

Center for Soft Matter and Biological Physics
Seminar

Prof. David Leitner

(University of Nevada, Reno)

“Watching energy transport in proteins: Identifying dynamics networks and thermodynamic properties”

Monday, October 8, 2018

4:00pm – 5:00pm

304 Robeson Hall

Energy transport in a protein mediates protein function and represents the early events following a reaction or photoexcitation. New time-resolved measurements, and a variety of computational and theoretical methods allow us to map out and describe energy transport in great detail. I will describe some of our theoretical and computational work on the nature of energy transport in proteins, with focus on what we can learn about protein dynamics and thermodynamics by watching energy flow in proteins. By coarse graining energy transport dynamics from the all-atom to residue level, we have identified a relation between conformational dynamics at equilibrium and rates of energy transfer across non-bonded contacts. Measurements of rates of energy transfer thus provide a window into equilibrium dynamics of proteins and entropy associated with the dynamics of the contact.