Theoretical Chemistry Lecture Series Presents

Michael Feig

Michigan State University

Insights into the Structure and Dynamics of Biomolecules in Cellular Environments from Computer Simulations

Biological macromolecules such as proteins and nucleic acids have become well-understood at the single molecule level but it is much less clear how the structure-dynamics-function paradigms established largely under dilute and homogeneous conditions hold up under realistic biological conditions where crowding, heterogeneity, and the presence of a diverse set of metabolites are important factors. Using computational approaches, we are exploring model systems of dense crowded systems ranging from simple spherical crowder models to concentrated protein solutions and a comprehensive model of a bacterial cytoplasm with all of the key components present in full atomistic detail. Simulations of these systems show altered dynamic properties, suggest the possibility of protein native state destabilization due to protein-protein and protein-metabolite interactions, altered solvent and metabolite behavior, and non-specific interactions between functionally related enzymes as a result of crowding. Some of the work described involves very large scale computer simulations that were enabled by methodological advances that will also be briefly discussed.

Wednesday, November 30, 2016
4:15-6:15PM at MIT (4-163)