

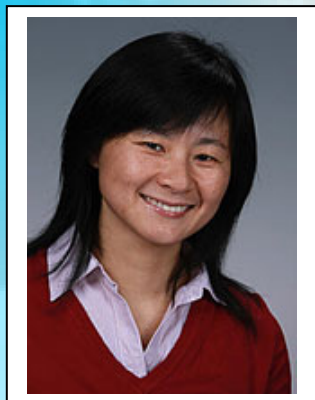
Physics Colloquium

Michigan Technological University

Thursday, November 29, 2012

4:00 pm

Room 139 Fisher Hall



Computational Modeling of Actinide Species in the Natural Environment

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Abstract: Actinides are of environmental and health concern due to their introduction into ground water and the natural environment via nuclear activities. The complicated electronic structure of actinide complexes leads to their versatility of chemical binding, reactivity, and spectral and magnetic properties. It is critical to have a fundamental understanding of the electronic structures of actinides in homogeneous and heterogeneous environments. In this talk, we will show that, complementary to modern experimental spectroscopic techniques, computational chemistry modeling has become an effective tool in providing a first-principle description yielding insight into actinides-ligand bonding interactions. Relativistic density functional theory (DFT) and time-dependent DFT have been applied to study the thermodynamic and spectroscopic properties of actinide complexes.¹⁻³ Furthermore, we study the dynamical behavior of actinide species interacting at a heterogeneous interface using *ab initio* molecular dynamics.⁴ Our calculations provide insights into the physico-chemical properties of actinide complexes in the natural environment, a step towards rational design of remediation technologies for environmental contaminants.

Biography: My research interests lie in computational studies of heavy element chemistry, biochemical systems, and energy conversion materials using combination of advanced first-principles quantum mechanical methods. I am especially interested in questions related to fundamental electronic structures, bonding interactions, reaction mechanisms, and magnetic and optical spectroscopic properties. I believe that close integration with experimental efforts is essential for mutual validation of results and exchange of perspectives.