



UNIVERSITY OF MINNESOTA
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Department of Chemistry

Seminar

9:45 a.m. Thursday, November 6, 2014 • 331 Smith Hall

Associate Professor

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University of Oregon



Thermodynamic Consistency and Other Challenges in Coarse-Graining Models

Research interests: the structure and dynamics of complex fluids, with the goal of developing novel theoretical (statistical mechanics) approaches to describing the structure and dynamics of complex (macromolecular) systems, while including the underlying molecular details.

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Abstract

Structural and dynamical properties of macromolecular liquids, melts and mixtures, bridge an extensive range of length- and time-scales. For these systems, the computational limitations of the atomistic description prevent the study of the properties of interest and coarse-grained models remain the only viable approach. In coarse-grained models, structural and thermodynamic consistency across multiple length scales is essential for the predictive role of multi-scale modeling and molecular dynamic simulations that use mesoscale descriptions. This talk presents a coarse-graining approach that conserves structural and thermodynamic quantities independent of the extent of coarse-graining, and describes a model for the reconstruction of the dynamics measured in mesoscale simulations of the coarse-grained system. Some of the general challenges of preserving structural and thermodynamic consistency in coarse-grained models are discussed together with the conditions by which the problem is lessened.

Host: Professor Ilja Siepmann

Refreshments will be served prior to the seminar.