CCT Colloquium Series

Using Computers to Discover Strange Behavior at Water Surfaces

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Ph.D.

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Abstract:
Interfaces can create an environment in which unexpected behavior that is not normally possible exists, which may spur specific regular chemical reactions through catalysis, or the realization of other unique properties. For instance, many atmospheric transformations occur at the surface of cloud and fog droplets, and any trace gas in the atmosphere will always come in initial contact with the surface of the droplet. Determining if species are present at the surface of these droplets, such as sodium or chloride ions in saltwater can be a very challenging task experimentally, and not always unambiguous. Computational studies, on the other hand, if using reliable molecular models, can bring significant insight into this, and in many cases can change our understanding of the mechanism for the creation and destruction of countless gases in our environment. Furthermore, an understanding of simple problems such as the acidity of the surface of neat water or if acids or bases are preferentially present at the surface will affect interfacial reactivity. Unfortunately, the most reliable methods and molecular models are too computationally expensive to tackle some of these problems. This requires the development of efficient computational methodology that incorporates the correct levels of physics in its models. With a combination of high performance computing and the efficient methodology, a new picture is emerging into the properties at the surfaces of water.

Speaker's Bio:
Collin Wick graduated from University of Minnesota with a PhD in Physical Chemistry in 2003 on a DOE computational science graduate fellowship, and received the first prize in the American Chemical Society administered IBM award in theoretical chemistry. After receiving his PhD, he did a one year postdoc in Greece under the NSF-MPS distinguished international postdoctoral fellowship. Then, he spent three years as a postdoc at Pacific Northwest National Laboratory. Since 2007, he has been an Assistant Professor of Chemistry at Louisiana Tech University. His research focuses on using molecular simulation with Monte Carlo and molecular dynamics for aqueous and polymer systems, and liquid interfaces. He has been an author in 33 refereed journal articles, including five that were featured on the cover.

Refreshments will be served.
This lecture has a reception.

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