**Proton-Coupled Electron Transfer in Catalysis and Energy Conversion**

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Proton-coupled electron transfer (PCET) reactions play a vital role in a wide range of chemical and biological processes. This talk will summarize the main concepts from our PCET theory and will present applications to catalysis and energy conversion. Our general theoretical formulation for PCET includes the quantum mechanical effects of the electrons and transferring protons, as well as the motions of the donor-acceptor modes and solvent or protein environment. This PCET theory enables the calculation of rate constants and kinetic isotope effects for comparison to experiment and the study of nonequilibrium dynamics. Applications to PCET in enzymes, molecular electrocatalysts, proton wires, nanoparticles, heterogeneous electrochemical systems, and photoreceptor proteins will be discussed. These theoretical studies have identified the thermodynamically and kinetically favorable mechanisms, as well as the roles of hydrogen tunneling, excited vibronic states, reorganization, electrostatics, and conformational motions. The resulting insights are guiding the design of more effective catalysts and energy conversion devices.