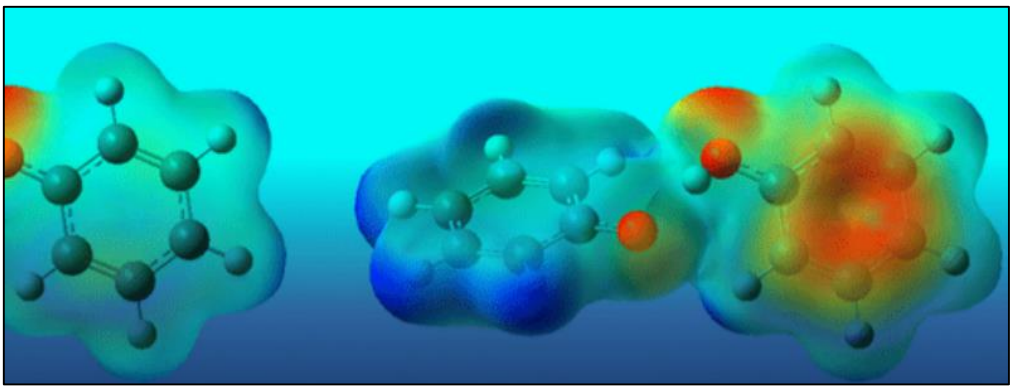

Proton-Coupled Electron Transfer in Catalysis and Energy Conversion

Proton-coupled electron transfer (PCET) reactions play a vital role in a wide range of chemical and biological processes. This talk will focus on recent advances in the theory of PCET and applications to catalysis and energy conversion. The quantum mechanical effects of the active electrons and transferring proton, as well as the motions of the proton donor-acceptor mode and solvent or protein environment, are included in a general theoretical formulation. This formulation enables the calculation of rate constants and kinetic isotope effects for comparison to experiment. Recent extensions enable the study of heterogeneous as well as homogeneous interfacial PCET processes. Applications to PCET in molecular electrocatalysts for water splitting, proton wires, photoreduced zinc-oxide nanocrystals, and proton discharge on a gold electrode will be discussed. In addition, recent developments of theoretical approaches for simulating the ultrafast dynamics of photoinduced PCET, along with applications to photoreceptor proteins, will be discussed. Overall, these studies have identified the thermodynamically and kinetically favorable mechanisms, as well as the roles of proton relays, excited vibronic states, hydrogen tunneling, reorganization, electrostatics, and conformational motions. The resulting insights are guiding the design of more effective catalysts and energy conversion devices.

DEPARTMENT SEMINAR

The Department of Chemistry and Biochemistry Presents

Sharon Hammes-Schiffer

John Gamble Kirkwood Professor of Chemistry,
Department of Chemistry,
Yale University

9 September
Zoom
4-5 PM (MST)