

# *COLLOQUIUM*

**Department of Physics, Temple University**

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

**Jeff Wereszczynski  
(IIT).**

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 mechanisms by which DNA is packaged and maintained in eukaryotic cells. In particular, I will discuss how protein modifications and “linker histone” binding affects the structure, dynamics, and energetics of the nucleosome and higher-order chromatin structures. 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.

**Monday, April 2, 2018 at 3:00 pm  
SERC, Room 116  
Refreshments will be served at 2:45 pm**