UTSA Geological Sciences

And

Institute of Water Research, Sustainability and Policy (IWRSP)

Seminar Presentation

By

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On

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4:00 P.M.

"Molecular Modeling in Environmental Chemistry"

James D. Kubicki
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Abstract
The connection between large scale environmental processes and molecular properties is critical to understanding and managing contaminants, but the complexity of natural systems makes it difficult to scale scientific research over orders of magnitude in the spatial and temporal domains. Collaboration among scientists working at different scales is key to identifying information that can be transferred across the various levels of natural processes. This talk will focus on studies in computational chemistry that have been designed to address questions generated by field and laboratory observations. Myriad techniques exist to simulate environmental chemistry. Verifying the accuracy of these simulations against experimental observables helps to build confidence in the model results and utilize the molecular-scale results to the real world. Two examples of this approach are the adsorption behaviors of phosphorous and polycyclic aromatic hydrocarbons (PAHs).

James Kubicki is currently Chair of the Department of Geological Sciences and the interdisciplinary Environmental Science program at UTEP. His academic pathway has taken him from undergraduate work at CSUF, a Ph.D. from Yale with research performed at the Carnegie Geophysical Laboratory (with Russell Hemley), postdoctoral appointments at Caltech (under Geoff Blake and Ed Stolper) and the U.S. Navy (under Sabine Apitz), and a faculty position at Penn State. Over this time, his research has ranged across high-pressure melt structure, melting, nucleation and volatiles in magmas, organic contaminant recalcitrance, bacteria-mineral adhesion, plant cell wall architecture, and nanoparticle surface chemistry. The overarching theme in all these studies has been to understand geochemical reaction mechanisms that control the rates of processes in the environment. To follow this path, Kubicki has relied upon computational chemistry and spectroscopy to learn details of molecular structure, especially in systems with significant disorder (e.g., glasses & melts, soot, and mineral-water interfaces). He enjoys a collaborative approach to combine the expertise of colleagues to obtain a more comprehensive view of the chemistry in the systems of interest.

Selected Publications

1. Ohno T., Kubicki J.D. (2020) Adsorption of organic acids and phosphate to an iron (oxyhydr)oxide mineral: A combined experimental and density functional theory study. The Journal of Physical Chemistry A, 124, 3249-3.
2. Ajayi O.A., Kubicki J.D. (2019) Interfacial energies of supercritical CO2 and water with 2:1 layered silicate surfaces: a density functional theory study. Applied Geochemistry, 104514.
3. Boettger J., Kubicki J.D. (2019) Evaluating computational chemistry methods for isotopic fractionation between CO2(g) and H2O(g). J. Chem. Inf. Modeling, 59(11), 4663-4677.
4. Soldoozy S., Trinh A., Kubicki J.D., Al-Abadleh H.A. (2020) In situ and real-time ATR-FTIR temperature-dependent adsorption kinetics coupled with DFT calculations of dimethylarsinate and arsenate on hematite nanoparticles. Langmuir, 35, 4299-4307. https://dx.doi.org/10.1021/acs.langmuir.0c00252.
5. Watts H.D., O'Day P.A., Kubicki J.D. (2019) Gibbsite (100) and Kaolinite (100) Sorption of Cadmium(II): a Density Functional Theory and XANES Study of Structures and Energies. The Journal of Physical Chemistry A, 123, 6319-63.