J. Clarence Karcher Lecture

◆ DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY ◆ THE UNIVERSITY OF OKLAHOMA ◆ NORMAN, OK 73019-5251 ◆ (405) 325-4811 ◆

Is Pleased to Announce A Seminar
Presented By
Christine Aikens
Kansas State University
Friday, October 25, 2019
4:00 pm
NWC 1313

Understanding Nanoparticle Properties using Theoretical Methods

Theoretical investigations of noble metal nanoparticles are important for determining the origins of the unique chemical and physical properties of these systems that lead to applications in photonics, sensing, catalysis, etc. Using DFT and TDDFT calculations, we have recently elucidated the optical absorption and photoluminescence spectra of Au$_{25}$(SR)$_{18}$ and related nanoparticles. Significant changes in the geometric and electronic structure of this system are observed upon photoexcitation. Small silver clusters encapsulated by DNA have been of interest for biotagging applications because they display fluorescence. The absorption and CD spectra of helical silver nanowires are computed and compared with experimental spectra. The agreement between theory and experiment suggests that the silver-DNA clusters have a helical arrangement.

Refreshments will be served at 3:45 pm
REMINDER ~ WEAR YOUR ID

(Bio on back)
Christine M. Aikens received a B.S. degree in Chemistry from the University of Oklahoma in 2000. Her graduate studies in Physical Chemistry were performed under the direction of Mark S. Gordon at Iowa State University and were supported by a National Science Foundation Predoctoral Fellowship. Upon receiving her Ph.D. degree in 2005, she began a postdoctoral research position in Theoretical Chemistry with George C. Schatz at Northwestern University. In 2007, she accepted a position as an Assistant Professor at Kansas State University. Prof. Aikens received a NSF CAREER grant in 2010 and was awarded an Alfred P. Sloan Research Fellowship and a Camille Dreyfus Teacher-Scholar Award in 2011. She became an Associate Professor at Kansas State in 2012 and a Full Professor in 2015. She was selected for the Journal of Physical Chemistry A Lectureship in 2015 and was chosen as a WCC Rising Star in 2019.