

Theory and Simulation of Biomolecular Systems: The Multiscale Challenge

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Abstract:

A multiscale theoretical and computational methodology will be discussed for studying biomolecular systems across multiple length and time scales. The approach provides a systematic connection between all-atom molecular dynamics, coarse-grained modeling, and mesoscopic phenomena. At the heart of the approach is a method for deriving coarse-grained models from protein structures and their underlying molecular-scale interactions. This particular aspect of the work has strong connections to the theory of renormalization, but it is more broadly developed and implemented for heterogeneous biomolecular systems. A critical component of the methodology is also its connection to experimental structural data such as cryo-EM or x-ray, thus making it “hybrid” in its character. Applications of our multiscale simulation approach to elaborate key features of complex processes such as protein-mediated membrane remodeling and the HIV virus capsid assembly will be presented as time allows.

Thursday, September 10th, 2015, 11:15

Seminar Room 227, PH II