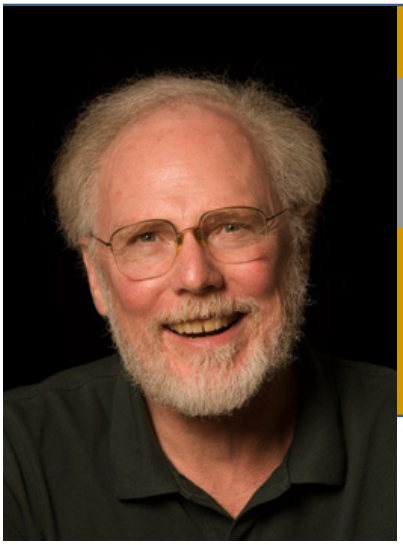

2016-17

Joseph O. Hirschfelder Lectures in Theoretical Chemistry

Professor J. Andrew McCammon
University of California – San Diego

Computer-aided Drug Discovery

Monday, September 26 2:00 p.m. Room 1315 Chemistry

This lecture will provide a general introduction to some of the ways that modern theoretical and computational chemistry are contributing to the discovery of new pharmaceuticals, with special emphasis on drugs for infectious diseases. The basic sciences and computing technologies involved have advanced to the point that physics-based simulations of drug targets are now yielding truly valuable suggestions for new compounds.

Biomolecular Thermodynamics

Tuesday, September 27 11:00 a.m. Room 1315 Chemistry

The selective character of molecular binding is critical for much of biology and chemistry. Computer simulations that yield free energies can be used quantitatively to interpret the selectivity of much molecular behavior. After a brief review of the use of thermodynamic perturbation methods, recent advances in enhanced simulation methods will be described, including both explicit and implicit solvent models.

Biomolecular Kinetics

Wednesday, September 28 2:00 p.m. Room 1315 Chemistry

The rates of a surprising number of biomolecular processes are diffusion controlled. Brownian dynamics simulations that treat the reactants explicitly allow calculation of the rates of many such processes, allowing for treatment of intermolecular interactions and other details. Simulations in which the some of the reactants are treated by continuum models are also helpful, and hybridization of the two approaches is a promising new area of work.