

Exploring the Relationship Between the Structure, Function, and Dynamics of Biomolecular Complexes

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Biological macromolecules such as proteins, DNAs, and lipids, perform diverse functions in the cell that are the foundations of life processes. These complex mechanisms are a result of finely balanced thermodynamic forces governing both inter- and intramolecular interactions, as well as kinetic processes that occur over a vast range of time and length scales. Understanding the fundamental driving forces of biomolecular functions, and how they can be altered to tune cellular mechanisms, is therefore a central problem in modern biophysics research. In this talk, I will discuss work in our group that utilizes molecular dynamics simulations to explore these processes at atomic-scale resolution. First, I will focus on simulations aimed at understanding the physical mechanisms underpinning gene expression and epigenetic regulation, with a particular emphasis on post-translational

modifications of histone tails and the mechanisms of linker histones. Second, I will discuss how we can use enhanced sampling simulations in conjunction with small angle X-ray scattering experiments and Bayesian inference to rigorously determine a minimal ensemble of states of flexible biomolecular complexes in solution.

Date: Wed, Jan. 16, 2019

Time: 4:30-5:30 pm

Location: 208 Clark Hall

Students, meet the speaker over coffee and cookies in the Bennett Conference room at 3:30 pm