Charge and energy transfer in a complex environment: The Marcus picture and its breakdown

Seminar

Wednesday, November 13, 2024

2:00 – 3:00 p.m.

Beaupre Center, Room 105

Electron transfer and electronic excitation transfer are ubiquitous processes in nature, underlying photosynthetic light harvesting, bioluminescence, and other instances of energy transfer in molecular systems. Successfully modeling charge or energy excitation transfer across a range of conditions demands consideration of nonadiabatic effects. When a complex environment effectively gates electron transfer, the coupling of nuclear and electronic degrees of freedom inverts the assumptions of the Born-Oppenheimer approximation. Marcus theory has been tremendously successful both in shaping our intuition around charge and energy transfer and quantitatively predicting the rates of such events. However, there are questions about nature of the reaction coordinate, the validity of the Condon approximation, and how to think about charge transfer in non-equilibrium contexts. Combining techniques from electronic structure, dynamics, and statistical mechanics, we investigate several prototypical systems, and begin to answer the above questions while providing solutions for when Marcus theory breaks down.

D. Vale Cofer-Shabica
Department of Chemistry
Princeton University

THE UNIVERSITY OF RHODE ISLAND

Department of Chemistry

Fall 2024 Seminar Series

Host: **Dugan Hayes**
Associate Professor
dugan@uri.edu
401-874-5516 (office)
617-785-4633 (mobile)