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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 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 PCET processes. Applications to PCET in molecular electrocatalysts, proton wires, photoreduced zinc-oxide nanocrystals, and proton discharge on gold electrodes will be discussed. In addition, recent developments of theoretical approaches for simulating the ultrafast nonequilibrium dynamics of photoinduced PCET, along with applications to photoreceptor proteins, will be discussed. The recently developed nuclear-electronic orbital (NEO) method for treating electrons and protons on the same level allows nonequilibrium quantum dynamical simulations beyond the Born-Oppenheimer approximation. 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.