



DEPARTMENT OF CHEMISTRY AND CHEMICAL BIOLOGY COLLOQUIUM

Presented by Professor Eric R. Bittner, University of Houston

Friday, April 5th, 2019, at 4:00pm in the Science and Math Learning Center, Room 102

Finding the Vibrations That Matter: Defining the Electron Transfer Coordinate in High-Dimensional Systems



Electron transfer between molecular donor and acceptor species is a fundamental mechanism for a wide range of chemical processes including photosynthesis, respiration, and detoxification. The cornerstone theory for this is from Marcus which gives the transfer rate between two redox centers in terms of the driving force, reorganization energy, and non-adiabatic

coupling. Lost in this description is a clear indication of specific nuclear motions that accompany the process. In my talk, I shall discuss an approach we have developed using a search algorithm to find the optimal combinations of nuclear normal modes that drive and couple intramolecular electronic transitions. I shall discuss our theoretical advances in light of experiments by Weinstein's group in Sheffield that probe energy transfer in Pt bridged donor/acceptor complexes.

