aggregation and settling (PEG-AuNPs in raw river water and COOH-AuNPs in filtered river water). This indicates that the physiochemical properties of the pristine AuNPs influence ENM behavior in river water, generally preventing their homo- and/or heteroaggregation. After aging, all the AuNP types underwent aggregation in the raw and filtered river water. Higher removal was observed in the raw river water compared to filtered river water, demonstrating that the aged AuNPs undergo heteroaggregation in addition to homoaggregation. Negligible removal of the aged AuNPs was observed in ultrapure water, revealing that the aging of ENMs in wastewater stimulates their aggregation and subsequent removal in natural aquatic systems. It is hypothesized that the impact of the initial engineered

surface coatings on the environmental fate of ENMs is largely masked by subsequent corona formation in wastewater treatment systems.

ENVR 176

Rare earth elements doping enhanced surface oxygen effect in MnO₂ for toluene decomposition at low temperatures

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For indoor air purification, low energy consumption requirement and low volatile organic compounds (VOCs) concentration call for catalysts that possess high catalytic activity at relatively low temperatures. Manganese dioxide (MnO₂) is one of the most attractive materials because of its rich surface defects, molecular adsorption, and regulatory structure etc. Generally, the surface oxygen vacancies of manganese oxides are beneficial for the lowtemperature catalytic activity in the removal of VOCs. Here, we have doped Ce, Sm, La, Y into MnO₂ by hydrothermal method to create surface active oxygenenriched MnO₂ nanocomposite that exhibited remarkably catalytic activity and high stability for toluene combustion at low temperatures. With little amount of rare earth elements doping, the catalysts can achieve almost 100% degradation of 10 ppm toluene (gas hourly space velocity: 60000 ml g⁻¹ h⁻¹) at room temperature and keep high catalytic stabilization at least for 15 hours. According to the element analysis of SEM, four kinds of rare earth elements uniformly distributed in the structure of manganese dioxide, and the surface area of the catalysts have significantly increased from 140 m^2/g to 185 m^2/g . 237 m²/g, 258 m²/g and 192 m²/g, respectively. Structure analysis by XPS revealed that the doping of rare earth elements can greatly increase the content of surface oxygen species of reactive the catalysts. Correspondingly, O2-TPD data also exhibited that the oxygen can be released at lower temperatures and the amount of active surface oxygen can be enriched by doping rare earth elements. ESR data also showed that there exist large amounts of oxygen defects in the structure of the materials in the presence of rare earth elements. And the enhanced hydroxyl radical in MnO₂ with rare earth elements doping, resulting in the higher low-temperature catalytic oxidation of toluene. The research show that the rare earth doped catalysts are applicable for the commercial non-noble metal catalysts used for the oxidative removal of VOCs in indoor air purification.

ENVR 177

Seasonal biogeochemical cycling of copper- and gold-based engineered nanomaterials in a freshwater wetland mesocosm

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Reliable predictions of the environmental fate and risk of engineered nanomaterials (ENMs) require a better understanding of ENM reactivity in complex, biologically active systems for chronic low concentration exposure scenarios. Here. simulated freshwater wetland mesocosms were dosed with ENMs to assess how their reactivity, and seasonal changes in environmental parameters, influence ENM fate in aquatic environments. Copper-based ENMs (Kocide), known to dissolve in water, and gold nanoparticles (AuNPs), stable against dissolution in the absence of specific ligands, were added weekly to mesocosm waters for 9 months. Metal accumulation and speciation changes in the different environmental compartments were assessed over time. Copper from Kocide rapidly transported to terrestrial soils and deeper sediment and associated to organic or sulfide phases. In contrast, Au accumulated on/in the macrophytes in the oxidized form, and over time transferred to the surficial sediment. A dynamic seasonal accumulation and metal redox cycling was found between the macrophyte and the surficial sediment for AuNPs. These results demonstrate the need for experimental quantification of how biological and chemical complexity of the environment combine with their seasonal variations, can drive the fate of metastable ENMs.

ENVR 178

Incidental nanoparticles in the environment: identification and their implications

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Incidental nanomaterials are produced unintentionally (more specifically, an unintended nano-byproduct of some anthropogenic process), and as a result commonly enter the environment very soon or immediately upon formation. We will discuss typical examples of incidental NPs in the environment. How to identify them and study their environmental implications. For example, we have discovered that TiO₂ minerals naturally present in coal quickly convert to titania suboxides, specifically Magnéli phases (Ti_xO_{2x-1} with $4 \le x \le 9$) during the coal's heating/burning in coal-fired power plants. This is a typical example of incidental NP with significant environmental risk. Moreover, engineered NPs are being produced in amounts large enough to make them a consequential nanocomponent of the planet. Taking silver NP as an example, we have found that Ag⁰-NPs are transformed into secondary biogenic NPs with the size less than 10 nm by sulfate reducing bacteria, showing more significant bioavailability and phyto-uptake.

ENVR 179

Role of nanoscale materials in environmental pollution and remediation

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Naturally occurring nanoscale materials in soils include clays, organic matter, and iron oxides and each can play an important role in contaminant transport and remediation. Incidental nanomaterials, including metals and plastic released through waste streams and agricultural processes, are emerging terrestrial pollutants of particular concern. In order to understand the behavior of natural and incidental nanomaterials, and to harness the potential to engineer them for contaminant sequestration, it is necessary to fully characterize these materials in terms of their structure and reactivity with various chemical/biological components in the environment. Within single particles, elemental distribution can varv from the interior to the surface, thus surface sensitive techniques must be employed. Here, we illustrate how the use of model materials, as well as field samples, in combination with high-resolution spectroscopic and microscopic capabilities, can be used to interrogate interfacial reactivity of nanomaterials, including with redox-active contaminants and at microbe-nanomaterial interfaces.

Palladium and platinum release from vehicle catalytic converter materials exposed to common environmental ligands

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Vehicle catalytic converters (VCCs) have been an essential application of nanotechnology since the 1970s, dramatically improving air quality by converting harmful engine emissions to more benign gases. The active components in VCCs are platinum group element (PGE) nanoparticles of palladium (Pd), platinum (Pt), and rhodium (Rh) as well as nanoparticles of oxides including ceria, alumina, and zirconia. Rising use of VCCs from increasing vehicle ownership continues to increase the input of PGEs to the environment. The fate of these solids is unknown, but one possibility of concern is dissolution of the PGE particles coupled to the formation of stable coordination complexes. We report results of our investigation into this possibility. Batch leaching studies were conducted mixing commercially-available VCC materials with solutions containing varying levels and combinations of environmentally-common ligands including chloride and ammonia, as well as cvanide (sourced from ferrocyanide in road deicing salt). Powdered VCC materials were exposed to varying concentrations of chloride (0, 1000, 4000, and 10000 ppm as NaCl), ammonia (0, 0.1, 1 and 2147 ppm as NH₄NO₃) and ferrocyanide (0, 1, 2 and 10 ppm as Na₄Fe(CN)₆) at pH 8 for 48 hours. Elemental analysis of leachates revealed a synergistic increase in Pd release when chloride was present at lower concentrations of ferrocyanide and ammonia but not at the highest concentrations. Platinum release followed trends similar to those of Pd but was limited. The results will be discussed in the context of coordination chemistry equilibria and a materials characterization included.

Nano-mineralogical study on the weathering of gunshot residue in soils of a shooting range in Ontario, Canada

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Gunshot residue is emitted as fine particulate matter during ignition in a firearm barrel. The particulates condense from a vapour phase and contain material from the Pb-Sb-Ba-bearing primer and the Pb-bearing bullet fragments. Shooters can inhale or ingest the fine particulates which also attach to their hands, clothing, and other surfaces. Estimation of the bioavailability of toxic Pb and Sb within the particulates requires detailed knowledge on the mineralogical composition of the particulates and their weathering products. For this purpose, particulates from gunshot residue have been collected from soils beneath a shooting position of a shooting range in Ontario, Canada. Transmission electron microscopy (TEM) shows for the first time that the particulates are composed of Pb-Sb alloys with minor unidentified Ba-bearing phases along the outer rim. Weathering of the particulates results in the formation of incidental nanoparticles of metallic Pb and massicot PbO. The mobilization of these nanoparticles within the soil grain suggest that their release during the weathering of bullets and gunshot residues contribute to the release of Pb into the environment. Hydrocerussite, Pb₃(CO₃)₂(OH)₂ is the major secondary Pb-phase in and around the altered particulates. The phase forms during the alteration of metallic Pb and massicot in a Ca-carbonate rich environment. Secondary Sb-bearing phases are valentinite, Sb₂O₃ and an amorphous Sb-Pb phase (Sb : Pb ratio = 3:1 - 4:1) that has partially replaced large proportions of the Ca-carbonates in the soil grain matrix. The larger abundance of the latter relative to the former phase indicates that its solubility most likely controls the release of Sb into the bulk soil.

ENVR 182

Crumpling versus puncturing: Biomechanical threshold for the cellular toxicity of silver nanowires

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The use of metallic silver nanowires in conductive transparent networks (CTN) could introduce new pathways for the interaction of novel fibers and human skin. We discovered that a material property, nanowire bending stiffness that is a function of diameter, controls the cytotoxicity of AgNW to non-immune cells from humans, mice and fish without deterioration of critical CTN performance parameters: electrical conductivity and optical transparency. Both 30- and 90-nm diameter AgNW are readily internalized by cells, but thinner NW are mechanically crumpled by the forces imposed during or after endocytosis while thicker nanowires puncture the enclosing membrane, release silver ions and lysosomal contents to the cytoplasm thereby initiating oxidative stress. This finding extends the fiber pathology paradigm and will enable the manufacture of safer products incorporating silver nanowires.



Pictured in grayscale is a virtual slice extracted from the 3D reconstruction of mouse fibroblast cells exposed to silver nanowires (NWs), acquired by coherent X-ray imaging at ID-16A of the ESRF under cryogenic conditions. Overlain on the central cell is a colorized image of elemental distributions showing internalized silver (red) nanowires, chlorine-rich (green) endolysosomes and phosphorus (blue) in the cell body. Lehmann et al., PNAS 116, 14893–14898 (2019).

ENVR 183

Plant interactions with engineered aluminum oxide nanoparticles

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The toxic effects of aluminum (AI) ions on plant roots were identified over a century ago. However, the effects of Al oxide nanoparticles (Al₂O₃ NPs) on plant growth and development are poorly understood. In the present study, plant interactions with Al₂O₃ NPs were systematically evaluated from seed germination and root growth to full maturity by measuring biomass and uptake of Al and nutrients of lettuce plants. The plants were grown in hydroponic solutions with varying concentrations of Al₂O₃ NPs (0, 0.4, 1, and 2 mg/mL) or AlCl₃ (0, 0.04, 0.4, and 1 mg/mL). The results suggest that Al₂O₃ NPs had a neutral or positive influence on seed germination and root elongation, whereas AICl₃ treatment resulted in a significant reduction in emerging root lengths. Upon harvest, lettuce plants exposed to Al₂O₃ NPs of 1 and 2 mg/mL showed 10.4% and 30.4% decreases in biomass, whereas exposure to AICI₃ of 0.4 and 1 mg/mL reduced plant biomass to 22.3% and 9.96% respectively. In both treatments, AI uptake by roots increased linearly; however, translocation of Al₂O₃ NPs into shoots was limited, whereas translocation of AICl₃ increased with increasing treatment concentration. Furthermore, significant adsorption and/or aggregation of Al₂O₃ NPs on the root surfaces appears to affect plant uptake of macronutrients, but not micronutrients. Calcium uptake was the most inhibited by AICl₃. The translocation of Al₂O₃ NPs from roots to stems and leaves were also visually confirmed by fluorescently-labeled Al₂O₃ NPs with fluorescence and confocal laser scanning microscopic techniques. These findings demonstrated that Al₂O₃ NPs behave differently from AI ions when interacting plants under hydroponic conditions. Thus, it is concluded that Al₂O₃ NPs pose less phytotoxicity than AlCl₃, primarily due to NPs role on stimulated root growth, significant adsorption/aggregation on roots, limited lateral translocation to shoots and leaves, as well as enhanced uptake of essential nutrients.

ENVR 184

High-throughput screening of engineered nanomaterials that enhance photosynthesis using mesophyll protoplasts

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Achieving and sustaining global food security will become increasingly difficult as a changing climate increases crop loss due to greater pest and pathogen activity. Certain engineered nanoparticles (NPs) have unique properties that have exhibited significant potential for promoting photosynthesis and enhancing crop productivity. Understanding the fundamental interactions between NPs and plants is crucial for the sustainable development of nano-enabled agriculture. Leaf mesophyll protoplasts, which maintain similar physiological response and cellular activity as intact plants, were selected as model system to study the impact of NPs on photosynthesis. The mesophyll protoplasts isolated from spinach were cultivated with different NMs (Fe, Mn3O4, SiO2, Ag, and MoS2) dosing at 50 mg/L for 2 hours under illumination. The potential maximum guantum yield and adenosine triphosphate (ATP) production of mesophyll protoplasts were significantly increased by Mn3O4 and Fe NPs (23% and 43%, respectively), and were decreased by Ag and MoS2 NPs. The mechanism for the photosynthetic enhancement by Mn3O4 and Fe is to increase the photocurrent and electron transfer rate, as revealed by photoelectrochemical measurement. GC-MS based single cell type metabolomics reveal that NPs (Fe and MoS2) altered that metabolic profiles of mesophyll cells during 2 hours illumination period. Separately, the effect of NPs exposure on photosynthesis and biomass were also conducted at the whole plant level. A strong correlation was observed with protoplast data; plant biomass was significantly increased by Mn3O4 exposure (57%). but was decreased (24%) by treatment Aq NPs. The use of mesophyll protoplasts can be a fast and reliable tool for screening NPs to enhance photosynthesis for potential nanofertilizer use. Importantly, inclusion of a metabolic analysis can provide mechanistic toxicity data to ensure the development "safer-by-design" nanoenabled platforms.



ENVR 185

Developing nanocarriers for delivery of double stranded RNA as a biological pest control agent

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There has been intense interest in using gene silencing technology for a wide variety of applications ranging from functional genomics to cancer therapeutics. One application that has received much attention recently is the use of double stranded RNA as a biological control agent for insect pests. Our research aims to develop nanocarriers which can protect dsRNA from degradation and deliver it to the cytoplasm of the gut cells of insects, where it can bind to the RISC complex and initiate silencing of target genes. A key challenge has been to develop materials that accomplish this goal without causing non-target toxicity. We have tested a variety of materials ranging from dsRNA-polyaminoacid polyplex to surface-functionalized nanoparticles inorganic nanoparticles in gut cells from the fall army worm (SF9 cells; (Spodoptera frugiperda)) and the model nematode Caenorhabditis elegans. Our presentation will describe how nanomaterial properties relate to efficacy, non-target toxicity, environmental stability, and mechanisms of action. The studies highlight the challenges of "safe by design" approaches.

ENVR 186

Investigating nanoparticles for sustainable fashion

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Nanotechnology is playing an increasing role in all industries, including fashion and design. In our approach, we are pushing the limits of nanotechnology and biofabrication to create prototype materials for use in the fashion industry and for biomedical applications. Studying these materials offers us new insights into a product's lifecycle impacts and the contribution of nanotechnology in the circular economy. Our studies include assessing the use of nanoparticles as flame retardants, as well as investigating their optical (including dichroism) and electronic properties. Here, we focus on incorporating nanoparticles in various matrices, such as cotton, wool, bioplastic and bacterial cellulose. Overall, this approach allows us to investigate new composite materials, advance knowledge in material science, and engage future leaders of the fashion industry in design with emerging materials, lifecycle assessment, sustainability and circularity.

ENVR 187

Engineered K-fertilizer derived from hydrothermally altered K-feldspar

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Global food security needs have led to an increased interest in the hydrothermal engineered production of K fertilizers using natural K-feldspars. To understand the mechanism of this process, sanidine, microcline and orthoclase feldspars were hydrothermally altered at alkaline conditions in a Ca(OH)₂ solution (pH 12.4) at 190 for 24 hours. Detailed analytical FESEM °C measurements and XRD-Rietveld refinements of the post-reaction products reveal that the original feldspar grains are surrounded by a several micron-thick rim of secondary crystalline phases, which include calcite, tobermorite, hydrogrossular phases, as well as abundant nanoparticles. High resolution TEM and TEM-EDXS also reveals the presence of a distinct K-enriched amorphous phase that forms directly at the interface with the Kfeldspar. This amorphous phase, as well as omnipresent nanoparticles, are the most likely phases that will release K in a soil pore solution. We hypothesize that the mechanism of feldspar alteration is most likely coupledinterfacial dissolution-reprecipitation (CIDR).

ENVR 188

Diabetes as an environmental risk factor: Critical role of artificial intelligence (A.I.) as a screening tool in diabetic retinopathy

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In India 70 million are diabetic and are at risk of diabetic retinopathy, which can cause blindness if left untreated. Increased levels of methylglyoxal (MGO), a dicarbonyl compound derived from glucose is linked to clinical microvascular complications causing nephropathy, retinopathy, and neuropathy. Our laboratory has studied

mechanistic details of inhibition of advanced glycation end products (AGEs) using natural bioactive compounds from plants (ACS 2012,2014-2018). MGO derived (AGEs) are responsible in causing macro-and micro-vascular complications in diabetes Type-2 patients. We are investigating target bioactive molecules found in Okra Seed Extract, bitter melon Peel for scavenging reactive oxygen species in diabetes Type-2 and cardiovascular disease patients which we believe could be potentially useful in fighting diabetic blindness. Molecular characterization of antioxidant bioactives (Lutein, chlorogenic acid from bitter melon and flavonoids from okra seed extract and their trapping efficiency of MGO, a potent neurotoxin was achieved. A critical role of Artificial Intelligence A.I.), a screening tool at an early stage for diabetic retinopathy identifying tiny lesions, hemorrhages, discoloration resulting in blindness will be described. Also a description of biological significance of metabolic inhibitors (metformin, phenformin and a monoguanide 2aminoguanidine) and their comparison with bioactives in inhibiting (AGEs) as well as their receptor will be discussed.

ENVR 189

Leaching of valuable metals from spent-lithium-ion batteries using organic aqua regia

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Lithium-ion batteries (LIBs) have increasingly been used since 1991 in diverse electronic products such as cameras, cellphones, laptops, and further for the electrical vehicle. The market of the cathode of LIBs is growing from \$7 billion in 2018 to \$58.8 billion by 2024. LIBs usually have 2-3 years of life span depending on materials. These electronic waste with high concentrations of metals and toxic organic solvents may negatively affect our environment and human health. Material recovery from the spent-LIBs system is not only necessary for environmental protection, but also important for resource conservation. Hydrometallurgy has been considered as the most efficient way to recover Li and Co from LIBs by using inorganic acids. In this work, we investigated the recovery of Co and Li using ten dilution times Organic Aqua Regia (OAR) without the separation of the cathode from Al foil which can reduce the complexity of the pretreatment process. OAR has been used as a high selectivity etchant to recovery noble metals such as gold (Au) and palladium (Pd) without leaving harmful residues. The metal leaching rate reached up to 0.035 mg-Li•ml⁻ ¹•min⁻¹and 0.29 mg-Co•ml⁻¹•min⁻¹depending on the metal species and other leaching conditions, which are comparable to the reported rates using other organic acids (i.e., succinic acid and malic acid). The result shows the leaching efficiency for Co and Li is over 80%, 2 wt.% H₂O₂under the temperature of 85°C for 60 minutes with

ultrasonication (120W). Moreover, we characterized the changes in the morphology of cathode materials before/after leaching by X-ray Diffraction, Raman spectrometer, SEM-EDS, and UV-vis to further understand the leaching mechanisms. This green chemical leaching method is aimed at improving the industrial recovery processes for LIBs.



ENVR 190

Characterization of hyperaccumulators for greener recovery of rare metals

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Phytoextraction is a promising green technique that can decrease the environmental hazards of chemical-based extractions during the recovery of critical and rare metals. The fundamental of this research is to establish the potential of renewable feedstock as a remediation bioprocess, and eventually reduce the environmental footprint caused by chemical utilizing methods. This study reports the identification and characterization of the hyperaccumulators and their response to various external stimuli and anthropogenic climate change. The plant samples in this research were used without any genetic modifications, and their response to induced physical or chemical stressors such as salinity, nutrient-deprivation, and acidity was observed. Our initial studies on the hyperaccumulators suggest that they can survive the severe environmental conditions and exposure to metalcontaining aquatic feed solutions. The preliminary results, demonstrated by the SEM- Energy Dispersive X-Ray Spectroscopy (SEM-EDX) and the Fourier-transform infrared spectroscopy (FTIR) to name a few, show that the hyperaccumulators have an effective biomechanism to withstand unforeseen or induced extremities. This overview highlights some salient points and perspective application of this green technology including waste minimization and recycling.

ENVR 191

Creating more efficient, less hazardous syntheses of pharmaceutical using the 12 principles of green chemistry

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We have used the 12 principles of green chemistry to redesign the syntheses of two classes of pharmaceutical compounds: 3,5-diarylisoxazoles and phenylmaileimides. Isoxazoles are a group of pharmaceuticals that are used as anti-convulsant, anti-epileptic and anti-inflammatory drugs. The conventional process used to make these molecules uses a number of hazardous chemicals and produces large amounts of waste. We have developed a more environmentally-friendly 4-step synthesis that yields multiple isoxazoles, uses less hazardous reagents, reduces waste, is more energy efficient, and is cost effective. Maleimides are essential building blocks for a number of pharmaceuticals and herbicides. We have developed a three-step synthesis for a variety of phenylmaleimide derivatives that has high atom economy, is energy efficiency, reduces waste and use of hazardous reagents and solvents, and is extremely cost effective.

ENVR 192

Withdrawn

ENVR 193

Techno-economic and life cycle analysis of biobased resin: Case study on acetoacetylated lignin resin

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Lignin is one of the primary components of plant materials and the second most abundant polymer on earth. Currently, lignin is produced as a byproduct of the wood and paper industries and to a lesser extent lignocellulosic biorefineries. Since, in most cases, the bulk of lignin is burned as a low value fuel, valorization of lignin into high value products can help create economic incentives for the producers and increase the economic feasibility of biorefineries, as well as contribute to a biobased economy. However, before an upgrading pathway for

lignin is recommended, full environmental and economic assessments are needed. One attractive route for upgrading lignin is functionalizing it for coating applications with comparable or better properties than conventional fossil-based coatings. The aromatic and aliphatic hydroxyl functional groups in lignin can be substituted with acetoacetate functionality to produce acetoacetylated lignin resin. This resin can be crosslinked with amines, polyisocyanates, or melamine-formaldehyde resins to get thermosets. The advantages of this process are 1) that the polyol used in the reaction mixture functionalizes with acetoacetate and acts as a reactive diluent while crosslinking the resin, and 2) avoiding the use of any solvents to solubilize lignin, so the process is waste free. In this study, we investigate the economic viability and environmental performance of lignin resin compared to its fossil-based counterparts. We use techno-economic analysis (TEA) to determine the major utilities, capital costs, and suggest areas that need to be optimized for higher economic value. Additionally, we use Life cycle assessment (LCA) method to assess the environmental impacts of the lignin-based resin compared to fossil-based counterparts and show whether the production of this resin is more sustainable than conventional coatings. The insights provided by the results from this study can provide valuable inputs in broadening the concept of integrated biorefineries.

ENVR 194

Paper-based fast and selective detection of lead in water

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The development of fast and selective methods for the detection of spectroscopically silent heavy metals such as lead (Pb2+) is important to prevent its exposure in drinking water. An efficient detection method can further facilitate effective remediation. Herein, cellulose filter paper-based simple, fast, and selective detection of lead (Pb2+) in water is reported. Sodium rhodizonate, a commercially available and cheap compound, was used as the probe molecule. When a microdroplet of Pb2+ solution was mixed with another droplet of sodium rhodizonate solution, it changed color to a deep red. This color change was found to be highly selective to Pb2+ and it could be easily detected by the naked eye observation. The limit of detection of Pb2+ was found to be about 1ppm in water. The mechanism and the kinetics of the detection of Pb2+ were further studied by UV-visible spectroscopy and Transmission Electron Microscopic (TEM) images.

ENVR 195

Enzymatic degradation of polyester plastics using a novel engineered biocatalyst

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Plastics have become the essential materials in daily life and industrial applications, due to their unique physicochemical properties. The extensive manufacture and use of plastic products have led to a tremendous amount of post-consumer plastic wastes globally, which is of increasing concern due to the hazardous impacts towards various natural environments and ecosystems. On the other hand, production of plastics consumes a large amount of fossil fuel resources and discarding plastics after only a single use is nonrenewable. Therefore, developing innovative and effective technologies for plastic waste recycling is of great significance to retain their economic value while minimizing the adverse environmental impacts. However, there are numbers of challenges and limitations in the existing plastic recycling approaches. The mechanical and chemical recycling approaches are usually energy intensive, have high cost, and yield downgraded lower value products. In contrast, biocatalytic approaches hold promise as a green chemistry alternative to depolymerize post-consumer plastics into building block molecules which can be either repolymerized to original products or converted into other value-added chemicals. In this study, we constructed a novel biocatalyst using synthetic biology for polyester plastic depolymerization. The engineered biocatalyst exhibited enzyme activity of 662 ± 42 U/g dry cell weight to *p*-nitrophenyl butyrate (PNPB), a standard water-soluble substrate for esterases. It could depolymerize polyethylene terephthalate (PET) film into its building block monomers, primarily the mono(2hydroxyethyl) terephthalate (MHET) and terephthalic acid (TPA), at 30 °C. Furthermore, pretreatment of PET plastic film with anionic surfactants prior to the biocatalytic reaction would significantly enhance the hydrolysis activity of the engineered biocatalyst by 10-fold compared with the reactions without surfactant treatment. The study provides proof-of-concept demonstration of effective depolymerization of plastics by exploiting biocatalysis and bioengineering technologies. Results are important for developing economical and eco-friendly strategies for sustainable plastic waste recycling.

Slow-release phosphate fertilizer using biochar

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Phosphate (PO₄³⁻) sorption onto biochar surface has been suggested as a means to produce enhanced soil amendment that can be land applied and recycle nutrients to agricultural soils. However, the unmodified biochar normally has low PO43- sorption capacity. The objective of this study is to tailor biochar for enhanced PO₄³⁻ sorption affinity by metal co-ordination reaction. This study focused on biochar produced from corn stover (CS) treated with 7.5 wt% FeSO₄ using autothermal (air-blown) pyrolysis at 500°C with high PO₄³⁻ sorption and low PO₄³⁻ desorption capacity for use as a slow-release fertilizer. Point of zero charge (ZPC) measurement of biochars indicated the dominance of acid functional groups in the Fe-impregnated biochar, as the pH_{ZPC} value shifted from 8.48 to 4.31 due to Fe impregnation. Our batch equilibration sorption isotherm results showed that the Feimpregnated biochar (CS-FeSO₄) has 48% more PO₄³⁻ sorption capacity relative to unmodified biochar (CScontrol) when challenged with 4.000 mg L^{-1} PO₄³⁻ solution. whereas the desorption isotherm rate was ~1/3 for CS-FeSO₄ biochar relative to CS-control. Further oxidation of biochar by post-pyrolysis air oxidation increased PO43sorption by 56% but did not change the PO₄³⁻ desorption rate. XRD and SEM-EDS analyses show the phosphate sorption mechanisms predominately involved surface complexation. XPS analysis shows the dominant oxidation state of Fe and phosphorus are +3 and +5. Column leaching trials will be carried out with simulated agricultural runoff and industrial effluent water to show the effectiveness of the biochar to act as PO₄³⁻ scavenger and slow-release fertilizer for phosphate recycling in soils.

ENVR 197

Microbial electrochemical treatment of biorefinery black liquor and resource recovery

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Biorefineries valorize waste biomass to biofuels and bioproducts, but the associated wastewater treatment is costly and energy-intensive. This study demonstrates that not only the recalcitrant black liquor generated from biorefineries can be treated using a microbial electrochemical process, but also value-added materials including lignin, chemicals, and H₂ can be separated to enable resource recovery. A lab scale microbial biomass recovery cell (MBRC) was developed to treat the actual black liquor from the deacetylation and mechanical refining (DMR) process, and the results show that 60.1-73.8% of organics, 52.0–54.6% of salts, and 30.8–49.5% of lignin were removed using different operational modes. Moreover, by utilizing the unique pH gradient generated between the different reactor chambers, tailored recoveries of lignin, chemicals, and H₂ were realized for the first time. The recoveries of lignin and salts were up to $61.2 \pm 2.7\%$ and $92.2 \pm 1.6\%$, respectively. Ion transfer and organic transformation were further analyzed to understand the reaction mechanisms and improve the system performance.

ENVR 198

Structural evaluation of humic acids and soil organic matter from integrated crop-livestock-forest systems

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The concern about soil quality has increased considerably due to environmental problems related to land degradation and demand on agricultural sustainable intensification. The current challenge in agriculture in Brazil is to maintain and advance the productive capacity of soils by using green technologies that are capable of promoting the sustainable expansion of agricultural production. Soil organic matter (SOM) plays an important role in environmental sustainability, due to contribution to biological, chemical and physical soil properties. Their main constituents are humic substances (HS) and their fractions (e.g., Humic Acids - HA, Humin). Among the different analytical techniques that could be used to characterize the humification index and chemical stability of organic materials we employed Nuclear Magnetic Resonance (NMR) and Laser Induced Fluorescence Spectroscopy (LIFS). In this work we examined SOM and HA from soils under Integrated Crop-Livestock-Forest Systems (ICLF) to establish a humification index. For this, samples of a dystrophic Red-Yellow Latosol (Oxisol) were collected from the experimental site of a research station called Embrapa Pecuária Sudeste (located in the Southeast of Brazil), five years after the implantation of the ICLF systems. Soil samples were extracted for HA following the protocol of the International Society of Humic Substances (IHSS). Also, whole soils, without any chemical treatment, were prepared for analysis by LIFS with excitation at 405 nm and emission scan from 465 nm to 800 nm. For ¹³C NMR a multi-CP/MAS approach was employed with a 400 mHz Bruker Avance II. Results showed that the humification index, determined by LIFS in the whole soils, are directly related to ¹³C NMR

aromaticity of HA with a Pearson correlation of R =0.65 and this aromaticity was higher in ICLF area than native vegetation area. So, in these integrated systems we observed an increase in organic matter stability, a promising result in line with agricultural sustainable intensification concepts; and that the LIFS technique provides an excellent alternative for structure determination of the SOM, without the need to perform chemical fractionation of soils.

ENVR 199

Things I learned from Prof. A. Lynn Roberts during the early years of research on contaminant degradation by zerovalent metals

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Many research groups began work on contaminant degradation with zerovalent metals in the early 1990s. and the first major papers from this work appeared in 1994. However, most groups first reported their results at a symposium on contaminant remediation with zerovalent metals in April 1995 at an ACS National Meeting in Anaheim, CA. This timeline meant that most of the early work on zerovalent metals was done in parallel, without much opportunity to learn from, and build on, the results of other groups. Many interesting examples of this can be identified from the extended abstracts of the symposium in Anaheim (DOI: 10.5281/zenodo.2561103), and the most significant of these became clear during the late 1990s, as more of this work was published. Two of these will be featured in this talk because they are the most significant of the many ways the Roberts group influence the work of my group on this system. The first concerns the pathways and mechanism by which zerovalent metals effect dechlorination of aliphatic hydrocarbons. In that case, we had chosen to focus on chloromethanes, thereby avoiding, and therefore missing, the profoundly significant role of reductive beta-elimination in the reaction of chloroethanes and ethenes with zerovalent metals. The second concerns the multiple uses of correlation analysis for interpretation of chemical reactivity data. In this case, we showed that a single structure-activity relationship could adequately describe reduction rate constants for all chlorinated aliphatics, whereas the Roberts group showed that better correlations could be obtained by partitioning the training set of compounds into structural groups. Comparison of these two approaches highlights some general principles of correlation analysis of chemical reactivity, which has become a theme in our subsequent work (e.g., 10.1039/C7EM00053G) and will be described in this presentation.

ENVR 200

Synergistic interaction between black carbon and sulfide in contaminant dehalogenation

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Anthropogenic pollutants, particularly those with halogen substituents, pose significant human health and ecotoxicity concerns due to their continued widespread occurrence in the environment. Many persistent organic pollutants, such as DDT, have accumulated in soils and sediments over the past decades, resulting in legacy sites. More importantly, a large influx of new organohalogenated contaminants continues to enter the environment through field applications, such as dichloroacetamide safeners that are commonly used in herbicide formulations to protect crops from unintended herbicide toxicity. This study will examine the fate of these chemicals in the subsurface environment, where black carbon and sulfide co-exist. Specifically. we demonstrated that graphite powder, a model black carbon, significantly accelerated the transformation of DDT and its metabolites (DDD and DDE), as well as three dichloroacetamide safeners (AD-67, benoxacor, and dichlormid) by sulfide. Chloride was formed for all target contaminants. For dichloroacetamides, an array of sulfursubstituted products was formed, which substantially increased their molecular weight and is anticipated to decrease their mobility in aquatic environments. Three operational reaction pathways might be involved for the accelerated rates of contaminant decay: (1) the electronaccepting capacity of black carbon can oxidize sulfide to elemental sulfur, which can further react with sulfide to form polysulfide, likely accounting for the observed accelerated transformation of dichloroacetamides; (2) the graphitic region of black carbon could shuttle electrons from sulfide to adsorbed DDE; and (3) the formation of surface-bound nucleophile could attach DDT and DDD. This research lays the groundwork for developing an alternative *in-situ*remediation technique for rapidly decontaminating soils and sediments to possibly lower toxic products under environmentally relevant conditions.

ENVR 201

Reduction of N–O containing compounds (NOCs) by soluble and surface complexed Fe(II)

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The release of nitrogen-oxygen containing contaminants (NOCs) into the environment is an important emerging water issue. The nitrogen-oxygen single bond is commonly found in organic contaminants ranging from aromatic N-oxides, hydroxylamines, to isoxazoles. Fell associated with either iron oxides or organic ligands (e.g., tiron) has been widely examined as environmental reductants in reducing organic contaminants. This research combined both experimental and computational approaches to examine the poorly understood reduction kinetics and mechanisms of various NOCs by soluble and surface-associated Fe(II) complexes. Results showed that the NOCs were reduced by both reductants at different rates. Reduction products of NOCs were mainly the deoxygenated or ring-opening analogs. Density functional theory calculations suggested that the elementary reactions, including protonation and N-O bond cleavage, were barrierless or having small energy barriers, indicating that the electron transfer was ratelimiting. Consistent with the theoretical results, the experimental kinetic isotope effects of the reduction of NOCs suggested that protonation was spontaneous, while the electron transfer was rate-limiting. Electrochemical cell experiments that separated complexation from electron transfer revealed that various types of complexes formed between NOCs and the reductant, leading to different reactivity and mechanisms. The electron transfer process was facilitated to different extents depending on the types of complexation. Overall, this project provided a wealth of new mechanistic information on the transformation of NOCs in model aquatic environments.

ENVR 202

What a long, strange trip it's been: Zero valent iron retrospective

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The use of zero valent iron in permeable reactive barriers (PRBs) to accomplish dechlorination of ground-water contaminants burst onto the scene in the early 1990s. It was clear that dechlorination was occurring, but rational design of PRBs languished in the absence of an understanding of reaction pathways and rates. Designs of laboratory studies varied widely as did speculations on reaction mechanisms. Lynn Roberts' group was one of a few to present a comprehensive framework for dechlorination pathways and mechanisms. This framework, coupled with experimental measurements of loss of parent chlorinated organics and production of a range of chlorinated and unchlorinated daughter products, brought a lucidity to this new field of research and practice. Mechanistic parlance such as "beta-elimination" became almost commonplace. This talk will review the discovery and development of ZVI as a reagent for dechlorination reactions, summarize major accomplish-ments and breakthroughs in mechanistic understanding, and relate this history to current understanding and practice. Chlorinated solvents such as chloroethenes will receive focus as aqueous contaminants. Throughout, the contributions and importance of the Roberts group's work will be emphasized.

ENVR 203

Redox properties of iron-ligand complexes in dissolved organic matter

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Electron donating and accepting capacity (EDC and EAC respectively) in dissolved organic matter (DOM) has long been attributed to guinone moieties that readily facilitate electron transfer in redox reactions. Further, the complexation of iron by organic ligands, such as those present in DOM, can alter the redox potential and reactivity of iron. In this study we assess the role of complexed iron as a component of the overall EDC and EAC of DOM. DOM samples were isolated from a freshwater stream in New Jersev (MacDonald's Branch. Pine Barrens, NJ, USA) with relatively high background total iron concentrations (10's of µM). Both the EDC and EAC of this isolated DOM were measured electrochemically by mediated electrochemical oxidation (MEO) with 2.2'-azino-bis(3-ethylbenzothiazoline-6-sulphonic acid (ABTS) and reduction (MER) with Diquat. Following measurements, DOM was treated with a cation exchange resin to remove complexed iron. Initial results show a decrease in EDC following treatment with the resin, indicating loss of electron donating components (i.e. Fe²⁺) associated with DOM. Removal of the naturally complexed iron from our sample did not, however, affect EAC. Additionally, we will add Fe2+ to various IHSS standard isolates to assess how it alters the electron donating and accepting capacity of DOM. Finally, DOM will also be profiled with multiple electron mediators to evaluate changes in the distribution of reducible moieties within DOM following iron addition.

ENVR 204

Reductive degradation using Mg-based bimetal: Transformation and fate of 2,4-dinitroanisole (DNAN) and nitroguanidine (NQ) in wastewater

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The production of energetic materials produces wastewater-containing residual levels of insensitive munition (IM) formulation constituents such as nitroguanidine (NQ) and 2,4-dinitroanisole (DNAN). Treatment of IMs using zero-valent metal or bimetal technology is well-studied, particularly iron-based treatment such as the use of zero-valent iron (ZVI). However, ZVI is usually effective only under acidic conditions. Mg-based reagents, on the other hand, remain effective without acidic conditions and offer greater reduction potential. In this work, the reductive degradation of pure NQ and DNAN in water by Mg/Cu bimetal was studied. Treatment of NQ produced two parallel reactions: nitroreduction led to aminoguanidine formation, or reduction of the encompassing nitramine group resulted in N-N bond cleavage forming guanidine. Additional byproducts identified were urea, cyanamide, formamide, and dicyandiamide. Experimental evidence on the degradation of NQ byproducts elucidated a complete reaction pathway, along with complete carbon closure from NQ byproducts. Results on conditions controlling reaction selectivity will be discussed. Conversely, treatment of DNAN in a solvent matrix resulted in subsequent nitroreduction: one nitro group was reduced (ortho or para) to form 2-amino-4-nitroanisole or 4-amino-2-nitroanisole (2-ANAN or 4-ANAN), and subsequent reduction of the other nitro group formed 2,4diaminoanisole (DAAN). However, in an aqueous matrix, adsorption to the bimetal was significant. A fraction of DNAN partially reduced to 2-ANAN and adsorbed to the bimetal. Concurrently, DAAN formed in the liquid phase, but in insufficient amounts, i.e. resulting in an open mass balance in the liquid phase. Adsorption to the bimetal increased with oxygenation. Subsequent experiments indicated DAAN was not necessarily the final product from Mg/Cu treatment. In oxygenated systems, DAAN degraded and led to adsorption of DAAN or DAAN transformation products to the bimetal. Complete mass balance and transformation products from DNAN and DAAN degradation will be discussed.

ENVR 205

Enhanced tribromoacetic acid (Br₃AA) degradation using pyrogenic carbonaceous matter (PCM)

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The interaction of natural organic matter and disinfectants such as chlorine and chloramine tend to produce a suite

of toxic chemicals, such as haloacetic acids (HAAs), which are currently under the Stage I and II Disinfectants/Disinfection Byproducts Rule by the United States Environmental Protection Agency (EPA). This study investigated the removal of HAAs using pyrogenic (PCM)-modified carbonaceous matter reductive electrochemical membranes (REMs) to enhance their adsorption. More importantly, we reported for the first time that PCM could accelerate the degradation kinetics of three HAAs, namely Br₃AA, BrCl₂AA, and Br₂CIAA, at pH 7. Detailed characterization of the degradation kinetics of Br₃AA and its subsequent product formation were performed in the absence and presence of our PCM model graphite. Br₃AA followed a pseudo-first order decay with a rate constant (k_{obs}) of (1.92 ± 0.29) × 10⁻³ h⁻¹ ¹ in the absence of graphite, which corresponds to a halflife $(t_{1/2})$ of 360.94 ± 2.39 h at pH 7.1. Graphite powder accelerated the degradation of Br₃AA with a shortened k_{obs} of (8.41 ± 0.70) × 10⁻³ h⁻¹ and $t_{1/2}$ of 82.40 ± 0.99 h. Product characterization indicated a 1-to-1 molar transformation of Br₃AA to CHBr₃, its corresponding trihalomethane. The formation of CHBr₃ suggests that the transformation of Br₃AA involves the decarboxylation pathway, where the deprotonated form of Br₃AA could dissociate into carbon dioxide and CHBr₃. To understand the role of PCM in accelerating the degradation of Br₃AA, the activation energy (E_a) of Br₃AA with and without graphite was quantified by measuring the Br₃AA degradation kinetics from 15°C to 45°C. Our results suggest that graphite significantly lowered the activation energy for the decarboxylation of Br₃AA to CHBr₃ from 25.7 ± 3.2 kcal/mol to 13.6 ± 2.2 kcal/mol, thus enabling the conversion of Br₃AA. These findings improve our understanding of the activity of HAAs with PCM under ambient temperatures and neutral pH, though the specific reactive sites on PCM require further characterization.

ENVR 206

Abiotic reduction of the munitions compounds DNAN and NTO by carbonaceous reductants and carbonrich soils

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Abiotic reduction is an important process that governs the fate of munitions compounds (MCs) in reducing environments and represents a potential approach to remediate MC-contaminated soil and groundwater. Organic carbon in soils contains redox-active functional groups that can behave like rechargeable electron reservoirs which, when reduced, can react with MCs. To understand the kinetics and mechanism of MC transformation by carbonaceous reductants, we

the reactivity of dithionite-reduced investigated anthraquinone-2,6-disulfonate (AQDS, a model quinone and surrogate of dissolved organic carbon), Leonardite humic acid (LHA), and two carbon-rich soils, Pocomoke and Rhydtalog, toward 3-nitro-1,2,4-triazol-5-one (NTO) and 2,4-dinitroanisole (DNAN), insensitive munitions constituents in the IMX-101 and IMX-104 formulations. NTO was reduced to 3-amino-1,2,4-triazol-5-one (ATO), and DNAN was reduced to 2,4-diaminoansiole (DAAN) through 2-amino-4-nitroanisole as the predominant intermediate. DAAN formation was transient, particularly in the presence of LHA, presumably due to further transformation. LHA exhibited measurable reactivity toward NTO and DNAN only when reduced above a threshold percent of its electron storage capacity (ESC), beyond which the reduction rates and extents of both MCs increased with LHA electron content. The reaction rates generally increased with pH, presumably due to the speciation of NTO and hydroguinone functional groups. The pseudo-first-order rate constant for NTO varied by ~2 orders of magnitude from pH 2 to 9.5 and increased by about 3 orders of magnitude for DNAN between pH 6 and 8.5. While the rates of MCs transformation increased with the extent of Pocomoke and Rhydtalog reduction (i.e., chemical enhancement), the mass balances worsen indicative of side reactions between reduced species in soils and the MCs. This study illustrates the reactivity and potentially important role of soil organic carbon in influencing the natural and enhanced attenuation of NTO and DNAN in munitions constituent-impacted sites.

ENVR 207

Modeling the reduction of nitroaromatics by humic acid using quantum chemically computed energies of reduction and oxidation half-reactions and quinone functional groups

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Nitroaromatic compounds (NACs) are common munition constituents that contaminate military sites and require extensive remediation efforts. For this reason, it would be desirable to develop models that can predict the kinetics of NAC reduction in the subsurface. Humic acid (HA) comprises a sizeable portion of the redox-active media in the subsurface and is therefore a critical reductant for building a predictive model for NAC reduction kinetics. Such a model would require the inclusion of the energies associated with both the reduction of the NACs and the oxidation of the HA. The heterogeneous and unknown structure of HA, however, has previously prohibited reliable determination of such oxidation energies. To overcome this limitation, the redox moieties of soil humic acid were modeled as a collection of quinones of varying

redox potentials. The reduction and oxidation energies of the NACs and hydroquinones, respectively, were then calculated quantum-chemically via a hydrogen atom transfer (HAT) mechanism. These are used in a recently developed linear free energy relationship (LFER) to predict second order rate constants. Furthermore, a relationship between the calculated oxidation energies and their respective standard reduction potentials of the quinones allows for the inclusion of hypothetical quinone functional groups that better represent the different redox moieties of the HA. To evaluate the validity of the model, the energetics and the concentrations of the guinone-like groups were fit to experimental HA reduction profiles, which characterize the potential as a function of the electron content of the humic acid. This was done concurrently with fits to the NAC reduction profile at various extents of HA reduction. Global fits were then performed across multiple NACs as a final determination of the energetics and distribution of the guinone-like groups in HA. The results indicate a potential solution for predicting the timescales of NAC reduction under realistic environmental conditions.

ENVR 208

Raman tweezers for small microplastics and nanoplastics identification in seawater

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Our understanding of the fate and distribution of microand nanoplastics in the marine environment is limited by the intrinsic difficulties of the techniques currently used for the detection, guantification, and chemical identification of small particles in liquid (light scattering, vibrational spectroscopies, and optical and electron microscopies). Here we introduce Raman Tweezers (RTs), namely optical tweezers combined with Raman spectroscopy, as an analytical tool for the study of micro- and nanoplastics in seawater. We show optical trapping and chemical identification of sub-20 µm plastics, down to the 50 nm range. Analysis at the single particle level allows us to unambiguously discriminate plastics from organic matter and mineral sediments, overcoming the capacities of standard Raman spectroscopy in liquid, intrinsically limited to ensemble measurements. Being a microscopy technique, RTs also permits one to assess the size and shapes of particles (beads, fragments, and fibers), with spatial resolution only limited by diffraction. Applications are shown on both model particles and naturally aged environmental samples, made of common plastic pollutants, including polyethylene, polypropylene, nylon, and polystyrene, also in the presence of a thin ecocorona. Coupled to suitable extraction and concentration

protocols, RTs have the potential to strongly impact future research on micro and nanoplastics environmental pollution and enable the understanding of the fragmentation processes on a multiscale level of aged polymers.

ENVR 209

Quantifying nanoplastic heterogeneity

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Colloidal nanoparticles are at the vanguard of commercial nanotechnology, while environmental contaminants ranging from nanoparticle products to nanoplastic byproducts are of grave concern. Quantifying the heterogeneous structures and properties of nanoparticles is fundamental both to optimizing product quality and to understanding byproduct dangers, but such measurements remain impractical. To solve this problem, we present a new measurement system which advances and integrates complex nanofluidic replicas, localization optical microscopy, and Bayesian statistical analysis. Our method enables dimensional and optical metrology of single nanoparticles with record precision, accuracy, and efficiency. We apply our system to measure polystyrene nanoparticles which sorb and carry hydrophobic fluorophores, quantifying the size distribution to within a few nanometers and revealing that fluorescence emissivity is heterogeneous far beyond current understanding. This elucidates a fundamental structureproperty relationship of probes and fiducials of primary importance in fluorescence microscopy and model nanoplastics of utmost concern as sorbents and carriers of toxic fluorophores. Our work informs the application of model nanoplastics and enables the characterization of environmental nanoplastics, which can be only more heterogeneous and less understood than laboratory standards for calibration and comparison.

ENVR 210

Detection and analysis of microplastics using Raman spectroscopy

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There is a rapidly growing interest in applying micro Raman spectroscopy to environmentally collected microplastics. The diversity of samples and collection points has made it difficult to have a consensus for a

standard sample preparation or analysis method. We propose and discuss a method for microplastic sample preparation, and the advances in Raman microscope instrumentation and analysis software that aids in the detection and identification of microplastics collected from bottled water samples. Raman spectroscopy (RS) is a non-invasive and non-destructive tool that can identify many polymer sample types. Raman spectroscopy becomes an important identification method as other characterization techniques struggle with microplastic particles smaller than 20 um. New research is suggesting that the majority of microplastics in drinking water are less than 5 um in size. A confocal Raman microscope system has an advantage in the identification of smaller particles and is applicable to sizes less than 1 um. The confocal Raman microscope is an ideal, fast, non-destructive characterization method of these small microplastic particles. Three methods are evaluated for identifying and isolating microplastics with good contrast on the filter substrates: white light imaging, Rayleigh mapping, and fast Raman imaging mapping using StreamLine. Renishaw's Particle Analysis Software is used in each contrast method to characterize the particle sizes, morphology, distribution, and to define the particle coordinate positions necessary for more detailed measurements. High resolution spectra of the microplastics are measured and compared to library spectra for the identification of the plastic type. LiveTrack allows analysis with automatic focusing on microplastic particles of differing heights with no loss in signal intensity. A suggested workflow for sample preparation, data collection, and sample analysis of microplastic samples is discussed.

ENVR 211

Methods to detect microplastics and nanoplastics in human tissue

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Multiple pathways have been established for exposure of humans to microplastics and nanoplastics but data on the burden of plastics in human tissues are still scarce. Studies on wildlife and animal models furthermore have established negative health effects resulting from macromicro-, and nanoplastic exposure, including linkages to infertility, onset of inflammation, and the development of

cancer. Exposure of mice to microplastics was documented to result in an accumulation of the foreign objects in diverse tissues but similar studies on human tissues and organs are still lacking. In order to advance the human exposure assessment for plastic pollutants, we created a workflow for the processing of human tissue for subsequent analysis using µ-Raman spectrometry. The resultant method was applied to different human tissue and organ types obtained from a large sample repository of brain and body tissues established for the study of neurodegenerative diseases. Method performance was evaluated in terms of recovery rates and detection limits as a function of plastic particle dimensions and tissue types. The study is among the first to establish the environmental background of plastic exposure detectable as a organ- and tissue-specific body burden in adult humans. The methodology may find future applications in the routine analysis of human biopsy and autopsy specimens for the determination of nanoplastic and microplastic exposure.

ENVR 212

Metrological framework supporting the characterization of nanoplastics

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The cumulative impact of nanoplastics on the environment-predominantly from fragmentation of plastic waste and possibly from consumer products-has become a major concern in recent years. Due to their small size and inherently diverse physical-chemical properties, detection and characterization of nanoplastics are challenging. Adaptation of analytical techniques established for size measurement of engineered nanoparticles, like dynamic light scattering (DLS), is often a feasible option for nanoplastics. For the development of new analytical techniques however and for toxicology studies, the need for model particle systems is pressing. This presentation articulates some of these challenges for nanoparticle sizing and standardization from the perspective of dimensional metrology, and proposes improvements to DLS data interpretation and analysis procedures relevant for the characterization of nanoplastics. Toward the development of realistic reference nanoplastics, we present an innovative emulsion polymerization method for the synthesis of highquality polystyrene spheres in the 100 nm to 300 nm diameter range. With the use of complex surfactant systems, we are able to control the width of the particle size distribution from highly monodisperse to polydisperse. These polystyrene spheres could then be readily functionalized for specialized applications in environmental investigations.

ENVR 213

Novel approach to Infrared spectroscopy and imaging for the routine characterization of microplastics in environmental samples

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When reading both scientific literature and general media today, it is abundantly clear the level of interest there is in microplastics in the Environment. While a recent WHO study identified there was insufficient information to conclude on the health impacts, more and more research is demonstrating the widespread nature of these plastics. While one branch of science will continue to work to determine the potential impacts of microplastics in the environment and the food chain, another branch will continue to work to understand the spread and sources of these. As this area of research expands and with the potential for it to move into a routine testing application, there is a clear need for faster and more robust testing methods. There is also a need to develop testing methods that provide rich information on the plastics present. It is no longer enough to simply give total particle counts or total mass of polymers present. To better understand this topic, researches need information on the size and shape of particles present in addition to the plastic-type. Vibrational spectroscopy is a useful technique and when combined with microscopy, it can be employed to explore particles down to the lowest micron level. FTIR and Raman microscopy has become the mainstay of most microplastics investigations and while they certainly have their advantages, they also have limitations that preclude them from providing the robust tool required for more investigations. Infrared large-scale spectroscopy combined with a bright coherent laser light source can overcome many of the limitations of these traditional techniques. The bright laser with a coherent beam allows all the light to be focused onto the smallest particles facilitating very rapid analysis without the fluorescence and sample damage issues of Raman spectroscopy and the huge data files needed for FTIR analysis. In this paper, we present results of studies several studies using an Infrared spectrometer utilizing a Quantum Cascade Laser for the characterization and quantitation of microplastics and we discuss the role this technology may have in the development of standardized methods for rapid and routine analysis of microplastics in various environmental samples.

Transition size in polymer fragmentation processes may slow down nanoplastics production in the environment

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The influence of the initial size on the fragmentation kinetics of polymers based on experimental results has not been deeply investigated so far. In this work, the fragmentation kinetics during photodegradation of polyethylene (PE) microplastics in abiotic water were investigated and compared to the fragmentation of macroscopic PE films with a surface of several square centimeters. In both cases, the weathering was performed in situ to avoid any contamination and the focus was on the detection of colloidal fragments, i.e. with sizes less than 1 µm. The chemical modifications associated with weathering and ageing were measured for the films using infra red and Raman spectroscopy. The results showed that colloidal PE particles do not fragment in smaller particles during weathering. However, during the same time of exposition, the macroscopic PE film was fragmented with the smallest fragments having a size of around 200 µm. No colloidal plastics could be detected in the water despite the fact that chemical oxidation of the film and modification of its crystallinity were found to have occurred during weathering. Once the water was dried, a few particles were detected that had the spectral signature of aged PE, but it is not clear in what form this PE was present in the water before drying (particles vs aggregation of short polymer chains). These results confirm that the fragmentation from macro to microplastics for a PE film exposed to photodegradation is quite rapid whereas, at the conditions of this study (no strong mechanical abrasion during weathering, abiotic conditions), PE nanoplastics were not formed in significant quantities implying that they are not produced or only at a rate slower than investigated here. Surfaceablation appeared also to be very limited. Nevertheless, such processes could be more important in natural environments through the presence of microorganisms at the surface or of abrasives. Bulk fragmentation did take place at larger length scales but the fact that micrometric PE particles did not exhibit any size decrease over more than 40 weeks of photodegradation suggests that the existence of a size limit below which the rate fragmentation of plastics would strongly decrease should be considered. The factors that may influence this size limit should be further investigated.

ENVR 215

Extraction, concentration, and quantification of nanoplastics using functionalized magnetic nanoparticles

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Significant knowledge gaps exist regarding the sources, transport, distribution and effects of microplastic pollution (plastic particles <5 mm) in the environment. Even less is known regarding nanoplastic pollution (generally considered to be plastic particles <1 µm). Due to their small size, nanoplastics pose unique challenges and potential risks. Yet, data on the extent of nanoplastic pollution is limited due to a lack of rigorous methods specifically designed to assess and quantify nanoplastics, which necessitate unique sample preparation and analytical considerations. The aim of this research is to develop and refine methods to selectively extract, concentrate, and quantify nanoplastic particles in environmental samples. Adapting a previously reported approach, testing is underway of an extraction and concentration technique which utilizes functionalized magnetic nanoparticles (FeNPs) that hydrophobically attach to nanoplastic particles, followed by a magnetic flow-cell system to separate and concentrate the particle aggregates. То quantify extraction efficiencies. polystyrene nanoplastic particles with a palladium-doped polv(acrvlonitrile) core (Pd-PAN@PS) are being used as model nanoplastic particles, thus enabling the use of ICP-MS to precisely measure nanoplastic recoveries. Batch experiments will evaluate adsorption kinetics and attachment of the functionalized FeNPs to the model nanoplastic particles under varying aquatic conditions that mimic relevant sample media, initially focusing on freshwater and marine environments. To separate the extracted nanoplastic particles from the FeNPs, enabling their subsequent characterization and guantification, a variety of sample clean-up methods will be assessed. These include the use of surfactants and longduration/low-concentration digestions to remove the FeNPs and tangential-flow filtration to recover and concentrate the extracted nanoplastic particles. Once refined, this overall method will be a component in a broader sample preparation scheme that first removes non-target bio- and geogenic colloids in actual environmental samples before isolating any nanoplastic particles that may be present. It is envisioned that this broader approach can be used to provide initial estimates

on the quantity and extent of nanoplastics in the environment.

ENVR 216

Development of active sampling technique for the analysis of atmospheric microplastics

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The recent discovery of microplastics in remote regions including the headwaters of rivers and remote mountain regions where there is minimal human influence has raised the question of the importance of atmospheric transport on the dissemination of microplastics. A number of recent studies have used passive sampling techniques, such as rain collectors, to quantify the deposition of microplastics at a given site. These techniques provide valuable insight into the influence of atmospheric deposition at the site. The deposition techniques, however, takes a long time to obtain a sample (weeks to months) and the does not provide atmospheric concentration. To improve temporal resolution and better understand sources of atmospheric microplastics we are working on developing an active sampling technique to sample whole air masses by pulling air through filters rather than simple passive deposition techniques. We have recently tested many variable to produce the best technique and will discuss the effect of different samplers, sample flow rates, and filter material has on sampling atmospheric microplastics. In addition, techniques to process samples and analyze samples using Raman microscopy, FTIR microscopy, and fluorescence using Nile red staining will be presented.

ENVR 217

Withdrawn

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Withdrawn

ENVR 219

Pulsed electric field (PEF) device: Design, performance and deployment in an elderly home for tap water disinfection

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The most common way of municipal water disinfection, i.e., chlorination, is now deemed inadequate given the emergence and spread of antibiotic-resistant bacteria. Reports about chlorine-induced antibiotic resistance and how chlorination increases the concentrations of antibiotic resistance genes in water, show the critical need for more innovative disinfection systems. This work addresses this concern through the development of a water disinfection device that utilizes pulsed electric field (PEF) to initiate cell permeability and irreversible electroporation on bacterium cell membrane that leads to cell death. The disinfection mechanism does not induce adaptation effects as it preserves the cell's nuclease activity or the provision of enzymes that will degrade the DNA. It then prevents the spread of resistance plasmids from antibiotic-resistant bacteria. The PEF device is composed of micro-engineered electrodes and a low voltage circuit which can either be battery-operated or plugged to a socket. Laboratory studies show that the PEF device can deliver as high as 2 log reduction against common gramnegative bacteria found in water (i.e. Escherichia Coli K12) in less than 1 minute of treatment. Prototypes were installed in the pantry faucets of a local elderly home. Field test results show that the bacteria present in the untreated tap water are mostly gram-negative nonlactose fermenting bacteria and that the current prototype can significantly decrease the tap water's bacterial concentration.

ENVR 220

Evaluation of persistent, bioaccumulative, toxic chemicals under the Frank R. Lautenberg Chemical Safety for the 21st Century Act

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Under the Frank R. Lautenberg Chemical Safety for the 21st Century Act, the Environmental Protection Agency (EPA) is required to make an affirmative determination on the safety of all new chemicals. Under this new law, there is particular interest in chemicals that are Persistent, Bioaccumulative, and Toxic (PBT), as these can pose significant risks to human health through the environment. Because of the hazards PBT chemicals can pose in surface water, identifying and regulating PBT chemicals has become a prominent focus under the new law, and the EPA continues to strive for accurate and pertinent chemical review of these new chemicals to ensure the safety of the environment and general population while allowing for continued chemical innovation.

Mapping the antibiotic footprint in Minnesota

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Antimicrobial resistance is considered to be one of the greatest global public health threats of the 21st century. The discharge of antibiotics into the environment may increase antimicrobial resistance as well as disrupt proper ecosystem functioning. Thus, evaluating the antibiotics present in Minnesota's environment as well as contributing factors to their presence in their environment will provide invaluable information for improving water quality and protecting human and ecosystem health. This goal is being accomplished through sampling water and sediment at field sites across Minnesota variably impacted by human and animal husbandry activity. Twenty-five antibiotics from various therapeutic classes used in both human and veterinary medicine have been quantified using liquid chromatography-tandem mass spectrometry to determine trends. Preliminary results indicate that antibiotics primarily used in animals are primarily found in sites impacted by animals while the same holds true for human antibiotics. As a general rule, the total quantity of antibiotics increased sampling points upstream of the wastewater effluent outfalls to those downstream. In total, tetracycline, doxycycline, oxytetracycline, and sulfadimethoxine were found most often. The results are being used to develop a geospatial model of antibiotic and antibiotic resistance in Minnesota's environment.

ENVR 222

Synthetic dithiols and superparamagnetic nanoparticles: Purification of contaminated heavy metal water

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A series of sulfhydryl compounds (L= AB9, MB9, EB9) was synthesized with the concern of discovering reagents with excellent accessibility, long term stability, and to bind targeted heavy metals (M= Cd, Hg, Pb, As). These ligands derivative from B9= 1,3-benzenediamidoethanethiol (Figure 1a); a compound irreversibly precipitates heavy metals (Figure 1b). New sulfhydryl compounds provide different inductive effects towards the thiol (SH), and multiple, concerted, bonding sites used in sequestration of heavy metal contaminants through strong S-M covalent bonds formation. Promising

advantages of these L-M compounds include their colorlessness, odorless nature, complete metal removal via immediate precipitation formation, and leaching resistivity over a wide pH range. Furthermore, thiol coupled magnetic nanoparticles (MNPs) were used in the removal of arsenite from water. The MNPs coated with the amine-functionalized silica surface, coupled to AB9= 2,2'-(isophthaloybis(azanaediyl))bis-3-mercaptopropanoic acid; (sulfhydryl compound with pendant carboxylate groups) used as the composite, Fe₃O₄-SiO₂-linker-AB9 (AB-MNP). Complete arsenic removal was achieved with As(III) solutions of 200, 500, and 1000 ppb resulting in detectable arsenic dropped to below 10 ppb. This single solid-composite immobilize As(III) by forming strong covalent As-S bonds producing "proposed" structure As(III)-AB9@MNP (Figure 2). The components of this new composite material are made from non-toxic, earthabundant elements, and rapid magnetic separation allows them to be used as an effective, affordable means of providing arsenic-free drinking water to at-risk populations around the world.



(a) B9, (b) B9-Hg structure



The proposed structure of As(III)-AB9@MNP

ENVR 223

Emerging environmental contaminants in water in Chennai, India: Comprehensive study on fate & occurrence

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The presence of pharmaceuticals, hormones, pesticides, perfluorinated compounds and industrial contaminants in wastewater has been well-documented in the USA, Europe, and many developed regions in the world over the last two decades. However, information on occurrence and fate is still lacking from many parts in India which is the second most populous country in the world. The goal of this study was to detect for the presence and concentration of twenty two emerging organic contaminants (EOCs) at 3 different wastewater treatment plants in Chennai which is one of the most densely populated regions in South India. The treatment plants selected were different in size and treatment capacity to mimic more urban and domestic settings. Three different sampling campaigns at different seasons were conducted at different locations in the wastewater treatment plants including the influent, primary, secondary and final effluent. The wastewater data indicated 11 EOCs were detected in every sample from every location at all sites, while only 5 EOCs were detected consistently in effluent samples. The effluent composition of the 22 EOCs were similar within the three WWTPs but quite different to those seen in the US, indicating the importance of region-specific monitoring. Diurnal trends indicated that variability is compound specific but trended within certain classes of compounds (artificial sweeteners, and pharmaceuticals). We also studied the treatment efficacy of the wastewater treatment plants for these emerging contaminants. Finally, 22 surface water sites upstream and downstream of the WWTPs were evaluated for presence of these EOCs to determine their fate and exposure to the population in the area.

ENVR 224

Analysis of dissolved organic matter and contaminants of emerging concern to detect leaking sewers in urban streams

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Sanitary sewer overflows (SSOs) are common in urban areas due to aging infrastructure. SSOs can introduce wastewater contaminants directly to urban watersheds, threatening public health and ecological systems. With approximately 550,000 residents, the Gwynns Falls and Jones Falls watersheds cover the western and central

areas of Baltimore City. The Baltimore City Department of Public Works tracks SSOs in these watersheds: however. the impacts of SSOs and other unidentified sewer leaks on urban streams are not well understood. We propose that characterization of dissolved organic matter (DOM) and measurement of contaminants of emerging concern (CECs) in urban streams can be used to locate leaking sewers. The objective of this work was to investigate DOM fluorescence signatures and CEC concentrations in urban streams and assess the potential input of raw wastewater. DOM was analyzed in water samples collected each month from 27 sites in these streams from March to December 2019. Absorbance spectra and fluorescence excitation-emission matrices (EEMs) were used to understand changes in DOM composition across the watersheds, and a parallel factor analysis (PARAFAC) was conducted with the 270 EEMs to identify fluorescent components. CECs were measured in water samples from four sites, including one urban and one suburban from each watershed, for July to December 2019. The investigated CECs included antibiotics, hormones, sucralose, and UV-filters. Sucralose, oxybenzone, and octocrylene were detected at concentrations as high as 417, 116, and 48 ng L⁻¹, respectively, and the highest concentrations occurred at urban sites in the Gwynns Falls. The EEM-PARAFAC component scores and regional volumes (e.g., tyrosine, tryptophan, fulvic acid, soluble microbial product, and humic acid likefluorescence) were compared to CEC concentrations and SSO data. Overall, this work will combine municipal data on SSOs with spatiotemporal analysis of DOM and CECs to improve identification of leaking sewers and their effects on urban streams.

ENVR 225

Modeling chromate removal using type 1 quaternary amine anion exchangers in drinking water applications

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Chromates have wide applications in the industry as corrosion inhibitors and oxidizing agents in various reactions. Unfortunately, they are carcinogenic at low concentrations. The chromates can be removed by quaternary amine anion exchangers. Using a series of collected data from literature, a dynamic Thomas isotherm was used to model and subsequently predict the effect of contact time, initial capacity, and anion exchange characteristics on the performance of the resin system. The parameters of the model were derived via a nonlinear programming algorithm where the objective function was the minimization of the least square errors between experimental and predicted values. The resulting model was used to predict the performance by instituting a major increase in chromate concentration up to 200 ppb. This demonstrated that the Thomas model can be used to accurately predict the resin performance in chromate removal even in the presence of competing ions like chlorides and sulfates.

ENVR 226

Withdrawn

ENVR 227

Urban stormwater chemistry: Quality characterization and recommendation for synthetic stormwater

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Increases in urbanization has led to excess stormwater production and mobilization of numerous pollutants from urban watersheds. Discharge of these pollutants leads to contamination of receiving water bodies. Chemical characterization of urban stormwater is necessary to gain deeper insights into the ecological impacts of urban runoff and to factors that influence possible treatment technologies. This project collected stormwater event mean concentration and particle size fraction data from field studies from peer-reviewed literature and national/international stormwater quality databases. A comprehensive characterization of urban runoff pollutants, including dissolved and particulate-bound, and their partitioning and speciation behavior. Solids, nutrients, metals, various organic pollutants, and pathogens (indicators) were evaluated. Due to limited data, metals evaluation is limited to Zn, Cu, Pb, Fe and Cr. A significant fraction of phosphorous, metals and organics are particle-bound. Metal speciation results demonstrated divalent ions (Zn, Cu and Pb) present predominantly as dissolved organic matter complexes, and trivalent ions (Fe and Cr) forming hydroxide complexes. Land use and EPA rain zones influenced the concentrations of many water quality constituents, while seasonal variation did not show high statistical significance. Further, as an outcome of our data analysis. a recommendation for synthetic stormwater is offered that can adequately represent field conditions in a lab setting to enable accurate and realistic results for use in lab-scale treatment research, to better scale up from lab to field. The urban stormwater recipe will account for particulatebound pollutants, incorporating different size fractions to accurately mimic urban stormwater.

ENVR 228

Raised versus inverted: Significance of bioretention underdrain configuration on denitrification in stormwater

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Bioretention basins are widely used to retain and treat stormwater runoff but field sites demonstrate variable performance with regards to total nitrogen (TN) removal. Bioretention design can include an underdrain to maintain an internal water storage layer (IWS), promote denitrification, and achieve TN reduction. However, the effect of underdrain configuration (e.g., raised vs. inverted) on solute mixing and N dynamics remains a knowledge gap. We employed computational modeling, 2-D laboratory column studies, and limited field monitoring to evaluate how underdrain height can improve hydraulic mixing and nitrate dynamics. VS2D modeling results demonstrate that mean hydraulic residence time (HRT) within an IWS layer can vary by 14% among different underdrain configurations and an elevated underdrain is more effective in enhancing IWS mixing. Longer HRTs are associated with higher denitrification rates; thus, underdrain height can improve system performance. 2-D laboratory columns with varying underdrain configurations evaluate mixina and denitrification under both steady state and intermittent storm conditions. Dual tracers were used as analogues to assess mixing between "fresh" and "old" stormwater. Additionally, IWS storage sample ports located at various heights and lateral distances enabled characterization of spatial and temporal water quality trends. Lastly, field data collected from two urban field sites with and without an underdrain in Philadelphia are compared to column results. Our field site without an IWS laver demonstrates TN and nitrate increase in filter media compared to influent stormwater runoff and nitrate on average comprised 35% of TN. Preliminary field data from field site with IWS and a raised underdrain show TN outflow concentrations equal to or less than influent runoff and dissolved organic nitrogen (DON) constitutes more than 80% of TN. Improved understanding of how hydraulic design choices impact bioretention TN removal is critical to achieving stormwater treatment objectives and advancing the sustainability of green-stormwater infrastructure.

Hydrologic and biogeochemical controls on seasonal soil nutrient dynamics in urban green spaces

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Humans dominate urban nutrient cycles – adding nitrogen (N) and phosphorus (P) through car exhaust, fertilizer over-use, and pet waste. N and P are transported to streams via stormwater runoff, where they ultimately create eutrophic conditions and reduced water quality. A leading tool to enhance urban watershed nutrient retention and to improve water quality is green stormwater infrastructure (GSI). GSI employs filtration, plant uptake, and biogeochemical processes to retain nutrients. These processes are highly variable, due to the influence of varying environmental conditions such as temperature, soil oxygen availability, and soil moisture as driven by rainfall duration and frequency. In order to better understand this variability and its implications for GSI performance, this work studies the seasonal variation in mobile nutrients and corresponding hydrologic and biogeochemical conditions in GSI soils. Over a 6-month period, ion exchange resins were used to capture the seasonality of soil nutrient availability. In addition, soil temperature, soil moisture, soil oxygen, and precipitation were monitored. Sites included a green roof, upland and lowland plots in a constructed wetland, and an urban garden. Across all sites, oxygen availability was lowest in the most frequently saturated soils. Further, increased precipitation, soil moisture, and temperature were associated with increased mobile nitrate. In contrast, mobile ammonium and phosphate had little to no response to precipitation, soil moisture, or temperature. These patterns indicate varying roles of hydrologic and biogeochemical drivers for N and P mobility in GSI. The observed relationships between environmental drivers and the quantity of mobile nutrients provide a better understanding of what biogeochemical process may be dominant in GSI systems under varying environmental conditions. This information can be used to better understand how GSI systems will perform as biogeochemical conditions change with the impacts of land use and climate change.

ENVR 230

Evaluating the efficacy of MnO₂ impregnated polypropylene fiber as a sorbent material to treat urban stormwater runoff

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Catch basin inserts are runoff-filters designed to be installed under an individual sewer grate with the goal of filtering particles and dissolved pollutants (e.g., nutrients and metals) from stormwater before entering a sewer system. Catch basin inserts usually consist of a sediment trap to remove particles, followed by various sorption media filters designed for various pollutants. Although catch basin inserts have been used widely as sediment traps near construction sites, they have not received a lot of attention as a potential pre-treatment step before introducing polluted stormwater into various green stormwater infrastructure (GSI). In this study, we are using the MnO₂ impregnated polypropylene fibers as the sorbent material to test its efficacy in treating various urban stormwater pollutants. Runoff water samples were collected and the concentrations of the potential contaminants were evaluated. Chemical sorption kinetics evaluated by conducting batch sorption were experiments. Various amounts of the sorbent material were added to 50 ml centrifuge tubes containing synthetic runoff and measured for concentration over time. The dosage of the sorbent material was varied in batch experiments for a better understanding of the sorption process. Different models (e.g., Freundlich, Langmuir, Temkin) were used to interpret the kinetics of the sorption process. The effect of temperature on adsorption kinetics was also evaluated. All measurements were in duplicate to reduce error.

ENVR 231

Decision framework for biochar selection to remove PCBs, PAHs, Cu and Zn from stormwater

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Stormwater is an important contributor of contaminants of concern (COCs) such as polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), Cu, and Zn to receiving water bodies. Although a fraction of these COCs bind to stormwater particulate matter, which can be removed through filtration by traditional media in stormwater control measures, the dissolved portion of COCs requires special attention, such as engineered treatment measures and media. Biochar is a highly porous sorbent produced from a variety of organic materials. It is gaining increasing attention as a stormwater geomedium due to its high potential for adsorption and simultaneously relatively low cost compared to activated carbon. However, biochar is not a uniform product and selection of an appropriate biochar for removal of specific contaminants can be a complex process. Biochars are synthesized from various feed

stocks and using different manufacturing methods (i.e., pyrolysis temperature and surface treatment) that can significantly affect biochar properties. These properties can affect the capacity of biochar to remove stormwater contaminants. The local availability of biochar products is another important consideration for the application of biochar in stormwater bioretention cells. To address these issues, we developed a decision framework to select readily available biochars based on criteria obtained from in depth literature survey to identify promising candidates for future laboratory and field testing. As an example, plant-derived biochars contain less nutrient and potential contaminants (such as heavy metals and micropollutants) than sludge and manure based biochars. This can affect the biochar capacity to remove or release nutrients in stormwater. Therefore, the sludge/manure based biochars are not suitable for stormwater treatment. Pyrolysis temperature is considered as the most significant parameter affecting the adsorption of contaminants. Increase in pyrolysis temperature favors ash content, microporous structure, fixed carbon content, pH, and surface area. Generally, biochar produced at low pyrolysis temperature (<400°C) is suitable for the adsorption of inorganic contaminants whereas, relatively high pyrolysis temperature (>700°C) enhances the adsorption of organic contaminants. Information about these basic characteristics have been applied to select suitable biochars for further laboratory experiments.

ENVR 232

Using rainfall measures to evaluate hydrologic performance of green infrastructure systems under climate change

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Green stormwater infrastructure (GSI) is increasingly used in urban areas to mitigate stormwater runoff and combined sewer overflows. However, as climate change continues to alter precipitation patterns in many areas, these installations may fail to perform as expected, with more stormwater discharged to sewers over time. To prepare for and adapt to these changes, city and regional stakeholders will be required to track GSI performance. This could be done using on-site sensors or hydrologic simulations; however, to understand GSI performance across an urban catchment, these site specific techniques may not be feasible. As an alternative approach, we propose that changes in GSI performance could be detected by monitoring annual rainfall measures. like the maximum daily rainfall each year. Correlations were established between annual rainfall measures and specific performance metrics, like the frequency of runoff discharged to the sewer, to estimate annual GSI

performance in seventeen cities across the U.S. Findings suggest that tracking rainfall measures can provide insight into the hydrologic performance of green infrastructure; however, the specific rainfall index used to track performance varies by location because the strength of correlations changes depending on regional rainfall patterns. Performance prediction accuracy was evaluated for the period 2020 to 2060 in two cities, Pittsburgh and Memphis. First, changes in hydrologic performance were estimated based on changes in rainfall from regional climate models and then these predictions were verified by simulating GSI system performance using the same regional climate models as input. The percent of rainfall captured by the system decreased significantly under both future climate scenarios and in both cities. Rainfall measures were able to predict the direction of this change in performance, as well as, the magnitude of change within 25 to 50% change, for the four performance metrics evaluated.

ENVR 233

Elevated levels of pathogenic indicator bacteria and antibiotic resistance genes after hurricane Harvey's Flooding in Houston

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Urban flooding can dramatically affect the local microbial landscape and increase the risk of waterborne infection in flooded areas. Hurricane Harvey, the most destructive hurricane since Katrina in 2005, damaged more than 100000 homes in Houston and flooded numerous wastewater treatment plants. Here we surveyed microbial communities in floodwater inside and outside residences, bayou water, and residual bayou sediment collected immediately postflood. Levels of Escherichia coli, a fecal indicator organism, were elevated in bayou water samples as compared to historical levels, as were relative abundances of key indicator genes of anthropogenic sources of antibiotic resistance (sul1/16S rRNA and int/1/16S rRNA) based on 6 month postflood monitorina. Quantitative polymerase chain reaction measurements showed that gene markers corresponding to putative pathogenic bacteria were more abundant in indoor floodwater than in street floodwater and bayou water. Higher abundances of 16S rRNA and sul1 genes were also observed in indoor stagnant waters. Sediments mobilized by floodwater exhibited an increased abundance of putative pathogens postflood in both residential areas and public parks. Overall, this study demonstrates that extreme flooding can increase the level of exposure to pathogens and associated risks.

Development of a parsimonious model for nitrate removal in woodchip bioreactors under dynamic hydrologic and temperature conditions

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Denitrifying woodchip bioreactors (DNBs) are appealing passive technologies for mitigating excess nitrate loads from stormwater, agricultural runoff, and decentralized wastewater treatment to prevent eutrophication downstream. DNBs utilize a woodchip supported biofilm community to reduce influent nitrate via denitrification and typically discharge treated water into nearby surface waters. Nitrate removal efficiency is primarily a function of hydraulic retention time (HRT) and temperature, both of which are dependent on local climate in passive DNBs. To better understand the seasonal performance of minimally managed reactors, we developed а mathematical model to predict nitrate removal over the course of a year utilizing water level and temperature data from a field scale reactor in central New York State. The reactor experiences cold winter temperatures, with a mean air temperature of -3°C between December and February. Water level in the outlet control structure was used to determine volumetric flow rates and HRT for timediscretized parcels of water. A simplified Arrhenius equation was used to estimate the temperature dependent zero-order reaction rate constant for the microbial community using a coefficient determined with laboratory batch experiments. A two-year dataset of longitudinal profiles of dissolved nitrogen species (nitrate, nitrite, and nitrous oxide) will be used to evaluate model performance and explore the impacts of hydrologic and/or temperature variability on the accumulation of the areenhouse gas nitrous oxide within bioreactors. Finally, we will use climate change scenarios to generate synthetic discharge and temperature datasets to assess impacts of hydroclimatic change (warmer winter temperatures and less frequent but more intense precipitation) on seasonal bioreactor performance.

ENVR 235

Bonechar as a potential sorbent for enhanced metal removal in green stormwater infrastucture

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Controlling stormwater runoff from impervious surfaces in urban areas such as Detroit, MI presents two main challenges: (1) handling a large volume of water in a short period of time and (2) removing contaminants. The solution in the early 1900's was to combine stormwater and sanitary wastewater in an underground network to be treated in a centralized treatment plant. Although Detroit has one of the largest wastewater treatment plants in the United States, large storm events can cause untreated sewage to be discharged to nearby water bodies in events known as combined sewer overflows (CSOs). As many abandoned structures in Detroit are demolished and replaced with vacant lots, Detroit has revisited the possibility for a more sustainable approach to stormwater management with the introduction of many tools such as raingardens, bioswales, and rain barrel storage. Bioswales are being constructed all over the city in an attempt to increase infiltration while providing a place to concentrate and/or remove suspended materials (e.g., silt, dirt) and pollution (e.g., automotive fluids, heavy metals) through mechanisms such as physical deposition, chemical sorption, and biogeochemical transformation. We investigated the potential to increase contaminant removal by amending bioswale soil with novel and inexpensive sorbents such as bone char (the product of heating animal bones to ~500 °C in the absence of oxygen). We collected soil cores from various bioswales, measured various parameters (pH, organic matter, electric conductivity, and texture), and measured hydraulic conductivities using Darcy's law and a constant head permeameter. We also analyzed copper transport through undisturbed soil cores with and without a surface addition of bonechar. Copper concentrations were measured by colorimetry and were confirmed with ICP-MS analysis. The effect of temperature on copper sorption kinetics was also tested in batch experiments where after 10 days, 5 °C, 25 °C, 40 °C samples had 21%, 28%, and 79% sorption, respectively (with mass loading of 64, 176, and 200 mg Cu/g bonechar, respectively). Bioswales with bone char amendments show promising results and better quantification of these mechanisms will enable improved designs to ensure economical, predictable, and reliable treatment of runoff from urban areas.

ENVR 236

Release of nanomaterial additives from automobile coatings and home siding during natural and artificial weathering

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Polymeric exterior materials are the outermost barrier between occupants of a home or automobile and the surrounding environment. Frequently, a variety of particulate additives from the nano to micron scale are incorporated into home vinyl siding and automotive acrylic coatings to confer desirable properties such as increased impact resistance, improved UV stabilization, or enhanced glossiness. While automotive and home exterior materials are engineered for different functions and performance standards, their polymer matrices share an inherent susceptibility to weathering, and particularly UV-driven photodegradation, during the use-phase of their respective lifecycles. Presently unknown is both the extent to which nano to micron scale particulate additives in each exterior material will regulate the kinetics of overall material aging and the degree to which such additives will release into the environment during polymer matrix degradation. To address these knowledge gaps regarding environmental exposure of automobile and home exteriors and the fate of their particulate additives, the effects of weathering on exterior performance, degradation, and nanomaterial release were investigated. First, the natural and artificial weathering of an automotive coating containing a nanoform pigment (i.e., Cuphthalocyanine) was examined and coating degradation and pigment release were compared after both weathering strategies. The nanoform pigment both improved coating resiliency against extensive photodegradation and its inclusion dictated release characteristics (i.e., release kinetics and form of released material) of the coating during weathering. Second, artificial weathering studies utilized both the NIST SPHERE (Simulated Photodegradation via High Energy Radiant Exposure) and a QUV Weatherometer to age commercially available vinvl siding. Vinvl siding samples were characterized spectroscopically and morphologically to track the rate of polymer degradation and monitor the emergence and exposure of embedded particulate additives that resulted from each exposure strategy. A key component of this study was the examination of how the differing spectral power distributions of the NIST SPHERE and QUV Weatherometer impacted the kinetics of vinyl degradation and particulate additive exposure. Collectively, these investigations inform the potential for weathering of exterior materials to result in nanomaterial release and exposure to humans and the environment.

ENVR 237

Evaluation of nanomaterials under the Frank R. Lautenberg Chemical Safety for the 21st Century Act

Alexandria Stanton, alexdstanton@gmail.com. Environmental Protection Agency, Washington DC, District of Columbia, United States The Toxic Substances Control Act (TSCA), recently amended as the Frank R. Lautenberg Chemical Safety Act, requires the Environmental Protection Agency (EPA) to make affirmative findings on the potential risk to human health and the environment posed by new chemicals entering the market. For newer classes of chemicals such as nanomaterials, this evaluation can be challenging new standards and test guidelines are currently being produced to accurately characterize these fascinating chemicals, making timely risk evaluations by EPA difficult. By participating in standards making and rule writing and working closely with industry, EPA continues to pave the way for thorough risk assessment and protective risk management strategies which allow for the growth of this new field and the protection of the environment.

ENVR 238

Ameliorative role of antioxidant therapy against chronic arsenicosis in humans

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Arsenicosis is a disease caused by the ingestion of arsenic contaminated ground water and millions of peoples of Ganga-Meghna-Brahmaputra river delta are worst sufferer of this disease. Despite the magnitude of this potentially fatal toxicity till date there is no available effective therapy for this disease other than chelation therapy. The potential role of oxidative stress in arsenic toxicity suggests that antioxidants may be effective against chronic arsenicosis. In our study, Antioxidant and placebo were distributed in a double-blind manner. Reactive Oxygen Species (ROS) generation in peripheral blood cells and the status of both, enzymatic and non enzymatic antioxidant defence molecules were monitored immediately before and after the antioxidant treatment. The decrease in ROS generation in peripheral blood lymphocytes was more significant in antioxidant treatment group rather than placebo treated subjects. This is the first ever report involving chronic arsenicosis patients. The changes of the status of enzymatic and non-enzymatic antioxidant defense molecules in antioxidant treatment group and placebo treated subjects are also in good agreement with the results of ROS generation in peripheral blood cells. On the basis of many signs and symptoms including typical raindrop pigmentation on skin and keratosis of palm and foot 'clinical scoring' was investigated. Arsenic concentration in hair and nail of all the participants of the study were also compared. Results suggest that antioxidant more effectively reduced clinical scores as well as arsenic content in hair and nails in comparison to placebo. The study reports that antioxidant

treatment mitigates arsenic intoxication-induced oxidative damage in chronic arsenicosis patients. The maximum chemoprophylactic efficacy was recorded with antioxidant treatment in combination with consumption of arsenic free safe water. Being a very good scavenger of free radicals, antioxidants can be very efficiently used in the treatment of chronic arsenicosis as an alternative to chelation therapy.

ENVR 239

Ammonium as structure-inducing ions to synthesize ultrathin birnessite-type MnO₂ nanosheets with excellent catalytic activity of ozone

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Two-dimensional nanomaterials have attracted great interests in the field of catalysis because of their high surface-to-volume ratio. Herein, ultrathin birnessite-type MnO₂ nanosheets have been synthesized under ambient condition without use of surfactants and templates, which have the lateral diameter of 300-500 nm and the thickness of 10-15 nm. We demonstrate that inorganic ammonium serving as structure-inducing ions play a vital role in the process of growth of ultrathin nanosheets. The adsorption of NH4⁺ on the (001) facet can significantly decrease the surficial energy, which inhibits the process of [MnO₆] layers self-assembly along the c axis, resulting in the growth of ultrathin nanosheets in two dimensions. The appearance of the huge nanosheets makes the high exposure of (001) facet with massive tri-coordination oxygen atoms, leading to more oxygen vacancies. In addition, unique hierarchical mesoporous structure and larger specific surface area deriving from self-assembled interconnected nanosheets are produced. Due to more oxygen vacancies, porous structure and enough surface acidity resulting from NH4⁺ adsorption on the surface, the as-prepared catalyst exhibits excellent catalytic ability to remove ozone, which can achieve the complete degradation of ozone for 36 h under the space velocity of 600 L/q_{cat}/h and 50% relative humidity. This work opens avenues for facile synthesis of ultrathin birnessite-type MnO₂ nanosheets and suggests the application for catalytic degradation harmful gas pollutants (ozone).

ENVR 240

Biocompatibility of two-dimensional transition metal carbides and nitrides (MXenes) and their potential in ophthalmic applications

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Due to their unique combination of properties including hydrophilicity, electrical conductivity, and optical transparency, two-dimensional (2D) transition metal carbides and nitrides (MXenes), developed in 2011 at Drexel University, have shown multidisciplinary potential. With tunable surface chemistry, MXene properties can be modified to alter their performance for specific applications. Biomedical applications have been considered for sensing and diagnostic imaging using mainly the most investigated MXene, Ti₃C₂T_x, this research however, remains in its infancy. In order to achieve a greater understanding of MXenes potential to be used in biomedical applications their biocompatibility must be further investigated as more than 30 MXene variations have been experimentally synthesized, there is scope to evaluate more than just Ti₃C₂T_x. This study evaluates the biocompatibility of several MXene variants by analyzing their biological interaction in ophthalmic environments. The investigation includes an assessment of cell viability and cytotoxicity, reactive oxygen species (ROS) stimulation, inflammatory cytokine expression and protein adsorption. From this analysis we expect to pave the way for more MXene compositions to be explored expanding their applications in the biomedical field. By taking advantage of the combination of mechanical, biocompatible and optoelectronic properties of MXenes, we have also presented one of the first ophthalmic applications of MXenes. Ti₃C₂T_x was used in an intraocular lens (IOLs) design in the attempt to recover the loss of accommodation as the natural intraocular lens is removed during cataract surgery.

ENVR 241

Construction of a bioinspired laccase-mimicking nanozyme for the degradation and detection of phenolic pollutants

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Nanozymes, defined as nanomaterials with enzyme-like activity, have attracted extensive interest in both fundamental and applied research. Laccases are members of the multi-copper oxidases, which are utilized as green catalysts in the environmental catalysis and biochemical industry. In this work, we report a facile strategy for the preparation of a new class of nanozyme (denoted as CH-Cu) with laccase-like activity inspired by the structure of the active site and the electron transfer pathway of laccase *via* the coordination of Cu⁺/Cu²⁺ with
a cysteine (Cys)-histidine (His) dipeptide. The CH-Cu nanozymes exhibit excellent catalytic activity, recyclability and substrate universality and have a similar K_m (Michaelis constant) and a higher v_{max} (maximum rate) than laccase at the same mass concentration. They are robust under a variety of conditions, such as extreme pH, high temperature, long-term storage and high salinity, which can cause severe loss in the catalytic activity of laccase. Higher efficacy of the CH-Cu nanozymes compared with laccase in the degradation of chlorophenols and bisphenols is also demonstrated in a batch reaction. Furthermore, a method for the quantitative detection of epinephrine by a smart phone is established based on the CH-Cu nanozymes. We believe that this nanozyme has promising applications in environmental catalysis and rapid detection and expect that combining key peptides as metal ligands with metal ions to mimic the structure of the catalytic center of a natural enzyme will be a general and important strategy for the design and synthesis of a new type of nanozyme that can be used in various applications.



We present a facile strategy for the preparation of a new class of nanozyme (denoted as CH-Cu) with laccase-like activity. This strategy is inspired by the structure of the active site and the electron transfer pathway of laccase *via* coordination of Cu^+/Cu^{2+} with a Cys-His dipeptide. Specifically, the CH-Cu nanozymes were synthesized through a hydrothermal method using Cys-His dipeptide and CuCl₂ as precursors.

ENVR 242

Release and transformation nanoparticle additives from surface coatings on pristine & weathered pressure treated lumber

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With the continued inclusion of engineered nanoparticles (NPs) in consumer products, a detailed understating their release during use is critical in determining their potential effect on human and environmental health. Of interests are commercially available NP-based surface coatings

including paints, stains, and sealants as they represent an area of direct contact between the product, the consumer, and the surrounding environment. In this study, pristine and aged (1-year outdoor) Micronized-Copper pressure treated lumber, were coated with ZnO NPs dispersed in Super-Q Water or commercially available wood stain. Coated surfaces were samples eight times consecutively using a modified method developed by the Consumer Product Safety Commission (CPSC) to estimate the release of NPs from the surface through dermal transfer. The total concentrations of Zn released during sampling was tracked through ICP-OES. Our results indicate that release is greatly affected by dispersion matrix (water vs. stain) and the age of the coated surface. Critically this study demonstrates this need to asses the intended use, and reasonably foreseeable misuse of nano-enabled products for proper risk assessment.

ENVR 243

Ferrihydrite dissolution at the root zone of crops under semi-arid condition controls the plant uptake of uranium and arsenic

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Ferrihydrite (Fh) dissolution at the root zone controls crop uptake of nutrients and a number of trace elements. This process has been previously demonstrated for flooded soils but is poorly understood for aerobic semi-arid irrigated soils prevalent in the corn belt of the US. The aim of this study is to clarify the effect of Fh dissolution and transformation for plant availability of arsenic (As) and uranium (U) under intermittently irrigated oxic soils. A greenhouse experiment was conducted utilizing an artificial soil mixture containing synthesized 2-line Fh coprecipitated with As and U, as the only form of iron (Fe) available to crops. Fh content in artificial soil was similar to field conditions in western Nebraska irrigated test plots. Irrigation was controlled to simulate semi-arid and primarily aerobic soil conditions. Soybean and corn (n=6) were grown for 60 days, leachate samples were collected and analyzed at 20 day intervals, and the soil Fe redox state was monitored. Crop samples were analyzed to quantify As and U uptake at the end of the study. X-ray photoelectron spectroscopy confirmed that the soil at the beginning of the experiment contained only Fe(III). After the experiment, soil was found to contain both Fe(II) and Leachates contained similar Fe(III). total Fe concentrations, but Fe(II) was higher for soybean than corn and Fe(II) positively correlated with concentrations of As and U in both leachates and crops. The data indicate that the reduction of Fe and Fh reductive dissolution plays

a critical role in controlling the bioavailability for a number of redox-sensitive nutrients and trace elements under semi-arid, mainly aerobic soil conditions. We postulate that dissolution of Fh controls mobilization of As and U in the soil pore water, and this process is driven by plant induced redox micro-zones at the root zone-soil-pore water interface.



Ferrihydrite dissolution at root zone-soil-pore water microzones generating reduced iron.

ENVR 244

Novel biomimetic system for the application of nanomaterials in water treatment: Implications and challenges

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Adsorption has emerged as a promising and costeffective water treatment method. Unfortunately, largescale adsorption technologies have failed to evolve as quickly as new nanomaterials have been discovered, and much of the industry still heavily relies on activated carbon and ion exchange resins. Given an ever-expanding list of contaminants and an increasing demand for clean water. an evolution of water treatment technology utilizing new materials is needed. Nano-adsorbents featuring high surface areas, strong sorption, and short intraparticle diffusion distances have the potential to revolutionize water treatment yet are difficult to implement in conventional packed-bed applications. A new biomimetic system has shown remarkable removal with its simple design. In bench-scale experiments, greater than 90% of heavy metals such as lead and arsenic have been removed using metal oxide nano-adsorbents manganese oxide and ferrihydrite - within three hours at environmental conditions. This system can also be adapted to remove a variety of contaminants using other nanoscale and 2D adsorbents. With efficient, low-cost manufacturing of the nanoadsorbents, this approach paves a path for a scalable and economical industrial treatment process. Current work focuses on evolving system design and overcoming technical challenges. Improvements promise to substantially increase removal efficiency and shorten treatment duration.

ENVR 245

Green engineering of gold nanoparticles

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Plants have been manipulated for the synthesis of nanomaterials (NMs), which can be an eco-friendly alternative to the chemical methods. We report a system using plant cell culture, which ensures control over the size of the particles. Isolated nanoparticles were characterized for their shape, size, and functions. The particles varied in shapes to exotic tetrahedrons, pentagons, and pentagonal prisms. Administration of cell culture-derived nanoparticles elicited milder inflammatory responses in mice compared to chemically synthesized NMs. These results envisage the utility of these particles for various biological applications.

ENVR 246

Myriad (nano)particulate phases emanating from hydrothermal vent and diffuse flow fluids fertilize the ocean

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Mixing between cold, oxygenated seawater and hot, anoxic hydrothermal vent fluids induce the formation and/or precipitation of (nano)mineral phases. Using the NanoEarth Facility at Virginia Tech, we demonstrate the occurrence and/or formation of a wide variety of chemical constituents as nano and submicron mineral phases in the mixing zone (first 1-2 meters from the vent orifice) between high-temperature hydrothermal fluids and ambient seawater and in diffuse flow waters at the 9° 50¢

N East Pacific Rise hydrothermal fields. Phases include pyrite, chalcopyrite, sphalerite, wurtzite, graphite, and silicates containing Mg and Fe (kaolinite, Fe-rich mica, and talc/lizardite). We find that silicate (nano)particles are ubiquitous in sampled fluids and are a previously undocumented source of Fe to the global ocean. Particle size and uniformity, in addition to the inclusion of Mg, suggests that these (nano)particles form from solution in rapid reverse weathering reactions rather than representing pieces of basement rock or chimneys entrained into the flow. The formation of hydrothermal silicates may be more widespread than previously documented and have an impact on the ocean's Si, Fe, and other element budgets. Thus, both nanoparticulate pyrite and metal-bearing (alumino)sili-cate phases can transport away from vent sites, and act as a source of Fe and other metals to the global ocean. In addition to SEM/EDS and TEM/EDS data, selected area electron diffraction patterns confirm the identity of these (nano)mineral phases. We define nanoparticles in the size range from 20-200 nm based upon filtering with 200 nm filters. Filters also trap these nanoparticles as they cooccur and aggregate during filtration indicating that ICP-MS data underdetermine the concentration of these nanoparticles as "dissolved" species. Analytical methods commonly used for determining DOC and POC indicate that graphite is measureable as DOC and POC. ICP-MS data suggest that, for Fe, nano-silicate particles may be more prevalent than nano-sulfides.

ENVR 247

Nanoparticle (and macroparticle) movement in the subsurface changes regolith chemistry

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It has been long known that colloidal particles move in the subsurface in different environmental systems. For example, metal colloids can cause contamination, clay particles can move from one horizon to another in soils, and organic matter can create colloidal particles through agglomeration. We have investigated the movement of particles in the subsurface of two critical zone observatories and discovered that such particle movement can change the chemistry of rock at depth in a shale in humid temperate climates and can move significant fluxes of material out of weathering corestones in guartz diorite lithologies under rain forest conditions. In particular, loss of micron-sized K-containing particles in weathering rock at meters depth, well below the soil, has been documented in the Rose Hill shale of central Pennsylvania while sub-millimeter-sized particles have been observed to move in large voids in the subsurface in weathering quartz diorite in the Luquillo Mountains of Puerto Rico. The former particles are almost exclusively illite in composition. In contrast, the particles moving through the quartz diorite consist of weathered biotite, weathered plagioclase, and quartz. In both cases, the weathered rock material that remains after particle movement is chemically different from the original (unaltered) rock. Such subsurface particulate transport may be geomorphologically important during weathering reactions especially in shale lithologies (where particle sizes are small) and in granitic rocks in the tropics (where large voids can form between corestones).

ENVR 248

Metal nanoparticle occurrence in nationwide municipal waters

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The presence and behavior of nanoparticles (NPs) in the environment is now widely studied due to increasing nanomaterials in consumer products and recent improvements in analytical methods, namely single particle inductively coupled plasma-mass spectrometry (spICP-MS). Published studies have examined NPs in natural and urban waters using spICP-MS, but are limited to discrete geographic locations. A survey of NPs in waters across widespread areas and over time would be useful for establishing and comparing their occurrence in different environments. Through a collaborative network of 20 municipal water treatment plants and analytical laboratories, we have obtained surface and groundwater samples spanning much of the U.S. with multiple time points over 6-9 months. Total mass concentrations indicate notable amounts of Au, Ti, and Ce in some samples which merit further investigation by spICP-MS to determine which occur as NPs. By comparing total mass concentrations, NP concentrations, and NP size distributions in different waters for these elements over several time points, we will examine the prevalence of nanoparticulate metals in varying aquatic environments.

ENVR 249

Mechanism of formation, stability, and toxicity of silver nanoparticles in aquatic environment

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Nanoparticles (NPs) exist in atmosphere, ores, rocks, ocean, hydrothermal vents, river, and wastewater. The presentation will first summarize the examples of

presence of different nanoparticles and their oxides/sulfides forms in different compartments of aquatic environment. The focus of the presentation will be on silver nanoparticles (AqNPs) to demonstrate their formation under different environmental conditions such as temperature, pH, and source of natural organic matters (NOMs). The influence of natural sunlight and types of NOMs (e.g., fulvic acid and humic acid) will also be discussed. Approaches used in elucidating the mechanism of the formation of AqNPs will be discussed. Formed AgNPs from NOMs are highly stable up to several months. Recent research on the potential interactions of AqNPs with metals, metal oxides, and carbon-based nanomaterials under natural environment will be shown. Finally, current understanding of the toxicity of naturally formed AgNPs will be presented.

ENVR 250

Sequential determination of microplastics and nanoplastics in environmental waters

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With their high production and wide application, large amounts of plastics are discharged and transformed into microplastics (MPs, with fragments < 5 mm) and nanoplastics (NPs, with fragments < 1 μ m) in the environment. However, little is known about their potential risks to organisms and human health. Investigation on their environmental behaviors and effects calls for the development of methods for separation and detection of MPs and NPs. By combining membrane filtration and cloud-point extraction (CPE) with pyrolysis-gas chromatography-mass spectrometry (Py-GC-MS), we developed a highly sensitive method for sequential determination MPs and NPs. After filtrating with a glass membrane of 1 µm pore size, MPs were trapped on the membrane, whereas NPs remained in the filtrate. The glass membranes with MPs were frozen, ground and vortexed. The NPs kept in the filtrate were concentrated by CPE and heated at 190°C for degradation the Triton X-45 used in CPE. Then, the concentrated MPs and NPs were subjected to Py-GC-MS determination. The method was validated by taking MPs and NPs made from polystyrene and polymethyl methacrylate as models. For samples prepared by spiking these MPs and NPs in water, the linear ranges were between 10 and 1000 µg/L $(R^2 \ge 0.99)$, and the recoveries and the detection limits were in the range of 72-118% and 0.10- 0.60 µg/L, respectively. The feasibility of the proposed method was verified by the detection of $1.6 - 2.7 \mu g/L$ of polystyrene MPs in river and sea waters; whereas the polystyrene MPs. and polymethyl methacrylate MPs and NPs were below their limits of quantification. This work provides an efficient approach for sequential determination MPs and NPs in environmental waters.

ENVR 251

Atomic force microscope enabled systematic evaluation of nanomaterial transformations

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Engineered, natural, and incidental nanoparticles are subject to transformation processes when exposed to aqueous environments. To develop a fundamental understanding of these transformations, we have systematically examined nanoparticle fate using an atomic force microscope (AFM). Uniform arrays of silver (AgNPs) and copper (CuNPs) were immobilized on glass substrates via nanosphere lithography. These arrays were then exposed to variable water chemistries and changes in AgNP or CuNP height and shape were quantified over time via AFM. This presentation will discuss work examining how changes in solution chemistry, surface coating, and nanoparticle size impact nanoparticle transformation rates.

ENVR 252

Density functional theory modeling of nanoparticles

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The career of Michael Hochella has covered numerous important topics, and the environmental impacts of nanoparticles has been one of the more well-known areas of study. His ability to bridge the field to molecular scales is remarkable, and Hochella continually demonstrates the need to understand chemistry in detail in order to assess health and environmental effects. This talk will review work on nanoparticles of rutile, anatase, ferrihydrite, goethite, and silica that has been conducted using the density functional theory (DFT) approach. Often, experimental data is enlightening but ambiguous or incomplete, so DFT can be used to help interpret observations and fill in details missing from various techniques. DFT can shed light on the nucleation and growth of particles, their sorption behavior, and potential mechanisms of negative health effects such as the generation of reactive oxygen species (ROS). In this presentation, the audience is encouraged to use computational chemistry methods to complement experimental observations as part of a toolbox for dealing with the complex and difficult to study world of environmental nanoparticles.

Nanophases in planetary processes

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Thermodynamic studies over the last decade have shown that differences in surface energies strongly affect phase equilibria at the nanoscale, sometimes stabilizing structures metastable in the bulk and changing the P-T positions of dehydration and redox reactions. Here I discuss three examples where such nanoscale effects may be important in a planetary context. (1) The condensation of solid particles from the solar nebula occurs from a dilute gas phase. Although temperatures may be high, the initial particles are likely to be isolated and initially small in size. The thermodynamics of condensation equilibria and therefore the sequence of phases formed on cooling may be changed by differences in surface energies. (2) Ultra cold environments abound on the surfaces of planets far from their suns. Nanoscale effects may dominate the chemistry of particles in the atmospheres, hydrocarbon lakes and surfaces of such icy planets and moons. (3) Impacts, including the Earth's possible moon-forming episode, produce short-lived hightemperature vaporization events. The rapid cooling and condensation of a mixture of gaseous, liquid and solid materials is likely a non-equilibrium phenomenon and may be dominated by the formation and further reaction of nanoparticles. These may form a much longer-lived sequence of metastable phases, which could be geochemical markers of such events.

ENVR 254

Impact of Fe-oxide nanoparticles on biogeochemical cycling of elements in a changing environment

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Iron oxide nanoparticles, e.g., ferrihydrite, have major impact on biogeochemical cycling of carbon and trace metals in soils. Climate and environmental change are having profound impacts on humankind. Rising seas and temperatures are causing increasing flooding, salt water intrusion, and melting of ice and permafrost soils. The impact of these processes on Fe-oxide nanoparticle interactions with carbon and metal(loid)s is not well understood. For example, how do rising seas affect transformations of Fe-oxides and As? Under changing climatic conditions, how will sequestration of C by Feoxide minerals be impacted, and resultant mobility of elements? This presentation will explore these questions, and others, over a range of spatial and temporal scales.

ENVR 255

From quantum confinement to global behavior: Overall state of nano-environmental and nano-geo research

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The sun, functioning solely as a quantum mechanical reactor, makes this planet, and us, who we are. Just so, the quantum behavior of Earth's natural, incidental, and engineered nanomaterials strongly influence all that occurs on this human-altered planet, as natural nanomaterials have since Earth's origin. Nanomaterial behavior and reactivity are the consequence of guantumcontrolled electron energy states dependent on size and shape, these size/shape factors often constantly changing among inorganic, organic, and mixed nanomaterials. The influence of gravity is completely replaced by van der Waals forces which are central at this scale, delicately dependent on size, shape, and tweaks in atomic structure. This dictates all-important dispersion/ aggregation factors. Overall, we have only begun to explore and understand the planet's nano-machinery. While progress is being made to fill in this last incomplete piece of the entire ultra-complex Earth puzzle, what we do not know will be emphasized in this talk.

