Physics Colloquium

Thursday, MARCH 21, 2019
At 4:10PM
in LL 316
Refreshments at 3:45PM

"Overcoming the Multiscale Challenge for Biomolecular Systems"

BY

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A multiscale theoretical and computational methodology will be discussed that can successfully describe biomolecular systems across multiple length and time scales. The overall 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, the actin-based cytoskeleton, and protein-mediated membrane remodeling will be presented as time allows.

Gregory A. Voth *is the Haig P. Papazian Distinguished Service Professor of Chemistry at the University of Chicago. He is also a Professor of the James Franck Institute and the Institute for Biophysical Dynamics. He received a Ph.D. in Theoretical Chemistry from the California Institute of Technology in 1987 and was an IBM Postdoctoral Fellow at the University of California, Berkeley from 1987-89. He is the author or co-author of more 500 peer-reviewed scientific articles that have been cited more than 38,000 times with a current h-index of 99. Voth is a Fellow of the American Chemical Society, American Physical Society, The Biophysical Society, and the American Association for the Advancement of Science. He has received a number of awards and other forms of recognition for his work, including most recently Joel Henry Hildebrand Award Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids from the American Chemical Society, the ACS Division of Physical Chemistry Award in Theoretical Chemistry, and Election to the International Academy of Quantum Molecular Science. He has mentored more than 175 postdoctoral fellows and graduate students. Professor Voth is a leader in the development and application of theoretical and computational methods to study problems involving the structure and dynamics of complex condense phase systems, including proteins, membranes, liquids, and materials.*