Chemistry and Physics Colloquium

Michigan Technological University

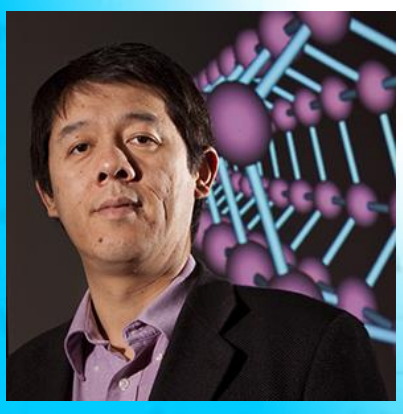
Thursday, April 2, 2015
4:00 pm
Fisher Hall Room 139

Computer-Aided Nanomaterial and Nanostructure Design: Nanoice, Gold-clusters, Superhydrophobicity, and 2D Materials

Prof. Xiao Zeng
Department of Chemistry
University of Nebraska-Lincoln
(Email: xzeng1@unl.edu)

Abstract: In this talk I shall report several research findings from my group over the past few years, including: (1) New phases of low-dimensional nano-ice and ice clathrate; (2) superhydrophobic phenomena at the nanoscale, e.g. Lotus effect at nanoscale; (3) growth pattern of small-sized gold clusters and gold nanocatalysis; and (4) novel 2D atomic-layer materials.

Understanding physical and chemical properties of confined water at nanoscale has implications for diverse phenomena at the intersection between chemistry, biological sciences, and physics, such as boundary lubrication in nanofluidic devices and synthesis of antifreeze proteins for ice-growth inhibition. Gas hydrates are solid-state materials typically consisting of a host ice frame with nanoscale cages that serve to trap small guest molecules such as methane. Methane hydrate is one of the most significant energy sources; and gas hydrate formation is also a critical issue in deep-water gas/oil pipelines. Molecular simulations of low-dimensional gas hydrate formation may bring new insights into bulk gas hydrate formation. Bulk gold is known to be catalytically inert whereas gold nanoparticles can exhibit exceptional catalytic properties towards CO oxidation. We have performed a systematic study of catalytic activities of sub-nanometer gold clusters, hollow-cage clusters in particular, with or without metal-oxide supports, using density functional theory (DFT) calculations. Lastly, I will present a recently predicted new 2D material that shows novel electronic properties.



Bio: Prof. Zeng is the Distinguished University Professor of Chemistry, and is Fellow of AAAS, Fellow of APS, and Fellow of RSC. He received his bachelor degree in Physics from Peking University in 1984 and his Ph.D. in Chemical & Condensed Matter Physics from the Ohio State University in 1989. He pursued his postdoctoral research in Physical Chemistry at University of Chicago (1989-1992) and UCLA (1992 – 1993). The most significant scientific discoveries from Zeng group include the 2D bilayer hexagonal ice ("Nebraska ice" – confirmed by experiments in 2009), 2D ice clathrate, multi-walled helical ice, one-dimensional ferroelectric ice, single-walled ice nanotubes (confirmed by experiments in 2003), hollow cages of gold (confirmed by experiments in 2006), and single-walled silicon nanotubes. These findings were featured in the New York Times, Omaha World Herald, Lincoln Journal Star, American Scientist Magazine, New Scientist Magazine, and National Public Radio.

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