ENVR 256

Using microscopy techniques to quantitate biological systems for improving wastewater treatment plant performance

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Many wastewater treatment plants (WWTPs) are managed/optimized through chemical analysis even though the systems are biological in nature. While there are a variety of biological analytical tests available to understand the microbiology of a WWTP, there use for monitoring to improve WWTP performance is somewhat limited due to their turnaround time. Microscopy is a common analytical technique used to understand the microbiology of a WWTP. Techniques in this area can give information into the type of microbes present along with information about the flocculation characters of the effluent. An issue with microscopic techniques is that there is usually a human element involved in both the imagine quality and imagine interpretation. This human element to microscopy can cause issues or decrease the effectiveness of long-term monitoring of the WWTP performance. With recent advances in microscopic imaging techniques, imagine recognition software and

mathematical modeling software programs there is now the ability to convert microscopic imagines of wastewater treatment effluent into numerical data that removes the human interpretation factor. The numerical data from this methodology allows for industrial users to monitor biological data through dashboards that were once only used only for chemical information. We will be demonstrating the use of this methodology in an industrial WWTP application.

ENVR 257

Producing and optimizing extracellular lipase for remediation of refinery wastewater

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Lipase was produced by a saprotrophic fungal strain, Aspergillus flavus isolated from crude oil contaminated soils. Optimization of selected environmental conditions and fermentation medium were performed using response surface methodology and factorial design. The results from factorial design reveal that agitation, substrate concentration, temperature and pH were the crucial elements affecting the production of lipase. The optimum medium conditions obtained for lipase production using response surface methodology were agitation of 150 rpm, substrate concentration of 2.75% v/v, temperature of 45 oC and pH 8.5. This model was authenticated by replicating the experiment under the established conditions, which led to maximum expression of lipase by the organism to 5.05 U/mg (predicted response 4.91 U/mg), hence substantiating the reliability of the model. This study reported significant efficiency of Aspergillus flavus, for lipase production and highlights the practicability of response surface methodology for the environmental conditions optimization of and fermentation medium for enhanced production of lipase.

ENVR 258

Treatment of textile sludge by coagulation and flocculation processes

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Coagulation and flocculation were found to be effective in alleviating pollution problems caused by sludge from textile industry. Composite samples of the sludge were characterized using some parameters like pH, solids

concentrations, oxygen demand, nitrogen, phosphorus and total bacteria counts. Samples were treated by coagulation and flocculation using alum, iron (III) chloride, lime, and polyelectrolyte. It was found that the method is effective in the treatment of sludge from the textile industry. Lime as a conditioner offers the best alternative for the treatment of sludge from textile factory. Its advantages over others are due to its complete odour prevention, disinfecting action, increase in the agricultural values of the sludge solids and its ability to neutralize heavy metals if present. Polyelectrolyte was found to be more effective in BOD and COD reductions. The percentage reductions were 92.6 and 92.8 respectively. Polyelectrolyte conditioned sludge were also observed to have less quantity of sludge solids (about 5% increase) as compared to the 15-30% increase recorded by other conditioners. pH was found to have a major influence on the stabilization of the sludge.

ENVR 259

Effects of reverse salt flux on the transport of disinfection byproducts in forward osmosis

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Forward osmosis (FO) is being considered as alternative or supplement technology to reverse osmosis (RO) for wastewater recycling due to its lower energy cost and less irreversible fouling than RO. Our previous study showed that the performance of FO in rejecting disinfection byproducts (DBPs), a critical aspect for wastewater recycling, was better than or comparable with that of RO. Because the current FO transport models, many of which were adopted from RO, overestimated DBP transport, it was hypothesized that the reverse salt flux from draw to feed, a phenomenon unique to FO, contributed to the improved DBP rejection. In this study, we tested this hypothesis by evaluating DBP transport through a commercial FO membrane (Aquaporin) under different reverse salt flux. Different concentrations and/or type of draw solute were used, including 0.2, 0.5, and 1 M sodium chloride, 1 M magnesium sulfate, and 1.5 M glucose. A total of sixteen DBPs including nine halogenated DBPs and seven nitrosamines were tested. For halogenated DBPs, DBP permeance was lower at higher reverse salt flux, suggesting retarded forward DBP transport by reverse salt flux. In contrast, nitrosamine permeance was independent of the reverse salt flux. To improve the prediction accuracy of the solution-diffusion model, hinderance factors were developed to represent the retarding effect of reverse salt flux on active laver (Ka) and supporting layer (K_b). The value of K_a was determined by

subtracting the free volume occupied by salt in active layer from the total free volume, while K_b was calculated based on the interaction between DBP and the polymeric matrix of the supporting layer. Preliminary results suggest that reverse salt flux exhibited a stronger effect in retarding DBP transport in the supporting layer than in the active layer. After incorporating K_a and K_b , the solutiondiffusion model showed improved accuracy in predicting DBP permeance through Aquaporin membrane. Lastly, the effect of reverse salt flux on DBP transport was evaluated on 4 other membranes being tested for FO applications.

ENVR 260

Imagine a world without environmental chemistry: Let's not

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This presentation will not articulate the doomsday scenario of an industrialized world without environmental chemistry. Rather, it will be full of hope, describing the myriad ways our health and wellbeing are promoted by efforts of diligent environmental scientists, who enable continual industrial and scientific innovation to advance in a green manner. We will specifically discuss how analytical instrumentation and application to industrial problem solving has evolved over the last few decades, and what positive impacts have been achieved. These advances have enabled a high integrity scientific framework for establishing important regulations to assure environmental and human health, along with the practical means to comply with them. We will highlight emerging technologies in environmental science, and opportunities for those eager to help drive continued technology and life science advancements, while still assuring good environmental stewardship.

ENVR 261

Rare earth element recovery from coal fly ash: Hydrothermal extraction and ligand-associated media sorption

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Rare earth elements (REEs) have many critical uses in components used in advanced technology (e.g., electric vehicles, industrial magnets) and the lack of a reliable domestic supply has been identified by the US DOE as a vulnerability to US economic security. We are working on developing an economical industrial process for extracting REEs from coal fly ash (the waste product left over after coal is burned for electricity generation) by coupling a hydrothermal extraction process with the enaineerina of a ligand-associated media for concentrating REEs from the extraction liquid. Traditional REE extraction requires large amounts of acids and organic solvents. Our process may provide an organic solvent-free and environmentally friendly method of extracting and recovering REEs. In addition, the residual material left after REE extraction will have most of the problematic toxic materials removed, which will allow the "beneficiation" of large amounts of fly ash to be used as building materials with less risk of metal leaching. We will discuss the process of collecting and characterizing fly ash and wastewater sludge feedstock from coal-fired power plants near Detroit, MI by scanning electron microscopy (SEM) and x-ray diffraction (XRD). Ash samples were then subjected to high pH hydrothermal conditions from 100-350 °C to produce a REE enriched leachate. Sorption media from commercially available sources and synthetic varieties have been successfully loaded to a commercially available organosilica media. Column experiments have been conducted to evaluate the optimal ligand/media ratio for repeat use cycling and this process is a promising application of green chemistry for extracting valuable materials from a waste product. We will focus on the connection between environmental chemistry and industrial applications by discussing costbenefits, availability of feedstocks, and the political influences around the industry of recovering REEs from coal fly ash and powerplant wastewater feedstocks.

ENVR 262

Impacts of interfacial tension and critical micelle concentration on emulsion stability in bilgewater

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Oil-in-water emulsions in shipboard generated bilgewater present a challenge to the water treatment equipment used to limit hydrocarbon discharge. Despite substantial research in emulsion behavior, bilgewater treatment continues to be unique due to its varied composition of surfactants, hydrocarbons, and suspended solids and water chemistry. Therefore, the properties of neat surfactants and common commercial cleaners were determined and the impact of said properties on bilgewater emulsion stability was evaluated. The effects of surfactant type, oil concentration, and homogenization energy on the relationship between critical micelle concentration (CMC) and equilibrium interfacial tensions (IFT) were examined using laser diffraction, optical microscopy, temporal evaluation, and surface tension measurements. The properties of IFT and CMC were found to correlate well with emulsion stability in neat surfactants. Commercial cleaners also showed this correlation, however their compositional heterogeneity increased variability in the results. The effects of specific surfactants will be discussed along with the potential of using IFT and CMC as indicators to predict emulsion stability in various bilgewater systems.

ENVR 263

Enhanced performance of carbon nanotube immobilized membrane for treatment of high salinity produced water via direct contact membrane distillation

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Membrane distillation (MD) is a promising desalination technology for the treatment of high salinity water. Here, we investigated the fouling characteristics of produced water obtained from hydraulic fracturing implementing a carbon nanotube immobilized membrane (CNIM) via direct contact membrane distillation. The CNIM exhibited enhanced water vapor flux 77% higher and antifouling characteristics compared to the pristine membrane. The normalized flux declination after 7 hr of operation was found to be 55% and 65% for CNIM and PTFE membrane, respectively. The addition of 1-hydroxy Ethylidene-1, 1- Diphosphonic acid (HEDP) antiscalant was observed to be effective in reducing the membrane fouling. The salt deposition was found 77% less in CNIM, which was further reduced to 135.4% with the addition of HEDP in feed, in comparison with PTFE membrane. The presence of CNTs on membrane surface facilitated the regenerability of the membrane. Results indicated that CNIM regained 45.46% of its initial water flux, whereas, the unmodified PTFE only reached to 59.45% of its initial flux after 5 days of operation.

ENVR 264

Adsorptive removal of Cr(VI) by zwitterionic surfactant coated manganese ferrite (MnFe₂O₄) nanoparticle: Equilibrium and kinetic study

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An efficient and new magnetic nanoadsorbent DDMAB coated MnFe₂O₄ nanoparticles were fabricated by coprecipitation technique. These nanoparticles were characterized using SEM, TEM, XRD, FT-IR and VSM. XRD and FT-IR confirmed the functionalization of the MnFe₂O₄ nanoparticles with the zwitterionic surfactant DDMAB. In this investigation, magnetic nanoadsorbent has been employed for the removal of Cr (VI) ions from aqueous solutions by a batch adsorption technique. In batch optimization studies, the maximum removal efficiency of 80% was obtained at optimal levels of pH 5, contact time 150 min, adsorbent dosage 2.5 mg/L and initial metal ion concentration 10 ppm. The equilibrium sorption data were fitted into Langmuir, Freundlich and Temkin isotherms. Of the three adsorption isotherms, the R² value of Langmuir isotherm model was the highest. The maximum monolayer coverage (Q_{max}) from Langmuir isotherm model was determined to be 75.76 mg/g. The adsorption of Cr(VI) by DDMAB coated MNPs follows the pseudo-second order kinetic model. The results of this study showed that the DDMAB coated MNPs were found to be cost effective and easily separable nanoadsorbent for efficient removal of Cr (VI).

ENVR 265

Reactivity and *N*-nitrosodimethylamine formation potential of betrixaban with monochloramine, chlorine, and ozone

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Betrixaban is an oral anticoagulant drug, recently approved by the Food and Drug Administration (FDA), for the treatment of Venous Thromboembolism. Its FDA approval is expected to exponentially increase its medical use which necessitates understanding its fate in the environment. This study investigated the fate of betrixaban during disinfection with monochloramine (NH₂Cl), free chlorine, and ozone as well as its *N*-Nitrosodimethylamine (NDMA) formation potential with these oxidants. Betrixaban revealed an NDMA yield of >1% upon monochloramination. An increase in NH₂Cl dosage, contact time, and pH significantly increased betrixaban degradation and NDMA formation. Although

the highest yield of NDMA was observed at basic pH, the formation of NDMA was still significant (yield ~0.3%) at circumneutral pH. This study revealed a new potent precursor of NDMA, indicating that monochloramination of waters containing betrixaban can lead to the formation of NDMA and other disinfection by-products (DBPs) such as dichloroacetonitrile (DCAN) and dimethyl-formamide (DMF). Moreover, betrixaban showed a complete degradation with 5 mM free chlorine over seven days with 0.01% NDMA yield. The degradation of betrixaban, in the presence of 0.3 mM ozone, increased from 40% after 1 minute to almost complete degradation after 6 minutes of contact time, with no observed NDMA formation. DMF was detected as a prominent DBP of chlorination and ozonation of betrixaban. The kinetic studies revealed that the reaction of betrixaban with NH₂Cl and ozone followed pseudo-first-order reaction kinetics while no reaction kinetics was obtained for chlorination of betrixaban due to its complete removal within initial two minutes of the reaction. As the use of betrixaban will widen, and its presence in the environment, including in wastewater and surface waters, will increase, its DBPs' formation risks in the environment will also increase. Our study highlights these risks and, through a detailed investigation of contributing factors, kinetics, and reaction mechanism, provides useful information to mitigate such risks.

ENVR 266

Insight into the interplay between graphitic carbon nitride aging and its photoreactivity

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Graphitic carbon nitride (g-C₃N₄) has emerged as a promising material in various areas, owing to its unique properties and low cost in manufacturing. However, g- C_3N_4 can be released into nature after use and degrade, which leads to the secondary pollution. As a photocatalyst, g-C₃N₄ can interact with contaminants in nature via photoreactions. Meanwhile, the material can degrade and age in natural environment during photocatalysis. which could further tailor its interactions with contaminants. Nevertheless, understanding environmental impacts of g-C₃N₄ on nature is still at its nascent stage. As the strongest oxidant in water, hydroxyl radicals commonly exist in natural aquatic environment. The interaction between hydroxyl radicals and g-C₃N₄ is expected to age the photocatalyst and produce organic and inorganic fragments. We systematically conducted the accelerated ageing experiments for two g-C₃N₄ nanosheet samples by photo-Fenton reaction and ozonation that produces hydroxyl radicals, and evaluated property change of the photocatalyst and its impact on contaminant transformation kinetics. After ageing, the samples were broken into small fragments, as characterized by transmission electron microscopy and

dynamic light scattering, releasing nitrate and dissolved organic species that will be quantified by high performance liquid chromatography-mass spectrometry. Zeta potential of graphitic carbon nitride became more negative, possibly suggesting the introduction of oxygen functional groups. Other photocatalyst properties such as band gap, band energy levels, surface functional groups, and bonding environment will be characterized. Aged g-C₃N₄ nanosheets also showed different reaction kinetics for degrading representative organic contamin-ants. Computational simulations will predict the interactions of aged g-C₃N₄ and the contaminants, including surface adsorption of the contaminants and direct electron transfer rate. Our study will shed light on the environmental impact of an emerging photoreactive material in nature, and it can also guide rational material design to achieve safer and more robust materials.

ENVR 267

Microcystins degradation kinetics during chlorination: Role of water quality conditions

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Microcystins produced during cyanobacteria bloom can contaminate the drinking water sources and pose threat to public health. Microcystin-LR (MCLR) is one of the most widespread and toxic microcystins, which is a cyclic heptapeptide containing a large amino acid moiety (Adda) and two variable amino acid moieties. Leucine and aRginine. The World Health Organization (WHO) has set a provisional guideline value of 1 µg/L for MCLR in drinking water due to its potent toxicity. Among the disinfectants typically applied during water treatment, chlorine was found to be effective for microcystins removal. However, the water quality conditions, especially the presence of dissolved organic matter (DOM), are believed to significantly affect the efficacy of chlorine in treating microcystins. Therefore, this work is intended to (i) evaluate the degradation kinetics of MCLR during chlorination under different water quality conditions, including pH, alkalinity, temperature, and dissolved organic matter (DOM), and (ii) construct a practical model to predict the decay of MCLR during chlorination of waters with various water qualities. In order to achieve these goals, the reaction kinetics of MCLR with free chlorine was first evaluated in synthetic waters only containing buffer (pH 7-9), and buffer intensity, alkalinity or temperatures were varied in certain cases. Here, a novel quencher, 1,3,5-trimethoxyl-benzene, rather than traditionally used strong reducing agents (e.g. sodium thiosulfate), was used to preserve the N-chlorinated products. Secondly, two natural organic matter isolates, Suwannee River Fulvic Acid (SRFA) and Grant Lake St. Marv's (GLSM), were added to assess the free chlorine consumption by DOM. These two isolates were selected

since they represent DOM from two distinct sources, terrestrial (SRFA) and microbial (GLSM). The results indicated that DOM is a strong scavenger of free chlorine, and the extent depends on the DOM properties (e.g. TOC, SUVA254 and E2/E3 ratio). The obtained reaction rates between MCLR and free chlorine ($k_{FC-MCLR}$), and between DOM and free chlorine (k_{DOM-FC}) were validated in real water samples from severe algal bloom-impacted lakes and water treatment plants. Overall, our results show that by incorporating the competition of DOM, the decay of MCLR by reaction with free chlorine can be predicted in a given water matrix.

ENVR 268

Permanganate oxidation: From dissolved organic matter (DOM) to model compounds

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Permanganate oxidation is commonly used in drinking water treatment and in-situ remediation. The efficacy of permanganate oxidation in these operations can be greatly diminished in the presence of dissolved organic matter (DOM). Previous work by our group has utilized Fourier transform- ion cyclotron resonance- mass spectrometry (FT-ICR-MS) to identify compounds that are likely to react with permanganate. We identified alkylbenzenes and nitrogen-containing aromatic compounds as being responsible for DOM scavenging of permanganate. However, rate constants and oxidation products for these types of compounds are unknown. Preliminary work with phenols showed that their reaction rate constants with permanganate followed similar trends as electrophilic aromatic substitution reactions with C-H bonds. Specifically, we observed that substituents that activate aromatic rings had faster rate constants while substituents that deactivate aromatic rings had slower rate constants. Alkylphenols had some of the fastest reaction rate constants but the product distributions are unknown. Permanganate could react either with phenols to form para-quinones or with alkylbenzenes to form benzoic acids. The alkylphenols studied, therefore, had multiple reactions sites; for example, permanganate could react with four different bond sites within trimethylphenol. Work is currently underway to identify oxidation products for alkylphenols. We expect similar trends with benzylamine compound substituents; however, we do not yet know the effect of amine order and work is underway to identify the effects and will be discussed. The characterization of these rate constants enables the development of quantitative structure-activity relationships to predict other permanganate reaction rate constants. These results suggest that permanganate could be used to remove pharmaceuticals in wastewater or drinking water treatment because many pharmaceuticals contain both alkylbenzene and amine-functionalities.

ENVR 269

Steric and electronic effects on reaction rates of substituted benzenes with often-overlooked brominating agents

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Chlorine used to disinfect drinking water can react with bromide and natural organic matter present in water sources, forming toxic disinfection byproducts (DBPs). Bromide can be oxidized by chlorine into free bromine which can subsequently react with organic compounds, forming brominated DBPs. Free bromine can be in the form of BrCl, Br₂O, Br₂, BrOCl, and HOBr (among others), but most previous studies assume HOBr to be the only relevant brominating agent in solutions of free bromine. The relative contributions of these brominating agents to overall bromination rates can be calculated after performing reactions with organic compounds under varying solution conditions, such as [Cl-], [Br-], and pH. The purpose of this research is to evaluate the role of steric and electronic effects in bromination of benzene, alkylbenzenes (ethyl, isopropyl, *tert*-butyl), and alkoxybenzenes (ethoxy, isopropoxy, tert-butoxy), and to elucidate the inherent reactivities of brominating agents towards these aromatic compounds. For monosubstituted alkylor alkoxybenzenes, bromine substitution occurs at the para- or ortho- positions. BrCl was the most inherently reactive brominating agent towards the examined alkyl- and alkoxybenzene species. Rate constants for reactions of aromatic nucleophiles with BrCl ranged from 5.7 \pm 1.3 M⁻¹ s⁻¹ (for benzene) to (6 \pm 2) × 10⁵ M⁻¹ s⁻¹ (for iso-propoxybenzene). For parasubstituted alkylbenzenes, overall reactivity increased from *tert*-butyl < ethyl ≈ isopropyl. For *para*-substituted alkoxybenzenes, reactivity increased from *tert*-butoxy < ethoxy < isopropoxy. In going from ethyl to tert-butyl and ethoxy to isopropoxy, unfavorable steric effects can attenuate the favorable electronic effects imparted by the substituents. When comparing unsubstituted benzene, alkyl-, and alkoxybenzenes, the structure of the substituent has a significant effect on rates and regioselectivity of bromination. Collectively, these findings indicate that steric effects, electronic effects, and brominating agents other than HOBr can influence aromatic compound bromination in solutions of free bromine.

ENVR 270

Environmental fate and transformation of herbicide safeners

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Herbicide safeners are bioactive agrochemicals included in many commercial herbicide formulations to selectively protect crops from herbicide toxicity. Despite their bioactivity, safeners are classified as "inert" from a regulatory perspective, and as such, minimal data exist describing their environmental occurrence, fate, and transformation. Yet, a growing body of literature suggests that some safeners, particularly those of the dichloroacetamide transform class. can over environmentally relevant timescales into products with increased bioactivity that may pose human and environmental health risks. To evaluate the persistence, fate, and transformation of safeners in aquatic systems. we quantified timescales (i.e., half-lives, sorption rates) for predicting safener persistence, elucidated novel transformation pathways and products for safener hydrolysis, and assessed the potential for differential sorption fate profiles between parent and product species. Furthermore, we developed a method to analyze a new safener, cyprosulfamide, and two of its degradates in water by hydrophilic-lipophilic balance (HLB) solid-phase extraction and liquid-chromatography/tandem mass spectroscopy. We employed the method to quantify cyprosulfamide concentrations in agricultural drainage waters.

ENVR 271

Pharmaceuticals and personal care product accumulation in terminal lakes receiving reclaimed wastewater

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Endorheic lakes or terminal lakes are common in the intermountain west. These lakes have no natural outlet other than evaporation and slow infiltration, but receive water from precipitation and anthropogenic sources, such as treated wastewater which is released to rivers that terminate in such lakes. Poor removal of pharmaceuticals and personal care products (PPCPs) at wastewater treatment plants results in the potential for PPCPs accumulation in lake water and sediment. This study

examined a suite of twelve PPCPs in soil, sediment and water of three terminal lakes receiving reclaimed wastewater and two lakes which were anthropogenically influenced but did not directly receive wastewater. The goal was to determine the extent of accumulation of PPCPs in terminal lakes. Initial results demonstrated that six out of twelve PPCPs (e.g., carbamazepine, DEET, diphenhydramine, primidone, sulfamethoxazole, and trimethoprim) were present in all terminal lake water samples. Primidone and carbamazepine are sometimes used as wastewater tracers in the environment, and both were detected in all water samples, indicating the ubiguitous distribution of these compounds. Primidone ranged from 345-1509 ng/L in the reclaimed wastewater influenced terminal lake and was <MDL to 360 ng/L in non-wastewater influenced lakes. A similar trend was observed with all other PPCPs being higher in reclaimed wastewater influenced terminal lakes as compared to non-wastewater influenced terminal lakes was observed. Ongoing research includes the quantification of these compounds in near-shore soil and sediments.

ENVR 272

Sorption of organic cations to organic matter: Use of molecular docking simulations to understand binding interactions

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The increasing ubiquity of charged organic contaminants in environmental systems has elevated the need for predictive sorption models. Current models for organic cation sorption to organic matter use an additive framework, predicting sorption coefficients based on sorbate size plus an electrostatic charge contribution. However, maps of the electrostatic surface potential of organic cations show electron distributions to vary across the whole molecule with the addition of neutral substituent groups. Thus, there is a need for predictive tools that incorporate the intrinsic electron distributions of charged compounds in determining sorption interactions. This problem is analogous to that of drug-protein binding predictions in pharmaceutical sciences for which effective computational chemistry tools have been applied. Here, we examined the extent to which molecular docking techniques can be applied for prediction of organic cation/organic matter binding affinities using an atomistic representation of the "Schulten humic acid" molecule with the software tool, AutoDock. Calculated sorbate binding affinities were correlated strongly with experimental measures of sorption coefficients for organic cations and Pahokee Peat organic matter, Further, computational tools allow for exploration of the importance of sorption energy contributions by hydrogen bonding, electrostatic attraction and van der Waals interactions. Primary, secondary, and tertiary amines interacted with organic

matter carboxylic groups via hydrogen bonds while positive charges on quaternary amine hydrogens are too weak to participate in interactions at organic matter charge sites. Secondary electrostatic interactions between organic cations and organic matter also gradually weakened with increasing amine order due to increasing charge delocalization. For compounds with the same amine order, sorption coefficients were correlated with van der Waals energy contributions, suggesting these interactions largely drive the extent of uptake; however, correlations were unique to amine order. Our work shows that molecular docking tools provide an efficient means for predicting binding mechanisms and affinities of cationic organic contaminants.

ENVR 273

Biotransformation of methoxylated polychlorinated biphenyls in whole poplar plants

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Polychlorinated biphenyls (PCBs) are still ubiquitous in a variety of environmental matrices, even though they were banned 30 years ago. The lighter, lesser chlorinated PCB congeners are subject to uptake and transformation by plants. It is important to study biotransformation of the parent compounds metabolites and to reveal environmental fate and effects of PCBs. Hydroxylated polychlorinated biphenyls (OH-PCBs) and PCB sulfates are well-known metabolites of PCBs. They are toxic to a variety of organisms and have raised environmental concerns. Generally, OH-PCBs are more toxic than their parent PCBs. OH-PCBs can interrupt brain function, reproductive processes and the endocrine system in mammals. OH-PCBs can be further transformed to PCB sulfates in various organisms including certain plants such as poplar. PCB sulfates have a potential activity as of endocrine signaling. Methoxylated disruptors polychlorinated biphenyls (MeO-PCBs) are metabolites of PCBs which have not been widely studied. They are likely more lipophilic and persistent than OH-PCBs. Thus, they have a potential chronic health risk and raise concern. MeO-PCBs were detected in sewage sludge of China. Information on demethylation of MeO-PCBs is quite limited. There are no reports on the transformation of MeO-PCBs to sulfate PCBs. In this study, poplar plants (Populus deltoides × nigra, DN34) were used as a model plant to investigate the biotransformation of MeO-PCBs in plants. Poplar cuttings (small trees) were hydroponically exposed to 4'-methoxy-4-monochlorobiphenyl (4'-MeO-PCB 3) for 10 days. After 10 days exposure, about 50% and 70% of the initial mass of 4'-MeO-PCB 3 were found in the exposure groups (plant tissues and solutions) and unplanted controls (solution samples), respectively. A 4'-hydroxy-4-monochlorohvdroxvlated metabolite. biphenyl (4'-OH-PCB 3), was detected in exposure groups. The transformation ratio (yield) of 4'-OH-PCB 3 was about 2% in exposure groups. The recovered 4'-MeO-PCB 3 in the exposure groups were much lower than that of unplanted controls, indicating that other metabolism pathways existed in exposure groups besides demethylation. We expect the sulfate metabolite, 4'-PCB 3 sulfate, of 4'-MeO-PCB 3 will be detected and account for the missing mass in exposure groups. This is the first work focused on the sulfate metabolites of methoxy-PCBs in an important trophic level, plants.

ENVR 274

Ecological and health risk assessment of organochlorine pesticides in an urbanized river network of Shanghai, China

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The concentrations, distribution and partitioning, ecological and health risk assessment of organochlorine pesticides (OCPs) in the urbanized river network of Shanghai were studied. The goal was to establish connections among OCP residues with their impacts on ecological and human health. Analytical results showed that the OCPs concentrations in the northern and southern regions of Shanghai were significantly higher than that in other regions, and OCP concentrations in suspended particulate matter (SPM) were higher than that in surface water. The Kp values of different OCP individuals varied widely, and that of Σ_{26} OCPs were negatively correlated with TSS contents (p < 0.01). The ecological risk was assessed according to the Risk Quotient (RQ) method, and some OCPs formed point-like areas with higher local ecological risks, which were concentrated in agricultural areas. The health risk assessment showed the rankings of incremental lifetime carcinogenic risk (ILCR) for dermal contact and mistaken oral intake according to age and gender. From the median, the ILCR for dermal contact in population groups were at low risk, except for male adults and female adults. whose ILCR were at moderate risk. The ILCR values caused by mistaken oral intake were all at very low risk. The non-carcinogenic risk hazard index (HI) values of both exposure routes were smaller than 1, indicating that OCPs in river waters didn't cause significant noncarcinogenic health hazards for most people.

ENVR 275

Microplastics as a novel air pollutant: Successes and challenges

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Microplastics are a complex class of heavily modified. synthetic organic particulates which contaminate a range of environments. Laboratory studies indicate they can negatively impact biota following exposure, primarily via oxidative stress and metabolic disruption. Recently, microplastics have been reported in atmospheric deposition, and indoor and outdoor air in major population centres. This has raised concern for public health due to the potential for exposure via inhalation. However, very little is known about airborne microplastics, including their concentrations, chemical composition and size distribution. Here we present two workflows developed for different air sample types. Using a combination of passive sampling and FTIR microscopy to detect microplastics in atmospheric deposition collected in central London (UK), we found fibrous microplastics were an order of magnitude more abundant than non-fibrous. An average deposition rate of 706 microplastics/m2/d was observed, with polyacrylonitrile forming the most common polymer. Through active sampling and automated micro-Raman analysis, we have improved limits of detection using a range of chemometric techniques. Microplastics down to 2 µm have been observed in ambient particulate matter (PM) samples from London, UK and we are now consolidating concentrations. As global pressure to reduce PM emissions from road transport and fuel burning increases, particle composition is likely to shift. In combination with a predicted increase in plastic use, especially in the textile sector (4%/year), the proportional concentration of airborne microplastics will become increasingly important. It is therefore timely to establish baseline knowledge of global airborne microplastic burdens and begin to understand what their potential role in PM-associated health effects might be.

ENVR 276

Organotin release from polyvinyl chloride (PVC) microplastics under photodegradation: Impacts from salinity, dissolved organic matter and light exposure

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Photochemical weathering leads to degradation of microplastics and releases chemical additives, polymeric fragments and/or byproducts. This study evaluated the release kinetics of organotin compounds (OTCs) from three different sized (10-300 µm) polyvinyl chloride (PVC) microplastics under UV and visible light irradiation. Four OTCs, dimethyltin (DMT), mono-methyltin (MMT),

dibutyltin (DBT) and monobutyltin (MBT), were found to release from PVC particles after 24-h leaching in darkness ranging from 2 to 20 µg/g-PVC. Under UV/visible light irradiation, only DMT and DBT were detectable, whereas MMT and MBT were not detected due to rapid photodegradation. The total tin concentrations (including organic and inorganic tins) in the aqueous phase monotonically increased under light exposure. By contrast, they reached plateaus after 24 h in darkness, confirming the photodegradation of OTCs. A release kinetics model was established and correctly interpreted the microplastics size effect on OTC release process. Finally, the impacts of salinity and dissolved organic matter (DOM) were investigated. The release and photodegradation of OTCs were both inhibited at high salinity conditions, probably due to the enhanced readsorption of OTCs on PVC microplastics and the formation of halogen radicals that were less reactive towards neutral OTCs. The presence of DOM, however, increased OTCs release probably because excited state triplet DOM (³DOM^{*}) formed and reacted with OTCs from PVC microplastics.

ENVR 277

Fate of microplastics and microfibers in bioretention cells

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Despite the fast-growing research on the distribution and quantification of microplastics in aquatic environments, little research has focused on urban stormwater runoff. In urban environments, low impact development green infrastructures such as bioretention cells are often implemented to collect, infiltrate, and treat urban runoff. Bioretention cells consist of a depression in the ground filled with engineered media and covered with mulch and vegetation. While they are typically designed to reduce flooding, they are also able to reduce the concentration of some contaminants such as total suspended solids. Given that microplastics are a type of particles, we hypothesized that bioretention cells would be efficient at removing microplastics from urban runoff. Our study site was located in Vaughan, Ontario, Canada. Stormwater samples were collected over two years from the inlet and outlet of a bioretention cell receiving runoff from a recycled-tire pavement parking lot. The samples were sieved to 106 µm and counted visually before analysis by micro-Fourier Transfer InfraRed spectroscopy. With careful protocol development and validation, we showed that current sample sieving practices result in large errors in assigning microplastics to a given size fraction. likely due to the dominance of fibers (>70%) in our samples. Our results demonstrated high percent decreases in microplastic concentrations between the inlet and outlet of the bioretention cell. All size fractions together, we

found an overall 67-% reduction from 248 to 65 particles/L. The larger size fractions (500 μ m – 1mm, and > 1 mm) exhibited higher concentration reductions than the lower 300-500 μ m size fraction. Microplastic concentration in the bioretention cell inlet was proportional to the number of antecedent dry days and inversely proportional to the rainfall amount. This is the first comprehensive study demonstrating the potential for bioretention cells to sequester a large portion of microplastics from urban runoff.

ENVR 278

Limiting interactions between nano/microplastics and water filtration membranes using plasma surface treatment

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The contamination of worldwide waters and ecosystems by plastic litter has turned plastic pollution into a serious environmental problem. Among all plastic pieces, microplastic fragments and fibers constitute a real threat for aquatic species and human health. Although a growing number of studies have investigated the environmental impact of nano/microplastics, knowledge on the occurrence and behavior of nanoplastics (NPs) and nanofibres (NFs) in water is limited. Common analytical methods are not appropriate to detect and analyze NPs and NFs due to their shape and nanometer size. The main concern relies on the fate of NPs and NFs through water treatment plants since processes used to treat water can be impacted by the presence of these nano-sized fragments and fibres, such as ultrafiltration membranes. Membrane can suffer from fouling due to the adsorption of species on their surface which decreases their filtration performance, however, the fouling mechanism of NPs and NFs remains unclear. Investigating the fouling of NPs and NFs on filtration membranes is therefore necessary to develop a solution preventing fouling from occurring and keep membrane performance to a high level. The present work aims at studying the fouling of poly(ethylene) fragments and textile poly(ester) fibres on commercial ultrafiltration membranes. The membrane surface was subsequently enhanced by plasma polymerization to induce the repulsion of fragments and fibres from the membrane surface. Fouling mechanism was followed by measuring permeate water flux and turbidity measurements were combined to optical imaging to quantify the amount of fibres in water. Nanoparticle Tracking Analysis was used to quantity the amount of fragments in water. Membrane surface properties such as roughness and hydrophilicity were assessed before and after filtration to understand the impact of NPs and NFs on the structural and chemical properties of the membrane. Results showed that the plasma layer reduced the fouling of NPs and NFs by decreasing the amount of NPs and NFs adsorbed on the membrane which kept permeate water flux decline to a low value.

ENVR 279

Physico-chemical properties of styrene oligomers as new pollutants in the environment

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Polystyrene (PS), one of the representative plastics, is an environmental concern. The monitoring of styrene oligomers (SOs) as a possible indicator of PS pollution is important issue. However, there appears to be no or very limited information on both monitoring of SOs in drinking water and the physicochemical properties of SOs. Hence. this study is monitoring of SOs and the prediction of their physico-chemical properties. All samples in drinking water were often found to contain SOs such as styrene monomer (SM), styrene dimers (SDs), and styrene trimers (STs), in which these concentrations were in the range of 4.2 ~ 15.78 μ g/L, and these concentration distribution was mostly in the order of $\Sigma STs > \Sigma SDs > SM$. In addition, this study investigates the physico-chemical properties of SOs via EPI suite program based on the computational method. At a result, this study will help to understand the behavior of SOs present in the environment.

ENVR 280

Quantifying the weathering of aquatic plastic debris and the influence of weathering on pollutant sorption

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Plastics are a ubiquitous part of everyday life and a central challenge in the environment. Environmental stresses such as sunlight, temperature fluctuations, wet/dry cycling or microbial forces affect the longevity or degradation of plastics. Assessing the fate of plastics under these stresses allows us to accurately predict the service lifetime of plastics used in infrastructure (e.g., power cabling/solar panels) or evaluate the extent of the plastic pollution problem. This talk details the work of quantifying photochemical and thermal degradation mechanisms of plastics commonly found in aquatic plastic debris: polyethylene, polypropylene and polyethylene terephthalate. In this talk, I will focus on the development

of a methodological framework for characterization of the rates and yields of the chemical transformations within polymers, moving beyond traditional materials characterization techniques, in addition to characterizing and quantifying microplastic formation. Beyond the transformations of the plastics, we also began to unravel the role plastics and plastic weathering play on the ecosystem health by monitoring the sorption of model micropollutants to weathered plastics. Ultimately, this work strives to quantify the transformations and fate of plastics so as to design a predictive model of plastic behavior in the environment, which has implications for accurately assessing the burden of plastics on the environment but also allows for new polymer design.

ENVR 281

Effect of fabric type, washing conditions, and aquatic environment on the fate of microfibers released during home laundering

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Microplastics are small plastic particles with a size below 5 mm. They are generated from the fragmentation and wear of plastic objects, paints, textiles, tires, etc., They have been observed in freshwater and marine environments all over the world. They have been found in seafood, beer, tap water, sea salt, and human stools. They can adsorb pathogens and pollutants on their surface, and they might affect the growth and development of aquatic fauna. About 700 thousand tons per year of synthetic microfibers are released into the ocean, which is equivalent to 70 billion plastic bottles, and microparticles from home laundering are thought to be the main route. For that reason, to address today's concerns about microplastics pollution, the understanding of the fate of microfibers generated during home laundering in aquatic environments is critical. In our research, we studied the number and mass of microfibers released from polyester, cotton, and rayon fabrics in both actual home laundering equipment and also with а LaunderOmeter, an accelerated laundering laboratory device. Additionally, biodegradation of these materials was evaluated in simulated aquatic environ-ments, a local wastewater treatment plant (WWTP), lake, and ocean water, and analysis on the microbial communities before and after the experiments were made. In general, all

fabric types released micro-particles. It is estimated that 700,000 particles are released per wash load. Cellulosebased fabrics release more microfibers than did the polyester textile. Fabrics less resistance to abrasion like cotton are more susceptible to microfiber release and a strong correlation was found. However, the cellulosic fibers were found to readily degrade, whereas the polyester fibers remained essentially unchanged during the biodegradation experiments. Finishes on the cellulosic fabrics with finishes degraded also but at a slower pace relative to the untreated cellulose fabric. The cellulosic fibers were highly assimilated by the bacteria in the environment, whereas the polyester microfibers are expected to persist for very long times. Cellulosic materials promoted a microbiome with enriched microorganisms that can process cellulose whereas the polyester fibers behaved inertly with respect to the microbiome.

ENVR 282

Sorption behavior of antibiotics in water by virgin and aged micro-plastics

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the appearance distribution Recently, and of microplastics, as a new type of pollutant, in the global aquatic environment have attracted increasing attention. Because of its small particles, strong hydrophobicity, large specific surface area and mostly organic materials. micro-plastics can adsorb heavy metals and organic pollutants in the process of water migration, and produce joint toxicity after being ingested by aquatic organisms. Moreover, the interaction between microplastics and pollutants is a very complex process, which is easily disturbed by various factors, microplastics type, particle size, and pollutant type all affect the adsorption process. In this paper, the adsorption behavior of some typical antibiotics, was systematically studied by using different kinds of virgin and aged micro-plastics particle. The results demonstrated that with the increase of particle size, the maximum adsorption capacity and adsorption coefficient of tetracycline (TC) show a significant decreasing trend, with a slight fluctuation in the middle, which can be attributed to the interaction of specific surface area, porous structure, and hydrogen bond of micro-plastics. The adsorption kinetics of TC on PE might be depend on both intra-particle diffusion and boundary layer diffusion. The presence of Pb2+, Cr3+, Cd2+, and Zn2+ could significantly enhance the adsorption of antibiotic by microplastics, and the presence of Cu²⁺ could reduce the adsorption of TC by PE. Therefore, the surface properties of micro-plastics and the chemical properties of aqueous solution played an important part in the adsorption of TC. The adsorption abilities of aged PS and PVC were more than 123.3% and 20.4% higher, respectively, than the

corresponding pristine microplastics, and the adsorption ability of CIP was in the order aged PS > aged PVC > PVC > PS. The partition, hydrogen bonding and electrostatic mechanisms were the main mechanisms for adsorption, and hydrogen bonding was especially important in the mechanism for aged microplastics. Moreover, the adsorption capacity dropped sharply when the salinity increased. The results presented here fundamentally improve our under-standing of the environmental behavior of aged microplastics with hydrophilic pollutants in aqueous ecosystems, which is important for research on the toxicity of microplastics in combination with organic pollutants in real environments.

ENVR 283

Characterization of the nanoplastics fate from soil to ocean: Coupling *in situ* measurement with experimental investigation

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Nanoplastics (NPs) are defined as colloids that originate from the unintentional degradation of plastic. They have recently been detected in the North Atlantic Ocean and are characterized by a continuum in sizes ranging from 1nm to 1µm, associated to asymmetrical shapes and Brownian motion (ter Halle et al., 2017, Gigault et al., 2019). Since these particles could pose specific ecological and health risks, it appears crucial to describe their global environmental fate. In the life-cycle of a plastic debris, the terrestrial compartment is the main source and water is the main vector. As their final destination is the ocean, their transportation pathways from soil to marine system need to be elucidated in order to better evaluate their final impact on the environment and human health. Within the frame of different national and International projects, the last five years we focused our research on the understanding of the environmental fate of nanoplastics. The objective of this presentation is to demonstrate the analytical strategy (nanoplastics standards and analytical methods) that we developed to characterize nanoplastics in the environment and how this strategy is relevant to assess the life cycle of nanoplastics in the environment based on in-situ measurement coupled to experimental approach. On the different systems investigated, I will focus particularly on Mangrove swamp and soil system. Using a combined approach of asymmetrical flow field flow fractionation (A4F) coupled to light scattering (SLS) and pyrolysis - gas chromatography - mass spectrometry (PyGCMS), we isolated and demonstrated the presence of nanoplastics in soil and in Manarove water/sediment from 50 up to 200nm. largely heterogeneous in composition (PS, PVC, PE) and heteroaggregated with the natural organic matter (NOM). These results confirm those ones obtained in laboratory by reproducing the environmental features (and their dynamics) of these both systems and using various NPs standards with in-situ detection (IS-DLS). Definitely, the nanoplastics composition, size and structure (opened-structure) play a key role in their dynamics in these systems. Our results also demonstrated that these properties control the nanoplastics "trojan horse" property, and more specifically for Pb(II) (Davranche et al., 2019). Based on these results new orientations of our strategy were made and would be presented/discussed during the ACS meeting.

ENVR 284

Forgotten fungicide: Detection of strobin fungicides in minnesota waters

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In 2015, 10,000 dead fish washed up on a three mile stretch of the shores of the Whitewater River in Minnesota. When state and federal agencies analyzed the river for the cause of the event, no single contaminant could be determined to be the cause. Three strobin fungicides, however, were detected. These fungicides are known to be toxic to non-target organisms. Strobin fungicides are used extensively in agriculture both to control fungi, as well as to increase crop yields. The goal of this study is to test water and sediment samples from three forks of the Whitewater River for strobin fungicides to determine their presence and concentrations. To further understand their movement in the environment, concentration data are compared with water quantity and quality variables under base flow conditions and during rain events to see if wash off from nearby agricultural fields is a source into aquatic environments. While all samples tested yielded concentrations of almost all strobins studied, no correlations with storm event hydrographs, date, total dissolved solids or nutrients was observed. Samples taken during a storm events, however, showed higher overall concentrations of strobins, in some cases reaching 149 µg/L.

ENVR 285

Effect of pH on polyacrylamide degradation and methane production

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Polyacrylamide (PAM), widely used as a flocculant in wastewater treatment process. The existance of PAM in sludge discharged a remarkable amount of its toxic monomer acrylamide (AM) in the atmosphere and impose serious threats for human beings and the environment. The aim of this work was to investigate the PAM degradation and improvement of methane production by mesophilic AD under optimum pH value. Sludge used in study was collected from the secondary this sedimentation tank of (G) Municipal Wastewater Treatment Plant (China). The sludge was firstly concentrated by settling for 24 h at 4 °C. The laboratory analysis was done by 1L glass bottles that were used as fermentation reactors in triplicate at different pH (e.g., from 5.0 to 11.0) for 15-days batch tests. the reactors were fed with 800 mL of PAM-added sludge. The reactors were purged with nitrogen gas for 3 min to displace oxygen, and inserted with rubber plugs and gas bags were operated at 35 ± 1°C in rotary shakers at 165RPM, Main Characteristics of the experimental sludge were pH 6.54. TS(q/L) 23.35 ±0.27, VS(q/L) 17.84 ±0.19, TSS(g/L) 21.72±0.20, VSS(g/L) 15.88±0.14. Polyacrylamide (PAM) degradation during mesophilic AD at pH 11 was observed to be rapid. 74.3% PAM degradation occurred at pH 11 during 15 days of mesophilic AD. Fig.1. showed the results for methane production. It can be seen from fig.1, that methane yield of 135.6 -141.7 ml/g VSS was achieved at pH 11 whereas it was only 80.3 ml/gVSS in control. Methane degradation of 98.7 and 118.4 ml/g VSS at pH 5 and 7 was achieved. The methane yield was increased at pH 11 while at pH 5 and 7 it was declined. Though results for methane production at pH 7 were higher than at pH 5. The pH 11 stood most suitable for higher methane yield and PAM degradation. PAM degradation at pH 11 during mesophilic AD was 74.3% with a higher methane yield of 135.6-14.7ml/gVSS.



Figure 1: Cumulative methane yield at pH 5,7,11

ENVR 286

Chemically modified surfaces for the separation of non-polar organic contaminants from the water

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The separation of the oil and the organic contaminants from the water is the area of high interest. The water is continuously being polluted from the oil and the organic contaminants due to rapid industrialization and high energy demands. History has also revealed numerous oil spill incidents that severely damaged aquatic life and human life. The oil and the non-polar organic contaminants can be separated by selectively adsorbing or filtering them from the water with the help of the superhydrophobic surfaces. The surfaces are defined as superhydrophobic if they displayed the water contact angle greater than 150°. We modified various surfaces such as meshes and polyurethane with various low surface energy materials to achieve superhydrophobic surfaces that display the water contact angle of greater than 150°. To generate the superhydrophobic surface, at first step the surface roughness was generated and in the second step the surface was functionalized with the low surface energy material. The polypyrrole was catalytically polymerized on the surface of the poly-urethane that produced the superhydrophobicity by interacting with the low surface energy material such as octadecyltrichlorosilane. The developed material has displayed the maximum absorption capacity of 34 times (w/w ratio) for various non-polar organic contaminants. The separation efficiency was observed greater than 99%.

ENVR 287

Sequential anaerobic and aerobic bioremediation of commingled contamination of trichloroethene and 1,4-dioxane

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Commingled contamination of trichloroethene (TCE) and 1,4-dioxane (dioxane) has been perceived as one of the most prevalent groundwater remediation challenges. Considering their risks to human health and natural biota, an effective and cost-efficient treatment for *in situ* remediation is desired. In this study, we developed a biotreatment train that integrates anaerobic dehalogenation of TCE by SDC-9 and aerobic cometabolism of dioxane using a propanotrophic isolate Azoarcus sp. DD4. Microcosms were prepared with groundwater and bedrock samples from a TCE and dioxane impacted site located in New Jersey. All TCE (~20 µM) underwent a stepwise dehalogenation by SDC-9 anaerobically within 4 weeks to cDCE, then completely converted to VC after 16 weeks. After air exposure, the system was then converted into aerobic condition (DO > 8.00 mg/L and ORP > 50 mV). The subsequent aerobic microcosm demonstrated that dioxane can be completely removed by DD4 with propane from the initial 20 µg/L to below our method detection limit (0.38 μ g/L) in 4 weeks. Even better, DD4 simultaneously co-oxidized cDCE and VC accumulated during the previous anaerobic treatment, although the presence of these cVOCs delayed the degradation of dioxane. Pure culture studies further revealed cDCE has a greater inhibitory effect to DD4 than VC. Overall, anaerobic SDC-9 bioaugmentation followed by aerobic treatment with DD4 exhibited high efficiency and feasibility to clean up the mixed contamination of TCE and dioxane.

ENVR 288

Detection of oxyhalides using ion chromatography system coupled with single quad mass spectrometry verus conductivity detection

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Disinfection treatment is used to protect municipal water from potentially dangerous microbes. The most common chemical disinfectants are chlorine, chlorine dioxide, chloramine, and ozone. These chemical disinfectants can react with natural organic and inorganic matter in the source water to produce disinfection byproducts (DBPs), including oxyhalides (e.g., bromate, chlorate, etc.), that are potentially harmful to humans. The combination of ion chromatography and mass spectrometry (IC-MS) for oxyhalide detection can maximize the benefits of both confirmation. chromatography and mass This presentation shows the benefits of mass confirmation and higher sensivity as compared to traditional IC conductivity methods.

ENVR 289

Extraction of uranium from contaminated seawater using pistachio shells

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Anthropogenic and natural environmental activities have led to the release of heavy and/or radioactive metals into the groundwater and soils, such as uranium-238 (U-238). A radioactive heavy metal with a relatively long half-life of 4.47 billion years, uranium, present in aqueous media as the uranyl cation UO₂²⁺, is detrimental to living organisms located near groundwater and soils. Inorganic materials such as ion-exchangers, extractants, and nanoporous sorbents have been previously investigated to remove U-238. However, with regards to the removal of heavy nonradioactive metals from aqueous solutions, recent research focuses on using biodegradable, recyclable, and organic biological wastes. This study aims to determine whether pistachio shells, which fit these criteria, can be used for the removal of uranyl ions from aqueous solutions. Batch sorption experiments were performed where the effects of pH, contact time, temperature, and initial uranyl concentration on uranyl uptake were investigated. In order to approximate the adsorption mechanism of uranyl by pistachio shells, the experimental data were fitted to kinetic models and to isotherm models. pH had a varied influence on uranyl uptake whereby high uptakes occurred at pH 4 and at a slightly alkaline medium. In addition, uranyl uptake by pistachio shells increased with greater contact time, initial uranyl and concentration, temperature, plateauing at approximately 2 h, 30 ppm U, and room temperature, respectively. The experimental data best fit pseudosecond-order and intraparticle kinetics models, and a Freundlich isotherm model. The pistachio shells were successfully demonstrated to be viable adsorbents for uranium in actual seawater samples, with trends observed to be similar to those that were achieved in the batch sorption studies.

ENVR 290

Estrogenicity and toxicity of environmentally relevant mixtures of endocrine active compounds

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The presence of endocrine active compounds (EACs) in wastewater, surface water, groundwater and even drinking water has become a major public concern worldwide. Exposure to a mixture of EACs has been predicted to result in additive or possibly synergistic effects, which is difficult to detect by chemical analysis. Bioanalysis, such as using *in vitro* or *in vivo* methods, has the advantage of measuring the mixture effects of EACs, but this has not been well studied using environmentally relevant mixtures of EACs. In a previous study, we

evaluated the estrogenic effects of 11 EACs of high environmental concern using the in vitro yeast estrogen screen (YES) method. The full mixture of all these chemicals at an environmentally relevant ratio also showed weak anti-estrogenic activity. Further, EE2 did not have a prominent contribution to the estrogenic activity of the mixture. The objective of the current study was to evaluate the in vivo response to exposure to eleven endocrine active compounds (EACs) commonly found in surface water globally. We evaluated the mixture toxicity of three naturally occurring estrogens (17βestradiol-E2, estrone-E1 and estriol-E3), one synthetic estrogen (17α-ethinyl estradiol–EE2), one phytoestrogen (genistein-GEN), three phenolic xenoestrogens (bisphenol A-BPA, nonyl phenol-NP, octyl phenol-OP) and three phthalates (dibutyl phthalate-DBP, butyl benzyl phthalate-BBP and bis(2-ethylhexyl) phthalate-DEHP) on the model aquatic organisms, zebrafish. This is the same set of EACs we used in the in vitro YES study. We followed the OECD 236 guideline and the U.S. Environmental Protection Agency (EPA) method EPA/600/4-91/002. The zebrafish embryos were exposed to 6 dilutions of the EAC mixture, varying from 0.1 to 100 concentrations. times the environmental This presentation will discuss our results, and provide a holistic evaluation of the toxicity and estrogenic activity necessary to evaluate the risk of exposure to a mixture of EACs in the environment.

ENVR 291

Understanding inhibition of anammox activity by nitrite, sulfide and recalcitrant carbonsat a functional gene level

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The need to remove nitrogen from wastewater for most wastewater treatment plants around the world. Conventional removal of inorganic nitrogen is completed by nitrification-denitrification processes. However, these processes carbon and energy intensive. The other alternative technology is anaerobic ammonium oxidation (Anammox). Since its discovery in early 1990s, Anammox the ideal treatment technology in removal of TIN in wastewater. Anammox is efficient both in removal of TIN and energy consumption as well as no requirement for additional carbon as Anammox takes place in anoxic environment and Anammox bacteria are autotrophs capable of using CO₂ as their carbon source. Anammox process shows a promising future in full deployment to remove TIN couples with conventional activated sludge process to remove organic carbon in wastewater treatment plants. However, Anammox technology is in development stage requires more research to fully understanding the process. Anammox bacteria are known for their slow growth rates and widespread inhibited by

different factors including various chemicals that are commonly found in wastewater. However. the mechanisms behind this chemical inhibition are not well understood, especially at the molecular level. There are discrepancies in reported inhibiting concentrations of the chemicals, like inhibition by NO2⁻ ranges from 5 to 280 mg N/L depending on different research groups. Our study focuses on mechanisms of the inhibition of Anammox by NO₂⁻, S²⁻ and recalcitrant carbons at the molecular level by investigate of gene expression and metagenomic of the Anammox during the stress tests under an NSF Results show that ammonia funded project. monooxygenase gene expressions increased where the ammonia oxidation (contrary to amoA gene expression) was inhibited under external perturnations listed above. On the other hand, the expression of hyzrazine synthase enzyme responsible for the final step in Anammox decreased substantially. Currently, serum bottle tests are being conducted to evaluate the kinetics and response of other flanking community members. Preliminary result has shown that with our setup. Anammox activity was not affected by NO2⁻ up to 30 mg N/L but partially inhibited beyond this concentration upto 100 mg/L.

ENVR 292

Magnetized Douglas fir biochar for fast adsorptive removal of emerging contaminants in aqueous solutions

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Magnetic biochar is increasingly recognized as a multifunctional material in environmental applications and proper synthesis methodologies further increase the efficiency of the application. In this study, the fabrication of commercially available Douglas fir biochar with iron oxide precipitation by Fe³⁺/Fe²⁺ upon NaOH treatment was employed to study the removal of pharmaceutical contaminants. The surface morphology of the modified biochar was examined by SEM. TEM. SEM-EDX. XRD. PZC, and surface area measurements. The adsorption of three emerging contaminants; a stimulant (caffeine) and two anti-inflammatory drugs (ibuprofen and acetylsalicylic acid) from aqueous solutions at different initial concentrations, temperature, contact time, and pH values through batch sorption were investigated. External magnet is utilized for separating the magnetized biochar from contaminated solutions. Remediated solutions were analyzed using UV-Visible spectroscopy. Adsorption follows Langmuir-type isotherm. The data fitted well with pseudo-second order ($R^2 > 0.99$) rather than pseudo-first order kinetics model showing a more complex mechanism. According to the experimental data, it can be inferred that the basic characteristics of the surface favor the adsorption of contaminants. Regarding

pharmaceutical adsorption, herein obtained magnetic biochar presents an excellent low cost and environmentally friendly adsorbent for fast removal of pharmaceutical contaminants from the water with high adsorption removal efficiencies above 95%.

ENVR 293

Fast determination of haloacetic acids in drinking water

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As a result of current government proposals and developments, haloacetic acids (HAA) are in the focus of modern water analysis. The established methods use gas chromatography with electron capture detection (GC-ECD) or mass spectrometry (GC-MS). However, the drawback of these methods is the need for timeconsuming derivatization and multiple extraction steps. Can the analysis be simplified? Can sensitive and rapid detection be achieved without sample pretreatment? These questions are answered based on current developments in IC-MS/MS.

ENVR 294

Challenges and successes of green stormwater infrastructure in Detroit

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sewer overflows (CSOs) Combined and aged infrastructure have led to heightened awareness of the burdens and perils of stormwater management in Detroit. Furthermore, the failure points for much of these aged systems affect residents and businesses in vulnerable. low-income neighborhoods. On August 11, 2014, Detroit received a 500-year storm event that attracted national attention, flooded major highways, and resulted in catastrophic damages. Detroit Water and Sewerage Department (DWSD) has enforced a significant drainage fee of \$750 per month per acre of impervious surface for non-residential properties to provide funds for maintenance to their aging stormwater management system. As a result, many small businesses are motivated to offset this impactful drainage expense by implementing Green Stormwater Infrastructure (GSI) practices on their properties. Detroit poses a unique set of issues for GSI implementation, most notably the spatial constraints of small urban lots (average lot size of 0.13 acres) and a hydrogeologic setting that is typically low permeability clays. Among other challenges are funding, historic

building issues, unknown utilities, legacy contamination, soil management, and permitting agencies that operate as silos. However, DWSD will award up to an 80% total drainage reduction through the use of GSI, which has a movement of grassroots helped stimulated stakeholders including local nonprofits, community and neighborhood organizations, and small businesses. The presentation will touch on challenges and pitfalls of the GSI design and construction processes in Detroit through two case studies: PizzaPlex Infiltration Gallery and Southwest Detroit Business Association Rain Garden. Each case study will track the project from idea through the design/build phase. In addition, each case study will present details on the GSI drainage credit process, unique funding opportunities, and two years of operation, maintenance and monitoring (OM&M), culminating with a comparison of predicted design performance versus real world performance metrics for both practices.

ENVR 295

Quantifying heterogeneity of microbial community structure and the potential to remediate stormwater contaminants under varied biological and chemical conditions

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Pathogens and nutrients are consistently top polluters of waterbodies in the US according to the USEPA National Water Quality Inventory Reports. Stormwater runoff is a major source of these pollutants, and proper treatment of stormwater, including the use of filtration media, has improved water quality. Microorganisms are an important part of this remediation strategy and previous work has demonstrated that biofilm microorganisms can differ substantially in their remediation potential. To understand the remediation potential of stormwater filtration systems in natural settings, we must understand how the structure of microbial communities in stormwater vary in space and time, how this variation affects the biofilm structure in stormwater filtration systems, and how much biofilm community variation affects remediation. Limited studies have investigated either the variation of the community in stormwater or tested remediation potential using natural communities that are representative of variation from different potential treatment locations. Here we analyzed the natural bacterial community structure variability with 16S rRNA gene sequencing at a variety of runoff locations during both wet and dry events. We inferred potential pathogens and organisms associated with remediation functions (e.g. denitrification) from their sequence classification. We also tested whether contaminant removal (e.g. pathogen and nitrate pollution) was sensitive to inoculum community composition in experimental sand columns. Overall, we found high variability in stormwater related bacterial community

structures between rooftop, roadway, and Municipal Separate Storm Sewer outfall baseflow samples, but substantially less variability in potential for contaminant remediation. Inoculation of sand columns by environmental stormwater microbial communities provided significantly better pathogen removal than biofilm-forming isolate P. aeruginosa or non-inoculated controls. We have confirmed that complex environmental biofilm presence can improve the removal of contaminants. Differences in bacterial community inoculum taxonomy did not influence significantly variable pathogen removal in environments with similar chemistry. These methods can be applied to other contexts, as the results could be similar for other pathogens of concern, varied chemistry and environmental conditions, and drinking, waste and other water treatment systems.

ENVR 296

Urban green roofs as new habitats for birds...and bacteria: Yearlong water quality assessment of storm water runoff of the Javits Center green roof

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The Jacob K. Javits Convention Center is home to 6.75acre green roof, one of the largest in the United States. In addition to its role in mitigating the volume and peak flow of stormwater runoff, the green roof is becoming an urban wildlife refuge to birds, bats, and honeybees. The impact of the nesting seabirds, specifically herring gulls, on the water quality of the green roof's runoff water was largely unknown. In this study, the chemical and biological composition of the runoff water from the green roof was analyzed and compared to rainwater precipitation. Samples of runoff and precipitation were measured for concentrations of common nutrients, such as nitrate, nitrite, phosphorus, total carbon (TC) and non-purgeable organic carbon (NPOC). Total coliform, E. coli, and Enterococcus were tested via culturing assay while the quantification of potential opportunistic pathogens, including Legionellaspp., Mycobac-teriumspp., Campylobacterspp., and Salmonella sp. via real-time quantitative polymerase chain reaction (qPCR). All samples were obtained from during major precipitation events over an approximately 1-year period. Although the levels of nutrients, TC, and NPOC in the runoff were higher than the rainwater, the concentrations of these chemical species were relatively low. The measured bacterial counts and concentrations of potential opportunistic pathogen in runoff samples, however, were high in the runoff samples. These results indicate that further studies are needed to more accurately assess potential public health associated these risks with elevated concentrations of bacteria and opportunistic pathogens and to determine if reducing or preventing the presence of nesting birds improves the water quality of the runoff.

ENVR 297

Biodegradation potential of PCBs in stormwater sediment

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Urban stormwater runoff is a major contributor of nonpoint source pollution. Many toxic contaminants of concern (COCs) are associated with stormwater, including persistent organic pollutants (POPs) and heavy metals. Many of these COCs bind to particulate matter (PM) washed off with stormwater in urban areas. These include polychlorinated biphenyls (PCBs), and heavy metals (e.g. copper and zinc). Dissolved and PM-bound pollutants are addressed using different treatment mechanisms. This work addresses both PM-bound and dissolved phase COCs with focus on PCBs, Cu, and Zn. The ability for a bioretention cell to filter out PM-bound COCs can theoretically be explained by the filtration equation. However, dissolved phase constituents of stormwater are not included in this equation and are thus not accounted for. PCBs typically remain in the PM-bound phase (>90%), thus are mostly retained at the surface of the bioretention cell. This study determines the potential for PCB biodegradation in stormwater sediments. It is hypothesized that most biodegradation activity occurs in the bioretention cell, and stormwater sediments have the potential to transport PCB organohalide respiring bacteria to the bioretention cell. Sediments are collected and spiked with PCB 116 (2,3,4,5,6-PCB) to determine PCB biodegradation potential in stormwater sediments at various points in transport of sediments to urban catchments in bioretention cells.

ENVR 298

Could fungi improve resilience of stormwater biofilters?

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Stormwater is the nonpoint source of many emerging and persistent pollutants, which can exhaust the adsorption capacity of adsorbents such as biochar. However, soil microorganisms such as bacteria and fungi can degrade some of the pollutants on the adsorbents and biologically regenerate their adsorption capacity. Compared to

bacteria, fungi are designed to degrade persistent pollutants by enzymic activity, and they may withstand harsh environmental conditions. In this study, we examine the performance of a biofilter stimulated with the fungal community on filter media compared to the bacterial community. Batch experiments were conducted in the laboratory to quantify the fungal and bacterial degradation rate of contaminants. Column experiments were used to evaluate the effectiveness of different waste-derived media (mulch, iron filings, and biochar) on the stimulation of the fungal and bacterial community, and to examine the effect of fungi and bacteria to regenerate the removal capacity of the media. Our results showed that, among tested filter media, biochar-fungal biofilter is most efficient at removing nitrate, phosphate and heavy metals because of three coupled processes: (1) biochar increases the sorption capacity of biofilter during a rainfall event, (2) biochar stimulates the growth of fungal community more than bacterial, and (3) fungal community is better than bacterial community at regenerating the sorption capacity of exhausted biochar during rainless periods. The results improved the understanding of how biotic and abiotic processes in a stormwater biofilter can be coupled to improve its long-term performance. Overall, the experiments showed that fungal amended biofilter is a feasible technology to increase the resiliency of a biofilter.

ENVR 299

Applied mycology and integrated soil management in stormwater treatment

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Emerging knowledge on the interrelated roles of fungi, bacteria and plants in soil and water health has implications for almost every field of environmental management. Planting appropriate vegetation has long been established as an environmentally sustainable water treatment technique for stormwater management, while the application of fungi and bacteria is often less explored even though they can improve the health and functionality of plants and soils, making them more tolerant and resilient to environmental extremes. This talk will begin with a discussion of the importance of fungi to the fate, transport and transformation of chemicals in the environment and how they can be utilized in land and water management. This will be followed by a case study of a stormwater treatment basin design in Greenville, SC that will test the use of native plants, fungi, microbial inoculation, and mineral fertilization to enhance the ecological health, resilience and treatment performance of the basin. A collaboration between landscape architects, mycologists and environ-mental scientists, this project will explore the use of interdisciplinary applied ecology to achieve contaminant treatment goals while improving biodiversity, enhancing soil health and establishing an aesthetically pleasing park like atmosphere. Projects like this point to the potential of acheiving multiple environmental and cultural benefits as well as performing novel research when designing municipal stormwater infrastructure.

ENVR 300

Presence of polycyclic aromatic hydrocarbons in stormwater sediment and bioretention cells

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Polycyclic aromatic hydrocarbons (PAHs) are widely present in the environment, and they are often recalcitrant compounds thus making biodegradation a difficult task. These recalcitrant compounds have been recognized as carcinogenic to humans and can bioaccumulate in the food chain due to their hydrophobic characteristics. As a result, PAHs are of significant environmental concern. Due to the mentioned characteristics, PAHs can adsorp to particulate matter (PM) thus enabling transport by stormwater to receiving bodies of water, where they can cause environmental issues and pose risks of toxicity for humans. Bioretention cells are a Best Management Practice (BMP), which contain soil, organic matter and plants, and function by infiltration and biodegradation to treat contaminated stormwater. The removal of 16 EPA priority PAHs by a bioretention cell and the presence of PAHs degrading bacteria in the bioretention cell media and associated with the transported PM are investigated in this research. To achieve the treatment goals, PAHs concentration analysis, DNA extraction, Polymerase chain reaction (PCR) and sequencing of DNA from microorganisms in the bioretention media were performed. This study will assess the removal efficiency of PAHs based on the spatial distribution of PAHs in bioretention cell. PCR will be based on the gene that encodes PAH-ring hydroxylating dioxygenases (PAH-RHD) and PAH-ring cleaving dioxygenases (PAH-RCD). Overall the results will be used to design geomedia with enhanced treatment efficiency for the 16 EPA Priority PAHs.

ENVR 301

Multi-tracer experiment in a bioretention cell to study the transport of trace organic stormwater contaminants

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Bioretention cells are known to effectively remove contaminants such as suspended solids, dissolved nutrients and trace metals, though with variable efficiencies. Limited research has investigated the fate of trace organic contaminants in bioretention cells, especially under field conditions. To fill this knowledge dap, we performed a tracer experiment at a bioretention cell site to obtain in situ field data at a high time-resolution with the goal of investigating the underlying transport, transfer and transformation mechanisms of various stormwater trace organic contaminants. A tracer mixture containing bromide, rhodamine WT, nitrate, phosphate, benzotriazole, and four organophosphate esters (OPEs) was injected as a pulse at the inlet of a bioretention cell located north of Toronto. Outflow samples were collected at different time points and analyzed to generate tracer breakthrough curves for these compounds. The results showed that the bioretention cell had a short retention time of less than 2 hours. The calculated effective volume ratio was 0.39 suggesting the presence of dead volume and/or preferential flow paths. The recovery rate was 95% for the water tracer bromide, and 35 and 51% for nitrate and phosphate, respectively, indicating removal of these nutrient species. Recovery of benzotriazole was 71%, consistent with this compound sorbing poorly to soil. Samples were analyzed by high-resolution liquid chromatography mass spectrometry – Orbitrap. Benzotriazole transformation products that were signatures of biotransformation and phytotransformation were found, suggesting potential for transformation between events. This field tracer experiment produced valuable information on the performance of the bioretention cell in mitigating trace organic chemicals. These results demonstrated the need to use new design strategies to effectively sorb or transform these contaminants, such as increasing the retention time, incorporating soil amendments, and selecting specific plant species for better treatment performance.

ENVR 302

Effect of natural organic matter on urban stormwater trace organic compound and metal removal by polymer-clay composites

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Stormwater runoff is a major component of the urban water cycle and acts as a large nonpoint source pollution due to elevated concentrations of trace contaminants. In water-stressed cities, urban stormwater could provide a local water source to augment existing water supplies. stormwater Unfortunately, existing management practices are not suited for contaminant removal. Lowcost engineered materials applied to low-impact infiltration developments can greatly reduce contaminant loads to receiving waters. We have developed and characterized polymer-clay composites as a potential urban stormwater treatment media. Montmorillonite clays, which are highly effective trace metal adsorbents, were functionalized with either polydiallyldimethyl-ammonium chloride (PDADMAC) or poly(4-vinylpyridine-co-styrene) (PVPcoS) to enhance organic compound sorption using a simple, scalable synthesis method. Seven representative trace organics and six trace metals were employed to assess polymer-clay composite performance against biochar, a carbonaceous adsorbent previously examined for stormwater treatment. Batch and column filtration studies were conducted in a simulated stormwater matrix in the presence and absence of Suwannee River natural organic matter (NOM) to gauge media reactivity and longevity under realistic conditions, and the effect of NOM on contaminant removal. In batch studies, polymer-clay composites exhibited similar removal of perfluoroalkyl substances to biochar, but exhibited low affinity for polar pesticides and tris(2-chloroethyl) phosphate. Cr[VI] removal was greatest for PDADMAC-clay composites, while PVPcoS-clay composites displayed over 95% removal of Ni. Cd. and Cu. NOM decreased all organic compound removal, yet increased trace metal removal on clay composites due to sorption of complexed metals. This finding was contradictory to previous studies reporting enhanced organic compound sorption via Aldrich humic acid complexes. Polymer-clay compositeamended columns displayed greater or equal trace metal removal to biochar, while biochar-amended columns exhibited superior removal for all trace organics. Polymerclav composites did however exhibit significantly higher saturated hydraulic conductivity relative to biochar which is advantageous to prevent clogging or when rapid infiltration is needed. We estimate that under typical urban stormwater conditions, the clay composites will remove contaminants for at least 20 years before replacement is required.

ENVR 303

Biofilter fingerprinting: Effluent suspended particles as indicator biofilter performance assessment

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Implementation of stormwater infrastructures, an integral part of urban water sustainability, is slow due to a lack of reliable diagnostic tools that can predict the performance of stormwater infrastructure. The performance of biofilters is typically assessed based on the removal of dissolved pollutants, which vary widely. This method is unreliable to predict both short-term and long-term removal. Unlike the concentration of dissolved pollutants, biogeochemical properties of mobile particles can vary predictably and slowly in response to the conditions they are exposed to. The aim of this study was to establish a mechanistic link between the removal of pollutants and the properties of particles mobilized from biofilters. To examine if the mobile particles carry the chemical and biological signature of the conditions in biofilter and removal processes, we examined a variation of mobile particle properties with particles in stormwater feed and the corresponding removal of pollutants. Results show that the surface chemistry and the microbiome on the colloidal material closely matched with that of the biofilter media, not the stormwater. These properties of the colloidal material were also unique to each type of media in the columns and their exhaustion state. Thus, the colloidal material can be used as an indicator of the biochemical processes that occur inside the biofilter. The results of this study will be used to develop a diagnostic procedure to map the properties of the colloidal material with the reasons for the loss in biofilter performance.

ENVR 304

Column and batch studies exemplifying the reductive decomposition of perfluoroalkyl substances by NiFe⁰ nanoparticles synthesized onto activated carbon

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In recent years, different reductive techniques have been evaluated for treatment of per- and polyfluoroalkyl substances (PFAS) particularly due to the limited to negligible ability of oxidative processes to attack perfluorooctane sulfonate (PFOS). Although UV-activated sulfite and similar approaches are showing reductive transformation of PFAS including PFOS, such approaches are not amenable for use in-situ. In addition, most of these reductive approaches like vitamin B12 can only target branched isomers of PFOS (Br-PFOS), and not linear PFOS (L-PFOS), the most dominant and resistant isomer to attack. We found that one of the most effective PFAS reductive transformation technology amenable with in-situ potential and capable to transform both L- and Br-PFOS is bimetal zero valent iron particles

(nFe⁰) with a Ni catalyst synthesized onto activated carbon (AC). Here we present data from both column and batch studies using nNiFe⁰-AC to mineralize perfluoroalkyl sulfonates C4-C8) (PFSAs, and perfluoroalkyl carboxylates (PFCAs, C4-C8) as well as 6:2 and 8:2 fluorotelomer sulfonates in single solute solutions and mixtures at temperatures up to 60°C. Batch studies were done in nNiFe⁰-AC:solution ratio of ~0.4 g:20 mL at reaction times up to 5 days. For column studies, columns were packed with a 1:10 nNiFe⁰-AC:sand mix and conducted with flow rates that translate to ~ 0.2 to 2 d residence times. In batch systems at 60 °C, ~50% of the PFAS initially presented was transformed with fluoride and sulfite generation with up to 90% being mineralized. Interestingly, batch experiments at 50 °C led to the highest PFOS transformation of ~90% which was confirmed by higher generation of fluoride and sulfite compared to 60°C. However, decreasing temperature further to 40°C led to no PFOS transformation. In addition to temperature, the ionic composition in mixtures also impacted PFAS transformation rates, which will be thoroughly discussed later. Overall, the experimental overview and results will be summarized for both batch and column studies including degradation magnitude for different PFAS, kinetic rates of decomposition for PFOA and PFOS, formation magnitude for fluoride and sulfite, screening for different organic transformation products, efficiency of PFAS degradation in batch versus column systems and the effect of the solution matrix on PFAS transformation.

ENVR 305

Influence of chemical structure on hydridefluorination activity of poly- and perfluorocarbons by zeolite supported Rh catalysts

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Poly- and per-fluorocarbons (PFCs) are manufactured and used for various purposes such as fire-fighting applications, medicine, cosmetics, lubricants, etc. With increasing industrial use of the fluorochemicals, there has been a growing concern for their impact on human health and fate in the environment. Their strong C-F bonds particularly make them recalcitrant in the water and wastewater treatment processes. Therefore, there have been many studies to remove C-F bonds from PFCs. Among them, catalytic hydrodefluorination is a promising way to sustainability treat PFCs. While C-F bonds in few fluoroarenes such as fluorobenzene are known to be reduced to C-H bond in the presence of aluminasupported Rh catalyst, the applicability of Rh-based catalyst for poly- and perfluoroalkyl groups is not explored. In this study, we have evaluated the applicability of a novel zeolite-supported Rh catalyst for their reductive treatment of a class of poly- and perfluoroalkyl group

substituted aromatics using H₂ as a reductant under mild aqueous conditions (1atm of H₂ and ambient temperature). First, we have explored the influence of solution pH on reaction kinetics and reduction pathway of fluorobenzene. While defluorination was the major reduction pathway at pH 7 with defluorination yield of 95.9%, increased concentrations of fluorocyclehexane was monitored at acidic condition (i.e., pH 2) suggesting hydrogenation also becomes an important reduction pathway as pH decreases. Second, we have also quantified the reaction kinetics and defluorination yield of fluoroarenes with various poly and perfluoroalkyl substituents such as difluorobenzene, difluoromethyl benzene, trifluoromethyl benzene, and pentafluoroethyl benzene. Kinetic results were used to develop a linear free energy relationships (LFERs) model to elucidate the relationship between catalytic reactivity and structure of perfluorocarbons.



ENVR 306

Reductive defluorination and removal of aqueous fluorinated pharmaceuticals using heterogeneous alumina supported bimetallic catalysts

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Fluorinated pharmaceuticals are of increasing interest among pharmaceutical industry because they have improved pharmacological properties compared to their non-fluorinated analogues without significantly altering their sizes and shapes. With their growing uses, fluorinated pharmaceuticals such as fluoxetine have been detected in natural and engineered water systems. While most pharmaceuticals can be transformed to recalcitrant products via advanced oxidation technology, C-F bonds in fluorinated pharmaceuticals do not readily break up and only limited study is available on toxicity and fate of fluorine-containing intermediates in the environment.

There is a need for a novel treatment process that can defluorinate and transform these contaminants. In this study, we firstly report the feasibility of heterogeneous bimetallic catalysts (i.e., Pd-Rh/Al₂O₃, Rh-Pt/Al₂O₃, Pd-Pt/Al₂O₃, Pd-Ru/Al₂O₃, Ph-Ru/Al₂O₃, and Pt-Ru/Al₂O₃) for reductive defluorination and degradation of four fluorinated pharmaceuticals (i.e., Fluoxetine (FLX), Flunixin (FX), Levofloxacin (LFX), and Sitagliptin (SGT)). Kinetic experiments of reduction and defluorination of fluorinated pharmaceuticals were conducted using monometallic catalysts of Pd, Rh, Pt, and Ru and bimetallic catalysts of combinations of these metals in the presence of H₂ as reductant. The degradation products and intermediates were determined using analytical instruments such as LC-MS and GC-MS. Different reduction pathways were observed for different metal combinations and Pd-Ru bimetallic catalysts exhibited fastest reduction kinetics compared to other catalysts. A series of characterization techniques such as fieldemission TEM, H₂-pulse chemisorption, and X-ray photoelectron spectroscopy were performed to investigate physicochemical properties of catalysts and their changes after the reaction. We have also investigated effect of various environmental parameters (e.g., metal loading, catalyst loading, and pH) on the catalytic activity as well as longevity of catalyst over repeated cycles of reduction experiments.

ENVR 307

Degradation of perfluorooctane sulfonate by subbandgap irradiation of hydrogen terminated detonation nanodiamond

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The extraordinary stability of the C-F bond imparts many commercially useful properties to poly- and per-fluoroalkyl substances (PFASs). Among the properties imparted by the stability of the C-F bond is a high resistance to degradation via traditional oxidative/reductive processes. As a consequence, PFAS is a persistent contaminant upon environmental exposure, especially in water. In this work, we examine the impact of nanodiamond photochemistry on the degradation of one of the more resilient in the class of PFASs, perfluorooctane sulfonate (PFOS). Using nanosecond transient absorption we find that hydrated electrons result by photodetachment from hvdrogen-terminated (negative electron affinity) detonation nanodiamond (HDND) suspensions in water upon sub-bandgap (266nm) irradiation. Hydrated electron photogeneration from oxygen-terminated (positive electron affinity) detonation nanodiamond (ODND), on the

other hand, is not observed. The transient absorption data suggest the presence of an interaction between PFOS and HDND and, more so, an interaction between PFOS and the hydrated electrons. Finally, we show that prolonged sub-bandgap (254nm) irradiation of aqueous HDND in the presence of PFOS leads to full decomposition of PFOS by reductive fragmentation, consistent with hydrated electron reductive chemistry.

ENVR 308

Degradation of main PFASs used as alternatives to PFOS/PFOA in China: Kinetics, intermediates and mechanism

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Despite of the fact that China is still producing and using PFOS and PFOA, various PFASs as the alternatives have been introduced into the Chinese market in recent years. Some of them are guite different in structure from those used in Europe and America. Several typical examples include: F-53B (CIC₆F₁₂OCF₂CF₂SO₃K, CAS no.: 73606-19-6) as the chrome mist suppressant, OBS (C₉F₁₇OC₆H₄SO₃Na, CAS no. 70829-87-7) as the surfactant in fire-fighting foams or recovery aids of acidfracturing fluid, hexafluoropropylene oxide trimer acid (HFPO-TA, C₉F₁₇O₄H, CAS no. 13252-14-7) and perfluoropolyether carboxylic acids (multiether PFECAs, $CF_3(OCF_2)_nCOO$, n=2-4) as the emulsifiers in fluoropolymer production. These alternatives will enter into the environment via the wastewater discharge from the above processes. However, these chemicals have not been registered in China, and their environment relevant properties are not available. Considering the persistence of PFASs, it's essential to investigate their degradability especially in aqueous phase. In the present study, these main China-specific alternatives to PFOS and PFOA were investigated for their degradation under the conditions of UV/persulfate oxidation and UV/sulfite reduction. Kinetics, intermediates and mechanisms were studied in detail. Quantum chemical calculations were executed for a better understanding of the degradation mechanisms and pathways of target molecules. For comparison purpose, some isomers of these chemicals were also included in the study. In most cases, the oxidative degradation was incomplete with stable intermediates as the endpoints, while the reductive degradation based on the hydrated electron generated in UV/sulfite can lead to nearly complete conversion of organofluorine into inorganic fluoride. The chain length, the oxygen atoms in the carbon chain, the side chain, and unsaturated bond have significant effects on the degradability. Matrix effects in raw wastewater (e.g. chrome plating wastewater) on the degradation can be overcome by the optimization of reaction parameters. UV/sulfite system seems to be promising to remove these alternatives at the industrial scale.

ENVR 309

Elucidating structure-reactivity relationships for the redox degradation of major categories of PFAS pollutants in water

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This presentation will summarize our recent progress on the elucidation of structure-reactivity relationships for the reductive and oxidative degradation of major PFAS categories (e.g., perfluorocarboxylic acids, perfluorosulfonic acids, fluorotelomeric acids, and perfluoroether carboxylic acids) in various chain-lengths. Reaction mechanisms and pathways are elucidated through PFAS degradation kinetics, theoretical calculations, and transformation product analyses. This talk will also discuss some previously proposed and frequently cited reaction mechanisms that are different from our experimental findings.

ENVR 310

Effects of geochemistry on photo-reductive treatment of per- and polyfluoroalkyl substances (PFAS) by hydrated electrons in groundwaters impacted by aqueous film-forming foam (AFFF)

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Recent studies have shown widespread contamination of per- and polyfluoroalkyl substances (PFAS) throughout the U.S. due to historical use of aqueous film-forming foam (AFFF) in fire training activities at military and municipal sites. Though AFFF effectively extinguishes hydrocarbon fuel fires, formulations contain PFAS, known to be highly recalcitrant, bioaccumulative, and persistent in the environment. Because natural biological and abiotic processes cannot effectively degrade PFAS and conventional technologies can become cost-prohibitive, developing advanced PFAS treatment strategies is critical. Photochemical approaches such as the UV-sulfite process (i.e., UV_{254} + Na₂SO₃) have recently been

explored for PFAS destruction. The UV-sulfite process produces highly reactive hydrated electrons (e_{ag} ; $E^0 = -$ 2.9 V) which have shown promising reactivity with PFOS and PFOA. However, little is known about efficacy in treatment of complex PFAS mixtures resulting from AFFF wherein over 50 PFAS classes and 100s of individual PFAS compounds have been discovered in formulations. Additionally, the impacts of the complex geochemical conditions in AFFF-impacted groundwaters on UV-sulfite treatment is poorly understood. In this study, the UVsulfite process was applied to multiple AFFF-impacted groundwaters to investigate the efficacy of PFAS treatment in relevant geochemical matrices. High resolution mass spectrometry was used to quantify a diverse set of PFAS structures. The effects of dissolved organic matter (DOM), cations (e.g., Ca²⁺), and oxyanion co-contaminants (e.g., NO3) on PFAS treatment will be discussed. Initial results show that PFOS and perfluorocarboxylic acids (PFCAs, including PFOA) are readily degraded during treatment. Additionally, results show PFAS reactivity can be enhanced or diminished in selected groundwater matrices depending on compound class. Relationships between constituent concentrations and degradation rates will be explored. Insights and challenges for future water treatment will also be discussed.

ENVR 311

Chemical destruction of PFAS sorbed on ion exchange resins: Solution to the PFAS pollution in water?

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Per-and poly-fluoroalkyl substances (PFAS) represent a family of emerging and persistent contaminants in water. Very few chemical and biological methods can efficiently remove them from water. Although adsorption with ion exchange resins or activated carbon is recognized as a technically effective PFAS treatment option, the processes are restricted, at a minimum, in two aspects: 1) they only transfer PFAS from one phase to another, but cannot provide an ultimate solution to the toxic contaminants; and 2) they suffer from costly regeneration. In this study, laboratory scale tests were performed to explore chemical destruction of PFOA, a representative PFAS chemical, sorbed on anion exchange resins through chemical oxidation using advanced oxidation processes (AOPs) or through chemical reduction achieved by advanced reduction processes (ARPs). PFOA saturated anion exchange resins (Amberlite IRA 910) were treated using a sulfate radical based AOP (heat/persulfate) and a UV/sulfite ARP system, separately. As the reactions proceeded, fluoride was released into water, indicating the destruction of sorbed PFOA. The extent of fluoride release replied upon solution

chemistry (e.g. pH) and operating conditions (e.g. chemical doses). Either of the chemical processes was capable of recovering the resin adsorption capacity for PFOA, so that the resin could be repeatedly used for continuously capturing aqueous PFOA. These encouraging results demonstrate that AOP or ARP is a promising on-site resin regeneration process, which can serve as a basis for the development of technically and economically efficient PFAS treatment designs.

ENVR 312

Degradation of short, medium and long-chain PFASs in water using high-frequency ultrasound and effect of process variables

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Per- and polyfluorinated chemicals (PFASs) are known to be environmentally persistent, toxic, bioaccumulative, and are being widely detected in the environment. A number of US state agencies have, or are in the process, of regulating these chemicals, and the US Environmental Protection Agency (EPA) has issued a drinking water advisory limit of 70ng/L for perfluoro-octanoic acid (PFOA) and perfluoro-octane sulfonic acid (PFOS). This study evaluates the effectiveness of high frequency ultrasound process for the removal of short-chain (PFPrA- C_3 , PFBA- C_4 , PFPeA- C_5), medium-chain (PFHxA- C_6 , PFHeA-C₇, PFOA-C₈), long-chain (PFNA-C₉, PFDA-C₁₀, PFUDA-C11, PFDDA-C12, PFTrDA-C13, PFTeDA-C14, PFHxDA-C₁₅, PFODA-C₁₈) and sulfonic (PFBS-CS₄, PFHxSA-CS₆, PFOS-CS₈) PFAS. Process parameters such as the presence of gases, temperature, frequency, power density, and initial concentration were evaluated. Sonolytic degradation was found to be dependent on frequency and PFAS chain length. High degradation of all the PFAS was observed at ambient temperature, neutral pH and without sparging any gas, and at a power density of 250W/L. More than 90% removal of all the PFAS (with an exception of PFTeDA (85%), PFBS (67%) and PFBA (75%)) was observed in 120 minutes using a power density of 250W/L. Experimental sonolytic activation energies were found to be significantly lower than the actual bond dissociation energy of the C-F bonds. This process could be very attractive for small volume waste treatment and could be further improved by optimizing the reactor geometry. Michaelis Menten models were developed for the sonolytic degradation of the PFAS, and will also be presented. Operating costs for the process will also be presented.



ENVR 313

Microwave-enhanced membrane filtration for degradation of PFASs

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In recent years per- and poly fluorinated alkylated substances (PFASs) have been increasingly studied as a new class of global pollutants due to the broad historic uses in diverse industrial products. PFASs are extremely resistant to natural weathering and degradation processes such as hydrolysis, photolysis, and microbial degradation. Microwave-assisted membrane (MWM) filtration was explored to facilitate the degradation of refractory PFASs from wastewater. Microwave-absorbing catalyst (e.g., BiFeO₃) coated on the ceramic membrane produced hydroxyl radicals that enhance oxidative degradation of PFASs (specifically PFOA as a model molecule). MW irradiation was selectively absorbed by catalysts and hydrogen peroxide to produce "hotpots" on membrane surface that promoted generation of nanobubbles, which prevented membrane fouling and assisted degradation of PFASs. The contributions from physical separation (size exclusion and sorption or chemical binding with ceramic membrane) and MW-Fenton-like degradation to the PFASs removal were analyzed and quantified by switching microwave irradiation "on" or "off". Furthermore, the LC-QQQ mass spectrometry was used to identify degradation byproducts (e.g., shorter-chain PFASs with C7, C6, C5, C4 and C3) and confirmed the transformation pathway of PFASs.



Figure: Experimental set-up for microwave-assisted membrane filtration system4

ENVR 314

Atom probe tomography (APT) and its potential applications in nanogeosciences

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Atom probe tomography (APT) analysis of materials is an established technique for atomic level compositional analysis. Extensive research has been performed on many alloys, compounds, multi-layered thin films, integrated circuits, and even polymers. The use of APT in Earth Sciences is still emerging, yet results are encouraging for multiple applications in nanogeosciences. The aim of this talk is to present a general introduction of APT, including principles and sample preparation, and to explore potential geoscience applications for nanogeochemistry based on published data and our work at the University of Alabama, mainly related to biomineralization processes.



APT 3D exploration of the distribution of chitin fragments inside a single calcite crystal

ENVR 315

Illuminating the connections between the environmental nanosciences and the trace element biogeochemical sciences

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The environmental and geoscience research community has invested substantial efforts over the past two decades in understanding the environmental health and safety (EH&S) risks of engineered nanomaterials. As the field has matured, researchers are now asking: What have we learned from all of this environmental nano research? What is next? Naturally occurring and engineered nanomaterials in the environment share similar processes that affect their distribution, transformation, and bioavailability. Moreover, research tools used in one context, such as evaluating the impacts of synthetic nanomaterials, can be directed toward understanding the environmental distribution and reactivity of naturally occurring and incidentally produced nanoparticles. This presentation will describe the broader relevance of EH&S research for nanomaterials, and in particular, how this work illuminates biogeochemical processes controlling trace elements in earth systems.

ENVR 316

Lateritic nanophases: Witnesses of the fragility and promises of tropical soils

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Laterites cover about one third of the Earth surface. corresponding to extreme weathering conditions under present and/or past humid tropical to sub-tropical climates. Leading to thick weathering profiles, such intense weathering causes a massive exportation of Si, soluble elements and reactive natural nanophases. This mobility is enhanced by the presence of organic matter (humic colloids), as illustrated in the Amazon basin: the concentration of AI- and Fe³⁺- bound organic nanos rises from soils to river colloids, with a specific spectroscopic signature. Such a translocation and massive exportation of chemical elements to rivers results in a progressive and irreversible degradation of tropical soils. On the other hand, surface reactions on lateritic minerals are at the origin of the concentration of strategic metals, such as heavy REE's adsorbed on clay minerals or Ni, Co, and Sc adsorbed on or sequestered within lateritic Fe- and Mnoxides (60-70% of the world's Ni resources). This has recently illustrated by the unusually high-grade Sccontaining laterites from Eastern Australia. Concentration processes are often mediated by Fe-oxide nanophases, but the surface reactivity and the intrinsic nanoscale porosity of lateritic minerals play also a major role. Such diversity underlines the importance of a multiscale approach based on various spectroscopic and microscopic approaches. This will be helpful to model and predict the concentration processes of strategic elements in this new kind of mineral deposits that will receive increasing attention due the growing demand of strategic metals.

ENVR 317

Influence of nanoparticle coatings on corona composition

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Upon introduction into environmental or biological fluids, nanoparticles rapidly aquire coatings of natural organic matter or biomolecules, commonly referred to as coronas. Acquisition of coronas alters the electrokinetic and hydrodynamic properties of nanoparticles and can affect their aggregation state. The surface properties of nanoparticles in environmental and biological milieus thus diverge from those that the nanoparticle was engineered impacting their to possess, interactions with environmental and biological surfaces. We have demonstrated that the initial surface chemistry of nanoparticles governs the ensemble of proteins that associate with them, which in turn influences subsequent interactions with model biological membranes. We will discuss recent work on the influence of nanoparticle surface chemistry on the composition of acquired coronas.

ENVR 318

Quantifying CeO₂-(nano)-particles from anthropogenic activities in sewage sludge samples

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Cerium (Ce) in sewage sludge originates from either anthropogenic activities (anthropogenic Ce, dominantly present as CeO₂), or from natural inputs (natural Ce, primarily associated with minerals such as monazite or allanite). In dried biosolids, Ce concentrations can range from a few tens to a few hundreds of milligram per kilogram. It has been suggested that the fraction of anthropogenic Ce in biosolids, often present in nanoparticulate form, can be separated from natural Ce based on the Ce:La ratio or based on the oxidation state of Ce in (bulk) biosolids. Using analytical electron microscopy, synchrotron X-ray absorption spectroscopy and bulk inductively coupled plasma mass spectrometry analyses, however, we reveal that neither the oxidation state of Ce, nor the Ce:La ratio in biosolids are sufficiently distinct to distinguish between anthropogenic and natural Ce. However, other rare earth elements (REE) such as Dysprosium, Erbium and Europium, which are also associated with Ce-bearing minerals, proved as much more robust tracers for natural Ce inputs into wastewater systems. Based on distinct Ce:REE ratios, anthropogenic Ce fractions ranging from 10 - 90% were calculated for biosolids collected from various wastewater treatment plants. Such results will allow an estimation of the amounts of anthropogenic Ce discharged to wastewater systems and may eventually be used to 'validate' or calibrate respective results from mass flow models.

ENVR 319

Investigating toxicity of particulate emissions from combustion power plants

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Thermal power plants using coal and biomass as fuel represent major sources of fine and ultrafine particulate matter (PM) in the atmosphere. The interactions of PM with the atmosphere and the solid Earth, its hydrosphere, and its biosphere, as well as the impacts on human health not only depend on particle size but also on other PM properties, including chemical composition, structure. surface area, and solubility of the individual particles, which therefore need to be characterized in detail. This presentation will give an overview of combustion-derived PM emissions and discuss their various environmental and health impacts. The focus will be on the characterization of select types of solid particles, which are common constituents of emissions from coal and biomass combustion (e.g., metal sulfates, magnetite), as well as on the in-vitro cytotoxicity, genotoxicity, and uptake/translocation of these particles in human lung cells (alveolar epithelial A549, bronchial epithelial BEAS-2B).

ENVR 320

Nano-scale mineralogy of a rare earth element-rich Manchester coal lithotype, Clay County, Kentucky

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Many Eastern Kentucky coals have high-REE contents. with lithotypes of the Pennsylvanian-age Manchester coal rivalling some of the richest concentrations in the Fire Clay coal, arguably the premier resource in terms of concentration and aerial extent. A >2000-ppm-REE (ash basis) Manchester coal lithotype, analyzed first by scanning electron microscopy, was selected for detailed transmission electron microscopy/ energy dispersive xray spectroscopy/ fast Fourier transform/ selected area electron diffraction investigation. The grains, seemingly fragments of one or more 2-3-µm spherical nodules, proved to have a phosphate (florencite?) rim with a light REE (La through Sm) and Gd association. The core of the nodule and the region surrounding the nodule is Al-Si rich but the mineralogy could not be determined. The nodule may have be a mineralized coprolite, the product of the microfauna inhabiting the peat.

ENVR 321

Withdrawn

ENVR 322

Still plenty of room at the bottom: Nanoscience in geochemistry beyond nanoparticles

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In writing about nanomaterials, Professor Hochella once wrote about how "There's plenty of room at the bottom: Nanoscience in geochemistry" (Hochella, 2002). I will show how nanoscale concepts are also important to other areas of geochemistry, with lessons for treating tank wastes and dealing with flowback water from hydraulic fracturing. For example, reactivity in complex aqueous solutions deviates from idealized solutions, even after accounting for status-quo activity-concentration relationships. This reactivity is hypothesized to be due to a change in the extended solvation structure around ions and leading to competition for water molecules and varying reactivity. Examples of changing reactivity include ion pair formation equilibrium constants, reaction mechanisms of ion association, induction times for precipitate nucleation and phase selection. In the second half of the talk, I will show how nanoporous materials are ubiguitous in the subsurface, and even constitute the majority of pores in shales. In a mirror image to nanoparticles, nanopores can have anomalous reactivity relative to their larger counterparts. Documented cases include nucleation of materials, ion selectivity, performing phase selection and inhibiting nucleation in cases. It is

hypothesized that the anomalous reactivity in nanopores is due to the high ratio of mineral-water interface area relative to fluid volume, and this drives changes in interfacial water structure within the nanopore, a similar effect to concentrated solutions. In both of these cases, nanoscale changes lead to macroscopic differences in reactivity. In other words, there's still plenty of room at the bottom!

ENVR 323

Reactive interfaces in engineered clay barriers

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Clays are natural nanomaterials used for many purposes, e.g. as engineered barrier in geological repositories for nuclear waste. There, swelling clays may be in contact with other materials (cement, steel) displaying high reactivity towards clay. This leads to complex interface reactions and structural and mineralogical changes affecting the sealing properties of clay barriers. To address this issue we have investigated iron/clay and cement/clay interfaces having reacted over several years (max. 18 years) in small-scale laboratory and large-scale field experimental settings using a multi-method approach. Both spatially resolved (SEM/EDX, µ-Raman, µ-XRD, x-ray CT) and bulk methods (XRF, XRD, Mössbauer) have enabled to quantify small-scale elemental and mineral compositions and to identify newly formed species on both sides of the original interface and microscale changes in the pore structure. On this basis reactive transport models have been developed to improve the understanding and prediction of the long-term evolution of engineered clay barriers.

ENVR 324

Development of heterogeneous advanced oxidation processes for the removal of contaminants of emerging concern in water and wastewater

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Contaminants of emerging concern (CECs) are increasingly being detected in drinking water supplies and treated wastewater effluent, which may pose risk on human and ecological health. Moreover, the transformation products of these chemicals during and after the water treatment processes might have greater cytotoxicity than the parent compounds. Various treatment technologies are developed to remove these

CECs from water and wastewater. Advanced oxidation processes (AOPs), which are based on the generation of reactive species, have been gaining significant popularity for the treatment of CECs. This presentation will introduce different types of heterogeneous AOPs catalyzed by nonmetal doped titanium dioxide (TiO₂), bismuth tungstate (Bi₂WO₆), and ferrites nanomaterials. The novel approaches for synthesizing these materials and their unique properties and enhanced activities will be discussed in detail. Kinetics of catalytic removal of several categories of CECs such as pharmaceuticals and personal care products (PPCPs), pesticides, herbicides, cyanotoxins, and industrial chemicals will be presented. In addition, degradation pathways and mechanism of pollutants removal by different heterogeneous catalytic systems will be shown. The generation of reactive species such as reactive oxygen species, reactive sulfur species will be illustrated. Finally, the influence of operation conditions and water parameters on the removal efficiency will be evaluated.

ENVR 325

Curious incidences of PFASs at environmental interfaces impacted by aqueous film forming foams

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Many per- and polyfluoroalkyl substances (PFASs) are surface-active-agents, designed to impart properties of oil and water repellency to surfaces of consumer products and to lower the surface tension of aqueous commercial solutions. Given their surface-active nature, PFASs naturally accumulate at interfaces including air-water and oil-water interfaces in the vadose zone of the subsurface and in surface water bodies. Recent experimental and modeling work quantifies the fluid-fluid interfacial adsorption coefficients (K_i) and the surface excess (Γ) at the air-water interface. Solution chemistry and PFAS structure impacts interfacial partitioning. Discharge of groundwater impacted by aqueous film forming foam (AFFFs) results in the release of PFASs to surface waters. Movement of PFASs from groundwater to surface with subsequent partitioning to the water-air interface results in the formation of surface microlayers and foams containing PFASs. Enrichment of long-chain PFASs in the surface microlayer and foams on surface water is due to the increasing molar volume and hydrophobicity of the longer-chain PFASs, which have larger K_i and Γ values. The presence and potential implications of PFAS in foams and surface microlayers will be discussed. Engineering foaming approaches that capitalize on the foaming

potential of PFASs will also be discussed as a remedial technology under evaluation for removing PFASs from AFFF-impacted waters.

ENVR 326

Combating the spread of antibiotic resistance in water systems: Surveillance and risk

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Antibiotic resistance is increasingly being recognized as an environmental problem and there is an urgent need to identify and quantify relative contributions of various sources to the emergence and spread of antibiotic resistant pathogens. Numerous studies have now documented the role of human activities in elevating various molecular-based and culture-based indicators of antibiotic resistance. However, formalized and coordinated surveillance efforts are needed in order to identify hot spots where there is potential for antibiotic resistance to emerge and spread and also where there is maximum likelihood of human exposure and risk. Risk assessment frameworks can aid in this endeavor, but must be appropriately adapted to take into account unique challenges associated with antibiotic resistance, such as the potential for horizontal gene transfer. Here we will compare various 'omics-based methods that are emerging to aid in this endeavor and can help inform a globally-coordinated surveillance of environmental sources of antibiotic resistance.

ENVR 327

Combating global expansion of toxic cyanobacterial blooms: Challenges posed by climate change

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Managing and mitigating the global expansion of toxic cyanobacterial harmful algal blooms (CyanoHABs) is a major challenge facing researchers and water quality managers. Various approaches, including nutrient load reduction, artificial mixing and flushing, omnivorous fish removal, algaecide applications and sediment dredging, have been used to reduce bloom occurrences. However, managers now face the additional challenge of having to address the effects of climate change on watershed hydrological and nutrient load dynamics, water temperature, mixing regime and internal nutrient cycling. Rising temperatures and increasing frequencies and magnitudes of extreme weather events, including tropical cyclones, extratropical storms, floods and droughts, all promote CyanoHABs and affect the efficacy of ecosystem

remediation measures. These climatic changes will likely require setting stricter nutrient (including both nitrogen and phosphorus) reduction targets for bloom control in affected waters. In addition, the efficacy of currently used methods to reduce CyanoHABs will need to be reevaluated in light of the synergistic effects of climate change with nutrient enrichment.



Toxic cyanobacterial bloom in Lake Taihu, China. Photograph by H. Paerl, UNC-CH



Cyanobacterial bloom near the city of Wuxi, Jiangsu Province, China

ENVR 328

Development of a three-dimensional electrochemical system using a blue $TiO_2/SnO_2-Sb_2O_3$ anode for treating low ionic strength wastewater

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Reducing energy use is crucial to commercialize electrochemical oxidation technologies. We developed a three-dimensional (3-D) electrochemical system that can significantly reduce the applied voltage and effectively degrade organic contaminants in low ionic strength wastewaters. The 3-D system consisted of a composite wire mesh anode (comprised of blue TiO₂ nanotubes covered by SnO₂-Sb₂O₃), a proton exchange membrane (PEM), and a stainless-steel wire mesh cathode, which were compressed firmly together. For the 3-D system, we placed the anode of a 3-D electrode toward the wastewater that flowed past the anode. Both the 2-D and the 3-D systems had the same anode and cathode. We found that the 3-D system could reduce the applied voltage 75.7% and EE/O 73% for 0.001 M Na₂SO₄. For Na₂SO₄ concentrations greater than 0.05 M, the 2-D system had a slightly lower EE/O. We also compared the EE/O of EAOPs to other AOPs (UV/H₂O₂, UV/Persulfate, O₃/H₂O₂, UV/ TiO₂ and UV/ Chlorine). We found that EAOPs have a much higher EE/O for low BA concentrations (20 mg/L) and a much lower EE/O for high BA concentrations (2000 mg/L).

ENVR 329

Disrupting desalination: Temperature swing solvent extraction for hypersaline brines

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Hypersaline brines, e.g., produced water from oil and gas extraction, are of growing environmental importance but are technologically under-served by today's desalination methods. In this talk, we present a radically different approach for hypersaline desalination, termed temperature swing solvent extraction (TSSE). The technology utilizes a low-polarity solvent that is immiscible with aqueous solutions to extract water from hypersaline brines. Because water solubility of the solvent is highly temperature-sensitive, a mild temperature swing causes the aqueous phase to demix from the solvent, yielding product water. We demonstrate the potential of TSSE to desalinate hypersaline brines with exceptional salt removal and showed high water recovery of actual brines. Capability of TSSE to treat high-scaling propensity feed streams is presented and prospects of the technology for zero liquid discharge is examined.

ENVR 330

Electrocatalytic reduction of nitrate using Pd-based reactive electrochemical membranes

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This research focused on the fabrication and testing of point-of-use Pd-based (Pd-Cu and Pd-In) catalytic reactive electrochemical membranes (REMs) for electrocatalytic nitratereduction. Results showed that the optimal performance was achieved using a Pd-Cu/REM and an upstream counter electrode. Under these experimental conditions, nitrate was reducedfrom an initial concentration of 1.0 mM to below the EPAs regulatory MCL (700 µM) in single-pass, flow-through mode operation, with a hydraulic residence time of ~ 2 s. The product selectivity was < 2% towards nitrite and ammonia. Additional experiments showed that nitrate reduction was not affected by dissolved oxygen, dissolved carbon, and carbonate species and was only slightly affected by scaling of divalent cations (i.e., Ca²⁺and Mg²⁺) present in a surface water sample. Energy consumption was between 1.1 and 1.3 kWh mol-1 for 1 mM nitrate in a surface water sample and decreased to 0.19 mol⁻¹ for 10 mM NaNO₃and 0.12 kWh mol⁻¹ for 100 mΜ NaNO₃solutions. Electrocatalytic reduction was significantly higher than catalytic reduction, where electrocatalytic reduction kinetics were an order of magnitude higher. Overall, the high conversion of nitrate, low energy consumption, and low nitriteand NH₃ formation demonstrates the extreme promise of using Pd-Cu/REMs for distributed water treatment.

ENVR 331

Roles of emerging reactive species in UV/chlor(am)ine and UV/permanganate processes

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The UV/chlor(am)ine and UV/permanganate processes are emerging advanced oxidation processes (AOPs) that produces both hydroxyl radical (HO^{*}) and emerging

reactive species, i.e., reactive chlorine species (RCS) or reactive manganese species (RMnS). However, the roles of these emerging reactive species for the abatement of micropollutants were largely unknown, due to the lack of identification methods and the unknowns of their reactivity toward most micropollutants. We developed the identification methods by using kinetic modeling and chemical probes to quantify the concentrations of reactive species. Then the roles of specific reactive species for the abatement of target micropollutants were differentiated with respects to kinetics and mechanisms. In UV/chlorine, RCS such as Cl^{*}, Cl₂^{*-} and ClO^{*}, played an essential role in the abatement of a variety of micropollutants, particularly those containing electron donating groups, which was verified by a good linear relationship between the RCS reactivity and negative values of the Hammett constant for aromatic pollutants. In UV/chloramine, besides HO* and RCS, the role of reactive nitrogen species (RNS) such as nitrogen oxide (*NO) was also proved to be very important. For UV/permanganate, we firstly reported the activation of permanganate by UV irradiation for the abatement of micropollutants, which may lead to a new advanced oxidation process relying on both HO^{*} and RMnS. The production of HO^{*} and emerging reactive species makes UV/chlor(am)ine and UV/permanganate processes AOPs more compatible for pollution control.

