“Modeling the Structure and Properties of Soft Materials”

Wednesday
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3:00 pm
Wu and Chen Auditorium
Levine Hall

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Abstract
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 challenging, 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 a set of molecular simulation techniques, which are useful for extracting phase behavior and material properties. In particular, I will discuss a powerful new algorithm we have developed which enables fast, on-the-fly free energy computations, and how we have applied molecular simulation techniques to the study of liquid crystalline materials and weak polyelectrolyte systems.

Bio
Jonathan (Jon) K. Whitmer is an Assistant Professor in the Department of Chemical and Biomolecular Engineering at the University of Notre Dame. Jon holds MS and PhD degrees in Physics from the University of Illinois at Urbana-Champaign, and undergraduate degrees in Mathematics and Physics from Kansas State University. Prior to 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 *of* Molecular Engineering at Argonne National Laboratory, as well as the University of Chicago, working in the group of Juan de Pablo on simulations colloids, polymers, liquid crystals and biomolecules. This followed graduate work in the group of Erik Luijten. 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 (**S**oftware **S**uite for **A**dvanced **G**eneralized **E**nsemble **S**imulations), which augments standard molecular dynamics simulations with free energy and reactive path calculations.

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