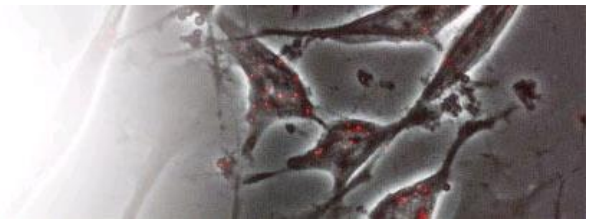
UCLA Engineering

Chemical and Biomolecular Engineering



SEMINARS IN CHEMICAL AND BIOMOLECULAR ENGINEERING

Thursday, May 23, 2019
10:00am - 11:00am
Boelter Hall 5436

Jonathan Whitmer

Assistant Professor
Chemical and Biomolecular Engineering
University of Notre Dame

"Probing the Assembly and Properties of Soft Materials with Advanced Sampling"

Soft Materials, encompassing (but not limited to) polymers, colloids, and liquid crystals are fascinating systems where molecular interactions often conspire to create new phases and emergent properties. Free energies provide essential information about the properties and structure of these materials, but calculations can be onerous, as the systems can be complex, and useful analytical expressions may not be present. Computations may elucidate these features but can be challenging, particularly if the associated landscape exhibits large, rapidly varying features and many competing metastable minima. In this seminar, I will discuss my group's work in developing and extending a set of molecular simulation techniques that are useful for extracting phase behavior and material properties. In particular, I will discuss our applications of these advanced sampling techniques to probe fundamental elastic properties of model liquid crystal systems, to elucidate the charging and complexation behavior of weak polyelectrolytes, and to examine more general physico-chemical equilibria in colloidal and macromolecular systems.

Jonathan K. (Jon) Whitmer is an Assistant Professor in the Department of Chemical and Biomolecular Engineering at the University of Notre Dame. Jon holds MS and Ph.D. degrees in Physics from the University of Illinois at Urbana-Champaign (where he worked in the group of Erik Luijten [now at Northwestern Universty]) and undergraduate degrees in Mathematics and Physics from Kansas State University. Before Notre Dame, he was a postdoctoral scientist in the Department of Chemical and Biological Engineering at the University of Wisconsin and later in the Institute for Molecular Engineering at Argonne National Laboratory and the University of Chicago working in the group of Juan de Pablo on simulations of colloids, polymers, liquid crystals, and biomolecules. Professor Whitmer's work specializes in the use of molecular simulations, particularly coarse-graining and free energy mapping techniques, to compute phase behavior and material properties of a diverse array of soft materials systems. Recent work has involved charge separation membranes, polyelectrolyte complexation, liquid crystal response and the development of free energy simulation methods. His group is also actively developing the broad-purpose molecular simulation software SSAGES (Software Suite for Advanced Generalized Ensemble Simulations), which augments standard molecular dynamics simulations with free energy and reactive path calculations, and is available for download at http://github.com/miccom/SSAGES-public.