Physical Chemistry Seminar

Tuesday, January 21, 2014 | **11:00 am** | **Room 1315 Chemistry Building**

Theory and Simulation of Biomolecular Systems: Surmounting the Challenge of Bridging the Scales

Professor Gregory A. Voth

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Host: Professor Jim Skinner

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. Important applications of the multiscale approach to study key features of large multi-protein complexes such as the HIV-1 virus capsid, actin filaments, and protein-mediated membrane remodeling will be presented as time allows.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8335