ENVR 332

Meet the editors of the ES&T family of journals

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Are you curious about how the Environmental Science & Technology (ES&T) family of journals handles manuscripts, evaluates reviews and reviewers, and select new editors or advisory board members? Or do you just want an opportunity to meet an editor of ES&T journals, and possibly the Associate Editor that handled your most recent manuscript? If so, then join us for this session on the ES&T family of journals, published by the American Chemical Society (ACS). ES&T celebrated its 50th year in 2017, and ES&T Letters is now in its 6th year. Over the years these journals have had a distinguished and dedicated series of Editors-in-Chief (EICs), Editors, and Associate Editors. In this session the current Editors-in-Chief will be present to provide their thoughts and vision for their ES&T journal, and alongside some of the Associate Editors, will be available to answer questions from the audience on all aspects of the ES&T family.

ENVR 333

Re-envisioning the American Chemical Society's role in environmental sustainability

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In 2020, the American Chemical Society will revisit its policy statement – and organization priorities – on sustainability in the chemical enterprise. This brief introduction to ACS' current policy agenda will identify key areas where our organization has the potential to push a new vision in the future of sustainability in the chemical enterprise and beyond and guide our panel's conversation.

ENVR 334

Sustainability metrics and environmental sustainability analytics for green chemistry from a life cycle perspective

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This presentation will discuss metrics and methods for environmental sustainability analytics of green chemical processes. Emerging tools on life cycle optimization for chemical processes and biorefineries will be briefly reviewed as well.

ENVR 335

Sustainable design for a circular economy: Bioenergy, bioproducts, and resource recovery systems

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With population growth, urbanization, and rapidly changing environments, challenges to meeting basic human needs for food, services, and infrastructure are becoming increasingly complex. This presentation will provide a framework to identify, prioritize, and pursue opportunities for innovation to advance technology and policy related to circular economies, with a focus on bioenergy, bioproducts, and resource recovery from bodily waste. By integrating experimental data and process modeling with techno-economic analysis (TEA) and life cycle assessment (LCA) under uncertainty, a quantitative sustainable design (QSD) framework will be used to identify technology targets and chart a path forward for innovation. For resource recovery specifically, a social ecological systems (SES) framework will also be presented to re-envision bodily waste management as part of the circular economy, with the goal of facilitating interdisciplinary collaborations and supporting the pursuit of broader environmental and societal goals for sustainability. Altogether, this presentation will demonstrate how to leverage fundamental insight from laboratory-scale experiments to advance systems-scale sustainability.

ENVR 336

Sustainability in the chemical process industries through process intensification and modular manufacturing

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The manufacturing sector accounts for a guarter of the total U.S. energy use, and the process industries (chemicals, petroleum refining, pulp and paper, iron and steel) are the largest energy consumers in the sector. Likewise, these industries significantly impact other dimensions of sustainability including water use, climate change, clean energy, waste management, and human health. Process intensification (PI) is an often radical rethinking of chemical processes to remove bottlenecks, improving productivity and safety while reducing waste, energy consumption, production cost, and carbon footprint. PI is often a shift from the conventional "unit operations" paradigm in chemical processing to a more integrative paradigm. Modular manufacturing, a complementary concept, is an approach to building chemical plants that favors assembly of pre-fabricated, standardized modules rather than conventional "stickbuilt" construction. Modular manufacturing also provides opportunities for distributed chemical manufacturing that utilizes stranded resources such as waste biomass feedstocks or renewable wind and solar power. Modular manufacturing also enables a shift from the bigger-isbetter paradigm in chemical production to a small, modular paradigm where economies of scale are replaced with economies of mass production. Both PI and modular manufacturing are tools that can be used to improve the sustainability of the chemical process industries, which are under pressure to change given recent shifts in supply and demand, the rise of inexpensive renewable power, and an increased need to reduce operational footprints. Our work uses research and education to promote better process technologies and to define appropriate metrics to capture the impact of these technologies on productivity and sustainability.

ENVR 337

Molecular farming, biomass valorization and platform chemicals: Sustainable and abundant materials from biosphere's molecular factories of renewable resources

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Biosphere's abundant biopolymeric contents such as cellulose, chitin, and chitosan possess highly desired traits namely renewability and biodegradability and especially the basic polysaccharides bearing amino group in chitin/chitosan that can generate unique chemical entities with much sought-after functional properties. From sustainability viewpoint, agricultural residues and seafood waste, not consumed by animals or humans, should be targeted which can exploit visible/solar light for processing in the field. Besides traditional biomassderived platform chemicals, sustainable materials from plants as green factories and their diverse use ranging from molecular factories for therapeutic proteins and metallic nanoparticles to biological scaffolds will be highlighted. The fusion of technological developments in the genetic engineering and nanotechnology fields may provide emerging high-value products. Examples will be provided for potential source of renewable feedstocks from these carbon-based materials which offer many options for production of sustainable products thus circumventing the traditional use of fossil-derived chemicals.

ENVR 338

Sustainability in the chemical enterprise: Renewable energy beyond the benchtop

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This presentation will discuss how renewable energy policy can affect environmental sustainability of chemical production and how it can be effectively utilized to help green chemical processes. We will cover recent examples of biomass and solar energy integration in process systems. The speaker will share her journey as chemist in the renewable energy field.

ENVR 339

Critical role of chemistry in efforts to achieve sustainability in agriculture on a global scale

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Agricultural science is at the forefront of addressing many of the UN Sustainable Development Goals. Dramatic advances in plant genomics have blurred the lines between chemistry and biology. For example, scientists can now design plants that produce proteins or doublestranded RNA to protect themselves from some insect pests, thereby reducing the need for chemical sprays. This provides an opportunity to use more selective chemistries that reduce risk to nontarget organisms. Farmers in developed countries now have access to sophisticated tools to track and increase productivity while protecting the health of their soils and sensitive areas like streams, wetlands, and pollinator habitat. However, challenges exist in achieving adoption of modern agricultural systems globally in time to meet the challenges of climate change and the food production needs of a growing population.

ENVR 340

Photochemical reactivity of dissolved organic matter in the Adirondacks lakes

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In sunlit aquatic systems, the quantity and quality of dissolved organic matter (DOM) control the formation of triplet excited state of DOM which serves as the main precursor of other reactive intermediates (RIs). These RIs play critical roles in both organic contaminant attenuation and global carbon cycling. In the present study, we quantified the steady state concentrations and apparent quantum yields of three RIs in the Adirondacks lakes. These lakes are undergoing chemical and biological recovery from reduced acid deposition. We hypothesized that recovery will lead to increased photoreactivity due to increasing inputs of dissolved organic carbon (DOC) (i.e., browning) into these lakes. We collected grab samples from 16 Adirondacks lakes in the summer of 2018. We studied the effects of acid deposition and recovery on the photoreactivity of DOM by adjusting the pH of samples from 4.5 to 8.5. In addition, we also evaluated the effect of high aluminum (AI) levels observed during the acid deposition era as well as the increasing ferric (Fe) concentration observed in lakes undergoing recovery. Our results indicate that the observed increase in lake pH promoted the formation of higher steady-state concentrations of RIs. Lakes with higher DOC concentrations produced higher steady-state concentrations of all RIs. Both aluminum and ferric decreased the steady-state concentrations and apparent quantum yields of triplet DOM and singlet oxygen, while the effect on hydroxyl radical production was more variable. The concentration of nitrate was a key

determinant for the formation of hydroxyl radical in these lakes. This work demonstrates that with increased recovery of Adirondacks lakes from the effects of acid deposition, the photoreactivity of DOM will increase but also vary depending on the chemical characteristics of the lake as well as the DOM quality.

ENVR 341

On the quantification of hydroxyl radical and lower energy hydroxylator from dissolved organic matter photoirradiation

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It is well known that in surface waters, the photoirradiation of dissolved organic matter (DOM) produces hydroxyl radicals (•OH). There are several hypothesis as to how •OH could be photochemically formed, including via reactions involving benzoic acids derivatives and through other excited state reactions. •OH play an important role in the fate of contaminants in surface waters as they have a high reactivity with most contaminants. Additionally to the formation of •OH, lower energy hydroxylators (LEH) are also produced during DOM photo-irradiation. These LEH are far less studied than •OH, but it is known that they have a lower reactivity when compared to •OH. One hypothesis regarding these LEH is that they are formed through exited triplet states of guinones. In this study, we present an investigation of potential methods to quantify and differentiate •OH and LEH. The first method is the use of a quencher such as isopropanol or methanol to guench all hydroxylating capacity in the system. The second method is to use a probe compound such as benzene or benzoic acid to quantify •OH and LEH. In the latter case, as LEH lifetime are limited in water, the concentration of the probe compound matters and it is possible to distinguish between •OH and LEH by varying the concentration of the probe compound. Literature results often presents the quantification of hydroxyl radical using probe compounds without distinguishing between •OH and LEH. As the quantification of LEH is dependent on the concentration of the probe, this has the important consequence that the determination of parameters such as the •OH quantum yield $(\Phi_{\bullet OH})$ can yield different results depending on the experimental condition used.
Photochemical formation and decay of superoxide radical in dissolved organic matter solutions

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The photochemical formation and decay rates of superoxide radical ions $(O_2^{\bullet-})$ in irradiated dissolved organic matter (DOM) solutions were directly determined by using a flow injection analysis system. Under simulated solar irradiation, uncatalyzed and catalyzed O2. dismutation account for only ~25% of the total $O_2^{\bullet-}$ degradation in air-saturated DOM solutions. Lightinduced O2. loss, which does not produce H2O2, was observed. Both the O2. photochemical formation and light-induced loss rates are positively correlated with the electron-donating capacities of the DOM, suggesting that phenolic moieties play a dual role in the photochemical behavior of O2... In air-saturated conditions, the O2. quantum yields of 12 DOM solutions varied in a narrow range, from 2.1‰ to 3.7‰, and the average was (2.6 \pm 0.5)‰. The quantum yield of O₂•- nonlinearly increased with increasing dissolved oxygen concentration. Therefore, the quantum vield of one-electron reducing intermediates (OERI), the precursor of O2., was calculated as (5.5 ± 0.4) %. High-energy triplets (³DOM^{*}, E_T >200 kJ mol⁻¹) and ¹O₂ quenching experiments indicate that high-energy ³DOM^{*} and ¹O₂ play minor roles in O₂^{•-} production. The aforementioned results are useful for predicting the photochemical formation and decay of O2. in sunlit surface waters.

ENVR 343

Dissolved organic matter composition and electrondonating capacity determine photochemical reactivity of diverse waters

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Photochemical reactions involving dissolved organic matter (DOM) yield a suite of photochemically produced reactive intermediates (PPRI). These species affect contaminant fate in aquatic environments and participate in reactions involving the flux between dissolved and atmospheric carbon. To investigate relationships between DOM composition and mechanisms for PPRI formation, we combine extensive water sampling with detailed DOM

characterization and evaluation of photoreactivity. We sampled oligotrophic, mesotrophic, and eutrophic lakes, dystrophic bogs, rivers and streams impacted by agricultural runoff and wastewater effluent, and waters in highly urbanized watersheds. DOM characterization includes molecular analysis using Fourier-transform ion cyclotron resonance mass spectrometry and bulk analyses including ultraviolet-visible spectroscopy and measurements of electron-donating capacity. Chemical probes are used to quantify steady-state concentrations formed during irradiation and quantum yields for tripletstate DOM (3 DOM), singlet oxygen ($^{1}O_{2}$), and radical species (e.g., hydroxyl radical; •OH). Surrounding landcover has significant impacts on DOM composition and on resulting PPRI formation. Samples from developed landscapes including agricultural and urbanized watersheds have higher quantum yields for ³DOM and ¹O₂, while water bodies receiving significant DOM inputs from forests and wetlands generate higher steady-state concentrations of PPRI and have higher quantum vields for •OH. Quantum vields for ³DOM and ¹O₂ formation correlate strongly in waters, while •OH shows opposing relationships to DOM character. Electron-donating capacities provide evidence that these trends are likely due to the mechanism of •OH formation.

ENVR 344

Comparing photoproduction rates of one-electron reductants and hydrogen peroxide in extracts and natural waters

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Photo-produced one-electron reductants within chromophoric dissolved organic matter (CDOM) have been shown to be likely precursors for formation of superoxide and therefore hydrogen peroxide. The current proposed mechanism involves photochemically produced one-electron reductants within CDOM reacting with dissolved oxygen to form superoxide, which dismutates to form hydrogen peroxide. Nitroxide radical probes have been used to trap one-electron reductants and their detection was previously performed using liquid chromatography with fluorescence detection. This method was modified to be achieved using a fluorescence spectrophotometer allowing for faster, easier, and more flexible measurements. The production rates of oneelectron reductants and hydrogen peroxide have been measured for a wide variety of samples from reference materials to natural waters and extracts. Based on the stoichiometry of the proposed mechanism, the ratio of the production rate of one-electron reductants to that of hydrogen peroxide should be equal to two. However, ratios obtained thus far range from six (natural waters) to fourteen (extracts). A value greater than two indicates that not all photo-produced superoxide is undergoing

dismutation to form hydrogen peroxide, suggesting that other reactions are competing with dismutation. In order to investigate the discrepancies in the ratios, various experimental factors were changed to see the resulting effects on the production rates of one-electron reductants and hydrogen peroxide. Some of the factors tested so far include irradiance wavelengths, concentration of CDOM, salinity, and addition of metal chelators. Results obtained from these experiments have shown that none of these factors affect the ratios observed. Interestingly, mixing reference fulvic acids with natural waters dampened oneelectron reductant production. For future work, superoxide production rates will be measured. This will provide more information on the relationship between the reactions in the mechanism discussed above. Measurements of all three species (one-electron reductant, superoxide, and hydrogen peroxide) have yet to be conducted collectively on the same sample.

ENVR 345

Determining the importance of NOM type and water composition on the photochemical formation of VOCs at the air-water interface

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Natural organic matter (NOM) is a naturally occurring, complex and ubiquitous component of aqueous environments. While its structural characteristics are widely variable, all NOM can absorb light, and undergo intersystem crossing to form the excited triplet state. The formation of volatile organic compounds (VOCs) over surface waters has been noted in both lab and field studies. There is evidence to suggest that the presence of the sea surface micro-layer and dissolved organic manner influence the concentration and identity of these volatile species. It has been shown previously that the photoformation of ³NOM* and ¹O₂ are slower in seawater relative to freshwater, and the changes to the formation kinetics may influence the formation of VOCs in different water bodies. This work focuses on how the formation of VOCs from either sea water or fresh water is affected by the presence of a model sea surface microlaver, using nonanoic acid, and the type of NOM, using Suwannee River and Nordic Reservoir Natural Organic Matter. We observe that for both NOM samples, the presence of the microlayer increases the number of VOCs species, and their concentrations. We also note that the formation of VOCs is different in sea water compared to freshwater. Given that the photochemical formation of VOCs happens at the air-water interface, we used Glancing Angle Fluorescence to determine the surface properties of Suwannee River and Nordic Reservoir Natural Organic Matter in seawater and freshwater. We report these results and our explorations of the mechanism(s) responsible.

ENVR 346

Leveraging breakthroughs in light-emitting diode technology to probe the photochemical reactivity of arctic permafrost dissolved organic matter

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Richard Zepp's research substantially improved our understanding of the photochemical degradation of dissolved organic matter (DOM) in aquatic ecosystems. Novel aspects of his research include assessments of the wavelength dependence, rates, reactants, products, and pathways of DOM photochemical degradation. Expanding on Richard's work, the first half of this talk will describe a new approach to measure the wavelength dependence of photochemical reaction efficiencies (quantum yields). The new approach exploits recent developments in highpowered, discrete waveband light-emitting diode (LED) technology. The design and performance of the custombuilt LED-based reactor will be presented, including results from a series of quality assurance and quality control tests (e.g., comparison of chemical actinometry vs. radiometry; reproducibility of the apparent guantum yield (AQY) spectrum of DOM photochemical oxidation). Overall, the LED-based reactor is highly reproducible, extremely cost effective, has high sample throughput, and is compact, lightweight, and durable, making it ideal for operation at remote field stations or at sea. The second half of the talk will describe the first application of the LEDbased reactor by an assessment of the photochemical reactivity of five different types of DOM draining arctic permafrost soils. All permafrost DOM was labile to photomineralization to CO2 at all wavelengths measured (278, 309, 348, 369, and 406 nm), and the AQY spectrum always decreased exponentially with increasing wavelength. The magnitude of the photomineralization AQY varied up to 8-fold among permafrost DOM samples and was significantly, positively correlated with the concentration of dissolved iron. The chemical composition of photo-labile compounds within permafrost DOM and the ¹³C and ¹⁴C isotopic composition of the CO₂ produced by sunlight were characterized. The results collectively support a mechanism of iron-catalyzed photodecarboxylation of lignin- and tannin-derived organic acids within old permafrost DOM. Kinetic modeling revealed that if more permafrost DOC is exported to

surface waters, photomineralization rates will increase. Therefore, photochemistry will continue to be an important component of the C budget in a future, warmer Arctic.

ENVR 347

Aqueous aerosol processing in real time

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We have developed the use of acoustic levitation of individual droplets to study atmospheric aerosol processing in real time. In our studies, acoustic levitation is coupled with spectroscopic techniques and imaging to provide detailed chemical and visual information of transformations within single and multi-component droplets. Owing to the large size of the droplets (mm diameter), the technique can be combined with other spectroscopic tools, such as Raman spectroscopy, to obtain more detailed chemical information on droplet processing in real time. In addition, pH changes during droplet processing may be monitored using the absorption of pH indicators, and gross morphological changes detected using imaging. During an aerosol lifetime, numerous chemical transformations including photochemical processes occur resulting in the formation of new compounds. Organic material present in aerosols can undergo transformations to form organosulfate compounds which are light absorbing and thus contribute to positive radiative forcing of the climate. In this presentation, we give results of preliminary experiments using direct absorption UV-Visible spectroscopy to study the formation of organosulfates in evaporating mixed component droplets of Ammonium Sulfate and Humic Acid, illuminated with a Xenon lamp. We discuss how the formation of organosulfate compounds in aerosol containing organic material can be followed using acoustic levitation coupled with UV-Visible spectroscopy.

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Global model for depth-dependent carbonyl photochemical production rates in seawater

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Acetaldehyde and glyoxal are ubiquitous, oxygenated volatile organic compounds in the troposphere wherein they affect the oxidizing capacity and secondary organic aerosol formation. The oceans are a potentially significant

source of these carbonyl compounds to the atmosphere. To date, large uncertainties persist regarding air-sea fluxes, primarily due to the lack of observations and an understanding of carbonyl cycling in the surface oceans. A photochemical model was used to quantify the global carbonyl photoproduction impact of in the photodegradation of marine dissolved organic carbon (DOC). As model input, wavelength- and temperaturedependent apparent quantum yields (AQY) for the photochemical production of carbonyl compounds were determined in seawater collected from the Northwest Atlantic Ocean. These AQY data and published AQY data from the North Pacific were used with remotely sensed seawater optical properties and solar irradiance data in a global model to calculate depth-resolved, mixed-layer photochemical fluxes of acetaldehyde and glyoxal in seawater. Based on this model, the annual global surface mixed-layer photochemical production was 119.4 Tg for acetaldehyde and 19.8 Tg for glyoxal. This work significantly improves our understanding of the impact of photochemistry on the cycling of DOC in the surface oceans. Low-molecular-weight carbonyl compounds represent the second largest carbon flux among all known carbon products that are produced during the photolysis of DOC. The annual photoproduction of carbonylcompound carbon is 151 Tg C, comprising 13% of the total carbon and 30% of the biologically labile carbon that are produced globally from the photolysis of marine DOC.

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Disinfection byproducts (DBPs) in mixtures: Is cytotoxicity additive and what are the toxicity drivers?

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Disinfection byproducts (DBPs) in chlorinated waters have been associated with adverse health outcomes such as bladder cancer. To quantify the toxic potency of various DBPs, cell-based in vitro assays using Chinese hamster ovary (CHO) cells have been conducted on >100 individual DBPs to obtain LC50 values of these compounds. As the contribution of a DBP to the toxicity of disinfected waters depends on both the concentration and toxic potency of the compound, previous studies have weighted the measured concentrations of individual DBPs by the LC₅₀ values of those DBPs. This approach has revealed that unregulated DBPs. such as haloacetonitriles (HANs) and haloacetamides (HAMs), may be more important toxicity drivers than are regulated DBPs. Furthermore, the sum of toxic potency-weighted DBP concentrations has been used as a metric to compare the guality of various conventional drinking and potable reuse waters. These calculations assume that

DBP-associated toxicity is additive rather than synergistic or antagonistic, but little information is currently available regarding the interactions of unregulated DBPs in complex mixtures of DBPs. To assess whether the cytotoxicity of DBPs in mixtures is additive, we prepared 9 defined mixtures (each containing 11 to 29 DBPs) based on concentrations that were measured in different waters. We compared the observed cytotoxicity of defined DBP mixtures on CHO cells with the additive cytotoxity calculated usina toxic potency-weighted DBP concentrations. This comparison shows that cytotoxicity is additive in most of the defined mixtures. Our results also confirm that unregulated DBPs contribute more significantly to the overall cytotoxicity of the mixtures than regulated DBPs. Overall, our findings support the validity of using the sum of toxic potency-weighted DBP concentrations as a metric to compare the DBPassociated toxicity of disinfected waters.

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Determination of low-level haloacetic acids, bromate, and dalapon in drinking water using IC-MS

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To ensure drinking water safety, the U.S. Environmental Protection Agency (EPA) have set Maximum Contaminant Levels (MCL) for toxic compounds in drinking water. Five of nine haloacetic acids (HAA5), bromate, and dalapon, are regulated by the EPA with MCLs of 60 µg/L for HAA5 (total for the five compounds), 10 µg/L for bromate, and 200 µg/L for dalapon. U. S. EPA Method 557 has been validated for the determination of nine HAAs, bromate, and dalapon. The EPA method uses ion chromatography (IC) coupled with tandem mass spectrometry (IC -MS/MS). This study evaluated an IC-MS method for determination of these analytes using a single quadrupole mass spectrometer. We used an anionexchange column that was developed after the publication of Method 557 and found that the IC-MS method was fast (40 min vs. 60 min in Method 557) and linear over the established analytical range for the 11 analytes with a r²-value range of 0.998 to 1. The method is sensitive for the determination of U.S. EPA regulated HAA5, bromate, and dalapon with MDL ranges from 0.03 to 0.67µg/L. The method is accurate for the determination of 10 of 11 analytes (not for tribromoacetic acid (TBAA)) in U.S. EPA Method 557 with recoveries ranging from 92% to 119% when spiked with 10 µg/L of nine HAAs, bromate, and dalapon in the Laboratory Synthetic Sample Matrix (LSSM). The method is precise with retention time precision below 0.1% and internal standard corrected peak area interday precision ranging from 0.7% to 4%. We believe this simple IC-MS method can be used to replace IC-MS/MS for monitoring regulated HAA5,

bromate, and dalapon in drinking water when an IC-MS/MS is not available.

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Improving our understanding of point and non-point sources of contamination in a rural to urban watershed

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Understanding drivers of freshwater contamination is essential for maintaining ecosystem functioning and preserving water supply. Although many studies have focused on contaminant delivery in areas downstream of major urban centers and agricultural areas, the associated flow pathways are poorly understood. Furthermore, there are a lack of studies evaluating water quality in systems that traverse multiple land uses, such as a rural to urban gradient, where both point and nonpoint sources can have an impact on water quality. This study addresses these knowledge gaps by examining the impact and delivery of both land use practices (i.e., urban, agricultural, pasture, etc.) and point sources (i.e., wastewater treatment plants) on streamwater metal, nutrient, salt, and sediment concentrations and yields in a mixed-use watershed. The efficacy of riparian buffers for reducing contaminant loading was also explored. Our preliminary results show a statistical link between streamwater specific conductivity (SPC) values and the percentage of roads, structures, and other impervious surfaces in upstream areas. Elevated streamwater SPC measurements during summer months suggest historical application of road salts has resulted in salinization of shallow groundwater, even in areas with lower population densities. Finally, the cumulative percentage of land use practices in upstream was a better predictor of water quality then those found within various stream buffer widths. Results of this study are of immediate relevance to local and state regulatory agencies seeking to establish more effective water quality regulations and land management strategies.

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Chemistry of surface waters in the agro-forested watersheds of Eastern Ohio experiencing unconventional natural gas exploration

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This paper investigates the changes in surface water chemistry and associated impacts on the stream quality from landscape disturbances and fragmentation of agroforested lands in eastern Ohio. The fragmentation over the last decade is occurring from the shale gas exploration using horizontal drilling technology. A single well pad along with its auxiliary infrastructure can convert approximately 20 - 30 acres of forested land into an impervious area. However, given the large number of well pads constructed in a short period of time, this exploration can lead to considerable forest fragmentation in the region, and further might result in land erosion, deterioration of regional surface water guality, and loss of healthy ecological habitats. The well pad inventory shows over 136 pads constructed between 2014 and 2018 in Muskingum watershed alone resulting in 2200 hectares of deforested land, which estimates to about 22.57 % forest loss calculated based on tree heights. Harrison and Carroll are the counties in eastern Ohio experiencing the most significant deforestation and undergoing the most intensive well pad construction, respectively, within the basin. Therefore, this project primarily focused on studying the changes in surface water quality in these two counties at the sub-watershed scale. Surface water sampling and quality analysis were carried out in two streams (Irish and Conotton) and one reservoir (Leesville) in Carroll and Harrison counties. Water samples were collected from 10 sites in the fall and spring of years 2018 and 2019. Our study analyzed total suspended solids, conductivity, chloride, and nutrients, Ba, Sr, Mg and Ca. The results showed only seasonal variations in key elemental levels in upstream water samples. Increase of nitrate contents were also observed from 0.06 to 1.6 ppm in stream samples.

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Seawater augmented reuse: Study of upstream blending for potable reuse

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As climate change and freshwater scarcity worsen, demand grows to secure new reliable sources of potable water, including desalinated seawater and recycled wastewater. During recent techno-economic а assessment, our research group identified significant overlaps between desalination and potable reuse treatment trains. Significant energetic benefits, without the capital cost, footprint, and other concerns associated with building a new plant, could be obtained by blending seawater and wastewater upstream of potable reuse treatment plants. In this work, for the first time, the technoeconomic ramifications of pre-treatment blending of seawater and treated wastewater for potable reuse applications are explored. The value of diluting either

stream with the other is guantified in two parts: (1) diluting seawater with wastewater to reduce specific energy demand in the reverse osmosis process, and (2) diluting wastewater with seawater to reduce public health risks associated with direct potable reuse. This study is ongoing; results both from modeling and experimental work will be presented. One critical consideration is the speciation of the oxidants formed during chlorine addition to prevent biofouling. Wastewater chlorination produces chloramines by ammonia oxidation, and seawater chlorination produces free bromine by bromide oxidation. Blending the two produces bromamines, which are associated with the formation of certain toxic byproducts such as NDMA. Bromamine formation is expected to be a function of which stream is chlorinated, and whether the disinfection happens before or after blending. In addition to chemical considerations, specific energy demand associated with the reverse osmosis process will be modeled as a function of membrane properties and recovery rate. Parameters including blending ratio, pH, pre-disinfectant choice, membrane type, and recovery rate will be determined based on the results from the modeling work. Finally, bench-scale testing results from these treatment trains under different blending scenarios will be presented. The chemical composition and water quality of the blended stream after each treatment step will be determined via mass spectrometry. The results from this study will provide new insights into the implementation and optimization of desalination and potable reuse systems.

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Evaluation for the fate and health impacts of trace organic chemicals in the reclaimed wastewater reused for agriculture

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Wastewater reclamation and reuse for agriculture has been attracting a great deal of interests, due to the increasing water demanding for growing agricultural crops. However, the application of treated wastewater for agricultural irrigation can lead to the bioaccumulation of trace organic chemicals in the agricultural crops and consequent human exposure. In this study, a mathematical model was developed to evaluate the fate of five trace organic chemicals, namely triclosan (TCS), carbamazepine (CBZ), naproxen (NPX), gemfibrozil (GFB), and fluoxetine (FXT) during wastewater reuse for agriculture, as well as consequent human exposure and health risk. Under the setup of a reclaimed-water-irrigated local farm, it took 100 - 535 days for the compounds to achieve steady-state concentrations of 1.41×10-3. 4.73×10⁻², 1.17×10⁻³, 1.53×10⁻², and 7.38×10⁻³ µg/kg for

TCS, CBZ, NPX, GFB, and FXT in soils, respectively. The soil concentrations were critically governed by the degradation rate of compounds in soils. The steady-state concentration of trace organics in plant (alfalfa) and grazing animal (beef) ranged $6.69 \times 10^{-5} - 9.30 \times 10^{-1}$ and $1.41 \times 10^{-8} - 3.65 \times 10^{-3} \mu g/kg$, respectively. Human exposure to these compounds was calculated to be $1.04 \times 10^{-21} - 4.40 \times 10^{-5} \mu g/kg/d$, much lower than the acceptable daily intake (ADI). Screening analysis showed that the compounds with relatively higher K_{ow} and lower degradation rates have a higher tendency to be transferred to human beings and cause health risks. Our study established a modeling method for evaluating the fate and human health effects of trace organic compounds in reclaimed water reuse for the agricultural systems.

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Phosphate adsorption properties of ZSM-5 modified by metal cation exchange

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Phosphorus is an essential macronutrient for plant growth and a key element in all biological systems, primarily through its importance in the structures of biomolecules (e.g., nucleic acids, phospholipids) and role in metabolic reactions (e.g., ATP, NADPH). Phosphorus extracted from the ground—phosphate rock—is increasingly being viewed as a critical, non-renewable resource in a similar vein to conventional oil. Though phosphorus as a macronutrient has no substitute, there are several alternative and renewable sources that are largely untapped, many originating from its status as an environmental contaminant. A common thread is that effective phosphorus recovery would require-in most instances at least-separation of dissolved phosphate phase. Zeolites—crystalline from an aqueous aluminosilicates amenable to modification through green chemical techniques— are one proposed class of material for the recovery of phosphate through reversible adsorption. Here, we present ZSM-5 zeolite modified by cation exchange to contain copper sites active for phosphate adsorption. Batch tests showed that adsorption is well-described by the empirical Freundlich model at room temperature and pH 7. The adsorption capacity of Cu-ZSM-5 was found to increase with increasing pH. We present a study of the phosphate adsorption mechanism and assess the material for application to other anionic environmental contaminants.

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Mineral precipitation for simultaneous toxic metal uptake from mining run-off and carbon dioxide fixation for reduction of greenhouse gases

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The extent of toxic metal contamination in waterbodies near mine tailings is severe, especially in countries like South Africa, where there has been uncontrolled release of mining operation and tailings run-off waters. Mining discharge waters contain high levels of metalloids and metals like arsenic and lead, and sources of high acidity such as sulfuric acid. Solving the water pollution problem consistently associated with mining activities is an important focus of many mining countries. In this work, a new strategy is proposed for toxic metal removal from waters. The strategy minina waste involves immobilization of toxic metals through precipitation and co-precipitation from solution with the addition of various sources of alkalinity, anions, and basicity from fly ash, seawater, high concentration CO₂, and bases. This strategy has the added benefit of carbon dioxide fixation, positively contributing to greenhouse gas reduction. Simulated mine tailings run-off waters were treated to show overall feasibility and CO₂ emission reduction geochemical potential through modelina and experimental work. We show direct evidence of coprecipitated solids, indicating effective immobilization of toxic metals. Detailed cost-analysis of different treatment options, and finding appropriate cost minimizing reagents were done. Significant insights are obtained for the waste water treatment of mine tailings of different composition and origin, based on experimental and geochemical modeling analyses.

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New insights to the degradation of 2,4dichlorophenoxyacetic acid when applied to wholelake treatments

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The herbicide 2,4-dichlorophenoxyacetic acid (2,4-D) is used in aquatic systems as a treatment for invasive Eurasian watermilfoil. However, the degradation rate and resulting lifetime of 2,4-D can vary widely, with complete degradation in Wisconsin lakes ranging from 70 to 150 days. This variability may increase the risk for off-target effects to fish and aquatic plants due to unintended long exposure times. We used a combination of laboratory and field-based studies to investigate the dominant mechanisms of degradation of 2,4-D in aquatic systems. Microbial and photochemical degradation were individually assessed using laboratory-based microcosms and irradiation studies, respectively. Additionally, field campaigns were conducted in six lakes to quantify 2,4-D loss following whole-lake herbicide treatments. Initial results suggest sediment microbial communities are instrumental to 2,4-D degradation at the sediment water interface. Furthermore, previous treatment of a lake with 2,4-D can shorten the lag time between initial 2,4-D exposure and the start of degradation, likely due to selection pressures favoring 2,4-D degraders. Irradiation studies show that 2,4-D is primarily susceptible to indirect photochemical degradation in the presence of sunlight. Additionally, the primary metabolites from microbial degradation undergo relatively rapid photodegradation, suggesting that both bacterial degradation and photodegradation contribute to the transformation of 2,4-D and its major products in aquatic systems. These results will be used to determine environmentally relevant degradation mechanisms to optimize the 2.4-D application of 2,4-D and support decision making related to whole-lake herbicide treatments.

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Advances and challenges for using advanced oxidation processes to eliminate cyanotoxins

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The quality of drinking water sources is greatly affected by agricultural runoff, industrial and municipal wastewater effluents. Coupled with climate change, harmful algal blooms (HABs) occur more intensively and severely in recent years. Certain cyanobacteria could produce cyanotoxins which are potent hepatotoxins, such as microcystins, cylindrospermopsin and nodularins, and neurotoxins, such as saxitoxin, and anatoxin-a. These cyanotoxins showed the potential to enter drinking water systems. In 2014, a water crisis affected half million people in Toledo, Ohio, which was caused by cyanotoxins breaking through the drinking water facilities. Recordbreaking HABs are becoming more frequent worldwide, which poses a serious threat to drinking water safety. Thus, it is widely accepted that a multiple-barrier

approach is needed to secure drinking water safety when experiencing HABs events. Advanced oxidation processes (AOPs) has been evaluated as an effective barrier for treating cyanotoxins containing water by oxidation of these organic contaminants with highly reactive radical species. In this presentation, Professor Dionysiou will give an overview of recent progress in the treatment of cyanotoxins using advanced oxidation processes (AOPs). Kinetics and transformation pathways of the destruction of various cyanotoxins, including several microcystin isoforms (MC-LR, YR, LA, RR) and cylindrospermopsin by hydroxyl radicals, sulfate radicals, chlorine related radicals, and other reactive species generated in various AOPs will be discussed. The effects of solution co-contaminants and halide ions in-field water samples will be emphasized, considering also potential application of some of these technologies in a treatment plan or a case-specific application. Finally, a comprehensive assessment of UV/chlorine process which could be potentially applied especially during HABs to prevent the cyanotoxins from entering the finished water will be provided.

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Roles of reactive bromine radicals in the abatement of micropollutants by UV based AOPs in the presence of bromide

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Reactive bromine species (RBS) such as Br*, Br2*- are inevitable during UV based advanced oxidation processes (AOPs) such as UV/chlorine and UV/H₂O₂ processes. This study investigated the roles of RBS in the degradation of micropollutants by using the UV/bromine process. RBS dominated the degradation of ibuprofen (IBP) and caffeine (CAF), but not benzoate (BA) in UV/bromine. The second order rate constants of IBP reacting with Br* and Br_2^{*-} were determined to be ~10⁹ M⁻ $^{1}s^{-1}$ and $\sim 10^{7}$ M⁻¹s⁻¹. The concentration of Br₂^{*-} was enhanced with increasing Br⁻ concentrations, resulted in the enhanced RBS contribution to IBP abatement. RBS reacted with IBP through hydroxylation, decarboxylation, side chain cleavage, and bromine substitution, where electron transfer by Br2*- took place followed by hydroxylation. This is the first study to demonstrate the roles and mechanisms of RBS in micropollutant abatement by the UV/bromine process.

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Light-driven degradation of Trace Organic Compounds (TOrC) by photosensitizing activity of Effluent Organic Matter (EfOM) for singlet oxygen production via indirect photolysis reactions

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Components of effluent organic matter (EfOM) present in been amply identified wastewater have as photosensitizers for singlet oxygen production that induces trace organic compounds (TOrC) transformations via indirect photolysis. Kinetic models based on known mechanisms have been used to simulate these degradation processes with few or no fitted parameters. but it remains necessary to fill gaps in the characterization of the EfOM photosensitizing behavior. Objectives of this study are: (i) to assess the light absorbance and quantum yield for singlet oxygen production of EfOM sensitizers, and (ii) to quantify the concentration of singlet oxygen produced bv light-driven reactions. То test photosensitizer activity, secondary effluent samples from the Agua Nueva Water Reclamation Facility located in Tucson, Arizona, were used to effect TOrC indirect photolysis, using furfuryl alcohol (FFA) and p-cresol as targets. Solar light. UVA (300-400 nm) and monochromatic light-emitting diodes (LEDs) were used as light sources to ascertain photosensitizer absorbance and guantum yield. Results showed that the TOrC targets were removed by singlet oxygen oxidation in a wide range of wavelengths. Bleaching effects of the photosensitizers have been analyzed and results show that singlet oxygen production ability decreases upon irradiation over a time scale longer than that necessary for significant degradation of the TOrC targets. These results highlight the need to fully characterize the photosensitizer behavior of EfOM so better models to predict its role in the degradation of TOrCs can be formulated.

Template free mild hydrothermal synthesis of coreshell Cu₂O(Cu)@CuO visible light photocatalysts for model pharmaceutical organics degradation

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Solar photocatalytic processes are a promising approach to environmental remediation, however their implementation requires improvements in visible light harvesting and conversion and a focus on low cost, Earth abundant materials. Semiconducting copper oxides are promising visible light photocatalysts for solar fuels and wastewater depollution. Here we propose the mild, hydrothermal (template-free) synthesis of core-shell Cu₂O(Cu)@CuO photocatalytic architectures for the visible light photocatalytic degradation of pharmaceutical organics as an emerging concern. Hollow and rattle-like core-shell nanosphere aggregates with diameters between 200 nm and 2.5 mm formed under different synthesis conditions; all comprised an inner Cu₂O shell, formed of 10-50 nm nanoparticles, surrounded by a protective corona of CuO nanoparticles. High reductant and structure-directing agent concentrations promoted the formation of a volk-like Cu₂O/Cu core, associated with improved photophysical properties, notably a high oxidation potential and suppressed charge carrier recombination, that correlated with the highest apparent quantum efficiency and removal rate. Trapping experiments demonstrated hydroxyl radicals were the primary active species responsible for organics oxidation to quinones and short chain carboxylic acids. Rattle-like core-shell Cu₂O/Cu@CuO and hierarchical nanospheres exhibited excellent physiochemical stability and recyclability for APAP photocatalytic degradation.



Withdrawn

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Reactivity of aromatic organic compounds to radical species under cobalt/peracetic acid advanced oxidation process

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Peracetic acid (PAA, CH₃C(O)OOH) has recently emerged as an oxidant for the radical-based advanced oxidation processes (AOPs). Compared to hydroxyl and sulfate radicals, carbon-centered radicals generated by activation of PAA have been limitedly studied, and their reactivity to organic structures is not well understood. Co/PAA is a unique AOP in that Co(II)/Co(III) can efficiently activate PAA to generate $CH_3C(O)O^{\bullet}$ and CH₃C(O)OO• radicals, with little formation of •OH. Meanwhile, Co(II)/Co(III) react sluggishly with H₂O₂ coexistent with PAA. This study utilizes the Co/PAA system to investigate a suite of aromatic organic compounds for their potential to react with carboncentered radicals generated from PAA. This study included two parts. First, the reaction kinetics of PAA with Co(II) and Co(III) were investigated. Then, the degradation of model contaminants (bisphenol-A, carbamazepine, naproxen and sulfamethoxazole) by Co/PAA was studied. The impacts of reaction conditions (pH, dosages of PAA, Co(II) and H_2O_2 , and water matrix) and radical quenchers were assessed. Results confirmed the major role of carbon-centered radicals for the contaminants' transformation, with little contribution from •OH. Second, similar study was extended to a total of 30 aromatic organic compounds with various structures and functional groups. The pseudo-first-order rate constants (k_{PAA}) of compounds' degradation by Co/PAA were measured, and 29 descriptors of compounds' properties were calculated. Based on the results, a quantitative structure-activity relationship was established, highlighting the importance of the number of ring atoms, E_{HOMO} , and E_{LUMO} - E_{HOMO} for a compound's reactivity to carbon-centered radicals generated from PAA. This study significantly advances the fundamental understating of (i) the oxidation conditions under the combined PAA and Co(II)/Co(III), and (ii) organic compounds' reactivity to carbon-centered radicals generated from activation of PAA. The results will be useful for further development of advanced oxidation technologies utilizing PAA.

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Removal pathway of hydrogen peroxide induced by dissolved organic matters under solar irradiation

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Hydrogen peroxide (H_2O_2) is a transient chemical species in surface waters where it is produced from the photochemical reactions of dissolved organics matters (DOM). H₂O₂ can affect the speciation of metals as well contributing to the degradation of organic as contaminates. The disproportionation of superoxide ions is considered as the primary source of H₂O₂ under solar irradiation, while its removal pathway has been seldom reported. Our study found that the loss rate of $H_2O_2(L_{H2O2})$ linearly increased with increasing of concentration of DOM under N₂-saturated conditions. The formation rates of hydroxyl radicals generated from H₂O₂ decomposition shows a strong correlation with additional DOM concentration indicates that the reactions between excited states of DOM (3DOM*) and H2O2 occurred. Based on observing the inhibitory effect of L_{H2O2} by borohydride reduction of the DOM and oxygen exposure, we propose that the aromatic ketones mojeties of ³DOM* react with H₂O₂ forming hydroperoxyl radical/superoxide (HO₂/O₂⁻) and reduced DOM (DOM⁻). The subsequent reaction between DOM⁻ and H₂O₂ leads a faster hydroxyl radical formation rate. By using model ketone compounds, the second-order rate constants of triplets with H_2O_2 are estimated to be ~10⁷ M⁻¹ s⁻¹. Our results reveal an important attenuation channel of hydrogen peroxide in sunlit surface waters that has been neglected in DOM photochemistry and it also provides a new sight of source of hydroxyl radical.

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Degradation mechanism of Benzophenone-3 during chlorination and UV/chlorination reactions

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Benzophenone-3 (BP3) is a potential phenolic endocrine disrupter that is widely used as a sunscreen and ultraviolet (UV) stabilizer. In this study, the degradation of BP3 in water during chlorination and UV/chlorination reactions was investigated. The degradation of BP3 by both reactions followed pseudo-first-order kinetics. The pH profile of the observed pseudo-first-order rate constants (k_{obs}) were bell shapes that depended on pH,

and the highest kobs values were obtained at a pH 8 for both reactions. The contribution of OH radicals on BP3 degradation under UV/chlorination conditions increased at acidic pH values, and the contribution of reactive chlorine species (RCS) such as CI radicals increased at neutral and basic pH conditions. The BP3 degradation rate was enhanced by the presence of HCO3- ions, but was inhibited by humic acid. A total of seven transformation products (TPs) of BP3 were identified during chlorination (TP-262, TP-296, TP-192, TP-226, and TP-118) and UV/chlorination (TP-244, TP-262, TP-278, and TP-296) reactions. Among the TPs, chloroform (TP-118) was only found in the chlorination reaction. The BP3 degradation pathways during both reactions were proposed based on these identified TPs. BP3 Degradation was mainly associated with electrophilic aromatic halogenation in both reactions. Finally, the toxicity of the TPs of the BP3 produced during the UV/chlorination reaction was lower than that of the TPs obtained during chlorination, implying that the additional oxidation of BP3 occurs by the reactive radicals produced during the UV/chlorination reaction. The results of this study can help to understand the behavior of BP3 during chlorination and UV/chlorination in the water and wastewater treatment processes.



Graphical Abstract

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Enhanced degradation of 1,4-dioxane by photofenton reactive ceramic membrane

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This study investigated the degradation of 1,4-dioxane using the photo-Fenton ceramic membrane filtration with goethite (α -FeOOH) as the photocatalyst. The effects of different concentrations of the H₂O₂, UV irradiation wavelength and initial 1,4-dioxane concentrations on the degradation efficiency were systematically investigated. 90% of 1,4-dioxane with an initial concentration of 10.77

mg L⁻¹ and α -FeOOH dose 1 g L⁻¹ were degraded within 12 h in batch experiments with the initial H_2O_2 concentration of 2 mM under UV254 irradiation at 2000 µW cm⁻². In the filtration studies, evaluation of 1,4-dioxane degradation was conducted with/without addition of H₂O₂, goethite coating and/or UV irradiation. Additionally, the total organic carbon (TOC), hydroxyl radicals and degradation by-products were both assessed under different degradation conditions to achieve deeper insight into the degradation mechanisms of 1,4-dioxane. Similar to the impact of the initial 1,4-dioxane concentration. increasing the influent flux essentially increases the level of the electron loading from the influent pollutant (J_e) and decreases the degradation rate of 1,4-dioxane. The removal efficiencies reached up to 15% when the influent flux is less than 12.46 LMH with the coated ceramic membrane. This study embarks on a novel demonstration of enhanced catalytic degradation processes via incorporation of photo-Fenton reactions into membrane filtration.



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Degradation of tetracycline by medium pressure UVactivated peroxymonosulfate process: Influencing factors, degradation pathways, and toxicity evaluation

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This study employed the medium pressure UV/peroxymonosulfate (MPUV/PMS), a new sulfate radical-based advanced oxidation process, to eliminate tetracycline (TTC) in water. At pH = 3.7, initial TTC concentration of 11.25 µM, PMS dosage of 0.2 mM and UV dose of 250 mJ cm⁻², 82 % of TTC was degraded by MPUV/PMS. The second-order reaction rate constants of TTC with SO₄•- and •OH were found to be 1.4 × 10¹⁰ M⁻¹ s^{-1} and 6.0 × 10⁹ M⁻¹ s^{-1} , respectively. Radical quenching experiments indicated that •OH played the major role in the degradation of TTC. Higher PMS dosage (0.1 mM~1.0 mM) and higher pH (3~11) could accelerate the TTC removal. Besides, the presence of Cl⁻ (0.1 mM~5.0 mM) and CO32- (0.05 mM~0.5 mM) could also promote the

reaction. Eight transformation products (TPs) were identified, and the potential degradation pathways mainly involved hydroxylation, demethylation and decarbonylation processes. The variation in the genotoxicity was investigated using the umu-test, and the results indicate that the genotoxicity of TTC after the MPUV/PMS treatment significantly increased during the initial stage. In addition, the ecotoxicity and mutagenicity of TTC and its TPs were predicted using quantitative structure-activity relationship (QSAR) analysis, and the results revealed that some TPs could have equivalent and even higher toxicity than TTC. MPUV/PMS showed better performance in TTC degradation in real waters than in Milli-Q water. MPUV/PMS is concluded to be an efficient method for removing TTC, but more attention should be paid to the changes of toxicity during this process.



Proposed degradation pathways of TTC by MPUV/PMS process.

Table 1. Toxicological data of TTC and its TPs as predicted by ECOSAR and T.E.S.T. In the case of ECOSAR, the results can be classified as very toxic (< 1 mg L³), toxic (1–10 mg L³), hamful (10–100 mg L³) and not harmful (> 100 mg L²) based on the Globally Harmonized

System of Classification and Labeline of Chemicals (GHS) [51]

				ECOSAL	R.			TEST
Compound	Acute toxicity (mg L ⁻¹)			Chronic toxicity (mg L ⁻¹)				
	Fish (96-h LC50)	Daphnid (48-h LC50)	Algae (96-h EC50)	Fish	Daphnid	Algae	ECOSAR Class	Ames Mutagenicity
TTC	27.088	2.866	5767.117	7.292		379.529	Vinyl/Allyl Alcohols	Positive
TP373	20.622	2.234	3301.278	4.486		235.711	Vinyl/Allyl Alcohols	Positive
TP416	35.394	3.458	19743.266	19.566	1.104	986.489	Vinyl/Allyl Alcohols	Positive
TP430	28.213	2.933	7415.485	8.89	0.66	459.471	Vinyl/Allyl Alcohols	Positive
TP432	26.683	2.815	5887.464	7.377		383.512	Vinyl/Allyl Alcohols	Negative
TP442	15.638	41.994	0.601				Acrylamides	Positive
TP458	16.866	2.014	832.317	1.523		83.201	Vinyl/Allyl Alcohols	Positive
TP460	16.45	1.978	745.544	1.394		76.362	Vinyl/Allyl Alcohols	Positive
TP466	1433.94	18.704	955.799	362.771	88.902	56.419	Phenol Amines	Positive

ENVR 368

Density functional theory calculations on the reaction pathways for the transformation of 6:2 fluorotelomer sulfonate to perfluoroalkyl carboxylic acids initiated by hydroxyl radical in aqueous phase

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Hydroxyl radical is the major oxidant in most advanced oxidation processes and can degrade various contaminants efficiently, but its reactivity for perfluoroalkyl acids (PFAAs) is very limited. Previous studies have shown that PFAA precursors that contain nonfluorinated groups can be transformed by hydroxyl radical into different chain length of PFAAs, but the reaction mechanism and pathways are not clear. In this study, we used density functional theory (DFT) calculations to investigate the hydroxyl radical-initiated transformation of one representative precursor, 6:2 fluorotelomer sulfonate (6:2 FTS) and illustrate the detailed reaction path. Different reaction pathways were proposed, and the free energy of the reactions was calculated at the M06-2X/6-311++G(2d,2p) level of theory using SMD as the solvation model. The kinetic feasibility of the reactions was compared by calculating the free energy of activation at the same level of theory and the optimal reaction path was then proposed. The results showed that the reaction started with a H-abstraction from the ethyl carbons of 6:2 FTS followed by a hydroxyl radical addition and a second H-abstraction. The addition of O₂ to the alkyl radical is critical as it generated the ketone radicals, which tend to capture any available electrons from adjacent functional groups and cause C-C cleavage. The C-C cleavage resulted in the formation of perfluoroalkyl or polyfluoroalkyl attached to carboxyl groups or aldehyde groups, and perfluorohexyl radical, which were further transformed to different chain length of perfluoroalkyl carboxylic acids (PFCAs). The rate constants of each step were calculated based on transition state theory. The product profile from DFT calculations were comparable with our experimental data where 6:2 FTS was efficiently transformed by hydroxyl radical into different PFCAs simultaneously, with perfluorohexanoic acid being the predominant product. The involvement of O₂ in the reaction path was verified experimentally and there was no reaction of 6:2 FTS under anaerobic conditions. The intermediates proposed in the optimal reaction path such as 6:2 fluorotelomer carboxylic acid and OH-substituted sulfonate and carboxylate were detected in the reaction solution by high resolution mass spectrometer. This study provides valuable insight into the degradation and transformation of precursors in hydroxyl radical-based oxidation processes.

Investigating the Influence of pH on persulfate mediated oxidation of perfluoroalkyl carboxylates using DFT and transient absorption spectroscopy

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The high stability and remarkable chemical properties of perfluoroalkyl carboxylates make them excellent for use in consumer products and industrial processes. Unfortunately, their widespread application led to environmental contamination on a global scale and they have been shown to bioaccumulate and cause physiological harm. Due to their inert nature, their environmental remediation is a contemporary challenge. Oxidation by sulfate radicals stands out as a promising approach to degrade these recalcitrant molecules. A major hurdle for transferring this technology to the field is the need for low matrix pH for efficient degradation, which is a poorly understood phenomenon. Clarifying the mechanistic role protons play in the oxidation of perfluoroalkyl carboxylates by sulfate radicals will provide insight into what conditions are necessary for field application of this technology. Results will be presented from computational and empirical techniques used to investigate the influence of pH on persulfate mediated oxidation of perfluoroalkyl carboxylates. Density functional theory was used to investigate specific interactions that influence kinetics and transient absorption spectroscopy was used to evaluate rate constants.

ENVR 370

Simple and Efficient Defluorination of PFAS in Wastewater by V_2C Nanosheets and H_2O_2

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Per-and polyfluoroalkyl substances (PFAS) in wastewater has become widespread and has attracted increasing attention due to its broad use in manufacturing and in industrial applications as flame retardants, and stain, grease and water repellants. However, if present in drinking water, PFAS are acutely toxic causing tumors, and kidney and liver diseases in humans as well as immunological effects in aquatic animals. Successful degradation of PFAS remains a key environmental challenge due to the extreme strength and stability of characteristic carbon-fluorine PFAS bonds. Therefore, developing an environmentally-friendly, mild and convenient approach for PFAS degradation is highly

desirable. Herein, a facile and green method is developed, which shows extremely efficient defluorination of PFAS in the presence of vanadium carbide (V₂C) nanosheets and H₂O₂ under physiological conditions. The as-prepared V₂C layered nanostructures were exfoliated into nanosheets resulting in a significant enlargement of V₂C surface area and reactive sites which facilitates the fast degradation rate of PFAS. Perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS) were selected as representative PFAS at initial concentrations of 50 µg/L. Defluorination reactions were conducted at pH 7 under aerobic conditions. PFOA and PFOS were first adsorbed to the carbon nanosheets, then defluorination occurred via singlet oxygen generation and the cooperative catalysis of the nearby vanadium nanosheets and hydroxyl radicals to effectively degrade PFAS. The V₂C-H₂O₂ defluorination mechanism is so effective, that over 80% PFOS and over 45% PFOA defluorination was observed with less than 0.15 mg/mL V₂C within 4 h of reaction at circumneutral pH and in the presence of dissolved oxygen. The findings from this work of high reactivity and efficiency of PFAS degradation employing V₂C nanosheets coupled with the addition of a mild oxidant under environmentally relevant conditions can translate to other applications in contaminant removal, such as degradation of halogenated disinfection byproducts.

ENVR 371

Rapid removal of poly- and perfluorinated compounds from investigation derived waste (IDW) in a pilot-scale plasma reactor: laboratory and field demonstration studies

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The U.S. Defense Department, along with numerous other agencies and entities around the world, are currently undertaking expansive portfolio-wide investigations of the extent of poly- and perfluorinated alkyl substances (PFAS) contamination. These investigations will continue for decades and result in copious amounts of liquid investigation-derived waste (IDW) primarily from development and purge water from the installation and sampling of monitoring wells. Current disposal options for liquid IDW at sites where existing treatment systems are not available are limited and costly due to off-site transportation costs. In this study, 4 L pilot scale plasma reactors installed into an 8 × 20 ft mobile trailer were used to treat IDW obtained from 13 different site investigations at Air Force installations in order to reduce perfluoroalkyl acids (PFAAs) concentrations

below United States Environmental Protection Agency's (USEPA's) health advisory concentration level (HAL). Before the treatment, PFAAs and their precursors in all IDW samples were characterized. In the raw water, numerous PFAS were detected in a wide concentration range. The concentration of total PFAS (12 perfluorocarboxylic acids (PFCAs) and perfluoroalkyl sulfonates (PFSAs)) in the 13 samples ranged between 2.7 and 1440 µg/L and the concentration of perfluorooctane sulfonate (PFOS) plus perfluorooctanoic acid (PFOA) ranged between 365 and 73700 ng/L. The treatment resulted in rapid PFAAs removal with faster rates for longer-chain PFCAs (C \geq 8) and PFSAs (C \geq 6) than for PFCAs and PFSAs of shorter chain length. In nine of the 13 IDW samples both PFOS and PFOA were removed to below USEPA's HAL concentrations in < 1 minute whereas longer treatment times (up to 50 minutes) were required for the remaining four IDW samples. Continuous treatment results of contaminated groundwater on-site at flowrates up to 1.2 gpm using our mobile treatment trailer will also be presented.

ENVR 372

Current use C6 aqueous film-forming foams (AFFF) containing per- and polyfluoroalkyl substances: Characterization and treatment options

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Per- and polyfluoroalkyl substances (PFAS) are chemical compounds that have been used in numerous industries, commercial applications, and extensively in aqueous filmforming foams (AFFF) for fire-fighting activities. They are environmentally persistent compounds and reported to cause adverse effects on human health. According to the USEPA, currently available industrial formulations of AFFF should be free from long-chain perfluoroalkyl acids (PFAAs) which are the most commonly found PFAS in the environment and reported to be the most problematic. This study characterized four industrially formulated and currently used AFFF samples to determine if they could be treated to remove PFAAs. PFAS precursors were preoxidized using various advanced oxidation processes (heat-activated persulfate. UV-activated (AOPs) persulfate, Fenton, UV-Fenton and UV-peroxide) and then subjected to plasma treatment. Preliminary measurements of 15 PFAAs and 10 precursors with an LC-MS/MS found high concentrations of short-chained

PFAAs (30 to 3000 µg/L), traces of long-chain PFAAs (40 to 60 µg/L), and a significant amount of PFAS precursors (70 to 50000 µg/L).The 6:2 fluorotelomer sulfonate (6:2 FTS) was present at high concentrations in three samples which ranged between 1000 and 50000 µg/L. The AFFF samples also contained high concentrations of total oxidizable precursors (TOP) in the range of 1500 to 10000 mg/L and total fluorine in the range of 400 to 6000 mg/L, indicating the presence of unknown PFAS precursors at high concentrations. The TOP assay (involving heatactivated persulfate oxidation) as developed by Houtz and Sedlak (2012) (DOI: 10.1021/es302274g), was only partially effective at oxidizing the precursors, hence the existing TOP assay was modified by optimizing persulfate dose, sodium hydroxide concentration and dilution factors for complete oxidation of precursors to PFAAs. With optimized conditions, it was found that the concentrations of short-chain PFAAs increased by 2-3 orders of magnitude with the appearance of some long-chain PFAAs. This optimized TOP method was implemented as the pre-oxidation treatment prior to plasma treatment for complete removal of PFAS from AFFF. We are currently extending this study by exploring other oxidation techniques and plasma destruction technologies for AFFF treatment.

ENVR 373

Regeneration of per- and polyfluoroalkyl substances (PFAS) contaminated granular activated carbon (GAC) using non-thermal plasma

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Per- and polyfluoroalkyl substances (PFASs) are an expansive set of organofluorine compounds that are now classified as emerging contaminants by the US EPA due to their potential human and ecosystem health risks. Due to contamination from various sources like firefighting foams and biosolids applied from wastewater treatment plants, PFASs are being detected in waterways all over the US. PFASs are recalcitrant to degradation by many traditional remediation strategies. Current PFAS removal techniques like ion exchange resins have limited effectiveness and can prove to be expensive. The objectives of this study were to (1) test the use of granulated activated carbon (GAC) as an adsorbent for different PFASs, and (2) explore the feasibility of the regeneration of PFAS-contaminated GAC using dielectric barrier discharge (DBD) plasma technology and its reuse. Adsorption densities of virgin and regenerated GAC were

measured using adsorption tests. Virgin GAC from initial adsorption tests was regenerated using DBD plasma and then reused in subsequent tests to measure its capacity to adsorb PFASs after treatment. Plasma parameters were adjusted to obtain the most effectively regenerated GAC. 30 minutes of plasma treatment at 14 W showed the best GAC regeneration results. The treated GAC achieved concentrations very similar to that of the virgin GAC. For example, at hour 45 of the adsorption tests, treated GAC reached a PFOA concentration of 0.018 mg/L while virgin GAC reached a concentration of 0.011 mg/L. Similar results were observed during tests conducted using PFOS. Regenerated GAC also adsorbed more PFOA than untreated, contaminated GAC. For example, at approximately hour 22 of the adsorption tests, untreated GAC reached a PFOA concentration of 4.617 mg/L while regenerated GAC reached a concentration of 1.265 mg/L. The results show that plasma treatment can be a promising technique for effectively regenerating PFAS-contaminated GAC for reuse. Further studies are in progress on the effects of regeneration on different types of GAC as well as other adsorbent media (e.g., ion exchange resins, clays, and zeolites).

ENVR 374

Efficient mineralization of fluoropolymers using subcritical water

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Organofluorine compounds show unique characters such as high thermal and chemical stability, high surface activity, no light-absorbing ability, high pharmacological effect, etc. While these chemicals show a variety of functionalities, some of them have environmentally negative features, e.g., high persistence in the aquatic environment and difficulty in waste treatments. Indeed, compounds such as perfluorooctanesulfonic acid (PFOS), perfluorooctanoic acid (PFOA) and their derivatives show non-ignorable bioaccumulation and health risks. Therefore, international regulations for their manufacturing, uses, export/import have already begun. Among organofluorine compounds, fluoropolymers have many industrial applications such as not only traditional uses (packing, tubes, sinks, valves etc.), but also ionexchange membranes, optical fibers, resists, energy devices, etc. While applications of these polymers are being spread, waste treatment techniques for the polymers are not well established, because these polymers are thermally and chemically stable, and incineration treatment generates hydrogen fluoride gas. which seriously damages incinerators. If fluoropolymers could be decomposed to fluoride ions (F-) by means of environmentally benign techniques, the established methodology for treatment of F⁻ could be used, whereby

 Ca^{2+} is added to the aqueous F⁻ to form CaF_2 , which is a raw material for hydrofluoric acid, and hydrofluoric acid is a raw material for all organofluorine compounds. Hence, the development of such a method would contribute to recycling of fluorine element. Herein we describe effective methodologies decompose cutting-edge to fluoropolymers (ion-exchange membrane polymer, polv(vinvlidene fluoride) (PVDF), ethvlenetetrafluoroethylene copolymer (ETFE), and VDF-related copolymers) to F⁻ ions in subcritical water by reductive or oxidative approaches. Formation of CaF₂ in the presence of Ca(OH)₂ in the reaction system is also reported.



Decomposition of PVDF and related copolymers in low-temperature subcritical water

ENVR 375

PFAS degradation in UV/BOHP photocatalytic system: Mechanisms and pilot-scale studies

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Destructive approaches for the removal of perfluoroalkyl substances (PFAS) from aqueous systems have always been a major challenge for environmental engineers due to the high energy of carbon-fluorine bonds in their structure. So far, various advanced oxidation and reduction processes based on UV/Photocatalysis as an alternative to insufficient traditional techniques have been successfully proposed for a wide range of recalcitrant organics, but in this case, poor performance and vague kinetic are impeding the practicality of photocatalysis technology for PFAS treatment. This study herein reveals the pivotal role of holes along with electrons and hydroxyl radicals in а simultaneous oxidative/reductive degradation mechanism of PFAS using a bismuth

phosphate-based semiconductor (Bi₃O (OH) (PO₄)2 or BOHP) as photocatalyst. Detection of shorter chain PFAS in the reaction solution suggested that they degrade to smaller PFAS by losing CF2 in a stepwise manner. Investigating the effects of carbon chain length (C4 to C10) on the degradation efficiency showed that as the chain length decreases, the degradation rate drops as well, which is likely attributed to the lower tendency of smaller PFAS to adsorb on the surface of the catalyst particles. Also, the individual effects of major coconstituents of AFFF-contaminated groundwaters, as the main target, were assessed on the kinetics of the reaction. Finally, the performance of the developed process was evaluated in a pilot-scale system (Photocat, Purifics Inc.) consisting of high turbulence annular rectors for treating tap water matrix samples spiked by PFAS as well as AFFF-contaminated groundwater samples. The results demonstrated a much faster degradation rate in comparison to the benchtop system, considering the actual residence time of the solution in the reactor.

ENVR 376

Treatment and removal of PFOA using an innovative technology of UV-vis/ $Zn_xCu_{1-x}Fe_2O_4$ /oxalic acid

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Per- and polyfluoroalkyl substances (PFAS) are a class of synthetic chemicals used to modify surfaces properties of fabrics, carpets and furniture, and as fire retardants, present a public health challenge due to the wide range of drinking water contamination. Exposure to PFAS, most notably perfluorooctanoic acid (PFOA) causes health risks including thyroid disease, and several cancers. PFOA is very stable, persistent in the environment, and hard to be decomposed by traditional technologies due to the strong covalent carbon-fluorine (C-F) bond. Considering the saturated electronic status of C-F atom in PFOA, the reductive conditions are preferred for degradation. Herein, we demonstrate an innovative technology for efficient removal of PFOA from the water using photocatalytic reduction approaches. Our protocol uses UV-vis light and scalable, low cost, magnetically retrievable and reusable heterogeneous ZnxCu1-_xFe₂O₄/oxalic acid for the treatment of PFOA. This accessible approach might lead to a new technique in PFASs treatment which will bring the industrial application of water purification at a reduced cost.

ENVR 377

Electrochemical mineralization of PFOA and PFOS

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Perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS) are per- and polyfluorinated alkyl substances (PFAS) linked to adverse health effects. Due to their recalcitrance to conventional treatment, alternate options have been explored. Electrochemical mineralization which employs direct current to transform PFOA/PFOS into bicarbonate, fluoride, and sulfate is a promising one but still has some gaps to be addressed. Most previous studies were not able to achieve full mineralization of PFOA/PFOS and complete fluorine mass balance. The goal of this research is to achieve full PFOA/PFOS mineralization by testing different anodes and current densities and validate complete fluorine mass balance. The study tested different anode materials such as boron-doped diamond, Ebonex-Plus, and Ti/RuO₂ for their mineralization efficiency of PFOA/PFOS at current densities ranging from 0.1 to 40 mA/cm². Mineralization efficiency was calculated as a ratio of fluoride at the end of reaction time to the amount of organic fluorine in the initial sample. The effect of applied current density was determined by studying the increase in PFOA/PFOS mineralization with increasing current density and arriving at an optimum based on the plot between PFOA/PFOS mineralization and applied current density. The complete electrochemical study setup consisted of the main reactor vessel containing PFOA/PFOS along with the supporting electrolyte and an absorption solution that captures PFAS and hydrogen fluoride gases produced during the degradation of PFOA/PFOS. To achieve complete fluorine mass balance at the end of treatment, first, PFAS compounds in samples collected from the reactors and absorption solutions were analyzed using liquid chromatography-mass spectrometry for PFAS compounds whose standards are available. These samples were also analyzed for adsorbable organic fluorine (AOF) to account for unknown PFAS compounds formed. Finally, fluoride in the reactor samples and those captured by the absorption solution were analyzed by ion chromatography thus completing the fluorine mass balance.

ENVR 378

Role of sulfur functionality in the production of photogenerated water-soluble compounds from surrogate and MC252 crude oils

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Photooxidation of surface oil has been implicated as a critical weathering process in the environment after major oil spills (e.g., Deepwater Horizon (DWH)) and has been demonstrated to produce oil- and water-soluble oxygenated compounds. After the DWH oil spill, many laboratory studies have been conducted to mimic petroleum weathering in the environment. Due to the low availability of oil directly from the Mississippi Canyon (MC) 252 well from which the DWH spill occurred, several studies use surrogate crude oil, which is collected from various nearby wells in the Gulf of Mexico. Although chemically similar to the oil spilled in DWH, previous studies have shown minor differences between surrogate and MC 252 crude oils and suggest the production of different photooxidation products. For example, one study observed differences in the carbon number range for photochemical transformation products between the two oils, suggesting differences in boiling point. Our initial studies involved laboratory photoirradiation of MC252 and surrogate crude oils, and we observed notable differences between the sulfur content in the photooxidized products; thus, we focus here on sulfur functionality. Although light sweet crude oils (e.g., surrogate and MC252) typically contain very low amounts of sulfur (<0.5%), the watersoluble fraction produced from irradiation of surrogate oil contained high levels of SO_x species. Furthermore, sulfurcontaining polyaromatic hydrocarbons from crude oil have been demonstrated to photooxidize and become water-soluble; however the role of sulfur chemistry in the formation of photogenerated water-solubles has not been extensively studied. Thus, surrogate and MC252 crude oil are separated into three fractions enriched in thiophene, sulfide, and thiol functionalities. Fractions are then irradiated in a solar simulator, which mimics photooxidation in the environment, and analyzed by ultrahigh resolution Fourier-transform ion cyclotron resonance mass spectrometry to reveal the sulfur functionalities of the water- and oil-soluble photooxidation products and allow for comparison of surrogate and MC252 sulfur-containing transformation products.

ENVR 379

Using high-resolution mass spectrometry to identify transformation products of synthetic progestins in environmental matrices

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Synthetic progestins are commonly used as human and agricultural pharmaceuticals; their environmental discharge induces endocrine disruption at trace concentrations. Despite the wide occurrence of synthetic progestins in wastewater influent, effluent, and receiving waters, their fate and transformation in these environmental matrices has not been well characterized. In particular, environmental fate and risk assessment should focus more on the potential for steroidal transformation products to retain the steroid skeleton and exhibit similar or altered endocrine disrupting potentials. Here, we evaluated the biotransformation and product identification of three largely used, yet understudied synthetic progestins: altrenogest, a veterinary medicine extensively applied in the US, and dienogest and drospirenone, two most consumed progestins in Europe acting as fourth-generation human contraceptives. Biotransformation was studied in environmentally relevant inocula, specifically agricultural receiving water for altrenogest (for 30 days, simulating its fate after agricultural runoff discharge), and activated sludge for dienogest and drospirenone (for 30 hours, simulating their fate in wastewater treatment plant). The identification of transformation products utilized high-resolution quadrupole time-of-flight mass spectrometry and structural elucidation via MS/MS spectra. More than ten transformation products were identified for altrenogest, including dehydrogenation, hydroxylation, oxidation, and dealkylation products. Transformation products (~10) observed for dienogest and drospirenone included hydrogenation, dehydrogenation, hydroxylation, dihydroxylation, isomerization, and hydration products. Dehydrogenation tended to be the major pathway for all the studied biotransformation processes, and the dehydrogenation products formed were recalcitrant to further degradation. Notably, steroid skeleton was conserved in most of the transformation products, which indicated potentials of retained bioactivity although the parent masses were eliminated.

ENVR 380

Application of HRMS in transformation of organic matters in the wastewater effluent

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High-resolution mass spectrometry (HRMS) is a novel technology that has been coupled with liquid chromatography (LC) to analyze complex environmental

samples. Although the structural information of the majority of compounds detected by HRMS was unknown, it is possible to investigate the transformation of unknown compounds based on the MS profile. This study introduces the application of HRMS in the environment process analysis. Firstly, we report the unequivocal identification of the products and the detailed pathways for the photodegradation of nicotine in an effluent matrix under simulated solar irradiation. Using the multivariate statistical strategies orthogonal partial least-squares discriminant analysis (OPLS-DA) and hierarchical clustering, 38 potential transformation products (TPs) of nicotine were successfully extracted from the water matrix via high-resolution ultra-high-performance liquid chromatography quadrupole time-of-flight mass spectrometry (UHPLC-QTOF-MS). Overall, 30 TPs, including 4 groups of non-separated isomeric photo TPs, were confirmed based on the MS² information of standard compounds and the isotope-labeling method (using rac-nicotine-2',3',3'-D₃, rac-nicotine-¹³CD₃, and rac-nicotine-D₄). Secondly, statistical analysis assisted HRMS was employed to investigate the phototransformation of nontarget features in wastewater effluents under various radical quenching/enhancing conditions. A total of 9694 nontarget features were extracted from the effluents, including photoresistant features, photolabile features and transformation products. Sixty-five percent of the wastewater effluent features were photoresistant, and the photolabile features could be classified into five groups: direct photolysis group (group I), HR/CR-dominated group (group II), ³OM*-dominated group (group III), photochemically produced reactive intermediates (PPRIs) combination-dominated group (group IV), and non-firstorder degradation group (group V). The reaction types that occurred in the phototransformation process were analyzed by linkage analysis. The results suggested that oxygen addition and dealkyl group reactions were the most common reaction types identified in the phototransformation process. Thirdly, we try to apply statistical analysis assisted HRMS to compare the efficiency and reaction of different radicals mediated advanced oxidation processes.

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Fate of agrochemicals during anaerobic digestion: Quantifying degradation and identifying transformation products using orbitrap mass spectrometry

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A wide variety of chemicals are applied in agricultural systems for animal and crop growth including antibiotics, antifungals, and insect repellents. Many chemicals within these classes pose serious human and environmental health risks, and technologies to reduce their emission into the environment are needed. Anaerobic digestion (AD) is a biological process that converts organic material (e.g. biosolids, manure) to valuable biogas, and is considered a key component to enhancing agricultural sustainability. AD may also be valuable as a technology for degrading agricultural chemicals prior to environmental release. While the effects of contaminants, in particular antibiotics, on biogas production have been investigated previously, little is known about the transformation of xenobiotics during AD. We used liquid chromatography coupled with high resolution mass spectrometry to measure the degradation of agricultural chemicals and identify transformation products formed in lab-scale AD batch reactors. Reactors were prepared following the Biochemical Methane Potential method and spiked with compounds individually and in mixtures. Digestion media samples were extracted using a modified QuEChERS method and analyzed using positive electron spray ionization in full MS mode with data dependent MS2 acquisition. Degradation kinetics were measured, and several transformation products were identified indicating the relevance of both biotic and abiotic transformation processes. The application of statistical tools including principal component and differential analyses demonstrated significant changes in the chemical composition of digested material between samples with and without contaminants added. Additionally, biogas production, pH, and volatile fatty acid profiles were observed to assess the impact of the contaminants on AD microcosm health.

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Withdrawn

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Applications of high-resolution mass spectrometry in large-scale emerging contaminant monitoring: Perand polyfluorinated alkyl substance testing network in North Carolina

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High-resolution mass spectrometry (HRMS) and nontargeted analysis (NTA) provide an analytical platform for

assessing occurrence of organic contaminants in aguatic environments across a broad swath of chemical space. Interest in using NTA in the context of large-scale monitoring efforts for evaluating chemical risk continues to grow. Here we present a case study on the use of NTA to evaluate the occurrence of per- and polyfluorinated substances (PFAS) in drinking water sources from more than 400 surface- and groundwater sites in North Carolina, USA. We developed and validated novel onlinesolid phase extraction (SPE) method that achieves low part-per-trillion detection limits for neutral, anionic and zwitterionic PFAS, using low-volume samples (10 mL). This method employs back-elution from a mixed-mode anion exchange column and peak focusing prior to ultraperformance liquid chromatography (UHPLC). We coupled online-SPE-UHPLC with electrospray ionizationultra-high-resolution mass spectrometry (Orbitrap Fusion Lumos) with internally calibrated full-scan HRMS and data-dependent HRMS². We have applied novel data treatment approaches to match analyses against databases of known PFAS chemicals as well as a custom PFAS MS/MS library. We have explored the utility of mass-defect filtering and defect-dependent analysis for elucidation of novel PFAS compounds. Furthermore, HRMS NTA results were integrated with sample-matched targeted quantitative analysis (UHPLC-QqQ) and compound-class specific endpoints (i.e., total organic fluorine) to evaluate co-occurrence trends and evaluate method coverage, respectively. Results indicate the widespread occurrence of emerging "ether-acid" PFAS compounds (e.g. GenX and related compounds) in the Cape Fear river basin of NC downstream of a major fluorochemical manufacturing facility as well as sporadic groundwater and surface water contamination from sources including firefighting foams and wastewater discharges. Our results represent the first state-wide map of holistic PFAS contamination in drinking water sources within the United States. Our discussion will focus on development and implementation of the NTA screening framework, with special consideration for chemical informatics tools used in developing and deploving the PFAS database and spectral library and establishing analytical figures of merit for identifications made in the absence of authentic standards, and report on the first completed round of sampling.

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Investigating poly- and perfluoroalkyl substances (PFAS) degradation in non-equilibrium cold plasma technologies treatment using HRMS suspect screening

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Poly- and perfluoroalkyl substances (PFASs), organofluorine surfactants, are an emerging class of water contaminants that are extremely recalcitrant to degradation by many conventional forms of treatment, including modern advanced oxidation processes. Here we demonstrate the ability of non-equilibrium (cold) plasma technologies to degrade perfluoroalkyl acids (e.g., PFOA, PFOS, PFNA, PFHxS) in aqueous solutions. time-of-flight Quadrupole high resolution mass spectrometry (QTOF HRMS) was used to quantify target analytes, and SWATH and Independent Data Analysis (IDA) were used to tentatively identify PFAS degradates during plasma treatment; a fluorinated compound library was employed for suspect screening. Additionally, data worksflows were developed to assess and rank the 1) chromatography and signal, 2) library match, and 3) temporal trends. Analysis of water spiked with perfluoroalkyl acids revealed that degradation of both sulfonate and carboxylate compounds yielded shorter chain length perfluoroalkyl carboxylic acids (quantified with targeted methods), and that other species were not observed to be created. Field-contaminated groundwater was treated with plasma, and HRMS results indicated that perfluorohexane sulfonamide (FHxSA) was degraded (non-target analysis) but that many PFAS, including PFCA, were created during plasma treatment. These results suggest that there are source PFAS that are not included in the library; non-target analysis is underway to try to identify potential compounds.

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Development of a non-target workflow for the identification of industrial chemical contaminants

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The pollution of the aquatic environment with products and intermediates from the chemical or related industry is a continuing challenge due to continuously changing chemical usage and the large number of unknown or undocumented chemicals being emitted. Non-target screening (NTS) using high-resolution mass spectrometry has proven to be a powerful method for the identification of previously unknown organic contaminants. However, in rivers, a large number of ubiquitously distributed waterborne compounds can be detected and their features must be filtered out to isolate specific substances. Therefore, the aim of this study was to develop a sampling and analysis workflow with filtering methods for the isolation and identification of industrial chemical compounds discharged into a river. This workflow was applied to the Nidda river basin located north of Frankfurt

am Main (Germany) in a ten-day sampling with 28 sampling locations. The analysis was performed using high-resolution LC-ESI-QToF-MS with RP chromatography followed by data processing using R and custombuilt functions. Features were prioritized when they were detected in a tributary a) exclusively at a sampling point (not upstream) and b) not in the receiving river upstream of the confluence. The filtering of ubiquitously detected features common to domestic wastewater was carried out by comparing the sample data to the NTS data of 16 investigated WWTP-effluents and removing features found in both data sets. The prioritization procedure led to a considerable reduction of data by 78%. Finally, three tributaries of the river basin were identified as a source of a comparatively high number of potentially industrialoriginating contaminants. In total, nine of the compounds specifically discharged by these three tributaries into the river could be identified. Six of them most likely originate from industrial processes. Among them were the UV stabilizer Nylostab S-EED and the vulcanization accelerator 1-(o-tolyl)-biguanide which are mainly applied in textile industry.

ENVR 386

Using high resolution mass spectrometry to uncover advanced oxidation and disinfection by-products in algal and wastewater-impacted drinking water

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Wastewater, from either municipal or industrial sources, can contaminate drinking water sources and impact human health. Municipal wastewater is treated prior to being introduced into nearby rivers and creeks, but conventional wastewater treatment does not completely remove halides or many contaminants, such as pharmaceuticals, hormones, per- and polyfluorinated alkyl substances (PFASs), flame retardants, UV filters, and pesticides. In addition, disinfection by-products (DBPs) can form from these contaminants when wastewaters are chlorinated prior to their release to surface waters. Moreover, environmental factors, like the presence of harmful algal blooms in source waters, can also impact drinking water and provide precursor material for potentially toxic DBPs. In our latest research, we have been investigating Lyngbya wollei algae and their toxins in a South Carolina lake that have the potential to impact downstream drinking water. We are using high resolution mass spectrometry to investigate DBPs from Lyngbya

wollei algae and their toxins, along with wastewaterimpacted waters that are treated with advanced oxidation and chlorine.

ENVR 387

Science and policy of POPs through passive air sampling

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Since the early 1990s. Kevin Jones et al., pursued research on biomonitors of air, including archived grasses and soils from long-term experiment stations in the UK. This was done to better understand the fate and transport of persistent organic pollutants (POPs) including their spatial and temporal tendencies. These unique data were applied to fugacity models to reveal the transient nature of POPs residues and the importance of secondary emissions to air, governed by properties such as KOA. Kevin expanded this line of work and tested synthetic passive air samplers such as semi-permeable membrane devices (SPMD), which were until then only applied in water, to conduct spatial transect studies that spanned national and regional scales. This work led to an improved understanding of secondary sources which is a key element of the global fractionation phenomenon by which chemicals are preferentially retained in different latitudinal predicted by Mackay and Wania. zones, as Kevin's scientific advances, coupled with the numerous advantages of employing simple, electricity-free, and relatively inexpensive samplers, triggered a whole community of researchers to undertake studies on POPlike chemicals in air using passive air samplers. This new direction, by-passed the limitations on spatial scale and replicate sampling sites that existed for conventional air sampling methods. In Canada, Kevin's research motivated the development of the polyurethane foam (PUF) disk sampler by Harner et al., and eventually, the Global Passive Air Sampling (GAPS) Network. The GAPS network, since 2005, has provided a unique global-scale context on POPs, that addresses the risk assessment and risk management needs of the Stockholm Convention on POPs. This plenary presentation will be a historical perspective of the PUF disk passive air sampler over the last 20 years - including motivation and early adoption that has led to its widespread use today at the intersection of science and policy.

ENVR 388

Importance of source inventories for our understanding of the global distribution of POPs

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The role of emission inventories is key to understanding and controlling the global distribution of POPs such as PCBs, yet their importance and the challenges putting them together is often overlooked. One of the first comprehensive estimates of historical global production for PCBs suggested that over 1.3 million tonnes of were manufactured and that 97% of PCB use occurred in the Northern Hemisphere. A follow-up study using a dynamic mass balance model approach estimated the resulting historical emission profile over a 70-year period. Additional updates have reduced uncertainty, increased future projections and taken into account global movements of waste such as discarded electrical products. These studies provided vital data for the global assessment of PCB transport and fate and have guided our understanding of what has become one of the most well characterised global contaminants. Models such as BETR-Global have utilised such estimates to provide valuable insights into dominant transport and fate processes, important sinks and long-term trends. The discussion of the dominance of primary and secondary sources can only really be addressed using such studies. Recent developments in China, which has experienced limited historical production and use of PCBs, identified a of on-going and increasingly important range unintentionally produced PCBs. This presentation will discuss the importance of the development of reliable emission inventories and their constant assessment and revision using global models and measurement datasets to understand the fate and effects of POPs. Focus may have shifted to other important chemical groups such as PFAS, but the questions and challenges remain the same.



ENVR 389

Probing sources of persistent organic pollutants in the atmosphere of China and nexus

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Persistent organic pollutants (POPs) is long-term challenge to mankind. While the Stockholm Convention list of industrial POPs keeps expanding, unintentionallyproduced POPs (UP-POPs) from industrial and municipal/agricultural waste burning and vehicular exhaust are ubiquitous. The shift of chemical production capacity, solid/electronic waste from the northern countries to the low-latitude developing regions in the last three decades, followed by a less sound industrial production and environmental management, may have been resulting in a 'southern tilt' or global shift of POPs emission sources to developing countries. Monitoring POPs in the air could provide timely and sensitive signals to probe source information; in particular the development and wide application of passive air sampling (PAS) technique enables comparison studies at regional/global scale. A recent PAS campaign was organized in China to look at the contribution of unintentionally-produced polychlorinated biphenyls (UP-PCBs) to the PCBs in the atmosphere, in which a dominance of UP-PCBs (>60%) was revealed in the Chinese atmosphere. PAS campaigns were also organized in several coastal cities along the 21st Maritime Silk Road (MSR), from Northeast/South/Southeast Asia to East/West Africa to investigate the current situation of POPs in the atmosphere, as well as their potential link to solid/electronic waste burning. It is suggested that an international collaboration on tracking and assessing the global 'southern tilt' of POPs emission regions and nexus could be of timely need.

ENVR 390

From Lancaster to the poles: Chasing POPs in one ocean, one air

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Some of the most notorious organic contaminants are persistent, bioaccumulative and hydrophobic, including PCBs and organochlorine pesticides, such as DDT. Yet many emerging contaminants in water possess very different physico-chemical properties and pathways. Perand polyfluorinated alkyl substances in particular are at least as persistent as PCBs, also bioaccumulate but are much more soluble in water. Both are of concern to humans near contaminated sites, but also pose risks in the remote Arctic environment. Using a combination of active water sampling and relying on passive sampling approaches, we investigated the presence of legacy and emerging organic contaminants in ocean basins, with a particular focus on the Arctic Ocean. For PFASs, the available evidence suggests that atmospheric transport is still more important than water mass transport, though we detected first signs of PFASs in Atlantic water masses reaching the Arctic Ocean. For PCBs, in contrast, mass flux estimates suggest that ocean transport is important, and that there are more PCBs entering the Arctic Ocean through the Fram Strait than being exported. Emerging contaminants are also found throughout the Arctic Ocean water column.

ENVR 391

Temporal trends of polycyclic aromatic hydrocarbons in the UK and the USA

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I first met Kevin Jones when he started at the University of Lancaster. He proposed that we collaborate on polycyclic aromatic hydrocarbons (PAH). He had several soil samples collected over the last 150 years from an agricultural research field station in the UK, and he wondered about the time-trends of deposition of PAH. We, of course, jumped at the idea, and Kevin ended up publishing a highly collaborative paper titled "Increases in the polynuclear aromatic hydrocarbon content of an agricultural soil over the last century," by K. C. Jones, J. A. Stratford, K. S. Waterhouse, E. T. Furlong, W. Giger, R. A. Hites, C. Schaffner, and A. E. Johnson, in Environmental Science & Technology (1989, 23, 95-101). In honor of that earlier work, this presentation will bring us up to date on measurements of PAH in the vapor and particle phase of atmospheric samples collected around the Great Lakes for 24 hours once every 12 days since 1990. We have analyzed about about 2000 concentrations of 22 different PAH using multiple regression of the form: $ln(C) = a_0 + a_1 t + a_2 sin(zt) +$ a_3 cos(zt) + a_4 log(pop) + a_5 ln(ws) + a_6 sin(wd) + a 7 cos(wd), where "t" is the sampling date, "z" =6.28/365.25. "pop" is the number of people within a 25km radius of the sampling site, "ws" is the average wind speed during sampling, and "wd" is the average wind direction (in radians) during sampling. There is a wealth of information in these fitted coefficients.

ENVR 392

Atmospheric deposition of polycyclic aromatic hydrocarbons and organohalogen compounds in high mountain areas of Europe

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Polycyclic aromatic hydrocarbons (PAHs), organochlorine compounds (OCs) and polybromodiphenyl ethers (PBDEs) were analyzed in bulk atmospheric deposition collected at four European high mountain areas, Gossenköllesee (Tyrolean Alps), Redon (Central Pyrenees), Skalnate Pleso (High Tatra Mountains) and Lochnagar (Grampian Mountains) between 2004 and 2006. The samples were collected monthly in the first three sites and biweekly in Lochnagar, providing the most comprehensive fallout description of these compounds in high mountains. The average PAH deposition fluxes were highest in Skalnate Pleso, 9700 ng m⁻² mo⁻¹. In Gossenköllesee, Redon and Lochnagar they ranged between 800 and 2100 ng m⁻² mo⁻¹. Parent phenanthrene, fluoranthene and pyrene were the dominant compounds (32-60% of total). Polychlorobiphenyls (PCBs) generally showed the highest OC deposition fluxes in the four sites, 112-488 ng m⁻² mo⁻¹, and hexachlorobenzene the lowest, a few ng m⁻² mo⁻¹. Endosulfans were found at higher deposition fluxes. 11-177 ng m⁻² mo⁻¹, than hexachlorocyclohexanes, 17-66 ng m⁻² mo⁻¹, in all sites except Lochnagar that was characterized by very low fluxes of this insecticide. The total PBDE fluxes ranged between 100 ng m⁻² mo⁻¹ (Alps) and 190 ng m⁻² mo⁻¹ (Tatras). These distributions were dominated by BDE209. Significant correlations between PBDE deposition and percent of North Atlantic backwards air mass trajectories were observed in the westernmost sites, Lochnagar and Redon, suggesting a transcontinental transfer of these pollutants from North American sources into Europe. Skalnate and, to a lower extent Redon, also recorded secondary emissions of the pentaBDE mixture from central Europe. A specific PBDE source was observed in United Kingdom and recorded in Lochnagar. Significant correlations between current-use OC pesticides and air masses flowing from the south were observed in Gossenköllesee, Lochnagar and Redon. No relationship between PCB deposition fluxes and air mass trajectories were observed. Photolytic degradation during transport decreased the relative abundance of BDE209 and modified the emitted pentaBDE technical mixtures by depletion of the relative composition of BDE99 and, to a lower extent. BDE47. The transformations were more intense in the sites located above 2000 m, Redon and Gossenköllesee, and particularly during the warm periods. These sites were also those with lowest relative fluxes of photooxidable PAH such as benz[a]anthracene.

Award Address. (ACS Award for Creative Advances in Environmental Science and Technology sponsored by Aerodyne and the ACS Division of Environmental Chemistry) POPs: Story of global pollutants

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This presentation will consider the global scale sources, fate, behaviour and processes governing persistent organic pollutants (POPs). I will discuss some of the key scientific concepts and their significance, such as longrange transport, cold condensation, and global fractionation, together with global mass balances, primary and secondary sources, and the scientific challenges of investigating them. I will advocate a 'whole system' approach to studying POPs, and the benefits of combining source estimation, lab studies, field measurement campaigns and modelling. This journey will take us from some of the early studies on POPs up to present day questions and priorities. I will highlight the importance and value of international collaborations and key colleagues in the field. The Stockholm Convention requires countries to conduct source inventories and to obtain spatial and temporal trend data. Timely work with passive sampling made it possible to start to assemble regional and global scale databases, and to assemble global, regional and national source and emission inventory data, together with time trend data, and to scrutinise this with multi-media fate models. This approach - global chemical mass balances and accounting - is now fundamental to underpinning chemicals regulations. A key scientific issue for POPs is whether ambient levels and exposures to POPs are controlled by primary (ongoing, 'fresh') sources or secondary (previously emitted compound re-cycling through the environment). This requires the search for evidence to distinguish primary and secondary source controls, to inform decision-makers, who are being challenged - 'is there more we can do to control these compounds?; is the Stockholm Convention working?'. China, India and some developing countries now provide some of the most important challenges for environmental monitoring and chemicals management, with issues such as e-waste export and disposal, use of pesticides and antibiotics, and where water, air and soils quality are now a critical focus.

ENVR 394

Environmental sustainability and routine organizational management

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The field of management has evolved throughout the past hundred years, encompassing mass production and operations research, social psychology, accounting, finance, information management, network management, globalization and now sustainability. As the planet's human population and level of material consumption has grown, managers have needed to pay more attention to their organization's use of natural resources and their impact on the natural environment. The concept of sustainability management has its roots in the field of sustainable development which was first defined in the 1987 Commission on Environment and Development, or the Brundtland Commission, which termed sustainable development as: "Development that meets the needs of the present without compromising the ability of future generations to meet their own needs." Sustainability management refers to the organizational management practices that result in sustainable development. It results in economic production and consumption that minimizes environmental impact and maximizes resource conservation and reuse. This presentation will discuss the opportunities presented by incorporating environmental sustainability into routine management decision making and the obstacles to doing so.

ENVR 395

Technological innovation and environmental regulation

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There is widespread agreement (at least among scientists and technologists) that science and technology should inform government action. But the coupling between technology and regulation can be distressingly weak. A recent example is the regulation of methane emissions from the oil and gas industry. Methane is a powerful greenhouse gas, and controlling its emission to the atmosphere is a relatively painless way to moderate global temperature increase. In the United States, methane emission control as a method of climate change mitigation dates only from 2016. Since 2017 the Environmental Protection Agency has proposed a series of measures that weaken the methane regulatory regime with the objective of reducing the regulatory burden on the oil and gas industry. A constant of policy, from 2016 to the present, is the acceptance of methane control regulations that are suboptimal with respect to both efficiency and effectiveness. Innovative technology can improve both efficiency and effectiveness, relieving regulatory burdens while improving environmental performance. However, the current regulatory regime is built into the Code of Federal Regulations and is not easy to change. Policy

makers and regulators need to be more aware of how scientific knowledge and technological innovation can help achieve cost-effective regulation. Scientists and technologists who interact with government mandates need to have a better understanding of the processes and constraints that control and influence the design of regulation.

ENVR 396

Strategic communication, social influence, and promoting sustainable behavior

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Misinformed perceptions, social identity, group pressures, and a lack engagement are all detrimental to promoting sustainable behavior. Strategic communication can help effectively counter such detrimental individual behaviors and lack of support for sustainable policy. This talk discusses specific cognitive biases and social processes that may hinder sustainability efforts and how strategic messaging can be used to overcome them. Informed by current research in science and risk communication, the talk presents communication and persuasion models that can inspire change and foster sustainable behavior.

ENVR 397

Prospects for plastic material recycling by chemical and biological technology

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Since the early 1950s, plastics production has generated a variety of material forms which have led to ubiquitous environmental contamination on a global scale. Over the last sixty years, plastic production has increased at a rate faster than that of any other manufactured material. The social value of plastic is easily seen in its myriad uses ranging from durable to single-use applications. Our overuse of disposable plastic items is a major problem with severe environmental consequences that tax resource management efforts. Recent decisions by many countries to cease accepting used plastics from elsewhere has disrupted international plastic material flows and triggered disposal crises in many countries. These changes to international recycling pathways have intensified demand and opened new opportunities for environmentally conscious recycling technologies. The repurposing of used plastics can be accomplished through technologies based on purification, decomposition, or conversion approaches to waste plastic utilization. Depolymerization technologies ranging for bench-scale demonstration to full scale implementation are becoming investment targets. Notable examples involve liquefaction, methanolysis, or cross alkane metathesis processes. Plastics-to-fuel strategies are prominent in the catalogue of processes under investigation. Clearly, it is important to provide sustainable management of used plastics while employing these emerging technologies. Closed supply chain constraints offer optimal solutions to the recycling needs of our society. Assessment approaches such as life-cycle evaluation can contribute to a more complete knowledge of used plastics recycling technology development.

ENVR 398

From assessing to scouting: Need for entropy indicators to identify plastics recycling opportunities

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Research and development efforts on plastics recycling are rising, driven by global awareness on ocean plastics, next to climate change and fossil resource scarcity. Yet, the investment climate (even for research) is insecure, given the many potential technologies and a multitude of plastic waste fractions existing. Although novel technologies such as chemolysis, pyrolysis or even multilayer delamination may be demonstrated technoeconomically at lab/pilot scale, it is often unknown whether the waste feedstock is available, at what quality, and more importantly what the environmental/economic cost of collecting and sorting would be. Moreover, in transitioning to a circular economy, the recycling sector should leverage such information to upstream virgin plastics manufacturers. Previous research recognized the advantages of ex-ante sustainability assessments; the earlier the assessment is done, the more degrees of freedom are available to change the design/pathway. Upon shifting these methods to initial research stages, they may even be used for screening the recycling potential from an investor's perspective, and additionally for informing policy in the transition towards a circular plastics economy. Nevertheless, at low technology readiness levels, most information to estimate lifecycle impact or cost of plastic waste sourcing is lacking, or in the best case calculated with very specific assumptions, hence not suitable in decision making support. This study outlines how ex-ante identification of feasible plastics recycling routes, prior to experimental work, can be done existing assessment methods, yet using usina fundamental proxy thermodynamic data as input. Expanding the framework for the use of entropy at a materials or process level, with a new 'societal' entropy indicator, upstream dispersion of plastics may be captured in ex-ante generic studies. The combined

entropy indicators may predict the energy and hence cost of collecting and sorting. Although mostly conceptual, the study also gives examples of the potential for various plastics.

ENVR 399

Sustainability: Why chemistry will have many ways to engage

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The role of chemistry in maintaining sustainability is planetary in scope. An understanding of the issues concerned with sustainability must now be part of educational curricula, especially those followed by nonscientists. In an age in which science and its practitioners will be held increasingly accountable, it becomes important for the general public as much as possible to be sufficiently informed. It is also important that perspectives of non-sustainability be considered particularly in making environments inhospitable for pathogenic organisms and for agricultural pests. There will be many barriers to achieving sustainability. Mostly these will arise from established economic, political, and sociological interests. One particular recurring problem is deciding to close industrial plants because of pollution problems. A second continual problem is dealing with runoffs from fertilizer treatments to improve crop yields. A new planetary concern is what is happening with the Amazon rain forest. Chemistry will be used to justify competing resolutions to environmental problems. Chemistry must ally with and be prepared to help practitioners of other scientific and engineering disciplines in achieving sustainability. If sustainability is to be considered worthwhile, it will require major commitments to resolve a vast array of issues from local to planetary.

ENVR 400

Comprehensive characterization of per- and polyfluoroalkyl substances (PFASs) in manufacturing wastewater

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Per- and polyfluoroalkyl substances (PFASs) are a class of chemicals that are of emerging concern. There are 1000s of PFASs with numerous industrial applications due to their thermal and chemical stability, which also contributes to their persistence and bioaccumulative nature. The objective of this work was to improve our understanding of the fate of known and unknown PFASs in manufacturing wastewater. We collected samples from different locations along the flow path of three electronic

manufacturing facilities and measured the wastewater samples by means of high-resolution mass spectrometry. We quantified the occurrence of 25 target PFASs and simultaneously performed a comprehensive nontarget analysis based on the presence of homologous series. We measured concentrations of the target PFASs ranging from below the limit of detection (0 ng/L) to more than 10 µg/L. We found that the highest concentrations of PFASs were present in the upstream samples from each of the facilities and that the concentrations decreased downstream as wastewater was diluted with onsite wastewater from other sources, whereas the loads actually increased along the flow path. To perform the nontarget screening, we used a datamining software to extract homologous series of CF2, C2F4, CF2O, and C2F4O and tentatively identified 41 homologs unique homologous series among the samples. We have found evidence of a number of perfluoroalkyl ethers, some of which have been previously reported and others that have not yet been reported in literature. We used a semiquantitative approach to demonstrate that the abundance and loads of untargeted PFASs were higher upstream than downstream along the flow path. This could indicate dilution but could also suggest that transformations of the untargeted compounds are occurring. Our data provide a comprehensive evaluation of PFASs in manufacturing wastewater and provide novel insight into the possible transformation products created during the manufacturing process.

ENVR 401

New odor and corrosion control technologies for drainage system

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Odor problem from the wastewater is one of the most frequently encountered issues in the densely populated urban area. Hydrogen sulfide (H₂S) as the primary source of the odor reported, originates from the anaerobic digestion of organic substances containing sulfur in wastewater. H₂S gas is further converted into sulfuric acid (H₂SO₄) by another strain of bacteria, i.e., Sulfur Oxidizing Bacteria (SOB), which induces the corrosion of the drainage concrete wall. This works focuses on two aspects, the laboratory research and field study. The former investigated the corrosion mechanism, concrete degradation rate and to develop the controlled-release hydrogel technology to inhibit the growth of both strains of bacteria for suppressing odor and corrosion problem. The latter was conducted in the drainage system in Hong Kong where the effectiveness of the hydrogel is measured in terms of the reduction in total H₂S generated. In

addition to the gas measurement, concrete coupons as a parameter to measure the corrosion rate are also deployed at each site and exposed for 2 periods with each period of 90days. Preliminary experimental result indicates that the corrosion rate in treatment site where 90% of the H₂S gas is reduced is only 0.1% of the rate in control site.

ENVR 402

Atomically precise membranes from molecular Legos

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This study aims at developing membranes with unprecedented atomically precise separation accuracy and efficiency through a bottom-up approach, which are radically different from current polymeric membranes. We construct the ultrathin membranes by assembling designed, chemically synthesized channel molecules into two-dimensional dense arrays. The ultimately thin barriers are envisioned to offer an exceptional permeability. The large rigid channel structures with welldefined shapes are assembled from unique "Molecular Lego" building blocks. These stereochemically pure and highly functionable building blocks (bis-amino acids) are coupled to each other through pairs of amide bonds to create spiro-ladder oligomers or "spiroligomers" with programmed shapes like building with Legos. We utilize microwave peptide synthesizer to assemble spiroligomers into channel molecules on solid support in a sequence-controlled way. With this methodology, we have successfully synthesized rectangular and triangular macrocycles exhibiting uniform intrinsic pore sizes. The fabrication of atomically precise membranes (APMs) is enabled by two techniques: 1) Interfacial polymerization: cross-linking amine-functionalized macrocycles with trimesoyl chloride on support membrane surface in a manner similar to preparing polyamide thin film composite membranes; 2) Langmuir monolayer: self-assembling surfactant-like amphiphilic macrocycles into monolavers in the Langmuir trough and cross-linking them in-situ to form single-molecule thick stand-alone films followed by transferring to support membranes. Filtration tests are ongoing to demonstrate the precise separation capability of APMs.

ENVR 403

Performance of a multifunctional odor control gel for H_2S abatement in drainage system

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Hydrogen sulfide (H₂S) is a common odorous gas produced in drainage system and is present in sewers and storm water drains. H₂S forms quickly in the drainage systems due to the presence of sulfate reducing bacteria (SRB) and besides causing malodor problem due to its low olfactory threshold, it also contributes to the deterioration of the drainage infrastructure by microbialinduced corrosion. There are numerous works on H_2S removal in sewer system including precipitation, redox potential and pH control and even catalytic oxidation processes. However, an efficient, reliable and costeffective process remains unrealized. This work reports the use of a multifunctional odor control (MOC) gel as a means to control H₂S malodor in drainage system. The MOC gel releases disinfectants and metabolic inhibitors in controlled dosage to effectively control the population and inhibit the activity of SRB and other anaerobic bacteria responsible for odor emissions. It also releases catalysts that capture and remove dissolve sulfides in the drainage water. Laboratory study showed that the MOC gel can suppress SRB activity and H₂S emission over a period of 35 days. A 12-month field study was carried out at a designated drainage infrastructure in Hong Kong through partnership with the Drainage Services Department of the HKSAR Government to examine the feasibility of applying MOC gel in storm drain nullah. The study involved continuous H₂S monitoring of the drainage infrastructure and analysis of the water samples for aerobic and anaerobic bacteria counts, COD and dissolved sulfides. The 12-month field study was divided into 60-day background establishment followed by 4 test period that consists of 60-day deployment and 60-day washout. The MOC gel is effective suppressing microbial population and H₂S emission as far as 2 km from the deployment point in storm water flow of 40 m³ per min. Only a modest amount of the gel (i.e., ≤ 1 Kg) is required to decrease H₂S concentration in the drainage infrastructure to below 0.01 ppm from the background values of 1 ppm (Furthermore, the anaerobic bacteria population was decreased by 85 % over the same period of time.

ENVR 404

Enhancement of anaerobic digestion by direct interspecies electron transfer

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Anaerobic digestion is a widely applied technology to produce bioenergy from waste streams. However, it suffering an inhibition of acetogenesis which limited its reaction efficiency and lead to the process failure. Direct interspecies electron transfer which was developed in recent years offered another perspective which provides a potential for alleviating the limitations in anaerobic digestion. This talk will review the recent advances revolving around mechanism of direct interspecies electron transfer on-going, current status of application on anaerobic digestion, and future challenges.

ENVR 405

Collection and speciation of gaseous and particulate nitrate for isotopic determination

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Reactive nitrogen species are emitted into the atmosphere from a variety of sources, including vehicles, biomass burning, agriculture, and industry. Ultimately, these reactive nitrogen species and their products have implications for quality of air, soil, water, and human health. Nitric acid (HNO₃) gas is most often a secondary product, existing in equilibrium with the particle phase. Speciation between the two phases is essential to understanding the chemistry of the atmospheric environment, and isotopes add a unique dimension of being able to track oxidation chemistry and primary emission sources. However, it is critical to determine the suitability of collection methods for consistent isotopic results that accurately reflect environmental values. Honeycomb denuders, coated with a selective solution, allows for capture of the gas phase while particles (<2.5 µm) continue downstream and collect on a Nylon filter. The literature debates the merit of using a Na₂CO₃ coating on denuders as it is more efficient for the collection of many acidic species, versus a NaCl coating, which may be more selective for strong acids. Neither of these methods, nor the use of Nylon filters to collect particulate nitrate (pNO3-), have been evaluated for quantitative determination of stable isotope ratios (¹⁵N/¹⁴N; ¹⁸O/¹⁶O). Evaluation and comparison of a Na₂CO₃ and a NaCl denuder coating for collection efficiency, operative capacity, and quantitative collection of isotopes was conducted. The Na₂CO₃ showed high operative capacity at 1,600 µg or 39.4 ppb_v HNO_{3(g)} over 24 h, but showed lower selectivity in comparison to the NaCl coating. The NaCl coating has a much lower operative capacity at 76 µg or 1.9 ppb_v HNO_{3(g)} over 24 h. Nylon Filters have been shown previously to collect pNO3⁻ quantitatively, and our results agree. Overall, both coating solutions and nylon filters yield highly reproducible isotopic results; showing no isotopic fractionation as a result of collection.

