

INTERDISCIPLINARY PHYSICS

SATE

December 2nd 2016, 1400 Biomedical Physical Sciences, 11:30 a.m.

Exploring Free Energy and Fitness Landscapes of Proteins for Molecular Recognition, Binding, and Allostery

Ronald M. Levy

Center for Biophysics and Computational Biology and Department of Chemistry, Temple University

My talk will review work in my lab over the last several years concerning the construction and analysis of free energy and fitness landscapes for protein-ligand binding and allosteric conformational transitions. Approaches based on molecular dynamics free energy simulations as well as those based on the construction of Potts models of sequence co-variation will be described. I will review some of the technical challenges involved in the construction of free energy landscapes and the development of computational tools to overcome these challenges, including stochastic methods for solving the WHAM equations. I will also describe some very recent work underway on the role of interfacial water in molecular recognition. Examples will be chosen from: host-guest model systems, HIV-1 proteins, and Kinase family proteins.

Email: ronlevy@temple.edu