

**SMS Spring 2021 Seminar Series**  
**Friday April 23 | 1:30pm | ZOOM\***

**Energy transport in biomolecules:  
Identifying dynamic networks and thermodynamic properties**

Energy transport in biomolecules contributes to function in a number of ways, including thermal regulation and chemical reaction dynamics. I will discuss some of our theoretical and computational work examining the influence of structure and structural dynamics on thermal flow and networks for vibrational energy transport in biomolecules. Thermal transport in systems of biomolecules helps regulate the temperature of the cell and involves an interplay between structure and anharmonic dynamics. Chemical reaction dynamics involves vibrational dynamics and relaxation, and I will also discuss the role of structure and structural dynamics on these processes. 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-covalent contacts. Measurements of rates of energy transfer thus provide a window into equilibrium dynamics of biomolecules and entropy associated with the dynamics of the contact.

**David Leitner, PhD**

*Professor, University of Nevada*

David Leitner is Reynold C. Fuson Professor of Chemistry at the University of Nevada, Reno. His current research interests include theoretical and computational studies of energy flow in molecules, particularly in biological systems, and its influence on chemical reaction kinetics and thermal transport. Other research interests include theoretical approaches to address thermal conduction in nanoscale systems, and computational studies of terahertz spectroscopy and dynamics of solvated biomolecules. He carried out undergraduate studies in Chemical Engineering and Chemistry at Cornell University and received his Ph.D. in Chemical Physics at the University of Chicago working with R. S. Berry. He was an NSF Postdoctoral Fellow at the University of Heidelberg, Germany, where he worked with Lorenz Cederbaum, and research associate at the University of Illinois at Urbana-Champaign, where he worked with Peter Wolynes. He joined the Chemistry Department at UNR in 2000.