ENVR 406

Withdrawn

ENVR 407

Roles of oxygen and Mn(IV) oxide in abiotic formation of humic substances by oxidative polymerization of polyphenol and amino acid

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The metal oxide-facilitated transformation of polyphenols and amino acids to humic substances (HS) is an essential process in soil and compost maturing processes. The objective of this research was to examine the specific roles of MnO₂ and O₂ in the formation of HS by oxidative polymerization between catechin (a polyphenol) and glycine (an amino acid). The results demonstrated that large amounts of fulvic acid (FA) and humic acid (HA) formed by O₂ only, MnO₂ itself only led to a small amount of HS generated, while the presence of both O₂ and MnO₂ significant enhanced HA formation, demonstrating their synergistic effects. The size of HA only increased in the presence of MnO₂. Two-dimensional correlation spectroscopy results suggested that the sequence of the formation of HA functional groups was: C-OH in carboxylic acids>C-O in phenolic-OH>amide II and aromatic C-C>amide and carboxylate C=O>COO->NH>hydrogen bonds. Finally, XPS spectra of the residual MnO₂ showed that the Mn(IV) content decreased from >99% to 89.98% and 80.89% while the Mn(III) content increased from <0.1% to 10.02% and 15.07% for the humification in MnO_2 with and without O_2 , respectively, suggesting the role of MnO₂ as both a catalyst and a direct oxidant. The results offered new insights into the abiotic humification process and can help developing treatment technologies for bio-wastes.

ENVR 408

Accelerated degradation of micro-pollutant by permanganate: Comparison of organic and inorganic activations

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Permanganate (PM) is an oxidant commonly used in water treatment. However, the reaction rate of micropollutants with PM is highly variable, mainly depending on the electron density of certain moieties of micropollutants. Using a pesticide (carbendazim, CBZ) as a

target micro-pollutant, this study compared the organic and inorganic activations of PM by benzoquinone (PM/BQ) and bisulfite (PM/BS), respectively. It was found that both the PM/BQ and PM/BS systems could accelerate the removal of CBZ; however, the former removed 96.6% of CBZ within 15 s, while the latter took 2 h to achieve a 95.7% removal. The optimal molar ratios of [PM]₀:[BS]₀ and [PM]₀:[BQ]₀ were determined to be 1:5 and 1:0.1, respectively. Interestingly, the removal of CBZ by both PM/BQ and PM/BS was highly dependent on the dissolved oxygen (DO) concentration. With 0.5 mg L⁻¹ DO, the removal of CBZ by PM/BQ and PM/BS was just 3.6% and 36.8% after 2 h, respectively, much lower than those with 9.1 mg L^{-1} DO (95.7% and 96.6%, respectively). The transformation products of CBZ in both PM/BQ and PM/BS were identified, and the degradation dehydrogenation, pathways including alkylation, carboxylation and hydroxylation were proposed. The inorganic activation of PM by BS exhibited a higher micropollutant degradation rate and a higher stability in various water matrices, indicating its good application potential for water treatment.

ENVR 409

Degradation of phenol by persulfate activated with zero-valent iron-biochar composites

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Two types of Fe(0)-biochar composites, Fe(0)-included biochar and biochar-coated Fe(0) were synthesized in a laboratory with different methods, and their catalytic role was investigated in the oxidative degradation of phenol by persulfate via a series of batch experiments. Compared with individual biochar-Fe(0)-persulfate systems, phenol was degraded more effectively by persulfate with less amount of the Fe(0)-biochar composites or persulfate. More than 95% of phenol was degraded in the Fe(0)biochar composites-persulfate systems with 2.08 mM of persulfate and 2400 mg of Fe(0)-included biochar or 5.20 mM of persulfate and 1200 mg of biochar-coated Fe(0). Electron paramagnetic resonance analysis showed that sulfate and hydroxyl radicals were involved in phenol degradation. A graphitic structure and oxygen-containing functional groups on biochar were responsible for enhancement of phenol degradation. Our study suggests that the addition of Fe(0)-biochar composites to persulfate systems may be a simple and effective remediation option to enhance the removal of phenol from natural and engineered aquatic systems.

ENVR 410

Optimization of the landfill leachate treatment process using *Musa sp* flower extract in the process of coagulation, flocculation and sedimentation

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One of the major challenges in the world is the treatment of municipal solid waste, which can lead to contamination of the ecosystem due to percolated liquids when improperly discharged. The novelty of this study is the use of biocoagulant extracted from the flower of Musa sp. This approach was promising in the sense of production of the extract as well as the cost associated to it. The extract is based on polyphenolic chains (cumaric and gallic acid) composed of a hydrolyzable part and a condensed one. The effectiveness of the extract is given by the organic matter and turbidity removal. This study aimed to reducing the organic load measured in terms of Chemical Oxygen Demand (COD) and turbidity of leachate from landfill with 3 years of operation. The experiments that demonstrated effectiveness in the removal of humic and fulvic substances were performed in Jar-Test standard equipment. The factors applied in this study were: rotation, coagulant dosage and pH. These factors were used in a model through a Central Composite Design (CCD) response surface. The coagulation process was performed in two stages, the first with rotation being established according to the CCD and the second was kept fixed at 40 rpm. The COD removal and turbidity levels were 50.15% and 92.2%, respectively.

ENVR 411

Persulfate activation towards organic decomposition and Cr(VI) reduction achieved by a novel CQDs-TiO_{2-x}/rGO nanocomposite

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In this work, a novel carbon quantum dots and Ti^{3+} comodified TiO_2 -graphene nanocomposite (CQDs- TiO_2 x/rGO) was successfully fabricated via a facile, relatively cheap and environmentally friendly process. The light absorption edge of CQDs- TiO_2 -x/rGO was significantly extended to 481.93 nm due to the formation of Ti^{3+} impurities and Ti-O-C bonds and the excellent photon

conversion function of CQDs. The presence of CQDs and rGO with an excellent conductivity provide dual channels for the transfer of electrons, leading to the rapid transportation and effective separation of charge carriers. To enhance the mineralization of organics in the water treatment, persulfate (PS) was introduced to the developed the CQDs-TiO2-x/rGO-Vis reaction system. Due to the excellent photocatalytic performance of the CQDs-TiO_{2-x}/rGO nanocomposite, PS was efficiently activated by CQDs-TiO_{2-x}/rGO to produce a large number of sulfate radicals and hydroxyl radicals under visible-light irradiation. As a result, 10 mg/L bisphenol A (BPA) and phenol were completely degraded and the mineralization efficiency was improved to 82% and 76% by CQDs-TiO2x/rGO (0.5 g/L) in the presence of PS (2 mM) in only 5 and 20 min, respectively. Additionally, the excellent performance of CQDs-TiO2-x/rGO was also exhibited by the efficient reduction of Cr(VI) under visible-light irradiation. The findings of the present study highlight the great potential of CQDs-TiO_{2-x}/rGO for environmental remediations.



ENVR 412

Enhanced catalytic reduction of aqueous bromate by metal-organic framework Ni(HBTC)(4,4'-bipy) in the presence of NaBH₄

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The occurrence of bromate during the ozonation process can cause serious health problems as it was suspected human carcinogen. There have been extensive environmental technologies developed to eliminate an aqueous bromate precursor and bromate itself before and after the ozonation. However, these approaches are considered as difficult and ineffective ways of removal of bromate accompanied by several drawbacks. The catalytic reduction of bromate in the presence of NaBH₄ is one of the promising techniques which not only removes the bromate, it also converts it to bromide. In addition, using solid H₂-generating compounds is

relatively safe and cost-effective. In recent times, metalorganic frameworks (MOFs) have attracted considerable attention having a variety of interesting structures and various applications in surface and groundwater. This investigated research study the reactivitv of Ni(HBTC)(4,4'-bipy) with NaBH₄ for the bromate reduction in an aqueous environment. The metal-organic framework, supporting with immobilized Ni porosity, was synthesized using 4,4'-bipyridine and 1,3,5-tricarboxylic acid in DMF at 100°C for 24 hours. MOFs in the presence of NaBH₄ have shown accelerated reduction kinetics and complete conversion of bromate to bromide in 1 hour with a rate constant of 0.140 min⁻¹. Moreover, the study found out that the increase in catalyst loading and NaBH4 loading resulted in further enhancement of bromate reduction. The above-mentioned results indicate that Ni(HBTC)(4,4'-bipy) with NaBH₄ could be a promising environmental technology for the removal of bromate in water and wastewater systems.

ENVR 413

Effect of nitrite ion, chlorine dose, and pH on the ammonia chlorination reactions and speciation in clean water matrices

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The effect of ammonia and nitrite ion concentrations, chlorine dose, and pH on combined chlorination was investigated at chlorine to ammonia molar dose ratios (MDR) of 0.30, 0.50, and 0.70, initial ammonia concentration of 0.214, 0.107, and 0.036 mM, nitrite to ammonia molar ratio (NDR) and pH ranging between 0.12 to 3.0, and 6.0 to 8.0, respectively. The results indicated initial chlorine partitioning between nitrite ion and ammonia under all experimental conditions. Rising NDR by decreasing ammonia concentration resulted in reduction of the fraction of chlorine combined with ammonia. In addition, lowering pH decreased the fraction of chlorine combined with ammonia. At NDR=0.50, initial ammonia concentration of 0.107 mM, and MDR of 0.50, observed fractions of chlorine combined with ammonia were found to be 0.21, 0.47, and 0.70 at pH=6.0, 7.0, and 8.0, accordingly. Nitrite ion was a significant factor in the kinetics of chlorine residuals decay at pH=6.0 and 7.0, while no such effect was observed at pH of 8.0. Figure 1 depicts the dependency of the fraction of chlorine dose combined with ammonia as a function of NDR as measured at reaction time of 0.1 minute at pH=7.0. In addition, although the pH decrease resulted into decreasing monochloramine concentration, it caused increase in dichloramine concentration. These results of this study have chlorine residual and stability implications for water matrices with varving concentration of nitrite ion under combine chlorination.



Figure 1 Chlorine fraction combined with NH₃ at increasing NDR($[NO_2^{-}/NH_3]$) in batch reactors dosed with initial ammonia concentration of ($[NH_3]_0$)=0.036, 0.107, and 0.214 Mm. MDR: ($[Cl_2]_0/[NH_3]_0$)=0.30 - 0.70, phosphate buffer = 0.10 mM

ENVR 414

Role of carbonate radicals in the advanced oxidation process (UV/H₂O₂ and UV/K₂S₂O₈) for removing PPCPs

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Carbonate radicals (CO3.-) is a powerful oxidant that is present in sunlit surface waters and in waters treated by advanced oxidation process. However, the the information on reactions kinetics and mechanism of carbonate radical with personal care products were relatively few compared with hydroxyl radical and sulfate radical. In the present work, the second-order rate constants of 20 selected PPCP compounds were determined by using laser flash photolysis and competition kinetic methods at a pH of 8.3 and 11.6. Carbonate radical exhibits guite high reactivity toward the electron-rich moieties of PPCPs, which has a similar rate constant ranging of 1×10^4 M⁻¹ s⁻¹ to 6×10^7 M⁻¹ s⁻¹ with their parent compounds. The correlation between rate constants of CO_3^- (k_{CO3-}) versus the Hamett coefficient $(\Sigma \sigma^{+})$ suggests that single electron transfer (SET) dominates the reaction process of CO₃⁻ with organic compounds. The fraction of CO3⁻ on the first-order degradation rate of PPCPs accounts for average values of 9-27% in UV/H₂O₂, while it significantly increases to 19-43% in UV/K₂S₂O₈ process in simulated effluent waters. The quantitative comparison model reveals that a lower ratio of sulfate radical to carbonate radical $(In_{kSO4.-/kCO3.-} = 3.1 \text{ and } In_{kHO./kCO3.-} = 4.5)$ promotes the oxidation of PPCPs by CO3⁻ and enhanced their removal efficiency at a higher level of organic pollutant concentrations. The present study helps prioritize PPCPs that are favorable to CO3⁻ based on the advanced oxidation process and provide general CO3⁻ reaction mechanisms.

ENVR 415

Arsenic(III) removal by the activated iron media system facilitated by O₂-initiated advanced oxidation reaction

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Arsenic, a pollutant often found in groundwater, affects drinking water of over 100 million people around the world. Iron-based technologies, including zero-valent iron (ZVI) technology, are one of the most effective methods for removing arsenic from water. Removal of As by ZVI was often attributed to surface adsorption and coprecipitation onto iron oxides, products of ZVI corrosion reaction upon its deployment. In this study, we investigate the fate and evolution of As(III) through its removal by the Activated Iron Media (AIM), an engineered ZVI-based media consisted of a mixture of ZVI powder, a reactive surface FeOx coating, and a discrete FeOx phase. The engineered FeOx of the AIM features mixed Fe(II)/Fe(III) crystalline with an inverse spinel structure that develops from a meta-stable, Fe(II)-rich green rust structure evolvina towards а Fe₃O₄-like structure. The effectiveness of AIM as media was compared with virgin ZVI, magnetite, alone or mixed under different conditions for arsenite removal. Composition and structure of FeOx, O₂, and labile Fe²⁺ are identified as the key factors that determine the media reactivity. In particular, we discovered that the AIM system with a O₂ and Fe²⁺ supply achieves best As removal, decreasing 50 mg/L As to below 1 ug/L within 30 min. In the AIM system operated under oxic condition (with O₂), Ar(III) was found to be partially oxidized to As(V), which can be more readily immobilized by FeOx. Under O₂ free environments, the immobilized As(V) within the AIM is gradually reduced to As(III) and then As(0) over time. Control tests with AIM+O₂ reveal that interaction of O₂ with AIM could generate a substantial amount of hydroxyl radicals, which is likely responsible for the oxidation of Arsenite to Arsenate, thus greatly accelerate As removal by the media. The presence of ZVI and the availability of labile Fe(II) may be essential in facilitating the production of hydroxyl radical by maintaining the favorable properties of the FeOx such as high electron conductivity, Fe(II)-rich nonstoichiometric and flexible structure, and thus sustaining its unique reactivities.

ENVR 416

Withdrawn

Degradation kinetics and toxicity reduction during UV/persulfate reaction of benzophenon-3

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Benzophenon-3 (BP3) is one of the most widely used organic UV filters in sunscreen products and also used as a plastic addictive to prevent discoloration from UV degradation. Therefore, BP3 can be directly released through swimming pools, shower, etc., and indirectly discharged to the environment through sewage and wastewater treatment plants. BP3 is considered to be an endocrine disrupting compounds (EDCs) due to the reported results of adverse estrogenic effects in organisms. In addition, it is reported that BP3 can react with chlorine to produce chlorinated transformation products (TPs) and disinfectant byproducts (DBPs) such as chloroform. BP3 and its chlorinated TPs can be persistent in waterbodies, because they are very stable when exposed to UV light. Therefore, a safe treatment process of BP3 is required to ensure safe water reuse and to prevent adverse effects on the aquatic environment. Recently, sulfate radical-based AOPs have received increasing research interests for the destruction of emerging micropollutants via the generation of sulfate (SO₄⁻) radical. In this study, UV/persulfate process was investigated to treat BP3 in water. The degradation of BP3 by UV/ persulfate reaction followed pseudo-first-order kinetics. The degradation rate of BP3 increased with increasing persulfate concentration. In addition, the degradation rate of BP3 tended to decrease with increasing pH, due to that SO4⁻ radicals are dominant in acidic and neutral pH regions and OH radical is dominant at higher pH. The second-order rate constant of BP3 with SO_4^- radical was 1.67 (±0.04) × 10⁹ M⁻¹ s⁻¹. During UV/persulfate reaction, while HCO3- ion, Br- ion, and humic acid inhibited the removal of BP3, NO₃⁻ and Cl⁻ ions enhanced the degradation of BP3. The bioluminescence inhibition of transformation products (TPs) of BP3 decreased with increasing reaction times. implying that the toxicities of TPs were less than BP3 itself. The results of this study suggest the UV/persulfate process as one of the ecologically safe treatments for BP3 removal in water.

ENVR 418

Selective {012} facet exposure of CuFeO₂ for efficient fenton-like degradation of antibiotic in water

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In this work, the effect of facet exposure on the Fentonlike activity of CuFeO2 was investigated by ofloxacin (OFX) degradation efficiency. It indicates that OFX degradation rate by CuFeO2 [012] is four times faster than that of CuFeO2 [110] (0.0408 vs. 0.0101 min-1). In CuFeO2 [012]-H2O2 system, OFX is completely removed at a pH range 3-10. The experimental results and theoretical simulations show that OH hydroxyl is preferentially formed from the reduction of absorbed H2O2 by electron from CuFeO2 [012] due to suitable elongation of O-O (1.472 Å) bond length in H2O2. By contrast, the O-O bond length is elongated from 1.468 Å to 3.290 Å by CuFeO2 [110] facet, H2O2 tends to be dissociated into -OH group and passivates [110] facet. New formed surface Fe2+ is responsible to the excellent long-term stability of CuFeO2 [012] nanoplates by accelerating the redox cycle of Cu and Fe species. Hence, suitable facet exposure is the key parameter determining the Fenton catalyst's activity.

ENVR 419

Enhanced transformation of emerging contaminants by permanganate in the presence of redox mediators

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In this study, а permanganate/redox-mediator (Mn(VII)/RM) system for enhanced transformation of a series of emerging contaminants was evaluated. The presence of various redox-mediators (i.e., 1-hydroxybenzotriaozole, N-hydroxyphthalimide, violuric acid, syringaldehyde, vanilin, 4-hydroxycoumarin, and pcoumaric acid) accelerated the degradation of bisphenol A by Mn(VII). Since 1-hydroxybenzotriaozole (HBT) exhibited the highest reactive ability, it was selected to further investigate the controlling reaction mechanisms and quantify the effects of important reaction parameters (HBT dosages and initial pH) and water constituents (inorganic ions and humic acid) on Mn(VII) reactions with bisphenol A (BPA) and bisphenol AF (BPAF). Interestingly, not only HBT accelerated the degradation of BPA, but also BPA enhanced the removal of HBT, which has a significant meaning for permanganate oxidation application in natural environment where the natural dissolved organic matters, or other alternative natural mediators present. As a broad-spectrum technique, Mn(VII)/HBT is effective for accelerating the transformation emerging contaminants with different moieties. Evidence for the reversible in-situ formation of HBT• radicals as the active oxidant for accelerated BPA and BPAF degradation was obtained by radical scavenging experiments and ³¹P NMR spin trapping techniques. Compared to transformation pathways of BPA/BPAF with Mn(VII) alone, the presence of HBT

totally inhibited self-coupling of BPA and BPAF and promoted b-scission, hydroxylation, ring opening, and decarboxylation reactions based on the high performance liquid chromatography/quadrupole time-of-flight/mass spectrometry (HPLC/Q-TOF/MS) analyses. Moreover, Mn(VII)/HBT is also effective in real waters with the order of river water > waste water treatment plant (WWPT) effluent > deionized water, indicating potential feasibility for Mn(VII)/HBT treatment processes.



Mechanisms of Mn(VII)/HBT system for accelerated oxidation of BPA

ENVR 420

Destruction of tetrabromobisphenol-a (TBBPA) by UV advanced oxidation processes

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Tetrabromobisphenol-A (TBBPA) is the most commonly used brominated flame retardant with global production exceeding 170 kilotons. Similar to other brominated flame retardants, there is concern about its potential to be an endocrine disrupting compound (EDC) due to its ability to leach out of materials and environmental persistence. We examined the photolysis of TBBPA by low pressure germicidal ultraviolet (LP-UV) light (254 nm). The breakdown of the compound was observed by HPLC at 290 nm. We observed about 61% removal of TBBPA in 20% MeOH solutions after a UV dose of 370 mJ/cm², or after 60 min of UV exposure. Preliminary experiments to assess the ability of advanced oxidation processes (AOPs) that employ UV in combination with H_2O_2 to generate OH-radicals reveal 50% destruction of TBBPA in 20% MeOH after 20 minutes with a UV dose of 370 mJ/cm3 at 0.02 ppm H_2O_2 . The photolysis breakdown products of TBBPA were determined by LC-MS. Direct-UV photolysis produces mostly tribromobisphenol-a, which appears to not degrade after more than 60 minutes of UV exposure. We are currently examining the breakdown products of H₂O₂/UV AOP processes by LC-MS.

ENVR 421

Rate constants and mechanisms of the reactions of CI and CI_2^- with trace organic contaminants

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Cl and Cl₂- radicals contribute to the degradation of trace organic contaminants (TrOCs) such as pharmaceutical and personal care products (PPCPs) and endocrine disrupting chemicals (EDCs). However, little is known about their reaction rate constants and mechanisms. In this study, the reaction rate constants of CI and Cl2⁻ with 88 target compounds were determined using laser flash photolysis. Decay kinetics, product buildup kinetics and competition kinetics were applied to track the changes in their transient spectra. CI exhibited guite high reactivity toward TrOCs with reaction rate constants ranging from 3.10×10⁹ to 4.08×10¹⁰ M⁻¹s⁻¹. Cl₂ was less reactive but more selective, with reaction rate constants varying from <1×10⁶ to 2.78×10⁹ M⁻¹s⁻¹ . Three QSAR models were developed, which were capable of predicting the reaction rate constants of Cl₂ with TrOCs bearing phenol, alkoxy benzene and aniline groups (Fig. 1). The reaction mechanism was proposed via observation of transient intermediates using time-resolved spectroscopy (Fig. 2). CI could react with TrOCs through multiple pathways since more than one transient intermediate was detected simultaneously. Single electron transfer was the major reaction mechanism of Cl2⁻ reactions with TrOCs bearing phenols, alkoxy-benzenes and anilines groups . Cl2 was found to play an important role in TrOC degradation, though it is often neglected in previous studies. The results improve understanding of the halogen radical involved TrOCs' degradation. chemistrv in



Fig.1 QSAR for phenols



Fig.2 (a-c) Time-resolved spectra of reaction of TrOCs with Cl and (d) \mbox{Cl}_2^-

ENVR 422

Risk control of antibiotic-resistant bacteria, antibiotic-resistant genes and disinfection by-products during UV/chlorination process

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This study investigated the reduction of one antibiotic resistance gene (ARG, sul1) and one integron (intl1) within a multiple-antibiotic-resistant bacterium (ARB), Pseudomonas. HLS-6, during UV, chlorination and UV/chlorination. This bacterial strain can be thoroughly inactivated by UV/chlorination, but reactivation occurred after chlorination alone. For the removal of target genes (sul1 and intl1), the degradation rate order was as follows: UV/chlorination > chlorination > UV. The log reduction of sul1 and intl1 by UV/chlorination can achieved more than 3.50 and 4.00 log, respectively. Among the radicals produced in UV/chlorination, only the reactive chlorine species (CI., Cl2. and CIO.) can degrade the target genes, while •OH has no influence. With low chlorine dosage, *sul*1 was easier to be removed than *intl*1 by UV/chlorination. The log reduction of both *sul*1 and *intl*1 decreased with pH increasing during UV/chlorination. In the presence of sulfamethoxazole, UV/chlorination showed more advantages than direct UV and chlorination in the simultaneous removal of antibiotics, ARBs and ARGs. As for the formation of disinfection by-products HLS-6 (DBPs) during the ARB disinfection. UV/chlorination enhanced the yields of trihalomethanes (THMs), haloketones (HKs) and haloacetonitriles (HANs) compared with chlorination alone. But in the coexistence of Br and I. the UV/chlorination of ARB could reduce the formation of THMs, HKs and highly toxic I-THMs compared with chlorination, especially in the condition of high Br-/I- molar ratio. Therefore, UV/chlorination should be an effective method for risk control of ARBs, ARGs and DBPs in drinking water disinfection.

ENVR 423

Simultaneous removal of ammonium and manganese from surface water in South China by manganese cooxide film: Application effect

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Compared with the treatment of the surface water in north China, the manganese oxidation film, when used to treat the surface water in south China. shows a finer catalytic oxidation behavior, and the effect of removing manganese and ammonium is remarkable. In this research, without any additional condition, only by relying on the performance of the abovesaid film, the rate of the synchronous removal of manganese and ammonium, when the temperature of water is 20°C.can come up to above 95%; and the maximum capacity of the removal of manganese can reach 3.5 mg/L, and the maximum capacity of the removal of ammonium can reach 3 mg/L. In addition, the effect of their removal is stable. It is discovered that, by contrasting the water quality in north China with that in south China, the PH value and the contents of alkalinity, calcium and aluminium in south China all are blew those in north China. When manganese and ammonium are removed by the manganese oxidation film, hydrogen ions are released, resulting in the consumption of the PH value and the alkalinity. Due to this phenomenon, the catalytic oxidation reaction of the abovesaid film is restricted. A careful comparison shows that when the alkalinity of the surface water in north China is 35mg/L, the rate of the removal of manganese and ammonium is 50%. While the alkalinity of the surface water in south China is 30mg/L, the rate of the removal of manganese and ammonium still can come up to 95%. Furthermore, the rate of the removal of manganese can come up to 99% with a proper increase of the alkalinity of influent water. As our experiment has proved, the presence of calcium and aluminium ions in water affects the removal of manganese and ammonium. The abovesaid film is characterized by using scanning electronic microscope, X-ray fluorescence spectrometry and X-ray photoelectronic spectroscopy; and by using XPS and EDS to conduct an analysis of the main elements one the surfaces of the filter media. it is noticed that calcium and aluminium ions are adsorbed on the surface of the abovesaid film and then part in the competition for the active parts on the surface of the abovesaid film, thus playing a role of restricting the catalytic oxidation reaction of the manganese oxidation film

ENVR 424

Manganese removal by iron-manganese co-oxide filter films under anaerobic condition in groundwater treatment

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Dissolved oxygen (DO) is a necessary and important influencing factor for the removal of manganese in water treatment. However, lately, it was found that an ironmanganese (Fe-Mn) co-oxide filter film could continuously catalyze oxidation to remove high concentrations of manganese from groundwater under low or even no DO condition, which has been developed manganese and ammonium removal from for groundwater by catalytic oxidation. In this work, a pilotscale filter treating real groundwater was adapted to explore the performance of manganese removal by the Fe-Mn co-oxide under three different DO conditions. Results indicated that the Fe-Mn co-oxide filter exhibited excellent manganese removal performance without consumption of DO under anaerobic condition, which may attribute to high pH. The morphology, composition, structure and manganese valence changes of the Fe-Mn co-oxide filter film have been studied in detail using scanning electron microscopy (SEM), high resolution transmission electron microscopy (HRTEM), Brunauer Emmett Teller (BET) and X-ray photoelectron spectroscopy (XPS) techniques. Mechanistic studies for the catalytic reaction have been conducted and related to the characterization results. The Fe-Mn co-oxide filter film under anaerobic condition has shown to be highly contact surface area and pore volume, possessing more adsorption sites and reaction channel for manganese removal. Combined the analysis of manganese species and relationship between manganese removal and DO consumption, it could be concluded that Mn(II) in solution should be mostly converted to solid phase Mn(II) of the Fe-Mn co-oxide under anaerobic conditions, since no DO consumption and high surface Mn(II) content. Finally, the mechanism of manganese removal under anaerobic conditions was proposed. This discovery reveals a new approach for manganese removal in groundwater treatment.

ENVR 425

UV/TiO₂ photoelectrocatalysis as a novel alternative to degrade estrogens in food production systems

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Supplementation of 17beta-estradiol (E2) into food production systems has increased concern of estradiol

and its metabolites in the environment. These estrogens have been proven to cause physiological changes in aquatic organisms at even low (i.e., ngL-1) concentrations, and, as such, must be removed or degraded before water can be safely discharged into the environment. UV/TiO₂ photoelectrocatalysis is an emerging technology that has shown promise in mineralizing a variety of contaminants of concern (COCs), including estrogens. It has been established that the morphology of TiO₂ photoanodes can be impacted by electrolyte aging time and anodization voltage. This study aimed to determine the impact of these factors on the photocatalytic performance of TiO₂ foils as a function of estrogen degradation in either pure or aquaculture wastewater. Titanium foils were anodized in an electrolytic cell using a graphite cathode and an electrolyte solution composed of ethylene glycol, H₂O (1% by volume) and NH₄F (0.2% by weight). Four different anodization voltages (30, 40, 50 and 60 V) and three different electrolyte aging times (6, 18, and 36 hours) were tested. Post-anodization, foils were annealed at a temperature of 500°C for a period of two hours and analyzed using scanning electron microscopy and X-ray diffraction. Annealed foils were further equipped into a photoelectrocatalytic (PEC) cell with a platinum cathode and stimulated by UV doses of either 250, 500 or 1000 mJcm⁻² and an external voltage of 0.5 V. Samples were analyzed using liquid chromatography with tandem mass spectrometry. This work will investigate fundamental approaches of PEC design to minimize power consumption while maximizing degradation of estrogenic substances. Attention will be drawn to interfering agents that may inhibit PEC application to enable an understanding appropriateness of of desian considerations.

ENVR 426

Kinetics of singlet oxygen indirect photolysis of trace organic compounds (TOrC) in wastewater effluent

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Removal of trace organic compounds (TOrCs) from wastewater effluent has been identified as one of the main challenges for water reuse applications. Exposure of wastewater effluent to solar light leads to the attenuation of TOrCs by indirect photolysis due to the generation of singlet oxygen by photosensitizers present in the wastewater. In this work, indirect photolysis removal rates were measured for TOrCs commonly found in wastewater effluent. The second-order rate constants for TOrCs with singlet oxygen were determined from laboratory experiments utilizing competition kinetics under solar light and UVA (300-400 nm) as light sources. Methylene Blue and Rose Bengal were used as singlet oxygen photosensitizers, whereas furfuryl alcohol, a probe compound for singlet oxygen, was used as a competition agent. In particular, results show that phenolic compounds, such as bisphenol A and p-cresol, which have singlet oxygen reaction rate constants in the order of 10⁸ M⁻¹s⁻¹, are sensitive to pH variations in the range usually encountered in wastewater effluents.

ENVR 427

Oxidized mercury compounds: Computational investigation

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According to the US Government Agency for Toxic Substances and Disease Registry, mercury is listed as the third most toxic element that continues to be released into the atmosphere and consumed through the food cvcle. Many studies show that both oxidized mercury and methylmercury are neurotoxins and can potentially result in irritability, fatigue, behavioral changes, tremors, headaches, hearing, and cognitive loss, etc. Elemental mercury is insoluble and does not readily enter the ecosystem; However, the oxidized mercury is very soluble and more likely to enter the ecosystem. Therefore, it is very important to understand the mechanism of atmospheric mercury oxidation. The purpose of this research study is to investigate the structural, electronic and spectroscopic properties of all oxidized mercury compounds both in gas and aqueous phase using computational chemistry techniques. We examined 16 oxidized mercury species: IHgCl, IHgBr, CIHgBr, BrHgOBr, BrHgBrO, BrHgOCI, BrHgCIO, BrHgOI, BrHgIO, HOHgBr, CIHgO₂H, CIHgNO₂ 1 double bond), CIHgNO₂ (2 double bond), BrHgNO₂(1 double bond), BrHgNO₂ (2 double bond), and BrHgO₂H both in the gas and aqueous phases. For example, below is the chart showing the three out of sixteen compounds that we have studied:

	Hg-X bond distance in Å				
Compounds	Gaseous phase	Aqueous phase			
BrHgOBr	2.406	2.504			
IHgCl	2.589	2.753			
BrHgOCI	2.405	2.494			

ENVR 428

Analysis of UV photodegradation of fluoroquinolone compound moxifloxacin

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Fluoroguinolone antibiotics are emerging water contaminants that are poorly removed by traditional water treatment processes. Moxifloxacin is a fluoroquinolone that is released to the environment primarily by incomplete metabolism by humans and animals. Causing unknown impacts to the environment and neurological damage in humans, this research investigates the UV photodegradation of moxifloxacin in order to improve water treatment of moxifloxacin-contaminated water sources. 0.15 mM moxifloxacin solutions were radiated under UV, UV/H₂O₂, or UV/H₂O₂/FeSO₄•7H₂O. Samples were collected at various time points and analyzed by HPLC. After discovering UV/H₂O₂/FeSO₄•7H₂O (photo-Fenton system) caused greatest degradation (k = 8.51 × 10⁻² s⁻¹), similar radiating methods were used to analyze the role of reactive species singlet oxygen and hydroxyl radical. Competition agents furfural and acetophenone and sensitizers rose bengal and H₂O₂ were used to evaluate rate constants for both reactive species. Hydroxyl radical may play a more significant role in degradation (k = 8.4×10^9 M⁻¹s⁻¹) than singlet oxygen (k = 6.7×10^4 M⁻¹s⁻¹). Steps in the future will investigate the concentrations of singlet oxygen and hydroxyl radical and the degradation of moxifloxacin when placed in solution with organic materials, analyzing the presence and toxicity of the products of degradation.

ENVR 429

Elucidation of imidazolium-based ionic liquid cations binding to iron porphyrin from a QM/MM framework

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Ionic liquids are composed of asymmetric organic cations while anions can be both organic or inorganic in nature. Highly articulated structures and low charge density on the ions frustrate crystal packing resulting in a large number of ionic liquids to exist as liquids at or below room temperature. Negligible vapor pressures and the availability of a large number of cations and anions to tune physicochemical and biological properties for a given chemical process have been the primary drivers for research in this field over the last two decades. Due to the near elimination of air emissions, ionic liquids are regarded as environmentally benign solvents. Unfortunately, many ionic liquids are water soluble and

can be toxic to aquatic microorganisms. Thus, recovery, recycling, and biodegradation of ionic liquids are of paramount importance to harness the green chemistry aspect of ionic liquids. Despite some experimental efforts at studying the biodegradation mechanism of ionic liquids, the molecular-level mechanisms by which ionic liquids are biodegraded in not well understood. In this presentation, we focus on the cytochrome P450 enzyme which plays a crucial role in in the oxidation of a wide range of aromatic molecules in different environments. Thus, to gain insight into the ability of P450 in oxidizing imidazolium-based 1n-alkyl-3-methylimdiazolium [Cnmim]+ cations, a hybrid approach of high-level quantum mechanical (QM) calculations and computationally efficient molecular mechanics (MM) is adopted. The catalytic site (iron porphyrine (FeP)) and the ionic liquids as substrate are considered at the QM level to describe chemical reactions while the effect of the protein environment is modeled at the MM level. Docking calculations are carried out to generate suitable starting conformations for cations of varving alkyl chain length; ethyl, butyl, hexyl, octyl, and decyl. We report the binding energy for forming the ionic liquid-FeP complex - pivotal in the subsequent steps for the biodegradation of ionic liquids. We will also present how the presence of ionic liquid alters the electrophilicity - the electron uptake ability of the catalytic cycle, which is the next step in the catalytic cycle of ionic liquid hydroxylation triggered by cytochrome P450. The implication of the results on the propensity for biodegradation of the imidazolium-based cations will be discussed.

ENVR 430

Removal of bisphenol F from water with UV/H_2O_2 advanced oxidation processes

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Bisphenol F (BPF) is an organic compound used as a replacement for bisphenol A (BPA) in plastics. We investigated the rate at which BPF photodegrades under UV-C light. The fluence was determined with periodate chemical actinometry. We exposed test solutions of BPF to UV doses (fluence) of 370 mJ/cm² to 2200 mJ/cm² (1 h to 7 h) with a low pressure germicidal UV lamp. These samples were then analyzed by HPLC to determine the concentration of BPF remaining after UV photolysis. Results reveal that after exposure to 2200 mJ/cm², only 22% BPF was removed from the solution, this indicates that BPF is difficult to degrade. We also examined whether the degradation of BPF can be enhanced with H₂O₂/UV advanced oxidation processes (AOPs). The results from this investigation indicate that BPF solutions reacted with UV/H₂O₂ revealed up to 41% degradation of BPF at a fluence of 370 mJ/cm². We are currently examining the effects of varied concentrations of H₂O₂ on BPF degradation rates. In addition, we are currently determining possible breakdown products of UV and H_2O_2/UV destruction of BPF by LC-MS.

ENVR 431

Comparison of the phosphate adsorption capacity of MgAI- and MgAIZr-LDH

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Phosphorous (P) in the form of phosphate is an essential nutrient and most of the P for fertilizer production is obtained by mining from phosphate rocks. However, phosphate rock is a limited resource that may be depleted within 50-100 years. Phosphate rich wastewater from wastewater treatment plants (WWTPs) could be alternative phosphate source due to the high concentration of phosphate (4-16 mgP/L). Thus, recovery of phosphate from wastewater using various adsorbents such as activated alumina, calcite, zirconium hydroxide, activated carbon, iron oxide and lavered double hydroxide (LDH) are tested. Among those adsorbents, LDH have been intensively studied due to their favorable properties such as high biocompatibility, high adsorption capacity, and high affinity for orthophosphate. Enhanced phosphate adsorption efficacy has been obtained for LDH doped with zirconium (Zr⁴⁺). However, it is unclear if Zr is incorporated in the LDH lattice or doped on the surface of LDH, which will impact the recyclability of the LDH filter material. Bimetallic (MgAI) and trimetallic (MgAIZr) LDHs were prepared using conventional coprecipitation followed by aging or hydrothermal treatment, which affects the LDH quality, to understand the effect of Zr doping on the atomic level. All MgAI-LDHs and MgAIZr-LDHs show hydrotalcite-like structure according to powder X-ray diffraction (XRD). The physicochemical properties of prepared samples were verified with SEM-EDS and zeta-potentiometer. Moreover, solid state ¹H and ²⁷AI MAS NMR (SSNMR) was used to understand the atomic level of structure of prepared LDHs. Subsequently. the phosphate adsorption capacity of MgAI- and MgAIZr LDHs were evaluated as a function of phosphate concentration, exposure time and pH using phosphate solution and waste water. The obtained solid products were analyzed with XRD, FT-IR, ²⁷Al and ³¹P SSNMR as well as the composition of the supernatant (ICP-OES) to quantify how the different phosphate binding modes (adsorption, intercalation, mineralization etc.) contribute to the P removal efficiency of LDH, as our recent study MgAI-LDH of showed that more phosphate is surface bound than intercalated.

Combining nanoparticles and foam transport in porous media for contaminated site remediation

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Wet foam is a complex fluid consisting of bubbles dispersed in a liquid-phase, with a volume fraction of the gas-phase can be up to 97 vol.%. Foam stability is significantly enhanced in the presence of nanoparticles opening opportunities for new applications such as enhanced oil recovery and remediation of contaminated sites. However, the mechanisms of particle-bubble interaction in porous media are not well understood and current models do not capture the overall multi-phase fluid flow and transport dynamics. Here, a study on the modeling and monitoring of the generation and evolution of a foam in porous media is presented. Experiments at the pore-scale were carried out and used to derived a constitutive equation of foam generation [1]. The mathematical equation was then coupled with a model of foam and nanoparticle transport in porous media [2] and used to describe laboratory tests at the continuum scale [3]. Anionic and cation surfactants combined with bare and functionalized nanoparticles were used to stabilized the foam. Measurements show that generation mechanism is not affected by the presence of nanoparticles; whereas the stability is remarkably enhanced in as much as the viscosity. Improving therefore the mobility control of the foam as well as of the nanoparticles. These results suggest that foam bubbles could be therefore used a carrier of nanoparticles in applications such as remediation of contaminated sites, where reactive particulate must be delivered to trigger reactions.



ENVR 433

Pressure drop and diffusion rate in 3D printed aerospace structure

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The purpose of this project is to successfully design, simulate, practice test, and finally produce functioning three dimensional (3D) printed structures applicable in aerospace applications. Various designs of pore structures were produced in a 3D design program for applications including gas- and liquid-phase filters. The fluid flow patterns and mass diffusion were simulated using the Comsol Multiphysics program. The pressure drop across the structure, permeability, porosity, and mass transfer rate were estimated in the simulation. The pore structure and size that produced the lowest pressure drop and highest mass transfer in the simulation were selected and printed out for laboratory flow tests. The 3D printed filter was installed in a flow system and deionized water was pumped in at different flow rates, e. g., 0.1, 0.5, 1.0 and 2 ml min⁻¹. Blue ink (Tracer) was injected at the entrance of the filter at 0.1 ml min⁻¹. The pressure drop and ink breakthrough curve were obtained at each flow rate. The results were compared with the commercial filters. The 3D printed filter with the spiral pore structure showed a higher mass transfer rate than that of standard filters while maintaining the pressure drop lower on average than that of standard filters.

ENVR 434

Unraveling nanostructures properties with potential environmental implications: *Ab-initio* study

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Some important properties of nanostructures incorporated in membranes for water treatment, as selectivity, water flux and nanoparticles release, still deserve attention. Several theoretical investigations on this topic can be find, nevertheless Density Functional Theory (DFT) based modeling on the aforementioned properties is desirable. The selectivity-permeability tuning of functionalized CNT-polymer membranes used for water treatment will be first showed. A new computational
method is presented in order to optimize the selectivitypermeability of ideal CNT membranes encompassing the advantages of vertically aligned CNTs. The intrinsic correlation between selectivity and permeability (selectivity increasing implies permeability decrease) was investigated from a fundamental point of view. A DFT modeling was used to improve the CNTs selectivity by functionalizing the tips of multiwall nanotubes with PIM-1 monomers, achieving simultaneously an increase in selectivity and water permeability. The modelling was performed without resorting any adjustable or empirical parameters, thus it is quite general and can be applied to other nano-porous materials with known inlet geometry. Moreover, contaminants adsorption on graphene faces of polyhedral multi-shell nanoparticles with external diameters between 1 and 4 nm will be examined. This is useful for designing NMs based sensors. The noncovalent interactions between polyoxometalates and ammonium surfactants were previously evaluated in the frame of DFT to predict the release of these inorganic nanoparticles in aqueous solutions. Polyoxometalateammonium surfactant complexes are used to increase hydrophilicity and antibacterial properties of membranes applied in water treatment. The modeling showed that monovalent anions, dissolved in water, cannot be exchanged with this nanosized polyanion in large extent. The theoretical conclusion was validated experimentally and the agreement between the theoretical prediction and the experimental data was remarkable. These findings can be considered quite general since achieved by an abinitio approach, then exploitable for other similar systems. Based on these encouraging results, the same approach has been used to model, at the nanoscale, the rejection of some cationic dyes and the consequent fouling of ionexchange membranes used for the treatment of textile wastewater.

ENVR 435

Synthesis, characterization, morphological study, photocatalysis application of Ag doped ZnWO₄ nanoparticles

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This study provides in-depth understanding on the morphology, particle size, and crystal structure of Ag doped ZnWO4 nanoparticulate. Monoclinic ZnWO4 and Ag dopped ZnWO4 nanoparticulate were prepared via a CTAB surfactant assisted hydrothermal method. Assynthesized nanoparticulate were investigated by ultraviolet-visible spectroscopy (UV-VIS), Fourier transform infrared spectroscopy (FT-IR), X-ray powder diffraction (XRD), X-ray photoelectron spectroscopy (XPS), energy dispersive X-ray spectroscopy (EDS), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). The effects of doping on the surface area also performed using Brunnauer-Emmett-Teller (BET) surface adsorption method. The effects of the reaction time, temperature, and changing reaction's solvent on the surface properties were investigated. Results show that the crystallinity was enhanced with the increase of the reaction temperature and time. Besides performing experiments, using ethylene glycol/water mixture as a solvent matrix was found to be effective in the enhancement of the surface morphology and the size distribution of the final product of ZnWO₄ nanoparticles. The photocatalytic activities for dye degradation will also be evaluated.

ENVR 436

Sub-nanocatalysis for efficient aqueous nitrate reduction: Effect of strong metal–support interaction

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Magnetic ferroferric oxide-supported bimetallic Pd-In cluster sub-nanoparticles were used for the first time for the catalytic reduction of nitrates. Due to the unique properties of the FeOx support, the PdIn active centers could be highly dispersed in both nano- and subnanoscales. A variety of characterizations and the charge density difference model confirm that a strong metalsupport interaction exists between the active sites and the support. The PdIn nanoparticles on FeOx show high selectivity toward nitrogen and excellent cyclic activity due to ferromagnetism, which broaden its prospect in practical water treatment. Moreover, the active centers in the subnanoscale are used in the nitrate reduction process for the first time and they show a distinct higher activity in denitration. The rate constant fornitrate conversion on PdIn sub-nanoparticles is larger than that for its nanometer counterpart based on the Langmuir-Hinshelwood model. High turnover frequency value and ammonia selectivity are achieved for the small-sized subnanocatalyst. The FeOx-supported PdIn nanoparticles and sub-nanoparticles have two application areas in water purification and ammonia recovery, respectively, Density functional theory calculations on the adsorption energies of elemental reactions are also performed, which shed some light on the catalysis mechanism and catalyst desian.



Figure 1. HAADF-STEM images of 10-PI/F in low (a) and high (b) magnification, HAADF-STEM images of 1-PI/F in low (d) and high (e) magnification. Nitrates conversion and products selectivity on 10-PI/F (c) and 1-PI/F(f) catalysts as a function of time , C0(NO3-)=50 mg/L. (g) Test of the Langmuir-Hinshelwood kinetic model. (h) Cycle tests of 10-PI/F catalysts. DFT study on the energy of thermodynamics for different reaction paths on Pd3In/Fe3O4 (i) and Pd4/Fe3O4 (j).

ENVR 437

Construction of $g-C_3N_4$ /carbon ring/TiO₂ nanocomposite by improved heterojunction contact for enhanced photocatalytic performance

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То realize high photocatalytic performance of photocatalyst, effective heterojunction interface contact is siginificant. In this study, with the improvement of heterojunction interface contact, a novel ternary g-C₃N₄/carbon ring/TiO₂ nanocomposite is constructed, in which the mixture of melamine and tetracycline is calcined to form the carbon ring grafted g-C₃N₄ and then it is coupled with TiO₂. The special in-plane carbon ring, which is anchored into g-C₃N₄ basal domains, plays a crucial role to achieve the sufficient ternary heterojunction contact in the prepared nanostructure system. The synthetic catalysts are investigated in terms of morphologies, composition information as well as optical and electronic properties via systematic characterization techniques. The g-C₃N₄/carbon ring/TiO₂ nanocomposite exhibits excellent photocatalytic activity under visible light irradiation. It is observed that 98.6% of methylene blue is degraded with a mineralization efficiency of 80.3%, which

is several times higher than that of pristine one. In addition, effect of catalyst dosage, water quality parameters, and scavengers of the reactive species on the degradation reaction is also analyzed. The enhanced photocatalytic capability can be ascribed to the effective heterojunction interface contact, which extends visiblelight absorption and incrases charge separation. Moreover, electron spin resonance assay and radical scavenging experiments demonstrates that the photogenerated hole, superoxide anion radical, and hydroxyl radical play crucial roles in degradation process. Importantly, this work may give new horizons to design ternary heterostructure with efficacious photocatalytic property and future applications in environment protection.

ENVR 438

Withdrawn

ENVR 439

Solar seawater evaporation based on hanging polyaniline-cotton photothermal fabrics

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Solar-enabled seawater evaporation has been considered to be an attractive, renewable and environmentally friendly way for desalination, alleviating the long-standing problem of freshwater scarcity without the consumption of fossil fuels. Till now, tremendous efforts have been devoted on the fabrication of photothermal membranes and floating them on seawater, generating water vapor under solar irradiation. This floating model suffers from three problems, including unavoidable heat loss, single-face evaporation (only top surface) and solid-salt separation. To solve these polyaniline-cotton problems, we have fabricated photothermal fabric and come up a hanging model that lifts the photothermal fabric away from seawater with only two fabric edges immersed in seawater. In the hanging model, top and bottom surfaces of the fabric are surrounded by air. Thus, the fabric can evaporate seawater on its two surfaces, effectively overcoming the limitations associated with the floating model. Meanwhile, the coverage of air makes the heat dissipation is only 16.8% of that from floating fabric, due to the extremely low conductivity (0.023 W m⁻¹ K⁻¹) of air. More importantly, the hanging fabric is arc-shaped, with its two edges higher than the center. Seawater is absorbed by the fabric from two sides to the center. With the progress of solar-driven seawater evaporation, the high-salinity brine is gathered at the lowest center of hanging fabric and finally dropped down for collection. Dropping brine takes away the salt in

fabric, and thus the solid salt separation can be completely avoided. Additionally, the brine is also meaningful for other industry applications, such as seasalt preparation or the chlor-alkali industry.



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New magnetic nanoscavengers to clean water

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Clean water is currently one of the main concerns of the humanity, since recycling has shown to be efficient but drinkable water conditioning still need to be improved. Among the water treatment technologies to eliminate pathogens and dissolved organic matter there are the advanced oxidation processes. AOPs: however, the post treatment conditions engage the water pH requiring postadjustment, making this process onerous. In this paper we show new nanoscavengers with high potential to improve recycle water quality. Two types ecofriendly magnetic nanoparticles were prepared using a powder. biopolymer (chitosan) and nanodimond respectively. Both of them were coupled with magnetite to obtain magnetic chitosan and magnetic nanodiamond. FTIR, FESEM, zeta potential, DLS and TGA studies have proven the binding between magnetite and the modifiers: chitosan and nanodiamond. In figure 1 FTIR show the raw materials and the supramolecular modifications. The FTIR spectra shows the characteristic peak from the bound Fe-O around the 500 cm⁻¹, present in raw magnetite and modified materials. All these spectra in conjunction with the other characterizations proved the correct modifications of the materials. The expectation is to use them as antibacterial and resistant materials to be used in water cleaning procedures with the possibility of recovering them to further uses and reduce the operation cost. All these characteristics allow to classify the prepared materials as sustainable nanomaterials.



Figure 1. FT-IR spectra for: a) Magnetite-Nanodiamond, b) Nanodiamond (dispersion), c) Magnetite-chitosan, d) Magnetite and e) Chitosan

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Controlled dissolution kinetics study of silver nanoparticles: Role of particle size

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Silver nanoparticles (AgNPs) are being widely used in various products due to the antibiotic property and increasing concerns are given to the potential adverse effects of AgNP release on humans as well as the environment. Dissolution is a critical step in determining the safety of AqNP and both internal and external factors have effects on this dynamic process. We fabricated small, medium and large sized AgNPs by nanosphere lithography (NSL) and electron beam evaporator. Dissolution experiments were conducted for each different sized AgNP in air-saturated phosphate buffer with different NaCl concentrations. Tapping-mode atomic force microscope (AFM) was used to measure changes in AgNP morphology over time. Higher dissolution were observed with increased NaCl solutions. Linear regression relationship was established between NaCl concentration and dissolution rate for each specific sized AqNP sample. Specifically, with the highest NaCl concentration (550mM), the measured dissolution rate for small, medium and large AgNPs were, 2.022 ± 0.12 nm. 1.69 ± 0.23 nm and 1.44 ± 0.098 nm per day respectively. Smaller AgNPs showed higher dissolution rates than larger AgNPs when the salt concentrations were the same. Moreover, the dissolution rate of bigger AgNPs is less dependent on the concentration of NaCl solution than smaller AgNPs. When we changed the temperatures for the dissolution experiments, the results show that temperature has a positive effects on the dissolution rate.

Electro-oxidation of trimethoprim using new electrode system based on graphite carbon paste modified with Au/Ag nanoparticles

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Pharmaceutical contaminants are causing a serious environmental issue, requiring adequate treatments. The present work deals about the electro-oxidation of trimethoprim (TMP) presenting in the pharmaceutical wastewater. Thus we developed graphite carbon paste electrode (CPE) having AgNP and AuNPs at different proportions, and then they were characterized by different analytical methods (XRD, FT-IR, SEM, TEM). The electrochemical performance of all the electrode systems was studied, and the results were compared with that of commercially existing electrode. Furthermore, in the electrochemical oxidation, the concentration of TMP measured was plotted against time, and analyzed the efficiency of oxidation by different electrode systems. The results show that there exists a considerable degradation of substrate, and observed the formation of intermediates determined by GC-MS. Interestingly, the electrode of CPE/Au/AgNPs oxidizes TMP efficiently than other electrodes (CPE/Au NPs, CPE/Ag NPs, and CPE) due to its synergic effect generated from Ag/Au with CPE than the individual systems.

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Application of copper nanomaterials to improve the resistance to root fungal disease in tomato (*Solanum lycopersicum*)

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With a projected global population of 9.7 billion by 2050, efforts to sustainably maintain global food security will become highly challenged. A changing climate and continued net loss of arable soil will present additional barriers. There has been rapidly increasing interest in the use of nanotechnology in agriculture, including the use of nanomaterials for fertilizers and crop protection. In both greenhouse and field studies, we applied two kinds of copper nanomaterials (commercial CuO nanoparticles and synthesized Cu₃(PO₄)₂ 3H₂O nanosheets), as well as two ionic/salt controls (CuSO₄ and Na₃(PO₄)), on a weekly basis to treat the tomato seedlings infested with the fungal pathogen *Fusarium oxysporum* f. sp. *lycopersici.* In an

ongoing greenhouse experiment, we found that repeated treatment with 50 mg L⁻¹ Cu₃(PO₄)₂ 3H₂O nanosheets, 31.25 mg L⁻¹ CuO nanoparticles, 63.25 mg L⁻¹ solubilized CuSO₄, 24.5 mg L⁻¹ Na₃(PO₄) had no impact on healthy seedlings. However, for the diseased plants both the Cu₃(PO₄)₂ 3H₂O nanosheets and the solubilized CuSO₄ increased plant biomass and decreased disease progress relative to the controls. The field experiment is currently on-going, but qualitatively, the treatments have had no significant effects on healthy tomato seedlings. In the diseased treatments, plants treated with 50 mg L⁻¹ Cu₃(PO₄)₂ 3H₂O nanosheets are larger and more vigorous than the other four treatments nearly two months into the growth cycle. Disease ratings, biomass. and element/nutrient content will be collected and presented for both the greenhouse and field trials. The findings not only suggest that in both greenhouse and field studies, repeated applications of Cu nanomaterials may significantly suppress fungal disease but also that the morphology and composition of the materials may be controlled to further optimize beneficial effects.

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Phosphate recovery from wastewater by engineered green synthesized iron/bentonite nanocomposite

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Phosphate can be removed from water using sorbents such as iron oxides, calcite, goethite, and activated carbon. However, these sorbents have very low sorption capacities. Nanoscale zero-valent iron (nZVI) particles have received much attention because of their unique reactive and sorptive characteristics in the last decades. Iron nanoparticles have a high affinity to aggregate into agglomerates which in turn decreases the reactivity of the particles. Hence, nZVI should be supported on certain materials to overcome clumping aggregation of nanoparticles and to enhance their separation and hydraulic conductivity. Bentonite is an abundant clay mineral and has unique characteristics which makes it suitable for hosting nZVI. It is well known that synthesis of the iron nanoparticles involves various parameters and each parameter has an effect on the resultant nanoparticle suspension. The aim of the study is to synthesize bentonite supported iron nanoparticles following a green route and evaluate the effectiveness of the composite material in the removal and recovery of phosphate from a synthetic wastewater stream. Synthesis variables are shown in Table 1. Preliminary results show that 55% phosphate adsorption is achieved with the nanocomposite C at all masses after a 6 h equilibrium period (Fig.1). When we compare the composition of nanocomposite B and C, we observe that iron mass does not have a significant impact on the adsorption efficiency. Although, nanocomposites B and D have exactly the same composition the effect of extract addition rate onto

the composite is clearly seen. Similar to adsorption results, nanocomposites C and D show the highest desorption percentages; 178% and 159%, respectively. Further studies are planned to include the determination of adsorption and desorption isotherms, kinetic modelling of the best nanocomposite, characterization of the nanocomposite using BET, XRD, FTIR and SEM before and after phosphate adsorption/desorption to understand the underlying mechanism of phosphate removal and recovery.



Table 1. Nanocomposites and composition

Name	Bentonite (g)	Iron (g)	Fe / Extract (V/V)	Extract addition speed
Α	2	1	1/1	Slow
В	2	2	1/0,5	Rapid
C	2	1	1/0,5	Rapid
D	2	2	1/0,5	Slow
E	2	1	1/1	Rapid

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Fluorescence microscopy of liposome-filled microwell arrays for studying interactions between laurdan-labeled liposomes and engineered nanoparticles

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Fluorescence microscopy of liposomes in a microwell array is applied as a method for quick determination of nanoparticle-membrane interactions to inform better nanoparticle (NP) design. Upon release into the environment, NPs may have a variety of adverse effects on organisms. Cellular membranes are commonly used systems in interaction studies for their impact on cellular function and organism health. Even if the membrane is not destroyed, we hypothesize that effects such as membrane phase change resulting from the interactions may negatively impact cellular function or potentially lead to programmed cell death. Fluorescence spectroscopy of laurdan-labeled phospholipid vesicles, or liposomes, has been used to measure the membrane phase of these model cellular membranes as quantified by the generalized polarization (GP). Preliminary spectroscopy results show that upon exposure to engineered NPs such as nickel manganese cobalt (NMC) and lithium cobalt oxide (LCO), the GP changes depending on the surface chemistry of the NPs and the mechanism of interaction. However, spectroscopy only yields an average of all the liposomes in a sample, requiring a high number of samples for statistical analysis. We anticipate that the same liposomes arranged in a microwell array and imaged in two-channel fluorescence microscopy will yield a greater distribution of data. A greater distribution would require fewer samples for statistical analysis and provide insights into a potential heterogeneity of NP-membrane interactions.

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Shape-controlled dissolution of faceted nanomaterials by hybrid scanning electrochemical microscope-atomic force microscope (SECM-AFM)

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Studies have shown that size, shape, surface coating, and solution chemistry all influence the dissolution process of nanomaterials, which in turn affects their stability, reactivity, and even toxicity toward aquatic organisms. In this study, we synthesized different shaped Ag and Cu₂O nanomaterials (such as wire, cube, plate and polyhedron) and evaluated the dissolution process using a hybrid scanning electrochemical microscopy atomic force microscopy (SECM-AFM). AFM-SECM simultaneously acquires topographic and electrochemical information on single nanomaterials at a local surface or facet level. Meanwhile, facet identification, indexing, and individual facet surface areas were determined statistically by High-resolution transmission electron microscopy (HR-TEM). Our results indicated that the dissolution behavior varied with shapes of the two nanomaterials. Particularly, the exposure facets (111) and (110) led to the fasted dissolution rates as observed morphological images. bv Furthermore. the electrochemical activity measurement indicates that these two facets had higher electric currents (200 pA) under -0.50 V applied voltages in 5 mM [Ru(NH₃)₆]Cl₃/0.1 M KCl solution. The results provide new insight into the facet dependent properties of nanomaterials, which is critical to understandings and development of functional materials such as catalysts.



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Mechanism of organosilanol compounds removal in water by adsorbent materials

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In the International Space Station (ISS), the National Aeronautics and Space Administration (NASA) has designed and established a water recovery system (WRS) intended to recycle and purify the wastewater that comes from crew urine and latent, and CO₂ reduction system in order to address the high costs associated to payload transport of water for long-term space missions. However, the WRS is presenting limitations to obtain highly purified water due to the presence of organosilanols compounds (OSC) such as dimethylsilanediol (DMSD), trimethylsilanol (TMS), monomethylsilanetriol (MMST), and dimethylsulfone (DMSO₂). They are difficult to remove from the WRS due to low affinity with the adsorbent materials. The goal of the project is to study the mechanisms of the OSC removal from water by the evaluation of different naturally porous adsorbent materials. Zeolite, activated carbon, limestone, carbon nanotubes and graphene oxide have been considered so far for preliminary analyses. Adsorption studies will be carried out at isothermal conditions with no flow (batch). The compiled data will be analyzed by using the Langmuir and Freundlich mathematical models to estimate the adsorbent capacity of the materials. Recent results evaluated by means of a total organic carbon (TOC) analyzer demonstrated above 60% of TMS removal for zeolite, activated carbon, and limestone adsorbent materials: however, a total adsorption (100%) was not achieved. Activated carbon demonstrate the highest adsorption removal with an approximate 87% efficiency after 6 hours of contact, an apparent desorption occurs after this time. The removal by the limestone is higher than the zeolite with an adsorption efficiency of 85% and 60%, respectively. Future work will include evaluating the behavior of the adsorbent materials for the other OSC in batch and a continuous system.

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Converting waste into worth: Fe_{1.72}Al_{0.28}O₃ nanoflakes harvesting from brown coal fly ash with crystal defects for enhanced water remediation

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The accumulation of coal ash waste is an environmental and economic obstacle. Herein, AI^{3+} -substituted α -Fe₂O₃ nanoflakes, with a nominal formula of Fe_{1.72}Al_{0.28}O₃ were successfully synthesized from brown coal fly ash waste. The synthesis yield reaches approximately 32 wt% on the basis of dried ash waste. During the hydrothermal process, the impure Al³⁺ replaced part of the Fe³⁺ in the hematite crystal, resultina in defect mediated Fe_{1.72}Al_{0.28}O₃ nanoflakes. The obtained nanoflakes possess a round-shape morphology with a diameter of around 300 nm and 50 nm in thickness. Results show that Al³⁺ partially substituted Fe³⁺ in α -Fe₂O₃, which is the root reason of the defects formation. In addition, the Al3+defects changed the original atomic structure of α -Fe₂O₃, causing a smaller first shell for an Fe-O bond distance of 1.95(0.21) Å, and a destroyed periodical symmetry for a smaller coordination number of 4.5(0.3)) for Fe. Owing to the introduction of defects, the resultant nanoflakes showed an enhanced adsorption performance for Cr(VI), As(V), As(III) and Congo red in waste water, with the maximum adsorption capacity of 68.3, 80.6, 61.1 and 213.8 mg g⁻¹, respectively. These values are around 3-5 times larger than that for the pure nanosized α-Fe₂O₃ synthesized under the same conditions.



Schematic illustration of the synthesis of Al³⁺-substituted α -Fe₂O₃ nanoflakes from Victorian brown coal fly ash.

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Withdrawn

Enhanced anti-fouling performance in nitrogen removing MBRs using nanocellulose coated membrane

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The application of MBR technology in industrial and domestic wastewater treatment is well-established. The major challenge of using MBR for nitrogen removal is to reduce membrane fouling and the corresponding maintenance cost. This obstacle is largely due to the interaction of inorganic and organic foulants with the membrane material. In this study, we compared the fouling behavior of a thin film nanofibrous composite (TFNC) membrane and a conventional polyvinylidene fluoride (PVDF) membrane using real wastewater samples collected from a treatment plant. Foulant characteristics and their interaction with the membrane surface were explored. Our results showed enhanced flux in the cellulose nanofiber (CNF) coated TFNC membrane compared with the PVDF membrane due to the super hydrophilic nature of the CNF surface. More specifically, the abundant carboxylate groups on the TFNC membrane surface enhance the negative surface charge. When real wastewater was applied to the membrane module, the flux of the CNF-coated TFNC membrane was almost twice that of the PVDF membrane, at both low (45 kPa) and high pressures (75kPa). The results at a constant pressure (45 kPa) showed the CNF-coated TFNC membrane was able to recover the initial flux by 98.5%, 94.5% and 92% after three consecutive mechanical cleaning processes. While the PVDF membrane's recovery rates were 43.5%, 30.5%, and 27% following the same treatment procedure. The SEM analysis of membranes confirmed a thinner foulant layer on CNF compared with PVDF. The enhanced rejection rate and more facile cleaning of CNF-coated TFNC membrane makes it a promising material to be utilized in membrane bioreactors for wastewater treatment.

ENVR 451

Voltammetric investigations of the sulfidation and dissolution of metal and metal oxide nanoparticles

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Metal and metal oxide nanoparticles are among the most common forms of nanoparticles in consumer products, raising concerns about the environmental implications of their widespread use. Voltammetry is an essential analytical tool that can be used to study various chemical transformations of this emerging class of contaminants to better anticipate potential transformations in the environment. The sulfidation of silver nanoparticles (Ag NPs) results in the formation of a stable silver sulfide (Ag₂S) product and may be an important removal mechanism of bioavailable silver from Ag NPs. Zinc sulfide (ZnS) was shown to undergo cation exchange reactions with silver, resulting in the liberation of Zn²⁺, which could be monitored in situ with anodic stripping voltammetry. It was found that the rate of sulfidation was strongly influenced by Ag NP size and small nanoparticles reacted more rapidly due to their greater surface area. A comparison of the sulfidation by ZnS of Ag NPs with various coating agents (citrate, lipoic acid, BPEI and PVP) revealed polymeric capping agents slow sulfidation somewhat, but no capping agent studied was found to completely prevent sulfidation from taking place. The dissolution of zinc oxide (ZnO) and copper oxide (CuO) nanoparticles was also assessed with anodic stripping voltammetry. ZnO and CuO NP dissolution were pHdependent with dissolution being favored under low pH conditions, consistent with the predicted solubilities of the bulk metal oxides. The role of metal ion complexation was also investigated using ligands with well-characterized binding constants for Zn²⁺ and Cu²⁺. The availability of ligands capable of forming stable complexes with increased the rate of NP dissolution and the equilibrium concentrations of both Zn²⁺ and Cu²⁺. The results demonstrate the presence of ligands of sufficient concentration and metal ion complexation capacity can control ZnO and CuO NP dissolution even at relatively high pH.

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Fabrication of Cu(II)/TiO₂/GO ternary composite for photocatalytic degradation of tetracycline hydrochloride

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Tetracycline antibiotics have the largest input and production capacity in livestock and poultry farming around the world. In this study, a novel Cu(II)/TiO₂/GO (graphene oxide) ternary composite was fabricated by the hydrothermal-dipping method. The morphological structure and physiochemical features were characterized by XPS, TEM, FT-IR and XRD. Cu(II), TiO₂

and GO were successfully combined, and the particle diameter of Cu(II)/TiO₂/GO is about ca. 11.1 nm. With tetracycline hydrochloride as a model pollutant, the photodegradation rate of Cu(II)/TiO₂/GO system under UV light was almost twice that of pure TiO₂ and the final removal ratio was 98.5%. Cu(II)/TiO₂/GO can absorb more visible light than TiO₂. The band gap of TiO₂, TiO₂/GO and Cu(II)/TiO₂/GO were calculated to be 3.13 eV, 2.84 eV and 2.83 eV. EPR study showed that the formation rate of superoxide free radical and hydroxyl radicals in the Cu(II)/TiO₂/GO ternary system was obviously higher than that in the pure TiO₂ and TiO₂/GO systems. Cu(II) and GO accelerated the separation of electron-hole pairs while slowing the recombination of holes and electrons, increasing the specific surface area and the absorption of dissolved oxygen, thereby synergistically accelerating the production of superoxide free radical, hole and hydroxyl radicals. After four cycles, the degradation rate of tetracycline hydrochloride can still reach 98.5%. In summarize, the utilization of visible light and the rate of active species production in the Cu(II)/TiO₂/GO ternary system are improved compared with TiO₂, which provides Cu(II)/TiO₂/GO a promising opportunity for making the contribution in the practical organic wastewater treatment.



ENVR 453

Application of nanostructured bimetallic catalyst for oxyanion reduction

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Noble metal (e.g., Pd, Ru, Rh)-based heterogeneous catalysis has emerged as a promising water treatment strategy for reductively destruction of a broad suite of waterborne contaminants. Oxyanions (e.g., BrO₃⁻, ClO₃⁻, etc.) are ubiquitous drinking water contaminants originating from both anthropogenic and natural sources

or generated during water treatment processes, and their presence may pose a threat to human health at even low concentrations. However, limited efforts have been devoted to investigating the application of bimetallic noble metal-based catalysts for the treatment of oxyanions. In the present work, nanostructured bimetallic catalysts were developed by decorating monometallic noble metalbased catalysts with a secondary promoter metal (e.g., Re, In) on functionalized mesoporous silica supports. The as-synthesized catalysts were extensively characterized for surface area, pore structure, charge, functionality, morphology, and metal dispersion. The impacts of noble metal type, secondary promoter type, and modified functional group on the performance of the bimetallic catalysts were investigated. Results showed that the bimetallic catalysts exhibit improved activity and considerable reusability for destruction of oxyanions in various water matrices. This presentation will focus on characterization, material synthesis, and activity evaluation under different environmental conditions.

ENVR 454

Selective adsorption and photocatalytic degradation of extracellular ARGs by partially molecular imprinted graphitic carbon nitride

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There is a growing pressure to mitigate the discharge of extracellular antibiotic resistance genes (ARGs) from municipal treatment systems. Here, guanine imprinted graphitic carbon nitride (g-C₃N₄) was synthesized for selective degradation of plasmid-encoded ARG (*bla*NDM-1) in secondary effluent. The molecularly imprinted g-C₃N₄ (CN-MIP) exhibited specific and efficient adsorption of ARGs, which improved the utilization of photogenerated reactive species by ARGs rather than background nontargeted constituents. Consequently, the photocatalytic degradation of *bla*NDM-1 in secondary effluent by CN-MIP $(0.030 \pm 0.002 \text{ min}^{-1})$ is 30 times higher than nonmolecularly imprinted g-C₃N₄ (CN-NIP, 0.001 ± 0.001 min⁻ ¹) under UVA irradiation (λ = 365 nm, 3.64× 10⁻⁶ Einstein/L*s). The molecular imprinting strategy changes the primary pathway responsible for the photocatalytic removal of ARGs. The photocatalytically generated hole (h⁺) is main specie responsible for ARG removal by CN-MIP due to improved contact between ARGs and specific binding sites on CN-MIP surface., whereas free radicals (i.e. \times OH and O₂⁻) play the key role in removing ARGs by CN-NIP. In addition, CN-MIP can significantly inactivate ARG by extensive fragmentation of ARG, eliminating the risks of ARG repair by transformed bacteria. Overall, CN-MIP can efficiently remove ARGs from secondary effluent. which holds the promise for mitigating the dissemination of antibiotic resistance from sewage treatment systems.

ENVR 455

Withdrawn

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Utilization of magnetic nanomaterials for remediation of arsenic contaminated wastewater

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The heavy metal toxic waste has become more abundant with the increase of energy demand for more than two decades, causing problematic global health and environmental issues. This research has been focused on the remediation of hazardous wastes (composed of AsO43- and CrO42-) using bio-encapsulated Fe3O4 magnetic nanoparticles (MNPs). These MNPs will be encapsulated with natural product extracts (such as polyphenols from pomegranate and chitosan from shrimp shell) to improve their biocompatibility and mitigate their toxicity. This talk will present three areas, 1) material synthesis and characterization to improve the robustness and coverage of MNPs; 2) removal efficacy of heavy metal ions from solid or aqueous waste to provide indepth understanding of the thermodynamics and interactions between AsO43- and/or CrO42- with Fe3O4 MNPs, and 3) mechanistic analyses using spectroscopic method(s) to determine the oxidation number change or bond vibration. Our results demonstrated the minimization of oxidative stress and cellular damage to the human retinal pigmented epithelium cells when the encapsulated MNPs were used. The fabrication variables of functionalized NMPs were optimized by a cost-effective colloidal chemistry. The high removal efficiency of As was obtained when sodium hydrogen arsenate (Na₂HAsO₄) and contaminated water sample were tested. The thermodynamics and interactions between NPs with the heavy metal ions affirmed that the mechanism of the metal removal was through electrochemistry reaction and physio-sorption approaches.



MNP synthesis, *a*: reverse micro-emulsion approach; and *b*: MNPs preparation using natural product extract.



Results of bioencapsulated Fe_3O_4 MNPs as analogies to demonstrate their nanostructural characterization using XRD, TEM and Lakeshore 7304 VSM instrument

ENVR 457

Graphene nanoplatelets in geopolymeric systems: New class of nanocomposites

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In this work, authors report the evidence of an electromechanical behavior in geopolymer/graphene nanoplatelets (GNPs) composites. Geopolymers without GNPs show a linear behavior of charge amplitude AQ versus load amplitude AP in the loads range 0 N ÷ 750 N and reaches a plateau in the AQ - AP plot for loads higher than 750 N. The former is due to a complex interplay that involves not-framework cations, framework and water contained in the material pores, while the latter is attributed to a charge saturation due to the limited amount of mobile cations Na⁺ contained into the material microstructure. The calculated charge coefficient d₃₃ is equal to 4.02 pC/N. Geopolymer mortar/1%wt. GNPs nanocomposites show, instead, a linear behavior from 0 N to 2500 N and a d₃₃ value of 11.99 pC/N. The presence of GNPs, thus, determines a change in the electromechanical behavior and an increase in the charge coefficient value of about 190%. The increase of charge coefficient d₃₃ in presence of GNPs, could be explained by assuming a combined interaction between GNPs and Na⁺. FT-IR spectroscopy and X-ray photoelectron spectroscopy were carried out to characterize graphene nanoplatelets and the nanocomposite. Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Spectrometry (EDS) were used to investigate the

microstructure and composition of the produced geopolymer/GNPs composite. The mechanical characterization of the nanocomposites is provided by using an innovative single test based on the combination of Brazilian disk test and Digital Image Correlation. The greatest increments in Young Modulus (E) and ultimate tensile strength (σ T), with values of 17.44 ± 0.67 GPa and 6.26 ± 0.05 GPa respectively, were measured when 0.5% wt of GNPs was used.



Charge amplitude A_Q versus load amplitude A_P of the plain geopolymer (black), and nanocomposite with 1% of GNPs (red).

ENVR 458

$Na_3V_2(PO_4)_3$ @C as faradaic electrodes in capacitive deionization for high performance desalination

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Among various desalination technologies, capacitive deionization (CDI) has rapidly developed due to its low energy consumption and environmental compatibility, among other factors. Traditional CDI stores ions within the electric double layers (EDLs) in the nanopores of the carbon electrode, but carbon anode oxidation, the co-ion expulsion effect, and a low salt adsorption capacity (SAC) block its further application. Herein, the faradaic-based electrode is proposed to overcome the above limitations, offering an ultrahigh adsorption capacity and a rapid removal rate. In this paper, the open framework structure Na₃V₂(PO₄)₃@C is applied for the first time as a novel faradaic electrode in the hybrid capacitive deionization (HCDI) system. During the adsorption and desorption process, sodium ions are intercalated/de-intercalated through the crystal structure of Na₃V₂(PO₄)₃@C while chloride ions are physically trapped or released by the AC electrode. Different concentrations of feed water are investigated, and a high SAC of 137. 20 mg NaCl g⁻¹

NVP@C and low energy consumption of 2.157 kg NaCl kWh⁻¹ are observed at a constant voltage of 1.0 V, a concentration of 100 mM and a flow rate of 15 mL/min. The outstanding performance of the Na₃V₂(PO₄)₃@C faradaic electrode demonstrates that it is a promising material for desalination and that HCDI offers great future potential.

ENVR 459

Nanoplastic identification and quantification in aqueous media

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Plastics constitute 60% of all floating oceanic debris. Although much attention has been devoted to the effects of macroscopic pollution, e.g., impact on visual aesthetics, injury and death due to indestion of plastic by aquatic-dependent species, micro- and nano-plastics are now believed to be an even greater environmental and biological hazard. Unfortunately, the simultaneous detection, identification, and quantification of nanoplastics (broadly defined as 1-100 nm in particle diameter) in oceanic and lacustrine environments is hampered by several factors: Diffraction-limited resolution and the complex nature of these solutions where naturally occurring nanoparticles (i.e., non-plastic) likelv outnumber plastic nanoparticles. Available techniques for nanoparticle characterization are predominantly focused on size characterization in simple matrices of known, and often, synthetically prepared compositionally uniform particles. However, the simultaneous determination of size and chemical composition of a targeted class of nanoparticles (i.e., plastics) in a complex matrix is still an unresolved major challenge. We prepared plastic nanoparticle solutions via the degradation of polyethylene and polycarbonate samples in tap and saltwater over the course of a few months. Particle size distributions were determined using nanoparticle tracking analysis and small-angle x-ray scattering methods. We then developed and optimized sample preparative and instrumental conditions to provide for the targeted detection of nanoplastics in our model solutions using both nano-IR and cryo-EM techniques. The efficacy of our method was tested on more complex natural sample matrices: light beer in glass and metal cans, and vodka in plastic bottles. Our results suggest that the method can be used for the targeted detection of nanoplastics in natural samples.

Photocatalytic degradation of pharmaceutical component a study with membrane reactor

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Recently deposal of pharmaceutical wastes has become a major problem globally. Therefore, it is necessary to removes pharmaceutical waste from the municipal as well as industrial effluents before its discharge. The convectional wastewater and biological treatments are generally failed to separate different drugs from wastewater streams. Thus. heterogeneous photocatalysis process becomes lucrative method for reduction of detrimental effects of pharmaceutical compounds. The main disadvantage of the process is the reuse or recycle of photocatalysis is a tedious job. In this the degradation of aqueous solution of work. chlorhexidine digluconate (CHD), an antibiotic drug, by heterogeneous photocatalysis was study using supported TiO₂ nanoparticle. The major concern of this study is to bring down the limitations of suspension mode heterogeneous photocatalysis by implementation of immobilized TiO₂ with help of calcium alginate beads. The alginate supported catalyst beads was characterized by scanning electron microscopy coupled with energy dispersive X-ray spectroscopy (SEM/EDAX) as well as the characteristic crystalline forms of TiO2 nanoparticle was confirmed by XRD. The degradation efficiency of TiO₂ impregnated alginate beads (TIAB) was compared with the performance of free TiO₂ suspension. Although, the degradation efficiency was reduced considerably using TIAB but the recycle and reuse of catalyst was increased quite appreciably. The kinetic parameters related to this work have also been measure. Moreover, to study the susceptibility of the present system photocatalysis of other three drugs ibuprofen (IBP), atenolol (ATL) and carbamazepine (CBZ) has been carried out using immobilized TiO2. The continuous mode operation in PBPR has ensured the applicability of alginate beads along with TiO₂ in wastewater treatment. The variation of residence time has significant impact on the performance of PBPR.

ENVR 461

Tannicacid-metalcomplexmodifiedMXenemembrane for water purification

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Two-dimensional (2D) material-based membranes are promising candidates for applications in water and wastewater treatment. Most of the previous studies adjust the membrane selectivity by tuning the interlayer spacing, which can be challenging since it is difficult to precisely control the interlayer spacing at the nanometer/subnanometer level. In the current study, we enhance the selectivity of 2D MXene membrane by coating a tannic acid (TA)-metal complex layer on the surface of the membrane. The coating layer has a low resistance to water permeance. After the addition of the coating laver. the membrane water permeability is 250-300 L/m²h bar, which is still about 10 times the value of conventional nanofiltration membranes. The TA-metal complex modified MXene membranes have low retention towards salt ions; however, they have much-enhanced rejection of the various contaminants. For example, the NaCl rejection of MXene-Fe is 3.7%; however, the membrane rejection of 4-hydroxybenzoic acid and Rhodamine B is 66.0% and 87.5%, respectively. Our analysis shows that the enhanced rejection performance of the modified membranes is due to the minimized mean pore size and increased surface hydrophilicity. The modified membranes are suitable for wastewater reuse and drinking water treatment, and this study proposes a new and facile strategy for adjusting the selectivity of 2D material-based membranes.

ENVR 462

Passive sampling of various emerging contaminants in air and water using electrospun nanofiber mats

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We developed electrospun nanofiber mats (ENMs) and their composites with embedded carbon nanotubes (CNTs) for use as passive samplers for various emerging contaminants in air and water. The majority of the work has been conducted with (i) polymer nanofibers of polyacrylonitrile (PAN), (ii) functionalized PAN composites with embedded carbon nanotubes (with or without surface carboxylic acid groups) and additives that impart surface charge (e.g. tetra-butyl ammonium bromide), and (iii) carbon nanofibers created from carbonization of PAN, using phthalic acid volatilization to create high surface area, macroporous materials. Various ENMs were tested in sorption kinetic and isotherm experiments toward a diverse suite of pesticides and pharmaceuticals, including pesticides like atrazine,

neonicotinoid insecticides (e.g.imidacloprid, colthianidin), acetochlor, metolachlor, 2,4-D, diuron, and chlorpyrifos as well as pharmaceuticals like sulfamethoxazole and carbamazepine, among others. We generally show that the rate and uptake of pesticides on ENMs can be controlled by tuning nanofiber properties, including nanofiber diameter, the amount and surface chemistry of embedded CNTs, and the presence of surface functional groups integrated into the ENMs via surface-segregating surfactants. Ultimately, their fast rate and high capacity uptake make these materials ideal for equilibrium passive sampling applications. For field validation, optimally performing ENMs were deplored in a nearby stream that contained agricultural runoff, revealing good agreement between results obtained with ENM passive sampling and more traditional grab sampling. ENMs were also deployed in air in residential areas and agricultural areas to measure these materials ability to also perform as passive samplers in air. In ongoing work ENMs have been deployed in a nearby wastewater effluent dominated stream to test the ENMs ability to sorb pharmaceuticals present in the stream. Together, this work shows the promise of electrospun nanofiber mats as a next generation, multi-media passive sampling technology.

ENVR 463

Patterned few-layer graphene (FLG) surfaces from plasma deposition

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Graphene was synthesized on transition metal scaffolding which serves as a catalyst. Plasma is used as a means for creating high-internal-energy structures such as graphene or single walled nanotubes. The plasma is created at about 10 Torr pressure with an Astex 1500. In lieu of a customized pattern deposited on a substrate, a Transmission Electron Microscopy (TEM) grid was used, 50-288-94 1000 mesh from Fisher Thermo Scientific. The result is Few-Layer Graphene (FLG) produced at a substrate temperature of 950 °C as estimated by optical two-color pyrometer. The graphene takes the form of freestanding walls, growing outward from the metal grid. The grid spacing was thus 25.4 microns, and the square perforation was about 10 microns. Using a mixture of hydrocarbons, a plasma was maintained for 10 minutes in order to create a uniform deposit of graphene with about 1.0 microns thickness, as shown by scanning electron microscopy. The plasma is contained in a guartz tube, the outside of which is cooled by water flowing in copper tubing. Energy Dispersive Spectroscopy (EDS) date shows a layer of titanium on the underside of the FLG layer, indicating strong adherence between the graphene and the metal. This may imply that the unpaired pibonding electrons in graphene are able to make much stronger chemical bonds than the Van der Waals bonds that are left on the surface of crystalline graphite. The ability to create highly patterned FLG has many applications, including the creation of ultra-black coatings. The photon absorbing properties of graphene make it of great interest for photovoltaic conversion, and in this case those attributes also make it of great interest to simply absorb broadspectrum photons and then dissipate the energy in the atomic plane.

ENVR 464

Identifying phenolic photoproducts after exposure of crude oil over water to sunlight

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Oxygen-containing phenol-like photoproducts were observed in the aqueous phase under crude oil exposed to simulated sunlight using dansyl chloride (DNS-CI) derivatization and high-performance liauid chromatography (HPLC). Oil samples were spread over water in a jacketed beaker held at 27.0 °C and exposed to simulated sunlight for various times. The aqueous phase was collected after irradiation and derivatized with DNS-CI, which selectively reacts with amines and phenols. Solid phase extraction was used to increase the photoproduct concentration prior to derivatization and HPLC analysis. Another derivatization agent, ophthalaldehyde (OPA), which only reacts with amines, was also used as a derivatizing reagent. By utilizing OPA, it was confirmed that the DNS-CI derivatives observed by HPLC were phenol-like compounds and not amines. Phenol concentrations were determined by HPLC with fluorescence detection. Water-extracted oil compounds were largely excluded from detection by careful wavelength selection, but compounds present in both dark and irradiated samples were eliminated from our analysis. Oxygen-containing phenol-like photoproducts were detected in the aqueous phase after irradiation but were not present in dark control samples. Concentrations of these compounds increased with irradiation time. Photooxidation of oil leads to the formation of these products. This method allows the identification of phenol photoproducts without interference from the immense number of other compounds in the oil. These results improve understanding of the impact that photochemistry has on the fate, transport, and toxicity of oil in the environment. Phenolic compounds have important toxic effects, so it is necessary to understand their formation from oil exposed to sunlight in order to fully comprehend the impact of oil spills.

Photoproduction and photolysis of acrylate in seawater

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The marine organosulfur cycle has received considerable attention since it was first proposed that dimethylsulfoniopropionate (DMSP), dimethylsulfide (DMS), and marine algae may affect the Earth's radiation balance and climate. It is evident from these studies that DMS(P) are quantitatively significant components of the carbon, sulfur, and energy flows in the oceans. By very little is known about acrylate contrast. concentrations, fluxes, or impacts in the oceans, even though it is produced during the conversion of DMSP to DMS, and its concentrations and fluxes should at times be substantial, especially in shallow-water coral reefs or during blooms of DMSP-rich phytoplankton that are common throughout the world's oceans and often harmful or toxic. Herein we show that acrylate is produced when 0.2-um filtered seawater is exposed to sunlight, an abiotic production pathway for acrylate that has not been previously documented. Photochemical production rates varied from samples collected in the Atlantic and Pacific Oceans and the Gulf of Mexico, with a strong positive correlation observed between the photochemical production rate and initial absorption coefficient at 330 nm (r = 0.87). The concentration of acrylate increased in proportion to the decrease in the absorption coefficient at 330 nm, suggesting the involvement of CDOM in its photoproduction. No photolysis was observed in this study for acrylate in pure water or seawater in contrast to that reported in previous studies, presumably due to the rapid relaxation of triplet excited state by collision with water or energy transfer to dissolved oxygen in airsaturated seawater. These results will be discussed to assess the role of sunlight in the cycling of acrylate and carbon in the upper ocean.

ENVR 466

Interfacial analysis of single aerosol particle

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A number of gas-particle reactions occur among the strongly acidic particles and atmospheric gases through homogeneous gas or aqueous phase reactions as well as through heterogeneous reactions on particle surfaces. The gas-aerosol particle interface is believed to

contribute to the growth of secondary organic aerosols in the atmosphere. Despite its importance, the chemical composition of the interface has not been probed directly because of a lack of suitable interface-specific analytical techniques. Here we developed the interface-specific SHS for in situ chemical analysis of molecules at the gasaerosol particle interface. As an example, we demonstrated coherent SHS signal of a new SHS probe, crystal violet (CV), from interface of aerosol particle. We found that the combination of a high repetition rate as high as 1 MHz reaches a large signal-to-noise SHS signals from the gas-aerosol particle interfaces. It has greatly improved the detection sensitivity of interfacial molecules by more than 2 orders of magnitude, leading to interfacial detectivity of singlet aerosol particle. To further understand how interface plays a role in the growth of aerosol particle, we have measured interfacial behaviors of molecules of aerosol particles under different relative humidity (RH) by the interface-specific SHS. Since RH can vary the concentration of solutes inside single aerosol particle and interfacial hydration in local regions, the particle size and the phase of the single aerosol particle can be impacted by the RH. Organic molecules were found to exhibit distinct behaviors at the interfaces and bulk on the single aerosol particle under different RH levels. Our quantitative analyses showed that the interfacial adsorption free energies remain unchanged while interfacial areas increase as the relative humidity increases. Furthermore, the surface tension of single aerosol particle decreases as the RH increases. These experimental results not only provided a thorough analysis of the SHS technique but also built a solid foundation for further development of a new vibrational sum frequency scattering (SFS) technique for chemical structures at the gas-aerosol particle interface.

ENVR 467

Photolysis of aqueous atmospheric aerosol mimics

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Aqueous reactions of small, water soluble aldehydes with amines or ammonium salts have been shown to be important for atmospheric brown carbon formation processes. The extent to which photolysis of these brown carbon compounds changes the chemical composition and light absorption of these systems is not well understood or characterized. We photolyze aged reaction systems of aqueous carbonyls (e.g., glycolaldehyde, glyoxal, methylglyoxal, and hydroxyacetone) and ammonium sulfate and monitor light absorption and chemical composition via UV-visible spectroscopy and mass spectrometry. Photobleaching and photobrowning varies with wavelength and aldehyde identity, while mass spectrometry shows that the chemical composition changes significantly upon photolysis.

ENVR 468

Identification of highly fluorescent components of dissolved organic matter via size exclusion chromatography

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Fluorescence spectroscopy has become very popular due to its ability to collect vast amount of data with very high levels of sensitivity. Fluorescence is now being used for numerous applications, including tracking dissolved organic matter (DOM) across geographical scales and to fundamentally investigate its composition. However, the clear chemical identity of some of the most important fluorophores remain a mystery. Because DOM samples are a complex mixture of compounds, it is extremely difficult to investigate fundamental fluorophores using only whole-water measurements. Instead, it may be useful to separate DOM samples into fractions to be considered individually. Size exclusion chromatography (SEC) is a form of liquid chromatography in which compounds are separated by size and has been previously been used to investigate the size distribution of DOM samples. This study sets out to develop a method to identify the size portions of DOM with the highest Fluorescent Quantum Yield (FQY, defined as the number of photons emitted via fluorescence per photons absorbed). To accomplish this, investigators used a liquid chromatography system outfitted with a SEC column, Diode Array Detector, Fluorescence detector, and Total Organic Carbon analyzer. The method was then used to analyze several DOM isolates, natural water samples from Boulder Creek (Boulder, Colorado) as well as wastewater effluent samples. Preliminary results indicate the highest FQY occurs in the medium to low molecular weights (>1000 Da). It is hypothesized that the DOM fractions with the highest FQY contain the highest number of fluorophores. This method can be used to identify these fractions to later be isolated for further analysis of their molecular composition, yielding insight into the most important fluorophores of DOM.

ENVR 469

Combined effects of dissolved organic matter, pH, and divalent cations on UV-254 phototransformation of tetracycline antibiotics

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Tetracycline (TC) antibiotics are commonly prescribed for human and veterinary health. These pharmaceuticals are not completely metabolized in the human body and, as a result, have been detected in wastewater treatment plants at concentrations up to 4 µg L⁻¹. TCs exhibit complex acidbase dissociation reactions, which influence interactions with dissolved organic matter (DOM) and divalent cations. such as Ca2+ and Mg2+. In this study, we investigated the individual and combined effects of these parameters on the photochemical properties of TCs, specifically doxycycline, meclocycline, and methacycline. In particular, UV-visible absorbance spectra at 200-600 nm were generated after a 24-h equilibration time in the dark for the following solutions: (i) 250 µM TC; (ii) 250 µM Ca2+ or Mg²⁺; (iii) 20 mg_c L⁻¹ DOM; (iv) 250 µM TC with 250 µM Ca²⁺ or Mg²⁺; (v) 250 μ M TC with 20 mg_c L⁻¹ DOM; (vi) 250 µM Ca²⁺ or Mg²⁺ with 20 mg_c L⁻¹ DOM; and, (vii) 250 μ M TC with 20 mg_C L⁻¹ DOM and 250 μ M Ca²⁺ or Mg²⁺. All solutions were tested at pH 2, 3, 5, 7, 9, and 10, although at 254 nm, solution pH had a minimal effect on TC absorbance, in the absence of DOM and divalent cations. For example, species-specific molar extinctions for doxycycline were 1.57×10⁴ M⁻¹ cm⁻¹ (ε_{0,254}), 1.20×10⁴ M⁻¹ 1 cm⁻¹ ($\epsilon_{1,254}$), 1.13×10⁴ M⁻¹ cm⁻¹ ($\epsilon_{2,254}$), and 1.52×10⁴ M⁻¹ cm⁻¹ ($\epsilon_{3,254}$). Solutions containing 5 μ M TC, 5 μ M Ca²⁺ or Mg²⁺, 10 mg_C L⁻¹, and 5 mM phosphate buffer were irradiated at 254 nm using a merry-go-round Rayonet reactor. The species-specific, fluence-based rate constants for doxycycline, DC were 1.68×10⁻⁴ cm² mJ⁻ 1 (k'_{p,0,254}), 4.68×10⁻⁵ cm² mJ⁻¹(k'_{p,1,254}), 7.44×10⁻⁴ cm² mJ⁻¹ $(k'_{p,2,254})$ and 1.21×10^{-3} cm² mJ⁻¹ $(k'_{p,3,254})$, for the cation, zwitterion, monovalent anion, and divalent anion, respectively. Impacts of DOM and divalent cations were determined relative to these direct photolysis rate constants. Experimental results indicated that environmental factors, such as pH, DOM, and divalent cations, influenced the photodegradation of TCs in engineered processes.

ENVR 470

Using fixed potential electrodes to quantify *in situ* iron redox in soils of the Susquehanna Shale Hills Critical Zone Observatory

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Iron redox exerts strong controls on carbon and nutrient mobilization but is difficult to measure in real time in soils. In well-drained soils, seasonal and periodic fluctuations in

soil moisture most often regulate these redox reactions. Recent work from the Susquehanna Shale Hills Critical Zone Observatory (SSHCZO) in Central Pennsylvania confirms the importance of water content to soil iron redox, indicating widespread iron redox cycling within these soils in response to precipitation. To explore the fine-scale temporal fluctuations of iron redox in response to environmental conditions, we installed electrodes fixed at a 100 mV (vs. SHE) potential at two depths in the valley floor and midslope soils of a shale watershed at the SSHCZO in March 2019. Electrodes fixed at 100 mV mimic iron oxides in the soil so that iron reduction and oxidation rates can be calculated by measuring the changes in the electric current over time. Alongside the electrodes, soil porewater chemistry, pCO₂, pO₂, moisture content, temperature, and precipitation are being measured. Initial results suggest aerobic conditions persisted in the soils throughout the early spring from March through April, with a slight signal consistent with iron oxidation measured from the electrodes. In May and June, as the soils warmed and respiratory demand for O₂ increased, we observed periodic iron reduction at both the midslope and valley floor in response to precipitation events. To characterize reactions at the electrode surface under different conditions, cyclic voltammetry was used to identify the range of redox reactions taking place at each electrode. This study is the first time that fixed potential electrodes have been used successfully to track fine temporal scale fluctuations in microbial metabolisms in situ in upland soils.

ENVR 471

Identification of Sb(V) reducing bacteria and their potential metabolic traits by the combination of stable isotope probing and metagenomics analysis

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Microbes are considered to play an important role in changing Sb speciation, mobility, and bioavailability. In this study. DNA-stable isotope probing (DNA-SIP) and metagenomics analysis were combined to identify potential Sb(V)-reducing bacteria (SbRB) and predict their possible metabolic pathways for Sb(V) reduction. Cultures inoculated from Sb-contaminated paddy soil demonstrated a capability to reduce Sb(V) by innate microbial communities. DNA-SIP identified bacteria belonging to the genera Pseudomonas, Lysinibacillus, and Geobacter and the family Enterobacteriaceae as putative SbRB. Metagenomic-binning was performed to investigate the metabolic potentials of the Sb(V)-reducing cultures with a focus on those identified as putative SbRB by DNA-SIP. Near complete draft genomes (>90% completeness) of bins affiliated with putative SbRB were obtained. Given the similar chemical structure of As and Sb and the lack of known Sb-related genes in the existing

databases, we focused our search on genes involved in As transformation, especially genes encoding As(V) reduction. Notably, bins affiliated with *Pseudomonas*, *Geobacter*, and *Enterobacteriaceae* contained the respiratory arsenate reductase (*arrA*) gene. In contrast, *arrA* was not detected in bins affiliated with *Lysinibacillus*. A shift of *arrA* genes to heavier DNA fractions in treatments amended by ¹³C-acetate and Sb(V) than those in controls suggested that the *arrA* genes were ¹³Clabeled and were probably responsible for Sb(V) reduction. This current work represents the first attempts of using DNA-SIP and metagenomic-binning to identify anaerobic SbRB and their metabolic potential and provides valuable datasets to link bacterial identities with Sb(V) reduction.

ENVR 472

Withdrawn

ENVR 473

Humans are exposed to more than just water when inhaling aerosolized drinking water from ultrasonic humidifiers

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Utltrasonic humidifiers, a popular consumer product, impact indoor air quality in more ways than humidification. Emission from room-sized ultrasonic humidifiers are potential pathways to inhalable particulates for humans who fill these units with tap water. Our research demonstrates that approximately 85-90% of soluble minerals and < 50% insoluble iron oxide or aluminum oxide particles in drinking water used to fill humidifiers are aerosolized and form sub-micron particulates in room air. Denser, settleable particles of 1.5 µm diameter of iron or aluminum oxides accumulated at the bottom of humidifier reservoir. Smaller, suspended metal oxide particles of 0.22-0.57 µm diameter and soluble ions are emitted as aerosols from humidifier. When using 75 mg/L TDS tap water to fill an ultrasonic humidifier and operate for 8 hours, particles mass and number concentrations reach 211 µg/m³-air and 56,500 #/cm³-air, respectively, with median diameter as 146 nm. A multi-path particle dosimetry model predicts the deposition fractions of 0.24 and 0.10 in human pulmonary region for 3-month child and adult, respectively. In addition, deposited masses are 59 and 200 µg as total minerals for 3-month child and adult, during a single 8-hour exposure period. Fill water quality influences the emitted particles in room air; the higher TDS fill water has, the more and larger particles

are produced. These results indicate human inhalation exposure to both soluble and insoluble drinking water constituents when tap water is used to humidify air with an ultrasonic unit, and thus following USEPA recommendations to use distilled or low-mineral water is advised.



Child and adult inhalation exposure to emitted waterborne constituents from ultrasonic humidfiiers during rest

ENVR 474

Controls on the leaching of mercury from contaminated soils

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Streambank soils within the East Fork Poplar Creek (EFPC) watershed have elevated concentrations of mercury (Hg) as a result of historic use and discharge of Hg into the system associated with activities at the Y-12 National Security Complex. Mercury can leach from these soils as a result of water level fluctuations and erosion of stream banks resulting in the soils acting as a source of Hg to the creek. Laboratory experiments were conducted to examine the amount of Hg leaching from two soil samples collected from EFPC and a soil sample collected from Hinds Creek, an uncontaminated creek used as a reference site. For these batch laboratory studies the amount of mercury leaching from the soils when exposed to water from EFPC was examined for two weeks with

samples collected every 3-4 days. After two weeks, solid phase sorbents were added to some of the samples and the amount of Hg leaching from the soils with and without sorbent addition was examined for an additional two weeks. The concentration of Hg in the reference soil was 0.027 µg/g and the two soils from EFPC had Hg concentrations approximately 200 and 10,000 times greater than the reference soil. After the two-week leaching period with creek water, the concentration of Hg in the aqueous solution was 5.3 ng/L in the soils from the reference site and approximately 24 ng/L and 440 ng/L in the aqueous phase of the contaminated soil treatments. The solid phase sorbents that were tested included Thiol-SAMMS[®], Organoclay[™] PM-199, Organoclay[™] MRM, SediMite[™] and a biochar. The addition of the sorbent resulted in a decrease in the Hg leaching from the sediment. SediMite[™] provided the greatest reduction in Hg leaching from the soils. In a separate experiment the impact of repeatedly wetting and drying the soil showed that this process increases the leaching of Hg from the soils. Results from this laboratory study will help evaluate the usefulness of solid phase sorbent materials as a remedial option for reducing the amount of Hg leaching from soils into East Fork Polar Creek.

ENVR 475

Revealing surface interactions between emerging pollutants and polymeric natural organic matter

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Natural organic matter (NOM) can play an important role in the transport and fate of organic contaminants. NOM, in general, consists of carbon-based polymeric compounds with a wide range of chemical functional groups. They can exist as dissolved or particulate matter and thus, their interaction with aquatic contaminants are often complex. The goal of this study has been to decipher the specific interactions NOM can exhibit with different types of pharmaceutical contaminants. Our approach has been two-fold: we investigated (1) interactions of humic acid (HA) and Suwannee River NOM with polymeric particle surfaces of different (e.g., carboxylic and amine) functional groups and (2) binding affinity of emerging pharmaceutical contaminants (e.g., ketoprofen, carbamazepine, and amlodipine) onto polymer and NOM coated surfaces. The binding studies have been carried out using a magnetic separation method in conjunction with UV-Vis spectroscopy. Adsorption isotherms and colloidal size and zeta-potential data, based on the dynamic light scattering technique, will be presented. It has been found that both HA and NOM exhibit preferential adsorption onto amine surfaces and their binding affinity depends on pH and the buffer solution used. Uptake of pharmaceuticals onto these

surfaces also appears to be dependent on the surface functional moiety. These findings, along with zeta potential measurement and particle size dependent adsorption studies, not only map out the specific interactions pharmaceuticals can have with polymeric surfaces but also open up the possibility to understand the active binding sites of colloidal NOM.

ENVR 476

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Toxicity of sunscreen active ingredients to *Thalassiosira pseudonana*

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UV-filters, which are the active ingredients in sunscreen and other personal care products, have been detected in the aquatic environment. For example, we previously reported almost 100% detection frequencies for homosalate, octisalate, octocrylene, and oxybenzone in water, sediment, and oysters collected throughout the Chesapeake Bay. We hypothesized that organic UVfilters pose a threat to photosynthetic organisms, such as algae and submerged aquatic vegetation, because these chemicals partition into lipids and absorb sunlight. Thalassiosira pseudonana are marine centric diatoms that comprise an essential role in the diet of Eastern oysters and, therefore, Chesapeake Bay ecosystem services. The objective of this work was to establish the baseline toxicity of five UV-filters covering the natural sunlight spectrum to T. pseudonana. In this regard, T. pseudonana were cultured at a constant temperature of 26 °C and exposed to artificial estuarine water containing 0.1-1000 µg/L of avobenzone, homosalate, octisalate, octocrylene, or oxybenzone and salinity relevant to mid-Bay conditions. Mixtures of these UV-filters were also assayed against T. pseudonana to elucidate potential synergism or antagonism. After a 72-h exposure period, the optical density and relative chlorophyll fluorescence were measured to determine growth and chlorophyll inhibition, respectively. The toxicity of each UV-filter was calculated as the half maximal effective concentration (EC₅₀), which is the UV-filter concentration required to inhibit the growth or chlorophyll fluorescence of T. pseudonana by 50%. The EC₅₀ of each UV-filter was compared to previously reported UV-filter concentrations in raw wastewater, wastewater effluent, and the

Chesapeake Bay to contextualize the relative risk to *T. pseudonana*.

ENVR 479

High-performance degradation of bisphenol A by NaCIO: Effect, dynamic process and mechanism

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The commonly used disinfectant NaClO was employed as an oxidant in this study to investigate the effect of degrading the endocrine disruptor bisphenol A (BPA). Regardless of the initial concentration of NaClO, the optimal result can be achieved at pH 9.0-10.0, which illustrated that the reaction rate between HOCI with BPAwas faster than that with BPA according to the speciation distribution of chlorine and BPA. With the increase of NaClO dose from 1.0 to 10.0 mg/L, the degradation efficiency was greatly enhanced from 23% to 98% at pH 9.5. Simultaneously, TOC removal efficiency experienced a rapid rise upon 10.0 mg/L NaClO was dosed. Combined with the UPLC & Q-TOF MS and the DBPs formation analyses, the plausible degradation mechanism was proposed. At the beginning, substitution reaction was dominant based on the comparison of low TOC removal efficiency and relatively high degradation efficiency. As the NaClO dose increased, substitution converted into oxidation, leading to the commencement of its real degradation. More small molecules were produced to further generate TCM and TCAA once the NaClO dose was excessive. It indicated that appropriate dose of NaClO can efficiently degrade BPA but also restrain the DBPs formation. Intriguing phenomenon was that the decline of BPA concentration and TOC content almost stabled after 30 s at a NaClO dose of 10.0 mg/L. Considering the short retention time and high performance of the degradation, this study provides new insights for the feasibility of the BPA degradation by utilizing low-cost NaClO in drinking water treatment plant.





ENVR 480

Mountain Valley Pipeline's impact on the water chemistry of surrounding streams

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Stream chemistry is delicate, yet a healthy stream is essential to the ecology of the stream and the organisms depending in it. Alkalinity, total water hardness, and quantification of ions and metals are four analyses that provide direct insight into the chemistry of streams. The changes in these analyses can be monitored over a period of years with samples collected during different seasons. The Mountain Valley Pipeline is a natural gas pipeline that is being installed in Roanoke County, Virginia and is the main focus of this research. The overall objective is to monitor surrounding streams and how they are affected by its installment. At this point two baseline data sets have been collected, fall 2018 and spring 2019. The alkalinity and total hardness tests were determined through titrimetric procedures. Ion Chromatography gave results quantifying anions in the stream water. Fluoride, chloride, nitrate, and sulfate were found in the samples; however, phosphate, bromide, and nitrite were not found in the baseline samples. The last analysis is Inductively Coupled Plasma (ICP), in which results showed only four of the eight metals analyzed appeared in the baseline stream samples.

ENVR 481

Effects of climate-induced increases in road salt contamination on dissolved organic matter in a northern Michigan wetland

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Wetlands are a significant terrestrial sink for carbon. In the soluble phase, much of the organic carbon is in the form of humic- and tannic acids, referred to collectively as dissolved organic matter (DOM). These compounds are known to react in brackish and saline conditions, with UV exposure, to form trihalomethane end products. In the context of the Great Lakes region, continued road salt application over the past century has resulted in measurably higher salinity in adjacent wetlands, converting these systems from freshwater to nearlybrackish water. Here, we performed an incubation experiment to determine whether the native DOM or an experimental proxy (tannic acid) were amenable to trihalomethane production at the level of salinity currently found in a nearby wetland, and at a 100-year estimated salinity assuming continued application. We also controlled for UV exposure and the presence or absence of photosensitizers (Fe) which are found in high concentrations in the study system. We found that all three treatments (UV, chloride, Fe) altered the DOM character, resulting in different chemical constituents, and even liberating peroxide ions, but failed to result in trihalomethane production.

