

FACULTY OF SCIENCE THE UNIVERSITY OF HONG KONG CIENCE 香港大學理學院

Department of Chemistry 香港大學化學系

HKU SCIENCE Distinguished Lectures

Electrochemical and Photochemical Proton-Coupled Electron Transfer

Professor Sharon Hammes-Schiffer

Sterling Professor of Chemistry, Yale University

Sharon Hammes-Schiffer received her BA from Princeton University and her PhD from Stanford University. She is currently the Sterling Professor of Chemistry at Yale University and will move to Princeton University in January 2024. She is a member of the American Academy of Arts and Sciences, the US National Academy of Sciences, and the International Academy of Quantum Molecular Science. She is currently the Editor-in-Chief of *Chemical Reviews* and is on the Board of Reviewing Editors for *Science* and the Editorial Board for *PNAS*.

Abstract

Proton-coupled electron transfer (PCET) reactions play a vital role in a wide range of chemical and biological processes. This talk will summarise the main concepts from the PCET theory developed by Professor Hammes-Schiffer's research team and will present applications to catalysis and energy conversion. The 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. This theory has been applied to PCET in enzymes, molecular electrocatalysts, proton wires, nanoparticles, heterogeneous electrochemical systems, and photoreceptor proteins. These theoretical studies have identified the thermodynamically and kinetically favorable mechanisms, as well as the roles of hydrogen tunneling, excited vibronic states, reorganisation, electrostatics, and conformational motions. The resulting insights are guiding the design of more effective catalysts and energy conversion devices.





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