



PHYSICAL SEMINAR

Understanding Nanoparticle Properties using Theoretical Methods

PROF. CHRISTINE AIKENS
KANSAS STATE UNIVERSITY
Host: Prof. Yang Yang

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 $\text{Au}_{25}(\text{SR})_{18}^-$ 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.

DATE: TUESDAY, March 1st, 2022

TIME: 11:00 am in the Learning Studio, Room 1435

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