ENVR 482

Contamination of Grovnes Peninsula in east Antarctica by persistent organic pollutants (POP's)

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Anthropogenic activity in east Antarctica has increased since the last 2-3 decades because of the various scientific expeditions. Additionally, global pollution due to various newly introduced pollutants like pesticides is on use since the past century and many factors contribute to contamination even in Antarctica. Persistent Organic Pollutants (POP's) are semi-volatile, toxic organic compounds which resist photolytic, chemical and biological degradation. POP's are persistence in nature and includes some pesticides, PCB's and dioxins. Due to volatile nature these contaminate are transported across the earth by "grasshopper effect". The study reported the occurrence of several POP's in the lake water samples collected from Grovnes Peninsula. which were Larsemann Hills, East Antarctica. A total of 45 lake water samples from fifteen different selected locations were collected, during 34th Indian Scientific Expedition to Antarctica (ISEA) in austral summer of 2014 to 2015. In these samples, twenty-seven compounds of POP's were estimated. POP's residue levels were found in the lake water samples from 10.00 pg/mL - 75.00 pg/mL in fifteen different lakes. Presence of p,p'-DDT was detected in all different lakes but high concentration found in L1E NG &

L5 SG lake water. It has been observed that the lakes of Grovnes Peninsula have a trace amount of POP's and it is an alarming situation which needs to be investigated further to maintain the pristine environment in Antarctica. The presence of POP's may be attributed to orographic effects, migratory birds, bio magnification and anthropogenic sources.

ENVR 483

Quantification of nonylphenol and 4-tert-octylphenol in drinking water using UHPLC-MS/MS

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Nonylphenol is alkylphenol compound and often detected in the environment. It is widely used as intermediate in industrial processes to produce pharmaceuticals, pesticides, detergents, paints, personal care products, plastics, to name a few, and released into the environment including the water supply. The 4-branched nonylphenol represents that found in environment best and is selected along with 4-tert-octylphenol as target analytes. The current health reference level (HRL) from Minnesota Department of Health for nonylphenol is 20 µg/L. In this study, the minimum reporting limit (MRL) that is far below the HRL was established for branched nonylphenol and 4-tert-octylphenol after a method for identification and quantification of both compounds in drinking water samples was evaluated, using Agilent 1290 Infinity II LC coupled to an Agilent 6470A triple guadrupole LC/MS system with Agilent MassHunter workstation software. The sample preparation consists of loading water sample onto SPE cartridge and eluting with acetone. The challenges including contamination, buffer selection, and solvent effect encountered during the LC conditions optimization are discussed. The method was evaluated and quantified with isotopically labeled internal calibration curve, showing satisfactory results, including identification, selectivity, linearity, MRL, accuracy, and precision.

ENVR 484

Detailing the mechanism of degradation of perfluoroalkyl substances by a cold atmospheric pressure plasma

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Cold atmospheric pressure (CAP) plasma can generate various oxidizing and reducing species at ambient temperature and pressure. Conventional wastewater treatment methods mostly rely on oxidative techniques. Recent studies have shown that the reducing species generated by plasma are responsible for the inactivation of perfluoroalkyl acids (PFAAs). The EPA has released a health advisory for PFAAs, present in wastewater and drinking water. PFAAs can accumulate in the body and cause adverse health effects, an environmental issue. A pin-to-water glow discharge DC plasma is being used as the CAP source. Work is being done detailing the oxidative and reductive species generated by our CAP in both positive and reverse polarities. Reversing the polarities changes the concentration of the chemical species and reducing species being injected into the water. Plasma was ignited in three different gases Argon, Argon + 20% Oxygen, and air to offer a diverse range of chemical species. Perfluorooctanoic acid (PFOA) and perfluorooctanesulfonate (PFOS) were added to distilled water respectively and subject to the plasma ignited in the three different gases in different polarities. The degradation of PFOA and PFOS was analyzed by HPLC, and LC-MS. The mechanism of degradation of PFOA and PFOS is being determined by our CAP.

ENVR 485

Determining the relationship between hydraulic fracturing activities and streamwater trace metal concentrations in North-Central Pennsylvania watersheds

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Unconventional gas extraction, particularly in the Marcellus Shale, has transformed our energy supply; yet this transformative process is not without controversy. To date, a limited number of studies in the scientific literature have documented localized stream and well water contamination due to improper disposal and/or leakage of flowback and produced waters from drilled wells. However, discerning impacts of hydraulic fracturing activities at a regional level has been hindered by the lack of baseline data and the lack of regional sampling networks. Here we attempt to address these knowledge gaps through the analysis of stream and groundwater samples collected from 40 small watersheds (<10 mi²) in north central Pennsylvania (Bradford, Wyoming and Susquehanna Counties) from 2013-2015. The samples were analyzed for the presence of Cr, Mn, Fe, Co, Ni, Cu, Zn. As. Se. Cd. Ba. and Pb using inductively coupled mass spectrometry (ICP-MS). Sample concentrations were statistically compared to a variety of factors for each watershed, including relative land use patterns, number of hydraulic fracturing well pads, spud dates, and number

of drilling related violations. A statistically-significant correlation between Ba concentrations and the number of wells spudded in each watershed was identified for the 2014 and 2015 dataset. In addition, many stream and groundwater samples exhibited metal concentrations in excess of USEPA guidelines for freshwater quality and/or drinking water. These results suggest more studies are needed to evaluate the impacts of hydraulic fracturing activities on surface water quality.

ENVR 486

Phosphate removal from polluted waters by Iron hydroxide adsorption

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Nutrient pollution in water systems can result in severe environmental problems like eutrophication which leads to relocation and death of aquatic animals. Certain pollutants, like phosphate, can enter drinking water systems and, if present in high levels, can cause eutrophication and mild to severe health problems. Iron (II,III) hydroxides, including green rust, belong to the double layered hydroxides (LDH) group and their layered structure allows for intercalation of ions which leads to adsorption of many charged species. Green rusts, which belong to the LDH group, have been found in natural environments and their structure and high reactivity not only allows for adsorption of other compounds but also reduction of many contaminants. In this research, iron hydroxide minerals (similar to GR) were synthesized using several iron redox states to test the adsorption of phosphate. Preliminary results are promising as they show that at room temperature and pH ranging from 6.5-8.5 (relevant to surface water pH), the developed iron minerals have high adsorptivity toward phosphate, decreasing the phosphate concentration present in the aqueous phase of a 1-mL sample by up to 90%. Samples were analyzed via UV-Vis using molybdenum blue colorimetry technique for phosphate detection and ascorbic acid colorimetry technique for iron detection. Our goal is to test other parameters such as temperature and pH to find the optimum conditions for phosphate adsorption on iron hydroxides. Another goal is to be able to regenerate this mineral and convert the phosphate recovered to a less hazardous form. This work will be relevant to current water remediation techniques with respect to phosphate pollution.

ENVR 487

Exploring the freshwater salinization syndrome along a gradient of suburban development

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Road salts are one of the most commonly used methods of deicing, particularly in the northeastern region of the United States where this method has been used for nearly a hundred years. Excess road salt from deicing ultimately enters local watersheds either by direct runoff or by first entering the groundwater, where it can have deleterious impacts on freshwater aquatic organisms. More recently, this excess salt has been associated with contaminant increases in pH, alkalinity, base cations (i.e., sodium, calcium, magnesium, and potassium) as well as several trace metals in streamwater due to ion exchange in the surrounding soils. This combined effect has been dubbed the "freshwater salinization syndrome." This study evaluated the impact of the freshwater salinization syndrome on dissolved metal concentrations in three suburban watersheds, each with a varying density of development: The Mill Creek, Indian Run Creek, and the East Branch of the Brandywine Creek. Watersheds were spatially delineated using Esri's ArcMap software and land use practices in each of the three systems determined were using the 2011 National Land Cover Database. Water samples previously collected during summer baseflow conditions were analyzed for selects trace metals (Cr, Co, Ni, Cu, Zn, As, Se, Sr, Ba, Cd, Pb) using an inductively-coupled plasma mass spectrometer (ICP-MS) and for chloride using ion chromatography. Positive, statistically significant correlations were identified between streamwater concentrations of chloride and lead, nickel, strontium, and zinc for all three creeks suggesting elevated salt concentrations resulted in more metals entering the system. In addition, the relative concentrations of metals in each of the three watersheds varied as a function of land use, with higher concentrations linked to increased development within the watershed. Although metal concentrations did not exceed applicable USEPA guidelines, this relationship is concerning for ecosystem health as the volume of road salt used continues to rise.

ENVR 488

H_2O_2/UV -ceramic ultrafiltration membrane system for the mineralization of micropollutants: Role of V₂O₅-TiO₂ nanoparticles

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 V_2O_5 -TiO₂ nanoparticles were incorporated on to the ceramic ultrafiltration membrane surface and inside of pores for the enhanced oxidation of micropollutants by H_2O_2/UV . After V_2O_5 was successfully coated on the membrane through filtration-coating method, the catalytic oxidation of micropollutants was conducted on a V_2O_5 -TiO₂ catalyst in the presence of H_2O_2/UV . It has been found that catalytic reactions between H_2O_2/UV and V_2O_5 can improve permeate water quality as well as mitigate the membrane fouling. Consequently, a more strategic use of hybrid V_2O_5 -TiO₂ catalyst-coated ceramic UF membrane for the micropollutant removal, which requires less amount of oxidants due to catalyst, approaches to be a more economical suggestion.

ENVR 489

Partitioning of chlorpyrifos and tetrabromobisphenol A to sediments and dissolved organic matter in arctic lakes

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Anthropogenic organic pollutants have been commonly detected in the Arctic and include new classes of brominated flame retardants (BFRs) and current use pesticides (CUPs). In this study, we focus on the environmental fate of chlorpyrifos (CUP) and tetrabromobisphenol A (TBBPA, a flame retardant). These two chemicals have been detected in various environmental compartments in the Arctic and are transported there by global distillation. One process that can limit exposure and bioaccumulation of these compounds is through their interactions with Arctic dissolved and particulate organic matter (DOM and POM respectively). We hypothesize that the presence of DOM in Arctic surface waters at sufficiently high enough concentrations (from 3 to > 10 mg/L) will bind these chemicals thereby making them less bioavailable. Solubility enhancement studies for chlorpyrifos and TBBPA were conducted with various types of Arctic DOM (Toolik Lake and a tundra seep adjacent the Sagavanirktok River). We report log KDOM values for chlorpyrifos of 3.7 for Toolik Lake, 3.3 for Suwannee River, 3.5 for Oksrukuyik River, and 3.6 for Sagavanirktok River DOM. These values are consistent with a calculated poly-parameter linear free energy relationship (pp-LFER) value of 3.7. Sorption of these analytes to POM were also conducted and our partition coefficients are in good agreement with those reported in the literature. Surprisingly, we observed loss of TBBPA in the presence of DOM, which may be the result of an unknown abiotic

degradation pathway. Experiments investigating this phenomenon are ongoing.

ENVR 490

Control of lead release from lead service lines with sodium silicate addition

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Lead service lines (LSLs) connecting water mains to households are a major source of lead in drinking water. More than 50% of LSLs that remain in use in the United States are in the Midwest and Great Lakes regions. While the replacement of LSL is an ongoing process, drinking water suppliers can adjust the water chemistry for corrosion control. Sodium silicates can be used as a potential corrosion inhibitor for lead. Long-term loop experiments were carried out to investigate the role of sodium silicate in limiting lead release from LSLs. Harvested lead pipes were procured from Buffalo, NY for this study. The pre-existing lead- and aluminum-rich scales in these pipes are representative of many scales on LSLs in the Great Lakes region. The pipes were recirculated with baseline water chemistry (dissolved inorganic carbon 24 mg/L C, pH 7.7, 1.1 mg/L Cl₂) similar to that provided in Buffalo. Conditioning of these pipes with baseline water was followed by treatment with 20 mg/L SiO₂ of sodium silicate. Lead in the water was analyzed using inductively coupled plasma mass spectroscopy (ICP-MS). Scale characterization was carried out using X-ray diffraction (XRD), scanning electron microscopy (SEM), and Raman spectroscopy. Within a few weeks of the treatment with sodium silicate, lead concentrations decreased to below 15 ppb. Periodic assessments of the scale by SEM found that the low lead concentrations were associated with the accumulation of silica in the pipe scales. In this study, several factors that can influence lead release in the presence of sodium silicate were also investigated. The results of these experiments provide insights into the mechanism of lead corrosion inhibition by sodium silicates and can guide recommendations for the use of sodium silicates for corrosion control.

ENVR 491

Social history of U.S. kerosene standards in the late nineteenth century

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By 1860, kerosene had replaced whale oil as the primary source of fuel for illuminating lamps. Following the distillation of kerosene from coal in 1846 by Canadian chemist, Abraham Gesner, the kerosene industry grew by leaps and bounds. By the early eighteen sixties, over sixty "coal oil" companies were producing nearly ten million gallons of kerosene annually, at great profit. However, the rapid growth in the use of kerosene came at a steep price. The lack of a common standard on the definition of kerosene and its constituent components resulted in the production of unsafe mixtures containing highly volatile compounds such as benzine and gasoline. Improper distillation techniques, as well as the deliberate adulteration of kerosene with gasoline, produced numerous fires and explosions in homes and businesses. Women and children were frequently the victims of horrific accidents in homes due to the gendered division of domestic labor. Newspaper articles and municipal health department reports decried the lack of safety standards in the production and sale of kerosene for domestic use. Public outcry led to state and federal legislation mandating minimum standards for the flashpoint and specific gravity of commercially produced kerosene. Though the flashpoint test became the dominant safety standard, there was widespread disagreement on the instrumentation and process needed to establish the temperature at which the kerosene vapor ignited. In this presentation, we investigate the socially constructed nature of kerosene standards and laws in the late nineteenth-century. Using patents, court cases. articles, municipal newspaper reports, scientific publications, and other primary and secondary sources, we explore the chemistry and history of American kerosene consumption in the early decades. The interplay between scientific standards, flash point technology and consumer use highlights the impact of kerosene safety standards that remain in use today.

ENVR 492

Effectiveness of raw versus activated coconut shells for removing arsenic and mercury from water

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Relatively inexpensive biosorbents, made from coconut shell, were explored as alternatives to high-quality activated carbon for use in small-scale, wastewater treatment in developing economies. Simple charring and

activation procedures were followed to produce CaCl2activated coconut shell charcoal and its effectiveness was compared with raw coconut shell powder for removal of mercury (Hg) and arsenic (As) from contaminated water. From atomic absorption spectroscopy analyses, the removal efficiency of As and Hg with the use of activated charcoal were 67% (vs 65% for the raw form), and 53% (vs 49% for the raw form), respectively, from their corresponding "artificially"-contaminated wastewater. These results suggest that despite the slightly improved removal efficiencies recorded for activated coconut shells, the raw version could equally be used in treating wastewater towards the removal of the toxic metals- As and Hg. In order to understand the chemistry of the adsorption processes, FT-IR spectroscopy was employed to study similarities and differences in chemical compositions of the raw versus activated coconut shells before and after the biofiltration processes. To further investigate the effect of this biofiltration process on the overall quality of water, the physicochemical parameters (pH, conductivity, colour, turbidity, TDS and TSS) were measured on river water samples, pre-treated with the biosorbents. For both the raw and activated coconut shell, there was general improvement, although the conductivity of the water treated with the activated version was slightly elevated, likely due to leaching of CaCl₂ that was used for activation.

ENVR 493

Impact of fuel additives on oil-in-water emulsion stability

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The removal of oil from bilgewater is necessary for compliance with national and international maritime regulations; however, the formation of stable oil-in-water emulsions makes oil separation difficult. Therefore, it is necessary to understand the physical and chemical properties of emulsions created in bilgewater. Recent experiments have demonstrated that synthetic bilgewater emulsions can be stabilized in the absence of surfactants or cleaners. Therefore, the objective of this study was to determine if the additives found in fuels and lubricating oils can significantly contribute to bilgewater emulsion stability. Interfacial tension, conductivity, emulsion stability, and LC-MS measurements were conducted to determine transportation of oil additives into the aqueous phase. Results revealed that the additives in a common shipboard lubricant were capable of migrating from the oil phase to the bilgewater. The concentration of these additives in synthetic bilgewater correlated strongly with the stability of simulated bilgewater emulsions. In addition, characterization of actual bilgewater samples revealed the presence of the unknown additives in all bilgewater samples tested. Overall, this work shows fuel additives can contribute to the stabilization of bilgewater emulsions and further research is needed determine the full impact of these additives.

ENVR 494

Monitoring water quality activity implemented in the ACS student chapter

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The Environmental Chemistry Division (ECD) from the American Chemical Society UPRB Student Chapter (ACS-UPRB) focuses in to learn and to teach about the environmental chemical issues and their impact in our community. Water quality is an important part of environmental monitoring. When water quality is poor, it could affect not only aquatic life but also its surrounding. In November 2018, the ECD initiated a partnership with a local, non-profit organization, "Arrecife Pro Ciudad Inc." to monitor the water quality of the Isla Verde Reef Marine Reserve. In February 2019, we received a workshop of how to monitor water quality using an instrument that measure parameters such as: pH, salinity, temperature, dissolved oxygen levels, turbidity, total dissolved solids and conductivity. During the months of March, April and May, we had the opportunity to monitor the water quality of several sections of the Isla Verde Reef Marine Reserve. We obtained and analyzed the data which confirmed that the values of salinity, conductivity, dissolved oxygen and pH of the reserve, corresponded to the levels observed in seawater. The water quality was good, no contamination or irregularity was found. Furthermore, we observed a slightly increase of the water temperature (0.2 to 0.4 units) as we moved from March to May, indicative that summer was approaching. A slightly increase in salinity, conductivity and total dissolved solids were also observed. The other parameters remained almost constant. The results were analyzed for the different sections of the marine reserve that shown variability between them. We continued performing monitoring the water of the Marine Reserve during the subsequent months and after analysis we will present if there are any change in the parameters that could be relevant for the study. With this activity, the students could learn how to monitor water guality and had the experience to be in contact with the environment and to understand the importance to take care of it.

ENVR 495

Preparation and reactivity of hydroxy-nitrate esters derived from atmospherically relevant terpenes

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We will describe our simple, safe and effective method to prepare nitrate esters of terpenes (carene, limonene, perilic alcohol, beta-pinene and alpha-pinene) which are key oxidation products in the atmosphere. These compounds are implicated in the formation of secondary organic aerosols. The compiled spectroscopic data will also be presented. In addition, we will discuss our preliminary investigations into the atmosphericallyrelevant reactivity of these compounds.

ENVR 496

Adaptive polyvalency in *Klebsiella pneumonia* NDM-1+ bacteriophage KL

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Bacteriophage KL is a highly lytic virus infecting Klebsiella pneumonia ATCC BAA-2146. This emerging pathogen carries the broad antibiotic resistance gene New Delhi metallo-\beta-lactamase 1 (NDM-1) and is resistant to most antibiotic therapies. Upon challenging variety of Klebsiella Pneumonia serotypes, KL was found to be polyvalent for the antibiotic sensitive strain Klebsiella Pneumonia ATCC® 13883, albeit with an initial infection efficiency of 18% as determined by one-step growth curve analysis. However, after several cycles of infection in the K. Pneumoniae antibiotic sensitive strain, a 100% infection efficiency is achieved. This is due to a mutation that arises in the tail-spike protein (analogous to the phage lambda receptor binding protein J) that alters the last 10 aminoacids the protein complex, fusing it in frame with a downstream tail-fiber protein. This mutation is revertible upon re-infection of the NDM-1 positive strain. The switching of host serotype specificities in this way is unusual, and other examples of polyvalency regarding infectors of this NDM-1 strain have thus far not been observed. Given that study and genetic manipulations of phage KL in the NDM-1 host strain is infeasible due to the inability to employ necessary selective markers, a suitable antibiotic sensitive host for such experiments is necessary.

lonic liquid-based air purification and disinfection systems

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Bioaerosols, particulate matter and volatile organic compounds (VOCs) are major indoor air pollutants. Air purification systems based on filtration and adsorption can effectively capture inorganic particulate matter and remove VOCs. However, microorganisms in bioaerosols can remain viable on air filtration media, and further grow to colonize the media, thus decreasing air filtration efficiency and posing the risk of secondary pollution. Many attempts have been made to combine conventional disinfection technologies including photocatalysis, plasma and silver nanoparticles with filtration and adsorption processes for air purification and disinfection, complicated system design and increased air flow resistance are main concerns. This work develops a new air purification and disinfection technology based on supported ionic liquids. The optimized air purification and disinfection systems can directly inactivate bioaerosols (e.g., bacteria, viruses) and remove molecular pollutants (e.g., VOCs and malodors). New ionic liquid-based systems also exhibited enhanced filtration efficiencies for inorganic particulate matter without increased air flow resistance. This work provides a cost-effective solution to complex air pollutants.

ENVR 498

Intact carbonic acid is a strong reactive carboxilic acid affecting all aqueous environments

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Intact carbonic acid exists in all aqueous environments which interacts with atmospheric CO_2 and carbonate and bicarbonate salts. As the CO_2 concentration in the atmosphere increases the concentration of intact carbonic acid increases concomitantly. This previously unappreciated factor affecting the environment is especially important in buffered aqueous systems such as the earth seas and oceans where the concentration of intact carbonic acid is larger than the concentration of the aqueous proton there. In our study we evaluate the acidbase reactivity of intact carbonic acid and discuss the effect of this considerable reactivity in diverse aqueous environments.

ENVR 499

Investigation of personal care products for UV screening components and parabens, and their photolysis products

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Much study has been conducted on the environmental effects and personal health effects of UV-screening components, particularly oxybenzone and derivatives, found in sunscreens. This study quantifies the levels of UV-screening compounds and parabens in other personal care products (PCPs) that may or may not be marketed as having a sun protection factor (SPF). Additionally, the degradation products after UV exposure have been identified and quantified.

ENVR 500

Withdrawn

ENVR 501

Withdrawn

ENVR 502

Wavelength dependence toxicity using various oils

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Since the Deepwater Horizon oil spill in 2010, a significant amount of work has been done to study the natural weathering processes of petroleum in the environment and how it impacts biological systems. To help assess the overall impact of petroleum on the ecosystem, a key consideration in understanding the mechanism of toxicity is examination of components produced from petroleum products through photochemical processes. Samples of water mixed with crude oil are called water accommodated fractions (WAFs) and are commonly used to mimic environmental conditions when an oil spill occurs. Over time, water soluble species separate from the insoluble water species of the oil and partition into the water phase of the WAF. The toxicity of the resulting water fraction is of great interest. The objective of the study is to observe toxicity effects due to photochemical weathering of crude oils. Previously, it was determined that a Surrogate oil was the most toxic of the oils that were tested, when filtered with green light (520-560 nm). Acidic and basic species formed in WAFs incubated under various light conditions were extracted using liquid/liquid extraction. The resulting fractions were examined for toxicity using bacterial growth response as a measure. Overall the oil fractions that were exposed to light showed a decrease in toxicity in comparison to oils that were kept in the dark.

ENVR 503

Withdrawn

ENVR 504

Facile formation of ternary MgTiSi compounds from asbestos-chrysotile's abatement

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Annually, asbestos exposure kills approximately 104,000 people, and causes lasting disabilities to 1.5M people. It is estimated that 125M people have been affected by this compound worldwide. However, it is also recognized from centuries to be one of the most unsurpassed fire-retardant materials. Therefore, it will be very beneficial to have a simple and facile way to transform such naturally occurring crystals into an inactive, biologically safe compound that still possesses the efficient fire-retardant properties. In previous research, asbestos was modified with great difficulties and lengthy, energy intense procedures. Here, we report the fast introduction of Titanium on the chrysotile surface, one of the most important crystal forms of asbestos, to form a new fiber based on Mg_xTi_ySi_z. The reaction is fast and simple to perform and can be quickly scaled-up for industrial asbestos' abatement. We will present data such as Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), x-ray powder diffraction, xray photoelectron spectroscopy, thermal gravimetric analysis, differential scanning calorimetry (DSC) and gas chromatography-mass spectrometry (GCMS) suggesting a new facile way to create a novel compound. Moreover, this new procedure can be used as a commercial analytical tool for asbestos/chrysotile in air.



ENVR 505

Development of engineered soil surrogates for predicting natural soil behavior

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With Continuously growing population, agricultural practices need to be improved to maintain the quality of agriculture land. In order to do that, the interaction between agricultural chemicals and natural soils need to be understood. This will aid in increasing the efficiency of agricultural chemicals, crop production and improving the chemicals design. However, natural soils are very complex and introduce a lot of unknown factors. Therefore, we are synthesizing soil mimics of increasing complexity referred to as Engineered Soil Surrogates "ESS". The main component of soils that plays a major role in interacting with chemicals is the "Soil Organic Matter" (SOM). SOM is mainly composed of lipids, lignin, and cellulose. Therefore, ESSs were designed to contain silica to represent mineral particles, different sizes of aliphatic chains to model lipids, phenolic oligomers to mimic lignin, and cyclic glucose to represent cellulose. Atom transfer radical polymerization technique was used to synthesize the ESSs block co-polymers. This technique is simple, easy to set up and allow precise control over final polymer molecular weight. Our first approach to attach the copolymers to silica was grafting-from, which showed some drawbacks because of the presence of the mesoporous silica in the reaction, so we shifted to more successful and controllable alternative approach, which is grafting-onto. The ESSs were characterized using thermo-gravimetric analysis and nuclear magnetic resonance. After that Norflurazon herbicide interactions with different ESSs were predicted through modeling sorption with Freundlich isotherm that is commonly used for soils.

Silica particle: model for mineral Particle size: 40-63 $\mu m,$ pore size: 60 Å



General Model for Engineered Soil Surrogate System

ENVR 506

Glyphosate as an underlying cause of increased dissolved reactive phosphorus loading in the Western Lake Erie basin

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Western Lake Erie has been experiencing increasing dissolved reactive phosphorus (DRP) loads since 1995, the causes of which are poorly understood. Changing agricultural practices are certain to have an effect on DRP loads. One recent change in particular has been the increasing use of the phosphonate herbicide alvphosate (RoundUp®). Glyphosate is known to displace phosphate from soil particles. potentially increasing DRP concentrations and loads. This study links glyphosate to the observed increase in Maumee River DRP loads since 1994 by examining phosphate desorption from Maumee River watershed soil samples in equilibration with glyphosate solutions. A geospatial model was constructed to quantify DRP losses across the watershed. From this, the contribution of glyphosate to increased DRP loads can be determined. Glyphosate's widespread usage contributes to DRP loadings and eutrophication in Western Lake Erie. These findings also suggest that glyphosate contributes to increased DRP loads in freshwater systems worldwide.

ENVR 507

High throughput methods for determining the formation parameters of struvite

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Precipitation of struvite (MgNH₄PO₄*6H₂O), a slowrelease fertilizer, provides a means of recycling phosphate from wastewater streams. Through the implementation of high throughput methods, many different precipitation parameters can be investigated at once. These reactions occur in small volumes (300 µL or less) in a 96 well plate over the course of 45 minutes. A high throughput platform allows for a minimal use of chemicals and a fast way to compare many reaction conditions. The formation of struvite was investigated by fitting absorbance at 600 nm over time to a first order model with induction time. The impact of various peptide additions was also examined to identify a promising peptide to modulate struvite precipitation. In the future, purity of precipitates will be analyzed via high throughput assays and morphology will be examined using optical microscopy.

ENVR 508

Assessing the potential of Markov state models in reducing the computational expense of estimating PMF, equilibrium constants and kinetics of reactions

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Estimating the potential energy surface is critical to the study of the thermodynamics and kinetics of environmentally relevant reactions and processes. Umbrella sampling using ab initio molecular dynamics (AIMD) to obtain the potential of mean force (PMF) of a reaction is computationally expensive. One approach to reduce this cost is to combine umbrella sampling and free molecular dynamic simulations and using Discrete Transition-based Reweighting Analysis Method (DTRAM) to estimate the Markov state model and obtain the PMF. The objective of this study is to i) identify the duration of short umbrella and free MD simulations necessary to generate equivalent PMF from 11 ns long umbrella simulations over 21 umbrella windows combined with 1 ns free MD simulations. ii) determine the equilibrium constant of the reaction, and iii) the reaction kinetics. Two separate systems, one with a NaCl molecule and another with a BaSO₄ molecule were investigated in this study. Both systems were solvated with 2000 water molecules. The general Amber Force Field was used to describe the NaCl and BaSO₄ molecular interactions and the SPCE model was used to describe the water. Each of the structures was minimized to remove bad contacts followed by molecular dynamics simulations of heating, constant pressure, and constant volume at 300K. Constant total energy classical thermodynamics was used for the simulations. 21 umbrella windows from 2 to 12 Angstroms spaced at 0.5 Angstroms were used for the umbrella simulations. Each short umbrella simulation was combined with 5 short free MD simulations, both of different time lengths. The results were analyzed with DTRAM using the PyEMMA library. The findings from this study can be used to assess uncertainties from short AIMD or QM/MM/MD simulations. The results showed that there are combinations of short free MD simulations on top of short umbrella simulations that improved the PMF estimation by reducing the standard deviation compared to PMFs with short umbrella simulations only. However, there are large discrepancies between calculated mean first passage times and association constants for short simulations compared to the long 11 ns simulations. This indicates that large uncertainties in estimated quantities using AIMD with short simulations can be expected.

ENVR 509

Performance loss of activated carbon electrodes in capacitive deionization: Mechanisms and material property predictors

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Understanding the material property origins of performance decay in carbon electrodes is critical to maximizing the longevity of capacitive deionization (CDI) systems. This study investigates the cycling stability of electrodes fabricated from six commercial and two postprocessed activated carbons. We find that the capacity decay rate of electrodes in half cells is positively correlated with the specific surface area and total surface acidity of the activated carbons. We also demonstrate that half-cell cycling stability is consistent with full cell desalination performance durability. Finally, we confirm that physical pore blockage by oxygen functional groups generated during cycling is the primary origin for the specific capacitance decay of activated carbon electrodes. Our findings provide crucial guidelines for selecting activated carbon electrodes for stable CDI performance over long-term operation. Our half-cell cycling protocol also offers a method for evaluating the stability of new electrode materials without preparing large, freestanding electrodes.

ENVR 510

Unlocking potential of "green" aluminum batteries: Pulsed, amplified and proton boosted systems

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Aluminum is a ubiguitous industrial metal with about 70% gravimetric energy density of lithium and a favorable environmental profile. Despite these merits, aluminum has still not reached the stage of large-scale industrial utilization in electrochemical power devices, although the concept of aluminum batteries was introduced more than 150 years ago. It appears that a set of unique technical challenges associated with aluminum as anode material is responsible for this technological underperformance. Unlike lithium, aluminum is a multivalent metal with rich and sophisticated coordination chemistry, which remains poorly understood even today. However, this complexity can be turned into advantage with technomimetic approaches by facilitating creation of novel types of alkaline aluminum batteries that operate in the deep nonthermodynamic equilibrium regime. Specifically, modification of aluminum hydroxide surface nanofilm with special electrolyte additives allows designing pulsed batteries which are capable of generating stable AC power out of two identical aluminum electrodes. These pulsed batteries are also capable of amplification of a trigger signal thus allowing control of a power output in pulse frequency modulation mode. As an additional bonus from the environmental perspectives, pulsed aluminum batteries are tolerant to impurities in recycled aluminum, since the energy is being generated only during active states thus preserving the anode from corrosion during inactive states. Neutral salt aluminum batteries are also attractive due to their eco-friendliness, but require novel approaches, such as air cathode proton boosting, since the native voltage of these batteries is substantially lower.

ENVR 511

Acting through environmental chemistry and the sustainable global goals in an ACS local chapter

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The Environmental Chemistry Division (ECD) was founded in our local ACS Student Chapter at the University of Puerto Rico at Bayamón (ACS-UPRB) in September 2018. Our goal is to educate and make awareness about the environmental issues happening globally, the chemical processes involved and their

impact on society. To work on that goal, we want to create spaces where the public, our local communities and undergraduate members can learn and teach about the effects of climate change, and other environmental issues. We also want to encourage the community to monitor and obtain information of the environment in order to implement innovative solutions. This division is also acting by encouraging the United Nations Sustainable and Development Global Goals in all its activities, creating a movement. The ECD currently impacts 12 of the 17 sustainable goals and we hope to continue working on these efforts. Guided by these goals we intend to: Build Knowledge and capacity to meet climate change (Target 13), Protect and restore water related ecosystem (Target 6), Conserve and restore terrestrial and freshwater ecosystem (Target 15), Ensure full participation in leadership and decision-making (Target 5), and many more with a focus on Environmental Chemistry. The ECD has partnered with "Arrecifes Pro Ciudad, Inc." a local, non-profit organization, monitoring water quality in the "Reserva Natural de la Isla Verde". We are currently working on analyzing all the data collected. This data analysis will elucidate more knowledge about the effects of temperature, pH, turbidity, conductivity, dissolved oxygen and salinity in the Coral Reefs at the reserve. The ECD is working on bringing more conferences, workshops, experimental demonstrations and research in the natural reserve that shares our goals and objectives. Finally, all our activities are enacted to reach one final goal, give undergraduate students and the community the tools they need in order to execute and apply changes that have the potential to change the world.

ENVR 512

Electrocatalytic and photocatalytic behavior of hybrid TiO_2 nanomaterials towards water removal of NSAIDS and selected dyes

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A hybrid nanomaterial based on TiO₂ and graphite oxide (TiO₂-GrO) was tested for the photocatalytic water removal behavior of ibuprofen and naproxen classified as non-steroidal antiinflamatory drugs (NSAIDS) and three azo dyes: methyl red, methyl orange and eriochrome black T under UV-light. The photocatalytic material was prepared via a hydrothermal synthesis. The same organics were electrolyzed on TiO₂ nanotubes decorated with highly dispersed PbO₂. These electrodes were prepared by anodization of titanium plates (2 cm²) at 30 V, in a glycerol-water medium containing sodium fluoride followed annealing at 500°C salt. bv and

electrodeposition of PbO₂ from a lead nitrate solution. The electrocatalytic experiments were performed under galvanostatic conditions at 30 mAcm⁻². For both photocatalytic and electrocatalytic experiments, the organics removal was monitored in both a 0.5 M sulfuric acid aqueous solution (pH 1.8) and in 0.2 M basic sodium sulfate (pH 9.0); and their concentration decay was mainly followed by UV-vis spectrophotometric analysis. For naproxen and ibuprofen, an increase in the analytical peak during both catalytic processes was observed, which is an indication of the preservation of the aromatic structure during the allowed reaction time. On the other side, for the selected dyes, in both catalytic processes, methyl red and methyl orange underwent almost complete discoloration during the allowed reaction time in acid medium, while for eriochrome black T only a partial discoloration was observed. In contrast, in basic media, complete discoloration was not achieved during the reaction time for the three azo dyes for both photocatalytic and electrocatalytic processes.

ENVR 513

Creating awareness in undergraduate students and the community with environmental chemistry: Way of acting

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The Environmental Chemistry Division (ECD) was founded in our local ACS Student Chapter at the University of Puerto Rico at Bayamón (ACS-UPRB) in September 2018. Our goal is to educate and make awareness about the environmental issues happening globally, the chemical processes involved and their impact on society. To work on that goal, we want to create spaces where the public, our local communities and undergraduate members can learn and teach about the effects of climate change, and other environmental issues. We also want to encourage the community to monitor and obtain information of the environment in order to implement innovative solutions. This division is also acting by encouraging the United Nations Sustainable and Development Global Goals in all its activities, creating a movement. The ECD currently impacts 12 of the 17 sustainable goals and we hope to continue working on these efforts. In September 2019, the ECD participated in the march about climate change, "Caminata: P.R. ante el Cambio Climático". In this event, ACS-UPRB members participated as volunteers, in the march and in the presentation of The Chemistry Behind Ocean teaching, through Acidification, experimental demonstrations, the effects of climate change. We impacted over 164 community members in this activity

and we hope to participate and host more activities like this one. The ECD has partnered with "Arrecifes Pro Ciudad, Inc." a local, non-profit organization, monitoring water quality in the "Reserva Natural de la Isla Verde". We are currently working on analyzing all the data collected. This data analysis will elucidate more knowledge about the effects of temperature, pH, turbidity, conductivity, dissolved oxygen and salinity in the Coral Reefs at the reserve. The ECD is working on bringing more conferences. workshops and experimental demonstrations that shares our goals and objectives. Finally, all our activities are enacted to reach one final goal, give undergraduate students and the community the tools they need in order to execute and apply changes that have the potential to change the world.

ENVR 514

Cave soil abiotic factors as an indicator of cave ecosystems

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Characterizing the soil is essential for knowing the nutrients available and learn about the fertility, structure and chemical activity of the sampled site. Two caves were selected for this study, Cristales and Dos/Tres Pisos Cave, located in the Cabachuelas Nature Reserve in Morovis, PR. The soil abiotic factors are necessary to determine if the cave soil is a favorable ecosystem for the cave fauna. Samples were collected in the different regions of two caves (entrance, twilight and dark zones) and then processed in the laboratory. Abiotic factors such as the soil water content (moisture), nutritional content (organic matter), acidity (pH) and mineral content has a major influence in the cave ecosystem. For the collected cave soil samples; i) the pH was measured for each sample using the EPA Method 9045D, ii) the moisture was measured by drving the soil sample, iii) the organic matter was measured by loss on ignition method and iv) the mineral content of the soil samples was determined by FTIR spectroscopy and Munsell color value analysis. Results are then analysis to verify if the caves are a favorable soil ecosystem. A favorable soil ecosystem is determined by a range of pH (4.8-7.5), moisture (30% -80%) and nutritional content (>40%). The acidity for both caves, in all regions, are favorable. On the other hand, for the majority of the regions, the moisture and nutritional content were below the necessary to be a favorable ecosystem. The mineral signature (i.e. clays, calcites, etc.) for each cave is completely different even though they are in the same geological formation. This study can help us quantify the likeliness of which caves or regions of caves are needed to be preserved in the Cabachuelas Cave system that is increasing in human impact due to an increment in tourist and educational activities.

ENVR 515

Characterization of pore structure of activated carbon manufactured from coffee waste

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Activated carbon is the most widely used material to adsorb dissolved contaminants in water and wastewater treatment. Activated carbon has a very strong affinity for a wide range of dissolved organic contaminants, including both hydrophobic and hydrophilic molecules. For this reason, activated carbon is utilized for the adsorption of dissolved organic contaminants from drinking water sources. The effectiveness of activated carbon as an adsorbent derives from its extremely large surface area per unit mass. Activated carbon pores are classified by their sizes as micropores, mesopores, and macropores. In the present study, activated carbon was manufactured from spent coffee grounds using three different chemical agents including H₃PO₄, NaOH, and ZnCl₂. The pore structures of activated carbon were then examined by scanning electron microscopy (SEM) in Marshall University, WV. Figure 1 and 2 show the SEM image of activated carbon manufactured with H₃PO₄ at two magnifications. The sizes of activated carbon pores were calculated using an open source image processing program, ImageJ. The image processing results showed that most pores of the manufactured activated carbon were macropores.



Figure 1. A SEM image (x30) of the manufactured activated carbon from coffee waste grounds via chemical activation using H_3PO_4 .



Figure 2. A SEM image (x4000) of the manufactured activated carbon from coffee waste grounds via chemical activation using H₃PO₄.

ENVR 516

Optical properties and nanotoxicology of fluorescent CdS quantum dots

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Semiconductor nanomaterials like cadmium sulfide have interesting applications, consequent to their sizedependent optical properties. This compound is used as a pigment in papers, paint and it can also be found in solar cells. Due to the great use of these nanoparticles in society, there is a great concern in the scientific community about the potential toxicity of these nanomaterials in aquatic environments. According to this main problem, we have a theoretical assumption that the CdS particles in the nanoscale are more toxic than those in macroscale and in a greater concentration means greater toxicity. To verify its toxicity in the aguatic environment, first, we need to make sure the nanoparticles are soluble in water. Based in the mentioned before, the objectives of this research were: (i) synthesize cadmium sulfide quantum dots in the aqueous phase in presence of biocompatible molecules like L-Glutathione and N-Acetyl-L-cysteine, (ii) characterize the quantum dots optically, structurally and morphologically, (iii) evaluate the toxicity of cadmium sulfide in biological systems. Energy dispersive x-ray spectroscopy evidenced the chemical composition of produced nanostructures. The results we obtained of the CdS nanoparticles showed that the main absorption peak was at ~396 nm, this was observed in the emission spectrum and the photoluminescence spectrum which demonstrates a higher intensity with the cadmium sulfide

N-acetyl-L-cysteine covered, with the main peak at ~550 nm. For the morphology and the size, we used samples of CdS N-acetyl-L-cysteine covered and there were carried out by high-resolution transmission electron microscopy (HR-TEM). In this way, nanoparticles were spherical and with a size around 3 nm. Previously, the presence of L-glutathione or N-acetyl-L-cysteine on the quantum dots surface was verified by Infrared spectroscopy. Therefore, the results evidence that the CDS covered with N-acetyl-L-cysteine had a negative interaction in marine organism at higher concentrations than 1000 ppm at 48 hours of contact with the nanoparticles. We concluded that the higher the concentration, the greater the toxicity. This studies of the toxicity in different life stages of biological systems will be of great impact to evaluate the physiologic development of marine organisms in the presence of nanomaterials.

ENVR 517

Effects of metal-containing SBA-15 materials on the aqueous photodegradation of acetaprimid

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Neonicotinoid compounds are an important family of insecticides which have attracted recent global attention in terms of environmental concerns due to their largescale applications. Photodegradation is a relevant approach in pesticide degradation in the environment, also related to one of the most important aspects of pesticides persistence in the environment. In this work, studies on neonicotinoids photodegradation/photostability modulation by the addition of metal-containing mesoporous materials have been attempted. The aqueous photodegradation dynamics of acetamiprid, investigated under ultraviolet light irradiation using Cu and Ag-SBA-15 materials, can be described with first order kinetics equation. The addition of the metal-containing mesoporous materials was found to extend the half-life of acetamiprid photodegradation in aqueous solutions.

ENVR 518

Fabrication of a composite nanostructured cellulose membrane for direct contact membrane distillation

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Over 2 billion people live in countries experiencing high water stress (UN, 2018) and water crisis has become one of the biggest challenges for the world. Current techniques desalination necessitate complex infrastructure and high operating pressures, making them impractical in poor and technologically underdeveloped regions. Membrane distillation (MD) is an emerging water purification technique capable of purifying highly saline or contaminated water, which can help to alleviate water stress especially for the off-grid community. It is a thermally driven separation process employing a porous hydrophobic membrane which allows the passage of vapor molecules only. Currently used polymeric membranes in water filtration techniques have a large carbon footprint which makes it imperative to find an environmental and sustainable solution without compromising performance. In this study, a composite porous nanostructured cellulose based membrane was fabricated using carboxymethylated fibers (obtained from wood and non-wood plants like jute). The top barrier layer in this composite membrane is hydrophobic which prevents liquid penetration followed by a hydrophilic layer. The carboxymethylated cellulose fibers were cross-linked with wet strength additives to improve wet-integrity and water retention properties. The hydrophobic layer was developed by introducing micro-scale roughness using minerals like precipitated calcium carbonate followed by sizing with alkyl ketene dimer giving high contact angle exceeding 140° to prevent wetting of the membrane. The porosity of the entire membrane is in the range of 70-80%. Different characterization techniques like infra-red spectroscopy, solid state NMR, scanning electron microscopy, thermo-gravimetric analysis, and contact angle were used to study membrane properties. The performance of composite membrane was evaluated using a laboratory scale direct contact membrane distillation (DCMD) system. Water flux and salt rejection were tested under a set of feed water temperatures ranging between 40-60°C keeping the permeate water temperature same at 20°C. Moreover, the performance of the fabricated cellulosic membrane was compared to that of commercial hydrophobic PTFE membrane.

ENVR 519

Exploring how to test the presence of bisphenol A (BPA) in various plastic water bottles through different analytical techniques

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Bisphenol A, or BPA, is a well-known chemical that has been used in the wide scale production of certain polycarbonate plastics since the early 1950's. Among other problems with plastics, BPA has been found to be toxic to the human body. Through the course, Instrumental Analysis at Texas Woman's University, chemistry students are exploring testing the possibility of leaching of Bisphenol A (BPA) through several analytical techniques. The goal of the research is to learn the history of plastics, understand the problem with plastic use in food and beverage, as well as the environmental impact. Possible solutions for this major problem will be underlined and the students can contribute to those solutions. BPA in plastic water bottles has been analyzed using UV-Vis spectroscopy, Raman spectroscopy, thermogravimetric analysis (TGA), and high-performance liquid chromatography (HPLC). These techniques allow for the sensitive detection the leaching of BPA from the water bottles. Through this research-based class, students are able to apply learned analytical techniques to help solve a real-world problem.

ENVR 520

Use of isothermal titration calorimetry and molecular docking to study cavity formation and desolvation effects in the binding of organic cations to organic matter

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The increasing ubiquity of charged organic contaminants in environmental systems has elevated the need for the development of predictive sorption models. Previous work from our group indicated that molecular docking models provide an efficient means to predict binding mechanisms and affinities in organic cationic contaminant/organic matter systems. To further improve these models, energy contributions from cavity formation and secondary interactions with explicit water molecules upon binding should be considered. Isothermal titration calorimetry is commonly used to study the thermodynamics of solvent rearrangement upon drug-protein binding in drug discovery. The tool was adapted herein to an environmental system to quantify the underlying thermodynamics (Δ H, Δ S, and Δ G) of solvent cavity formation in systems of Pahokee Peat and Benzylamine derivatives. Resulting isotherms were reproducible, but enthalpies of binding were too low to be detected by the instrument (K_D << M⁻¹ - Malvern) for tertiary and quaternary amines indicating sorption of these compounds is largely entropically or partition driven. The entropy-enthalpy trend from the primary amine systems indicated sorption of larger, more hydrophobic compounds is more entropically favored while sorption of smaller compounds with polar moieties is more enthalpically-driven. This data was paired with molecular

docking outputs of organic cation/organic matter systems using explicit molecules. The outputs confirmed partitioning of tertiary and quaternary amines into hydrophobic pockets and primary amines with additional hydrogen donors or acceptors were able to participate in weak hydrogen bond interactions with neighboring water molecules. The primary entropy-enthalpy trend may provide insight to the relative number of hydrogen bonds that must be disrupted upon cation binding. Previous reports of analytical and computational studies place the penalty of losing a neutral hydrogen bond in the range of 0.34-1.72 kcal/mol. The relative differences in enthalpies of these primary amines could be reflecting the relative energetic penalties with increasing water hydrogen bond breakage. The results indicated that incorporating energy contributions from hydration effects with explicit water molecules in molecular docking approaches could serve to improve binding prediction.

ENVR 521

Identification and bio-reactivity of chemical components of indoor dust and aerosol in palliative care clinic

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People are consistently exposed to different concentrations of biological and non-biological particles. Aerosol and dust are currently understudied, despite their potentially significant role as a cause of infectious and allergenic adverse health effects. This is especially true for indoor dust and aerosol as people spend majority (~90%) of their lifetime in indoors. Indoor air quality in palliative care is important as the center optimizes quality of life by anticipating, preventing, and treating suffering when "curative" therapies are futile. Indoor air quality is affected by resuspension/deposition of hospital dust with their aerodynamic size or/and particle type, and further influenced by different activities (e.g., cleaning). In this work, the MTT Assay was used to determine the cell proliferation rate and the reduction in cell viability of the collected fine particulate matter/dust samples. Reactive oxygen species was quantified by fluorogenic probes for measuring generalized oxidative stress in cells. Energydispersive X-ray spectroscopy (EDX) was applied for elemental analysis and chemical characterization of the samples. Bacteria and mold suspended in air (bioaerosol) and deposited on surface (dust) were identified and compared in order to deduce the location characteristics. Further chemical analysis was performed to identify chemical components by using gas chromatographymass spectrometry and thermal gravimetric analysis. Bioassays such as acute toxicity and estrogenicity were used to distinguish the differences in the present/absent of disinfectant and the sample characteristics at different locations.

ENVR 522

Ionic liquid - MOF composite materials for VOC capture from polluted air

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The unique properties of ionic liquids (ILs), such as excellent affinity and sorption capabilities towards volatile organic compounds (VOCs), negligible vapor pressure, and chemical and thermal stabilities, make them promising candidates for targeting VOCs in polluted air. However, their relatively high viscosity and low air partition coefficients limit their direct application. Confining ILs into metal organic frameworks (MOFs) can overcome these drawbacks and presents an innovative alternative to support ionic liquids for efficient VOC capture. Here we synthesize a series of novel composite materials by cladding [BMIM][FeCl₄] ionic liquid into porous structures of MIL-101(Cr) through a postimpregnation method. The results showed that the ionic liquid was successfully confined into MIL-101(Cr) for a favorable VOC capture without damaging framework structure. The optimized composite materials exhibited much higher toluene sorption capacity than commercial activated carbons (AC) and AC fibers by 40-90%, Y-Zeolite by 4 times and pristine MIL-101 (Cr) by 3 times, especially at lower toluene concentrations ($P/P_0 < 0.1$ at 20°C). Sorption kinetics of toluene was also improved in the presence of ionic liquid, leading to 3.5 times higher sorption rates and toluene diffusion coefficients compared to pristine MIL-101 (Cr). This work demonstrates great potential of IL-MOF composites for VOC treatment.

ENVR 523

Quantification of trihalomethanes produced during chlorination of synthetic saline waters

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Chlorination of natural waters containing organic matter can produce chloroform, bromodichloromethane,

dibromochloromethane, and bromoform (collectively, trihalomethanes, THMs). THMs are monitored and regulated in municipal drinking water systems due to their potential health risks, which include bladder cancer and birth defects. Chlorination of saltwater swimming pools or ballast waters in seafaring ships also generate THMs. High bromide levels in these waters promote the formation of brominating agents (e.g., HOBr) during chlorination, which may increase production of brominated THMs. Chloride, despite its common classification as a "spectator ion", can contribute to increased rates of both chlorination and bromination by enhancing the formation of reactive halogenating agents such as Cl₂ and BrCl. The significance of this effect is not well established under saline conditions. The purpose of this investigation is to examine the effects of chloride ion concentration on THM formation at ionic strength and bromide concentrations comparable to seawater. Reactions are were conducted at pH 7 with fixed concentrations of bromide and an organic precursor (Suwannee River NOM extract or resorcinol). Chloride levels were varied while maintaining a constant ionic strength. Reactors spiked with free chlorine (as NaOCI) were held at 20.0 °C in a water bath and were sacrificed at fixed intervals. Free halogen residuals were quenched by the addition of excess 1,3,5-trimethoxybenzene. The quenched, aqueous solutions were extracted into methyl tert-butyl ether prior to analysis by gas chromatography coupled to a micro-electron capture detector. Typically, the most abundant THM formed was bromoform, followed by dibromochloromethane, chloroform and dichlorobromomethane. High ionic strength promoted volatilization of THMs from the aqueous phase, reinforcing the need to perform reactions in the absence of headspace. Choice of organic precursor strongly influenced overall THM yields but varying the chloride concentration (at fixed ionic strength) did not appreciably influence THM yields or speciation from NOM or resorcinol. This suggests that changes in halogenating agent speciation (resulting from changes in chloride ion concentration) do not substantially affect THM production in these systems.

ENVR 524

Selective adsorption and separation of dyes by dialdehyde cellulose and cationic dialdehyde cellulose

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In this study, bamboo-achieved cellulose is functionalized and upcycled into efficient bioadsorbents for dye adsorption and separation. Dialdehyde cellulose (DAC) was prepared through the chemical oxidation on cellulose surface via sodium periodate. Then, cationic Girard's reagent T was covalently crosslinked onto the backbone of cellulose molecules to form the cationic aldehyde

cellulose (cDAC). The chemical structure and morphology of two bioadsorbents were characterized. The adsorption behaviors of the functionalized DAC and cDAC to anionic Congo red (CR) and cationic Bismarck brown Y (BBY) were investigated systematically. The results showed that DAC could adsorb BBY more effectively while cDAC has a much higher adsorption capacity towards CR, this is due to the adsorption was dominated by both the static electric force and the chemical reaction between dyes and adsorbents. The adsorption process was found to follow the pseudo-second-order model. Both DAC and cDAC could maintain a high adsorption capacity under a wide pH range. Furthermore, the adsorption performance of six different dyes onto DAC and cDAC were studied, separately. Their adsorption capacities varied significantly on CR, BBY, Brilliant cresyl blue, Acid green 25, Acid brown M and Alizarin red S, and exhibited strong abilities for separating dye mixtures.

ENVR 525

Bromination of halosalicylates: Kinetics and product characterization

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In the presence of free chlorine, bromide can be oxidized to form free bromine species. Free chlorine and free bromine can react with natural organic matter to form chlorinated and brominated disinfection byproducts (DBPs). This process is common in aqueous systems such as drinking water and wastewater, in which free chlorine is used as a disinfectant. Many DBPs pose hazards to the environment and human health, with brominated DBPs generally found to be more genotoxic and carcinogenic than their chlorinated counterparts. Salicylic acid (SA) is a model DBP precursor capable of generating chlorinated and brominated products on timescales relevant to drinking water and wastewater treatment. In the presence of free chlorine and free bromine, SA can form four monohalogenated products, which can then react further with free chlorine/bromine to form dihalogenated salicylates and additional uncharacterized products. The purpose of this project is to identify the effect of chloride concentration and pH on bromination rates of monohalo- and dihalosalicylates, as well as to characterize the associated reaction products. Batch kinetic experiments were performed to assess reaction rates. Time course samples were analyzed by reversed-phase high-performance liquid chromatography (HPLC). Unknown products were characterized by gas chromatography-mass spectrometry (GC-MS) and liquid chromatography-mass spectrometry (LC-MS). The results show an increase in pseudo-first-order rate constants as chloride concentration increases at $pH \le 7$. These findings implicate BrCl as an active brominating agent in these systems. These results also suggest that chloride can potentially catalyze DBP formation when bromide-containing waters are disinfected with free chlorine.

ENVR 526

Stability of pharmaceuticals and personal care products in agricultural samples: Case study investigating effect of shipping and long-term storage on concentrations

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The necessity for the improvement of food security and access to clean water is a global demand, primarily in arid regions facing impacts of climate change. Because of this, alternative techniques which reuse waste products for the conservation of precious resources while simultaneously improving farming techniques have become an important topic. Wastewater irrigation and biosolid amended soils are two common practices which decrease the demand for fresh water and minimize nutrient deposition in surface waters respectively. In addition to providing a sink for waste products of treatment facilities, these reuse systems also decrease costs associated with the production of bulk synthetic fertilizers while also minimizing use of clean water for crop irrigation. However, one consequence of these nutrient reuse systems is the introduction of new contaminants into food sources. Previous studies have investigated uptake of organic contaminants in crop tissue due to pesticide application, showing that crops can accumulate as well as metabolize organic contaminants. Because of these findings, studies investigating waste reuse systems have also investigated crop uptake of pharmaceuticals and personal care products (PPCPs), which are abundant in wastewater and biosolids. Stability of PPCPs vary in different matrices and environmental conditions, thus, sample shipment from field to the laboratory as well as storage associated with these studies should be investigated for potential degradation of analytes prior to extraction. A study analyzing PPCPs in carrot, lettuce, soil, and water samples was completed over one week and one month time increments to evaluate analyte loss. Results from this study suggest that some targeted analytes are lost prior to sample analysis using liquid chromatography with tandem mass spectrometry (LC/MS/MS) after 1 week. These findings highlight the importance of spiking isotopically labelled standards for quantification before sample storage, to compensate and correct for degradation of analytes in order to obtain more accurate quantification of PPCPs in agricultural samples.

ENVR 527

Investigation of functionalized metal-organic framework/polybenzimidazole mixed-matrix membrane for gas separation

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Metal-organic framework (MOF) is a common material used as filler in polymer membranes. Such composite membranes, known as mixed matrix membranes (MMMs) perform better than neat membranes in gas separation applications. Functionalization of MOFs is an important method to improve the fabrication of MMMs. Functional groups enhance the gas separation and interaction between MOF and polymer surface to avoid the formation of defects. For instance, NH2-UiO-66/PIM-1 composite showed interfacial adhesion due to H-bonding interaction at the polymer surface. In this work, we used UiO-66, amino-, and nitro-modified variants to investigate the effect of functional groups between Zr-MOFs and polybenzimidazole (PBI), and we determined 10 wt % MOF loading in the polymer in order to avoid sedimentation agglomeration and of particles. Furthermore, XRD characterization was used to determine the crystallinity of the MOF structure; EDS mapping images were used to investigate the dispersion of particles in the matrix; SEM images showed the level of interaction between filler and polymer; TGA analysis indicated the structural stability and the decomposition of the composites; finally, gas permeation test demonstrate the gas transport properties and selectivity of the membranes.



ENVR 528

Biofuels and slow release fertilizers for sustainable farm & food production waste management

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As the human population continues to grow, the need to develop new sustainable approaches to meet rising global food and energy demands, while minimizing the adverse impact on the environment, presents a major challenge. One promising solution is to utilize agricultural and food waste as renewable energy sources by converting waste biomass into more usable forms of energy. Previous studies have demonstrated that pyrolysis and hydrothermal carbonization (HTC) may be used to convert biomass into solid biochars and hydrochars, respectively. The highly structured biochars represent ideal candidates for use as soil amendments, and hydrochars exhibit the properties of a potential slowrelease fertilizer. However, neither material alone represents a perfect energy source. The goal of this study was to generate a new thermochemical conversion pathway by combining HTC and pyrolysis to produce an improved hybrid fuel source that retains the beneficial properties of both biochar and hydrochar. This new pathway used the co-pyrolysis of HTC cow manure and raw agricultural feedstocks to produce biochar and bio-oil. Thermogravimetric analysis was conducted to evaluate the thermal stability of the biochar and raw biomass. Inorganic nutrient bioavailability and organic extraction experiments were performed to assess the biochar's potential to control nutrient losses to the soil. In addition, surface area analysis was used to determine the structural properties of the biochar and evaluate its potential as a soil amendment.

ENVR 529

Speciation, quantification, and release of arsenic bound to titanium dioxide (TiO₂, anatase) drinking water filter waste: Case study from the field to molecular scale

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Titanium dioxide (TiO₂, anatase) is used to remove contaminants such as arsenic from drinking water supplies. The TiO₂ solid phase becomes enriched with

arsenic as it removes arsenic from the water. Often, the source of arsenic is geogenic in nature, but it still causes problems for humans and the environments that are exposed to it. Adverse health effects due to arsenic consumption in humans can include kidney disease, cardiovascular problems, and several types of cancer. This research aims to identify and quantify arsenic speciation mobility from TiO₂ particles from field samples used to remove arsenic from drinking water. The field samples were obtained from the Bagaces area of Guanacaste, Costa Rica, where geogenic arsenic concentrations in aqueduct waters has been found at levels ranging from 31-80 ppb, and there is an estimated exposure of up to 12,000 people. During the dry season, high winds in this region also produce a risk of dust inhalation from these arsenic enriched TiO₂ sediments and soils, where the filter product was distributed in the environment. Results presented here include solid phase characterization and wet chemical analysis of arsenic -enriched TiO₂ water filter waste products using several determine speciation of arsenic. methods to quantification, and evaluation of its mobility and bioavailability. In addition, water retention curves from affected soils will be presented. Initial results from X-ray absorption near edge structure (XANES) spectroscopy indicate arsenic is present in the pentavalent (5+) oxidations state, which is the less mobile phase. Samples with the highest arsenic concentrations contained up to 600 ppm arsenic in the filter waste. There was a high correlation between arsenic and titanium (>0.96). In addition, TiO₂-enriched worm castings contained up to 530 ppm arsenic, indicating a possible biotic pathway for arsenic into soil organisms.

ENVR 530

Carbon isotopic insights into processing of marine organic matter and transfer to sea spray aerosols

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The content and speciation of organic matter in sea spray aerosols (SSA) affects climatically relevant properties of these aerosols such as hygroscopicity, reflectivity, and cloud seeding ability. A mesocosm phytoplankton bloom experiment was conducted to assess the effects of biological activity on processing of marine organic matter and transfer of this material into the aerosol during SSA formation. In this study, carbon isotopic compositions (d¹³C) of marine organic matter and size-segregated SSA were measured to elucidate changes in organic speciation during ocean-aerosol transfer and evaluate how organic speciation varies for submicron and supermicron SSA sizes. These measurements shed light on the timescales and extent of marine organic matter processing as well as transfer of these compounds into SSA of various sizes.

ENVR 531

Dominance of unintentionally produced PCBs in the air of China

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Polychlorinated biphenyls (PCBs) were not widely manufactured or used in China before they became the subject of international bans on production. Recent work has shown they have reached China associated with imported wastes, and that there are considerable unintentional sources of PCBs that have only recently been identified. As such, it was hypothesized that the source inventory and profile of PCBs may be different or unique in China, compared to countries where they were widely used and which have been widely studied. For the first time in this study we therefore undertook a complete analysis of all 209 PCB congeners and assess the contribution of unintentionally-produced PCBs (UP-PCBs) in the atmosphere of China, using polyurethane foam passive air samplers (PUF-PAS) deployed across a wide range of Chinese locations. \sum_{209} PCBs ranged from 9 to 6800 pg/m³ (median: 95 pg/m³) during three deployments in 2016-2017. PCB 11 was one of the most detected congeners, contributing $33\pm19\%$ to Σ_{209} PCBs. The main sources to airborne PCBs in China were estimated and ranked as pigment/painting (34%), metallurgical industry/combustion (31%), e-waste (23%) and petrochemical/plastic industry (6%). For typical Aroclor-PCBs, e-waste sources dominated (>50%). Results from our study indicate that UP-PCBs have become the controlling source in the atmosphere of China and an effective control strategy is urgently needed to mitigate emissions from multiple industrial sources.

ENVR 532

Evaluating phenyltrimethylammonium as a probe compound for quantifying heterocyclic amine cation exchange to soils

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Fate of contaminants, such as veterinary antibiotics, pesticides, and pharmaceuticals, depends on the extent of sorption to environmental solids. Recently, we advanced a predictive model for organic cation sorption that uses as a mechanism-specific probe

(phenyltrimethylammonium (PTMA), that offers a combined measure of both site abundance and a baseline driving force for sorption via cation exchange) and structural scaling factors derived from literature; we showed that PTMA was an effective probe for non-heterocyclic amine sorption. This work is focused on heterocyclic amines, important substructures of several pharmaceuticals. We explore the sorption of several heterocyclic amines, such as 1,2,3,4- and 5,6,7,8-tetrahydroisoquinoline, onto 30 well-characterized soils and evaluate whether our PTMA-based model can be used to also predict the sorption of heterocyclic amine cations.

ENVR 533

Efficiency of polyhydroxyalkanoate (PHA) production from wastewater sludge

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Nowadays, over 6,300 million tons of fossil-fuel plastic has been generated, with only 9% of it being recycled and 79% ending in landfills. Plastic persistence in the environment is causing serious environmental problem such as white pollution, entering the food chain and threatening the life of animals and plants. As the demand of plastic production keeps increasing, expected to be 12,000 million tons by 2050, there is a need to promote alternative materials for biodegradable plastic production. This project aims to develop a new process to produce bioplastic from the biopolymer polyhydroxyalkanoate (PHA) using activated sludge from wastewater. This process is expected to decrease the production cost to compete with the fossil-fuel based plastic in the market and to promote a better waste management using green technologies. Polyhydroxyalkanoate (PHA) is a candidate of alternative of non-degradable, traditional plastic. It has similar properties as fossil-fuel based plastic but also has capacity to completely biodegrade in the environment condition. In this project, PHA is synthesized by endogenous microorganisms found in wastewater activated sludge. In order to enrich the PHA accumulating in the microorganisms, the sludge is cycled through anaerobic (volatile fatty acids, VFA, generation) and aerobic (PHA accumulation) conditions. Different than the industrial PHA production, which is cultured and recovery from pure culture strains (i.e. Azohydromonas lata), our research is using a mixed culture from activated sludge containing various VFA producers and PHA accumulators. The efficiency of PHA production is being evaluated with changing operational parameters such as pH, temperature, retention time absorbent and bacterial community. The produced PHA will be analyzed for the chemical, mechanical and thermal properties using gas chromatography - flame ionization detector (GC-FID) for VFA and PHA concentrations, thermogravimetric analysis
(TGA) to evaluate the PHA thermal properties, and nuclear magnetic resonance (NMR) to identify the PHA main functional groups which affect the main properties of the bioplastic, and it will be compared with PHA produced by the pure culture *A. lata.* This study is expected to enhance the PHA production by using waste and estimate the properties of mixture culture produced PHA.

ENVR 534

Seasonal distribution of heavy metals in *Lemna minor* from a natural wetland

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Heavy metals are considered main sources of pollution in the environment. The analysis of macrophytes and sediment samples helps in evaluating pollution status in aquatic environment. In this study, accumulation of Pb, Cu, Cd, Mn, Fe, Ni and Cd in water, sediments and an aquatic plant species. Lemna minor, were investigated in a water stream located in a natural wetland in the northern part of Puerto Rico. Seasonal distribution of these heavy metals was performed to evaluate for possible contamination due to anthropogenic activity and pollution from nearby industries affecting its aquatic ecosystem. Aquatic macrophytes, like Lemna minor, act as good biofilters by accumulating heavy metals from the surrounding environment and hence aid as indicators of heavy metal contamination in aquatic ecosystems. Levels of the previously mentioned metals were evaluated in all four seasons. Treatment of samples included the use of acid digestion methods. For checking the accuracy, reference materials were subject to the same treatment that the samples and are included in the overall analytical process. The quantification of metals was performed by using a Flame Atomic Absorption Spectrometer. The concentrations of heavy metals in the three studied compartments showed a general trend as the following: sediment>plant>water. The concentrations of heavy metals in the sediment samples were in the order of Fe>Mn>Ni>Cu>Pb>Cd. The order of metal levels in Lemna minor tissue plants was Fe>Mn>Cu>Ni>Pb>Cd. Manganese (Mn) and Lead (Pb) levels are within the toxic critical level. Mn exhibited high BCF value in Lemna minor plant. The concentrations of heavy metals in the water were found in the following samples order: Fe>Mn>Cu>Pb>Ni>Cd. Bioconcentration factor (BCF) were recorded: 2.62-4.44 and 0.48-0.98, respectively for Mn and Pb. The aquatic macrophyte Lemna minor acts as an imperative plant for pollution remediation.

ENVR 535

Impact of surface oxidation on black carbon aerosols

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Black carbon (BC) particles are released into the atmosphere by combustion processes (e.g. burning wood), leading to poor air quality and unknown effects on climate. These particles are of concern due to their small size and heterogeneity caused by emissions from various sources and ignition processes, which complicates the study of their environmental impact. In addition, previous research has shown that BC contributes to droplet formation in clouds and can form cloud condensation nuclei (CCN), or small particles that water vapors condense on. Although BC particles are modeled to be hydrophobic and insoluble, the impact of hydrophilic functional groups (e.g. -COOH) on the surface has not been widely studied. In this study, the surface chemistry of BC particles was modified using different oxidation methods to impart hydrophilic functional groups. The surface chemistry of the particles was examined using Xray photoelectron spectroscopy (XPS), while the comparison of the particle size in solution and the particle size when aerosolized was determined using dynamic light scattering (DLS) and scanning mobility particle sizing (SMPS), respectively. Additionally, the role of surface functionalities on the particles in relation to the hygroscopicity parameter (k) for BC was investigated. Overall, this study provides insight on how the heterogeneity of BC is important to understand because the slightest surface chemistry modification can have a measurable impact on climate effects.

ENVR 536

Electrospinning of graphene and graphene oxide polymer composite membranes for water remediation

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Graphene and graphene oxide polymer composite membranes have been shown to effectively remediate wastewater streams. These types of membranes are

favorable for their good filtration and for their antimicrobial properties. This study involved the assembly of novel graphene and graphene oxide membranes into nonwoven fiber mats using electrospinning techniques. Geological studies were conducted to choose the polymer concentrations most likely to succeed in producing suitable fibers by electrospinning. Once electrospun produced, the morphological, membranes were mechanical, thermal, and hydrophilic properties were determined using various analytical and spectroscopic techniques such as SEM, XRD, FTIR, and Raman. The antimicrobial properties were tested against sewer sludge and cyanobacteria. The properties of electrospun membranes were compared to cast membranes using the same polymer composites. Once characterized, the electrospun membranes were challenged by a suite of simulants to investigate membrane performance for water treatment.

ENVR 537

Quantification of estrogenic compounds by SPE-GC-MS in New Jersey natural and wastewater sources

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Estrogens are known endocrine-disrupting agents which have emerged as a class of pollutants that pose danger to aquatic organisms at low concentrations. Among their negative impacts on aquatic life is their effect on reproductive behavior, which can ultimately move up trophic levels of the ecosystem resulting in a compounding environmental effect. Estrogenic compounds detected in wastewater effluents and surface water at nanogram to picogram per liter concentrations estrone (E1), 17β -estradiol include (E2), 17αethinylestradiol (EE2), and estriol (E3). Despite their known risks, concentrations in the Northeastern United States have remained largely unknown. We have developed and validated an SPE-GC-MS method for the quantification of these estrogenic compounds in the Whippany River and Loantaka Brook (NJ, USA). Estrogens extracted from water samples via SPE are subsequently derivatized using BSFTA + 2% TMCS and successfully separated and quantified at ppb levels using this GC-MS method.

ENVR 538

Absorption of estrogenic pollutants onto microfiltration membranes

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Estrogenic pollutants, like 17α -Ethinylestradiol (EE2), a compound with high endocrine-disrupting potency and high resistance to biodegradation in the aqueous environment, attracts increasing concern in the past decade. As a consequence, the elimination of EE2 is becoming a hot topic in recent researches. In this work, adsorption of EE2 was comparatively assessed on four types of microfiltration membranes at different pH, salinity, methanol content and concentrations of EE2 in feed solutions. Adsorption experiments performed in aqueous solution at different pH values showed that adsorption of EE2 by nylon membrane drops drastically along with the dissociation of EE2 with pH increasing from 9 to 11. Series of experiments on salinity (1.75-35g/L NaCl) effect were also performed at constant pH value, and the results indicated that adsorption of EE2 on nylon membrane increased with increasing salinity. Then, simulated brackish water prepared from a sequence of diluted seawater was employed to study the adsorption of EE2 in brackish water. The results matched with those in previous salinity effect study. Presence of methanol in feed solution significantly reduced nylon membrane adsorption of EE2.

ENVR 539

Strategies for the photoreduction of Tc-99 pertechnetate to low valent Tc by Keggin polyoxometalates

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Technetium-99 (⁹⁹Tc) is a high yield (~6%) product of Uranium-235 fission and is a weak beta emitter (b_{max} energy of 0.29 MeV) with a half-life of 2.1×10^5 years. When exposed to air, ⁹⁹Tc is most prevalent in its oxidized (Tc(VII)) form, which exists predominantly as pertechnetate (TcO4⁻). The immobilization of ⁹⁹Tc in the

environment has usually been achieved via reduction of the prevalent TcO_{4^-} anion to relatively insoluble TcO_2 , Tc(IV) species. We have been studying the use of small metal-oxide clusters called Keggin polyoxometalates (POMs), $XM_{12}O_{40}^{n-}$ (X= P, Si, Al, n=3, 4, 5) to act as both reducing agent and chelator for ⁹⁹Tc to lower valent species. The reduction potentials of Keggin POMs are a function of the central heteroatom that dictates the overall charge of the ion and its reduction potential. Under UV and visible light in acidic conditions they promote reduction of TcO_{4^-} to Tc(IV) in the form of $TcO_{2}\bullet 2H_2O$ and $Tc_2(\mu-O)_2$ ⁴⁺ species. The examination of Keggin POMs to photocatalytically reduce TcO_4^- will lead to investigation of solid-state materials for photocatalytic reduction of TcO_4^- .

ENVR 540

Novel TA acid-metal complex coating layer for forward osmosis membrane with enhanced antifouling property

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A novel tannic acid-metal complex coating layer was added on a commercially available cellulose triacetate (CTA) forward osmosis (FO) membrane. The coating process is facial and fast and can be finished in about only 90 seconds. Characterizations such as fourier-transform infrared spectroscopy (FTIR) and x-ray photoelectron spectroscopy (XPS) were used to confirm the successful deposition of the coating layer onto the membrane. The water permeability of the coated membrane was almost the same as that of the pure FO membrane since the water resistance of the coating layer is very small. When using NaCl solution and DI water as the draw and feed solutions, respectively, the water flux of the coated membrane in FO was the same with the pure FO membrane. In our 12-hour fouling test, the relative water flux (the ratio of the final water flux to the initial water flux) for the membrane without coating decreased from 1 to about 0.4. For our membrane with coating layer on the supporting layer side, the relative water flux was higher than 0.5 after the test meaning that our coated membrane has an enhanced antifouling property. Therefore, we provide a potential coating method to solve the common trade-off problem between water flux and antifouling property in osmotic pressure driven membrane processes.

ENVR 541

Chlorine-free disinfection of water contaminated with *E. coli* by combination of electrolysis, ultrasonic and photochemical treatment: Role of hydroxyl radical formation and generation of singlet oxygen

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Deionized water, highly contaminated with E. coli was treated using a non-chloride electrolyte solution such as sodium sulfate by pumping it through an electrochemical cell at low current (from 0.2 to 0.4 A) and initial voltage demand of 15-40 volts (close circulating system). The influence of additional water treatment with ultrasound (20 kHz) applied during electrolysis was evaluated together with effect of simultaneous generation of singlet oxygen during irradiation of polymer-based active photolayers containing insoluble in water form of fluorescent dyes. We have determined that hydroxyl radicals are the reactive species responsible for the sanitizing effect of the electrolytic treatment. It was shown that designed photolayers can be successfully used for disinfection of contaminated water through generation of singlet oxygen by their irradiation with visible light of low intensity. We have found the experimental conditions that provide the most effective combinations of singlet oxygen generation and generation of hydroxyl radicals through chlorine-free electrolytic processes and through ultrasonic treatment, superior to each applied individually.

ENVR 542

Dissolved organic matter percolated from periphyton in the Everglades: Characterization and interaction with mercury

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When organic matters of various kinds decompose partially, dissolved or soluble organic matters can form. The organic matters are usually produced from plants, soil, bacteria, algae, and living organisms. The wetland of Everglades is rich in dissolved organic matters. The quantity and quality of these dissolved organic matters have significant impact on environmental factors such as biogeochemical activity, transport, absorption, complexation, and more specifically the speciation and geochemical cycling of toxic metals such as mercury (Hg). Everglades wetland is abundant in periphyton which can also be responsible for dissolved organic matter

percolation and production. The DOM from periphyton, in particular when freshly produced and released into the water, would have a profound effect on mercury species present in the water, e.g., by forming mercury-DOM complexes. This experiment is designed to perform quantitative and qualitative analysis of DOM produced by periphyton and the complexation of mercury with the produced DOM from periphyton in molecular level. In addition to organic carbon analysis, the samples will be analyzed for optical properties by using a spectrofluorometer for information on the sources, types, and reactivity of DOM. Studies will be done with addition of inorganic and methyl mercury of different concentrations in leached DOM samples from different types of periphyton by observing fluorescence quenching for Hg-DOM complexation using 3D Excitation Emission Matrices Fluorescence Spectroscopy. Water samples from different types of periphyton will be differentiated by measuring different functional groups of DOM; such as total protein, carbohydrates, and thiols; including Chlorophyll-a and nutrients quantitatively using some standard protocols. Measurement of specific types of DOM from periphyton quantitatively will be performed by observing periphyton biomass response for interaction with mercury using Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy. The project will improve the understanding of the relation between DOM and periphyton and the environmental processes of Hg impacted by periphyton in the Florida Everglades.

ENVR 543

Coral's response to climate change: Characterization of coral's metabolome under varied pH conditions

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Ecosystems around the planet are facing increasing amounts of stress due to climate change caused by anthropogenic activities. Coral reefs are one of the most vulnerable ecosystems and are diminishing rapidly due to declining pH coupled with increasing sea surface temperature. To better understand the changes occurring in reef building corals, metabolomics can be employed as a tool to assess how the physiological state of the corals is affected by their surrounding environment. Coral samples (Porites rus) were collected near a hydrothermal vent in the Pacific Ocean off the coast of the island of Maug at low (7.94 ± 0.051) , mid (7.98 ± 0.027) and background (8.04 ± 0.016) pH sites. Twenty total P. Rus samples were analyzed. Metabolites were extracted from freeze dried coral tissue using a solvent system of chloroform/methanol/water and polar metabolites were

isolated for analysis by ¹H NMR. Metabolic profiles across the experimental samples were all metabolically similar (PCA Analysis). However, univariate analysis (ANOVA) identified specific metabolite differences between sites. Fourteen metabolites were annotated in the *P. rus* metabolic profile. While there have been previous studies that have analyzed the coral metabolome and demonstrated the effectiveness of ¹H NMR as a tool, this is one of the first studies examining how the metabolome of the coral responds to ocean acidification with the utilization ¹H NMR.

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Phosphate removal by lanthanum-containing materials: Effect of alkalinity and pH on treatment effectiveness

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Build-up of phosphorus, an important nutrient, in environmental waters can lead to diminished water quality. Orthophosphate (PO₄) is the most bioavailable source of phosphorus and is a key target for remediation efforts. Trivalent lanthanum (La) is known to effectively bind PO₄. At least one commercial La-containing product has been developed and evaluated for PO₄ removal in field settings. However, few studies used controlled experiments to examine the impact of background water matrix constituents, such as alkalinity and pH, on the performance of these materials. This study aimed to evaluate the impact of pH and dissolved inorganic carbon (DIC) on (1) the effectiveness of two La-containing materials, La₂(CO₃)₃ and La-modified bentonite, on PO₄ removal and (2) La leaching into water. Batch experiments were conducted at pH 6 and 8 and with DIC additions of 0, 12, and 60 mg/L as C. Aqueous concentrations of PO₄ and La were measured over time until equilibrium was reached. Equilibrium-model and experimental results revealed that PO₄ removal did not measurably vary at the tested pH and DIC treatments. However, the removal kinetics for La2(CO3)3 were pHdependent. At pH 8, the reaction was slower, regardless of DIC, 250% more time to reach 80% removal. Additionally, equilibrium-model and experimental results revealed that La leaching decreased with increasing DIC. Overall, increased DIC did not measurably impact PO₄ removal and decreased La leaching, while increasing pH led to slower PO₄ removal and increased La leaching such that La levels in filtrate were above 4 ug/L La, the level at which ecotoxicological concerns arise.

Use of gadolinium to track sewage effluent through the Poughkeepsie, New York water system

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Over the decades, there has been an increase in micropollutants in waterways around the world. Many pollutants are released into the environment from wastewater treatment plants. Current facilities are incapable of removing many of these chemical contaminants. As a result, these chemicals are released into the environment where they can accumulate. Several methods have been developed for the detection of wastewater including bacterial analysis, nutrient analysis, chloride analysis, and the direct detection of pollutants. There are, however, several flaws with these methods. An alternative method involves the use of gadolinium, a rare earth metal used primarily as contrast dye in MRI procedures. This study investigated the usefulness of gadolinium as a method of detection compared to Enterococci and chloride analysis. Samples were taken from four locations located over a six-mile stretch of the Hudson River near Poughkeepsie, NY; a sewage treatment plant, a water quality monitoring station, and the intake and effluent from a water treatment plant. Sampling occurred during June and July 2019. Enterococci analysis was conducted using the IDEXX Enterolert system. Chloride content was determined using the Mohr titration method. Lastly, gadolinium was analyzed using Inductively Coupled Plasma Mass Spectrometry. Enterococci analysis consistently demonstrated high values in wastewater and very low values in the water treatment plant effluent. However, the bacteria levels in open water locations were inconsistent between location and sample day. Chloride concentrations consistently decreased from the wastewater treatment plant to the monitoring station and the water treatment plant intake. However, chloride content appeared to increase after water treatment likely due to the decomposition of sodium hypochlorite. Gadolinium analysis showed a content averaging approximately 500 ng/L in the sewage treatment plant effluent, followed by a drastic decrease due to dilution at the monitoring station and water treatment plant intake, averaging 15 and 29 ng/L respectively, and a final decrease during the water treatment process to an average of 5 ng/L. When compared to chloride analysis, gadolinium appears to be comparable in effectiveness. With a single anthropogenic source and a low analysis cost, gadolinium has the potential to replace other methods for tracing wastewater in waterways.

ENVR 546

Wildfires give rise to conditions encouraging disinfection byproduct formation

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Wildfires serve an essential role in forested ecosystems by influencing nitrogen cycling, creating bio-reactive charcoal, and thinning accumulated fuel loads. However, surface water quality is also impacted by an increased transport of natural organic matter (NOM), most notably organic carbon and organic nitrogen, via overland runoff. The acuteness to water quality is largely attributed to the heating duration and temperature terrestrial NOM is exposed to during a wildfire. Although much of the carbon rich detritus in the O-horizon is mineralized during a burn event, A-horizon NOM experiences an increase in solubility due to heat induced physiochemical changes. The increase in NOM solubility not only effects a stream's ecological functions, but also creates complications for downstream communities that rely on burned watersheds for water resources. Disinfection byproducts (DBPs) are harmful halogenated compounds formed through reactions between NOM and chlorine during the disinfection phase of water treatment. Past research has found that formation potential (FP) of regulated carbonaceous DBPs (C-DBPs) and unregulated nitrogenous (N-DBPs) decreases and increases, respectively, with increasing burn severity. Moreover, our early results have found that five C-DBPs (CHCl₃, CHCL₂Br, DCAA, TCAA, 1,1,1-TCP) and two N-DBPs (DCAN, TCAN) exhibit higher FP at moderate burn temperatures (250-350 °C) in a controlled laboratory setting. These results suggest that communities affected by wildfires could experience a heightened risk of exposure to C/N-DBPs; most notably to unregulated and highly toxic N-DBPs. As wildfire intensity and severity continues to rise as a result of climate change, there is impetus to understand wildfire's continual effects on drinking water resources. Therefore, this project attempts to further our understanding of C/N-DBP FP as a function of burn temperature. Soils were collected from a variety of areas throughout Colorado's Front Range and heated in a muffle furnace to simulate wildfire burning. The heattreated soils were leached into water and chlorinated to simulate the disinfection phase of water treatment. FP of Sixteen C-DBPs and four N-DBPs was measured with gas chromatography and electron capture detection (GC-ECD). Additionally, the hydrophobic and transphilic fractions of heat-treated NOM were isolated through high performance liquid chromatography, chlorinated, and had C/N-DBP FP measured with GC-ECD.

High performance of honeycomb-supported natural soda ash in the removal of hydrogen chloride gas

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On the basis of a recent IEA world energy outlook, the world primary energy consumption in 2040 will be about 1.5 times that of 2014, and most of the increase is expected to be covered by fossil fuels, such as oil, coal and natural gas. It is thus likely that the development of clean carbon technologies which target zero emission is important. As is well known, a coal-based integrated gasification combined cycle (IGCC) system can achieve higher power generation efficiency compared to conventional pulverized coal-fired power plants; thus, the use of IGCC is expected to contribute to a reduction in CO₂ emission. However, raw fuel gas formed in coal gasification contains hydrogen chloride (HCI) at dozens to hundreds of ppm, which would corrode the gas turbine materials in the IGCC. Many researches on the removal of HCI have thus been carried out, and the method can be classified into cold gas cleaning and hot gas cleanup. Although the former method is well established, it is likely that the advancement of processes for the hot gas cleanup is extremely important for further improving the efficiency of the IGCC system. In this study, we examined the HCI absorption performance of cheap natural soda ash loaded on a honeycomb support as a hot gas cleanup method. The honeycomb-supported soda ash drastically improved the HCl absorption extent at the 1-ppm breakthrough time compared to the result without the support; thus, the use of the support was justified. The HCI removal performance of the honeycomb-supported soda ash depended significantly on temperature (573-873 K). Under the present conditions, the absorption extent at 1-ppm breakthrough time was maximized at 773 K. This absorption extent increased as the HCI concentration in the supplied gas decreased, and it was assumed that this absorbent was suited to actual coal gasification processes. No change in the HCI absorption extent (60-65 %) was observed for Na₂CO₃ loading between 33 and 65 mass%.

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Determination of glyphosate, glufosinate and their metabolites concentrations in surface water along the Red River, northern Vietnam

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Herbicide residues represent environmental threats including water contamination. There is a need to improve analytical methods for assessing the spread and the impacts of aquaculture herbicides residues in surface water. In this study, we developed a method to simultaneously quantify concentrations of glyphosate (GLYP), glufosinate (GLUF) as well as their main metabolites aminomethyl phosphonic acid (AMPA) and 3-(methylphosphinico)-propionic acid (MPPA) in natural waters. For this purpose, we use ultra-high-performance liquid chromatography coupled to tandem mass spectrometry (UPLC-MS/MS). These compounds were analyzed directly - without derivation steps - by cation exchange chromatography (Dionex ionPAC CS12A IC column) combined with tandem mass spectrometry compatible with isocratic mobile phase including water, acetonitrile and formic acid. Detection was through negative electrospray ionization with multiple reactionmonitoring mode. Solid-liquid extraction with a Chelex 100 sorbent was used for purification. Resulting recovery rates in spiked samples vary between 75 and 120%. The limits of quantifications at the optimum conditions for glyphosate and other herbicides in five different water matrices (pure, natural river, tap, estuary, and marine waters) range between 0.3 and 5.6 μ g/L. The method was applied successfully to water samples collected during dry (February and March) and wet (June and July) seasons in the Red River (northern Vietnam). More herbicide residues were found in water samples collected during wet season than dry one. The highest concentrations reported are 8.21 ± 1.81, 4.09 ± 0.70, 5.83 ± 1.34 and 1.46 ± 0.26 mg/L for AMPA, GLYP, MPPA and GLUF respectively, with higher concentrations in the Red River passing through the Delta region. To our knowledge, this is the first quantification of GLYP, AMPA, GLUF and MPPA concentrations along the Red River, with high performance of pre-concentration and analysis steps without derivation. Further work will be to look at the interactions between herbicides and colloids.

Analysis of short, medium and long-chain PFAS in municipal wastewater effluents and environmental matrices

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Per- and poly-fluoroalkyl substances (PFAS) are produced since the 1950's and are known to be environmentally persistent, toxic, bioaccumulative and are widely distributed in the environment. PFAS are persistent in environmental matrices due to their higher stability, resistance to thermal or biological breakdown and their high water-solubility. Soils and municipal biosolids may not only contain PFCs, but also a variety of chemical precursors that transform into PFAS over time. Due to the potential human health risks, the US-Environmental Protection Agency (EPA) has recently issued a drinking water advisory limit of 70ng/L for perfluoro-octanoic acid (PFOA) and perfluoro-octane sulfonic acid (PFOS). Additionally, EPA has set residential soil screening guidance values for PFOA and PFOS at 16 mg/kg and 6 mg/kg, respectively (US-EPA 2009). There is a need to develop robust analytical methods and extraction procedures for all the PFAS in different environmental matrices. A quantitative method for the determination of PFAS was developed using liquid chromatography (UPLC) tandem mass spectrometry (MS/MS) and applied to environmental matrices. Solidphase extraction method detection limits ranged from 0.57 – 1.5 ng/L with quantitation limits ranging from 1.7 – 25 ng/L. Method accuracy ranged from 70 - 130% with a relative standard deviation of <15% for all of the PFAS. This study evaluates the presence of short-chain (PFPrA- C_3 , PFBA- C_4 , PFPeA- C_5), medium-chain (PFHxA- C_6 , PFHeA-C7, PFOA-C8), long-chain (PFNA-C9, PFDA-C10, PFUDA-C₁₁, PFDDA-C₁₂, PFTrDA-C₁₃, PFTeDA-C₁₄, PFHxDA-C₁₅, PFODA-C₁₈) and sulfonic (PFBS-CS₄, PFHxSA-CS₆, PFOS-CS₈) PFAS in municipal wastewater effluents, municipal biosolids, groundwater, soil, and surface water. Several different extraction methods were tested for the analysis of municipal biosolid samples. The recovery efficiencies of PFAS from biosolids ranged from 65 - 150% with an RSD of <15%. Compared to other reported studies, this method has advantages as it employs a single chromatographic separation with a shorter runtime (8 min) while maintaining high accuracy, stability and the separation of the PFAS.

ENVR 550

Developing software to connect aerodynamic and microscopic measurements on soot particles

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Soot, a pollutant from incomplete combustion of fossil fuels and biomass burning, has a highly complex morphology as aggregates of primary spheres that are 10-50 nm in diameter and made of elemental carbon (EC). Soot particles absorb the solar radiation efficiently and can significantly increase the total radiative forcing by retaining the incoming solar energy. There are currently two major research communities to determine the morphological characteristics of soot. One based their measurements on aerosol aerodynamics and the other uses primarily electron microscopes. The connection between the results from the two communities are not direct and the data transformation is often not trivial. Therefore, new python-based software is developed to address such need in soot research. Our software offers customizable input options to allow various source data input, including measurement conditions and mobility diameters from instruments based on aerosol aerodynamics. Using the user input, the software generates a three-dimensional image of a sample soot particle based on the fractal theory and a Monte Carlo process. Our software can also analyze the twodimensional projection of the generated soot particle, therefore linking the aerodynamic results with the microscopic images. The product offers soot researchers a convenient way to interpret and communicate their research results using different scientific approaches.

ENVR 551

Aqueous bromate reduction by NZVI supported monometallic catalysts

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Water contamination with bromate is a serious environmental issue due to its carcinogenic nature. Aqueous bromate can form during the ozonation in the presence of bromide in a water treatment system. Filtration, biological degradation, adsorption, and electrochemical treatment are widely used technologies to remove the bromate in an aqueous environment. However, these technologies have drawbacks such as the generation of secondary byproducts including sludge, low efficiency, and high cost. Catalytic bromate reduction can be an effective alternative method to reduce aqueous

bromate to less harmful bromide. The removal efficiency, cost, recyclability of the catalyst heavily depend on the selection of proper materials. Nanoscale zero-valent iron (NZVI) is a cost-efficient and abundant material and thereby, was selected for the catalytic reduction of bromate. Metal loading on the surface of the support (NZVI) can increase the reactivity further. Therefore, several combinations of NZVI-supported catalysts (Sn, Cu, Ni, In, Zn, Pd on NZVI) were synthesized and tested in a batch reactor for the reactivity of bromate reduction by finding out the most efficient materials for the catalvst. All catalysts demonstrated complete removal of bromate to bromide. However, the Sn/NZVI catalyst demonstrated the fastest removal (0.47 min⁻¹) among other catalysts (0.13 min⁻¹ for Cu/NZVI and 0.40 min⁻¹ for Zn/NZVI, for example). The removal efficiency was in the order of Sn>Zn>Cu>Ni>In. SEM-EDX characterization study of Pd/NZVI revealed a uniform distribution of metal doping on the catalyst's surface. The results show that Sn/NZVI is a cost-effective and sustainable solution to treat the water and wastewater contaminated with bromate.

ENVR 552

Solar induced emulsification of petroleum in neat films and films on water

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The impact of sunlight on crude oil emulsification ability was evaluated following exposure to simulated sunlight for up to 48 hours. The oils chosen for analysis included Deep water horizon oil (Macondo well), surrogate from a nearby well, and heavy fuel oil (NIST 2717a). The selected oil types ranged from light-sweet to heavy sour crude oil. Emulsification capabilities were analyzed for sunlight exposed neat petroleum, petroleum over pure water, and petroleum over sea water via a bottle test. Irradiated samples were compared to both a dark control and a heated (50°C) neat control. Although each oil behaved differently, qualitative measures revealed that emulsion stability was positively correlated with exposure time for all oils. The time-dependent emulsion stability varied between oils, and for some oils, observable emulsification was generated with as little as one hour of simulated sunlight. Studies in which oil volume was varied over a fixed surface area elucidated a concentration dependence of emulsion stability such that smaller oil volumes produced greater emulsification capacity. Upon comparison of oil over sea water irradiations to oil over pure water exposures, it was demonstrated that sea water had an inhibitory effect on photogenerated emulsification ability. These results indicate that sunlight, in combination with factors such as irradiation time, oil type, oil thickness, and water type, is important in the emulsification of crude oil as observed in marine environments. Since emulsions impact the fate, transport, bioavailability and toxicity of spilled oil, a deeper understanding of the factors impacting crude oil emulsification is imperative.

ENVR 553

Characterization of polar compounds released in urban runoff from three formulations of sealcoat

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Sealcoat is a commercial coating product applied to parking lots and driveways to protect against surface weathering. Numerous studies conducted over the past 15 years have shown that sealcoat containing coal-tar pitch is a potent aquatic toxin and a major source of polycyclic aromatic hydrocarbons (PAHs) to urban streams. Three formulations of sealcoat products are in use: those containing coal-tar (CT) pitch, those containing steam-cracked petroleum (SCP) residue, and those containing petroleum asphalt (PA). In this study, we examined the composition of runoff from asphalt disks treated with three brands of petroleum asphalt (PA) sealant during a 20-day field experiment. The acidic, neutral, and basic constituents in sealcoat runoff were selectively isolated using strong-anion and strong-cation solid-phase extraction cartridges. Preliminary results show that the isolated compounds are additives such as pre-polymers, surfactants, and other unregulated compounds. Given heightened interest in protecting scarce water supplies, the implications of finding these compounds in surface runoff are considered.

ENVR 554

Pesticides concentrations in the atmosphere of an urban area in Brazil: Risk assessment for human health

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In the last few years, different types of pesticides have been detected in the atmosphere in rural and urban areas around the world. These are chemical compounds used in agriculture to avoid plague, rodents, fungi and unwanted plants. Besides that, they are often used in public health to kill vectors of disease, such as mosquitoes. Some studies have showed the relations between pesticides exposure and some diseases, such as autoimmune and cardiovascular diseases, and respiratory problems. An attempt to investigate the composition of PM in the neighbor atmosphere of an industrial complex has been proposed in the last years due to the high rate of thyroid diseases in the population living near this region. In this work was determined the

concentrations of pesticides in samples collected between 2015. 2016 and 2017 at an industrial and urban area. The assessment of the risk caused by inhalation of these compounds was calculated. Samples (n=42) were extracted and 11 pesticides were determined by gas chromatography coupled to a mass spectrometer. Samples collected in 2017 showed the higher concentrations. Pesticides such as malathion and permethrin, used in the control of domestic pests, presented the highest concentrations (537 pg m⁻³ and 625 pg m⁻³ respectively) due to the wide use in this area. The highest values of daily inhalation exposure were for heptachlor in infants, 2 x 10⁻⁴ mg kg⁻¹ day⁻¹. All values of the hazard quotients are lower than 1.0 indicating that there is no danger to human health by inhalation. Cancer risk was found for heptachlor in adults, infants and children in the three years.



Average concentrations of pesticides found in 2015, 2016 and 2017

ENVR 555

Characterization of soil carbon in native prairies and prairie restorations

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Soil organic carbon (SOC) can be defined as the fraction of soil carbon composed of plants, animals and microbial deposits at various stages of decomposition. Soil organic carbon is a significant carbon pool in the environment. Carbon is dynamic in the environment and readily changes oxidation states as it transitions through living, atmospheric, and soil systems. Increases of atmospheric carbon dioxide have raised concerns regarding global warming. A potential method to reduce atmospheric carbon dioxide is to sequester it as SOC. Restoration of farmland to prairie conditions in the Midwestern U.S.A. is ongoing by both private agencies and state governments. The restoration of land to near-native conditions should increase SOC content by sequestering atmospheric carbon. Soils of native prairies, restored prairie and analogous conventionally farmed lands were extensively

sampled. The samples were analyzed for SOC content and humic acid (HA) content. The HA was spectroscopically analyzed to determine structural characteristics. The SOC analysis indicated more carbon is retained in the native prairies and restored prairies than analogous conventionally tilled soils. Differences in SOC between prairie restorations and conventionally tilled soils were not always significant. The HA content of the native prairies was significantly greater than the prairie restorations and the conventionally tilled soils. The HA from native prairies, prairie restorations and the controls showed similar functional moieties in the 13C-NMR and IR spectra. The major differences observed in the 13C-NMR and IR spectra was peak intensity but not peak position. These results indicate that prairie restoration may be beneficial in reducing atmospheric carbon dioxide by allowing the soil to act as a carbon sink.

ENVR 556

Simultaneous removal of radioactive Cs^+ and Sr^{2+} ions from wastewater by facile solid-state alkaliactivation of montmorillonite

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Despite the fact that the nuclear power industry has been greatly developed at present, the nuclear power plant is considered a danger due to a large amount of radioactive material leaked from the nuclear accidents such as in Fukushima. In particular, radionuclides such as cesium-137 and strontium-90 were the most damaging in the Fukushima accident, since they have long half-lives (30 years) and emit strong gamma rays. In order to minimize the volume of these radionuclides generated in large quantities, it is necessary to develop a practical adsorbent able to selectively remove for both. For the synthesis of the effective adsorbent for both cesium and strontium ions, we demonstrate an effective modification of montmorillonite (MT) using solid-state NaOH thermal treatment at 300°C. Through this facile activation by desilication, porosity was enhanced and abundant surface functional groups for ion-exchange were generated. It was possible to optimize the adsorption performance of the activated montmorillonite (NaMT) by adjusting the mass ratio of NaOH (unity to MT). The adsorption mechanism analysis from XRD and XPS studies showed that cesium ions were mainly exchanged with intercalated cations in MT, and strontium ions were adsorbed on the surface functionalities (Si-O-Na⁺). As a result, the enlarged BET surface area (117 m²) and functional groups enabled adsorption of strontium (capacity of 185 mg/g, pristine MT: 16 mg/g), and cesium adsorption capacity was also increased (137 to 291 mg/g). In addition, NaMT exhibited the simultaneous

removal of cesium and strontium ions, and selective removal of them under groundwater conditions where competing cations exist, such as sodium, potassium, and calcium. Furthermore, it showed stability under a wide range of pHs (3-11) and following irradiation of gammaray (at 6 Gy/h for 30 min). This improvement removal performance of adsorbent synthesized from cost-effective montmorillonite has increased the applicability to realistic conditions.

ENVR 557

Impact of shale gas extraction and other anthropogenic activities on surface water quality

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The land adjacent to the Beaver Run Reservoir in Westmoreland County, Southwestern Pennsylvania, currently has seven unconventional natural gas drilling pads comprised of 47 Marcellus shale gas wells and four Utica shale gas wells. The majority of these pads sit within 1000 ft of a man-made reservoir that provides municipal water to over 130,000 customers of the Municipal Authority of Westmoreland County (MAWC). Since May 2011, our group has been collecting and analyzing quarterly water samples from watersheds upstream of and in the reservoir to assess the impact that natural gas extraction and other anthropogenic activities may have on surface water quality. Field data and lab results from eight years of study are presented, including total dissolved solids (TDS), alkalinity, anionic salt components, and metals.

ENVR 558

Surface proclivity and interaction of emerging contaminants at the lipid monolayer membrane

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Recent years have seen a rise in detection of pharmaceutical compounds and personal care products (PPCPs) within the aquatic environment. PPCPs generally enter the water systems via human and animal excretion as well as through industrial and agricultural processes. While they are detected in trace levels, over a long period of time these emerging contaminants (ECs) can have adverse effects on fish population and human health. However, limited information is available with respect to the interaction of these ECs can have with

biological and other environmental surfaces. In particular, the interaction between ECs with lipid membranes is of interest since aqueous-lipid interface is a common feature to living organisms. In this study, we have explored the effect of different ECs on model lipid membranes made of zwitterionic 1, 2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) monolayer at the air-water interface. Using Langmuir-Blodgett Trough (LBT), the surface pressure versus molecular area isotherms of DPPC in the absence and presence of varying EC concentrations have been measured. Interaction with the DPPC membrane was found for all ECs explored. While all of these contaminants displayed a concentration dependent destabilizing effect on the lipid monolayer, differences in the DPPC phase transition behavior was found to be dependent on the charge characteristics of the ECs. For instance, neutral ECs, including but not limited to, carbamazepine and β -estradiol, did not show modification of the DPPC phases, whereas charged species of amlodipine and triclosan led to significant deviation in DPPC phase domains. The complete set of LBT data, along with fluorescence study, mapping out the influence of ECs on DPPC phase behavior and the energetics of DPPC-EC interactions will be presented. It will be demonstrated that the interaction strength of ECs with biological membranes, and thereby their fate and transport in the aquatic medium, is dependent on the molecular identity of the contaminant. The study further shows the suitability of LBT method in generating surface pressure versus molecular area isotherms as a technique to detect and categorize EC-lipid membrane interactions.

ENVR 559

Poly(*N*-acryloylmorpholine)-grafted porous silica hybrid material for removal of organic dye from aqueous solution

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A new organic-inorganic hybrid material was fabricated by grafting poly(*N*-acryloyImorpholine) onto porous silica by free radical polymerization. The aim of this work is to prepare an adsorbent capable of efficiently removing organic dye from aqueous solution. The prepared poly(Nacryloylmorpholine)-grafted porous silica was characterized by Fourier Transform Infrared spectroscopic analysis, Elemental analysis, Scanning Electron Microscopy and Brunauer-Emmett-Teller analysis. FT-IR analysis confirmed grafting of organic polymer onto porous silica, while elemental analysis revealed the presence of nitrogen in the hybrid material due to grafting. Brunauer-Emmett-Teller analysis showed a decrease in the specific surface area that proved the introduction of polymer onto the silica surface. The performance of this hybrid material as adsorbent was

evaluated by removing methylene blue from aqueous solution. Effect of pH, adsorbent dosage, contact time, initial concentration of methylene blue were investigated to determine the maximum adsorption capacity. Adsorption isotherm studies were carried out to investigate the compatibility of the experimental data with mathematical models like Langmuir, Freundlich, Temkin and Dubinin-Radushkevich equation. Langmuir Isotherm showed an impressive maximum adsorption capacity of 270.27 mg/g. Adsorption kinetics revealed the mechanism involved in the removal of the dye by this hybrid material. This new organic-inorganic poly(Nacryloylmorpholine)-grafted porous silica could lead to a new way of eliminating organic pollutants from the environment.

ENVR 560

Quantifying and imaging of membrane fouling using Raman chemical imaging

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There is a wide range of application for Membrane based separation technologies such as wastewater treatment, water purification, food and beverage processing to pharmaceutical applications. In this study Raman chemical imaging was introduced as an easy, fast and nondestructive method that can be used to survey membrane fouling. This study focuses on imaging of fouled membranes with organic salts after membrane The distillation process. surface of the Polytetrafluoroethylene (PTFE) membrane was imaged by Raman chemical imaging before and after fouling and detailed information about concentration and location of three different salts (CaSO₄, BaSO₄ and CaCO₃) was achieved. Critical characteristics about distribution of the salts was established from Chemical images and it was observed that agglomerated CaSO4 was placed on specific areas of the membrane. On the other hand, BaSO₄ and CaCO₃ were distributed all over the membrane surface. Raman appears to be a powerful tool for mapping the membrane fouling which is major challenge in water treatment.

ENVR 561

Characterization and photoreactivity of chromophoric marine-dissolved organic matter

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Marine-dissolved organic matter (m-DOM) is a diverse assortment of compounds in seawater that includes proteins, fatty acids and aromatics that originate from microbiology and the decay of plant life. Although it has been studied for years, even with high resolution analysis, its composition still remains uncertain. Recently, the chromophoric component within m-DOM has been highlighted as a possible driver for photochemical reactions. When irradiated with solar light, chromophoric m-DOM at the sea surface layer can absorb photons between 280 and 500 nm. Once excited into a singlet state, there is rapid intersystem crossing into a lower energy triplet state which can then react with other organic species, facilitating photochemistry in the marine environment. In this study, bulk sea water has been collected from three bloom cycles in a months long experiment performed in a unique ocean-atmosphere facility at various times to better understand the temporal changes of bulk m-DOM in a marine bloom. The m-DOM was analyzed using heated electrospray ionization Orbitrap mass spectrometry, infrared spectroscopy, and excitation-emission matrix spectroscopy. In this study, we also compared the photoreactivity of m-DOM across a phytoplankton bloom.

ENVR 562

Determination of the equilibrium for 2-butanone with ice surfaces via static and dynamic experiments

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Methyl ethyl ketone (MEK), otherwise known as 2butanone has been found in low concentrations in snow and ice. Henry's law constants for MEK in liquid water have been determined, but its behavior over the surface of snow is unknown. Complicating these interactions, it has also been shown that the surface of snow and ice with impurities has a patchy coverage of liquid water. Two different experiments, static and dynamic, have been used in order to measure the equilibrium of MEK over artificial snow. For the static experiment, a closed system of snow with MEK is allowed to reach equilibrium and then headspace gas measurements are taken via gas chromatography - mass spectroscopy (GC-MS) over a range of temperatures from -30°C to +15°C. The concentration of MEK solutions were varied as well as the size of the artificial snow grains. In addition to the static experiment, a dynamic flow tube experiment is used in conjunction with mass spectroscopy in order to observe small ketones desorbing from ice surfaces. The equilibria observed by both methods will be quantified and compared.

