FALL 2021 CHEMISTRY SEMINAR SERIES

DR. GLEN HOCKY

Department of Chemistry

New York University
New York, NY

HOST: DR. KINZ-THOMPSON

ALL THOSE INTERESTED ARE WELCOME TO ATTEND

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Department of Chemistry
73 Warren Street, Olson Hall
Newark, New Jersey
https://sasn.rutgers.edu/chemistry

"What can I get for one piconewton? How biological molecules respond to thermal scale mechanical forces"

Friday, November 5, 2021, 11:30 AM
Life Science Center II, Room 130

Biographical sketch: I am currently an Assistant Professor in the Department of Chemistry at New York University, as part of the NYU Theoretical Chemistry Group. My research interests broadly involve using (and developing new) techniques from statistical mechanics and computational modeling to better understand how molecular interactions give rise to large scale collective phenomena. My research interests lie at the intersection between chemistry, physics, biology, and materials science. Prior to NYU, I was a postdoctoral fellow in the James Franck Institute at the University of Chicago and a Graduate Student in Chemical Physics at Columbia University. As a postdoc, I mainly used theory and simulation to study proteins that regulate the mechanics and dynamical features of the actin cytoskeleton. During my Ph.D., I used model glass-forming liquids to study the structural origin of dynamical arrest in supercooled liquids.

Abstract: A major goal of our research is to predict the response of biomolecules to the small, thermal scale, mechanical forces they experience within cells. Active processes in biological systems such as the motion of molecular motors produce piconewton-scale mechanical forces on supramolecular assemblies, and many proteins have evolved to sense and respond to these forces. Yet these forces are very small, and we would not expect them to have a large effect on a protein's conformation or conformational ensemble. Hence, robustly predicting the response of these mechanosensors at the molecular level is a challenge. I will present our efforts to develop enhanced sampling protocols that can allow us to make testable predictions about molecular mechanosensing mechanisms. Our efforts are broadly divided into two areas: predicting the change in conformational ensemble at constant force at equilibrium, and predicting the dissociation rate of protein-protein complexes under force. I will present the challenges and successes we've encountered in our methodological work on test systems as well as application to real mechanosensing proteins.