2014-15

Hirschfelder Lectures in Theoretical Chemistry

Professor George C. Schatz
Northwestern University

Silver and Gold Nanoparticles

Monday, October 6 2:00 p.m. Room 1315 Chemistry

Silver and gold nanoparticles have a history that dates to the Roman empire and before, as well as detailed work by Michael Faraday in the 1850s. However these particles have been given new life (and applications) in the last 40 years through a number of scientific advances. This talk will provide an overview of these advances, including new methods for making them, new spectroscopic techniques for measuring their properties and the properties of molecules near the nanoparticle surfaces, and new optical applications in sensing, photochemistry, photonic materials, solar cells and optoelectronic devices which continue to drive research in the field. An emphasis of this talk will be on the use of theory to understand the unusual optical properties of these materials, in which collective electronic excitations (plasmons) cause the colors of these particles to depend on their size, shape and arrangement. The cornerstone of this work is computational electromagnetics, which provides a simple but accurate description of many optical properties of these particles. Also important is the combination of classical electromagnetics with quantum mechanics, and its use in understanding plasmon enhancement effects in spectroscopy and photochemistry.

Using self-assembly to make functional materials

Tuesday, October 7 11:00 a.m. Room 1315 Chemistry

Self-assembly of amphiphilic molecules provides a well-known way to make nanoscale (and larger) supramolecular structures including micelles, ribbons, sheets and aggregates. Recently there has been growing interest in the coupling of this self-assembly chemistry with silver and gold nanoparticles, and with dye chromophores, leading to a new generation of materials of interest for optical devices and biodetection. This talk describes the self-assembly modeling and optical properties of two classes of these materials: DNA-linked nanoparticle superlattices and peptide amphiphile fibers and ribbons with embedded dyes or nanoparticles. The presentation will present a novel coarse-graining strategy for describing the assembly of DNA-linked superlattices, and models of the optical properties of the resulting structures, leading to new classes of plasmonic metamaterials, and photonic structures.

Challenges with harnessing the properties of carbon nanotubes and graphene for making strong materials

Wednesday, October 8 2:00 p.m. Room 1315 Chemistry

This talk describes theory, computational studies and related experiments aimed at understanding the mechanical properties of carbon nanotubes and related graphene structures, including the properties of individual nanotubes, small bundles, and fibers composed of millions of nanotubes. We begin by assessing the fracture strength of individual carbon nanotubes, showing the amazing strength and toughness of these structures provided that they aren't significantly defected. We then switch to shear interactions, where we find that intermolecular forces play a crucial role, which means that the shear interactions can be modified by nanotube functionalization in a way that can be predicted by theory. However there are still important questions as to how best to use nanotubes to make threads and fibers for practical applications. We finish by talking about the carbonization of polyacrylonitrile, where theory has provided new insights as to fundamental chemical processes at high temperature.