ENVR 563

Biodiesel production from waste cooked oil based on microwave irradiation and SrO catalyst

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An optimized method in the transesterification of cooked oil to biodiesel based on microwave dielectric irradiation as a driving force for the transesterification reaction and SrO as a catalyst. This combination has demonstrated excellent catalytic activity and stability. The transesterification was carried out with and without stirring. According to H NMR spectroscopy and TLC results, this combination accelerates the reaction, maintaining a very high conversion and high efficiency. The optimum method decreases the cost of biodiesel production and has potential for industrial application in the transesterification of cooked oil to biodiesel that considered an energy efficient and environmentally friendly source.

ENVR 564

Switchable hydrophilicity solvents: Single-droplet studies of CO₂-mediated solvent extraction in an intensified flow reactor

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Most chemical processes are currently heavily dependent on harmful volatile solvents and energy-intensive distillation due to its ease of separation. Recently, switchable solvents have emerged as a promising energy-efficient (green) alternative for solvent recovery. Switchable solvents offer facile reversible tuning of the physiochemical properties of the solvent triggered by carbon dioxide (CO₂) under moderate conditions (i.e., room temperature and atmospheric pressure), In particular case of switchable hydrophilicity solvents (SHSs), SHS shows dramatic change in hydrophilicity in presence and absence of CO₂ and water, which provides a promising alternative green strategy to various fields including recycling of mixed plastic and extraction of algae oil. Despite intriguing characteristics of switchable solvents, the time- and labor-intensive nature of conventional flask-based screening methods have hindered the adoption of SHSs by chemical industries, due to the lack of comprehensive understanding of thermodynamic characteristics and separation efficiencies of CO₂-mediated SHSs. In this project, we developed and utilized a time- and material-efficient microfluidic approach for accelerated in situ studies of CO₂-mediated SHSs. The single-droplet microreactor utilizes a tubular membrane reactor which significantly increases the gas-liquid interfacial area for CO₂ injection into the SHS mixture, removing mass transfer limitation in conventional batch reactors. Utilizing the developed microfluidic platform, we studied in detail effects of molecular structure of SHSs and its concentration on efficiency and kinetics of SHS extraction under different process parameters such as CO₂ pressure and reaction time. The fundamental understanding and the intensified continuous flow reactor developed in this work will accelerate the development of distillation-free solvent removal and recovery strategies towards achieving a green and sustainable chemical processing.

ENVR 565

Partitioning of 1-pentanol and ethanol to artificial snow surfaces

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Small organic compounds such as alcohols have been detected in snow and in the gas phase above snow. The purpose of this experiment is to analyze how alcohols partition between the gas phase and snow surfaces. The two methods used were a static headspace gas experiment and a dynamic flow tube experiment. For the static method, gas chromatography-mass spectrometry (GC/MS) was used to quantify 1-pentanol vapor in the headspace gas over artificial snow and liquid solutions (-15.0°C to 15.0°C). The equilibrium of pentanol between the gas and snow surface varied with surface area and temperature. The pressure of 1-pentanol over artificial snow that had been doped with alcohol increased with temperature. For large snow grains, the average pressure increased as the temperature increased. For smaller snow grains, the average pressure decreased from -5.0°C to -2.0°C, possibly due to more liquid covering the snow surface. In the dynamic method, gaseous ethanol in air was flowed through artificial snow in a flow tube while the gas phase was monitored by mass spectrometry. After removing the gaseous ethanol flow, the decay of ethanol signal over time was monitored, similar to a bubble column Henry's Law experiment. Comparison of data from both methods will be discussed. Snow-atmosphere chemistry models can be improved by using empirical measurements of organic gas partitioning like the ones presented here.

Bactericidal activity and mechanism of pulsed blue LED light

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Hospital-acquired infections (HAI) cause mortality and morbidity in hospitals. Although frequent cleaning with disinfectants can effectively prevent the contact transmission of microorganisms, surface corrosion, microbial tolerance and potential harmful residues resulting from ordinary chemical disinfectants are main concern. Pulsed blue LED lights are recently reported with obvious bactericidal activity. This study works on the bactericidal activities and mechanism of two types of pulsed blue light-470nm and 405nm. Results show that pulsed 470nm and 405nm blue LED lights not only save energy but also effectively reduce the gram positive and negative bacteria, and also have excellent performance on MDROs. By measuring the sub-lethal rate, DNA and Protein leakage from the bacteria, it reveals that 405nm light can deconstruction of the bacteria membrane. Genotoxicity test explain the bactericidal mechanism of 470nm light which is destroy the structure of bacterial DNA.

ENVR 567

New technology for controlling biofilm formation in water distribution system

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Water quality is related to human health. Microbial contamination not only seriously threatens water system but also increase the water treatment coast. Microbial growth and biofilm formation in water distribution system are main concern. This work develops a new durable anticorrosion and anti-biofouling coating for water pipes and pumps. The new coating is composed of epoxy matrix and antimicrobial material (i.e., polymer-based colloidal suspension). Studies show that the new coating exhibits contact-killing and anti-adhesion activities to effectively prevent biofilm formation on different substrates including metal, ceramic, glass and plastics. The coated surface can maintain better than 2 log reduction (99 %) for both E. coli and P. aeruginosa and avoid surface colonization even in the presence of scaling and fouling agents. Accelerated ageing test result indicates the coating can be stably operated under flow rate of 5 m/s for 30 years. Moreover, the new coating also obviously decreases friction loss of water pipes, which benefits energy efficiency of water distribution system.

ENVR 568

Co-evolution of iron and phosphorous speciation during anaerobic digestion with inter-stage hydrothermal treatment of sewage sludge

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Anaerobic digestion (AD) with inter-stage hydrothermal (HT) treatment of sewage sludge (i.e. AD-HT-AD) is a promising technique for energy recovery and nutrient recovery/recycling. Both AD and HT treatments impose significant impacts on the reclamation/recycling of critical elements, such as iron (Fe) and phosphorus (P). However, the co-evolution of these elements and their transformation mechanisms during the combined AD-HT-AD treatment of sewage sludge is poorly understood. This study conducted AD (15 days) - HT (90, 125, 155 and 185 °C) - AD (73 days) and investigated Fe and P speciation in the raw sludge, AD solids, and HT-derived hydrochars using complementary chemical extraction, Xray absorption spectroscopy, and X-ray diffraction analyses. A significant fraction (41%) of Fe is present as vivianite in the digested solids from the first stage AD treatment of sewage sludge. After the inter-stage HT treatment of the digested solids, the fraction of vivianite in the HT-derived hydrochars decreased with increasing HT temperature and with the precipitation of more strengite. This is possibly due to the oxidation of vivianite by oxygen introduced from the headspace in the HT treatment reactors. After HT and in the subsequent AD treatment of HT-derived hydrochars, much more vivianite was formed. which can be attributed to the microbial reduction of strengite and other Fe(III) species. The results from this work suggest that Fe plays important roles in controlling P mineralogy during AD and HT treatments of sludges. This work also provides insights into the reaction mechanisms during AD-HT-AD treatments of sludges and can help evaluate the nutrient recycling and reclamation options for sludges.

Electron-ionization gas chromatographic analysis of environmentally relevant chlorinated phenols

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The fast (30 s) and practical derivatization of three chlorinated phenols: 2,4,6-trichlorophenol, triclosan and pentachlorophenol for their subsequent detection by El-GC-MS is presented. The protocol involves the use of the eco-friendly difluoromethylating agent diethyl (bromodi-fluoromethyl) phosphonate (DBDFP) and results in the efficient labeling of the phenols with the difluoromethyl (CF₂H) group. In addition, the protocol works at room temperature thus eliminating the need of heating as in more conventional methods (e.g. silylation with BSTFA).

ENVR 570

Enhanced reduction of doxycycline by sucrosemodified NZVI

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Pharmaceutical pollution of environment is closely related to the growth of drug consumption. It is proved that these pharmacologically active substances, even in trace amounts are expected to have a negative impact on human health. Doxycycline (DOX) is one of the widely used antibiotics for the treatment of human and animal diseases. The high concentration of DOX in drinkingwater can cause health issues such as drug-resistant microorganisms. There are several approaches to treat DOX in drinking water such as filtration, sedimentation, chlorination and degradation. In fact, the degradation of DOX is an effective technology that fully mineralizes into less harmful substances. Currently, NZVI has attracted considerable attention in removing organic and inorganic contaminants from wastewater and groundwater. It has large surface area and small particle size which can be a good technology for the removal of antibiotics from wastewater. Although it is highly reactive, it agglomerates in conventional systems that considered as its one of the main drawbacks. To overcome the agglomeration and oxidation of NZVI, this research work investigated the metal loading and modified methods of NZVI that can support or stabilize particles in the liquid phase during the synthesis process. In addition, it simultaneously improves its reactivity through reducing the particles and their reducing capacity. NZVI supported monometallic and

sucrose-modified NZVI catalyst were synthesized and used for the degradation of aqueous DOX. The sucrosemodified NZVI shows degradation with high rate constant 0.35 min⁻¹ compared to that of Cu/ZNVI and Sn/NZVI, 0.14 min⁻¹ and 0.16 min⁻¹, respectively. The results showed the complete degradation of DOX in 30 min by sucrose-modified NZVI. Conditions of batch experiments were at neutral pH, room temperature, and 10 mg/L of catalyst loading. According to the results the studies provide a potential remediation technology for doxycycline polluted groundwater and wastewater.

ENVR 571

Comparative laboratory studies of NO3 radicalinitiated oxidation of monoterpenes

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Secondary Organic Aerosol (SOA) formation from the NO3 radical-initiated oxidation of monoterpenes is studied using chamber and flow-tube experiments at the Reed Environmental Chamber (REC) and the University of California, Irvine (UCI). The NO3 radical plays an important role in the production of SOA and organonitrates from monoterpenes, however, differences in yields between monoterpenes are still poorly understood. SOA and organonitrate yields from α -pinene are typically low compared to the relatively high yields from other monoterpenes such as 3-carene, which is attributed to differentially preferred reaction pathways. Chamber studies at REC have observed substantial pinonaldehyde formation and low SOA yield from apinene + NO3. α -Thujene, the only naturally-occurring monoterpene with the secondary ring in the same position relative to the double bond as α -pinene, has also displayed a low SOA yield when oxidized by NO3, demonstrating the importance of the secondary ring position in relation to SOA vield. Additional studies to be carried out at REC and UCI will further analyze oxidation products using thermal desorption chemical ionization mass spectroscopy for particle-phase measurements, spectroscopy time-of-flight mass for gas-phase measurements, and thermal dissociation cavity ring-down spectroscopy for bulk organonitrate concentrations in both phases.

Interaction of small ketones with artificial snow surface

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Snow chemistry is important because of the impact chemical reactions in snow have on health and the environment. Two complementary experiments were designed to gain quantitative data on the surface-to-air equilibrium of 3-pentanone and acetone in artificial snow as a function of temperature. The data collected will be compared to Henry's Law constants for gas in equilibrium with aqueous solutions. In one experiment, a gas spectrometer chromatograph-mass (GC/MS) and headspace gas bottles were used to analyze the air over artificial snow made with 5.0 × 10⁻² M 3-pentanone in water while the temperature of the snow was regulated by a low-temperature thermostat (-30°C to 15°C). Two different sized snow grains were used. It was found that as temperature increased, the concentration in the gas phase also increased. Additionally, there is a greater concentration of 3-pentanone in the gas phase over snow compared to when the snow has melted. The main results from these static experiments is that there is equilibrium between gas and the surface, and the surface area of snow influences the equilibrium. A dynamic experiment was also developed to monitor the desorption of acetone from artificial snow over time at different air flow rates using a mass spectrometer. Both the static and dynamic experiments were conducted to quantify the equilibrium of ketones with snow surfaces and the results will be compared to between the two experiments.

ENVR 573

Investigating algae-derived reduced graphene oxide membranes for ionic and molecular nanofiltration

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Recent advances in nanomaterials-based membranes shows great promise in efficient filtration and purification of compounds. Selectivity and permeability issues arise in many industrial applications of membranes. Carbon derivatives such as graphene oxide and reduced graphene oxide (RGO) have received increasing attention due to their interesting properties and potential for enhancing the performances of the membranes for wastewater purification with reduced energy costs. In this work, algae derived RGO carbon nanostructures were synthesized with multiple steps: *Nannochloropsis Oculata* and *Tetraselmis* algae cells were cultured, harvested, and

treated with the template tetramethyloxysilane. After heat annealing at 500°C under nitrogen gas and vacuum and the removal of the resulting SiO₂ template with NaOH, the final product is the carbonized cells (cCells) in the RGO form, which is further suspended in aqueous solution. Experiments were performed at various RGO concentrations in fabricating the membranes by vacuum filtration and were conducted to determine and adjust the pore sizes and interlayer spacings of RGO in membranes. The resulting samples were characterized by TGA, XRD, SEM, TEM, XPS, FTIR, and Raman. The efficiency and the permeability of the membranes for filtration of urea and NaCl, the key ingredients in wastewater from urine, were measured by UV-visible, IR, and electric conductivity measurements. With earth-abundant, renewable and sustainable algae resource, our research holds great promise for large scale use of the membranes for water purification.

ENVR 574

Radiological and non-radiological leaching assessment of alkali-activated materials containing ground granulated blast furnace slag and phosphogypsum

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Alkali-activated materials (AAMs) based on ground blast furnace slag (GGBFS) granulated and phosphogypsum (PG) were investigated in order to quantify leaching of naturally occurring radionuclides (NOR) and inorganic non-radiological elements according to an up-flow percolation column test as described in CEN/TS 16637-3. Gamma spectroscopy and neutron activation analysis (NAA) were applied for radiological characterization, inductively coupled plasma optical emission spectrometry (ICP-OES) and ionchromatography (IC) for chemical characterization. Upon leaching, ²³⁸U, ²²⁶Ra, ²¹⁰Pb, and ²²⁸Ra were retained very well. Both for ²³²Th and ⁴⁰K, a decrease in activity concentration was observed due to leaching and their release was influenced by the use of different alkali activators, which was also the case for the leaching of non-radiological elements. Only a small amount of AI (0.5-0.8%). Ca (0.1-0.2%) and Si (0.1-0.3%) was mobilized. while highest release was observed for K (56-94%), Na (49-88%) and S (71-87%). At first glance, drinking water is not endangered by leaching of NOR following the requirements of the European Drinking Water Directive.

From the results for porosity, obtained with mercury intrusion porosimetry (MIP), it was concluded that both the porosity and formation of multiple leachable and nonleachable complexes are determining factors for the release of elements from AAMs.

ENVR 575

Improved resolution of inorganic anions and oxyhalides in the presence of ethylenediamine

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Ethylenediamine is sometimes added to drinking water samples as a preservative and can react with carbonate to produce artifacts that interfere with early eluting analytes such as fluoride. This method minimizes this interference by increasing the separation between fluoride and the EDA carbamate artifact, allowing better integration of the fluoride peak. In comparison to other methods, this one features unique selectivity and much higher column capacity to enable separation of fluoride from the EDA carbamate artifact as well as separation of carbonate and sulfate for better quantification of sulfate.

ENVR 576

Pefluorooctanesulfonate induces hepatomegaly and lipoatrophy in mice through phosphoenolpyruvate carboxykinase-mediated glyceroneogenesis inhibition

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Perfluorooctansulfonate (PFOS) as a persistent organic pollutant has attracted extensive attention for its lipid metabolism disrupting effects. Exposure to PFOS can cause hepatomegaly and lipoatrophy in BALB/c mice, indicating the disturbed triglyceride (TG) homeostasis in liver and white adipose tissue (WAT), albeit with unknown mechanisms. Considering that glyceroneogenesis is the essential pathway for balancing the TG cycle between WAT and liver, we speculate that PFOS act via glyceroneogenesis inhibition to alter TG metabolism in the two tissues. Combining gene expression, enzyme activity assay and molecular docking analysis, we report here that PFOS can interact with cytosolic phosphoenolpyruvate carboxykinase (PEPCK), the rate-limiting enzyme of glyceroneogenesis. Specifically, by repression on PEPCK, PFOS can inhibit the glyceroneogenesis process

and thus decrease the glyceroneogenesis-derived glycerol level, leading to the reduced re-esterified triglyceride level and causing atrophy in WAT. Moreover, in PFOS-exposed liver tissue, despite that free glycerol and fatty acid released from WAT were being used for triglyceride synthesis, the export of triglyceride was slowed down. This eventually resulted in the continuous lipolysis of WAT and lipid accumulation in the liver. PEPCK can be used as a key biomarker to assess the lipid metabolism disorders induced by other conventional and emerging per- and polyfluoroalkyl substances.



ENVR 577

Legacy phosphorus desorption from U.S. Mid-Atlantic agricultural soils

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Phosphorus (P) is an essential nutrient for all life forms and plays a vital role in a variety of fundamental reactions within organisms. Plants in particular need P for photosynthesis, nitrogen fixation, and seed development. Due to its key role in plant nutrition, in US Mid-Atlantic agricultural soils, P is applied to fields in the form of chicken manure and fertilizers. The repetitive addition of P leads to a buildup of the nutrient and results in soils with excessive levels of legacy P. Through leaching, erosion, and runoff, P makes its way into bodies of water where it may contribute to eutrophication. Eutrophication is caused by the over enrichment of nutrients, promoting algae growth whose decomposition leads to anoxic and hypoxic conditions that can cause fish kills. There are many different P species found within soil, each having differences in solubility and bond strength. By introducing soil taken from agricultural fields throughout the Mid-Atlantic region of the US to various extracting solutions,

we can, to an extent, mimic the ionic strength of soil pore water (KCI extractable), acid rain (HNO3 extractable), and ligand exchange mechanisms (0.1 mM SiO4 2extractable) to determine the rate at which P desorbs. By pairing the phosphorus desorption data with Mehlich-III extractable P, total P, and soil textural classification, we can begin to understand legacy phosphorus mobility in these soils. Additionally, we compared these bulk, wet chemical data with high resolution, micro X-ray fluorescence (µ-XRF) maps of the soil to determine P colocation with other elements of interest (Si, P, S, Al, Fe, Mn, Ca, and Mg). We then used micro X-ray absorption near edge structure (µ-XANES) spectra of P hotspots to help determine the solid phase P speciation at the micron scale. Comparison of the u-XRF maps with µ-XANES spectra show that the majority of P species probed in the soil are associated with Ca, potentially in the form of fluorapatite. Understanding the legacy P mobility and speciation in soils will help inform improved P management practices and reduce negative environmental impacts.

ENVR 578

NMR-lipidomics measurement of Great Lakes mussels as an ecotoxicological assessment of areas of concern

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The National Oceanic and Atmospheric Administration's long-established Mussel Watch Program (MWP) uses freshwater mussel, Dreissena spp, as a bioindicator species to track the impact of pollutants on coastal ecosystems in the Great Lakes. Recently, metabolomics analysis has been used to evaluate the physiological response of mussels inhabiting areas of concern. In these studies, metabolomic analyses were applied to the polar extracts of mussel. In an effort to understand the biochemical effect of pollution more broadly, an investigation was made into lipid changes using nuclear magnetic resonance (NMR). The objective of this study was to determine how the mussel lipid profile varies based on collection season, location and handling method (caged vs in situ). To represent the given parameters, six sets of ten mussels were collected from two different sites in Lake Michigan (n=60), north Milwaukee harbor (LM-04) and one reference site (LM-05). Collected mussels were lyophilized whole and in-shell, individually homogenized and extracted with chloroform/methanol/water. The lipid profile was measured by 1H NMR. Principle component analysis (PCA) of the NMR spectra found no distinguishable difference between site, time of collection or handling method, similar to the findings of a previous study at these sites assessing the polar metabolome. However, univariate analysis of the spectra revealed triacylglyceride, diacylglyceride, phosphatidylcholine, and phosphoenolamine glycerol protons, in addition to an unknown peak, varied between sampling sites and time of collection. These preliminary results suggest NMRbased lipidomics can provide lipid class information as an ecotoxicological tool to understanding health and help guide future targeted investigations into the biochemical impact of areas of concern.

ENVR 579

Photophysical characterization of phycocyanobilin to predict *in vivo* cyanobacteria health

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Monitoring cyanobacteria and cyanotoxins has become increasingly important in Michigan's Great Lakes. Cyanobacteria, also known as blue-green algae, produce hepatotoxic microcystins that are being found in natural waters and drinking water supplies, causing severe risk to ecosystems and human health. High exposure to microcystin causes acute liver failure and even low exposure can lead to tumorigenesis. Whole cell cyanobacteria are harmless to drinking water supplies as they are large enough to be removed by simple filtration. However, upon apoptosis, the cyanobacteria release intracellular microcystin that is more difficult to treat. Monitoring cyanobacteria health and predicting cell death is therefore imperative to most efficiently treat drinking water supplies. Herein, we report the photophysical characterization of phycocyanobilin, which is the component of a chromophoric cyanobacteria's phycobiliprotein involved in its photosystems. This characterization ex vivo will be correlated to intracellular fluorescence in vivo throughout the cyanobacteria's lifecycle to probe the ability of using phycocyanobilin fluorescence to predict apoptosis. Phycocyanobilin extraction from wild Great Lakes cyanobacteria, purification, and photophysical characterization will be discussed. Measurements of fluorescence properties of phycocyanobilin in whole cells are reported and these data are compared to ex vivo fluorescence data.

ENVR 580

Controlling the pore sizes of graphene oxide nanostructures through hydrothermal reactions for efficient water purification

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As human population continues to increase on earth and human exploration on Mars is occurring, there is an urgent need to pay much attention on the guality and the sustainability of the basic unit of life: water. Several technologies have been employed in the past to sustain the quality of water, including reverse osmosis, which is energy-intensive with current methods. In this work, we have synthesized 3-dimensional (3D) reduced graphene oxide (RGO) decorated with and without metal ions (Ni 2+ and Fe³⁺) and organic ligand dipotassium naphthalene-2,6 dicarboxylate, which can form metal-organic framework (MOF), for water filtration membranes. To synthesize the 3D-RGO nanomaterials, one-step hydrothermal reaction was used to control the pore sizes and interlayer spacings of RGO by varying temperatures, reaction times and pH levels. For 3D-RGO, the pH of GO suspension was adjusted to near neutral, then was transferred to an autoclave, reacted at 180-200°C for 6-12 hours, resulting 3D-RGO foam. Similarly, 3D-RGO-NiFe and 3D-RGO-NiFe-MOF nanomaterials were synthesized in the presence of Ni²⁺, Fe³⁺ and dipotassium naphthalene-2,6 dicarboxylate. The nanomaterials were used to prepare filtration membranes by vacuum filtration method. The membrane structures were analyzed by TGA, XRD, XPS, SEM, FTIR, etc. The filtrations for NaCl and NH₄NO₃ were carried out and the efficiency and the permeability of the membranes were evaluated by IR, UVvisible, and electric conductivity measurements. Our current work may lead to low-cost, highly efficient water filtration membranes for seawater desalination and wastewater purification.

ENVR 581

Determining the pH of frozen and annealed acetic acid and sodium chloride solutions using infrared spectroscopy

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The purpose of this experiment is to better improve chemical models of reactions that occur at the surfaces of snow and ice by determining the pH changes at the microscopic layer of liquid that forms on ice. Some reactions which occur at the interface of this liquid and the

atmosphere alter the composition of the atmosphere and are acid-catalyzed. The change in pH upon freezing was measured by mixing solutions of water and acetic acid which were frozen and monitored by infrared spectroscopy. The temperature was varied between -20 and -6 degrees Celsius and spectra were taken at the different temperatures. The pH was then determined by comparing the ratios of absorbance between the acetic acid and its conjugate base acetate. The experiment was repeated with the addition of sodium chloride (0.5 M) to see if the addition of a solute would change the observed trends. The salt only caused the solution with a room temperature pH equal to the pK_a of acetic acid, 4.7 to decrease in acidity upon freezing and return to the room temperature pH as more of the solution became liquid. The added salt did not change the acidity of the solution with a room temperature pH of around 3.7. Solutions were also frozen top-down, as compared to bottom-up freezing that occurred in all other trials. Top-down freezing caused acetic acid solutions to start at a slightly more acidic level and gravitate above the room temperature pH as the temperature increased. Solutions with artificial sea salt were compared to the solutions with sodium chloride.

ENVR 582

Estimation of community drug use by detection and quantification of pharmaceuticals in wastewater using SPE and LC-MS/MS

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Pharmaceuticals are a significant group of micropollutants that, over time, has expanded to include substances of abuse. In Tennessee, from 2013 to 2016, all drug overdose deaths increased from 17.8 per 100,000 to 24.6 per 100,000 citizens. Sewage forensic epidemiology allows information about exposure to foreign agents and disease in population groups to be collected from wastewater. Chemical analysis of local wastewater allows us to detect both legal and illegal substances present in the population either by consumption or direct release into the sewage system. This research is focused on both the optimum preservation and hold times of wastewater samples and on the impact of a temporary increase in population to the presence of pharmaceuticals in wastewater. Influent and post-UV effluent samples were collected from a municipal wastewater treatment plant. Samples were filtered and extracted over a three-day period, with a portion of the samples acidified to pH <2 to determine if pH played a role in preservation. Influent and effluent samples were also collected before, during, and after the county fair, in order to determine if there was an increase in

pharmaceuticals detected. All samples were analyzed by the LC-MS/MS for opioids, amphetamines, and cocaine.

ENVR 583

Reduction rate of the hexavalent chromium in the presence of ascorbic acid: Kinetic study

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Ascorbic acid has been considered as a strong antioxidant indicating a potential reductant for the source of electrons. In this study, the hexavalent chromium [Cr(VI)] reduction rate in the presence of ascorbic acid was examined. Different amount of ascorbic acid was introduced to 25mg/L of Cr(VI) solution, and the concentration of Cr(VI) was monitored as a function of time. The amount of Cr(VI) in the solution was determined directly using an Aguamate 8000 UV-Vis spectrophotometer at 352.0 nm. Most experiments were performed at room temperature without pH control. To study the pH effects on the Cr(VI) reduction rate by ascorbic either 0.01M acid. 2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonic acid (HEPES) buffer or 0.0025M hydrochloric acid (HCI) solution was used. It was observed that the hexavalent chromium was reduced in the presence of ascorbic acid following pseudo first order reaction. The initial concentration of the introduced ascorbic acid and the solution pH are the major factors controlling the Cr(VI) reduction rate.

ENVR 584

Mineralogical characterization of Fe(II)-oxidizing bacterial stalks

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Neutrophilic, microaerobic Fe(II)-oxidizing bacteria (FeOB) from marine and freshwater environments are known to generate twisted ribbon-like organo-mineral stalks. These structures, which are extracellularly precipitated, are susceptible to chemical changes in the environment once synthesized. Here, we characterize the minerals associated with freshwater FeOB stalks to evaluate microbe-mineral mechanisms involved in biomineral formation and ageing processes. Based on

observations made by micro-Raman Spectroscopy, Electron Microscopy and Scanning Scanning/ Transmission Electron Microscopy combined with Dualrange Electron Energy-Loss Spectroscopy we propose a model that describes the crystal-growth mechanism, the Fe-valence state, and the mineralogical evolution of the stalks, as well as the biogenic contribution to these characteristics and processes. Our study suggests that the main crystal-growth mechanism includes nanoparticle aggregation and dissolution/re-precipitation reactions, which are dominant near the organic exopolymeric material produced by the microorganism and in the peripheral region of the stalk, respectively.

ENVR 585

Graphene oxide-MoS₂composite membranes for arsenic and lead polluted water purification

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Water plays an essential role in our lives. It is used by all parts of our body to help regulate temperature and maintain other bodily functions. Pollution caused by industrialization and population growth has led to water shortage and it is affecting humans by lowering their quality of life. One of the main solutions for this challenge is water purification. In this study, we have used a costand energy-efficient novel material, two-dimensional (2D) graphene oxide (GO) to fabricate promising water purification membranes alongside with another 2D material, molybdenum disulfide (MoS₂). GO has unique physicochemical properties including high surface area, mechanical durability, and nanosized pores, making it excellent water filtration membranes. GO can also decrease energy use in terrestrial and space applications. These characteristics makes GO extremely special by making it efficient in water purification on both earth and outer space. In comparison, MoS2also shows great promise for water filtration. When forming composites with GO, the water fluxes might vary significantly while the reliable structure and properties of MoS₂nanochannels in the composites are largely unknown. In this work, we have focused on the structure-filtration relationship of graphene oxide-MoS₂composite membranes for purifying wastewater containing arsenic and lead ions. The GO-MoS₂composites were synthesized by hydrothermal reactions and the composite membranes were prepared by vacuum filtration method. The structures of the membranes were examined by various methods including TGA, XRD, and SEM. The efficiency and the permeability of the membranes for arsenic and lead ion filtration were measured by electric conductivity measurements. The discoveries from this research may have a great impact on water reuse on both earth and outer space.

ENVR 586

Detection of toxins from harmful algae blooms: Identifying markers for Microsystin-LR

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Freshwater lakes can experience harmful algal blooms (HABs) of cyanobacteria that produce toxins which can affect human health. HABs have grown in frequency due to nutrient runoff and will continue to grow due to more favorable conditions in a warming climate. Most HAB studies have focused on the health consequences due to ingestion, but less is known about exposure resultant of toxin inhalation as a consequence of aerosolization. A field study was conducted to assess the potential for toxins to be aerosolized at Grand Lake St. Marv's due to its intense and consistent HAB coupled with its use for recreation. The samples collected during the field study were used to explore markers for the HAB toxin Microcystin-LR. An aerosol time of flight mass spectrometer (ATOFMS), a single particle mass spec that collects dual polarity mass spectra in real time, was used to analyze Microcystin -LR standards and lab-generated aerosols of HAB lake water. Possible mass spectrometry markers were identified, which will be used in future studies and field work to determine the conditions associated with the aerosolization of toxins from HABs. These data will help develop a greater understanding of the effects of these HABs on their surrounding environment and their potential transport of aerosolized toxins.

ENVR 587

Exploring the relationship between the properties of biochar and heavy metal sorption

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Studies have shown that biochars, a type of material produced from a carbon-rich organic matter that has undergone pyrolysis, can perform heavy metal sorption from lead-contaminated water. The amount of heavy metal adsorbed is determined by the surface properties of biochars. However, few studies have explored the surface properties quantitively. To address this, samples of biochars originating from two different coffee grounds were charred at 25° C, room temperature, and at charring temperatures of 350° C, 450° C, and 650° C. The biochars were then placed in various concentrations for a time range of 1 hour – 24 hours. The amount of lead adsorbed by the biochars were measured by the ICP-OES. As the charring temperature increases, the amount of lead adsorbed increases. The complete results of this research will be presented.

ENVR 588

Melting point determination using a solar irradiation heat source

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The recognition of the irreversible damage done to the environment through man-made materials and the desire to avoid the burden of pollution clean-up has inspired scientists to attempt to transform typical synthetic procedures into more environmentally friendly procedures. Since fossil fuels are used for the majority of electrical energy, the amount of electricity required to complete an experiment has recently become to emerge as an environmental concern. Parabolic solar reflectors have been proposed as an effective means for minimizing the amount of electricity needed to drive chemical reactions to completion. The solar reflectors were developed by covering satellite dishes with reflective tape, giving the dish reflective properties when directed at the sun. The ability to use the solar reflector as the sole heat source for high-temperature synthesis reactions has been extensively analyzed. However, analysis of the products synthesized through the use of the solar reflector still require electricity to operate the instrumentation. The ability to exchange traditional chemical analysis methods using electricity for solar sources is not only beneficial to our environment but it can also be useful to those with limited resources without the capacity to perform traditional analysis methods using electricity. A method has been developed in which the melting point of a compound can be taken with a high level of accuracy using solar energy as the sole heat source. A comparative study was conducted using an electrical and solar heat source to take the melting point of a series of compounds consisting of a wide range of melting points.

Industrial water corrosion control with nutrient free chemistries to minimize algal blooms and meet current and future discharge limits

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Phosphate and phosphonate chemistries for deposition and corrosion control have dominated industrial cooling applications for several decades. The ubiquitous use in the industry was a result of regulations eliminating the use and direct discharge of heavy metals such as chromium and instituting strict limits on the use of molybdate and zinc. Phosphorus-based corrosion control programs are non-toxic versus the metal alternatives. Unfortunately, phosphorus chemistries are a micronutrient that can cause algal blooms when discharged, biofilms within the industrial system, and dangerous microbiological growth such as Legionella. Phosphorus discharge limits are becoming more stringent to the extent that no added phosphorus is being required based on discharger permits. Presented here is a nutrient-free industrial cooling corrosion control program that was designed to engineer specific surface passivation films to meet regulation and performance criteria. The insight provided by understanding the surface chemistry connection between water quality and chemical treatments has allowed the development of engineered film technology.





Algae Blooms – Phosphonate-based Program

Algae Blooms Mitigated – Non-P Program

ENVR 590

Role of inorganic chemistry in improving the sustainability of heterogeneous catalysts for oxyanion reduction

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This presentation will report our recent results on heterogeneous catalyst development and discuss with sustainability researchers on the challenges and opportunities of using new reactions and materials for oxyanion pollutant treatment in water and wastewater. Examples will include how our new catalyst designs achieved the critical goals suggested by previous life cycle assessment (LCA), additional factors that may need to be included in the LCA, and new technology systems and components that can be evaluated before experimental works are accomplished.

ENVR 591

Is urban gardening safe in residential properties built prior to 1978? Field-assessment in the city neighborhoods of Rochester, NY

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Contamination of residential soil used in urban gardens causes exposure to lead (Pb) through consumption of produce. Urban gardening is otherwise beneficial to the local community and can be conducted safely with proper assessment of soil. Currently, the Environmental Protection Agency (EPA) sets limits for allowable soil-Pb in children's play areas, but no limit is defined for soils used for gardening. Our overarching goal is to demonstrate the need for assessment of potential garden sites. This will allow restriction of gardening to safe areas of the property, thus preventing lead exposure through consumption of contaminated produce. Our objectives were to: determine safe locations for urban gardens in residential properties, assess how produce absorbs and stores Pb from contaminated soil, and investigate the presence of Pb in commercially available produce and spices. Four residential locations were tested with an X-Ray fluorescence analyzer (XRF) to determine soil Pb contamination levels and compared with a control location. Plant samples were collected from these urban gardens. Produce and spices were collected from grocery stores and community farmers' market. Plant samples, produce, and spices were analyzed for lead concentration in a Microwave Plasma-Atomic Emission Spectrometer (MP-AES). Results show that lead contamination in residential soils is extremely heterogeneous and varies widely by location with respect to the number of sources, distance from the source(s), slope, and type of soils. Lead was detected in all four residential soils at varied amounts and was absent in the control location. Data obtained so far showed the absorption and storage of Pb in different parts of plants collected from the contaminated soils. Some of the edible parts were found to contain lead, which indicates high risk of exposure. The results establish the need for a case by case assessment of Pb

in every property that is being considered for urban gardening. Assessment of residential properties prior to setting up an urban garden will help to determine the safe location, within which the garden should be restricted. The contaminated area of the property can be further categorized into high and low risk zones and appropriate remediation processes should be implemented.

ENVR 592

In situ synthesis of magnetic Fe₃O₄@plant polyphenol composite particles for *Chlorella vulgaris* harvesting

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Magnetic separation is a promising and sustainable technology for rapid algal harvesting. In this work, the Fe₃O₄ particles coated with natural plant polyphenol (PP) were synthetized by in situ solvothermal method, towards the harvesting of Chlorella vulgaris from the medium broth. After PP coating, the dispersion of Fe₃O₄ improved and particle size was reduced from 230 nm to 180 nm. Fe₃O₄@PP had a higher saturated magnetization and thermal stability than Fe₃O₄. The influence of dosage, algal density, initial pH and reuse on harvesting efficiency were systematically investigated. The Fe₃O₄@PP achieved 98% harvesting efficiency at the dosage of 2.0 g/L, algal density of 2.0×10^{10} cell/L, and pH 8.0. The Fe₃O₄@PP was more efficiently detached from the harvested cell aggregates than Fe₃O₄ by alkali solution with ultrasonic treatment and realized 95% quality recovery. The reused Fe₃O₄@PP maintained more than 80% of harvesting efficiency after five recycles.

ENVR 593

Analysis of pesticide residues in strawberries: Multiresidue QuEChERS-LC-MS/MS method

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This study aimed to determine pesticide residues in strawberries from Pennsylvania retail stores during 2019-2020. A multiresidue method was developed for analysis of 10 pesticide molecules using SCIEX QTRAP UPLC/MS/MS. The strawberry samples (peel and whole fruit, separately) were extracted by QuEChERS and followed by dispersive solid-phase extraction (dSPE) for clean-up. Results showed that boscalid, tetrahydrophthalimide, cyprodinil, pyroclostrobin and myclobutinil were the most detected pesticides in strawberries. Peels of strawberries were detected with higher levels of the pesticides than blended fruit for most of the samples.

ENVR 594

Properties analysis and quality comparative study of PET used plastic bricks

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The methods in common theme of mixing together plastic and river sand to produce their composite material, however, due to the scarcity of river sand, preserve the ground water and riverine soil and its environment, the desert sand are used for the production of plastic brick with polyethene terephthalate (PET) which is prepared from used water bottles. PET and Sand is mixed with the ratio of 1:3, 1:4, 1:5 and 1:6, Each component is heated separately at 260 degrees Celsius which is the melting point of PET, the components are then mixed evenly, and the temperature of the fire is lowered until fuming ceases which is around 250 Celsius then mixture then becomes like putty. The mix is poured into a mold and compacted and pressed into it as it cools to prevent air pockets from forming. After 1 hour the brick is demolded and cooled at room temperature for 1 day before testing phase. The produced bricks have been taken into testing laboratory for the analysis of compressive strength, heat test, soaking test, alkali test, acid test and finally such properties are compared with the quality of standard bricks like first class, second class and common bricks. Result shows that the compressive strength N/mm² is 6.36, 7.64, 6.30, 3.22 with respect to PET and sand ratio. Similarly, heat test shows in (g) that for 1:3, initial weight 485 final weight 485, 1:4 - 612-612g, 1:5-713-713g, 1:6-679-679g without any weight change. Soaking test shows that 1:3- 485-488g, 1:4- 612-613g, 1:5 ratio shows 713-719g, 1:6 - 679-686g with minor change. The alkali test result shows no deviation from the initial weight 488g, 613g, 719g and 686g, the acid test shows slight decrease in quantity like 488g, 611g, 718g, 682g. The comparative study shows that the 1:4 ratio performed better than a second class brick but not better than a 1 st class brick. Buildability shows that the 1:4 and 1:5 ratio had the best workability and consistency when mixing, the 1:3 ratio had issues where it was very runny having lots of bubbles and escaping fumes and the 1:6 brick had the worst workability and high rigidity even past 260° Celsius. The advantage is that PET is essentially free and desert sand is available in plenty hence it is highly cost effective and other way reduces pollution.

ENVR 595

Promising FeOCI material for wastewater treatment: Controllable synthesis, modification and the investigation of H_2O_2 activation behavior

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Solid catalytic materials, especially iron-based materials, have attracted tremendous attention in the oxidative removal of pollutants using H₂O₂ as oxidant due to their high stability, low-cost and non-toxic nature. Among all iron-based materials, FeOCI exhibits excellent H₂O₂ activation ability, whose hydroxyl radical generationrate is 1-3 orders of magnitude higher than traditional iron-based materials. The coordination structure of iron sites on the surface FeOCI directly affected the generation of hydroxyl radical from H₂O₂. Thus, the controllable synthesis of FeOCI with more reactive crystal planes is important for enhancing its heterogeneous Fenton activity. We prepared FeOCI with abundant exposed crystal planes by using small sized Hematite nanoparticles as precursor, showing the higher activity than traditional FeOCI, in which the size of Hematite was controlled by high energy ball milling method. The growth of inert (010) plane on the as-prepared FeOCI is suppressed compared to the platelike structure of traditional FeOCI, and the ratio of exposed (100) and (110) planes with rich iron sites increased, leading to the significant improvement of its Fenton activity. In addition, based on the typical layered structure of FeOCI, we further modulated the coordination environment of iron sites by the surface modification (etching) and structural modification (intercalation). These modifications can create new reaction space on the FeOCI surface (or interlayer surface) for the conversion of pollutants. More importantly, phenolic compounds are no longer degraded into small molecular products in the treated FeOCI system, but are coupled to polycyclic polymers, which is very similar to the oxidative coupling process catalysed by peroxidases. This may indicate that the H₂O₂ activation pathway is changed from the homolytic cleavage of O-O bond to the heterolytic cleavage of H-OOH bond. The transformation of H₂O₂ activation behaviour has provided an excellent example to understand the reactivity of H2O2 on the surface of solid iron-based materials, which is of great significance for the design and development of highly efficient ironbased solid catalysts.

ENVR 596

Brown carbon aerosol systems

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Recent studies demonstrate that fine Particle Matter (PM) damages the human respiratory tract via intracellular redox reactivity between lung antioxidants and reactive oxidant species (ROS). Evidence continues to build that excess ROS generated by PM chemical components trigger oxidative stress biochemical mechanisms, leading to cellular/tissue injury, inflammation, and related systemic challenges, including cancer. Brown carbon (BrC) compounds are aerosol phase pollutants that are expected to oxidize PM in secondary organic aerosols (SOA). We use a DTT assay on an automated plate reader to quantify oxidant formation and characterize oxidative potentials for BrC species in local SOA systems.

ENVR 597

Fate of nanoparticles in simulated gastric fluid studied using single particle-ICP-MS

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The broad and increasing application of the nanoparticles (NPs) will end up in a biological system, intentionally and unintentionally. The first stop for NPs is the stomach after being ingested with water and food by human. It is important to know the fate of the NPs in gastric fluid before entering into other parts of the body. The objectives of this study are to study the fate of the most widely used AgNP, AuNP, CeO₂ NP, and ZnNPs in simulated gastric fluid (SGF) under room and body temperatures for different contact times by SP-ICP-MS. The results showed that ZnO-NPs (50-70 nm) dissolved very rapidly in SGF; CeO₂-NPs (30-50 nm) did not change significantly; mean sizes, size distributions, and particle concentration of AuNP (40 and 80 nm) and Ag-NP (40 and 70 nm) were affected by NP concentrations, original sizes, contact times, and temperatures.

ENVR 598

Clean air: Critical review of benefits of the U.S. Clean Air Act Amendments of 1990 and worldwide implications

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Promulgation of Clean Air Act Amendments of 1990 have been revolutionary and provided anticipated benefits not only in the US and showed the proven clean air pathway to both developed and developing countries. The Title V, Permits, program including the 'synthetic minor'

permitting is proven in that effective control of air pollution with certified air-compliance has along been accomplished. Moreover, the coordinated effort on airshed attainment and compliance has been observed utilizing the requirements as stipulated via the said Clean Air Act Titles I, II, III, IV, and VI. Those accomplishments on control of criteria air pollutants, hazardous air pollutants and, acid deposition, and the stratospheric ozone protection are significant. The air pollution control programs via budgeting, such as on NO_X, and intra-orinterstate trading within the designated airsheds have proven effects toward a cleaner air and resulting airsheds. The 'new source review' and 'prevention of significant deterioration' programs or rules of the clean air act brought the required attention, verification, implementation, and accomplishment on air pollution control. The airsheds have been continually assessed on attainment and non-attainment status with respect to the criteria air pollutants - particulate-matter, lead, sulfurnitrogen-dioxide, ground-level-ozone, dioxide. and carbon-monoxide - where, more and more airsheds are coming into attainment. This accomplishment in the US via clean air requirements included applications of green engineering, principles of circular economy, industrial evolution and advancement, and, sustainability and resiliency. The proven clean air program(s) must be required, and benefits be observed worldwide. This presentation will include: an explanation of critical elements of the air pollution control program(s); observedsustainability and resiliency via the air-attainment verification; a verification of US clean air act elements and benefits, using field-examples; and, the pathways to accomplishing on clean air worldwide.

ENVR 599

Water recovery from human urine by air gap membrane distillation (AG-MD)

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As a potential solution to overcome water shortage challenges, membrane distillation (MD) offers a possibility for alleviating the water demand in water scarce countries. In the field of urine treatment, air-gap membrane distillation (AG-MD) enables simultaneous recovery of water and nutrients (e.g., nitrogen) for potable or non-portable use such as irrigation and toilet. The performances including the membrane flux as well as the ammonia-nitrogen (NH₄⁺-N) and chemical oxygen demand (COD) concentration, and conductivity of distillates were studied experimentally. Our AGMD achieved a maximum water recovery of 31.9%~48.6% from human urine samples at pH=6.5 and 40° C, which

yielded a temperature difference of 20°C between the human urine and the surface of the code condenser at 20°C. AGMD process operated at a loading flux of 4.2 kg m²h⁻¹ and achieved high COD removal efficiencies of 99.3%~99.5% and the removal efficiencies of NH₄⁺-N of 40.6%~75.1%. This suggests that AGMD can directly use the heat from the fresh human urine on the feed side to achieve water and nutrient recovery.



ENVR 600

Antimicrobial air purification systems for effective improvement of indoor air quality in palliative care facility

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Airborne transmission is one of the major routes of respiratory infections and ranks in top ten causes of death worldwide. People spend more than 90% of their lifetime in indoor environments. Poor indoor air quality can cause adverse health impact and disease outbreak, particularly in healthcare facilities (e.g., elderly homes) where patients are vulnerable. The filtration technology is the most viable method for air purification and disinfection in healthcare facility. Yet the existing commercial air filtration devices have limitations such as recontamination and microbial emission from contaminated air filters. To tackle

the problem, new coating was developed to provide filters a sustained antimicrobial and filtration functions. An optimized antimicrobial particulate air filters is capable of 95% reduction in viable microorganisms by combining "release-killing" biocides, "contact-killing" reactive dyads and anti-adhesion polymers to target different cellular sites in the microorganism along different inactivation pathways. This work evaluates indoor air quality (i.e., bioaerosol, particulate matters and volatile organic compounds (VOCs)) and the effectiveness of antimicrobial particulate air filters. Computational fluid dynamics (CFD) simulation was used to determine the best placement of air purifiers for a wardroom configuration and dynamics. The results showed that the application of antimicrobial particulate air filter in healthcare center mitigated indoor air pollution, thus improving the elderly home residents' health conditions.

ENVR 601

Photophysical properties of coumarin-1 and coumarin-2 in water

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Coumarins, are widely used as dyes in different industrial processes and are found in wastewater as contaminants. Coumarins possess significant photophysical and photochemical properties and good solubility. Therefore, fluorescence spectroscopy can be an effective tool for its identification water. All chemicals including Coumarin-1 (4 - Methyl-7-Diethylamino coumarin) and Coumarin-2 (7-Ethylamino-6-methyl-4-methyl coumarin) was purchased from Sigma Aldrich of high purity. The fluorescence was examined by fluorescence spectrophotometer (F2700, Hitachi, Japan). The computational simulations were calculated by Gauss View-6 software, and Gaussian 16, to generate the molecular structures. The TD-DFT and DFT theory for fluorescence was done by 6-31 G (d,p) basis set & the B3LYP functional. These compounds demonstrated longer EX wavelength from 350nm and longer EM wavelength over 430nm. The difference of fluorescence EX and EM wavelengths for all compounds is represented as coumarin-1. EX/EM 375nm/456nm. coumarin-2, EX/EM 365nm/470nm (Fig.1). The EX/EM

wavelength region for coumarins, is displayed in humiclike region with strong fluorescent signals. The fluorescence coumarins in aqueous solution showed a good linear correlation between concentration and fluorescence intensity with value of R² as 0.999. The fluorescence EX/EM peak location remains same at all concentrations (µg/L) in water. The substitution of methyl group substitution on the heterocyclic ring at coumarins tends to maintain excitation from 340nm to 375nm and emission wavelength remains 440nm to 470nm. These results indicate that ethylamino substitution at the aromatic ring with methyl amino tends to produce longer excitation and redshift the emission wavelength. This phenomenon is due to the difference in electron donner ability ($C_2 H_5 > C H_3$). The theoretical results are in line with experiments. The photophysical properties of these compounds are helpful in its identification in water.



Fluorescence and electronic details

ENVR 602

Oil/water separation by using the photopolymerized porous hydrophobic and oleophilic materials

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The water pollution due to oil and organic contaminants has emerged as a major environmental issue. Oil and organic pollution are contributed by various industries, household activities, and offshore oil production. History has witnessed some major devastating oil spill incidents during the rapid offshore oil movement. The oil-related contaminants can stay for a longer time and have a severe adverse effect on marine and human life. The conventional methods are facing problems due to their high cost, inefficiency, and source of secondary contaminants. There is a dire need to develop new efficient materials that can effectively separate the oil from water and has the capacity to scale up. One of the

possible ways to separate the oil contaminants from the water by using porous hydrophobic and oleophilic surfaces. The hydrophobic and the oleophilic surfaces allow the passage of oil or non-polar organic contaminants from the water. The challenge associated with the development of hydrophobic surfaces is the complexity in synthesis and its stability. Synthesis of material through the naturally available sources is always attractive. The natural sunlight is an abundant natural source that carried out the great potential to drive the chemical reactions under a certain set of conditions. We built an amazing cost-efficient synthetic route by harvesting the natural sunlight to develop the hydrophobic surfaces that allowed the fast passage of the oil and prevented the water to pass. This was achieved by introducing the glass reactor and the suitable monomer that display the capacity to polymerize under the sunlight radiations. In brief, hydrophobic surfaces were prepared by harvesting the natural sunlight that initiated the polymerization of the styrene on the selected porous substrate in a glass reactor. This provides an extremely cost-effective route to prepare the hydrophobic surfaces. The surface area can be improved by adding various nanomaterials. The surfaces prepared by through this route can display the contact angle in the range of 126 ± 4° to 161° ± 2° according to the functionalities. The separation efficiency can be achieved for the various oil/water-based system in the range of 96 to 99 %. The developed porous materials can be used for the continuous separation of the oil spills and the spot absorption of the oil from the water.

ENVR 603

CO₂ conversion by high-dose rate electron beam irradiation

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The reduction in CO₂ emissions is an important issue across many industries. Inspired by extraterrestrial organic matter formation, we herein report a CO₂ conversion approach based on high-dose rate electron beam (EB) irradiation of an acid-decomposed CaCO₃/additive EtOH mixture (Figure 1). With ¹³C-CaCO₃, ¹²C-EtOH and 100 kGy s⁻¹ EB, H₂, CO, CH₄, C₂H₆ and organic acids are simultaneously produced within a few seconds, except for 2,3-butanediol formation from excess EtOH. According to the organic analysis results, CO and organic acids contain ¹³C carbon derived from ¹³C-CaCO₃. The high-dose rate EB gives increased CO₂ conversion products compared to the low-dose rate EB. The CO₂ conversion yield/energy efficiency (product energy/input electrical energy) at 300 kGy is 1.51/0.50% in total (CO: 0.03/0.01%, formic acid: 1.31/0.29%, acetic acid: 0.05/0.04% and propionic acid: 0.12/0.16%), and the total radiation energy efficiency (REE, product energy/net radiation energy) of CO₂ at 300 kGy is 51.5% (CO: 0.90%, formic acid: 30.3%, acetic acid: 3.71% and propionic acid: 16.6%). The CO₂ conversion yield is ~15 times larger than that of the only known CO₂ gas radiolysis (0.1%, CO only). Furthermore, the REE at 100 kGy is also ~15 times higher than that obtained in the absence of EtOH. The energy input for the 100% conversion yield is estimated to be 38000 GJ per t-CO2. The combination of the high-dose rate EB with organic additives facilitated CO₂ capture by radicals to afford improved CO₂ conversion efficiency/yield.



Figure. 1. (a) Proposed CO2 conversion approach by high-dose rate EB irradiation with organic additive. (b) EB irradiation overview of the glass vials used in the experiments.

ENVR 604

Green approach for the synthesis of silica nanoparticles

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The most routinely methods for the synthesis of nanoparticles are chemical and physical. However, these approaches are complicated, expensive and cause potential environmental and biological hazards. On the other hand, the emerging trend of green synthesis of nanoparticles with the help of plants and microbes as reducing agents is an efficient, cost effective, fast and eco-friendly is another option. This Green approach of synthesis of nanoparticles plays pivotal role in different fields such as medicine, pharmaceutical, electrical, technology and other science research areas. The present study reports on a green approach for synthesis of silica nanoparticles (SiNPs) from combination of Pochonia chlamydosporia and rice husk. Little research has been carried out on Green Synthesis for the synthesis of SiNPs from plants, microbes, algae and no research is undertaken so far from fungus P. chlamydosporia. Hence, the present work has been undertaken to synthesize SiNPs from *P. chlamydosporia*. It was found that the fungus P. chlamydosporia may be used to bio-transform amorphous silica present in rice

husk into highly crystalline silica nanoparticles. Characterization of those SiNPs was done by using different analytical tools like FT-IR, UV-Visible spectrophotometry, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM). The biological activity of fabricated silica nanoparticles has been tested in respect to germination of cowpea seeds.



Schematic representation of green synthesis of silica nanoparticles from rice husk

ENVR 605

Seasonal distribution of heavy metals in biotopes nearby the "Cavernas del Río Camuy" National Park

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Heavy metals are generally defined as a group of chemical elements, commonly associated to the transition metals that are characterized by their high atomic weight, by having a specific gravity greater than 4.0, and a density greater than 5 g/cm³. One of the most important characteristics of heavy metal is that it exhibits the potential for toxicity when it accumulates in living tissue. Heavy metals are relatively rare natural components in the earth's crust and are naturally introduced to the environment by geochemical activities; however, almost all human activities have the potential to introduce heavy metals into the environment through industrial waste. Since heavy metals cannot be degraded, they have the potential for bioaccumulation in distinct trophic levels in a food chain, which affects the overall health of the ecological region. In this research, the presence and abundance of cadmium, copper, iron, lead, manganese, and nickel in water bodies, sediment samples and flora present in the biotopes from the "Cavernas del Rio Camuy" National Park were evaluated. The sediment and collected water samples were treated in the laboratory following EPA Methods 3050B and 200.2, respectively.

Samples of plant tissue were digested using open-beaker acid treatment. Analyses will be carried out by means of a flame atomic absorption spectrometer. Plants of interest include T. zebrina, P. aquilinum, and U. barbata. During previous research, it was observed that the sampled plants had a cosmopolitan present in the ecology of the region. Such observations compelled us on expanding sampling these plants at a distant elevation within the cave system and compare the concentration of heavy metals within the analyzed samples. This will help us understand further how distinct physical-chemical parameters, like the exposition of light, affected the concentration of heavy metals in the plants. Another factor that we take into consideration from previous research is seasonal sampling since the climate in Puerto Rico has a wet season and a dry season. By sampling during this season, we could determine if other physicalchemical parameters, such as temperature or humidity, affect the concentration of heavy metals in the region. The results of this study will allow a better understanding of the environmental quality of the studied ecosystem and can help in future management measures specifically aimed at tracking pollution and contamination by metals in the cave system.

ENVR 606

Environmentally friendly clay filtration in the oil industry

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In the Permian Basin, there are about 188k oil and gas wells. This makes us the largest area in oil production in the United States. The wells require fracking which utilizes about 42,500 cubic meters of water for every well. The result of this method is about 80k cubic meters of flowback and produced water. Most of this produced water cannot be used again since it contains heavy metals and salts that seep into the ground, contaminating the aguifers in our area. Techniques for filtering this water are flocculation and chemical treatment, which is found to be lacking and expensive. Therefore, we have developed a multi-layered clay filter used to filter the produced contaminated water, so it is able to be reused as gray water. The structure consists of a pressurized system made of raw earthenware clay mixed with Fe₃O₄ and coated with Humic Acid which is used to remove the heavy metals from the water. A cleating agent is utilized on the layers to remove any possible contaminants from the clay. In addition, porcelain and stoneware clay filters complete the filtration to the cleanest composition with minimal leeching. Atomic Absorption Spectroscopy and Inductively Coupled Plasma-Optical Emission Spectrometry is used to analyze water before and after filtration

to determine metal ion contaminants present. Currently, results show an increase of iron, potassium and calcium and a decrease in levels of barium and zinc. The permeability, porosity, and rate flow as well as additional metal analyzation of produced waters from different sources will be presented.

ENVR 607

Bioaccumulation of heavy metals in West Texas

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The bioaccumulation of heavy metals has a dangerous impact on our environment with the amount of air and water pollution it can cause. While this pollution is increasing throughout the world, it is already a reality in West Texas. With the amount of oil and gas production, the groundwater that becomes our tap water has increasing amounts of heavy metals. On the University of Texas Permian Basin's campus, we have multiple gas wells including ones that are still in production. Soil samples were taken outside of a working well to be treated and analyzed for traces of Lead, Manganese, Chromium and Nickel. Using a grid of ten squares, three ten-centimeters soil samples were taken from each spot and treated with acid and placed in a digestion block. The results were taken using Atomic Absorption Spectroscopy and showed low concentrations of heavy metals.

ENVR 608

Fabrication of novel azo-linkage ion-exchange adsorbent based on green polymers for nitrate removal

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The amount of reactive nitrogen in terrestrial and aquatic ecosystems has been increasing due to the intensive use of synthetic nitrogen-containing fertilizers and animal farming. This excess level of nitrogen causes significant environmental and health issues. Here, we present a practical approach to synthesize ion-exchange materials using emulsion polymerization and synthesize polymer networks with enhanced selectivity for nitrate adsorption from water resources. We designed and synthesized new para-vinyl crosslinkers, forming a nitrogen cage, and performed emulsion polymerization to create crosslinked polystyrene networks. We demonstrate enhanced nitrate entrapment and removal efficiency in a batch operation. Additionally, we illustrate the effect of packing, operating parameters, and regenerating of the adsorbents when used as packed materials in an ion-exchange column.

Scalable and green synthesis of metal and metal alloy nanoparticles in a solid matrix

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This research develops a green synthesis approach without using organic solvent, toxic reducing agents and chemicals to obtain size controllable metal and metal alloy nanoparticles. A salt matrix, NaCl, is utilized as the medium for dispersing metal salt/complexes and plays a role in preventing the formed nanoparticles from severe sintering. The reduction of metal salt/complexes can be obtained under a reducing gas, such as H₂/N₂, in a conventional electric tube furnace at normal pressure. The resulting nanoparticles can be easily purified and collected after dissolving the matrix in water. Using the method, nanoparticles of Fe and its alloy have been synthesized. The synthesis parameters such as temperature and time, the weight ratio of metal precursors and salt matrix, and the synthesis steps have been investigated. These factors have an impact on particle size and uniformity where in a higher salt ratio and a lower temperature results in smaller particles with higher uniformity. It is also found that the resulting nanoparticles are stable in air, which then can be attributed to the surface coating layers comprising metal oxides, C, and decomposed ligands. The source of the surface C is from the metal complex precursors or the added ligand. Further, the nanoparticles exhibit magnetic properties, making them a potential candidate for various applications. Thus, the method is advantageous for green synthesis and applications of nanoparticles in term of cleanness, scalable capability, and its general applicability for various types of metal, metal oxides, and metal alloys.

ENVR 610

Coenzyme vitamin B₁₂ enhancing methane production during anaerobic digestion of food waste and mechanisms

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The enhanced methane production during two-stage anaerobic digestion of food waste was achieved by the addition of vitamin B_{12} which was an excellent catalyst and electron mediator. In the acidification stage, the accumulation of volatile fatty acids (VFAs), increased from 2961.52 mg COD/L to 3798.42 mg COD/L with the increase of vitamin B_{12} from 0 to 50 mg/L, suggesting 30% of promotion of VFAs yield. No obvious further enhancement of VFAs was observed when vitamin B_{12}

increased to 100 mg/L. The similar results were obtained in the methanogenesis stage, methane yield was improved by 49.8% at a vitamin B_{12} dosage of 50 mg/L. Although some vitamin B_{12} was biodegraded in the anaerobic digestion process, the methane generation from vitamin B_{12} was negligible. Mechanism investigations showed that the presence of vitamin B_{12} augmented the production of butyrate, propionate and acetate, due to the improved activities of key enzymes involved in acidification. Vitamin B_{12} also increased the activity of hydrogenotrophic methanogens by 47.7%, which might be owing to accelerating the electron transfer process. With a tremendous amount of food waste generated, adding vitamin B_{12} gives a new approach to improve methane production and energy recovery.

ENVR 611

Investigation on methane production by threonine with L- and D-configurations

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As a significant anaerobic digestion intermediate of protein, threonine can be applied for two-stage anaerobic digestion for methane production. In this research, the two-stage anaerobic digestion of threonine with L- and Dconfiguration was compared, and obvious significance was observed in both stages. In the acidification stage, it was found that the maximum VFAs yield was obtained at pH 8 with 4444.2 mg COD/L in L-threonine digestion reactor, while it was observed at pH 7 with merely 624.6 mg COD/L in D-threonine digestion reactor. By examining the VFAs component, both acetate (52.6%) and propionate (29.7%) presented as predominate products during L-threonine digestion, compared with only propionate during D-threonine digestion. As a result of the differences in VFAs concentration and composition accumulated in acidification stage, considerable gap between methane production from L- and D-threonine was recorded, and which were 64.8 mL/g COD and 5.6 respectively. mL/a COD. Mechanism studies demonstrated that the configuration of digestion substrates contributed to remarkable difference on key enzymatic activities, specifically, the key enzymes activities including threonine deaminase, phosphortransacetylase, acetate kinase and propionate kinase in L-threonine were 5.4, 6.8, 8.0, 7.9 and 7.6 folds higher than that in D-threonine reactor. In the long-term operation, the amino acid decomposition associated genuses in L-reactor were Aminicenantes (30.6%) and Acidaminobacter (17.4%), which also take obvious advantage over that in D-reactor, namely, Cloacimonetes (20.6%) and Aminicenantes (17.6%). Besides, the methanogens in L-reactor were affiliated to Methanobacterium (48.3%) and Methanosarcina (44.3%). While in D-reactor, there was predominantly Methanobacterium (41.7%) and Methanosaeta (29.1%). Overall, this study provided an insight into the effect of configuration of amino acid on methane production performance.

ENVR 612

Life cycle assessment and techno-economic analysis of epoxidized sucrose soyate: Novel biobased adhesive

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In the past few decades, there has been a growing demand for renewable and sustainable polymeric materials due to 1) their ability to provide enhanced functionality, and 2) increasing environmental concerns from fossil-based products. Epoxidized vegetable oils and their derivatives are alternative sources for petroleumbased resins. Among epoxidized vegetable oil-based resins, epoxidized sucrose soyate (ESS) has gained great interest as it has shown to significantly enhance the mechanical properties as an adhesive in a wide range of applications including composites and coatings. In our study, we investigate the environmental and economic performances of the ESS resins. We use laboratory and pilot-scale data to model the process of preparing ESS resin in industrial-scale using Aspen Plus software. Additionally, we use life cycle assessment (LCA) method to assess the environmental impacts of making this resin. We use Simapro software and TRACI 2 method (including ten environmental impact categories e.g. global warming) to compare the environmental performance of ESS with commercially available petroleum-based epoxy resins. The results from the process simulation including material and energy balances are also used to evaluate the production cost of ESS. The combination of environmental and cost performance data of the ESS will provide decision-making information for its commercialization and allow us to identify hotspots in the production process and recommend possible synthesis improvements that can help this novel resin compete with commercially available resins in the market. To our best of knowledge, this is the first research that investigates the cost and environmental impacts of ESS.

ENVR 613

Creation of a new fluorogenic estrogen-detecting sensor through computational modeling

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The presence of endocrine disrupting in water, which are estrogenic, are known to cause feminization of fish and amphibians. This process adversely affects the ecosystem as the hormonal imbalance in theses that makes unable to reproduce and reduces the population which adversely affects ecosystems globally. The current methods of detecting the presence of endocrine disruptors are inefficient as the gold standard Yeast Estrogen Assay (YES) takes 4 days. We have developed a computation model for a new sensor which is even faster in detection as it is predicted to take less than 2 hours. The sensor is in vitro and when the estrogen enters, it creates a conformational change that reconstitutes T7 RNAP and causes it to transcribe and translate the 32 base pairs of the fluorogenic aptamer mango-III. The G-Quadruplex structure of the mango aptamer allows it to fold around the TO1-biotin dye and constrain it which causes it to emit its energy in the form of a fluorescent signal with a 535nm wavelength. The sensor will be more sensitive relative to prior iterations of the estrogenic biosensors. The experimental data will be used to validate the predictions from the model and adjust it as necessary. There is vast potential for this sensor which can guickly create sensitive measurements of estrogenic compounds present in water.

ENVR 614

Investigating the enhanced solubility of carbon dioxide in nano-confined ionic liquids

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Ionic liquids (ILs) confined within nanostructures show non-ideal properties. Recently, we reported on the enhanced carbon dioxide solubility in encapsulated ILs within a fluoropolymer matrix. Here, we developed a new method based on quartz crystal microbalance (QCM) to measure the solubility of carbon dioxide, at medium pressures (up to 15 bar), for ILs confined in the polymeric domains. We systematically investigated the effect of the composition of IL/polymer mixture, pressure, temperature, and nanomaterials additive to the system to address the scientific question behind non-ideality of confined ILs. The results showed that by tailoring the material interfaces and creating interphase domains between the ILs and polymer, the gas solubility in these mixtures could be enhanced by 2 folds, demonstrating a synergistic effect from IL/polymer system in gas sorption.

ENVR 615

Copper ferrocyanide functionalized with MIL-125 composites for Cs⁺ removal from aqueous solution

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For removal of radioactive Cs⁺ in aqueous solution, MIL-125 based MOF materials was functionalized with copper ferrocyanide (abbreviation as MIL-125/CuFC). The adsorption capacities was achieved at 174.79 mg/g via the Langmuir isotherm model. However, behavior of Cs+ adsorption was fitted better to Freundlich isotherm model. Through the kinetic adsorption tests, it is confirmed that the adsorption was reached at equilibrium very quickly and followed the pseudo-second order reaction. The MIL-125/CuFC has also a high adsorption capacity over a wide pH range. In addition, It has good properties as a adsorbent such as high specific surface area and thermal stability by SEM, FT-IR, BET and TGA analysis. Therefore, the MIL-125/CuFC was synthesized successfully for the removal of Cs⁺ in aqueous solution.

ENVR 616

Morphology and adsorption removal of ^{110m}Ag in the radioactive waste liquid of the pressurized water reactor nuclear power plant

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^{110m}Ag is an important radionuclide in the radioactive effluent of nuclear power plant. Efficient removal of ^{110m}Ag nuclide in radioactive wastewater is an urgent problem to be solved. Based on the different hydrochemistry characteristics, the existent morphology of ^{110m}Ag was analyzed by theoretical analysis, model calculation and simulation experiments. The results show that ^{110m}Ag exists in Ag⁺/surfactants or Ag⁺/complexing agents complexes form, colloidal form, and free form. In our experiment, the adsoption of silver colloid and silver complexes were much lower than that of silver ions. According to the morphology of ^{110m}Ag nuclide, a treatment method combined advanced oxidation and inorganic adsorption technique was proposed and its feasibility was studied.



The oxidation properties of UV, H_2O_2 and UV/ H_2O_2 methods on the silver colloid.

ENVR 617

Assessing polyamide degradation kinetics by peracetic acid and chloramine using quartz crystal microbalance

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Membrane separation plays an important role in water reuse and desalination systems developed to supplement the dwindling global freshwater supplies. A major challenge of membrane process is biofouling. Although strong disinfectants such as chlorine can suppress biofouling, they can also degrade polyamide - the topmost, selective layer in many commercially-available nanofiltration and reverse osmosis membranes. In this study, we are evaluating a new disinfectant, peracetic acid (PAA), in terms of its polyamide compatibility using quartz crystal microbalance (QCM). Polyamide film was deposited on guartz crystal using molecular layer by layer (mLBL) deposition of trimesovl chloride (TMC) and mphenylenediamine (mPD). A film with 15 bi-layers and a thickness of ~ 19.1±1.4 nm was deposited on the silica substrate. The initial results show a significantly small mass loss of polyamide-coated crystals exposed to 1000 ppm of PAA after 20 hours. This is in sharp contrast to the rapid polyamide degradation when exposed to free chorine reported in literature: 20 hours of exposure to 250 hypochlorite solution completely degraded ppm polyamide. Desorption kinetics of polyamide exposed to PAA and monochloramine (NH₂Cl), the most common disinfectant used in full-scale advanced treatment systems for potable water reuse, under varying disinfectant concentrations, pH, and in the presence of Fe(II) are being investigated and compared. The findings of this study will generate an understanding of the impact of the disinfectant on polyamide degradation kinetics at molecular-length scales and hence will enable identification and design of an efficient disinfectant for membrane processes.

ENVR 618

Adsorption of zwitterionic and neutral per- and polyfluoroalkyl substances (PFASs) on differently charged cyclodextrin polymers

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Per- and polyfluoroalkyl substances (PFASs) are a class of thousands of fluorinated chemicals that persist in water resources around the world. There is an emerging need to develop novel cost-effective solutions to treat PFASimpacted waters due to correlation of PFAS exposure and adverse health effects. Adsorption technologies are of particular interest due to their ability to rapidly remove PFASs from water. However, existing adsorbents are known to remove relatively few of the thousands of PFASs, despite the known presence of other PFASs that are of increasing concern in water resources. In this study, we evaluated the performance of conventional and novel adsorbents to remove diverse types of PFASs from water. We conducted kinetics and isotherm experiments with a commercially available anionic exchange resin and 3 emerging cyclodextrin-based polymers (CDPs), and evaluated the removal of 11 PFASs which included 6 anionic, 2 neutral, and 3 zwitterionic PFASs. Two of the CDPs were modified to carry a positive surface charge, and 1 CDP was modified to carry a negative surface charge. Our studies demonstrated that the anionic PFASs were removed faster and to a greater extent by the positively charged CDPs, zwitterionic PFASs were best removed by the negatively charged CDP, and the neutral PFASs were not removed by any of the adsorbents. The anionic exchange resin removed only the anionic PFASs, as expected, though more slowly and to a lesser extent than the positively charged CDPs. The rate and extent of removal by all the adsorbents increased in experiments conducted at lower pH. Ongoing studies aim to evaluate the performance of these adsorbents in natural water matrices. Overall, these findings demonstrate the efficacy of CDPs for removing diverse types of PFAS from water and provide insight into adsorption mechanisms that determine the uptake of PFASs on CDPs.

ENVR 619

PFAAs identification and further classification through pKa analysis

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In recent years, long-chain perfluoroalkyl acids (PFAAs) that are commonly used in industrial production have been found to pose major health and environmental threats. Due to this a switch to a shorter chain of the compound has been initiated. The main purpose of this investigation of what will be classified as a PFAAs is to be able to identify physiochemical properties. To accomplish this density functional theory (DFT) calculations in conjunction with COSMO-RS calculations of already identified PFAAs and their anions are used to calculate the pKa of these compounds. By seeing the range of the pKas more information on a new way to classify PFAAs is being developed.

ENVR 620

Rapid and low energy degradation of PFAS in aqueous solutions by reverse vortex flow gliding arc plasma

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Poly- and perfluoroalkyl substances (PFASs) are a diverse set of organofluorine surfactants that are of great concern to the United States Department of Defense (US DoD) as emerging contaminants due to their potential human and ecosystem health risks. PFASs are persistent in the environment and are recalcitrant to degradation by many traditional remediation strategies. Across industrial sites, military sites, solids applied from water treatment plants, and other sources, there have been widespread contamination leading to large amounts of both solid and liquid wastes. The objective of this project was to demonstrate, as a proof-of-concept, the application of non-thermal plasma technologies for the treatment of PFASs from investigation derived wastes (IDW) from these sites. Specifically, this project focused on degradation of perfluoroalkyl sulfonates (PFSAs), perfluoroalkyl carboxylic acids (PFCAs), and fluorotelomer sulfonates (FtSs) by non-thermal air plasma in lab generated PFAS solutions, synthetic PFAS contaminated matrices, and PFAS contaminated IDW. In the liquid system, which used reverse vortex gliding arc discharges, we demonstrated greater than 90% removal within 60 minutes of treatment for a significant number of PFAS compounds tested. The percent degradation and percent defluorination of the tested PFFASs in the liquid system tended to decrease with shorter chain length

PFAAs and FtSs, but minimal differences were observed amount PFCAs, PFSAs, and FtSs with identical perfluoroalkyl chain lengths. In both the solid, which used dielectric barrier discharges (DBD), and the gliding arc liquid treatment systems, shorter chain PFAAs were generated. The promising results from the use of nonthermal plasma for treatment of PFAS contaminated matrices is promising in effectiveness as well as energy efficiency, requiring less than 500-900 kJ/L to achieve the PFAS degradation observed.

ENVR 621

Bioelectrochemical treatment of per- ad Polyfluoroalkyl Substances (PFAS) using *Acidimicrobiaceae* sp. Strain A6

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Per- and polyfluoroalkyl substances (PFAS) are widely used in consumer products and have posed a concern for public health because of the evidence of their adverse human health effects. Recent studies have shown that an autotrophic bacterium, Acidimicrobiaceae sp. strain A6 (A6 from here on), has the ability to defluorinate PFAS under anaerobic conditions. As an iron reducing bacterium, A6 is able to use solid ferric iron compound as the extracellular electron acceptor and has shown electrogenicity. Due to this characteristic, bacterium A6 has been grown in the microbial electrolysis cells (MECs) successfully with the anode as electron acceptor and has produced current while removing ammonium. To investigate the defluorination of PFAS by A6 in bioelectrochemical systems, PFAS were introduced into A6-inoculated MECs as well as microbial electrolysis continuous-flow reactors. Graphite plates and stainless steel meshes were used as electrode materials in the MECs, while granules of graphite with stainless steel mesh and Pt-coated carbon clothes were placed in the microbial electrolysis reactor to ensure larger anode surface area and to catalyze the cathodic reaction. Preliminary results show that fluoride and acetate were produced when FPAS were added into the MECs inoculated with A6. This indicates that degradation of PFAS through defluorination by A6 occurred in the MECs. In addition, A6 still produced current in the presence of PFAS, meaning introducing PFAS as electron acceptor into MECs does not fully suppress the electron transfer to the anode from A6. As continuous flow can provide fresh medium constantly, higher current production and better PFAS degradation are expected. With the ability to degrade PFAS with simultaneous ammonium removal under anaerobic condition, the A6-inoculated MECs and microbial electrolysis reactors have good application

prospects for PFAS contaminated water treatment and remediation.

ENVR 622

Rational material design for rapid capture and detection of perfluoroalkyl species

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Per and poly-fluoroalkyl substances (PFAS) are persistent organic pollutants, adversely affecting the environment. The strong carbon-fluorine bonds of PFASs make them resistant to physical and metabolic degradation leading to bioaccumulation, which can have serious effects on human's health, wildlife and ecosystem. The conventional analytical techniques for the quantitative determination of PFASs in environmental matrices are HPLC, GC-MS, etc. Despite their high reliability and accuracy, these laboratory-based techniques are expensive and can analyze only a limited number of samples, which impedes their broad applicability. To advance analysis and fast screening of samples, there is a critical need to develop cost effective, sensitive, easy to handle and portable methods for field detection of PFASs. This presentation will describe rational design of materials with specific and characteristic binding abilities for PFAS that can be incorporated into passive samplers and sensors for on site detection. The interaction of several materials with selected PFAS species and their incorporation into passive samples and an electrochemical sensing design will be discussed. This approach provides a new method for achieving qualitative and quantitative analysis of PFASs in the field. The developed method has potential for the onsite, selective, and sensitive detection of PFASs.

ENVR 623

Design and application of a biological system for detection, sequestration, and degradation of polyand perfluorinated alkyl substances

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Per- and polyfluoroalkyl substances (PFAS) are widely used commercial and industrial chemicals containing strong carbon-fluorine bonds which cause resistance to biological degradation. Along with being an emerging environmental contaminant, PFAS are known to accumulate in the human body leading to numerous health risks including reproductive deficits, hormone disruption, and cancer. Current wastewater PFAS remediation techniques involve adsorption on matrices

and subsequent degradation through incineration or chemical oxidation which often have limited efficacy. A biological strategy for detection, sequestration, and degradation of PFAS in aqueous environments is to engineer human liver fatty acid binding protein (LFABP) variants with high binding affinity which can then be used as a framework for the design of a fluorescent biosensor and enzymatic degradation system. This study focuses on the development of a survival-based screening technique of high binding affinity LFABP variants as well as initial study of tryptophan mutations as a fluorescent probing mechanism for further biosensor design. Preliminary screenings of perfluorooctanoic acid (PFOA) toxicity utilizing E. coli cell types found no apparent cell death up to 1000 ppm PFOA for BL21 (DE3) cells. However, E. coli strain AS19 showed significant loss of colony formation at lower levels of PFOA. This suggests success in future cell-survival screenings using AS19. Fluorescent assays were employed to characterize binding of several LFABP mutants as well as to assess the use of fluorescent mutations of LFABP as a biosensor for PFAS. Initial binding affinities of PFOA to wild type LFABP and mutants were characterized by using displacement of fluorescent probe 1-anilinonaphthalene-8-sulfonic acid (ANS), and the PFOA inhibition constants (Ki) were determined. Fluorescence spectra of tryptophan containing mutants were also obtained after titration of PFOA. The results discussed here set the groundwork for future research in the creation of a biological system capable to detecting and treating PFAS in aqueous environments.

ENVR 624

Assessment of isotherm fittings on co-removal of trace concentration 14 per- and polyfluoroalkyl substance by various resins in groundwater matrix

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Among several physicochemical technologies, ion exchange adsorption is a mature technology for the treatment of per- and polyfluoroalkyl substances (PFAS). In this study, six ion exchange resins and one granular activated carbon (GAC) were assessed for their ability to removal 14 PFAS compounds, at environmental relevant concentrations, from a groundwater matrix. Isotherm batch experimental concentrations were fit with linear, Langmuir, Freundlich and Temkin models. Our result indicates that in groundwater, when the PFAS concentration is low compared with the resin capacity, the resin isotherm performance will be best fit by a linear isotherm. As a general trend observed, PFAS removal efficiency generally improved as the aliphatic chain length increased, and this was observed for PFCA, PFSA, and FtS compounds. For the same chain length, PFSA exhibited greater media-water distribution coefficients, followed by FtS, and PFCA. Among the tested resins, A 694 E displayed the best sorption performance on all 14 PFAS tested. In addition, for an individual PFAS isotherms (e.g., PFOA as a single PFAS solute), single PFAS isotherm and PFAS suite isotherms were similar, suggesting that competition is not important at tested concentration ranges. Upcoming resin regeneration and column breakthrough experiments will be compared to predicted results based on isotherm performance.

ENVR 625

Assessment of endocrine disrupting effects of per- or polyfluoroalkyl substances on the H295R adreno-carcinoma cell line

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Per- or polyfluoroalkyl compounds (PFASs) are a broad class of synthetic chemicals used in a variety of industrial and consumer applications such as in fire extinguishing agents and hydrophobic surfactants. The multiple carbonfluorine bonds contribute to these compounds being chemically and thermally stable. Many treatment processes are being explored to remove PFAS in the aquatic systems. To assess efficiency of treatment processes, biological tests are needed to assess the changes in the toxicity of the PFAS-contaminated water after treatment. Accumulation of PFASs in humans has been linked to decreased levels of testosterone and increased levels of estrogens. Therefore, this study will determine the feasibility of using an adrenocarcinoma cell line, H295R, as a bioassay to reflect the endocrine disrupting effects of PFAS mixtures because H295R can produce 17 endogenous hormones including estrogens and androgens. The mechanism of PFASs toxicity is largely unknown with respect to which forms of PFASs may cause adverse effects, and whether the toxicity of these compounds is additive, synergistic, or antagonistic. The effect of the structural features of the different forms of PFASs, such as branching in the chemical structure, chain-length of the carbon backbone, or the type of head groups on the elicited response is poorly understood. The specific aim of this study is to determine the relative endocrine disrupting effects of model PFASs, perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS) in a model cell line, H295R. In this study, H295R were grown in a hormone free supplemented media. H295R cells were then exposed to nontoxic concentrations (1uM and 10uM) of PFOS and PFOA for 24 hours before the cellular media was collected. Solid phase extraction (SPE) was performed using an Oasis HLB cartridge to reduce matrix effects and to concentrate the hormones in the samples. Quantitative analysis of these hormones was performed using an optimized liquid chromatography tandem mass spectrometry method. This approach can successfully detect hormone concentrations in the cellular media to at least 1 ng/L, which can be used to determine changes in hormone concentrations in H295R cells caused by exposure to PFAS. This bioassay can potentially be useful for assessing changes in the endocrine disrupting effects of water that contain mixtures of PFAS without a *priori* knowledge of the chemical composition

ENVR 626

Application of electron beam for the degradation of short and long chain polyfluoroalkyl substances in drinking water

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Per and polyfluoroalkyl substances (PFASs) are a large group of anthropogenic substances that have been extensively used for over 60 years. These compounds can resist heat, oil, and water, and hence have been used as coatings in non-stick cookware, carpets, clothing, furnishing, paper as well as stain repellants and in firefighting foams. Due to their widespread use and resulting emissions, PFASs have been detected in surface water, groundwater, fish, birds, mammals, and humans worldwide. PFASs are highly persistent and resistant to degradation and have been associated with reproductive toxicity, reduced growth metrics in newborns and elevated cholesterol levels in humans. Conventional water treatment techniques such as coagulation, flocculation and sedimentation have shown to be ineffective in removing these substances. Although techniques such as reverse osmosis (RO), granular activated carbon (GAC) and nanofiltration (NF) have been shown to be effective in removing PFASs, these processes result in the generation of concentrated waste streams that requires further treatment and/or proper disposal. Hence, there is a need to identify techniques for destructive removal of PFASs from contaminated environments. In this study, we used the Accelerator Application Development and Demonstration (A2D2) tool located at the Illinois Accelerator Research Center (Fermi National Accelerator Laboratory) to investigate the efficacy of electron beam in the decomposition of PFASs in drinking water. Preliminary results have shown that this technique is effective in breaking down the persistent long chain (perfluorooctane sulfonate (PFOS) PFASs and perfluorooctanoic acid (PFOA)) due to the formation of

highly reactive species including hydrated electrons and hydroxyl radicals. Work is currently ongoing to (i) investigate the decomposition and defluorination efficiencies of long and short chain PFASs at environmentally relevant concentrations (ng/L); (ii) monitor subsequent byproducts formation during treatment, (iii) test the effects of various chemical additives on the overall PFAS removal efficiencies, and (iv) test the technology's effectiveness for treating PFASs mixtures and simultaneous removal of a co-contaminant, 1,4-dioxane. Results from this study will assess process feasibility and compare the performance of e-beam technology with other commercially available technologies (e.g. advanced oxidation processes) for water treatment.

ENVR 627

Rapid removal of poly- and perfluorinated compounds from high conductivity water in a batch-scale plasma reactor

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A batch-scale plasma reactor (1.5 L) was used to rapidly and effectively degrade poly- and perfluoroalkyl substances (PFAS) from ion exchange (IX) brine solution obtained from ECT₂ Inc. In the IX brine solutions, numerous PFAS were detected in a wide concentration range (~0.002 to 4 mg/L; total oxidizable precursors (TOP) ~46 mg/L, and total fluorine by combustion ion chromatography (CIC) ~99 mg F/L). The mean concentration of total perfluoroalkyl acids (PFAAs) (5 perfluorocarboxylic acids (PFCAs) and 4 perfluoroalkyl sulfonates (PFSAs) was 1.1 ± 1.2 mg/L (range 0.002 to 4 mg/L), and the concentrations of two identified PFAS precursors: 6:2 fluorotelomere sulfonate (6:2 FTS) and 4:2 fluorotelomere sulfonate (4:2 FTS) were 3.3 and 0.11 mg/L, respectively. Plasma-based water treatment resulted in rapid perfluorooctanoic acids (PFOA) (50 mg/L) degradation from 1.5 L synthetic water sample with faster rates in higher conductivity solutions (80 > 60 > 40)> 22 mS/cm). A faster rate of PFOA removal was found for higher delivered power (capacitance values 12 >8 > 4 nF). Several linear chain perfluoroalkyl carboxylic acids (PFCAs) (C4 to C7) were identified as byproducts of PFOA treatment, whose concentrations first increased and then decreased during 60 minutes of plasma treatment except for perfluorobutanoic acid (PFBA) whose concentration did not decrease during treatment. At the end of the treatment, 60% defluorination of PFOA was achieved with the remainder of <1% F associated

with remaining PFOA and its organic byproducts, and rest PFOA could be sorbed onto reactor walls and submerged diffuser. In real IX brine samples, the concentrations of long-chain PFAS (PFOA and PFHxS) were efficiently decreased by >99% in 120 minutes. Among the shortchain PFAAs near 100% removal of PFHpA, 75% removal of PFPeS, 60% removal of PFBS, 55% removal of PFHxA, and negligible removal (<5%) of PFPeA and PFBA was achieved. Among the precursors, complete removal for 6:2 FTS and 67% removal for 4:2 FTS was found. Overall, 76% of the TOP present in the IX brine sample was removed or chemically transformed to PFAAs during the treatment. The fluoride concentration increased from 1 to 12 mg/L after plasma treatment, indicating significant defluorination of PFAAs and their precursors. Overall, the results indicate that plasmabased water treatment is a viable technology for the treatment of PFAS-contaminated IX brine solutions.

ENVR 628

Removal of per- and polyfluoroalkyl substances by anion-exchange fibers

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Per- and polyfluoroalkyl substances (PFAS) are a broad class of fluorinated aliphatic compounds that have been widely used in diverse products, including fire-fighting foams, insecticides, stain-resistant fabric, food contact paper, and packaging. Due to the chemical and thermal stability of the C-F bond, PFAS are recalcitrant to drinking water and wastewater treatment processes and persist in the environment. At least six million US residents are supplied with drinking water exceeding the 70 ng/L PFAS lifetime health advisory level established by the US Environmental Protection Agency. New treatment approaches are needed to address this situation and safeguard public health. The objective of this study was to investigate the use of an ion-exchange fibers (*e.g.*, Mion AK-22 and Smopex-108) for removal of 12 chemically diverse PFAS, including perfluoroalkyl carboxylates, perfluoroalkyl sulfonates, fluorotelomer sulfonates, and perfluorooctane sulfonamides. The advantage of anionexchange fibers over resins stems from the shorter diffusive pathlength, which provides faster PFAS uptake and enables better utilization of the overall anionexchange capacity before breakthrough. Batch sorption tests were conducted with environmentally relevant PFAS concentrations in 10 mM NaCl and real groundwater solutions. The aqueous- and fiber-phase PFAS concentrations were used to calculate selectivity coefficients for PFAS anions over chloride. Relative trends in selectivity coefficients were explored by class and chain-length. To determine the ability of anionexchange fibers to treat PFAS in continuous-flow scenarios, columns were packed with anion-exchange fibers and a fraction collector was used to collect effluent samples as a function of bed volumes treated. The results showed that anion-exchange fibers can successfully treat diverse PFAS.

ENVR 629

Determination of occurrence and levels of per- and polyfluoroalkyl substances (PFASs) in deer tissue

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Per- and poly-fluoroalkyl substances (PFAS) are a broad class of more than 5,000 substances used in a variety of industrial and consumer applications because of their unique ability to modify surfaces, and their high chemical and thermal stability. PFASs are used in non-stick cookware, cleaning and personal care products, food packaging, and several other consumer products. Consequently, they have become ubiquitous environmental contaminants; they are also persistent and known to cause adverse health effects to human and wildlife. Several researches revealed presence and high levels of PFASs in different organisms consumed by humans. This work focuses on the optimization of PFASs extraction from deer tissue and applying the optimized method to determine occurrence and levels of PFASs in deer, which is regularly hunt down in Western New York. Results of the study showed that only four PFASs compounds with concentrations ranging from 1.0 - 20.0 ng/g were detected in eight deer samples analyzed for the study.

ENVR 630

Transformation of the neonicotinoid insecticides, thiamethoxam and imidacloprid, by select bacterial species

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Neonicotinoid insecticides, including thiamethoxam (THM) and imidacloprid (IMI), have become increasingly popular due to their specificity as insect neurotoxicants. However, neonicotinoids have been implicated as a potential contributing factor in Colony Collapse Disorder (CCD), the widespread disappearance of honey bees, which contribute to global produce production. The environmental persistence of neonicotinoids underscores the importance of developing a sustainable, ecologically-

friendly remediation technique to remove residual THM. This study assessed the THM bioremediation potential of six bacterial species: Pseudomonas fluorescens, Pseudomonas Pseudomonas putida, aeruginosa, Alcaligenes faecalis, Escherichia coli, and Streptococcus lactis. P. fluorescens, P. putida, and P. aeruginosa were able to utilize THM over IMI as a sole carbon or nitrogen source, with better growth when THM was used as the sole nitrogen source compared to carbon. Significant (p<0.0001) reductions in THM concentration in aqueous media were observed for P. fluorescens (67%), P. putida (65%), P. aeruginosa (52%), and A. faecalis (39%) over 24 days, and for E. coli (60%) and S. lactis (12%) over 14 days. The time required to remove 50% of the THM in the media was: E. coli (12d), P. fluorescens (18d), P. putida (19d), and P. aeruginosa (23d). Neither A. faecalis nor S. lactis achieved 50% removal during the study periods. Maximal thiamethoxam removal occurred at 30°C for all bacterial species assessed. HPLC chromatograms of P. fluorescens, P. putida, and E. coli cultures revealed that as the area of the THM peak decreased over time, the area of an unidentified metabolite peak increased. Identification of the metabolite is currently underway. If the metabolite is found to be less hazardous than thiamethoxam, testing will follow to evaluate this bioremediation technique in the field.

ENVR 631

Photo-induced Fenton chemistry of naturally occurring ferritin

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Photoexcitation of the native iron semiconductor housed within the cage-like protein, ferritin, in the presence of a sacrificial electron donor releases soluble ferrous iron (Fe²⁺), which can be used for environmental remediation reactions. To potentially enhance remediation efforts, photoexcitation reactions with ferritin were completed in the presence of hydrogen peroxide to observe if Fenton chemistry could be induced. The desired reactive product, hydroxyl radicals, was monitored through the use of an insitu probe, coumarin, which produces a fluorescent product after reaction with the species, as a function of wavelength, pH, and concentration. Results indicated that hydroxyl radical production, arising from reactions with ferritin, increased with decreasing pH and in the presence of the sacrificial electron donor, tartrate. Further, the production depended more on the concentration of H_2O_2 than Fe(II). The stability of ferritin exposed to hydroxyl radicals was studied using transmission electron microscopy (TEM), dynamic light scattering (DLS), and gel electrophoresis (SDS-PAGE). Preliminary results indicate that the protein cage is stable under this Fenton
chemistry, and potential remediation applications of the photochemical system will be discussed.

ENVR 632

Manganese loaded ferritin for hydrogen peroxide decomposition

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The ferritin protein cage has been used to host metal oxide nanoparticles other than the native ferric oxide for various chemical applications. Many of these strive to improve environmental remediation strategies, a similar aim in this research where we investigate the role of manganese loaded ferritin (MnFtn) for the catalytic decomposition of hydrogen peroxide (H₂O₂), which generates oxygen gas (O₂). The manganese core was synthesized in apoferritin (ApoFtn) under basic conditions (pH 8.9) by oxidation and precipitation. The structures were characterized by UV-Vis, transmission electron microscopy (TEM), inductively coupled plasma optical emission spectrometry (ICP-OES), and dynamic light scattering (DLS) and compared to ApoFtn to confirm Mn loading in the protein cage. The decomposition of hydrogen peroxide was carried out in a closed system where O_2 generation was followed by a luminescent dissolved oxygen probe. The effectiveness of MnFtn in the decomposition of hydrogen peroxide was determined by comparing the sample to ApoFtn, birnessite (δ -MnO₂), and an amorphous manganese oxide (A-Mn). Additionally, H₂O₂ decomposition was studied as a function of manganese loading. The preliminary results indicate that O₂ generation was successful when H₂O₂ was exposed to MnFtn and is potentially more active compared to an equimolar concentration of mineral.

ENVR 633

Geospatial distribution and fate of microplastics in the Hudson-Raritan estuary

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Microplastics have become an increasingly large environmental concern due to the risks they may pose to

aquatic ecosystems, as well as terrestrial species and humans as microplastics are transferred up trophic levels. This study aims to confirm the presence of microplastics (MPs) in surface water and zooplankton samples collected at ecologically and geographically significant sites in the Hudson-Raritan Bay area. Furthermore, MPs are enumerated for each sampling site using visible microscopy and characterized through the use of vibrational micro-spectroscopic techniques: Fourier Transform InfraRed (FTIR) and Raman. The use of these complementary techniques enables confirmatory MP identification. In some cases, copolymers or surface contamination or weathering can be observed. For some sample size classes (<250 microns), challenges include locating MPs on sample substrates and lengthy spectral data collection. These concerns will be discussed including the difficulty in identifying heavily weathered polymers and the high variability in sample properties (fragile nature, opaque vs. transmissive, etc.) and strategies to circumvent such issues will be suggested. For example, the use of an FTIR microscope with a focal plane array (FPA) detector has allowed for the relatively quick, automated collection of spectra across the surface of the sample substrate. This technique is particularly advantageous when examining MPs such as thin films that would be difficult to detect using a single-point detector due to their very low contrast and visibility against the sample substrate. Results will be presented on the relative concentrations of MPs found at each and correlations sampling site with relevant hydrodynamic properties, such as salinity. Additionally, results from zooplankton studies, including MP types, sizes and morphologies, will be discussed. These results will provide key insight into ingestion of MPs by biota, as well as regions of concern with regards to MPs entering the food chain.

ENVR 634

Evaluation of microplastic load in a waste water treatment plant (WWTP)

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Production and demand for single-use plastic materials is at an all-time high, resulting in increasing concerns about the proper disposal and end of life treatment of these materials. Plastics can accumulate in the environment and degrade over time into smaller fragments known as microplastics. Microplastics have a diameter of five millimeters (5 mm) or less and can easily be transported across different environmental compartments and trophic levels of the food chain. The aim of this study is to determine the microplastic content of influent, effluent and sludge (watered and de-watered) samples from the WWTP in Cookeville, Tennessee. Grab samples will be collected and passed through three sieves with different mesh sizes. All remaining solids will be digested by wet peroxide oxidation to remove all biological material and separated according to their densities via a saturated sodium chloride solution. Resulting particles will be oven dried, weighed and identified using Fourier Transform Infra-red Spectroscopy. Particle sizes will be measured using a laser diffraction particle size analyzer.

ENVR 635

Investigating the fate and biological impacts of polystyrene nanoplastics on *Shewanella oneidensis* MR-1

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The design of plastic materials, while resulting in highly useful and marketable products, has led to a challenging, long-term environmental problem. As advancements have been made in determining the fate and environmental role of plastic materials, the field of nanoplastics has gained increasing interest when considering their potential impact on local ecosystems. This work explores the impact of nanoplastic materials on viability and functionality of a model bacterial species. Specifically, Shewanella oneidensis were exposed to polystyrene(PS) nanoplastic particles and monitored for changes in viability using a growth based viability assay. The cell function of riboflavin secretion, a molecule secreted to serve in the terminal electron transport chain during metal reduction, was monitored with liquid chromatography. Upon exposure 4, 8 or 12 hours of exposure, the viability of the S. oneidensis indicated no significant changes, while the amount of riboflavin secreted increased and was directly correlated with increasing concentrations of PS nanoplastic exposures. The localization of the nanoplastics within or on the surface of the cells will be pursued with electron microscopy and mass spectrometry. Through this work we will provide valuable insight on the fate of nanoplastics in biological systems by investing the physical interactions between PS nanoplastics and S. oneidensis.

ENVR 636

Aqueous photochemistry of polyolefins

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Polypropylene (PP) and polyethylene (PE) are commonly used polyolefins in a variety of applications, which have resulted in their accumulation in the environment. Once in the environment, these polymers undergo various chemical and physical transformations as the result of environmental stressors including sunlight. During photodegradation, PP and PE undergo reactions such as oxidation, crosslinking, and chain scission that are induced from UV light; yet, there are key gaps in knowledge on the phototransformations that occur under aqueous conditions. Therefore, it is the goal of this project to characterize the phototransformations of PP and PE in simulated natural water conditions. This work focuses on PP and PE thin films with 25 and 30 mm thicknesses, respectively. The polymer films were irradiated with 254 nm and 350 nm UV light in air, ultra-pure water, and solutions of dissolved organic matter (DOM) (10 mgC/L Suwanee River natural organic matter) to simulate natural systems. For comparison, the films were subjected to natural weathering over the course of Summer 2019 in Duluth, Minnesota, Irradiated plastics were then evaluated for a variety of chemical transformations. It was observed using Fourier Transform Infrared Spectroscopy (FTIR) that oxidation occurred both in air and aqueous environments, with oxidation in aqueous environments happening at a slower rate. Using gel fraction analysis crosslinking was observed to occur in both air and aqueous environments with a higher crosslinking fraction occurring in aqueous environments. Through this work, we have gained a more clear perspective on the chemical weathering of materials found in aquatic plastic debris, which will allow us to predict the behavior of these materials, including the breakdown into microplastics.

ENVR 637

Release and transformation of organic additives from polymers in aqueous media

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Additives are organic or inorganic chemicals added to a polymer matrix to enhance the physiochemical properties of a plastic product. When a plastic reaches the end of its consumer lifetime and is discarded, immersion and degradation mechanisms such as UV photolysis in surface waters result in the release of additives to the surrounding environment. Unfortunately, these additives may pose significant health and environmental risks including endocrine disruption, birth defects, and cancer. Despite ever-growing presence in plastic products, a detailed understanding of the factors controlling the rate of additive release from polymers in aqueous environments remains undetermined. To address this challenge, the release and transformations of polymer additives was investigated in a variety of environmental exposure scenarios. Additive-modified polymers were prepared using solution blending techniques to create a suite of plastics that exhibit systematic differences in composition and properties. The resultant polymers were immersed in water and also exposed to accelerated weathering techniques, including high intensity UV irradiation, aggressive oxidation, and thermal cycling. High resolution-mass spectrometry was used to quantify the concentration of released additives and identify the extent of additive transformation.

ENVR 638

Comparison of different filter media materials for metals removal from urban stormwater runoff using green stormwater infrastructure

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The metals found in urban stormwater runoff have the potential to detrimentally impact ecosystem and/or human health. Infiltration based green stormwater infrastructure (GSI) is increasingly being employed to address both water quantity and quality concerns. This study evaluates sorbent media amendments to improve contaminant removal. Batch experiments were performed to determine the adsorption capacity of five potential soil amendment materials derived from affordable and abundant sources (Biochar (BC), Iron amended biochar (FeBC), Iron chips (FeCh), Scrap tire (ST) and Coir coconut (CC)) for six common toxic metals (Pb, Cu, Zn, Cd, Cr and Ni). Adsorption isotherms and kinetics were investigated, and it was observed that the isotherms of metals were fitted well by both Langmuir and Freundlich model, and the kinetic data were described well by the pseudo-second order for all selected adsorbents and metals, so adsorption process was assumed to be due to chemisorption. The extent of adsorption and removal of metals was found to be dependent on the type and concentration of metal as well as the filter material, as CC and FeCh showed high removal efficiencies of all desired metals (90-99%), but ST (20-99%) and BC (2-97%) had varying removal efficiencies of selected metals with no Zn removal by ST. Finally, FeBC had the worst performance removing only Pb and Cr (20-93%), and no removal of Cu, Ni, Zn and Cd. The adsorption mechanism of these adsorbents was mainly attributed to the interaction between metal ions and surface functional groups of adsorbents such as hydroxyl, carboxyl and carbonyl groups, so adsorption capacities of adsorbents varies based on the diversity and number of functional groups of their surfaces. The ongoing study is going to evaluate the effect of different parameters (pH, ionic strength, and dissolve organic carbon) on removal efficiency of selected

adsorbents. For the future work, surface characterization of adsorbents will be investigated using scanning electron microscope (SEM) and Fourier-transform infrared spectroscopy (FTIR). Moreover, bioretention columns will be designed using six different filter media to evaluate the effect of different media on hydraulic conductivity and removal of pollutant.

ENVR 639

Fe-OM coprecipitation and its effects on bioavailability of Cu and OM to denitrifying organisms

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Treatment wetlands and riparian zones undergo chemical and biological reactions that are sometimes at odds with environmental treatment goals. Active zones of iron coprecipitation with organic matter at the oxic-anoxic interface typically retain trace metals but can alter microbial activity. Specific microbial processes such as denitrification require Cu as an enzyme cofactor to reduce nitrous oxide, a more potent greenhouse gas, to nitrogen gas. The impacts of these geochemical reactions on microbial activity are not well understood. We used soil slurry mesocosms to examine how Fe-OM coprecipitation and sorption reactions influences the factors that control N₂O vields and rates. Through a series of treatments applied to soil slurries that control Cu and OM availability under fixed oxygen and nitrate concentrations, soil moisture, and pH, we assessed a series of conditions that altered Cu and OM availability through providing excess Fe, glucose as readily available carbon source, and humic acid (HA) as a coprecipitate for Fe. We hypothesized that there would be a net decrease in total denitrification (N2 + N₂O) when OM is not available to the organisms and an increase in N₂O yield [N₂O/(N₂O +N₂)] when Cu availability is limited in the environment. In mesocosms where excess Fe and humic acid coprecipitated and reduced bioavailable Cu, N2O rates decreased significantly compared to controls. Scenarios where just humic acid was present to limit Cu availability to organisms through metal binding, had less of a decrease in N₂O production. Additional experiments are in progress to explore ratios of Cu to Fe and OM to more specifically link Cu availability to denitrification processes.

ENVR 640

Determination of optimum dosage of chemical coagulant/flocculants needed for sludge treatment

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The efficiency of sludge treatment by physicochemical method is highly dependent on the accurate use of the optimum dosage of coagulants/flocculants needed for such treatment. In this work, the optimum dosages of coagulants/flocculants needed to effect proper treatment to sludge obtained from four industries; aluminium extrusion, brewery, pharmaceutical and textile processing factories were determined. For quick analysis, COD was chosen to assess the degree of treatment as there is a relationship between COD on one hand and BOD, Suspended Solid (SS), and total solid (TS) on the other hand. It was found that treatment of these sludges were most effective at coagulants doses of 3-5g/l for alum, and iron (III) chloride, 15-20g/l for lime and 400-700mg/l polyelectrolyte. It was also found that, the higher the doses of alum, iron (III) chloride and polyelectrolyte, the more acidic the sludge medium. The efficiency of treatment increased with increase in lime dosage and the most efficient treatment was achieved between the pH of 11 and 12. pH was found to be a major factor affecting coagulation of sludge and hence its treatment.

ENVR 641

Metabolization of tire wear products in synthetic stormwater by three model white rot fungi

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Extracellular white rot fungal enzymes have broad specificity, targeting a wide variety of structurally complex compounds such as lignin, polycyclic aromatic hydrocarbons, and pesticides. One situation where fungi could be used is within engineered natural treatment systems to treat the myriad of contaminants often present in urban stormwater. Tire wear products (TWP) are emerging contaminants of concern in stormwater. Tire wear particles are generated from the mechanical abrasion of tires with road surfaces. Tire particles can then be washed into surface water during rain events, allowing TWP to leach into streams and rivers and subsequently impact aquatic health. TWP have been implicated as possible drivers of acute coho mortality following rain events among other ecological impacts, meriting novel treatment strategies such as fungal bioremediation to address the complex mixture of contaminants. To assess treatment potential of fungi for

tire wear products in stormwater, we conducted batch experiments with three different white rot fungi species and select tire wear products. We quantified fungal removal of four tire wear products in synthetic stormwater: acetanilide, 1,3-diphenylguanidine, hexamethoxymethylmelamine, and n,n'-dicyclohexylurea. To measure changes in concentration of TWP over time, we used liquid chromatography coupled with diode array detection or mass spectrometry. We probed enzymatic pathways by inhibiting the intracellular enzyme, Cytochrome P450 and measuring removal of TWP over time. Ongoing work includes untargeted metabolomics approach to identify fungal metabolic products. These results indicate the potential of using white rot fungi to target select TWP in stormwater in engineered natural treatment systems such as bioretention cells.

ENVR 642

Dissolved organic matter as a photochemical source of reactive species: Current challenges and implications for the fate of aquatic contaminants

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The photochemistry of dissolved organic matter (DOM) has been studied for at least four decades, still many aspects of the photochemical activity of DOM, with particular focus on the consequences for the fate of organic contaminants in aquatic systems, remain to be explained. Most photochemically produced reactive intermediates (PPRIs) that are produced upon irradiation of DOM, with the exception of singlet oxygen $({}^{1}O_{2})$, cannot be observed directly by spectroscopic methods, and probe compounds are required for their detection and quantification. This contribution reviews the use of probe compounds to quantify primarily the steady-state concentration of reactive transient species. This task is very complex in the case of transient intermediates that are constituents of the photo-excited or photochemically modified DOM, such as excited triplet states of chromophoric moieties in the DOM, "lower-energy" hydroxylating species, and other organic radicals, which possibly comprise phenoxyl, semiquinone and peroxyl radical moieties. To illustrate this topic, a few examples of DOM-derived PPRIs are discussed and recent studies on the characterization of organic radical oxidants are presented.

Investigation of the phototransformation mechanisms of benzotriazole in surface waters using compound-specific isotope analysis

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Benzotriazole is part of a larger family of benzotriazoles which are widely used as antifreeze, corrosion inhibitor and UV-stabilizers in many commercial and industrial applications. It is frequently detected in urban runoff, wastewater, and receiving aquatic environments. In surface waters, benzotriazole is typically resistant to biodegradation and hydrolysis, but can be transformed via direct photolysis and photoinduced mechanisms, e.g., by reactive species formed from dissolved organic molecules. Compound-specific isotope analysis (CSIA) is a promising tool to track and quantify contaminant transformation in the environment. Due to the highly reaction-specific isotope fractionation patterns, CSIA can provide direct evidence of contaminant transformation and has the potential to provide insights into transformation mechanisms. In addition, measuring changes of isotope ratios of more than one element can help identify the relative contribution of different reaction mechanisms. Therefore, the aim of this study was to characterize the phototransformation processes of benzotriazole using multi-element CSIA. The direct photolysis of benzotriazole resulted in significant ¹⁵N fractionation, which were -3.4±0.4‰ at pH 5, -7.0±0.8‰ at pH 7 and -4.7±0.6‰ at pH 9, respectively, indicating a N-N bond fission yielding imine is the rate-limiting step. The identified transformation products of aniline, 3aminophenol and phenazine further supported that the vield imine was rapidly stabilized via two routes: nitrogen elimination followed by hydroxylation and a dimerization process. The formation of hydroxybenzotriazole during indirect photolysis suggested an oxidative attack by OH radical on the benzene ring. The significant ¹³C fractionation and non-detectable ²H and ¹⁵N fractionation in the UV/H₂O₂ system revealed that the formation of O-C bond at the benzene ring was the rate-limiting step of the indirect photolysis. The results of this study highlight the great potential for multi-element CSIA application to track benzotriazole degradation in complex environments.

ENVR 644

Investigating the photodegradation of triclosan's photodegradation products: Chlorinated dibenzo-pdioxins and hydroxylated biphenyls

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Triclosan, an antibacterial agent that has been incorporated into numerous consumer products, including hand soap, toothpaste and textiles, is capable of undergoing direct photodegradation. The phenolate $(pK_a=8.1)$ is the photoactive form of triclosan. During its photodegradation, the formation of 2,8-dichlorodibenzop-dioxin and hydroxylated polychlorinated biphenyls ((OH)₂PCBs) occurs, which also pose a risk to aquatic organisms. In this work, we explore the photodegradability of these transformation products by direct photolysis. The results show that these compounds are capable of being degraded in ultraviolet B (UVB, 280-315 nm) and ultraviolet A (UVA, 315-400 nm) light with relatively high guantum yields. Understanding the environmental fate of these compounds is not only important for determining the ultimate impact of triclosan occurrence in the environment, but also because chlorinated dibenzo-p-dioxins and hydroxylated PCBs have other sources that contaminate environmental systems (i.e., historical contamination from industrial wastes).

ENVR 645

Fluorinated photoproduct formation from photolysis of pharmaceuticals and agrochemicals

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Use of fluorine in agrochemical and pharmaceutical design has increased since the first fluorinated pharmaceutical came to market in 1957. Fluorine changes the physical properties, including lipophilicity, solubility, conformation, pKa, and metabolic stability of compounds, making its use appealing. Motifs of fluorine in common pharmaceuticals and agrochemicals include: -CF3 and -F groups bonded directly onto an aromatic or pyrazole ring, -CxHyFz aliphatic groups, and -SFz groups. Photolysis of these compounds is a potential source of new fluorinated compounds into the environment. Depending on the chemical structure and fluorine motif, fluoride and/or other organic fluorine compounds are produced and released into surface waters. With the potential of organic fluorine products, such as fluoroacetic acid, monitoring of product formation during photolysis of various fluorinated motif types is needed. To determine fluorinated products, selected pharmaceuticals and agrochemicals with varying fluorine motifs were subjected to photolysis in four aqueous conditions: pH 7, pH 10, 250 µM H2O2 at pH 7 to form hydroxyl radicals, and 1 mM

sulfite at pH 10 to form e-aq. Ortho, meta, and parafluorophenol as well as ortho, meta, and paratrifluoromethylphenol were also subjected to photolysis to determine if ring placement varies product formation. Product identification and fluorine quantification was conducted using a 600 MHz 19F-NMR and complemented by LC-HRMS, and rates of parent compound loss were monitored on an HPLC. Preliminary results suggest that fluoride is one of the most common products, but certain motifs show the formation of trifluoroacetic acid and other organic fluorine molecules. Results will help the design of fluorinated compounds to have the same functionality with the forethought of reducing harmful photoproducts.

ENVR 646

Initial photochemical fate of dissolved amino acids in natural aquatic environment by coupling theoretical calculations and experiments

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In aquatic systems that receive municipal wastewater, effluent organic matter (EfOM) containing soluble microbial products and dissolved organic nitrogen (DON) plays a major role in the biogeochemical uptake of carbon, nitrogen, and phosphorus. The EfOM also contributes to the fate and transport of various water constituents including trace elements, nutrients, and synthetic organic contaminants. Dissolved amino acids (both free and combined amino acids), which comprise a significant fraction of DON in EfOM, are major sources of nitrogen and carbon in freshwater systems. Combined amino acids account for approximately 10-20% of wastewater DON. The rare abundance of free amino acids in freshwater systems and the large energy cost of synthesis make free amino acids essential to aquatic biota. Abiotic photochemical oxidation is a major transformation pathway of amino acids in sunlit waters. Photochemical oxidation occurs through direct photolysis of amino acids and indirect oxidation by dissolved photochemically produced reactive intermediates, such as excited triplet state of chromophoric dissolved OM (³CDOM^{*}), singlet oxygen, hydroxyl radicals, and hydrogen peroxide. Goal of this current project is to elucidate the photochemical fate of free amino acids in freshwater systems. In this talk, we use ab initio and density functional theory quantum mechanical methods to predict the initial photochemical elementary reactions of photo-viable three amino acids: tyrosine, histidine, and methionine in the presence of structurally known welldefined DOM photosensitizers. We theoretically

calculated the aqueous-phase free energies of activation of each indirect oxidation elementary reaction pathway to investigate the kinetics. We also calculated the aqueousphase free energies of reactions to examine if each pathway is thermodynamically feasible. The contributions of each pathway to an overall photochemical degradation were validated with our own laboratory-controlled benchtop experiments. This is the first study to couple theoretical calculations and experiments to elucidate the initial photochemical fate of free amino acids.

ENVR 647

Interactions of light and chemical reactions in the aquatic environment: Kinetic and mechanistic aspects

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The importance of photochemical reactions in aquatic environments has become increasingly evident in the last fifty years. Here I discuss examples of: 1) direct and sensitized aqueous photoreactions of contaminants and natural compounds, including emerging materials such as nanomaterials and their composites with polymers; 2) the effects of photochemistry on microbial availability and toxicity of contaminants; 3) aquatic photochemical sources of atmospherically-important trace gases; 4) photobleaching and its impact on aquatic optics and the remote sensing of ocean color; 5) the role of photochemistry in biogeochemical cycles of carbon, nitrogen, and sulfur; and 6) links between photochemical and biological processes, including photoinactivation of pathogens and related indicators. A key focus is on the role played by the colored component of dissolved organic matter (CDOM) in controlling the availability of solar UV radiation in aquatic systems and initiating indirect photoreactions. Upon irradiation, CDOM and other natural substances (like nitrate) produce excited state and reactive oxygen species such as triplet states, singlet oxygen, superoxide/hydrogen peroxide and hydroxyl radicals that mediate indirect photoreactions in aquatic environments. I will discuss approaches to studying and modeling these intriguing photoreactions in the laboratory and field.

ENVR 648

Photochemical production of dissolved inorganic carbon from terrestrial organic matter: Significance to the oceanic organic carbon cycle - then and now

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Photochemical oxidation of dissolved organic carbon (DOC) is now recognized as a significant and ubiquitous process in surface waters, occurring everywhere chromophoric dissolved organic matter (CDOM) absorbs solar UV radiation. In 1995, Miller and Zepp published a first rough estimate of the degree to which photochemical production of dissolved inorganic carbon (DIC) and carbon monoxide (CO) controls the lifetime of terrestrial DOC in the ocean, concluding that "photo-oxidation of DOC by sunlight should be considered a dominant removal mechanism of organic carbon from the ocean." Considerable effort has been spent since then to quantify this process on regional and global scales. Direct DIC photochemical rates have been virtually impossible to measure in blue waters with vanishingly low CDOM absorbance, forcing the extrapolation of coastal DIC rates and quantum efficiency curves using optics and photochemical proxies to model the global significance of DOC photooxidation. A new and novel method using moderate DIC isotope enrichment (MoDIE) has potential to directly examine the validity of these extrapolations and directly test chemical proxies. Here we report MoDIE results that directly compare DIC photoproduction using concentrated DOM isolated from coastal to blue waters by solid phase extraction, re-dissolved in in a blue water matrix to have the same starting absorbance, and irradiated in matched solar simulators. Preliminary results suggest blue water DOC isolates, collected in July, are less efficient than those from coastal and inshore stations; and there may be a seasonality to DIC photoproduction in the open Atlantic ocean. From this, and using coincident measurements of HOOH, we examine the validity of photochemical proxies, the fundamental optical extrapolations used routinely in regional and global models for photochemical rates, and reevaluate the premise that "photo-oxidation of DOC by sunlight should be considered a dominant removal mechanism of organic carbon from the ocean."

ENVR 649

Coupling of multivariate statistics and advanced analytical techniques for understanding the composition of terrestrial organic matter and its changes during photo-irradiation

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Photochemistry of dissolved organic matter (DOM) has gained a lot of momentum in the last two decades. It is well-known as a highly impactful chemical process to DOM being a significant sink for carbon but also able to

produce various by-products. Only recently through the development of advanced NMR and ultrahigh resolution mass spectrometry it was possible to start elucidating the compositional changes occurring during photo-irradiation processes and identify structures of the involved molecular species. Commonly used techniques in photochemical studies are ultraviolet-visible and fluorescence spectroscopies, specific tools for lightreactive species that drive photochemical changes within DOM. The fractions of DOM that are evaluated using these techniques, chromophoric and fluorophoric DOM (CDOM and FDOM, respectively), are operationally defined, and lack information on their molecular composition. For addressing these gaps, we have collected a suite of nine terrestrial blackwater samples to characterize DOM composition, and to evaluate structural changes after photo-irradiation in a solar simulator. We observe high variability in the degrees of photodegradation, and also a formation of unidentified fluorophore components. Through the use of Principal Component Analysis (PCA), Parallel Factor Analysis (PARAFAC), and Spearman's Correlation Analysis, we have coupled the optical (UV-VIS and fluorescence spectroscopies) and compositional techniques (NMR spectroscopy and mass spectrometry) to obtain better understanding of the composition and reactivity of CDOM and FDOM in sunlit aquatic environments, providing more information in regards of their biogeochemistry.

ENVR 650

Sunlight converts polystyrene to carbon dioxide and dissolved organic carbon

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Numerous international governmental agencies that steer policy assume that polystyrene persists in the environment for millennia. Here, we show that polystyrene is completely photochemically oxidized to carbon dioxide and partially photochemically oxidized to dissolved organic carbon. Lifetimes of complete and partial photochemical oxidation are estimated to occur on centennial and decadal time scales, respectively. These lifetimes are orders of magnitude faster than biological respiration of polystyrene and thus challenge the prevailing assumption that polystyrene persists in the environment for millennia. Additives disproportionately altered the relative susceptibility to complete and partial photochemical oxidation of polystyrene and accelerated breakdown by shifting light absorbance and reactivity to longer wavelengths. Polystyrene photochemical oxidation increased approximately 25% with a 10°C increase in temperature, indicating that temperature is unlikely to be a primary driver of photochemical oxidation rates.

Collectively, sunlight exposure appears to be a governing control of the environmental persistence of polystyrene, and thus, photochemical loss terms need to be included in mass balance studies on the environmental fate of polystyrene. The experimental framework presented herein should be applied to a diverse array of polymers and formulations to establish how general these results are for other plastics in the environment.

ENVR 651

Nanoprobes for surface-enhanced Raman spectroscopy (SERS) based pH sensing in confined microenvironments

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pH is a critical trait that dictates chemical and biological reactions, partitioning, and reactivity in confined microenvironments, including aerosol droplets and biological cells. Quantification of pH in confined microenvironments experimentally is challenging because of their inaccessibility to conventional pH probes. To address this issue, nanoprobes that are functionalized by pH-sensitive molecules have been designed for pH surface-enhanced measurements by Raman spectroscopy (SERS). 4-mercaptopyridine (4-Mpy) is a pH reporter molecule commonly used to functionalize nanoprobes for SERS based pH measurements. However, nanoprobes functionalized by 4-Mpy alone have low pH sensitivity and are subject to interference by halide ions in sample media. To improve nanoprobe pH sensitivity and reliability, we functionalized gold nanoparticles (AuNPs) with both 4-Mpy and bromide ion (Br⁻). Br⁻ electrostatically stabilizes protonated 4-Mpy, thus enabling sensitive SERS detection of the protonation state of 4-Mpy as a function of pH while also reducing variability caused by external halide ions. Through optimization of the functionalization parameters, including suspension pH, [4-Mpy], and [Br-], the developed nanoprobes enable monitoring of pH from 2.1 to 10 with high SERS activity and minimal interference from halide ions within the sample matrix. As a proof of concept, we were able to quantify the pH levels and image the pH distribution inside individual aerosol droplets and cancer cells. This study provides a novel way to engineer reliable 4-Mpy-functionalized SERS nanoprobes for the sensitive analysis of spatially localized pH features in halide ioncontaining microenvironments.

ENVR 652

Nanomaterial-based portable sensor for phosphate detection in eutrophic water

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Phosphorus is an essential nutrient for living organisms. It is found in the structure of cell membranes, genetic materials, and is important for energy production. Phosphorus is mainly used as fertilizers in agriculture. While beneficial for living organisms, its excessive use and discharge in the aquatic ecosystem leads to water eutrophication, causing algae bloom formation, oxygen levels reduction and an overall poor quality of drinking water supplies. In order to maintain water quality and safety and minimize the cost and effects of eutrophication it is important to develop strategies for monitoring and managing phosphorous levels in the environment. This presentation will describe the design and development of methodology nanomaterial-based for phosphate detection. The nanomaterial has oxidase-like activity and upon phosphate being adsorbed on the surface, it alters its activity. The detection is based on incorporation of redox dves in the system which demonstrates a colorimetric response dependent on the phosphate concentration. This method could be adapted to portable platforms (e.g. paper-based sensor) for rapid onsite detection and assessment of the extent of water eutrophication in water bodies.

ENVR 653

Chemical fingerprinting applied to environmentally relevant media

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Our group has been developing polymer-based chemical fingerprinting systems to target multiple analytes of environmental relevance, including organophosphates, heavy metal cations, and polycyclic aromatic hydrocarbons. We will report on our recent progress towards making some of these systems compatible with high-salinity environments (for monitoring in sea- and brackish waters), as well as towards the inclusion of simpler assay formats (paper-based assays), and detection methods (electrical signals).

Sensitive detection and identification of antibiotic resistance genes (ARGs) enabled by surfaceenhanced Raman scattering (SERS) and multiclass support vector machine (MC-SVM)

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Antibiotic resistance is continuing to develop around the world due to the overuse of antibiotics and is acknowledged as a serious threat to human health. In this context, antibiotic resistance genes (ARGs) are emerging bio-contaminants that enhance the likelihood that antimicrobial resistance will spread through the environment. There is an urgent need for a rapid and sensitive detection technique for ARGs. In this study, surface-enhanced Raman scattering (SERS), a sensitive analytical tool that enables single-molecule detection, was used to detect a proxy ARG, mecA, with different concentrations. mecA is an ARG that enables the development of methicillin-resistant Staphylococcus aureus (MRSA). To create SERS active hot-spots, a slippery liquid-infused porous SERS (SLIPSERS) platform was used to concentrate water droplets containing gold nanoparticles (AuNPs) and a mecA segment. Isolation was achieved via free-pinning droplet evaporation on a hydrophobic porous PTFE membrane. With this SERS substrate, detection of low concentrations of the target down to 10⁻²³ M were achieved. A linear trend was observed between the logarithmic concentration of mecA segment and the normalized intensity of the corresponding peak in the Raman spectrum. We collected different Raman spectra of mecA segment (86 base pairs) and its base mismatches (2, 6, 10, 20 bases mismatched) to investigate if different shape profiles of Raman spectra of the gene reflect sequence differences. Using the collected Raman spectra, a multiclass support vector machine (MC-SVM) model was generated and trained. The results showed that MC-SVM model had 87.8% overall accuracy to predict the correct *mecA* segment and its analogue. To further improve the accuracy of the model, additional training data sets are being collected.

ENVR 655

Genetically programmed optical biosensor for pointof-care pathogen detection

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Water contamination by pathogenic bacteria is a major public health concern throughout the world. Monitoring

microbial contamination in water is becoming vitally important to inform consumers about water safety, identify source water problems, and facilitate decision-making to minimize human health risks. Pseudomonas aeruginosa (Pa), an opportunistic human pathogen, has emerged as one of the top causative agents of a wide range of infectious diseases (causing a total of 51,000 healthcare infections in the USA per year) and represents a critical public health concern worldwide. Current detection methods of Pa are either based on conventional culture techniques, which are time consuming and labor intensive, or based on molecular techniques, which require sample preprocessing, expensive reagents, specialized equipment and technical personnel. These methods are not suitable for contamination monitoring in a timely manner and are difficult to implement in underdeveloped areas. In this study, we developed an affordable, rapid and robust biosensor that detects Pa and the pathogens that share similar habitats as Pa by targeting the relevant quorum sensing signal molecules. The biosensor provides a visible, reagent-free readout through an engineered lycopene synthesis pathway in the cell, generating a bright red pigment to enable on-site pathogen surveillance. The quorum sensing signals produced from Pa and some similar pathogens can be quantitatively measured at nanomolar levels using our engineered biosensor device. In addition, we created a dipstick prototype that can be used in varied water samples, including tap water, and hospital drinking water and municipal wastewater. The developed biosensors can provide an economical and rapid detection platform for monitoring the pathogens in water systems under various clinical and environmental settings.

ENVR 656

Development of a colorimetric sensor for detection of PFOA and PFOS in water

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Per- and polyfluorinated compounds (PFASs), such as PFOA and PFOS, have been reported in the environment. The widespread applications in various industries including paints, surfactants, coatings, emulsifiers, fire retardants, firefighting foams, and others inevitably lead to the release of PFASs into the water environment. Chromatographic techniques (LC/MS/MS) are commonly used to detect PFASs, however, they are timeconsuming, expensive, require complicated pre-treatment steps and result in high costs. In order to minimize the usages of chromatographic analytical methods and reduce analytical costs, the goal of this research was to find an easy to use colorimetric method for the presence/absence test for PFASs at low aqueous concentrations. A number of colorimetric dyes were evaluated. The effect of dye concentration, PFAS concentration, and mixing time was examined. The color change of the dye-PFAS solution was quantified with a UV-vis spectrophotometer. The study provided promising results for PFAS detection, and the results will be presented. It may be possible to further improve the sensitivity of the presence /absence PFAS sensor method.

ENVR 657

Characterize the chemical moiety and pH distribution at dynamic environmental interfaces with Raman spectroscopy

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Environmental Interfaces, such as air-water interfaces and air-ice interfaces, are ubiquitous in the environment. For large systems, such as the sea surface, the surface to volume ratio is small, which makes the interface negligible. However, for small systems, such as aerosols and small domains within the ice and snow structures, the surface to volume ratio is large, thus the significance of interfaces can no longer be overlooked. Chemical and physical properties at interfaces could be thoroughly different from bulk phase properties. Such unique properties enable environmental interfaces to affect all kinds of environmental processes, such as ice and cloud nucleation, the formation of secondary aerosols as well as the reactivity of chemical processes. Chemical and physical properties at interfaces are critical to environmental processes yet understudied due to limited characterization approaches. In our study, we attempted to characterize: 1) the chemical moiety distribution using Raman spectroscopy, 2) pH distribution by applying pH enabled surface-enhanced nanoprobe Raman spectroscopy (SERS), at different types of interfaces. The interfaces include the air-water interface of the aerosol droplets as well as the air-ice interface of frozen aerosol droplets, frozen bulk solutions and snow. The droplets and solutions consisted of environmentally abundant inorganic electrolytes such as ammonium salts and sodium chloride. For micron-size aerosolized droplets, a 2D Raman map with a spatial resolution of 1 µm² was generated for single droplets. The distribution of each chemical moiety within the droplet can be represented by the contour map generated according to the corresponding peak. The pH inside droplets was measured by putting a SERS-active pH nanoprobe into the droplet and generating a 2D pH map. Droplets were frozen by a temperature-control stage to observe the distribution change during the phase transition. Frozen bulk solutions and snow field sample was studied by the combined system of the temperature-control stage and the Raman microspectroscopy. The characterization method for chemical moiety and pH distribution was the same for droplets. The distributions within small domains of ice crystals and snow were observed. A localized distribution of chemical moieties and pH values indicated the interfacial effect was observed in this study. Such observation can provide molecular-level implications for the interfacial effects on environmental processes.

ENVR 658

Magnetic and electrically conductive polypyrrole nanoparticles as highly effective materials for heavy metal removal and sensing

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Heavy metals such as arsenic, cadmium, chromium, nickel, and lead are a well-known source of air, water, and soil pollution. Their presence in the environment can cause harmful effects in plants, animals, and humans. To address the consequences of heavy metals pollution, there is a need for technology to detect, capture and remove heavy metal contamination from the environment. This presentation reports the synthesis and characterization of polypyrrole (PPy) - magnetite (Fe₃O₄-PPy) nanoparticles, prepared via a chemical oxidative polymerization process, using polyvinyl alcohol as a surfactant. The Fe₃O₄-PPy nanoparticles have spherical shape and size ranging from 110 to 220 nm and are characterized by high magnetic properties and electrical conductivity. The particles displayed high sorption capacity for arsenic and show promising characteristics for use as sorbent for the removal of heavy metals from contaminated water. Their high affinity for heavy metal contaminants also provided a platform to develop a highly sensitive electrochemical method for low cost detection of heavy metals using the principles of nano-impact electrochemistry. The synthesis and characterization of the magnetic nanocomposite, along with the performance evaluation of the novel nano-impact method to detect heavy metals will be discussed.

ENVR 659

Electrochemical determination of copper ions in water using polyacrylic-graphene-thiourea modified electrode

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Graphene based nanomaterials have shown interesting applications in electrochemical sensors due to its superb electron transfer properties and excellent electrochemical catalytic activity. Thiourea derivative is known to serve as heavy metal extractants because of their complexation capacity with various metals. Based on the unique electronic properties of reduced graphene oxide (rGO) as well as the selective interaction between bis-thiourea (BT) derivative with Cu(II) ions, a novel electrochemical sensor for the detection of Cu(II) ions using poly(n-butyl acrylate)graphene-(bis)thiourea [poly(nBA)-rGO-BT] modified electrode was proposed. The response current of the prepared electrochemical Cu(II) ions sensor was measured by differential pulse voltammetry(DPV). The effects of the composition of bis-thiourea derivative, accumulation potential, and accumulation time on the Cu(II) ions sensing properties (response) of the sensors were investigated to determine the optimal conditions for detecting Cu(II) ions in water. Other parameters such as pH, linear range, repeatability, stability and interference studies which influence the response of the measurement were optimized for the copper determination. The utilization of poly(nBA)-rGO-BT composite film has enhanced the performance of the electrochemical copper sensor in terms of broader detection range, lower detection limit, and favorable long-term stability. The modified electrode was successfully applied for the determination of Cu(II) ions in water samples.

ENVR 660

Chelating agents that offer insight into the speciation and reactivity of unusual oxidation states of manganese, iron, and copper

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Pyrophosphate as a chelating agent for Mn(III) and phenanthroline as a chelating agent for Fe(II) and Cu(I) are well known. But can we go further? Much of what chemists know about manganese +III, +IV, and +V, iron +IV, and copper +I comes from their existence and reactivity within catalytic sites of enzymes. A common approach within the field of bioinorganic chemistry is to synthesize simpler, biomimetic chelating agents that coordinate metal ions in a manner analogous to protein structures within enzymes. While most metal ionbiomimetic chelating agent complexes require organic solvents (which mimic enzyme interiors), a handful are stable in aqueous solutions and hence "reporter chelating agent" candidates, i.e. useful for trapping particular oxidation states and moderating their reactivity. Enzymatically-inspired chelating agents can tell us about transition metal ion involvement in the oxidative breakdown of biological signaling compounds in soils, the oxidative alteration of natural organic matter, disinfectant consumption during water treatment, and medium stability/product quality issues in cell growth media. By changing functional groups and molecular structure, chelating agents can also be re-purposed and optimized for particular technological applications. Manganese- and iron-bearing complexes that serve as peroxide-based bleach catalysts, for example, have been developed over the past thirty years. Tethering complexes to support media is possible. Chelating agent structure-reactivity relationships provide useful, albeit indirect, insight into metal ion reactivity.

ENVR 661

Enhancing water supply with ferrate(VI)

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Ferrate(VI) is an emerging treatment agent with a potential to revolutionize water treatment, reuse, and emergency water supply in the aftermath of natural disasters. It is a strong chemical oxidant with a redox potential up to 2.20 V. Accompanied with Fe(VI) reduction, Fe(III) is continuously in-situ produced to initiate coagulation and precipitation. The multiple treatment mechanisms enable an efficient, resilient, compact, and modular water treatment design. Recent advances in ferrate(VI) chemistry discovers that ferrate(VI) can "naturally" produce numerous iron oxide nanoparticles in water. If properly harnessed, these nanoparticles can broaden ferrate(VI) applications. This presentation will summarize our recent fundamental and applied research on ferrate(VI) for water treatment and reuse, including: 1) ferrate(VI) alleviation of phosphorus in municipal wastewater, including organic phosphorus; 2) interactions of natural organic matter (NOM) with ferrate(VI) versus ozone; and 3) the potential of ferrate(VI) for treatment of biologically treated municipal wastewater for agricultural water reuse.

ENVR 662

Assessment of activated ferrate oxidation for wastewater reuse

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Ferrate (Fe(VI)) is one of the more promising emerging water treatment technologies, but there has been limited

research on potential benefits in a water reuse paradigm. Fe(VI) has a relatively high oxidation potential and is known to inactivate waterborne pathogens. The ferric iron resulting from Fe(VI) reduction could support downstream coagulation processes. The California Code of Regulations Title 22 "Water Recycling Criteria" (CCR 22) has identified key pollutants that must be transformed for new recycled water oxidation technologies to be accepted. Recent literature has shown that Fe(VI) oxidation could be enhanced by "activation" with the addition of low molar ratios of reductants or acid. This study examined the impact of sodium sulfite-activated Fe(VI) in laboratory prepared solutions as well as spiked municipal wastewater effluents with the goal of meeting the 0.5-log (69%) removal of the organic contaminants, such as 1,4-dioxane, outlined in CCR 22. Additionally, the formation of brominated disinfection byproducts (DBPs) [e.g. brominated THMs] by activated Fe(VI) were examined. Bench-scale, batch experiments assessed treatment effectiveness by analysis of Fe(VI) decay over time and contaminant transformation under varving activation conditions. Optical and X-ray transient absorbance methods were also deployed to elucidate the role of intermediate iron radicals (e.g. Fe(V)) in aqueous media. Results presented will show the effectiveness of activated Fe(VI) to oxidize contaminants and the generation of DBPs relative to the benchmarks of CCR 22. In particular, the relative importance of reaction intermediates will be discussed. Generally, the results indicate that activated Fe(VI) seems viable for water reuse with possible achievement of CCR 22 guidance in full-scale applications.

ENVR 663

Development of fluorescence surrogates to predict the iron(VI) oxidation of pharmaceuticals in wastewater effluents

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Abstract: The occurrence and transformation of pharmaceuticals and personal care products (PPCPs) in the aquatic environment have gained great attention from environmental scientists and engineers. The effluents from municipal wastewater treatment facilities are one of primary sources of PPCPs due to the incomplete removal by existing biological treatment processes. Therefore, advanced treatment processes for the PPCPs attenuation in effluents need to be evaluated. As an alternative oxidant, ferrate (Fe^{VI}) has received much more attention as an environment-friendly chemical due to its dual functions. In the current study, total 13 PPCPs were selected due to their widespread existence in wastewater effluents. Our results suggested that the Fe^{VI} exposure dose and bimolecular reaction rate constant are not reliable for predict the removal efficiency of PPCPs in the effluents. Therefore, fluorescence spectroscopy of effluent organic matter (EfOM) was used as an alternative surrogate to predict the removal efficiency of PPCPs. Moreover, the surrogate was applied to five natural water bodies to verify the reliability. The surrogate proposed in this study can provide a new method to monitor the ferrate oxidation of PPCPs in the wastewater effluents.

ENVR 664

Withdrawn

ENVR 665

Redox reactions of iron and manganese oxides in complex systems

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The redox reactions of Fe- and Mn-oxides play an important role in the fate and transformation of many contaminants in natural environments. Due to experimental and analytical challenges associated with complex environments, there has been a limited understanding of the reaction mechanisms in real environmental systems, and most of the studies so far have only focused on simple model systems in the fate of contaminants. In order to bridge the gap between simple model systems and real environmental systems, we have started to increase the complexity of the model systems to approach real environmental systems. In this work, we primarily focused on (1) the oxidative reactivity of manganese and iron oxides and (2) the reductive reactivity of Fe(II)/iron oxides in complex model systems toward contaminant degradation. The effects of common metal ions such as Mn²⁺ and Ca²⁺, ligands such as natural organic matter, and second metal oxides such as AI, Fe, Si and Ti oxides on the redox reactivity of the systems were systematically studied. Results showed that the interaction mechanisms in the complex mixtures varied from heteroaggregation, surface complexation, competitive adsorption, soluble complex formation, to ternary surface complexation, and the contaminant degradation was largely inhibited in all systems expect in mixtures of Fe²⁺, goethite and TiO₂, where inter-particle electron transfer occurred to facilitate contaminant reduction.

ENVR 666

Oxidation of H-phosphonate and other overlooked P(III)-containing oxyanions: Interconnections between speciation and reactivity

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Despite its heavy use on agricultural lands and as a postharvest fruit and vegetable treatment, transformation reactions of H-phosphonate ("phosphite", HPO32-) are poorly documented. Distinguishing H-phosphonate from structurally-related pesticides (e.g., its ethyl ester), impurities (e.g., pyrophosphite and isohypophosphate), (orthophosphate and oxidation products and pyrophosphate) is an extraordinary analytical challenge. We have developed capillary electrophoresis with indirect photometric detection for this purpose. Oxidation of all the P(III)-containing compounds listed above to corresponding P(V) compounds by oxygen, iron and manganese oxyhydroxides, and even some organic moieties (e.g., benzoquinones, alpha-keto carboxylates) is thermodynamically favorable. Properties of P(III)containing compounds affecting aqueous speciation, e.g., oxyanion Lewis basicity that controls protonation, metal ion coordination, and adsorption, largely explain differences in oxidation rates. Much of what we've learned can be used to help understand technologies employing P(III)-containing species (e.g., metal plating, corrosion control, polymer stabilization) and shed light on sources and sinks across redox gradients in the environment.

ENVR 667

Formation of nitromethane during wastewater ozonation and implications for direct potable reuse

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We recently found that application of ozone, commonly employed in wastewater reuse before either membrane filtration (to control biofouling) or biological activated carbon (to break down larger molecules into digestible fragments) produces large quantities (up to ~50 µg/L) of nitromethane in wastewater effluent. Nitromethane itself is unlikely to be a major human health concern, however in this work we show that the nitromethane formed during wastewater ozonation can be transformed to chloropicrin, a highly genotoxic unregulated disinfection byproduct, at nearly 100% yield during subsequent chlorination. We further demonstrate via standard addition assays that nearly 100% of the chloropicrin formation in ozonated wastewater during subsequent chlorination (as would likely happen in a direct potable reuse scenario) can be attributed to nitromethane. A search for potential precursors to this reaction lead to N-methylamine stimulant drugs, including methamphetamine and ephedrine, which have been routinely measured in wastewater and which contain an N-methylamine functional group anticipated to serve as an efficient precursor. We found that these N-methylamine drugs ubiguitously form nitromethane upon ozonation, generally at high molar yield (>50%) and are currently quantifying the contribution of each to the nitromethane precursor pool. Finally, we examined the removal efficiency of nitromethane during advanced treatment as practiced during water reuse. We found removal to be very poor by reverse osmosis at both the bench and full scale (< 50% removal), likely because nitromethane is small, polar, and uncharged. Transformation rates by advanced oxidation were also poor (<50%), because nitromethane is a poor chromophore and its reaction rate constant with hydroxyl radical is low. These results are potentially troubling for future direct potable reuse scenarios in which recycled wastewater directly becomes a drinking water source. However, we found that biofiltration (including during O₃/BAC) may be a useful treatment technique for removing nitromethane.

ENVR 668

Impact of dissolved organic matter composition on the formation of regulated and novel disinfection byproducts during chlorination

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Dissolved organic matter (DOM) is a heterogeneous mixture of organic compounds derived from plant and microbial residues. DOM interacts with chlorine-based disinfection agents during water treatment to form potentially carcinogenic disinfection byproducts (DBPs). However, known DBPs such as trihalomethanes (THMs) and haloacetic acids (HAAs), make up only a fraction of the total organic halogen load present after disinfection. Additionally, the role of DOM composition in forming both regulated and novel DBPs is unknown. This study applies ultrahigh resolution mass spectrometry to investigate the formation of high molecular weight DBPs in DOM, which are of particular concern due to a lack of characterization as well as the potential for adverse health impacts. Specifically, we analyzed the chemical composition and DBP formation potential of DOM from 17 drinking water sources across the state of Wisconsin which includes 13 utilities that draw primarily from groundwater and 4 that draw primarily from surface waters. Known DBPs. including THMs and HAAs, were quantified following chlorination. Bulk characterization of DOM, performed using ultraviolet-visible spectroscopy, yielded information about aromaticity and molecular weight. Fourier transform-ion cyclotron resonance mass spectrometry (FT-ICR MS) was used to evaluate the molecular compositions of DOM samples. Chemical formulas were assigned to data generated from the FT-ICR MS, giving information on the chemical composition of DOM samples, as well as DBP formation. Of the unique chemical formula assignments, up to 10% of the assignments contained halogens and may be considered novel DBPs, indicative of the need to better understand DBP formation potential. This study provides insight into the role of DOM composition in the formation of novel and

regulated DBPs, which is essential for addressing the challenges of DBP formation in drinking water.

ENVR 669

Application and prospects of UV-LED disinfection in drinking water treatment

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Ultraviolet light-emitting diodes (UV-LEDs) are promising alternatives to conventional mercury lamps, mainly because they contain no toxic mercury, have adjustable emission wavelengths and operation modes, and have a potential for less energy consumption and longer lifetime. Pulsed UV-LED shows a higher disinfection efficiency than continuous mode for some bacteria in water treatment. Compared with low-pressure mercury lamps (LPUV) with 254 nm, UV-LEDs at 265, 275 and 285 nm can accelerate the free chlorine photolysis and produce more active radicals (such as hydroxyl and chlorine radicals), which can improve the degradation of organic contamination during UV/chlorination process. Meanwhile, 275 nm UV-LED/chlorine process can produce less highly toxic disinfection by-products than 254 nm LPUV under high UV fluence. Besides, better arranged LEDs according to computational fluid dynamics models can optimize the absorption of photons, and thus improve reaction efficiency of UV reactors. Therefore, UV-LEDs have great application prospects in future as novel UV sources in water disinfection.

ENVR 670

Improved solid phase extraction of perfluoroalkyl substances using automation

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Per- and polyfluoroalkyl substances (PFAS) are a group of man-made chemicals that includes perfluorooctanoic (PFOA), perfluorooctyl sulfonic acid (PFOS), and hexafluoropropylene oxide dimer acid (HFPO-DA, which is part of GenX process). PFAS compounds have been manufactured since the 1940s. These chemicals are very persistent in the environment and accumulate in the human body over time. It is well documented that exposure to PFAS can lead to adverse human health effects. The US EPA office of Ground Water and Drinking Water has developed a method specifically for the analysis of PFAS in drinking water, EPA 537, which is based on solid-phase extraction (SPE) followed by LC-MS/MS detection. The sample preparation required can be time consuming and laborious. The use of an automated instrument improved the sample prep process for these compounds.

ENVR 671

Development of a rapid PFAS screening tool for drinking water

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Particle-Induced Gamma-ray Emission (PIGE) spectroscopy has been used to screen consumer products and environmental samples for total fluorine, as a surrogate for PFAS. Since there are few natural sources of inorganic fluorine in most consumer products and ground water/biota, a total fluorine measurement that is spectroscopic provides rapid identification of samples that have PFAS. PIGE has been used successfully to screen food-packaging and textiles in commerce, as well as ground water, biota and soil samples at aqueous filmforming foam impacted sites. However, solid-phase extraction is required to pre-concentrate PFAS in aqueous samples to attain concentrations that can be measured by PIGE. We report here on the development of a novel method used to pre-concentrate heavy metals in aqueous solutions that can be adapted to work on PFAS found in drinking water samples. A two-liter soda container can be fit with a low-cost "cap" with a commercially available carbon felt insert that sensitively extracts PFAS from drinking water by gravity filtration. The carbon filter can be returned for PIGE analysis which yields quantitative total fluorine measurements that are linear with concentration and sensitive down to the EPA health advisory limits of 70 ppt. In addition, the screening is non-destructive and if positive for fluorine, the same sample can be extracted for full LC-MS/MS identification of specific PFAS analytes. Ideal for groundwater and well water supplies, fluoridated municipal water supplies can also be screened with an additional fluoride removal rinse step. This technology has significant applications to both drinking water screening efforts for PFAS as well as for rapid testing of remediation technology for the sequestration or destruction of PFAS contaminants.

ENVR 672

Volatile per- and polyfluoroalkyl substances released from aqueous film-forming foam

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Per- and polyfluoroalkyl substances (PFAS) are class of thousands of synthetic fluorinated organic chemicals that have unique beneficial chemical and mechanical attributes including chemical and thermal stability. Thus, they have been used in a wide variety of industrial and commercial applications including aqueous film forming foams (AFFFs). Use of AFFFs by firefighters to extinguish hydrocarbon fires tends to contaminate water and soil with PFAS near application sites. Furthermore, several groups of PFAS have been detected in the blood serum of firefighters that have been exposed to AFFFs. Exposure to PFAS can lead to adverse health outcomes in humans. Although dermal exposure may be one route for their presence in the serum, inhalation of volatile PFAS could be another major contributor, however, less is known about the volatile PFAS released by AFFFs. The primary objective of this study is to determine the presence of volatile PFAS in the headspace of AFFF concentrates. We investigated the presence of volatile PFAS in the headspace above agitated AFFF using two analytical techniques. One method utilized polyurethane foam and XAD resin with liquid chromatography mass spectrometry to quantify 30 PFAS. A second, more exploratory approach used a thermal desorption sampler and gas chromatography mass spectrometry to measure 22 PFAS. 16 PFAS were detected in the headspace including 5 fluorotelomer alcohols (1.1 to 38.1 ng/L), 10 perfluorinated carboxylic acids (1.2 to 13,668 ng/L) and 1 fluorotelomer sulfonate (72.1 ng/L). The most abundant PFAS detected in the headspace was perfluorooctanoic acid (13,668 ng/L). Additionally, a total of five saturated, iodinated, and ethenyl fluorocarbons were identified, which may be derived in the AFFF manufacturing process as precursors to other PFAS. The results of this research provide novel information about identity, concentration and rate of volatile PFAS released by AFFFs concentrates.

ENVR 673

Application of COSMO-RS-derived octanol-water partition coefficients in characterizing emerging perand polyfluoroalkyl substances

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The COnductor-like Screening MOdel for Realistic Solvents (COSMO-RS) was used to calculate the octanolwater partition coefficients (Kow) of Per- and Polyfluoroalkyl Substances (PFASs). The Log Kow values calculated from COSMO-RS were found to have a logarithmic relationship to the experimentally determined retention times from liquid chromatography-mass spectrometry. Predicted retention times were found to be within 0-13% of their experimental retention times for the unknowns. This simple approach could be useful in the identification and prediction of sorption behavior and mobility in the environment of the new and emerging PFASs that lack reference standards.



ENVR 674

Per- and polyfluoroalkyl substances: Computational insight

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A broad series of short- and long-chain per- and polyfluoroakyl substances have been investigated, including phased-out species and their replacement compounds to consider their binding characteristics, and other properties that will be of aid in determining effective mitigation strategies.

ENVR 675

Structural dependence of microbial reductive defluorination of per- and polyfluoroalkyl substances

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Due to the distinctive properties such as fire resistance and water/oil repellency, per- and polyfluoroalkyl substances (PFASs) are playing irreplaceable roles in manufacturing and industrial applications. However, environmental because of their persistence. bioaccumulation, and toxicity to human health and ecosystems, PFASs are of emerging concern globally over the decades. Thus, it becomes an urgent issue to address PFAS contamination efficiently and costeffectively. While many efforts focus on adapting physical and/or chemical approaches to remove and destroy PFAS residuals from contaminated water and soil, the design of more biodegradable and environmentally friendly alternative PFAS structures can be another solution. In this study, by investigating the biodegradability of structurally diverse PFASs, we discovered microbial reductive defluorination of certain per- and polyfluorinated compounds and found the specific structures that are crucial for anaerobic PFASs (especially for the perfluorinated ones) biodegradation. Furthermore, suspect and non-target analytical approaches are applied to identify the transformation products and the biotransformation pathways of PFASs. This study provides significant insights into the design of alternative PFASs, the evaluation of the environmental fate of PFASs, as well as the development of cost-effective PFAS treatment strategies.

ENVR 676

Biotransformation and biodefluorination of FTCAs by actinomycetes

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Fluorotelomer carboxylic acids (FTCAs, e.g., 6:2FTCA and 5:3FTCA) have been widely detected in the environment, especially in landfill leachates since they are common ingredient compounds of surfactant industry and metabolic intermediates essential for the biotransformation of various PFASs precursors. Aerobic degradation of FTCAs generates an array of perfluorinated carboxylic acids (PFCAs, e.g., PFHxA and PFBA) that are highly persistent and bioaccumulative. In this study, we investigated the biotransformation and biodefluorination of 6:2 FTCA and 5:3 FTCA in 7 selected Actinomycetes. including Mycobacterium dioxanotrophicus PH-06, Mycobacterium smegmatis mc²-155, Rhodococcus jostii RHA1, and 4 more Rhodococcus strains. RHA1 exhibited the best 6:2FTCA biotransformation activity than the other 6 species. free However, monitoring of fluoride and biotransformation metabolites revealed distinct biodefluorination potentials and pathways between 6:2FTCA and 5:3FTCA. After 48 hours of exposure, complete 6:2FTCA removal was observed by RHA1. In the interim, free fluoride in the media mounted up to a

concentration of 0.116 mM. We further analyzed the biotransformation metabolites using High-Resolution Mass Spectrometry (HRMS) equipped with the nanoelectrospray ionization (Nano-ESI) injection. More than 10 PFASs were detected as the metabolites of 6:2FTCA biotransformation, such as shorter chain PFCAs, FTUCAs, 5:3FTCA and α-OH5:3FTCA. Detection of these less fluorinated metabolites supports the observed defluorination. However, mass balance based on total fluoride revealed the existence of unknown intermediates accounting for the dominant products resulted from 6:2FTCA biotransformation. In contrast, minimal fluoride release (<0.001 mM) was detected during 5:3FTCA biotransformation by RHA1, though over 90% of 5:3FTCA removal was identified. Accordingly, no conventional defluorination metabolites of 5:3FTCA were significantly detected, suggesting some non-defluorinated metabolites were formed during 5:3FTCA biotransformation. We are in the process of untangling these unknown metabolites of FTCA biodefluorination using non-target HRMS workflow. Our research is of fundamental scientific value to advance our understanding of biodefluorination mechanisms and promote the development of costefficient biological treatment strategies to remove FTCA contamination with optimized defluorination and minimized accumulation of PFCAs and other persistent compounds.

ENVR 677

Sorption and desorption behavior of PFOS and PFOA onto a gram-positive and a gram-negative bacterial species

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Little is known about the environmental behavior of many per- and polyfluoroalkyl substances (PFAS). In this study, used experiments we batch to measure (PFOS) perfluorooctanesulfonic acid and perfluorooctanoic acid (PFOA) sorption onto Grampositive Bacillus subtilis and Gram-negative Pseudomonas putida bacterial cells as a function of time and pH, and we measured PFOA and PFOS desorption behavior as well. Sorption was quantified by analysis of total fluorine in the aqueous phase using particle induced gamma-ray emission spectroscopy. PFOA and PFOS sorption was rapid and showed no significant change with time. PFOS sorption was pH dependent, with more sorption occurring onto both bacterial species at pH 4 than pH 6. In contrast, PFOA sorption onto *B. subtilis* was pH independent, and PFOA sorption onto *P. putida* was negligible under all conditions studied. B. subtilis exhibited a greater sorption capacity than P. putida for

both PFOA and PFOS, suggesting that cell wall structure influences sorption capacity significantly. PFOS desorption, promoted by an increase in system pH, was rapid for both bacterial species, with sorption in each case exhibiting complete and rapid reversibility. These experimental results place constraints on the nature of the PFAS-cell interactions. The rapid reversibility of the sorption reaction indicates that sorption is likely a cell surface phenomenon with no internalization occurring, and that the process can be modeled as an equilibrium reaction. The pH dependence to the sorption behavior suggests that sorption involves both electrostatic and hydrophobic components. The increased sorption with decreasing pH suggests an electrostatic component to the sorption, as the bacterial surface becomes less negatively charged at lower pH, possibly enabling positively charged amino groups to bind the negatively charged PFAS molecules. The lack of a pH effect on PFOA sorption suggests that hydrophobic binding also occurs and can control the sorption behavior of some PFAS molecules.

ENVR 678

Interactions between Lemna minor (common duckweed) and PFAS intermediates: Perfluorooctanesulfonamide (PFOSA) and 6:2 fluorotelomer sulfonate (FTSA)

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Aqueous film-forming foam (AFFF) is a highly complex mixture. Once released to the environment, some degradation products or intermediates from PFAS precursors may persist in the environment for a long period of time. For example, perfluorooctane sulfonamide (PFOSA) is a known product of aerobic microbial transformation of sulfonamide containing compounds such as N-ethyl perfluorooctane sulfonamide ethanol (N-EtFOSE) and a metabolite of numerous sulfonamidecontaining precursors in humans and biota. PFOSA is known to be easily degraded by soil microbes, plants and earthworms. But the mechanisms of plant transformation of this chemical are unclear. 6:2 fluorotelomer sulfonate (6:2 FTSA) could have been produced from fluorotelomer thioamido sulfonates in Ansul AFFF or fluorotelomer sulfonamide betaines and amines in AFFF manufactured by National Foam. In four wells at Tyndall Air Force Base, the concentrations of 6:2 FTSA all exceeded 1,000 µg/L, much higher than 50 µg/L initially in AFFF. Whether this chemical can be further degraded or not is an unaddressed question. In this talk, we will present our recent study on understanding the interactions between Lemna minor (common duckweed) and the two PFAS intermediates. Results in terms of uptake of the target compounds by duckweed and the stresses caused by the chemicals will be discussed in detail.

ENVR 679

PFAS distribution in contaminated soils and impact on rhizosphere and plant microbiota

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Environmental contamination is usually made of complex mixtures of metals and organic compounds. Furthermore, these contaminants can interact with indigenous mineral phases and organic matter, a unique microbiome, and local vegetation. Rhizosphere horizons are particularly susceptive to heavy metals and organic contamination, including per- and polyfluoroalkyl substances (PFAS), due to their specific biogeochemical processes. A comprehensive understanding of the mechanisms controlling PFAS effect on plant growth and microbial community changes, in order to prevent or attenuate the effect of a changing environment and predict potential human exposure routes. The main objective of this project is to evaluate the distribution of PFAS in plants exposed to mixed contaminants, and their effect in the rhizosphere and in planta microbial community. Field measurements are combined with hydroponic experiments using the model plant Arabidopsis thaliana to assess the mechanisms of PFAS plant translocation and microbiome changes. This work focuses on the Ringwood/Ford Superfund, NJ site where lead, arsenic, chloroethane, benzene and 1,4-dioxane are the main contaminants of concern. However, PFAS have been measured in water, sediments and plants at different locations. PFNA, PFOA and PFOS have been analyzed in 8 locations, and elevated PFAS concentration was found in one location downstream a paint sludge disposal area (PFOS 445 ng/L, PFOA 23.78 ng/L, PFNA 25.69 ng/L). PFAS were also measured in sediments (PFOS 2.18 ng/g), rhizosphere (PFOS 2.45 ng/g) and plants (PFOS 0.811 ng/g roots). Hydroponic investigation on PFAS uptake by Arabidopsis thaliana shows PFOA preferred accumulation in roots, and a direct relationship with PFAS solution concentration. The changes in microbial communities are being evaluated using next-generation DNA Illumina sequencing. This work is expected to provide a holistic understanding of the fate and transformation of PFAS within the various environmental compartments, and it will inform future remediation strategies and exposure prevention alternatives.

Efforts to determine best practices for using metabolomics for environmental monitoring

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Metabolomics is used to discover biomarkers and probe the metabolism of samples by providing information on thousands of metabolite concentrations (the metabolome) for each sample. Recent advances in LC-MS based metabolomics have furthered understanding of metabolism in a variety of systems. Despite the power of this technique, biological and technical challenges hinder the use of metabolomics to interrogate microbial communities sampled from their natural habitat as wells as to relate these results to studies performed in the lab. Herein, our efforts to circumvent these challenges and apply this emerging systems biology technique to natural microbial communities will be discussed. Using an untargeted metabolomics method employed on an UPLC-Orbitrap Exactive Plus MS. 90-250 known metabolites and ~1.500-10.000 spectral features arising from molecules with unknown structures have been detected from the consortia of dechlorinating microorganisms, SDC-9. In the lab, sampling for metabolomics often utilizes vacuum filtration followed by immediate extraction and quenching of the sample at low temperatures. While this is believed to be necessary as metabolism can shift rapidly in response to perturbations, such sampling techniques are difficult to implement in the field. In order to make metabolomics more amenable for environmental monitoring, we set out to determine whether degradation alters the metabolome if the sample is not collected rapidly and immediately guenched at low temperature. To address this, SDC-9 samples were collected on 3 filter types and quenched and/or stored at each of three temperatures (-80°C, 4°C, rt), and the generated metabolomes were analyzed to determine collection and storage induced changes. Other studies to determine whether the metabolome of SDC-9 could be used to determine the progress of both cis-dichloroethene and vinyl chloride consumption and informing monitoring remediation efforts were also conducted.

ENVR 681

Impact of chlorinated compounds on natural organic matter analysis by ultrahigh resolution-mass spectrometry

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Ultrahigh resolution-mass spectrometry (UHR-MS) has become a common technique to analyze complex environmental mixtures, such as natural organic matter (NOM). Ion suppression is a major limitation to the study of NOM by UHR-MS and results in peak intensity not being reliably related to compound quantity. Additionally, ion suppression can lead to the misidentification of reactants or products in transformation studies. Ion suppression can occur via competition for charge or by preventing ions from entering the gas phase during electrosprav ionization (ESI). Based on previous work on ion suppression of metabolites in biological mixtures, we suspect that certain compound classes may be more susceptible to ion suppression than others. Specifically, we were interested in how the presence of chlorinated compounds would suppress or enhance ions because UHR-MS is increasingly used to identify disinfection byproducts and understand the impact of chlorination on NOM. We prepared a solution of Grand Lake St. Mary's NOM isolate and a second identical solution with compounds. includina chlorinated chlorinated benzylamines and quinones. Preliminary results using negative mode ESI and a 15T Bruker SolariXR Fourier transform- ion cyclotron resonance- mass spectrometer showed a 10% decrease in the number of chemical formulae that could be identified when chlorinated compounds were present in the mixture. Aromatic, ligninlike components appeared most susceptible to ion suppression. There was some evidence of ion enhancement, but the statistical significance of the results is still being investigated. Interestingly, the chlorinated compounds were not ionized by negative mode ESI, which suggests that the chlorinated compounds alter the solvent evaporation process rather than competing for charge. Results using positive mode ESI, negative mode laser desorption/ionization (LDI), and positive mode LDI are being obtained and will be discussed. This work will help provide a more nuanced analysis of NOM by UHR-MS.

ENVR 682

Online gas chromatograph with thermal desorption preconcentrator and high-resolution time-of-flight mass spectrometric detection for measurement of volatile organic compounds

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The introduction of organic contaminants to the environment from anthropogenic activities such as oil and

natural gas production, vehicle emissions, and the use and disposal of volatile chemical products is an issue of growing concern. These compounds can contribute to the formation and growth of atmospheric aerosols, participate in photochemistry that cause ozone formation, and can be environmentally persistent and accumulate in soils and natural waters where their degradation products form through unknown mechanisms. To understand the consequence of these emissions in terms of human exposure, climate forcing, and environmental burden analytical methods are needed to identify and quantify the contaminants in a range of environments with high sensitivity, specificity and sufficient time resolution. We have developed an online gas chromatograph (GC) equipped with thermal desorption (TD) preconcentration and high-resolution time-of-flight mass spectrometry (HR-ToF-MS) for the measurement of VOCs and OVOCs in a rugged, field-deployable package. The TD-GC has been coupled to both an electron-ionization (EI) HR-ToF-MS and Vocus proton-transfer-reaction (PTR) HR-ToF-MS to take advantage of the high-resolution spectra for both the compound's fragmentation pattern (EI-ToF-MS) and its intact protonated molecular ion (Vocus PTR-ToF-MS). Here, we will present one month of continuous field measurements of biomass burning tracers in the western U.S., results from a recent indoor air campaign, and examples from laboratory experiments to demonstrate that through the use of chromatographic separation and high resolution analysis this system has a novel ability to detect and quantify compounds that are of environmental concern. This includes VOCs and OVOCs described by the U.S. EPA as ozone precursors (PAMS) and air toxics (TO-15), polycyclic aromatic hydrocarbons (PAHs), and environmental transformation products like dimethyl silanediol (DMSD). The latter of which is thought to be a soil degradation product of polydimethylsiloxanes (PDMS) which are introduced to the environment in applications such as personal care products, food additives, and industrial cleaning.

ENVR 683

Analysis of persistent organic pollutants (POPs) by high-resolution GC/MS

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Persistent organic pollutants (POPs) like Dioxins, Furans and Chlorinated paraffins (CPs) are regulated and restricted from production globally as declared by the UN Stockholm Convention. CPs are complex mixtures of polychlorinated alkanes with alkane lengths C10 to C30 and various degrees of chlorination, typically 30 to 75%. Short Chain Chlorinated Paraffins (SCCPs, C10-C13) are bioaccumulative and persistent in the environment.

Analysis of these compounds represents substantial challenge due to their self-interference as well as an interference with other components of complex industrial matrices. Therefore, to ensure both high selectivity and high sensitivity for the analysis of the SCCP with wide range of chlorination, we used a high-resolution GC/Q-TOF operated in two ionization modes: negative chemical ionization (NCI) as well as low energy electron ionization (low energy EI). The pure congener standards were first used to evaluate the individual spectra. NCI spectra of SCCPs exhibited minor fragmentation with no significant breakdown of the carbon backbone. Low energy EI data indicated higher degree of fragmentation of the SCCPs as compared to negative CI. However, using this technique allowed the sensitive detection the SCCP species with low number of chlorine atoms. Both NCI and low energy El techniques were later applied to analyze complex SCCP mixtures.

ENVR 684

Benefits of sharing chemical structure data from commercial spectral databases for improved curation and chemical identification

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The identification of chemical contaminants in the environment utilizing high resolution mass spectrometry, either by targeted or non-targeted analysis, is assisted by access to various types of databases. These include commercial, highly curated collections of spectral data, open spectral data collections (e.g. MassBank) and large online databases such as PubChem, ChemSpider and the US EPA CompTox Chemicals Dashboard. The Dashboard (https://comptox.epa.gov/dashboard) is an open chemistry resource and web-based application containing data for ~900.000 substances and has been used to support structure identification using mass spectrometry. A specific type of data mapping in the database uses "MS-Ready" structures, a way to process all registered substances to separate multi-component chemicals into their individual components, remove stereochemical bonds and desalt and neutralize structures. MS-Ready structures have been shown to enhance database searching of unknowns. Curated lists Dashboard chemical in the (https://comptox.epa.gov/dashboard/chemical lists) support specific applications by providing pre-selected structures for non-targeted screening in easily downloadable formats. Examples include environmental toxins (algal toxins in harmful algal blooms, mycotoxins and microcystins), disinfection by-products, flame retardants, and other lists of candidates monitored around the world.

This presentation will provide an overview of how commercially available databases from Agilent Technologies have been collaboratively curated to improve data quality and added as lists to the CompTox Chemicals Dashboard. These databases as focused separate collections in the Dashboard can provide benefits in terms of supporting structure identification and non-targeted analysis in environmental monitoring and remediation.

ENVR 685

Determination of pesticide occurrence in private wells by high-resolution mass spectrometry

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Approximately 30% of North Carolinians rely on private wells as their primary source of drinking water. Because private wells fall outside of the purview of the Safe Drinking Water Act, occurrence data for pesticides are lacking. Additionally, standard EPA and USGS methods target only a limited number of pesticides and do not adequately target pesticides that are currently used in high volume in North Carolina or the United States. Over 3,000 pesticides have been registered with the US EPA, and while the list continues to grow, analytical methods have not evolved at a similar pace. To address this gap, my research aims to 1) develop robust non-targeted workflows for identifying LC-amenable pesticides and pesticide degradates and 2) investigate the occurrence of pesticides, as well as other common contaminants, in 150 private wells across five counties in North Carolina. A liquid chromatography - quadrupole time-of-flight mass spectrometry (LC-QToF MS) system was used to develop a large volume injection (200 uL) workflow. Pesticide mixtures containing a total of 31 compounds were used to develop 4 acquisition methods each in both positive and negative electrospray ionization (ESI) modes: one MS method and three Auto-MS/MS methods at collision energies of 10, 20 and 40 eV. For approximately 90% of the pesticides in the test mix, limits of quantitation were in the 10-25 ng/L range. Samples collected from 150 private wells are being analyzed with the developed workflow. Sample preparation includes the addition of methanol (2% v/v) and the addition of internal standards. MS data are analyzed using a workflow previously developed by the US EPA, which pairs Agilent identification algorithms with an online WebApp and Competitive Fragmentation Modeling for Metabolite Identification (CFM-ID). This presentation will introduce the developed workflow and present results for a subset of analyzed private wells.

ENVR 686

Pesticide exposure in drinking water and biomarker detection in human urine using high-resolution orbital ion trap mass spectrometry

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Exposure to pesticides is a global health concern. To better understand health risks associated with pesticide exposure, monitoring of one's environment (exposure characterization) and biomatrices (human biomonitoring) is essential. In addition to providing proof of internal allows investigation biomonitoring exposure, of endogenously formed compounds resulting from pesticide exposure. For example, potentially carcinogenic pesticide-associated *N*-nitroso compounds (PANNs) may form in the acidic environment of the stomach following exposure to nitrosatable pesticide residues in drinking water. Despite the advancement of technology used to identify a wide range of environmental pollutants and biomarkers, methods have not yet been developed for screening of PANNs in drinking water and urine. In this work, a comprehensive analytical method was developed for detecting nine nitrosatable pesticides and metabolites, as well as their PANNs, in groundwater and human urine using high-resolution orbital ion trap mass spectrometry. The novel sample preparation approach resulted in a suitable method for extraction of target analytes from urine: mean recoveries ranged between 96 to 116% (%RSD \leq 10). To assess PANN formation in groundwater, target analytes were individually reacted at environmentally relevant concentrations ($\leq 20 \ \mu g \ L^{-1}$) with sodium nitrite and hydrochloric acid in water. Only ethylenethiourea (ETU) participated in PANN compound formation as evidenced by the tentative identification of Nnitrosoethylenethiourea (N-ETU); tentative identification was achieved by matching the accurate masses of theoretical and experimental N-ETU molecular ions with a mass error tolerance of 5 parts per million. N-ETU formation was then assessed in a pooled groundwater sample collected from an intensive agricultural region of Prince Edward Island, Canada. Evidence of N-ETU formation in the groundwater sample was observed in under 30 minutes at a pH value of 2.5 and at concentrations 20, 10, and $7.5 \ \mu g \ L^{-1}$, but not at 5 $\ \mu g \ L^{-1}$. This work resulted in a single method capable of detecting PANN compounds and their parent pesticides in both groundwater and human urine. The results of the study show that ETU reacts with nitrite to form *N*-ETU at environmentally relevant concentrations and that endogenous *N*-ETU formation may be a concern for individuals exposed to low concentrations of ETU.

ENVR 687

Characterizing organic micropollutants in Onondaga Lake sediment traps using energized dispersive guided extraction coupled to liquid chromatographyhigh resolution mass spectrometry

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Organic micropollutants (OMPs) are a diverse group of synthetic organic compounds including pesticides and pharmaceuticals. OMPs have proven to be very persistent and have the potential to bioaccumulate in organisms. The long-term health and ecosystem impacts include endocrine disruption, induction of antibiotic resistance and aquatic toxicity. Following entry into natural water systems, more hydrophobic organic compounds partition to suspended solids and eventually accumulate in sediments. Sediments have long been analyzed to characterize highly hydrophobic legacy compounds, but limited studies have analyzed OMPs in sediment traps. Compared to sediments, sediment trap samples permit quantification of downward contaminant flux at high temporal resolution, making them important archives of past contamination that can be exploited for reconstruction of environmental changes over time. Onondaga Lake, located northwest of Syracuse, NY, was historically the most polluted lake in America because of raw sewage and industrial byproduct contamination. The lake has since undergone extensive remediation, industrial activities have been cut back, and the wastewater treatment plant has been upgraded. In this study, we analyze archived sediment trap samples collected by the Upstate Freshwater Institute from Onondaga Lake to identify and quantify the plethora of OMPs that are not yet targeted by environmental regulation or pollution prevention initiatives. We will optimize a semi-automated method based on energized dispersive guided extraction (EDGE) to extract OMPs from Onondaga Lake sediment trap samples. Different solvent combinations and temperatures will be tested to maximize the extraction efficiency of OMPs. We will screen for OMPs in the sample extracts against an inhouse compound database using liquid chromatographyhigh resolution mass spectrometry (LC-HRMS). Results from this project will provide new knowledge about the local history of environmental contamination patterns with respect to OMPs.

ENVR 688

PCB congeners in air and food of rural and urban communities in the United States midwest

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Over more than a decade, we have measured PCB congeners in air of two midwestern communities: a rural community in Iowa and an industrial community in northwest Indiana. As part of the AESOP Study, we recruited community members to host polyurethane passive air samplers inside and outside of their homes and schools. We also collected samples of the food they consumed, and we deployed emission samplers to collect direct emissions from indoor surfaces. We analyzed the samples for PCB congeners in a consistent manner using solvent extractions, solid/liquid and acid cleanup, and capillary gas chromatography with tandem mass spectrometry. The result is a uniform and comparable set of PCB congener concentrations that present compelling evidence of specific and variable sources and potential for human exposure. Here we summarize our findings for a suite of more than 150 PCB congeners and compare to historical reports. We find that the highest air concentrations are due to building materials that contain or are contaminated with Aroclor PCB mixtures. We detected congeners that indicated the presence of Aroclor 1254 (often used in window and masonry sealants) and Aroclor 1016 (often used in fluorescent light ballasts). We also detected congeners found in modern paint pigments and the emission signal from this source is widely prevalent in school air and homes that were recently constructed or remodeled. We find that foods consumed by our study participants have very low PCB concentrations. We found a variety of PCB congeners in most food samples, but at much lower concentrations than had previously been reported. We found higher chlorinated congeners in tuna and salmon, and PCB11 (3,3-dichlorobipheny) in tilapia. Our measurements from these communities in the United States Midwest suggest that remediation of schools may be have the greatest impact in reducing human exposure.

ENVR 689

Electronic waste recycling by the informal sector is a potential source for a cocktail of hazardous organic compounds in Indian cities: Atmospheric transport and risk assessment

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Following a trajectory of rapid economic development, an increasing demand for electronic equipment in India inevitably generates large amount of domestic electronic waste (e-waste) in addition to the dumped e-waste from developed nations. Because the rate of e-waste accumulation is startling and the combinatorial effects of toxicants are complex we aimed to investigate hazardous organic compounds (HOCs) in the surface soil and atmosphere of informal e-waste recycling corridor and nearby dump sites of Indian cities: New Delhi in the north; Kolkata in the east; Mumbai in the west and Bangalore and Chennai in the south. Incomplete combustion and pyrolytic processes in e-waste recycling workshops might have contributed in the emission of high levels of HOCs viz., polychlorinated dibenzo para dioxins and furans (PCDD/Fs), polychlorinated biphenyls (PCBs), phthalic acid esters (PAEs) and polycyclic aromatic hydrocarbons (PAHs). With positive matrix factorization (PMF) as a source-receptor modelling technique, we could identify metal recovery process as a specific factor for loading of dioxin like PCBs. A significant correlation was obtained between soil bis-2-ethyl hexyl phthalate (DEHP) and PCB- 126 (R²> 0.9, p<0.01) in shredding and metal recovery sites where burning of plastic cables was prevalent. Furans, PAEs and carcinogenic PAHs were higher in the acid leaching sites of New Delhi thereby leading to the highest toxicity equivalents (TEQs) for PCDD/Fs among all the cities. Although HYSPLIT model localized sources outputs indicated but subtropical/tropical climate in these cities have profound implications for the atmospheric transport of these semivolatile HOCs away from the source regions.

ENVR 690

Towards integrated monitoring and holistic process understanding of pollutants

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Obtaining appropriate and representative samples that reflect the real environment is a critical step for environmental research and monitoring. Many different sampling techniques have been developed to provide more accurate measurements of contaminants and essential elements in the environment, including metals, nutrients and a large array of organic compounds. This presentation examines the characteristics, strengths and

weaknesses of several of the most commonly used and techniques, includina approaches discrete. continuous and a variety of passive sampling techniques. It then selects one, namely DGT (diffusive gradients in thin films), to explore in more detail how it can be used in environmental monitoring and advanced research. Although DGT has been considered as a passive sampling technique for monitoring, it directly measures fluxes resulting from DGT's perturbation of chemical equilibrium and has been classified by physical chemists as a dynamic technique. DGT can be used simply to measure chemical concentrations from in situ deployments, without the need to calibrate on site or to include internal reference compounds. Moreover, it can be used to measure a much wider range of analytes than other techniques because its construction allows for easy fabrication of many different binding agents. DGT measures labile forms of compounds and it can provide information on chemical speciation and bioavailability. One example is that the in situ DGT deployments in lakes and rivers have advanced our understanding of the interaction, the dynamic processes and the kinetic signature of metals and organics, including dissolved organic carbon and biotic ligands. As well as being easy to deploy in natural waters, it can be deployed directly in soils and sediments. In soils it is possible to obtain kinetic information of soil solution and solid phase interactions, but most importantly DGT measurements of an analyte are often a good predictor of its bioavailability. Multiple, spatially separated high resolution measurements, can be obtained from a single sediment DGT probe. Undoubtedly, novel and useful information will be obtained. The challenge is to use a technique like DGT intelligently so that we can fully harness the new information and new knowledge to advance our holistic understanding of biogeochemical processes.

ENVR 691

Living the impossible dream: Measuring environmental mixture toxicity by combining equilibrium passive sampling and dosing

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Biological effects due to environmental organic pollutants are generally caused by mixtures rather than single compounds. When measuring these effects using toxicity bioassays, the initial sampling of the mixture is a critical first step. Ideally, this should sample all mixture components and specifically target their bioavailable dissolved levels. Passive sampling is attractive here: it is practical, allows *in situ* sampling and targets the dissolved compound levels. However, interfacing passive sampling

with mixture toxicity testing remains challenging due to the mixture profile accumulated in the sampler being different to that in the field. For kinetic sampling this is due to compound-specific differences in sampling rates. For equilibrium sampling this is due to compound-specific differences in partitioning ratios. Therefore, sampler extraction and spiking inevitably leads to a different mixture profile in the toxicity test and is further accompanied by poor exposure control during the test. One way to robustly sample, reproduce and maintain field mixtures in toxicity tests is by combing equilibrium passive sampling and dosing. This permits the in situ bioavailable mixture profile in the environment to be sampled, and subsequently to be faithfully reproduced and maintained in the toxicity test. The approach can even be extended to the concentration-response testing of environmental mixtures by loading onto larger/smaller polymer volumes. There remain, however, significant challenges associated with equilibrium sampling and dosing. These are related to the impractically long sampler equilibration times and a lack of polymers with suitable properties for handling of both polar and non-polar contaminants. Nevertheless, progress is being made here and this will be reviewed in this contribution.

ENVR 692

Investigation of legacy and emerging organic contaminants in top predators and their prey to support chemicals management

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Analysis of target contaminants in top predators plays a key role for understanding their conservation but also their

potential use as sentinels in environmental monitoring studies due to their high trophic position in food webs. Under the framework of the EU funded LIFE APEX project (www.lifeapex.eu), it was possible to bring together sample collections and analytical laboratories in order to produce a guide for generic sample preparation and analysis, characterize predominant chemical mixtures in the environment, improve chemical risk management, and strengthen EU regulation and mitigation measures. Liver from apex predators (buzzards, otters, seals, harbour porpoise) and muscles from prey (breams, roaches, eelpouts and herrings) have been provided from European Specimen Banks, research collections and Natural History Museums and selected to provide a spatial distribution across selected sites in Northern Europe (UK, DE, NL, SE). 67 samples were analysed for the presence of PCBs, HCB, PBDEs and emerging contaminants (ECs) using established methodologies. In particular, we focused the attention on dl-PCBs and indicator PCBs, and the main congeners of the three commercial mixtures. PCB and PBDE PBDE concentrations showed higher levels in prey than in predators and different contamination for each country. In general, the otters were the most contaminated animal species for all countries. Results exceeded from a hundred to a thousand times the EQS for penta-BDE (2013/39/EU) in few of our samples. Except bream samples from Germany, HCB concentrations did not exceed the EQS established from the same EU Directive. Furthermore, the wide-scope target screening results indicated the presence of hundreds of ECs in the tested samples, like plant protection products, stimulants, sweeteners, industrial chemicals, pharmaceuticals and psychoactive drugs. Numerous transformation products from various classes of compounds were also detected in livers from apex predators, underlying the power of widescope target screening. In total 15 out of 30 target perand polyfluoroalkyl substances were detected in the samples with wide-spread occurrence and high potential of bioaccumulation through the food chain, since their concentration was orders of magnitude higher in apex predator in comparison with their prey. PFOS was the most abundant compound of this class, especially in otters from all tested countries, and was the compound that presented a 100% frequency of appearance.

ENVR 693

Interactions between anthropogenic dissolved organic carbon and marine microorganisms: Implications at regional and global scales

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Thousands of organic pollutants reach the open ocean through atmospheric deposition and oceanic currents causing a ubiquitous pollution by anthropogenic dissolved organic carbon (ADOC). Microorganisms play a major role in the breakdown and mineralization of some ADOC compounds, allowing, at least, their partial elimination from seawater, but this oceanic sink of organic pollutants remains largely unquantified. Despite thousands of organic pollutants have been reported in seawater, large fractions of ADOC remain uncharacterized, including the chromatographically unresolved complex mixtures (UCM). Moreover, most of the genes involved in microbial degradation of anthropogenic compounds remain uncharacterized, neither under which conditions degradation occurs in the oceans. We performed field experiments at all oceans (Arctic, Southern, Atlantic, Pacific and Indian Oceans, and NW Mediterranean) to elucidate the mutual influences between bacteria and organic pollutants. We challenged marine microbial communities from these contrasted environments with the ADOC obtained from the hydrophobic dissolved organic matter fraction in seawater at oceanic relevant concentrations and analyzed the bacterial activities and gene expression profiles through metatranscriptomics and other physiological approaches. Additional experiments were performed with specific families of pollutants such as perfluoroalkyl substances, organophosphate ester flame retardants and plasticizers, and polycyclic aromatic hydrocarbons. We taxonomically identified the main degraders and the main metabolic routes involved in the responses to cope with ADOC, including the nutritive and the toxicological effects. In order to know if biodegradation is relevant at oceanic scale, in addition to exposure field experiments, we performed an assessment of the large data set on hydrocarbons and emerging pollutants generated during the Malaspina circumnavigation expedition. These observations showed the relevance of microbial degradation depleting the bio available dissolved aromatic and aliphatic hydrocarbons, as well some emerging organic pollutants. Our different approaches show that microorganisms are key players driving the fate of ADOC in the ocean and simultaneously, ADOC influences the functionality and structure of marine microbial communities.

ENVR 694

Trait driver ecological theory predicts complex responses of phytoplankton exposed to chemical stress

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Understanding the processes shaping the structures and functioning of ecosystem is key to assess their vulnerability and predict their development under stress. The trait-driver theory (TDT) was recently introduced to

relationship between describe the organisms' characteristics (traits), their assembling in communities and the emerging ecological functions. In so, it mechanistically details the processes underpinning response capacity (RC), the efficiency of a system in maintaining functionality by changing structures when conditions change. Despite being a fundamental concept in resilience theory, no direct measurements of RC has been drawn from empirical observations, so far. Furthermore, a detailed experimental assessment of TDT predictions is missing too. We ran *in situ* experiments with two distinct lake phytoplankton communities stressed for the first time with a mixture of micropollutants at environmentally realistic concentrations. We drew TDT expectations on community responses using an individual-base model, compared formally elaborated theoretical expectations with the results of the experiment, and found that TDT successfully predicts changes in size distribution, functional group turn-over and functional responses of the two communities. We also provide empirical evidence and a measure of their RC by looking at the rate of change of phytoplankton traits and its correlation with production. An empirical assessment of ecosystem RC is presented here for the first time. RC emerges as a trait-based measure of community responses linked to the maintenance of ecological functions under environmental changes.

ENVR 695

Reactive nitrogen species: Neglected radicals in the UV/monochloramine process

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The UV/monochloramine (NH₂Cl) process is being considered an emerging advanced oxidation process in water treatment. Free chlorine and UV are widely used for water treatment, and the common presence of ammonia in water lead to the de facto UV/chloramine scenarios. The kinetics and mechanism of ibuprofen (IBP) and naproxen (NPX), two pharmaceuticals, by the UV/NH₂CI process was investigated. Typical radicals such as hydroxyl radical (HO•) and chlorine atom (Cl•) were identified in the process, unexpectedly, we found that reactive nitrogen species (RNS) also played important roles in the transformation of pollutants. Electron paramagnetic resonance (EPR) analysis proved the production of •NO as well as HO•. The concentrations of HO•, CI• and •NO in UV/NH₂CI remained constant at pH 6.0-8.6 and increased with increasing NH₂Cl dosage. The contribution of RNS to the degradation was quantified, and modelling results also supported the formation of RNS. Products containing nitroso-, hvdroxvl- and chlorine-groups were detected during the degradation of IBP and NPX by UV/NH₂Cl, further indicating the important roles of RNS in this process. This study firstly

demonstrates the involvement of RNS in the transformation of pollutants in UV/NH₂Cl.

ENVR 696

Improved UV degradation of microcystin-LR by a novel KrCl excilamp

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To optimize UV-C treatment of cvanobacterial toxins, we treated microcystin-LR (mc-LR) with 222 nm emitted by a novel KrCl excimer lamp compared to 254 nm emitted by a conventional low-pressure (LP) mercury vapor lamp. Because mc-LR has higher absorbance at lower UV wavelengths, we hypothesized the novel excimer lamp would be more effective than LP lamps. Degradation of mc-LR spiked into distilled water was compared to degradation of mc-LR spiked into natural water samples from the Cuvahoga River and Lake Erie to quantify the extent that natural organic matter interfered with mc-LR degradation. Before and after UV exposure, toxin concentration in samples was quantified by ELISA (enzyme-linked immunosorbent assay) and UPLC (ultraperformance liquid chromatography). These methods with different detection mechanisms were used to compare the degradation of mc-LR from two chemical perspectives. In distilled water spiked with 50 ppb mc-LR and exposed to the highest UV dose (160 mJ / cm²), the excimer lamp degraded mc-LR to 15% and 7.5% of the original concentration (measured by ELISA and UPLC, respectively), while the LP lamp degraded mc-LR to only 50% and 40% of the original concentration. In spiked natural samples, mc-LR degradation by the excimer lamp was similar in Lake Erie water (6% and 9%) to Cuyahoga River water (10% and 8%), which was slightly greater than in distilled water. Overall, the novel excimer lamp was approximately as effective as the conventional LP lamp at degrading microcystin-LR. These results indicate the promise of low-wavelength UV emitted by KrCl excilamps as a feasible option for treating harmful algal blooms, even in natural water samples with high background absorbance and organic matter content.

ENVR 697

Development of quinine as a fluorescent probe compound for quantifying hydrated electron

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There has been increased interest in hydrated electron (e_{aq}⁻) for its use in chemical synthesis, as a reductant in natural aquatic systems, and as a reactive species in water treatment technologies. Recent laboratory studies have assessed the ability of e_{aq} to degrade inorganic and organic contaminants, including oxyanions, selenium, vinyl chloride, and, more recently, per- and polyfluoroalkyl substances (PFAS). Much of the work in this area has employed eag⁻ sensitizers activated by UV light (e.g., sulfite, iodide) from a low-pressure mercury lamp. Despite the growing interest in this technology, results from these individual studies are not readily comparable due in part to the lack of standardized method for quantifying the photoactive species, e_{aq}-. This study presents a method for quantifying e_{ag} in steady-state irradiation experiments using quinine as a probe compound. The relevant physicochemical data for quinine were determined including spectral properties, direct photolysis quantum yield, and second-order rate constant with eaq⁻. The utility of quinine is tested by measuring e_{aq}- steady-state concentrations, [eag-]ss, under a variety of conditions typically encountered in engineering applications and comparing these values to those calculated from kinetic modeling. Taken as a whole, our results are supportive of quinine as a probe compound for e_{aq}-, which will aid in the development of engineering technologies for the degradation of recalcitrant contaminants.

ENVR 698

Modeling the kinetics of UV/peracetic acid advanced oxidation process

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Peracetic acid combined with UV (i.e., UV/PAA) has emerged as a novel advanced oxidation process (AOP) for water disinfection and micropollutant degradation, but kinetic modeling for this AOP was lacking. In this study, a comprehensive model was developed to elucidate the reaction mechanisms and simulate reaction kinetics of UV/PAA process. By combining radical scavenging experiments and kinetic modeling, accurate quantum yield of PAA under UV₂₅₄ (Φ = 0.9 mol Einstein⁻¹) was determined via simultaneously quenching •OH and $CH_3C(O)O^{\bullet}$ with 2,4-hexadiene. The comparison between experimental observations and model predictions over a wide range of conditions allowed estimation of the rate constants of PAA with •OH ($k_{\bullet OH/PAA} = 1.1 \times 10^9 \text{ M}^{-1}\text{s}^{-1}$) and HO₂• ($k_{\text{HO2}\bullet/\text{PAA}} = 2.0 \times 10^2 \text{ M}^{-1}\text{s}^{-1}$) with good accuracy. With derived Φ , $k_{\bullet OH/PAA}$, and $k_{HO2\bullet/PAA}$, the kinetic model accurately predicts PAA decay under UV₂₅₄ photolysis

across varying PAA and H_2O_2 concentrations and water pH (5.8-7.1). Meanwhile, the model reveals that UV/PAA generates a lower •OH concentration than UV/ H_2O_2 at equivalent conditions, with $CH_3C(O)OO^{\bullet}$ as the most abundant carbon-centered radical. This study significantly improves the knowledge of reactive species generation and reaction kinetics and mechanisms under UV/PAA, and provides a new model tool for this degradation process for water contaminants.

ENVR 699

Wavelength dependence of E.coli photoreactivation in the presence of DOM

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UV disinfection has been utilized for many years in water treatment plants as an alternative method to conventional disinfection with chlorine. UV disinfection provides disinfection without any chemical costs and minimal DBP formation risk. With recent advances in the production of UV-LEDs, there is a great opportunity to change the current practice of using mercury lamps to the new UV-LEDs for advantages such as wavelength diversity and quicker start-up time. Given that the regrowth after treatment for mercury lamp is a known issue, it is critical to check UV-LEDs for the possibility of having the same issue with regrowth. The inactivation of two indicator microorganisms (E. coli and MS2) was studied under 254 nm, 278 nm and 305 nm doses in this research. Results demonstrated higher doses required to obtain 3.0 log inactivation than the amount needed for the 254 nm Hg Lamp. Furthermore, results illustrated DOM did not significantly impact disinfection kinetics for all the wavelengths. Regrowth experiments, including dark repair and photoreactivation, were conducted. Results showed DOM can enhance in several cases. Importantly, it was observed for the first time that the photoreactivation mechanism was exhausted after a given fluence followed by the inactivation phase which stresses the importance of light exposure. Moreover, the result indicated that different wavelength has different effects on the photoreactivation with visible light having more regrowth compared to UVA reactivation.

ENVR 700

Impact of sunlight on the fate of oil spilled in aquatic environments

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Sunlight has been shown to be an important factor in the fate of pollutants present in environments that are subject to solar exposure. Energy provided by absorption of solar photons can overcome activation barriers and initiate a wide range of reactions, including direct and indirect photolysis. Oil spills represent a recurring opportunity for contamination of aquatic, terrestrial, and atmospheric environments with petroleum compounds, predominantly linear and branched alkanes, aromatics, and alkyl aromatics. Once released into the environment, sunlight plays a major role in oxygenating these compounds, which results in dramatically different fate, transport, and toxicity behavior. Polycyclic aromatic hydrocarbons present in the oil are strong chromophores in the UV and visible regions. These compounds can undergo direct photolysis or can participate in the formation of reactive transients such as singlet oxygen and hydroxyl radical. High resolution mass spectrometry measurements have demonstrated that oil oxygenation occurs across a wide range of carbon numbers, double bond equivalencies, and heteroatom content, indicating that photochemistry impacts most if not all of the compound classes present. The oxygenated oil photoproducts partition between the oil, water, and gas phases as well as the interfacial regions. Interfacially active photoproducts support emulsification of oil and water, resulting in mousse that is more difficult to remediate or degrade naturally. Furthermore, the aqueous phase photoproducts are bioavailable and can either be metabolized or cause toxicity to microorganisms; hence, there is an important connection between photochemistry and biological utilization of spilled oil. Studies on oil photoproducts have identified a range of oxygen containing functional groups, including aldehydes, ketones, carboxylic acids, and alcohols. These photoproducts are observable on a short time scale (minutes), demonstrating that photochemistry is a more rapid process than microbial action. While sunlight has long been recognized as a factor in the fate of oil spills, our studies over the last decade have provided greater detail into the controlling factors. intermediates, and time frames for these processes.

ENVR 701

Photoaging of atmospheric particulate matter in the aqueous phase

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Particulate matter (PM) is produced by a variety of anthropogenic as well as natural processes and is a particularly important research topic due to their

detrimental impacts on human health. We present here investigations on the photoaging of these PM in the aqueous phase and particularly on the effects of hydroxyl radical (•OH) production, which is one of the major species driving to the photoaging of the PM. A sampling campaign from an urban, a rural and a mixed urban-rural site was done in the Denver area, Colorado. Following collection, part of the samples was extracted into water and photoaged using simulated sunlight. The optical properties and the potential of the PM aqueous extracts to generate •OH were measured, it was observed that the light absorbance capacity was higher in the urban site than in the rural one and that the decrease in light absorbance properties during photoirradiation was correlated with the iron and the nitrate content of the extracts. These observations correspond to a scenario where the PM are mostly produced in the urban site and are transported to the rural one, with a mean age of the PM higher in the rural site. This work should help to understand the parameters that influence the photoaging of PM in the atmosphere, as well as the influence of trace elements on this process.

ENVR 702

Impact of halogen radicals on dissolved organic matter transformation during chlorine photolysis

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Organic contaminants, such as pharmaceuticals and personal care products, are ubiquitous in drinking water sources, but are not removed by conventional water treatment processes. Chlorine photolysis, which relies on the photolytic cleavage of hypochlorous acid and hypochlorite, is an emerging water treatment method that degrades organic contaminants via a suite of reactive oxidants. Hydroxyl radical is the primary oxidant, while ozone, chlorine radical, dichloride radical anion, and other reactive chlorine species are also formed. In natural waters, these oxidants can react with dissolved organic matter, potentially forming halogenated disinfection byproducts. Two major classes of known disinfection byproducts, namely trihalomethanes and haloacetic acids, are regulated in drinking water to protect human health. This study investigates the impact of dissolved organic matter on the formation of reactive oxidants and the production of regulated and novel disinfection byproducts under multiple treatment conditions (i.e., pH 6.5 and 8.5, and photolysis at 254, 311, and 365 nm) using traditional analytical techniques and ultrahigh-resolution mass spectrometry. The presence of dissolved organic matter decreases the steady-state concentrations of both hydroxyl radical and chlorine radical due to guenching.

Chlorine photolysis forms less trihalomethanes and haloacetonitriles than dark chlorination but increases the formation of haloacetic acids. The formation of halogenated dissolved organic matter is also enhanced during chlorine photolysis under all conditions. The role of halogen radicals in the formation of these novel DBPs is investigated using quencher studies. This study provides insight into the potential of DBP formation during chlorine photolysis.

ENVR 703

Photochemical transformation of Fe in the presence of natural organic matter (NOM): Implications to Fe availability and NOM transformation

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Iron is a critical micronutrient in natural waters. In natural waters, iron exists principally in two oxidation states, namely, as ferric (Fe(III) and/or ferrous (Fe(II) iron. The rates of transformation of Fe between these oxidation states generally control Fe availability in natural waters. In this work, we investigated the mechanism of Fe redox transformation occurring in the presence of natural organic matter (NOM). In particular, we determined the rate and mechanism of (i) Fe(III) reduction in dark and irradiated conditions and (ii) Fe(II) oxidation in dark and irradiated condition using a comprehensive experimental data set. We also investigated the associated NOM oxidation occurring as a result of interaction with reactive oxygen species (ROS such as hydroxyl radicals) generated on Fe redox transformation and/or NOM photochemistry. The presentation will highlight the main findings of our studies, in particular, (i) The presence of native reduced organic groups in NOM which oxidizes to form stable organic specie on irradiation. The reduced organic group present intrinsically in NOM is capable of reducing Fe(III), while the oxidized organic specie formed irradiation is a strong Fe(II) oxidant. on (ii) Photogeneration of short-lived organic moieties, that is capable of oxidizing Fe(II), on irradiation of NOM. (iii) The influence of pH on the lifetime of the photogenerated organic moeties that are involved in Fe(II) oxidation. (iv) No significant influence of pH on the steady-state Fe(II) concentration (and hence Fe bioavailability), which is traditionally assumed to vary significantly with pH due to changes in Fe(III) solubility and Fe(II) oxygenation rate with variation in pH. (v) The influence of Fe(III) speciation (iron oxides versus organically-complexed Fe(III)) on the main pathways of Fe(III) reduction. (vi) Hydroxyl radical generation on Fe(III) photoreduction and the associated oxidation of NOM present.



Mechanism of Fe redox transformation in dark and irradiated conditions

ENVR 704

Effects of sunlight on haloacetonitrile formation potential from wastewater effluents

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The presence of wastewater effluents in source waters can increase the formation of haloacetonitriles (HANs), a group of nitrogenous disinfection byproducts exhibiting 10–100 times higher cytotoxicity and genotoxicity than the trihalomethanes and haloacetic acids regulated by the U.S. Environmental Protection Agency. Sunlight plays an important role in transforming effluent organic matter as it travels downstream, but its effect on the HAN formation potential of wastewater effluents has not been thoroughly investigated. In this study, 16 secondary effluent samples were collected from 4 wastewater treatment plants over 29 months, disinfected in the laboratory by chlorine or UV to simulate wastewater disinfection, and then irradiated under simulated sunlight. Among four evaluated HANs, dichloroacetonitrile (DCAN) and bromochloroacetonitrile (BCAN) were detected in all samples. Sunlight preferentially attenuated BCAN formation potential (BCAN-FP) over DCAN-FP. For chlorine disinfected samples, 8 h irradiation (equivalent to 2-3 d of natural sunlight) did not decrease the DCAN-FP for most samples, but removed BCAN-FP from two thirds of the samples. The calculated cytotoxicity contributed by all dihaloacetonitriles was also reduced in most samples after 8 h irradiation. Similar behavior was observed for a mixture of wastewater and surface water (volume ratio 1:1). Experiments using model precursors tryptophan, tyrosine, and fulvic acid showed that BCAN-FP was more likely to exhibit a decrease than DCAN-FP upon irradiation. Fulvic acid best approximated the behavior of the authentic effluent, likely serving as a photosensitizer to degrade other HAN precursors. Lastly, we observed that, for wastewater samples disinfected by UV, the higher the UV dose, the more likely the reductions in DCAN-FP and BCAN-FP by sunlight, a phenomenon also observed for Tryptophan. Experiments suggested that the UV photoproducts of tryptophan have high yields of excited triplet state, which can promote the attenuation of HAN precursors.

ENVR 705

Development of a poly(*N*-isopropylacrylamide)-based sensor for persistent per- and polyfluoroalkyl substances

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Per- and polyfluoroalkyl substances (PFAS) have pervaded the environment as a consequence of predominantly unconscious domestic and industrial use in contaminated cleaning supplies, stain-resistant coatings, and aqueous film-forming foams, which, when viewed in concert with increasing knowledge of their negative impact on the health of effected biota, raises concern for their facile detection in suspect water sources. Bulky analytical equipment, such as liquid chromatography with tandem mass spectroscopy, is the current gold standard for precise and selective determination of PFAS pollution, however, the necessity of complementary extraction and isolation encumbers the equipment's ready use for in-field sampling. To this end, an approach for measuring contaminant concentration utilizing thermoresponsive poly(N-isopropylacrylamide) is proposed herein as a simplistic method to identify the level of perfluorooctane sulfonate (PFOS) in solution. Polymers containing fluorinated comonomers were characterized with X-ray photoelectron spectroscopy and Fourier-transform infrared spectroscopy and employed to exploit fluorinefluorine attraction amongst the gels and contaminants to enhance the gels' sensitivity. Results indicate significant swelling of up to 3,759% by mass in the presence of 1 mM PFOS with respect to water, and efforts are currently focused on improving the precision of the method through functionalized microcantilevers.

Development of a simple analytical method for determination of Arsenate using FAM-labeled DNA and cerium oxide nanoparticles

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Since arsenic (As) is extremely toxic metal, its contamination of drinking water sources was estimated to affect human health over 144 million people around the world. The traditional methods for As detection require sophisticated, expensive and bulky equipment, specialize expertise for operation, have a high operating cost. They are not suitable for on-site analysis. Hence, there is a need for a simple, low-cost, and on-site technology to determine As. As has two common oxidation states: arsenate (As(V)) and arsenite (As(III)). Most of the simple analytical methods and sensors have been developed to detect As(III) or total As. While it is more challenging to detect As(V), there are a few studies to detect As(V). However, in these studies, As(V) concentration in environmental water has not been determined because of the lack of selectivity. In this study, we developed a simple and selective analytical method for As(V) using a carboxyfluorescein (FAM)-labeled DNA and cerium oxide (CeO₂NPs) and nanoparticles determined As(V) concentrations in groundwater. CeO2NPs has been used to adsorb DNA and quench FAM. As(V) could be adsorbed onto NPs, desorbed DNA and recover FAM. The optimal concentrations of CeO2NPs and FAM-labeled DNA and incubation time were determined to be 15 ug/mL, 40 nM and 6 min, respectively. Under the optimal conditions, a calibration curve of our method was created. The LOD was calculated to be 25 µg-As/L. According to the selectivity test, our method had a high selectivity toward As(V). Using the calibration curve, we determined As(V) concentrations in groundwaters (Fig.1). The relative errors in the As(V) concentrations determined by our method and ICP-MS were within 30%. Therefore, we concluded that our method might be applicable to As(V) monitoring in groundwater with a variety of ions at high concentration.



Fig.1: Relationship between concentrations of As(V) in groundwater samples determined by ICP-MS and those determined by our method. The samples were taken at 8 different sites.

ENVR 707

DNA-based tracers for hydrologic characterization

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Complex hydrogeological regimes such as karstic aquifers are difficult to characterize with conventional tracers such as chemical dyes, elements and streamflow gain and loss measurements. The limited options for different tracers, toxicity and watershed memory of past inputs limit the identification of multiple flow paths at once using conventional chemical tracers. To overcome these limitations, an engineered DNA-based tracer system is being developed. Synthetic DNA-based tracers are advantageous because they are cost effective, have a low detection limit, have thousands of possibilities for unique tracers and can be used to identify multiple flow pathways. Five unique DNA sequences were designed using an online random sequence generator. The sequences were designed to be 200bp in length with a GC content greater than 50% and no repeats longer than 4bp. The sequences were checked for similarity with naturally occurring DNA sequences using the NCBI Basic Local Alignment Tool. Primers were developed for the sequences using IDT PrimerQuest tool. The tracers will be injected in an acrylic column filled with alluvial aquifer media with water pumped to the top to keep the column saturated. The tracers will be recovered and guantified PCR usina Droplet Digital and Nanodrop Spectrophotometry. Once the tracers have been successfully recovered in the laboratory, they will be deployed near the headwaters of Helotes Creek. Samples will be collected downstream and transported to the

laboratory for detection and quantification. The tracers will then be introduced into three suspected points of recharge of Helotes Creek and samples will be collected from live-water reach. The samples will be transported to the laboratory for detection and quantification. The results of this project are expected to demonstrate the advantages and effectiveness of DNA-based tracers for hydrologic characterization and the advancement of our understanding of the natural environment.

ENVR 708

Did we really use the intrinsic fluorescent properties of nitro-factualized metal-organic frameworks (MOFs) to realize H₂S detection in an aqueous system?

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Hydrogen sulfide (H_2S), known as an odor of rotten eggs, is widely spread across industries including iron smelters. landfills, food processing plants, and breweries. The extreme toxicity of H₂S in the environment makes H₂S of significance for safety and human health. Various Nitrofunctionalized metal-organic frameworks (MOFs) have been designed and synthesized to realize H₂S detection based on the "turn-on" effect, where the -NO2 groups are reduced to -NH₂ groups and the fluorescence enhancement is observed after being exposed to H₂S treatment. Most researchers ascribed such a "turn-on" effect to "local transformation" of MOF in aqueous suspension (i.e., solid-state MOFs are dispersed in liquid evenly) using NaHS or Na₂S as the H₂S source. However, no direct evidence was given to the existence of -NH2 groups attached to the MOF surface. In addition, peak broadening phenomenon in XRD patterns was observed in previously reported Zr-based, Ce-based, and Al-based MOFs, which indicated all these MOFs experienced partial degradation and crystal consuming during H₂S treatment. No researchers noticed such peak broadening phenomenon and it is still unclear whether these -NH2 groups attached to the surface of MOFs or the free ones released in the solution that really contribute to the fluorescence enhancement. To explore the real fluorophores in MOF itself or in the solution, AI-MIL-53-NO₂ was utilized as a model MOF in this study. Specifically, the supernatant and the undissolved particles separated from AI-MIL-53-NO₂ suspension after being exposed to H₂S were analyzed systematically. The results indicated that it is the free BDC-NH₂ (2aminobenzene-1, 4-dicarboxylic acid) in the solution rather than the Al-MIL-53-NH₂ that gives rise to the "turnon" effect. During the H₂S detection, the crude Al-MIL-53-NO₂ was partially degraded by OH- attack in the solution and then the shedding BDC-NO₂ (2-nitrobenzene-1,4dicarboxylic acid) was reduced to BDC-NH₂. In addition, with the existence of fluorophores BDC-NH₂ dissolved in the solution, the supernatant can be used for quantitative H₂S detection as well. The result of this work unravels the origin of the "turn-on" effect of Al-MIL-53-NO₂ in H₂S sensing and provides new insights into the ways of fluorophore location in probe-consuming sensing application.

ENVR 709

Cross-linked UIO-66-NH₂/PIM-1 sensors for room temperature CH_4 detection

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Methane (CH₄), the main composition of natural gas, is considered as a greenhouse gas with a global warming potential greater than CO₂ per molecule, which could significantly contribute to undesired global warming through even moderate amounts of leakage. CH₄ is also explosive for concentrations above the lower explosive limit. For the purpose of both safety and environmental concerns, a strong interest and need exist for CH₄ leak detection. Unfortunately, current sensing technologies do not meet all practical requirements for widespread deployment and accurate measurement of low-level methane leaks or in-pipe gas composition monitoring. Thus, the development of advanced gas sensing devices of sufficiently low cost and which can be interrogated remotely over long distances would be highly beneficial. In this study, our proposed method seeks to develop polymer/MOF composite sensors based on the optical fiber platform. Zirconium metal-organic framework (UIO-66-NH₂) is chemically cross-linked with polymers of intrinsic microporosity (PIM-1) to exploit the excellent gas sorption capability of the porous MOF and the polymer. The PIM-1 acts as binder materials to keep the welldispersed composite mixture on the optical fiber surface and enables ease of scalability to km-length optical fibers, while the MOF particles could significantly mitigate the aging issues of the PIM-1 thin film. The limit of detection of the sensor achieved 3% of CH₄ at RT with full reversibility. The sensors also demonstrated high stability under ambient conditions and showed comparable sensing response after 45 days. A variety of characterizations are performed to investigate the physical/chemical/morphological properties of the composites and unravel the fundamental understanding of the sensing mechanism.



Figure 1. CH_4 sensing data of a UIO-66-NH₂/PIM-1 coated optical fiber sensor. CH_4 with different concentration is sensed by monitoring the change in light transmission at 760 nm. The inset is the zoom-in of low concentration CH_4 sensing.

ENVR 710

Bioenergetics by Lehninger coupled with "horizontal" nutrient transfer and "real time" spectrophotometric sensors offers an alternative explanation for algal blooms

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Spectrophotometric and other sensors at stream gaging stations on the Passaic River in New Jersey, principally USGS 01389005 provide "real time" data for nitrogen, carbon, dissolved oxygen and other nutrients necessary for chlorophyll synthesis. However, the replication rate of algal biomass during an algal bloom, for example, of blue green "algae" cyanobacteria, more energy than could be available solely through photosynthesis to synthesize cell mass at the supposed replication rate. Analysis of data gathered at that USGS station, and at nearby wastewater dischargers and water supply purveyors suggests that the contents of algal cells that leak or remain after cells die may allow the replication rates to be achieved without synthesis from scratch.

ENVR 711

Self-immolative systems for the disclosure of reactive electrophilic alkylating agents

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The design of self-immolative systems has been based upon a stable bond between trigger and reporter groups, the stability of which is sensitive to particular agents and environments. Chemically specific triggers have been realised for a diverse range of applications spanning drug delivery, biological and chemical sensors, diagnostics and degradable polymers. 'Classical' self-immolative chemistries operate by activation or deprotection of the trigger group by nucleophiles (e.g. fluoride, RSH) to render the immolative unit labile via generation of an electron rich, nucleophilic centre that then initiates a cascade of electrons and culminates in the release of the reporter group. To date, only limited use of selfimmolative linkers in the disclosure of electrophilic species such as chemical warfare agents (CWAs), fumigants, pesticides, pharmaceuticals and other environmental hazards, has been reported and that by the vicarious generation of a nucleophile to trigger the selfimmolative pathway. The challenge in generating a colorimetric disclosure system for reagents of this reactivity type under ambient conditions is to create a triggering system that responds to an electrophilic reagent in such a way as to allow indirect generation of a nucleophilic electron-rich centre in the trigger event. In this presentation, we report how we met this challenge by designing a series of disclosure molecules (see Figure 1) that represent the first examples of selective selfimmolative systems triggered by a non-acidic electrophilic species such as methyl, allyl and benzylic halides as distinct from a proton, for the avoidance of false positive results. These systems provide a visual colorimetric response to such electrophiles, following exposure to mild, basic conditions, without the need for analytical instrumentation and thus there is great potential for the use of these reagents for the visual disclosure of toxic electrophilic alkylating agents.



Figure 1. The design of the self-immolative disclosure systems **1–3** for non-acidic electrophiles.

Use of airborne and ground-based physical and chemical sensors for monitoring tidal wetlands enhancement projects

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Beneficial use of dredged material is the placement of dredged material to enhance, create, or restore a variety of estuarine habitats, as opposed to the usual practice of disposing of it in an upland confined facility. In 2013, the New Jersey Department of Environmental Protection (NJDEP) and multiple federal and state partners initiated three pilot projects to evaluate the concept of beneficial use of dredged material on existing, but stressed and vulnerable, salt marshes. Three deposition sites and two background sites were identified in salt marshes of southern New Jersey. The continuing project goal is to improve their structure, ecological functions, and resiliency, thus helping them to persist into the future in the face of sea level rise. Multiple sensors were deployed during the monitoring of the project. Water chemistry was monitored post placement using EXO[™] sondes to evaluate surface pools and a series of monitoring wells that were installed throughout each site. Both the enhanced and reference sites were monitored during times of flushing and times of stagnation in order to see if the variability in the water quality chemistry at the enhanced site was within the normal range for that parameter. Multiple measurements were made by the Wetlands Institute and NJDEP Division of Science and Research to assure the quality of the measurements. Survey grade RTK-GPS and ground based lidar were used to map the changing elevations at the sites. The high-precision GPS 3-D coordinates provided location data that was utilized to correct the information that was collected by programmed drone overflights that were conducted at various times during the seasonal growing periods to identify and assess the vegetative recovery of the estuarine habitats. The high-resolution drone images were post processed to create a geographical information system project layer using ESRI™ Drone to Map software so that the partners could utilize the layer to determine the changes in the study area with time. A continuouspressure sensor network has been deployed throughout the study area with local air reference stations, monitoring well locations near ground elevation reference points, and submerged in channels within the study areas to document tidal height variability. In combination, these data can be used to explore relationships between elevation, inundation, water chemistry, and vegetative recovery of salt marsh habitat enhanced by dredged material.

ENVR 713

Design and performance of a portable device for characterizing indoor and outdoor air

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Air pollution is one of the leading causes of adverse acute and chronic cardio-respiratory problems, worldwide. Poor indoor air quality is a rising concern as humans spend >90% of their lives indoor. To better study indoor air quality in such environments, a low cost, portable, IoT sensor-based device was built and deployed at the indoor and outdoor locations at two sites - a university and a hospital. The device was designed to monitor the concentrations of aerosol particles (0.3 - 10 µm) in real time and simultaneously collect particles using the principle of electrostatic precipitation for off-line analysis. Our goal was to obtain baseline information about the size-resolved aerosol concentrations at high spatial and temporal resolution, and their correlation to the airborne microbial population. At both the university and hospital, aerosol particle number concentrations positively correlated with the human occupancy and activities. The number concentration trends showed a striking commonality at all the ten indoor sites of both the university and hospital. Further, the influence of outdoor PM to the indoor sites was found by analyzing the I/O (indoor-outdoor) concentration ratios and with the statistical analysis such as Pearson correlation and principle component analysis (PCA). While human and soil associated airborne bacteria such as Bacilli (25%) and Actinobacteria (20%) was found to be relatively abundant in all the indoor sites, few notable clinically relevant airborne bacteria (~5%) belonging to the class Burkholderia and Pseudomonas, known to cause healthcare associated infections (HAI) were found in the hospital air samples. We will present the device design details and the findings from lab performance tests and field measurements.

ENVR 714

Remediation with zerovalent metals more strongly reducing than iron

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During the 25 years since zerovalent iron (ZVI) became the most widely studied of all environmental reductants, there has been a much smaller number of studies that investigated other zerovalent metals (ZVMs) that are similarly, or more strongly, reducing than ZVI. The most promising of these are zerovalent zinc (ZVZ) and zerovalent magnesium (ZVMg) because they-like ZVIundergo oxidative dissolution to products that are not of great environmental concern (e.g., their respective cations). In contrast to ZVI, the very low reduction potentials of ZVZ and ZVMg can result in rapid reduction of water, so much so that ebullition of hydrogen can cause operational problems like over-pressurized bottles in laboratory batch experiments. This has led to the presumption that rapid aqueous corrosion of ZVZ and ZVMg will make these metals impractical for remediation due to insufficient allocation of electrons to reduction of contaminants and blockage of pore space with hydrogen gas. However, our recent work with ZVZ and ZVMg has demonstrated that excessive reactivity is not a problem (at circum-neutral and higher pH's) because passivation of these metals tends to be strong. In fact, it appears that the oxide film that forms on these metals in air breaks down very slowly when immersed in water, so much so that aggressive pretreatments are needed to obtain the rapid contaminant degradation rates that are expected because of the low reduction potentials of these metals. This combination of effects poses a challenge to control passivation of the metal to maximize contaminant reduction and minimize the reaction with water. This paper will summarize some old, but mostly new, results on the dechlorination of organic contaminants and sequestration of metal oxyanions by ZVZ and ZVMg, with emphasize on how the competition among reactions of these metals might be managed to make practical processes for remediation.

ENVR 715

Degradation of triclosan by reduced nano-biochar

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Reductive dechlorination is one of the most important reactions for eliminating trace amounts of organohalogen contaminants in natural and engineering systems. This study targets dehalogenation by nano-scaled biochar (n-BC) (with size < 0.45 μ m) using a common organohalogen pollutant, triclosan (TCS). Five different types of n-BC were used and compared to activated carbon. In our experiments, n-BC was reduced biologically in a 24-h pre-incubation with *Shewanella putrefaciens* CN32, prior to reaction with TCS. We found that TCS can be anaerobically degraded by reduced n-

BC, with a pseudo first-order degradation rate constant of 0.0011-0.0105 hr⁻¹. The degradation rate of TCS correlated significantly with the number of n-BC-bound electrons available for TCS reduction. Reducing capacity of n-BC can be partially attributed to the semi-quinone functional groups in n-BC, detected by electron paramagnetic resonance analysis. In addition, the more n-BC was reduced, the more completely TCS can be degraded. Our results show that reduced n-BC can reductively dehalogenate organohalogen contaminants, with potential applications for wastewater treatment and groundwater remediation.

ENVR 716

Highly efficient Au@3-D carbon nitride nanocomposites for ultrafast recyclable reduction of nitroarenes

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In this study, we have demonstrated a simple and facile synthesis method for the fabrication of Au@3-D carbon nitride (C₃N₄) nanocomposite with 0.5 – 3 wt% Au loadings for highly recyclable reduction of nitrophenols. The small Au nanoparticles (NPs) with an average diameter of 5 nm are highly dispersed and anchored firmly on 3-D C₃N₄ in the presence of SBA-15 as the template, which can homogeneously disperse the Au nanoparticles onto the porous surface. The large surface area, wellordered porosity and highly dispersed Au NPs make Au@3-D C₃N₄ an excellent nanocomposite toward nitroarene reduction. The EIS and ORR results indicate that the strong interaction between 3-D C₃N₄ and Au NPs improve the electrochemical properties as well as accelerate the conversion efficiency and rate of nitroarenes such as nitrophenols and 1-chloro-4nitrobenzene. The electron transfer number is in the range of are in the range of 2.5 - 3.2, which is higher than the theoretical 2-electron reduction process. The kobs for 4-nitrophenol reduction over 2 wt% Au@3-D C₃N₄ nanocatalysts can be up to 3.56 min⁻¹ in the presence of NaBH₄. Moreover, nitroarenes with electron-withdrawing substituents such as 1-chloro-4-nitrobenzene exhibit high efficiencies and rates of reduction. The Au@3-D C3N4 also shows good reusability in the reduction of 4nitrophenol and 1-chloro-4-nitrobenzene for at least 10 consecutive catalytic cycles without considerable loss in catalytic activity. The detection of H radical adducts indicates that Au NPs adsorbs BH4- ions and forms Au-H species to accelerate the reduction of nitroarenes via direct hydrogenation route. Results clearly demonstrate that Au@C₃N₄ is a promising catalyst with a wide application, which can provide a new venue for tailoring

metal/metal oxide-based nanomaterials for green catalytic reactions in water and wastewater treatment.

ENVR 717

Degradation efficiency of chlorinated hydrocarbons by a novel functionalized iron nanoparticle for improved remediation of contaminated sites

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Nanoscale zerovalent iron (nZVI) can degrade various chlorinated hydrocarbons (CHCs), but the passivation of nZVI by water significantly reduces its reactivity, which prevents the commercial-scale application of nZVI. Modification of nZVI with sulfur, a process termed as sulfidation, has been shown to dramatically improve the reactivity and selectivity of nZVI. However, most studies have focused on trichloroethene (TCE), and only one or two concentration levels, which are not representative of conditions at contaminated sites where various CHCs are present as mixtures and as both dissolved plumes and nonaqueous phase liquids. In this study, we synthesized sulfidated nZVI (S-nZVI_{co}) by co-precipitating FeS and Fe⁰ and evaluated the degradation of various CHCs by S $nZVI_{co}$ under both Fe⁰ limited and Fe⁰ excess conditions. We used TCE as a model compound to test the reactivity of S-nZVI_{co} under a series of stoichiometric ratios between CHCs and Fe⁰. We found that the degradation kinetics of TCE by S-nZVI_{co} were comparable at TCE/Fe⁰ ratios of 0.1-2, but the degradation capacity increased with increasing presence of TCE because of the loss of electrons to water at lower ratios. The reactivity of S $nZVI_{\infty}$ for 1,1,1-trichloroethane, trans-1,2-dichloroethene, and chloroform were either higher than or comparable with TCE, and perchloroethylene, cis-1,2-dichloroethene, 1,1,2-trichloroethane, and 1,1-dichloroethane showed less degradation rate. The degradation intermediates and products were identified, and the degradation and transformation of the intermediates were evaluated to establish reaction pathways. We further applied quantum chemistry simulation by density functional theory calculations to estimate the activation energy of the first electron transfer step for the CHCs to explain their difference in reactivity. The results will fill an important data gap on the reactivity of S-nZVI for priority chlorinated solvent contaminants and contribute significantly to the feasibility of the commercial remediation potential of SnZVI and the assessment of the applicability of S-nZVI in situ.

ENVR 718

Catalytic degradation of p-nitrophenol by nano zerovalent iron (nZVI) supported bimetallic catalyst

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p-Nitrophenol (p-NP) is a widely known toxic nitroaromatic chemical compound with poor biological degradability. The source of the p-NP release to the natural environment has several sources of industrial activities such as the production of pharmaceuticals, rubbers, dyes, electronics, and textiles. The central nervous system, kidney, and liver can be damaged by p-NP, causing various symptoms such as eye and skin irritations, blood disorders, confusion, loss of consciousness. Hence, p-NP was claimed to be one of the most hazardous waste products and a priority toxic pollutant by the US EPA, and its maximum concentration in natural water bodies was established to below 10 ng/ml. We investigated catalytic degradation of p-NP using different types of promoter metals (Cu, In, Zn, Ni, Sn) on the nZVI surface. First, control tests were conducted to show that p-NP cannot be degraded by photolysis and cannot be adsorbed on the reactor wall. Among different promoter metals, Zn and Cu shows the complete removal of p-NP in 5 min. Reaction kinetics follows pseudo-first-order reaction with rate constants equal to 1.58 min⁻¹ and 0.82 min⁻¹ for Zn and Cu, respectively. Zn/nZVI and Cu/nZVI catalysts showed higher removal efficiency than the NaOH treated coal fly ash supported ZVI and nZVI with NaBH₄ (1.28 and 0.31 min⁻¹, respectively). Since Zn showed faster kinetics, it was chosen as representative promoter metal for further experiments with the bimetallic catalyst with Pd as a noble metal. Moreover. SEM-EDX analysis of synthesized bimetallic catalyst showed 50-100 nm nZVI particles and uniform distribution of promoter and noble metals on nZVI surface. The study shows that nZVI supported bimetallic catalysts might be one of the promising environmentally benign technologies, which has high efficiency and potential to mineralize p-NP. Also, our experimental results can provide a basic understanding to develop the novel remediation and treatment technologies for the reclamation of contaminated surface and groundwater.

ENVR 719

Continuous improvements on advanced reduction technologies for challenging oxyanions and fluorinated chemicals

Jinyong Liu, *jinyong.liu*101@gmail.com, Changxu Ren, *Jinyu Gao, Tianchi Liu, Michael J. Bentel*. Chemical and Environmental Engineering, University of California, Riverside, Riverside, California, United States This presentation will summarize our recent progress on the development of several advanced reduction technologies- the reduction of oxyanions with heterogeneous metal catalysts, defluorination of PFAS with bioinspired metal complexes or with hydrated electrons. The focus of this presentation will be on the understanding and design of advanced reduction processes from the angle of molecular structures and chemical reactions.

ENVR 720

Potential application of metallic Mg milling scraps as a green and powerful contaminant reductant

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Mg metal (zero-valent magnesium, ZVMg, Mg⁰) is currently of interest as a strong reductant of environmental contaminants. Developing a cost-effective means of ZVMg utilization is one of the most critical issues for the practical application of ZVMg in the contaminant treatment processes. We obtained metallic Mg milling scraps (MS-ZVMg) from a die casting factory and compared the reactivity with those of three reagentgrade ZVMg (RG-ZVMg) particles using Cr(VI) as a model contaminant. Batch experiments were conducted by reacting 1.0 g/L of the MS-ZVMg or the other three RG-ZVMg particles from different commercial vendors with 19.5 μ M Cr(VI) at the initial pH of 6.24 ± 0.15 in the presence of the atmospheric oxygen. The MS-ZVMg effectively reduced Cr(VI) within 24 h and showed competent reactivity compared to those of the RG-ZVMg. Sonication of MS-ZVMg substantially enhanced its reactivity by about 3 times but not those of RG-ZVMg particles. FT-IR analysis of the ZVMg particles suggested that the removal of residual lubricant oil from the surface of MS-ZVMg particles was accounted for the increasing reactivity. In addition, sonication effectively sustained the reactivity of every type of ZVMg particles up to 6 cycles. The increasing reactivity of MS-ZVMg was also achieved by washing it with an organic solvent. Our results successfully demonstrated the potentiality of practical and cost-effective application of ZVMg in the treatment processes of contaminants.

ENVR 721

Development of quantitative structure activity relationships (QSARs) for abiotic reduction of organic chemicals

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Quantitative Structure Activity Relationships (QSARs) are necessary for the prediction of rate constants of dominant transformation pathways controlling environmental fate of organic chemicals for the purpose of conducting accurate exposure assessments. The rates of reduction for a large variety of organic chemicals were measured with Fe(II)tiron as the reductant. These chemicals contain at least one of the known reducible functional groups, including halogenated aliphatics. substituted azobenzenes. substituted nitroaromatic benzenes, substituted hydroxyl amines, substituted phenyl alkyl sulfones, substituted phenyl alkyl sulfoxides, substituted phenyl alkyl nitrosamines, substituted isoxazoles, and substituted oxime carbamates. Normalization of the rate constants to the same conditions is necessary for the development of accurate predictive models. Base on the linear correlation between $logk_{obs}$, where k_{obs} is the observed rate constants, and log[FeL26-], where [FeL26-] is the concentration of 1:2 Fe(II)-tiron complex, the rate constants and [FeL₂⁶⁻] can be calculated at any given condition. This is particularly useful given that the kinetic experiments were conducted under diverse conditions to accommodate the wide range of reactivity of the chemicals examined. Ongoing work develops QSARs based on poly-parameter linear free energy relationships (pp-LFERs) and many other variables such as reduction potential, HOMO energy, and electron affinity.

ENVR 722

UV/sodium percarbonate for the degradation of bisphenol A

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Sodium Percarbonate (SPC) is a common alternative to liquid hydrogen peroxide (H_2O_2) due to its stability for transportation and storage. It has been comprehensively used in chemical synthesis and household products, however, its application for environmental remediation is limited. Most conducted studies are mainly focus on the activation of SPC by various valent irons; little information is available for the activation of SPC by UV (UV/SPC). Moreover, previous studies assess the performance of UV/SPC for water and wastewater treatment mainly from the aspect of hydroxyl radical generation; the contribution

of carbonate radical anion has been overlooked. Therefore, this study systematically investigated UV/SPC for the degradation of bisphenol A (BPA) with comparison to UV/H₂O₂. In this study, the degradation efficiency of BPA in UV/SPC was found to be comparable to that in UV/H₂O₂ at the equilibrium concentration of H₂O₂. The possible reason for such phenomenon was proposed as the generation of carbonate radical anion in UV/SPC which was supported by the result of identification of reactive species and the determination of their steady state concentrations. Influences of matrix parameters were evaluated, and real wastewater matrices were used. The unique transformation products of BPA in UV/SPC were identified and the transformation pathways were proposed accordingly.

ENVR 723

Efficient bromide removal from produced water by peroxymonosulfate for controlling disinfection byproduct formation in downstream water supplies

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Shale gas extraction has contributed notably to lower oil and gas prices in the United States in recent years. However, this process produces a significant amount of produced water with a high level of bromide ions, which are hardly removed during the treatment. Once it is discharged into the receiving water, it may significantly increase the bromide level in the drinking water sources, resulting in the formation of toxic brominated disinfection byproducts (Br-DBPs). Due to the presence of chloride at much higher levels, the selective removal of bromide is challenging. In this study, we examined a simple but costeffective way to selectively oxidize bromide using unactivated peroxymonosulfate (PMS). A kinetic model that considered all the major reactions was developed and could describe this process very well. More than 95% of bromide was removed by PMS in less than 10 minutes under weak acidic conditions, without the significant formation of Cl_2 (g) even when the chloride concentration was more than two orders of magnitude higher than that of bromide. The tests in both batch and continuously stirred tank reactors resulted in high bromide removal rates and neutral final pH. After the treatment, the harmful effect of bromide on Br-DBP formation in impacted water supplies was significantly reduced. Overall, this study provided a simple but promising approach to selectively remove bromide from produced water with high efficiency, low cost, and simple system setup.

ENVR 724

Electrosorption of perfluoroalkyl substances onto activated carbon

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Per- and polyfluoroalkyl substances (PFAS), a class of ~5,000 compounds that are toxic and persistent, have been detected in drinking water across the country. Activated carbon (AC) is a widely used sorbent to remove PFAS. One challenge of using AC is its limited adsorption capacity for some PFAS, especially short-chain species. Manipulating the electrical behavior of AC may provide a solution to overcome these limitations. At environmentally relevant pH values, many PFAS occur as anions and are highly soluble in water. We therefore hypothesized that applying a small voltage to AC would increase adsorption capacities of anionic PFAS. Our results show that compared to uncharged controls (open circuit voltage), treatments with an applied voltage (1 V) always improved PFAS adsorption. The increase was dependent on PFAS chain length and acidic functional group (i.e., sulfonate or carboxylate). For example, with an applied voltage, adsorption increased upwards of 2.4 times for perfluorobutanesulfonic (PFBS; C4; sulfonate), but only up to 1.3 times for perfluorononanoic acid (PFNA; C9; carboxylate) compared to the no-voltage control. Preliminary tests with the background anion chloride (Cl⁻) were conducted to determine the competitive effect of this common environmental matrix component. In the presence of low-levels of CI⁻ typical of most groundwaters (1 mM), PFBS adsorption was enhanced up to 2.7 times with an applied voltage when compared to the open circuit control. At higher Cl⁻ concentrations, however, an enhancement was not observed suggesting that the competitive effect of CI⁻ was concentration dependent. In summary, these results indicate that small inputs of electricity can enhance the adsorption of PFAS onto activated carbon, but that the degree of enhancement is dependent on PFAS species and background matrix components.

ENVR 725

Sorption behavior of perfluoroalkyl substances (PFASs) using on organic surface functionalized metal oxide nanoparticles

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Perfluoroalkyl and polyfluoroalkyl substances (PFASs) are emerging contaminants of concern as they are recalcitrant to chemical and biological degradation treatment due to strong carbon-fluorine (C-F) bonds. Advances in nanoscale engineering and material science now allow for novel approaches for high capacity, tailored sorbent strategies, which utilize not only high surface area nanoparticles designed for targeted adsorption, but also for subsequent (magnetic) recovery. In this study, we applied surface functionalized metal oxide nanoparticles to effectively sorb/remove the perfluorooctanesulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) in aqueous environments. We prepared metal oxide nanoparticles via thermal decomposition of iron oleate (Fe-oleate) and manganese oleate (Mn-oleate) with specific ratios to achieve precise particle size and composition(s) and then functionalized with a series of organic surfactants. Sorption isotherms for PFOS and PFOA were evaluated with respect to the particle core size, organic coating, core structure, and solution chemistry. Nanoparticles coated with positively charged organic coatings such as polyethyleneimine (PEI) showed high performance for both PFOA and PFOS sorption and thus removal. In addition, we applied quartz crystal microbalance with dissipation (QCM-D) to assess the real-time sorption behaviors of PFASs on these nanoparticles, correlating results with batch test isotherms.

ENVR 726

Sorption of PFOA and PFOS on organic-modified Camontmorillonite: Effect of modifier structure

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The contamination caused by per- and polyfluoroalkyl substances (PFAS), particularly perfluorooctanoic acid (PFOA) and perfluorooctane sulfonates (PFOS), is a big concern worldwide due to their persistence in the environment. Removal of PFAS represents a special challenge for water/wastewater treatment because of their unique chemical/physical properties that include high water solubility, high stability of C-F bond, and varied chemical structures. In this study, we reported a nondestructive treatment method to remove PFOA and PFOS from contaminated water using Ca-montmorillonite amended with various novel organic modifiers. The successful intercalation of organic modifiers was verified with X-ray diffraction (XRD), scanning electron Fourier-transform microscopy (SEM), infrared spectroscopy (FTIR), zeta potential measurement and elemental analyzer, which also revealed the performance difference among materials modified with various organic structures. The sorption of PFOA and PFOS on modified Ca-montmorillonite with optimal organic functionality reached equilibrium within 30min. The optimal modified clay also showed high PFOA and PFOS removal efficiency in environmental relevant matrices. Functionalized montmorillonite is a promising material for environmentally friendly and sustainable applications in PFAS pollution control.

ENVR 727

Anion-exchange membranes for passive sampling of per- and polyfluoroalkyl substances

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The ubiquitous presence of per- and polyfluoroalkyl substances (PFAS) in water, sediment, and air have highlighted the need for more effective and robust monitoring tools for these unique chemicals. The large sample volumes required for analysis have limited understanding of spatiotemporal variations in PFAS concentrations in the environment and during remediation. To overcome this limitation, we developed new passive samplers comprised of anion-exchange membranes. The objective of this work was to apply anion-exchange membranes as passive samplers for 12 chemically diverse PFAS, including perfluoroalkyl carboxylates, perfluoroalkyl sulfonates, fluorotelomer sulfonates, and perfluorooctane sulfonamides. Three different anion-exchange membranes were tested: AMI-7001 (Membranes International Inc.); FAA-3-PK-130 (Fumatech); and, FAP-450 (Fumatech). Batch sorption tests were conducted with environmentally relevant PFAS concentrations in 10 mM NaCl and real groundwater solutions to determine the time required to achieve equilibrium. In 10 mM NaCl, equilibrium was achieved within 48 h, highlighting the relative advantages of anionexchange membranes over both anion-exchange resins and traditional polymeric passive samplers. Aqueousand membrane-phase PFAS concentrations were measured at equilibrium, and the selectivity coefficients for PFAS were calculated with respect to background electrolytes, such as chloride. The batch sorption tests indicated that selectivity coefficients for PFAS over chloride varied by class and chain-length (e.g., 14.8±1.8 for PFBA, 287±32 for PFBS, 52.5±1.0 for PFHxA, and 1010±80 for PFHxS), but the relatively tight range of selectivity coefficients allowed simultaneous measurement of both short- and long-chain PFAS. Following extraction of PFAS from the anion-exchange membranes using methanol and inorganic or organic bases, the passive samplers were redeployed to determine reusability. Overall, the results highlight the potential use of anion-exchange membranes as passive samplers for chemically diverse PFAS.

Ionic fluorogels as for PFAS remediation from water

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Per- and polyfluorinated alkyl substances (PFAS) are a class of fluorinated compounds that are widely used as surfactants in the production of poly(tetrafluoroethylene) (Teflon), water and stain repellant coatings, and fire retardants. Recently, PFAS contamination of water supplies has generated significant concern, as these substances are known to adversely affect human health, including posing risks to the immune, metabolic, and endocrine systems. Conventional technologies to remove contaminants from water, including activated carbon and ion-exchange resins, have proven inadequate for sorption of the diverse class of PFAS. The primary challenge for developing a sorbent to remediate PFAS from water is that non-fluorinated organic contaminants are present in ground and surface waters at three to six orders of magnitude higher concentration than PFAS, causing saturation of typical resins. In this lecture, I will detail our group's efforts toward the realization of high capacity sorbents selective for PFAS in complex water matrices. The lonic Fluorogels we have developed outperform commercial sorbents in terms of equilibrium PFAS absorption, PFAS capacity, and kinetics of PFAS absorption. Key structure-property relationships will be outlined that enable the remediation of both legacy and emerging PFAS from North Carolina water supplies to below the EPA health advisory limit.



ENVR 729

Determination of adsorbable organic fluorine as a surrogate to total PFASs in water samples

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Perfluoroalkyl and polyfluoroalkyl substances (PFASs) are a large group of synthetic organic compounds which include thousands of compounds. Various types of PFASs have been reported in water samples worldwide. Qualifying and quantifying the individual PFAS in water samples is a challenge because of the lack of standards or available analytical methods. Therefore, an analytical method that can determine the total organic fluorine is necessary as a surrogate to fully estimate the extent of

total PFAS contamination. In our study, we have validated a method that utilizes activated carbon to adsorb PFASs from water, then completely burn the adsorbent to convert all the organic fluorine into fluoride and finally measure the fluoride level by Ion Chromatography to determine the total adsorbable organic fluorine (AOF) concentration. We utilize a carbon that contains a fluorine background level at about 0.4 µg/g (corresponding to 0.1 µg/L AOF in water samples) to conduct the analysis. The recovery of reference PFASs of various chain-length ranges from 68% to 106%. The interference from inorganic fluoride in water samples up to 100 µg/L can be effectively removed by a 5 g/L nitrate rinsing solution, while the influence of fluoride at higher levels needs to be corrected using the calibration curve between fluoride concentrations and false-positive AOF readings. This AOF method is applied for testing drinking water sources in North Caroline, aiming to identify possible PFAS contaminations in combination with targeted and non-targeted analysis. The AOF method is a very useful approach to estimate the total PFAS contamination level and also to understand the fate and transport of total PFAS in water.

ENVR 730

Development of a predictive model for ion exchange treatment of mixtures of per- and polyfluoroalkyl substances (PFASs)

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Currently, drinking water treatment of per- and polyfluoroalkyl substances (PFASs) is primarily accomplished by granular activated carbon (GAC) sorption of PFAS. However, rapid PFAS breakthrough in GAC beds and a growing concern around short-chain PFAS compounds not well removed by GAC have contributed to the emergence of ion exchange as a promising alternative treatment technology. Some anion exchange resins (AERs) are associated with higher PFAS selectivity (e.g., KPFOS/CI values up to 108) and capacity relative to GAC, but their longer operational lifetimes prohibit rapid assessment of resin performance in benchscale experiments. Therefore, a predictive model is needed to translate results from short-term batch experiments to practical treatment operations, estimate

relevant design parameters (e.g., resin regeneration/replacement frequency), and inform decision-making for resin selection, optimal resin combinations, and combined treatment technologies. While many current models rely on coupling experimental breakthrough data with theoretical equations to determine situation-specific operational parameters, here we describe a model that has been developed to predict compound breakthrough in ion exchange columns based upon PFAS/CI⁻ selectivity, maximum PFAS adsorption capacity, and kinetics data obtained in batch experiments rather than manipulated best-fit parameters. Batch selectivity coefficients, sorption kinetic rate constants, resin PFAS capacities, and compound diffusivities are utilized in these models, which are assessed for predictive accuracy based on preliminary column data. We will also describe plans to calibrate and validate the model with pilot- and full-scale treatment data for a range of PFASs measured in groundwater impacted by historical agueous film-forming foam (AFFF) used.

ENVR 731

Evaluating the efficiency of various anion exchange resins for removing legacy and emerging per- and polyfluoroalkyl substances (PFAS)

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The increasing concerns of per- and polyfluoroalkyl substances (PFAS) in drinking water sources are not only because of their ubiquitous presence but also due to the challenge of PFAS removal. Since PFAS commonly carry negatively charged functional groups in water phase, anion exchange has been a promising treatment process in removing legacy PFAS. However, whether anion exchange is capable of efficiently removing emerging PFAS, such as GenX and other perfluoroalkyl ether acids, remains uncertain. In this study, we tested nine commercially available anion exchange resins for their removal of 40 legacy and emerging PFAS, regeneration recovery, and the effect of water matrix. Bench-scale batch experiments were conducted by using groundwater collected near a fluorochemical manufacturer in North Carolina. The result shows that five of the tested nine anion exchange resins were able to remove more than half of the 40 spiked PFAS compounds over 90% in 2 hours. Resins with polystyrene-DVB matrix performed better than other polymer matrices. These five resins were further examined for regeneration under practical The regeneration strategies conditions. were systematically evaluated, including the effect of cation, anion, salt concentration, and pH, as well as the percentage of organic solvent. By evaluating the

capability of regeneration under practical applications, three resins were chosen for further determining the effects of water matrix on PFAS removal, including pH, competing anion concentration and natural organic matter.

ENVR 732

Effective adsorption removal of short-chain polyfluoroalkyl and perfluoroalkyl substances (PFASs) using biochar

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Polyfluoroalkyl and perfluoroalkyl substances (PFASs) are a class of environmental contaminants widely found in water, sediment, soil, air and biota. Their extreme recalcitrance and profound bioaccumulating potential have raised significant concerns regarding their imminent risks to the human health and natural biota. Unfortunately, PFASs have been detected in drinking water in the US and alobally at relatively high concentrations exceeding the EPA health advisory level (i.e., 70 ng/L for PFOA and PFOS together). Since 2002, short-chain PFASs, such as PFBA and PFHxA, have been developed by several major manufacturers as the replacement of their conventional C8 or higher homologues. Adsorption by granular activated carbon (GAC) has been widely employed to remove PFASs in water in general. However, GAC is not effective in adsorbing short-chain PFASs given their reduced hydrophobicity and increased tendency for micelle development. Biochar is an economic and green alternative for GAC and other manufactured carbonaceous adsorbents as it is made from biological wastes via pyrolysis. It has received increasing attention due to its unique feature such as high carbon content and cation exchange capacity, large specific surface area and stable structure. In this present research, we synthesized novel biochar and investigated their adsorption efficiencies to remove short-chain PFASs (C4 to C6). Two different biochar materials (A and B) synthesized in our lab displayed greater removal efficiencies for PFBA than GAC. Biochar A and B can remove over 80% of initially dosed PFBA. In contrast, the PFBA removal efficiency was as low as 20% by GAC. Based on the isotherm characterization, the adsorption capacity of Biochar A was 2 times higher than that of GAC and Biochar B displayed a rapid adsorption when PFBA concentration was low in the range from 10 to 1000 µg/L. Even better, both Biochar A and B demonstrated better performance on removing PFASs of different chain lengths (e.g., PFHxA and PFOA) and/or functional groups (e.g., PFOS). The specific surface areas, particle size distribution, and surface chemistry were characterized to exploit the adsorption mechanisms of different synthesized biochar. Thus, our synthesized biochars are promising as novel, low-cost,

and green adsorbents to treat water impacted by commingled PFASs.

ENVR 733

Adsorption of PFAS by granular activated carbon: Scale-up of bench-scale data and factors controlling GAC use rates

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Health implications associated with long-chain per- and polyfluoroalkyl substances (PFASs) have led to a shift towards production and use of shorter-chain PFASs and fluorinated alternatives. Fluorinated alternatives include perfluoroalkyl ether carboxylic acids (PFECAs) and sulfonic acids (PFESAs), in which ether oxygen atoms are incorporated into the fluorinated alkyl chain. Short-chain PFASs and many PFECAs/PFESAs are likely less bioaccumulative than long-chain PFASs, but many are still persistent and toxic. Detection of short-chain PFASs and fluorinated alternatives in source waters is of concern because many water treatment processes are not effective for their removal. One treatment option that can be effective is granular activated carbon (GAC) adsorption. Our research aims to 1) identify a rapid smallscale column test (RSSCT) design [e.g. constant diffusivity (CD), proportional diffusivity (PD)] to predict field-scale GAC performance, 2) elucidate PFAS properties controlling adsorbability to GAC, and 3) identify GAC properties that yield effective PFAS removal. RSSCTs were conducted to compare PFAS removal by four GACs from two surface waters and a groundwater. Samples were analyzed by LC-MS/MS for 24 PFASs, including 13 PFECAs/PFESAs. With the PD-RSSCT design, bed volumes to 10% PFAS breakthrough were a factor of ~3 greater for most PFASs than with the miniCD-RSSCT. Similarly, the PD-RSSCT yielded adsorption capacities for most PFASs that were about double those obtained with the miniCD-RSSCT. Bed volumes to 10% breakthrough increased with increasing PFAS chain length for both non-ether and ether containing PFAS. Compared to linear PFASs, branched counterparts were less adsorbable. Reagglomerated, sub-bituminous coalbased GAC was more effective than enhanced coconut GAC, likely due to the larger mesopore volume of the former. Background organic matter concentration strongly influenced PFAS removal. Especially for longer-chain PFASs, bed volumes to 10% breakthrough were substantially greater when treating groundwater (TOC <0.5 mg/L) compared to coagulated surface water (TOC = 1.3 mg/L).

ENVR 734

Use of biochar from biosolid pyrolysis for PFAS management in landfills: Technical and economic feasibility

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The use of carbon-based and non-carbon-based soil amendments for immobilization of PFASs has been the focus of many researchers. However, the majority of available literature is solely limited to laboratory-scale studies. The remediation industry commonly employs activated carbon as an effective and affordable treatment for communities affected by PFAS-contaminated soil or water. There are alternative treatment technologies that offer more or less removal efficiency for a broader suite of PFASs. Economic feasibility, longevity, and removal efficiency are important factors selecting a remediation practice for PFAS-contaminated leachate and soil. Biochar, having similar properties to GAC, has been studied and used to remove organic compounds. However, the state of development for PFAS removal is immature, and full-scale in-situ studies on PFAS sorption or immobilization by biochar are almost nonexistent. Pyrolysis of biosolids has been employed as an alternative process to traditional landfilling and incineration. The advantages of pyrolysis are using less energy, creating less gaseous emissions, destroying pathogens, and generating biochar. A sustainable pyrolysis process can be developed to destroy PFAS in biosolids. Additionally, the generated biochar, using biosolids as a feedstock, can be used to immobilize PFAS in landfills. This work reviews the technical viability and economic feasibility of biosolid pyrolysis for both destructions of PFAS in biosolid and biochar generation to immobilize PFAS in contaminated soil.

ENVR 735

Design of porous MOF/polymer composites for selective and enhanced chemical separations in aqueous media

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The discharge of toxic contaminants or commodities such as heavy and precious metals into the environment are of great concern. Drinking water contamination with lead is a persistent problem worldwide with grave public health consequences. As such, many strategies are under intense investigation for the extraction of such chemical species from their relevant mixtures. Recently we have developed a methodology to introduce extrinsic porosity

to intrinsically non-porous polymers using MOFs as a template. Here we illustrate how we take advantage of unsaturated open metal sites inside of MOFs to facilitate in situ polymerization adhering the polymer to the pore surface. The result is a number of new porous composites with significantly enhanced properties for chemical separations in aqueous media. Fe-BTC/PDA exhibits rapid, selective removal of large quantities of heavy metals, such as Pb²⁺ and Hg²⁺, from real world water samples [1]. The composite binds up to 1634 mg of Hg²⁺ and 394 mg of Pb²⁺ per gram of composite and removes more than 99.8% of these ions from a 1 ppm solution, vielding drinkable levels in seconds. Designing novel MOF/Polymer composites for selective metal remediation from water with high energetic efficiency is of great importance and offers a significant challenge from a materials design perspective. In this work, the blueprint to synthesize MOF/Polymer composites that exhibit interesting host-guest properties for environmental contaminant remediation will be shown.



ENVR 736

Speciation of legacy P in soils using multi-modal $\mu\text{-}XRF$ mapping and $\mu\text{-}XANES$

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As an essential plant nutrient, phosphorus (P) is often applied to agricultural fields in the form of animal manure or fertilizer. Excess P can become detrimental to aquatic ecosystems by causing eutrophication. Extensive research about general P pools in soils using sequential extractions, such as the Hedley extraction, has been done over the years. The Hedley extraction is a critical method used world-wide, therefore understanding the P speciation removed with each extraction is crucial. However, sequential extractions cannot directly identify the individual solid phase P species within the general P

pools and how they may vary. This is information bioavailability determine Р necessarv to and environmental susceptibility. By utilizing multi-modal micro X-ray fluorescence (µ-XRF) mapping to determine P elemental collocation with Al, S, Fe, Ca, and Mn followed by micro X-ray absorption near edge structure (µ-XANES) spectroscopy of P hotspots in this research, we will present a direct speciation of the P pools in sequential extraction residues from each step of the Hedley method. The spectroscopic data will be compared to wet chemical data to identify what locally causes the differences in bulk solubility of P species.

ENVR 737

Understanding and application of genetically induced bacteriophage/nano-particle interactions in the environment

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The interactions between bacteriophages, the viruses as prokaryotes as their host, and engineered nanomaterials has been least studied even if bacteriophages co-exist with prokaryotes in high number. This research evaluated these interactions with specific application of phages to carry engineered nanomaterials for further applications. Negatively charged Engineered Nanomaterials (ENMs) have been shown to bind to bacteriophages (figure 1) via local positive charges present on the surface of some phage capsids. This was determined by comparative analysis of the infection efficiencies (one-step growth curves: figure 2) of a variety of phage/host species after exposure to 1-10mg/L silver and gold nanoparticles and TEM. Bacteriophage P22, which lacks a positively charged surface and which does not normally bind to silver or gold nanoparticles, was induced to do so by addition of positively charged amino acid residues to the C-terminus of the capsid protein. The fold of the capsid protein, which makes up the DNA encapsulating shell of a virus, is structurally conserved in most phages. These nano-particle binding P22 mutants, with silver nanoparticles attached, produce no observable affect upon infection. In some phages, naturally possessing positive surface charges silver nanoparticle attachment has been shown to negatively affect viral infection by as much as 95%. These inhibitory effects partly derive from silver ions, shed continuously from the nanoparticles, interfering with Outer Membrane Proteins (OMPs). This was determined by the construction of OMP gene knockouts of phage hosts and infection experiments in the presence of Ag⁺. This is the first study depicting a mechanistic understanding on phage-nanoparticles interactions.



Figure 1: Images made using 1x10¹¹ phage in 10 mg/L, 10 nm AgNPs (a.) *Delftia* Phage RG2014 with cloud-like structures (shown with arrow) present from bare AgNPs. (b.) RG2014 with bare AgNPs. (c.) RG2014 with PVP AgNP (d., e.) *Klebsiella* Phage KL with PVP AgNPs.



Figure 2: (a) One step growth curve phage RG2014 after incubation with 10 mg/L 10 nm silver nanoparticles (b) One step growth curve phage KL after incubating with 10 mg/L 10 nm Silver nanoparticles nanoparticles.

ENVR 738

Remediation of crude oil contaminated soil: Comparison of normal and microwave pyrolysis

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In Nigeria, over three million barrels of crude oil have been spilt into the environment contaminating 840 acres of land. The oil content of the soil (> 1 %) is higher than the safe disposal limit for soil contaminated with oil (<1 %). This research compares the efficacy of microwave (MW) pyrolysis to traditional pyrolysis, investigated using a Gray-king (GK) retort, for removing hydrocarbons from contaminated soil. For batch wise microwave pyrolysis, the influence of incident power, time, specific energy (function of MW incident power) were studied. Hydrocarbons from the untreated, GK and MW treated soils were recovered in dichloromethane/methanol mixtures denoted as soluble hydrocarbons. Reduction of organic carbon (OC) in soil was used to estimate absolute release of hydrocarbon. In GK retorting, at heating rate of °C/min, 100 % solvent soluble hydrocarbon 5 contaminants were removed at 500 °C, representing OC of 66.43 % ±0.93. In comparison, MW process operated at frequency of 2.45 GHz, 94 % soluble hydrocarbons were removed at incident power of 0.8 kW and optimum treatment time (7 min) representing OC of 60.28 % ±0.99. Soil quality obtained at optimum MW treatment conditions was similar to GK pyrolysis treatment time of 125 min at 400 °C. At specific energies < 700 kWh/tonne C_{16} - C_{22} alkanes were recovered compared to C10-C30 alkanes at > 1800 kWh/tonne. Polyaromatic hydrocarbons (PAHs) naphthalene, acenaphthylene, such as fluorene. fluoranthene and pyrene at specific energy > 1800 kWh/tonne) were minor components recovered due to MW selective heating. Hydrocarbon recovered after GK pyrolysis composed mainly of C10-C30 and unresolved complex mixture of PAHs. This finding suggest that MW pyrolysis process reduces contaminated soil treatment time and the heating mechanism of the two techniques (GK and MW) has a role to play with regards to liquid product quality.

ENVR 739

Harnessing the power of stannous for trace metal remediation

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Tin, generally considered non-toxic, has been used in alloys in dental fillings, in lead-free solder, as a food preservative, and most recently, to remediate trace metals from contaminated water sources. Tin is an attractive reagent for trace metal remediation because of its reductive power and the insoluble nature of the reduced tin species, tin dioxide (SnO₂). This insoluble byproduct can simply be filtered out after treatment. Stannous can be applied to remove hexavalent chromium from groundwater, passivate lead/copper in service lines, passivate iron in cooling systems, recover selenium and mercury from industrial wastewater, and remove and inhibit biofilm growth in cooling systems to reduce corrosion and risk of legionella outbreaks. An innovative in situ stannous generator has been developed to harnesses the power of this highly effective chemical reagent; before this invention, there was no method for delivering a controlled dose of stannous reagent (Sn²⁺) to water treatment applications. Generating a stannous reagent onsite is a far more cost-effective treatment solution compared to traditional alternatives since tin and electricity are the only consumables with this novel approach. The stannous reagent is generated on demand using non-toxic, food-grade reagent precursor material. As a result, there is no shelf life of the reagent and operational costs are drastically reduced since shipping and handling of hazardous chemicals associated are entirely avoided. Traditional tin reagents such as stannous chloride (SnCl₂₎, are a caustic, unstable material requiring specialized handling. The stannous reagent generator incorporates proprietary continuous, real-time monitoring of contaminant levels at the influent and effluent to ensure optimal treatment and compliance with regulatory and operational targets 24/7/365. There are presently no similar applications that integrate a low lifetime cost contaminant treatment system with real-time performance controls. Case studies from this novel *in situ* stannous generator will be presented.

ENVR 740

Role of solvent polarity and hydrogen bonding on nitrate radical reactivity

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Oxygen centered radicals serve as important atmospheric cleansing agents with hydroxyl radical serving as a daytime "detergent" and nitrate radical operating throughout the night. To understand these radicals fully, it is important to study these compounds both in the gasphase, and in solution to simulate their effects in the atmosphere, on and within water droplets, and on aerosols surfaces. Previous work on the hydroxyl radical has shown that solvent polarity and hydrogen bonding stabilize the transition state and accelerate the rate of hydrogen abstraction in solution. Based on preliminary calculations we proposed that a similar effect might occur for the nitrate radical, because it is such a strong oxidant both in the gas-phase and in solution. Rate constants for hydrogen abstraction reactions from hydrocarbons, alcohols, and ethers by the NO3 radical in acetonitrile and water were determined by laser flash photolysis. These results were also compared to gas-phase experiments. Despite calculations predicting a polar transition state that should facilitate hydrogen bonding in the gas-phase, experimental evidence shows that rate constants in water were slightly lower than in CH₃CN. Further, the solutionphase reactions exhibit rate enhancement with respect to their gas-phase counterparts, consistent with the notion of a polarized transition state that can be stabilized in a polar solvent. We are doing calculations to full understand the role (if any) of hydrogen bonding in both the ground and transition states.



ENVR 741

Effects of affinity and aqueous speciation on uranium(VI) removal by ion exchange drinking water treatment processes

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Ion exchange treatment processes are designated as best available technology for removal of several contaminants in drinking water, including uranium (VI). For users of private drinking water wells, ion exchange units provide a commercially available solution to address water quality concerns. Common co-solutes in ground and surface water with elevated uranium concentrations include carbonate, hydroxide, and phosphate anions. These constituents simultaneously react and persist in soluble complexes with the uranyl cation and demonstrate preferential affinity over uranium species for ion exchange resins. Abundant dissolved natural organic matter in solution forms large, highly soluble, and negatively charged uranium species. Furthermore, uranium is the largest naturally occurring element, and the uranyl cation is strongly hydrated. This combination of physiochemical characteristics limits the treatment of uranium in drinking water. To elucidate the function of ion exchange affinity on uranium removal, we have developed a suite of functionalized electrospun polymeric sorbent materials to understand the influence of uranyl speciation in the presence of model organic ligands and inorganic anions on ion exchange processes. Polymeric materials functionalized with quaternary ammonium salts Aliquat-336 and tetra-n-butyl ammonium bromide display weak electrostatic affinity for elevated and environmentally relevant concentrations of dissolved uranyl citrate and uranyl oxalate and do not release respective counteranions chloride or bromide with uptake. For the model inorganic anion nitrate, complete removal and counteranion exchange is demonstrated with these novel membrane materials. Because mixtures of multiple cationic, anionic, and neutral uranium species exist in groundwater, electrostatic interactions ultimately govern the extent of coordination of soluble uranium with ion exchange membranes and resins. Improved ion exchange unit processes, especially for consumer devices, should move towards employing multi-step treatment to effectively remove large, reactive uranyl complexes in source water.

ENVR 742

Withdrawn

ENVR 743

Interfacial properties and crystalline transformations of doped MgO and MgCO₃ particles during nutrient (N and P) recovery from aqueous solutions

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Very low aqueous solubility magnesium containing mineral surface conversion into slow release fertilizer, MgNH₄PO₄ (struvite) crystals, utilizing simulated, N and P nutrient-containing, anthropogenic wastewater will be presented. The in situ experiments were utilized to understand fundamental processes, including reactive intermediates, their growth mechanisms and kinetics. These all take place during solid magnesium crystalline surface (MgO and MgCO₃) conversion in the presence of simulated wastewater solutions. In particular, the presented work provides new insights into the relationships among the struvite formation under varying N:P concentrations, dissolved organic matter amount, calcium ion concentration and solution pH. The diffusionlimited fundamental data are obtained from flat, semiinfinite model single crystal surfaces. These surfaces are then be propagated into tailor made Fe and Ca functionalized MgO nanoparticles to monitor struvite growth under interface limited growth conditions.

ENVR 744

Investigation of the production of hydroxylating species from DOM model sensitizers

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The photochemical production of hydroxylating species (e.g., hydroxyl radical (OH)) from dissolved organic matter (DOM) has been well documented. Quantum yields for the production of these species have been quantified in previous studies and are in the order of $10^{-5} - 10^{-4}$ depending on the source of the organic matter. These quantum yields are, partially, independent of photo-Fenton chemistry, and represent hydrogen-peroxide independent production of these species. It has been shown that lower energy hydroxylating species, in addition to free OH, are present upon the photolysis of DOM. The source of these lower energy hydroxylating species has been attributed, in part, to the presence of quinones in DOM. This study explores the DOM structural moieties responsible for its hydroxylating capacity in two ways. First, by testing the ability of various DOM model sensitizers to photohydroxylate commonly used probe compounds and then by exploring the ability of methanol to guench free OH in comparison to other species thought to be lower energy hydroxylators. The main classes of sensitizers tested were aromatic ketones, guinones, and hydroxybenzoic acids, which were selected to cover a range of molecular structures, triplet state one electron reduction potentials, and triplet energies. Results indicate that only quinones and hydroxybenzoic acids have the capacity to hydroxylate OH probe compounds when photolyzed, with quinones having the highest quantum yields.

ENVR 745

Sunlight photodegradation of pharmaceuticals in land-applied biosolids: Case study of ibuprofen and naproxen

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Biosolids produced in wastewater treatment plants can be applied to agriculture fields as fertilizers or soil amendment. However, the presence of pharmaceuticals in biosolids has raised concern on the long-term ecological impacts of biosolids land application. Sunlight photodegradation is an important dissipation pathway for pharmaceuticals in water and on soil. However, this process has not been considered in biosolids, a reaction environment enriches in organic matter with high moisture. In this study, two anti-inflammatory drugs present at high concentrations in biosolids, ibuprofen and naproxen, were selected as model compounds to sunlight photodegradation evaluate the of pharmaceuticals in biosolids. Reactions were conducted in water and on kaolinite surfaces, and the effects of dissolve organic matter extracted from biosolids (BDOM) were evaluated. In water, ibuprofen did not undergo direct photolysis whereas naproxen exhibited rapid decay (0.72 h⁻¹), consistent with their respective sunlight absorption spectra. In the presence of 5 mg C/L BDOM, ibuprofen degradation was observed (0.003 h⁻¹), but naproxen degradation was not affected. On kaolinite, the presence of BDOM accelerated ibuprofen and naproxen degradation by 1.5 and 1.1 times, respectively. These kinetics results suggest that BDOM can induce pharmaceutical decay both in water and on solid surface. A comparison of the excitation emission matrix (EEM) spectra of BDOM and soil-DOM showed that BDOM contains a more diverse range of fluorophores and has fluorescence stronger signals in the regions corresponding to humic acid-like and aromatic protein. On kaolinite with BDOM, ibuprofen degraded 1.3 times faster in the deoxygenated reaction environment suggesting the triplet DOM plays an important role during the photolysis reaction. Work is underway to evaluate the decay of ibuprofen and naproxen in authentic biosolids sample, and probe compounds will be applied to illustrate the important reactive species generated by the biosolids in the photolysis reaction.

Photochemical stability and degradation of carbon dots

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Carbon dots are an environmentally sustainable nanomaterial with optical properties similar to quantum dots. However, unlike quantum dots, carbon dots do not contain toxic metals and can be produced from renewable sources like agricultural waste or discarded plastic bags. In this study, we investigated the photochemical stability, degradation, and transformation of carbon dots throughout their lifecycle. Aqueous solutions of carbon dots were exposed to natural sunlight, UVC light (254 nm), and hydroxyl radicals, to mimic the lifecycle of carbon dots from their use and application to release, concluding with degradation caused by exposure to reactive oxygen species and advanced wastewater treatment processes. Carbon dots are rapidly photobleached with exposure to natural sunlight but remain intact and do not degrade. In contrast, exposing carbon dots to UVC light or hydroxyl radicals leads to degradation, but through distinctly different mechanisms.

ENVR 747

Photochemical fate of disinfection by-products formed during seawater desalination processes

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Desalination of seawater is becoming increasingly important for supplying drinking water, with desalination plants already operating in many coastal locations around the world. However, disinfection by-products (DBPs) formed during seawater chlorination are expected to be very different from those formed during freshwater chlorination due to differences in dissolved organic matter (DOM) composition and the much higher concentrations of iodide and bromide in seawater. Because discharge of the concentrated reject water from the reverse osmosis (RO) process into seawater is a viable disposal option, the molecular composition and environmental fate of DBPs in reject waters needs to be evaluated. To that end, we analyzed raw/intake waters and RO reject waters

collected from several desalination plants using absorbance and fluorescence spectroscopy and nontargeted ultra-high resolution mass spectrometry (HRMS). To evaluate the photochemical fate of DBPs, samples were exposed to simulated sunlight in a custombuilt flow-through system that allows for pH and temperature control and prevents oxygen starvation. During all experiments absorbance and fluorescence were monitored semi-continuously whereas DOM/DBP molecular composition was analyzed for discrete time points. Results highlight that RO reject waters contain hundreds of yet to be identified brominated and iodinated DBPs. When exposed to sunlight DBPs are rapidly degraded, so that both the toxicity of DBPs and their photodegradation products should be evaluated in the future.

ENVR 748

Investigating effect of pH and ionic strength on surface adsorption of natural organic matters on TiO₂ nanoparticles

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As a photocatalyst, TiO₂ has been widely studied in water treatment applications. The use of TiO₂ in a disinfection process with ultraviolet has shown an outstanding inactivation of viruses. The main complication of using TiO₂ outside laboratory conditions has been the presence of dissolved organic matter (DOM), which contributes to the low inactivation rate of microorganisms due to the scavenging of •OH radicals. The interaction dynamic between TiO₂ and DOM was investigated by using different types of probes including pCBA and MS2 bacteriophage. Further, the effect of pH, ionic strength, and organic matter concentration on the agglomeration of TiO₂ nanoparticles were studied using Dynamic Light Scattering. To evaluate the effect of DOM on the photocatalytic process photodegradation experiments were conducted using different conditions by adjusting pH and lonic Strength. The results showed improvement in the photodegradation of pCBA with low pH and high ionic strength. The results of the experiment indicated that there is a strong inhibitory effect in high pH regardless of organic matter concentration. It was concluded that high pH can induce high inhibition due to electrostatic interaction between target compounds and inhibition of •OH radicals' generation. By using these results, this research will discuss that various target compounds such as MBR effluent have different adsorption behavior which makes the different photodegradation kinetics.

Photochemical fate of triphenyltin hydroxide in natural and engineered water systems: Reaction kinetics, transformation products, and residual toxicity

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Triphenyltin hydroxide (TPTH) is an organotin fungicide that appears on the EPA contaminant candidate list and causes endocrine disruption and reproductive malformation in aquatic organisms. The objective of this study was to determine the photodegradation kinetics, identify transformation products, and measure the residual toxicity of TPTH for irradiation in natural (i.e., 365 nm and solar simulator) and engineered (i.e., 254 nm) systems. The effective quantum yield of TPTH was 3.0 (± 0.1) $\times 10^{-2}$ mol Ein⁻¹ for direct photolysis at 254 nm; however, the quantum yields were less than 3.9×10⁻⁵ mol Ein⁻¹ for 365 nm and simulated solar irradiation. The effects of solution pH (e.g., 4-10), ionic strength (e.g., 0.001-0.1 M), and photosensitizers (e.g., hydrogen peroxide, nitrate, and dissolved organic matter) on TPTH photodegradation were explored to simulate natural and engineered conditions. Solution pH and ionic strength had a negligible influence on measured rate constants. Enhanced TPTH degradation was observed in the UV-H₂O₂ process due to reaction with hydroxyl radicals. The apparent second-order rate constant for TPTH reaction with hydroxyl radicals was 5.5×10⁸ M⁻¹ s⁻¹. Primary phototransformation products were identified by highresolution mass spectrometry and used to elucidate the reaction pathways involved with direct and indirect photodegradation of TPTH. The biological activity of TPTH and its phototransformation products was measured using bacterial growth inhibition assays with Staphylococcus sp. (ATCC 14389). TPTH inhibited the growth of Staphylococcus sp. with an observed IC50 of approximately 400 µg L⁻¹. The antibacterial activity of phototransformation products was assessed using the potency equivalents approach, and the results indicated that both direct and indirect photolysis generated antimicrobially-active transformation products. The reported results highlight the light-dependent reaction kinetics and the importance of photodegradation products on the removal of TPTH-related toxicity in different water systems.

ENVR 750

Carbonate radical oxidation of cyanotoxins and its environmental application

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Cyanotoxins, in the form of cyanobacterial secondary metabolites, are a group of emerging contaminates that widespread in waterbodies throughout the world. It has led to not only livestock deaths but also several cases of human hepatoenteritis and even deaths. Microcystins-LR (MCLR) and cylindrospermopsin (CYN) are among the most frequent toxins produced by cyanobacteria. Due to the high toxicity and risk to the aqueous environment, the remove of cyanotoxins in nature surface water and water treatment systems are receiving extensive attention. Numerous studies focused on the major radicals generated in these processes, such as HO, O₃, SO₄-. Compared with those radicals, information on the carbonate radical (CO3-) oxidation of cyanotoxins is limited. CO₃⁻ is a powerful oxidant that is omnipresent in sunlight surface waters and in waters treated by advanced oxidation processes. The primary aims of this study were to conduct kinetic and mechanistic studies focused on the carbonate radical oxidation of cyanotoxins and its role in the environmental transformation of cyanotoxins. Phenol was chosen as the competitor to determine the apparent rates constant of CYN (k_{CYN} ^{app}) and MCLR (k_{MCLR} ^{app}) with CO₃⁻. The result suggested that the reaction of CYN and MCLR with CO3.- are pHdependent, the values of k_{CYN} app and k_{MCLR} app both increased as a function of pH. These pH dependencies of k_{CYN} ^{app} and k_{MCLR} ^{app} can be attributed to the combination of effects derived from CO3⁻⁻ react with dissimilar CYN and MCLR species. The species-specific second-order rate constants were calculated using the least-squares regression of the experimental. The second-rate constants were calculated as $1.7 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ and $2.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ 10^8 M⁻¹ s⁻¹ for CYN and CYN⁻, respectively. ~ 2.18 ± 0.74 $\times 10^{7}$ M⁻¹ s⁻¹ and 1.50 ± 0.51 $\times 10^{9}$ M⁻¹ s⁻¹ for MC-LR⁻ and MC-LR²⁻, respectively. Furthermore, we reported the detailed pathways for the degradation of CYN/MCLR by CO3⁻. Finally, the contribution of CO3⁻ on CYN/MCLR photodegradation was estimated.

ENVR 751

Withdrawn

ENVR 752

Fundamental studies of the singlet oxygenation of Melanin model compounds: Product and mechanistic studies

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Melanin, a vital natural pigment, plays a protective role against UV and reactive oxygen species damage, including singlet oxygen. We studied the singlet oxygenation of pyrroles as models for Melanin backbone subunits. We have established Melanin model compounds are highly reactive towards ¹O₂, producing very distinct and stable pyrrolones. In D₂O, singlet oxygenation of pyrroles with methyl ketone versus aldehyde at the alpha carbon yielded the same single product, but significantly different bimolecular rate constants of 12 x 107 M⁻¹s⁻¹ and 2.3 x 107 M⁻¹s⁻¹, respectively. The analogous hydrogen substituted pyrrole, however, yields a mixture of products with a slower reaction rate constant. The presence of 1Hpyrrole-2,3,4-tricarboxylic acid (Py-TCOOH) is commonly used as a maker to assess melanin pigments photodamage. Our results demonstrate Py-TCOOH is readily degraded by ¹O₂ and thus can lead to an underestimation of the UV degradation. The products identified in our study likely can serve as accurate markers for assessing the ¹O₂-mediated damage to Melanin. Our results provide fundamental mechanistic insight on the singlet oxygenation and photodamage of melanin model compounds in aqueous media which may contribute to better assessment of Melanin aging and the development of melanin-based photoactive materials.



ENVR 753

Withdrawn

ENVR 754

Chitosan crosslinking into magnetic multi-walled carbon nanotubes beads for efficient Cr(VI) removal

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Biopolymers (chitin, chitosan) like potential adsorbents are often challenged by weak stability, poor dispersibility, low adsorption, and difficulty of recovery. This work demonstrates the synthesis of an adsorbent in the form of CS/MWCNTs/Fe beads by combining chitosan and sodium alginate with magnetic iron oxide-doped MWCNTs. The prepared composite beads were then used for the adsorption of Cr(VI) from water samples. The physicochemical properties of CS/MWCNTs/Fe beads were characterized in detail by using FTIR, XRD, FE-SEM, EDS, and TGA. The outer to inner core structural characterization of composite beads found that the magnetic iron oxide-doped MWCNTs coated with chitosan were uniformly dispersed inside the alginate beads, making their shape as a spherical shell. During the adsorption experiments, CS/MWCNTs/Fe beads showed robust performance in Cr(VI) removal and could separate easily by using external magnet from the aqueous sample having the initial concentration, solution pH and temperature as critical factors to control their removal performance. We demonstrated that these beads can achieve a high Cr(VI) removal performance with an optimized chitosan and alginate contents. The pseudosecond-order model showed the best fit with experimental data, suggesting the rate-limiting factor of the adsorption. Langmuir isotherm with a maximum adsorption capacity of 11.74 mg/g characterized the Cr(VI) removal behavior. Moreover, the composite beads showed up to 76% of Cr(VI) removal efficiency after five cycles of adsorption. The synergistic impact in this process suggests the promising potential of CS/MWCNTs/Fe beads for the elimination of contaminants from the water bodies.



ENVR 755

Hydroxyapatite is not an adsorbent: Shifting the paradigm on how HAP removes fluoride from water

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High fluoride (F⁻), >2 mg/L, in drinking water causes chronic fluorosis. Groundwater aquifers around the world contain toxic F⁻ levels that disproportionately affect poor,

rural populations who lack access to technically involved, financially prohibitive, or otherwise inappropriate treatment technologies. As of 2008, it is estimated that 200 million people worldwide have or risk incurring fluorosis because they consume water above WHO's recommended level of 1.5 mg/L. Calcium hydroxyapatite (HAP, $Ca_5(PO_4)_3X$, where X = OH) is an appropriate F⁻ removal technology that has been in use in various forms and places for the past 70+ years. Throughout this time researchers have consistently labelled HAP as an adsorbent, a process characterized by contaminant accumulation limited to the surface of the sorbent. This assignment must be reassessed for HAP in light of the dominant F⁻ removal reaction (Ca₅(PO₄)₃OH ↔ Ca₅(PO₄)₃F) as well as its crystal structure. HAP NCs contain OH- ions in a three-dimensional array. That is, HAP OH- ions are located at both surface and bulk sites of HAP NCs. Given the thermodynamic favorability of a fluoridated apatite at both surface and bulk X sites, a system in which HAP NCs are initially placed in a fluoridated solution should proceed with a host-quest OH-F ion exchange. More specifically, F- ought to first accumulate at the HAP NC surface by exchanging with surface apatite OH ions (adsorption) and then migrate into the NC interior, a process we call internalization. Regardless of the mechanism(s) at play, if F could internalize into HAP NCs to utilize bulk OH- lattice sites, it would result in an order of magnitude increase in uptake capacity compared with adsorption only. In this presentation we will address the methods and results designed to prove that F- internalization into synthetic HAP NCs does occur. Batch tests of five different HAP variants were subjected to fluoridation for 36 days. Using both time-resolved Brunauer-Emmett-Teller specific surface area over the course of batch testing as well as a detailed particle size distribution analysis using TEM images and evidence-based understanding of the apatite crystal habit, the concentration of surface OH sites was quantified for each variant and directly compared with measured F⁻ uptake. For some variants, the amount of F⁻ removed (at 36 days) is more than double the conservative surface site concentration quantities, and all variants remove F⁻ in excess of those values.

ENVR 756

Rapid photocatalytic degradation of glyphosate by palladium-decorated *m*-BiVO₄/BiOBr nanosheets

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Glyphosate, N-(phosphonomethyl) glycine, is the most widely used herbicide for weed control that is commercialized as Roundup. Although glyphosate (GLP) is classified as low toxicity pesticide, several reports have demonstrated its side effects on non-target plants and organisms. Furthermore, the persistence of glyphosate in

the environment resulted in increased adverse effects on terrestrial and aquatic organisms. Moreover, recent studies have found a link between glyphosate and indirect adverse health effects on the human and animal organs, such as the liver and the kidney, and has been linked to Lymphoma cancer. In this presentation, we describe the light-activated catalytic degradation of glyphosate by Pd/m-BiVO₄/BiOBr photocatalyst. We prepared m-BiVO₄/BiOBr nanosheets and the ternary composite photocatalyst Pd/m-BiVO₄/BiOBr, according to our previously reported one-pot synthesis. The bare m-BiVO₄/BiOBr and the Pd-decorated particles, with various Pd content, were employed in the photocatalytic degradation of glyphosate and subsequently aminomethylphosphonic acid (AMPA), under simulated sunlight irradiation. The kinetics of the photocatalytic degradation reaction was studied by monitoring the concentration of glyphosate and its degradation products by ion chromatography. Complete degradation of glyphosate by Pd/m-BiVO₄/BiOBr was achieved within 5 minutes of the reaction. The stability of the photocatalyst for multiple degradation cycles and the mechanism of the reaction are demonstrated. Our mechanistic studies displayed that the holes and superoxide radicals are the main species involved in the degradation of glyphosate. The catalyst stability study revealed that the nanocomposite maintained over 75% of its activity after six cycles of the degradation of glyphosate. Such results could lead to the development of sustainable catalytic technologies to minimize the global impact of glyphosate.

ENVR 757

Developing best practices for combining fluorescence microscopy and water flux measurements to elucidate biofouling mechanisms

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With the increasing need for drinkable water, the push is rising to make water purification technologies more efficient. Techniques that are dependent on membranes for purification, though, are limited due to biofouling, the restriction of membrane pores from the reversible and irreversible build-up of biological material. While varying one parameter at a time with a model system has elucidated the importance of different parameters on biofouling, these experiments are limited. By not being able to see the surface of the membrane, the mechanism of how biofouling occurs still remains largely unknown. We have approached this problem by combining two techniques: traditional water flux studies and fluorescence microscopy. As this has not been done before, we worked to determine the best practices for gathering and interpreting data. This included photophysical tests to ensure the presence of the dye did not affect the fouling nature of the protein. After ensuring we had proper membrane handling and cleaning procedures, fluorescein-labeled BSA samples were prepared as a model system. Flux data in conjugation with fluorescent images of the membrane were collected to observe how fouling occurred throughout a run.

ENVR 758

Removal of amoxicillin using activated carbon manufactured from coffee waste

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Amoxicillin (AMX) is one of the derivatives of penicillin that is commonly used for human prescription medicine. Recently, the fate and transport of AMX in wastewater and the receiving environment have been studied thoroughly due to their potential problems such as the toxic effects toward susceptible microorganisms. While several methods are available for the removal of AMX from wastewater, activated carbon adsorption is one of the effective methods even at low concentration of AMX. Because commercial activated carbon is expensive and consumable, a cost-effective alternative is desirable. One possible option is to utilize coffee residue for adsorption processes. In the present research, waste coffee grounds were collected at a local coffee shop in Marshall University in Huntington, WV. Activated carbon was manufactured from collected coffee waste via chemical activation using H₃PO₄ and NaOH in the laboratory. Pore structures were evaluated by scanning electron microscopy as shown in Figure 1. A series of isotherm tests were then performed to understand the kinetics and equilibrium of adsorption of AMX onto manufactured activated carbon as shown in Figure 2. The adsorption capacity of the produced activated carbon for AMX was comparable to reported values of commercial activated carbon. These results confirmed that coffee waste can be recycled as a base material for manufacturing activated carbon that effectively removes AMX from water.



Figure 1. A SEM image of manufactured activated carbon from waste coffee grounds.



Figure 2. Variation of adsorption capacity depending on activated carbon concentration with initial AMX concentration of 100 mg/L.

ENVR 759

Micromixers with bi-directional flow enhancing features to minimize scaling effects on reverse osmosis membranes

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Three-dimensional (3-D) printing was utilized to manufacture micromixers directly on membrane swatches. To enhance performance, a two-dimensional computational fluid dynamic model was used to select the optimal geometry and pattern of 3-D printed micromixers. The optimal geometry selected created unhindered flow between 0.2 m/s and 0.3 m/s, using an inlet flow velocity of 0.104 m/s, across 40% of the membrane surface. Laboratory experiments were conducted to evaluate the

performance of micromixers and compared to unmodified membranes with a standard 20 mil (0.508 mm) mesh feed spacer. Pure water flux and salt rejection were found to be similar to standard membranes, indicating the 3-D printing process did not damage intrinsic membrane properties. Calcium sulfate scaling experiments were conducted. Scale initially began to form within 2 hours of treatment resulting in a flux decline of approximately 10% for both modified and unmodified membranes. Over 14 hours, an average flux decrease of 24% was observed for modified membranes compared to an average flux decrease of 78% for the unmodified membranes. This demonstrated the improved resistance to fouling created by the open channel design with optimal flow conditions. Based on the open-channel flow paths created using 3-D printed micromixers, improved scale removal by reverse flow cleaning procedures was evaluated. The modified membranes showed more removal for calcium sulfate compared to the unmodified membrane utilizing a 20 mil (0.508 mm) mesh feed spacer. Following cleaning, all three unmodified membranes and feed spacers had significant remaining scale, while all three modified membranes showed minimal scale. Micromixers printed directly to the membrane surface offers the ability to optimize feed channel hydrodynamics, reduce scale formation, minimize flux decline, and allow for reverse flow cleaning of fouled membranes, representing a significant advancement in membrane technology.

ENVR 760

DPPC liposomes reveal their remarkable capacity to entrap an emerging class of environmental pollutants

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Persistent organic pollutants (POPs) are organic compounds that have the ability to bioaccumulate in a wide variety of biological and ecological environments due to their resistive nature to chemical, thermal and photo degradation. Polychlorinated biphenyls (PCBs) are a class of man-made POPs that saw wide-spread use in commercial and industrial infrastructure as both an insulator and coolant in electrical transformers and capacitors. 2,2',3,3',4,4'-hexachlorobiphenyl (HCBP) was one of the most widely produced PCBs. As these mechanical structures fail or are discarded, PCBs are released into the soil, migrate to the water table, and eventually spread to nearby ecosystems by rain and wind. The stability of POPs and specifically PCBs leave few options for environmental waste removal. Conventionally, liposomes have been used for their drug delivery capabilities, but here we have chosen to investigate their potential for the removal of this class of emerging environmental pollutants. Liposomes are small, nonpolar lipid bi-layered aggregates capable of capturing a wide variety of both polar and nonpolar compounds.

Dipalmitoylphosphatidylcholine (DPPC) is a well characterized lipid that can be derived from natural sources. It is a phospholipid typically found as a major component of pulmonary surfactant mixtures. To assess the utility of liposomes prepared with pure DPPC in capturing PCBs, they were prepared using probe-tip sonication for both direct and passive incorporation of the HCBP compound. Assimilation of HCBP was assessed using differential scanning calorimetry and UV-Vis spectroscopy. For direct incorporation in the presence of HCBP, it was apparent that liposome stability generally decreased compared to pure DPPC liposomes based on a corresponding decrease in the phase transition temperature, T_m, from 40.8 °C to 37.4 °C. Additionally, an analysis of passive incorporation by UV-Vis spectroscopy showed an increase in the incorporation of HCBP proportionate to the length of exposure time up to 24 hours. Both the decrease in T_m and increase in absorbance are indicative of PCB incorporation and further demonstrates the remarkable potential for their use as a new method of sustainable environmental cleanup.

ENVR 761

Rational design of cerium-based metal-organic framework for the efficient uptake of phosphate from water

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Phosphate-based fertilizers are in widespread use around the world to increase agricultural yields and sustain food production. Plants utilize only a fraction of the phosphate added to the soil, the excess is lost from agricultural fields through erosion and surface water runoffs and accumulates in waterways. The excess phosphate causes a rapid growth of algal blooms and low oxygen (hypoxic) zones affecting the entire aquatic ecosystem (eutrophication). To mitigate the effects of eutrophication, there is a need to develop technology that can remove phosphate from water bodies. This presentation will report a cerium-based metal-organic framework sorbent that has exceptional stability, high surface area, microporous structure, and the ability to bind strongly with phosphate through cerium nodes supported experimental results and DFT calculations. The work demonstrates for the first time the ability of this material to remove phosphates from water with a removal capacity of 168 mg/g in less than 4 minutes. The remarkable adsorption capacity and fast kinetics provide a significant improvement over the current state-of-the-art crystalline porous materials, and the conventionally used activated carbon. The study suggests that cerium-based metal-organic framework are highly effective and durable sorbents and can be used to develop next generation technologies to address challenges related to water eutrophication.

ENVR 762

One-step tailoring surface roughness and surface chemistry to prepare superhydrophobic polyvinylidene fluoride (PVDF) membranes for enhanced membrane distillation performances

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Superhydrophobic polyvinylidene fluoride (PVDF) membrane is a promising material for membrane approaches for preparing distillation. Existing superhydrophobic PVDF membrane often involve separate manipulation of surface roughness and surface chemistry. Here we report a one-step approach to simultaneously manipulate both the surface roughness and surface chemistry of PVDF nanofibrous membranes for enhanced direct-contact membrane distillation (DCMD) performances. The manipulation was realized in a unique solvent-thermal treatment process, during which a treatment solution containing alcohols was involved. We demonstrate that by using different chain-length alcohols in the treatment solvent, surface roughness can be promoted by creating nanofin structures on the PVDF nanofibers using an alcohol which has moderate affinity with PVDF. Meanwhile, surface chemistry can be tuned by adjusting the fraction distribution of crystal phases (nonpolar α phase and polar β phase) in the membrane using different alcohols. PVDF membranes with different surface wetabilities were used to evaluate the effects of surface roughness and surface energy on the DCMD performances. Combining both low surface energy and multi-scale surface roughness, pentanol-treated PVDF membrane achieved best anti-water property (water contact angle of 164.1° and sliding angle of 8.1°), and exhibited superior water flux and enhanced anti-wetting ability to low-surface-tension feed in the DCMD application.



Schematic illustration of one step manipulation process



DCMD applications with the pristine, treated PVDF membranes

ENVR 763

Vertical profiles of therapeutic opioids and other pharmaceutical chemicals in sediment cores obtained from tidal marshes and river embayments in the Potomac River estuary, Virginia-Maryland, USA

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Therapeutic opioids and other pharmaceutical chemicals (often termed PPCPs) represent emerging contaminants in the tidal freshwater Potomac River (TFWPR) that are frequently detected in fluvial and estuarine sediments.

The TFWPR receives discharge from seven large wastewater treatment plants (WTP), representing a region where PPCPs are a concern in water quality. The depositional histories of PPCPs in riverine and estuarine sediments were evaluated by collecting sediment cores from large marshes and tributary shoals near WTP discharge. Cores (1-m depth) were obtained using a Vibecore mini, split vertically, sectioned into 2-cm segments, and analyzed by LC-MS/MS following QuEChERS extraction and cleanup for the presence of 90 PPCPs. PPCP concentration-depth profiles in the cores were compared to Cs-137 (where possible) and legacy insecticides (e.g., ΣHCHs). Approximately 30 PPCPs (including 5 opioid painkillers) were detected in the core sediment samples ranging from 0.5 to 245 ng/g dry weight. The vertical core profiles of the PPCPs differed from the legacy insecticides, in that the PPCPs did not display concentration maxima prior to the 1963 Cs-137 timeline. Furthermore, the PPCP concentrations were relatively more concentrated in the surface lavers. The marsh sediment cores showed PPCP depth profiles that reflected their unique hydrology relative to the open river cores.

ENVR 764

Computational study of THz spectra of fentanyl and its analogs

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Fentanyl is one of the most potent synthetic opioid pain reliever. However, the misuse and abuse of fentanyl leads to the death in the U.S. Terahertz (THz) spectra provides the information of matter conformation without damaging the sample. In this study, we investigated THz spectra of fentanyl and its analogs in solid state by PBEh-3c/def2mSVP density-functional theory (DFT) method to understand the normal mode between 20 and 90 cm⁻¹. Since the vibration is the breathing of the whole conformation, THz spectra become a fingerprint of each fentanyl, which is beneficial for the design of warfare agent detection. Structure-property relationships of THz spectra of fentanyl and its analogs is performed by substituting one hydroxyl (BIYTAF), one methyl (3methylfentanyl), or both (ohmefentanyl). For comparison, THz spectra of carfentanil and its analogs (4methoxylmethylfentanyl, sufentanil, and alfentanil) are performed as well. The substitution of single bond or one aromatic group lead to specific pattern of THz spectra. This study makes it possible to develop a database of spectra and predict the spectrum of fentanyl analog with similar conformation.

ENVR 765

Near real-time determination of the prevalence of illicit drugs, cannabinoids, cathinones, and synthetic opioids in four rural counties in Illinois using wastewater-based epidemiology

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Unregulated new psychoactive substances (NPS) in "pure" or "preparation" forms are designed to mimic the effects of controlled substances, and are introduced and reintroduced in the market as a cheap substitute of established regulated drugs in guick succession to loophole the law enforcement efforts on combating drugs. For example, carfentanil, a synthetic opioid activates the opioid receptors similar to morphine, but it is astoundingly potent compared to a typical drug of abuse (100 times more potent than fentanyl and 10,000 times more powerful than morphine). Based on the cost- and timeintensive forensic analysis, National Drug Early Warning System reported a total of 2023 identifications of NPS opioids/analgesics, 81 including 1783 synthetic cannabinoids. 55 cathinone identifications in the mid-vear 2019 in the USA. The UPLC-MS/MS based analytical technique was developed capable of determining trace level NPS in wastewater. The cost-effective, comprehensive, and near-real-time approach, wastewater-based epidemiology, was used for the first time in the U.S. to determine the prevalence of 43 NPS in four U.S. communities. Methcathinone, 5-IT, MAB-CHMINACA, 4methylamphetamine, 1-(3-chlorophenyl) piperazine (mCPP), 4-methyl pentedrone, 2-methyl-4'(methylthio)-2morpholinopropiophenone, alpha-ethylaminohexanophenone, carfentanil, methoxyacetyl fentanyl, and valervlfentanvl were the most abundant NPS. The prescription opioids and methamphetamine were more prevalent in communities with per-capita-income whereas the cocaine was found more prevalent in a university town.

ENVR 766

Development of an *in situ* self-template strategy for highly efficient PVDF/Cu-BTC composite ultrafiltration membrane

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Highly efficient PVDF/Cu-BTC composite ultrafiltration membrane was fabricated in situ on a poly (vinyl difluoride) through a facile self-template method at room temperature. The template of copper hydroxysulfates was

pre-grown on PVDF membrane, served as the source of metal ion and in situ transformed into Cu-BTC crystal in the precursor solution of ligand, which avoided the selfnucleation of MOF in the solution and formed an ordered MOF array. The as-synthesized PVDF/Cu-BTC was fully characterized by SEM, FTIR, XRD, XPS and EDX. And its performances including hydrophilicity, porosity, pure water flux and antifouling were also investigated. The result showed that the newly developed PVDF/Cu-BTC composite ultrafiltration membrane exhibited a declined water contact angle of 48° and an increased porosity of 80% comparing with pure PVDF ultrafiltration membrane. Meanwhile, the resultant membrane showed a high pure water flux up to 480 L/(m²*h) and maintain a high BSA rejection rate of 99%. The self-template synthesis approach provides new idea and means for the development of advanced PVDF/MOF composite ultrafiltration membrane in wastewater treatment application.

ENVR 767

Nexus of natural and engineered nanomaterial: Biofilm eradication using magnetic phagenanocomposite conjugates

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Biofilms, which are very difficult to eradicate from water treatment, distribution and reuse systems, can cause a variety of safety, aesthetic and corrosion problems. This underscores the need for effective and sustainable biofilm-eradication technologies. Here, we covalently loaded natural antimicrobial nanoparticles (phages) with optimized orientation onto Fe₃O₄-based magnetic nanocomposites. Compared with free phage treatments, immobilization mitigates phage dilution by the medium to maintain high phage concentrations locally, and ensures that phage tail fibers are exposed to the hosts for easier infection. Pushed by a weak magnetic field, phagenanocomposite conjugates (PNCs) targeted the dominant species at the base of the biofilm and de-anchored it within six hours. This combined experimental and computational study revealed that smaller PNCs enhanced biofilm bottom clearance with significant horizontal dispersion, while larger PNCs exerted more significant vertical biofilm disruption. Our study highlights the role of PNC size on biofilm eradication patterns and advances the scientific basis for nanotechnologyenhanced, phage-based strategies for biofilm control. Potential applications include membrane biofouling control and biocorrosion mitigation.

ENVR 768

Withdrawn

ENVR 769

Alternative to analytical chemistry for assessing disinfection byproducts in potable water reuse

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With more than 600 identified disinfection byproducts (DBPs), chemical analysis of all compounds in a water sample is not feasible. In addition, analysis of individual chemicals does not account for toxicological effects of complex mixtures. In recent years, bioanalytical tools such as in vitro assays have been used as alternatives to analytical tools to assess water quality for potable reuse. Unlike in vivo assays with whole organisms, in vitro assays are often faster, require fewer resources, and work well for screening purposes. Therefore, in vitro bioassavs could prove valuable for screening disinfected water samples. This work presents results from a recent study focused on bioassays suitable for screening disinfection byproducts (DBPs). Multiple bioassays (e.g., Chinese hamster ovary cytoxicity, Cell-Titer Blue, Mitochondrial Membrane Potential, umuChromotest and Glutathione-Glo) were evaluated for rapid screening of four classes of DBPs: trihalomethanes (THMs), haloacetic acids (HAAs), nitrosamines (NAs), and haloacetonitriles (HANs). These compound classes were chosen because they are regulated (THMs, HAAs) or proposed for regulation (NAs, HANs) due to significant toxicity. Bioassay responses varied; all assays exhibited a positive response for HANs and most exhibited a positive response for HAAs and THMs, while nitrosamines did not elicit bioassay responses. Additional results include effective concentrations (EC50) for individual chemicals, and an assessment of mixtures to determine if bioassay responses showed additive or antagonistic effects.

ENVR 770

Low cost polyamine-modified graphene composites for effective mercury remediation in water

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This work focuses on the engineering of graphene oxide (GO) using multi-amine precursor to achieve a low-cost and effective adsorbent decorated with N-containing to adsorb mercurv in water. Various aroups characterization outcomes including X-ray photoelectron spectroscopy (XPS) analysis confirmed successful modification of the graphene composite using polyamine precursor with 5.47% N content recorded. The polyamine functionalized graphene composite demonstrated high affinity towards mercury in broad range of pH (pH 4-9) and rapid adsorption rate with equilibrium attained within the first 10 minutes. This material was found to follow Freundlich isotherm and pseudo-second order models with 63.8 mg/g sorption capacity. It also showed remarkable selectivity in both its dispersed (~86%) and solid forms (~79%) towards Hg(II) compared to existing commercial adsorbent (~16% in solid form) in multimetallic solution. This material has also proven its outstanding outcome in regeneration test and mercury spiked natural waters environment which is promising for real remediation application. A low cost and effective polvamine functionalized graphene adsorbent has been successfully developed to mitigate mercury pollution issue. All the performance assessments exhibit potential conversion of this material for scalable application to remove mercury from the polluted waters.



ENVR 771

Rapid transformation of H₁-antihistamines cetirizine (CET) and diphenhydramine (DPH) by peroxy-monosulfate (PMS)

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Advanced oxidation processes (AOPs) have received tremendous attention for water treatment. Relatively few studies have been reported on peroxymonosulfate (PMS) mediated water treatment processes, despite its potential to generate two powerful oxidants, hydroxyl radical and sulfate radical. We herein report PMS leads to the rapid degradation of target H₁-antihistamines, cetirizine (CET) and diphenhydramine (DPH). These compounds are problematic and commonly found in drinking water sources. Detailed product and kinetic studies were conducted using HPLC, NMR, and LC-MS/MS. Selective quenching agents were added to the reaction solutions to identify the primary reactive species responsible for the degradation. Our results indicate direct oxidation of the target compounds by PMS is the predominant transformation pathway. Influence of pH, presence of common anions (NO₃⁻, Cl⁻, Br⁻, l⁻, HCO₃⁻, CO₃²⁻, and/or phosphate buffer solution (PBS)), initial PMS concentration, and initial CET concentration was examined on both the degradation kinetics and the transformation of the H₁-antihistamines. The outcome of this study contributes to the fundamental understanding of PMS mediated oxidation, which is critical to the development of PMS based water treatment technologies.

ENVR 772

Advancing heterogeneous catalytic ozonation for water treatment and reuse

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Ozone (O₃) has long been used in water/wastewater treatment as an oxidant and/or disinfectant, ascribed to its high oxidation potential (2.07V) and bactericidal properties. Ozone-based AOPs (e.g. O₃/UV, O₃/H₂O₂) have the advantages of simplicity, strong oxidation potential, and no toxic residual in the treated water. In particular, heterogeneous catalytic ozonation has attracted much attention due to the high efficiency for the removal of refractory organic compounds compared to ozonation alone, and easy catalysts separation compared to homogeneous catalytic ozonation. However, the application of heterogeneous catalytic ozonation on a full scale is still very limited due to many challenges, such as the surface properties and/or stability of the catalyst, the effect of water matrices, limited catalytic reactivity, and formation of toxic byproducts. In order to advance heterogeneous catalytic ozonation processes in water/wastewater treatment, we have systematically investigated the stability of solid catalysts during ozonation, effects of water matrices commonly-used in laboratory studies, and development of a novel plasmonenhanced catalytic ozonation process. Metal/metal oxides are the most commonly-used ozonation catalysts. Here we rigorously examined the stability of representative metal oxide catalysts and the results showed that the homogeneous catalytic effects resulting from the leached metal ions were significant. We also demonstrated that the catalyst stability can be improved by Atomic Layer Deposition (ALD) overcoating. Further, studies on heterogeneous catalytic ozonation usually start with well controlled water matrices to facilitate mechanism investigation. While this seems to be a

rational and valid research approach, the different solution chemical conditions of different controlled matrices need to be carefully examined. Our study indicated that the water matrices not only provide the buffering capacities, but also affect the catalytic ozonation process in various aspects. Lastly, we aim to enhance the efficiency of catalytic ozonation processes by utilizing surface plasmon resonance of plasmonic metal based catalysts. The promising performance of plasmonmediated catalytic ozoantion for the elimination of recalcitrant organic pollutants suggests this could be an effective strategy to advance heterogeneous catalytic ozonation processes for sustainable water treatment and reuse.

ENVR 773

Advanced oxidative destruction of cyanide by radicals generated from an activated iron media/O₂ system

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The activated iron media (AIM) consists of a mixture of zero-valent iron (ZVI) powder and specially formulated iron oxides (FeO_x) in forms of a surface coating on ZVI and discrete FeO_x particles independent of ZVI. The iron oxide component of the AIM is characterized with an inverse spinel crystal structure and non-stoichiometric Fe(II)/Fe(III) in the lattices that features high electron conductivity and flexible structure enriched with labile Fe(II), which endow the AIM with unique chemical reactivities. The AIM was better known for its effectiveness in reductive transformations and immobilizations of contaminants including nitrate, selenate, and various heavy metals/metalloids from water. In this study, we demonstrate that by a process as simple as aerating the AIM, the AIM system could be converted into an advanced oxidation reactive system that can generate large quantities of hydroxyl radicals for oxidative destruction of contaminants. In batch tests using cvanide as the target contaminant, we showed that when exposed to the AIM, cyanide (CN-) combined rapidly with labile Fe^(II) in the AIM to form Fe(CN)₆⁴⁻ without further degradation; but with aeration, [CN-] could be completely oxidized to cyanate (OCN-), which then degraded through hydrolysis and released NH4⁺ that was subsequently oxidized to N₂. When AIM was replaced with ZVI, no significant oxidation of CN was observed with or without aeration. When benzoic acid was added as a hydroxyl radical scavenger in the AIM-O₂ system, no CN⁻ oxidation was observed. We postulate that hydroxyl radicals may be generated at certain surface reactive sites of the FeOx upon contact with O₂. The unique electron conducting capability and the abundant e- from ZVI may play an essential role in this process. The co-presence of Fe(II) and Fe(III) and the ready Fe(II)<-->Fe(III) cyclic conversion within the AIM structure may catalyze reactions of O_2 -initiated hydroxyl radical production. The finding that O_2 can be used as an oxidant to efficiently generate hydroxyl radicals at ambient temperature and near neutral pH conditions may lead to development of a low-cost advanced oxidation technology for water treatment.

ENVR 774

Solar photoelectrochemical production of reactive oxidants as a sustainable method of water treatment

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The photoinduced electron transfer process occurring on the semiconductor surface is being extensively investigated for water purification. Metal oxides such as TiO₂, WO₃, and Fe₂O₃ and polymeric carbon nitride that consist of earth-abundant elements are the most practical base materials for photoelectrochemical (PEC) conversion systems. The interfacial engineering of the semiconductor electrodes can optimize the production of reactive oxidants such as hydroxyl radical, reactive chlorine species, and hydrogen peroxide in PEC systems. In this talk, the development of semiconductor electrodes and their applications to PEC water treatment via generating OH radicals and reactive chlorine species will be introduced and discussed. The PEC production of H₂O₂ through dioxygen reduction has been also investigated as an in-situ generation method of this ecofriendly oxidant. A PEC cell in which H₂O₂ is produced on both photoanode and cathode under visible light irradiation was successfully demonstrated without using any external bias, which can be directly applied to solar water treatment processes.

ENVR 775

Oxygen vacancy promoted heterogeneous fentonlike degradation of ofloxacin at pH 3.2-9.0 by Cu substituted magnetic Fe₃O₄@FeOOH nanocomposite

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To develop an ultra-efficient and reusable heterogeneous Fenton-like catalyst at a wide working pH range is a great challenge for its application in practical water treatment. We report an oxygen vacancy promoted heterogeneous Fenton-like reaction mechanism and an unprecedented ofloxacin (OFX) degradation efficiency of Cu doped Fe3O4@FeOOH magnetic nanocomposite. Without the aid of external energy, OFX was always completely removed within 30 min at pH 3.2-9.0. Compared with

reaction Fe3O4@FeOOH, pseudo-first-order the constant was enhanced by 10 times due to Cu substitution (9.04 /h vs. 0.94 /h). Based on the X-ray photoelectron spectroscopy (XPS), Raman analysis, and the investigation of H2O2 decomposition, OH radical generation, the pH effect on OFX removal and H2O2 utilization efficiency, the new formed oxygen vacancy from in-situ Fe substitution by Cu rather than promoted Fe3+/Fe2+ cycle was responsible for the ultra-efficiency of Cu doped Fe3O4@FeOOH at neutral and even alkaline pHs. Moreover, the catalyst had an excellent long-term stability and could be easily recovered by magnetic separation, which would not cause secondary pollution to treated water.

ENVR 776

Transformation of emerging contaminants during oxidation processes: Paying more attention to toxicity variation

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Emerging contaminants (ECs) in aqueous systems are mostly unregulated compounds, which can affect water quality and potentially impact drinking water supplies, ecosystem and human health. As conventional municipal water treatment plants are not able to entirely degrade ECs in ng-µg L⁻¹ concentration, various oxidation processes (e.g., permanganate, chlorine dioxide (CIO₂), ferrate and UV/chlorine) become attractive options to further eliminate ECs during water treatment. However, structural transformations of ECs by oxidation do not mean simultaneous reduction of their toxicities, which is supported by many examples. Oxidation of dichlorvos by permanganate was pH independent with rate constant determined to be 25.2 \pm 0.4 M⁻¹ s⁻¹ at pH 7.0, while luminescent bacteria test showed that the acute toxicity of dichlorvos solution evidently increased after permanganate oxidation. Although the oxidation rate constant between CIO₂ and methiocarb rapidly increased from 0.56 to $4.5 \text{ M}^{-1} \text{ s}^{-1}$ as the solution pH increased from 6.0 to 9.1. a significant increase in toxicity was observed after CIO₂ oxidation. Moreover, some functional groups in ECs (e.g., nitro-, amine- and iodine-groups) may become precursors of highly cytotoxic and genotoxic disinfection by-products (DBPs) after oxidation and disinfection processes. Enhanced formation of nitrogenous DBPs during UV/chlorine treatment of chloramphenicol was observed, and both the simultaneous formation and 24-h halonitromethanes formation potential were positively correlated with the reaction time. Oxidation of iopamidol, an iodinated X-ray contrast medium, by ferrate could induce the formation of highly toxic iodinated DBPs. All these results indicate that when selecting an oxidation process for water treatment, more attention should be paid to the toxicity-directed elimination of ECs and their by-products.

ENVR 777

Electrocatalytic degradation of short- and long-chain perfluoroalkyl substances (PFASs) at boron doped diamond (BDD) and Ti/RuO₂ electrodes: Effect of operational parameters and water matrix

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Per- and polyfluoroalkyl substances (PFASs) are a group of synthetic chemicals that have recently received significant regulatory attention. Among the PFASs, perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS) have been subjected to more intense research due to their toxicity, stability, and potential of This long-range transport. study investigates electrocatalytic degradation of several short and long chain PFASs. Electrocatalytic degradation has numerous advantages such as easy operation, cost-effectiveness and high degradation efficiency. Anode material and optimization of the operational conditions are important for improved degradation efficiency. This paper analyses electrocatalytic degradation of short and long-chain PFASs including PFOA and PFOS using different electrode materials, namely, boron doped diamond (BDD) and Ti/RuO₂. Our findings showed that BDD electrode provided more than 90% degradation of PFOA (at initial concentration of 200 µg L-1) with the applied current density of 25 mA cm⁻² at pH of 7 while PFOS was completely degraded under these conditions. The results for the degradation of short and long-chain PFASs at Ti/RuO₂ electrode will also be presented during the presentation. The effect of operational parameters (supporting electrolyte, applied current density and initial pH) were investigated at BDD anode. For example, acidic and neutral pH (3, 5 and 7) values provided much higher removal rates of PFOA compared to alkaline values (9 and 11). In the case of PFOS, much higher defluorination efficiency was gained at BDD anode. The degradation of long-chain PFASs (C≥7 for PFCAs and C≥6 for PFSAs) occurred rapidly during the first 30 min of reaction. Fluorinated intermediate products were initially formed but were subsequently mineralized to CO₂ and HF on BDD electrode. On the other hand, increase in chainlength affected significantly the degradation of short-chain PFASs (C<7 for PFCAs and C<6 for PFSAs). The removal of C3 and C4 was significantly lower (~40%) than C5 and C6 (~70%) PFCAs. The results also showed that water matrix did not significantly affect the degradation of short-chain PFASs. In contrast, the order of defluorination ratio of long-chain PFASs was found to be DI water>

WWTP effluent> river water. The comparison of single and multi-component systems for the degradation of short-chain PFASs will also be presented since the behavior of single-compound system could be different from multi-compound system.

ENVR 778

Withdrawn

ENVR 779

Effect and mechanism of NaCIO-Fe(II) conditioning on the treatment of cyanobacteria-laden water and the dewatering performance of cyanobacteriacontaining sludge

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Cyanobacteria blooms due to the eutrophication of surface waters have become a worldwide problem. To efficiently treat cyanobacteria-laden water and enhance the dewaterability of the cyanobacteria-containing sludge for its further resource utilization, NaClO-Fe(II) was employed as a chemical conditioner herein based on the oxidation property of NaCIO and the flocculation ability of in-situ formed Fe(III). Results showed that the algae and DOC removal rate achieved nearly 100% and 90% respectively after NaClO-Fe(II) conditioning. With the increase of NaClO dose, the sludge dewatering performance was firstly improved and obtained the optimal effect at 1.5-2.0 mg/L NaCIO dose whereas significantly deteriorated upon NaClO dose was excessive. The better aggregation effect and more compact floc structure resulting from the promotion of charge neutralization can account for the improvement of dewaterability. measurements Additionally, EEM indicated that the decline of protein-like substances in the soluble extracellular polymeric substances (S-EPS) was favorable for cyanobacteria-containing sludae dewatering. Moreover, the deterioration of the dewatering performance can be ascribed to the excessive oxidation of algae cells causing cell lysis and undesirable release of algal metabolites. Overall, appropriate NaClO dose with the in-situ Fe(III) can enhance the treatment of cvanobacteria-laden water and the dewatering performance of cyanobacteria-containing sludge, which illustrated the practical feasibility of applying widely-used reagents NaClO-Fe(II) into cyanobacteria-laden water treatment.



of algae with different NaClO dosages. Fe(II) concentration was controlled at 1.0 mmol/L.

Fig. 1 Effect of NaClO dosage on cyanobacteria-containing sludge dewatering behavior



Fig. 2 EEM fluorescence spectra of soluble EPS and bound EPS fractions

ENVR 780

Modulations of Bi₂MoO₆ for photocatalytic performance enhancement under visible light illumination

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Bi₂MoO₆ is one of the simplest members of the Aurivillius family, which is composed by [Bi2O2]²⁺ layers sandwiched between MoO₄²⁻ slabs. It had been found that the internal electric field formed between the [Bi2O2]2+ and MoO42could effectively lavers in Bi₂MoO₆ separate photogenerated charge carriers, while the hybridization between its O 2p and Bi 6s states could narrow its band gap to enable the absorption of visible light. Thus, it had drawn research attentions as an efficient visible-lightphotocatalyst for various applications. activated In this talk, two material modulation strategies will be presented for the photocatalytic performance enhancement of Bi2MoO6 under visible light illumination. Theoretical calculation based on density function theory

(DFT) discovered that the internal polarization in Bi₂MoO₆ could be increased by shortening its crystal lattice parameter b. Subsequently, a simple, one-pot templatefree solvent-thermal process was developed for the synthesis of Bi₂MoO₆ photocatalyst, and the addition of NaOH in the reaction solution was found to be effective to shorten its crystal lattice parameter b. With shortened crystal lattice parameter b, the Bi₂MoO₆ photocatalyst demonstrated improved photogenerated charge carrier separation efficiency due to its increased internal polarization, and subsequently possessed a largely enhanced photocatalytic performance as demonstrated in its photocatalytic degradation of organic pollutants and disinfection of staphylococcus aureus bacteria under visible light illumination. Next, rich oxygen vacancies were introduced in Bi₂MoO₆ nanosheets through a postsynthesis etching treatment by NaOH aqueous solution at room temperature. Without changing their crystal structure, morphology, optical properties, and energy band structures, a series of Bi₂MoO₆ nanosheet samples with different oxygen vacancy concentrations were synthesized to provide a model photocatalyst to examine the charge carrier separation role of oxygen vacancies on its photocatalytic performance without interferences from other factors. Bi2MoO6 nanosheets with rich oxygen vacancies demonstrated an improved separation efficiency on photogenerated electron-hole pairs due to the existence of oxygen vacancies, and subsequently they demonstrated largely enhanced photocatalytic activities as demonstrated by their effective sulfamethoxazole degradation and Escherichia coli bacteria disinfection under visible light illumination.

ENVR 781

Delivering an integrated data hub for opioid and cannabinoid chemicals via the US-EPA CompTox Chemicals Dashboard

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There is increasing interest in the environmental impact of opioid and cannabinoid chemicals and the aggregation of related data provides both agency and public access to support research. The US-EPA's CompTox Chemicals Dashboard (https://comptox.epa.gov/dashboard) is a publicly accessible website providing access to data for ~880,000 chemical substances, including hundreds of opioid and cannabinoid chemicals and associated data. The dashboard provides access to a wide array of experimental and predicted physicochemical properties, *in vitro* bioactivity and *in vivo* toxicity data, product use information and integrated linkages to a growing list of literature, toxicology, and analytical chemistry websites. The assembly of data associated with a collection of opioids and cannabinoids requires significant levels of manual curation and data checking to deliver segregated chemical lists of interest. This presentation will provide an overview of the dashboard, the ongoing expansion of the opioid and cannabinoid chemical lists, their mappings to both *in vivo* and *in vitro* data, and discusses how the assembly of data can be utilized to support identification of these chemicals in the environment by mass spectrometry analyses, specifically non-targeted analysis approaches.

ENVR 782

Coupled transformation of iron and phosphorous speciation during anaerobic digestion with hydrothermal pretreatment of sewage sludge

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Anaerobic digestion (AD) of sewage sludge with hydrothermal (HT) pretreatment have emerged as a sustainable technique for energy and nutrient recovery. The distinct treatment conditions can significantly impact elemental speciation. Yet, the speciation evolution of iron (Fe) and phosphorous (P) as well as involved reaction mechanisms during combined HT-AD treatment of sewage sludge still remain unclear. In this study, the reactions products from HT treatment at different temperature (90, 155, and 185 °C) and subsequent AD process (73 days) were investigated for Fe and P speciation. Complementary sequential chemical extraction, X-ray diffraction (XRD), and Fe and P K-edge X-ray absorption spectroscopy (XAS) analyses were conducted. Compared with the raw sludge, a large amount of vivianite was formed in the solid hydrochar after HT treatment at low temperature, while more strengite was precipitated at higher HT temperature. This suggests that HT treatment at high temperature prohibits Fe(III) reduction. During the subsequent AD of the derived hydrochar, microbial reduction of strengite and other Fe(III) species led to the formation of more vivianite, with concurrent P release to the solution phase and adsorption onto other minerals. These results suggest that the speciation of Fe and P are strongly interconnected during HT and AD processes, affecting the solubility and bioavailability of each other. This work has important implications for understanding the nutrient speciation and availability in sludge-derived hydrochars and AD solids, and also provides fundamental knowledge for the selection and optimization of HT pretreatment conditions for enhanced energy and nutrient recovery.

U(IV) adsorption onto montmorillonite in an anoxic environment

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Uranium is widely used as nuclear fuel for power generation throughout the world. Spent nuclear fuel, primarily composed of U(IV) oxide, is generated as waste in nuclear fission process. Storage of spent nuclear fuel in deep underground repositories under anoxic condition potential long-term management strategy. is а Montmorillonite, because of its low hydraulic conductivity, self-swelling capacity and generally high ion adsorption capacity, is being considered as a buffer material for packing between the canisters bearing spent nuclear fuel and the host rock in such repositories. While U(VI) adsorption to montmorillonite has been studied over a range of conditions, our understanding of U(IV) adsorption to montmorillonite is very limited. At the conditions of many geologic repositories, U(IV) will be the dominant form of uranium that would interact with a montmorillonite barrier. In this study we focused on the mechanisms of U(IV) adsorption to montmorillonite as a function of pH and background sodium concentration. Montmorillonite is composed of two types of adsorption sites: (1) edge sites and (2) fixed charge basal sites. The affinity of metal binding to edge sites is pH dependent, while the availability of binding to basal sites is affected by the ionic strength of the solution. We examined the extents of U(IV) adsorption for total U(IV) concentration of 15 to 25 nM, a montmorillonite loading of 1 g/L and sodium chloride concentrations of 10 or 100 mM. The montmorillonite was preequilibrated with anoxic deionized water to ensure removal of an interlayer trace amount of oxygen. A non-electrostatic surface complexation model was developed to interpret the adsorption results obtained under these conditions.

ENVR 784

Determining the growth capability of airborne methanotrophs

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The growth and activity of microbes has been heavily studied in nearly every environment on Earth, but there have been limited studies focusing on the air. In the air, microbes are present at 10⁴-10⁵ cells/m³ air and the air contains various compounds that could serve as simple microbial growth substrates at sufficient concentrations. Previous laboratory studies have demonstrated that airborne Serratia marcescens was able to grow in water droplets. However, most of the atmosphere does not contain water droplets. When not associated with water droplets, airborne Sphingomonas aerolata NW12 synthesized more ribosomes when provided a carbon substrate and synthesized new proteins. This activity suggests the potential for microbes to grow in the air outside of water droplets on volatile compounds such as CH₄. To examine airborne microbial communities, we aerosolized cultures into 320 L rotating gas-phase bioreactors and assessed the half-lives and distributions of the particles. We investigated the ability of airborne methanotrophs to grow on CH₄ using DNA-stable isotope probing (DNA-SIP). The cultures were aerosolized into the gas-phase reactors and amended with 1500 ppmv ¹³CH₄ or ¹²CH₄. The cells were suspended in air for five days, harvested, and analyzed for ¹³C incorporation into DNA by gradient fractionation/gPCR methods. Some results demonstrated ¹³C incorporation into DNA, indicating growth in air, and other experimental replicates did not. We conclude that methanotrophs outside of water droplets in the air can potentially grow under certain conditions. Based on our data, low biomass is the main limitation for utilizing the DNA-SIP method for detecting activity of airborne methanotrophs. Current work is investigating this and other limitations, as well as further exploring the potential activity of airborne microbes.

ENVR 785

Dibenzopyrenes and Benzo[c]fluorene as strong candidates for an extended list of priority pollutants

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Polycyclic aromatic hydrocarbons (PAH) are among the most widely investigated and monitored compounds in the environment. Much work is centered on a list of 16 PAHs as priority pollutants that was introduced by the Environmental Protection Agency (EPA) in 1976 to monitor the quality of U.S. waterways. However, since then this compilation of PAHs has become the standard even for toxicological assessments of environmental samples, a task for which it was never intended and is not particularly well suited. A scientific discussion on adding more relevant compounds is ongoing. Such compounds would belong to classes so far not represented, *i.e.*, larger PAHs, heterocyclic aromatic compounds and substituted

PAHs well-recognized of carcinogenicity. A strong case can be made for including several isomers of the dibenzopyrenes. They frequently are found in environmental samples and some of them are known to be much stronger carcinogens that benzo[a]pyrene. Their toxic equivalence factors vary between 1 and 100, i.e. they are 1-100 times as potent as dibenzo[a]pyrene. Thus they would have a decisive influence on the toxic equivalence (TEQ) of the sample but despite that they are not routinely measured today. Literature examples of environmental samples indicate that they can be contribute twice as much of the TEQ than the sum of the 16 EPA PAHs. Benzo[c]fluorene is another PAH with similar characteristics as the dibenzopyrenes; it shows a toxic equivalence factor of 20 and may therefore, from a toxcicological standpoint, be of major concern. Besides the toxicity, other factors should also be considered before deciding on an extension of a mandated list. Analyzability is among them and so is the bioavailability that strongly influences the relative amount of a compound that an organism actually takes up from the sample and thus exerts an adverse health effect.

ENVR 786

Validation testing of disinfection and environmental parameters in ISO 30500: New international standard for chemistry-driven onsite sanitation systems

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ISO 30500 "Non-sewered sanitation systems --Prefabricated integrated treatment units -- General safety and performance requirements for design and testing" was published in October 2018. It aims to enable the testing and verification of design, functionality, and performance requirements of an onsite sanitation system that "collects, conveys, and fully treats [human excreta] to allow for safe reuse or disposal of the generated solid, liquid, and gaseous output" without being connected to a "sewer or drainage system". In this paper we present the field measurement of E. Coli, MS2 Coliphage, and Clostridium Perfringens spores removal by large-scale (100 L) batch electrolysis from an onsite sanitation system tested in Durban, South Africa.

ENVR 787

Nutrient removal from blackwater using natural zeolites

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Anthropogenic nutrient pollution of surface waters has severe negative impacts on the environment, human health, and the economy. In particular, algal blooms caused by eutrophication due to high levels of nitrogen and phosphorus (primarily as ammonium and phosphate) pose immediate risks to wildlife and human populations. and it can cost millions of dollars to treat a single body of water once a bloom occurs. A major source of nutrient pollution is inadequately treated sewage, especially from non-sewered sanitation systems (NSSS) which are not designed to remove nutrients before discharge into the environment. Biological methods of nutrient removal work well at large scales (e.g. municipal wastewater treatment plants), but scaling down for NSSS may be challenging or prohibitive in many use cases. Alternative, non-biological approaches are required for effective nutrient removal in small-scale NSSS while maintaining affordability, reliability, and sustainability. Here, we will present recent efforts to upgrade our blackwater treatment process, which was developed in response to the Bill & Melinda Gates Foundation's "Reinvent the Toilet Challenge", to include nutrient removal capabilities. The natural silicatebased zeolites clinoptilolite and polonite were identified as promising materials for capture of ammonium and phosphate, respectively. Evaluating adsorbant performance with real wastewaters is critical for successfully translating sanitation technologies from the laboratory to prototype field testing. Batch and column adsorption experiments were carried out using raw blackwater and blackwater pre-treated with granular activated carbon and/or ultrafiltration. Both clinoptilolite and polonite were effective in removing their target ions from raw and pre-treated blackwater. We will discuss zeolite performance and process design in the context of meeting the newly adopted ISO 30500 standards for water reuse in NSSS, which require 70% and 80% reductions in total N and P, respectively. We will also present results on zeolite regeneration and reuse, as well as strategies for nutrient recovery.

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Beyond Wood's metal: Low melting alloys made from it

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The well-known low melting alloy Wood's metal was named after its creator, in the mid-nineteenth century. We have undertaken a series of experiments in which the amounts of tin and lead metal can be added to samples of Wood's metal, while the melting point still remains below that of boiling water. The results, and environmental implications of them, will be presented.

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Accurate quantitation of ethanolamines in oil and gas wastewaters

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The high salinity and organic content in oil and gas wastewaters can cause ion suppression during liquid chromatography mass spectrometry (LC/MS) analysis, diminishing the sensitivity and accuracy of measurements in available methods (e.g., ASTM D7599). This suppression is severe for low molecular weight organic compounds such ethanolamines as (e.g., monoethanolamine (MEA), diethanolamine (DEA). triethanolamine (TEA), N-methyldiethanolamine (MDEA), and N,N-ethyldiethanolamine (EDEA)) which are compounds of interest to energy producing companies. Here, we deployed solid phase extraction (SPE) for desalting, mixed-mode LC, triple quadrupole MS with positive electrospray ionization (ESI), and suite of stable isotope standards to correct for signal suppression by organic matter, SPE losses, and instrument variability. The method was evaluated in real produced waters from Italy (NaCl salinity = 8110 - 18100 mg/L; diesel range organics = 5.1 - 7.9 mg/L) and showed good matrix spike recoveries of 87 - 115% for all compounds, as compared to previous ASTM method that gave low recoveries (e.g., <5% for MEA) in the produced fluids. Using the improved method, produced water samples contained 37(±1) -646(±6) µg/L total ethanolamines, with DEA and MEA as dominant species. Possible ethanolamine sources (e.g., corrosion inhibitors and biotransformation) and natural attenuation potential during storage were also investigated. The developed method enables further understanding of the fate of low molecular weight organic additives in oil and gas development and provides an enhanced ability to evaluate risks associated with chemical release to the environment.