

# PROTON-COUPLED ELECTRON TRANSFER FROM MOLECULES TO NANOMATERIALS

James M. Mayer, Benjamin Groff, Justin Lee, Noah Gibson, and Saeed Saeed

Department of Chemistry, Yale University, New Haven, United States

Many redox reactions of transition metal complexes, enzyme active sites, and material surfaces occur by proton-coupled electron transfer (PCET), reactions that can often also be described as hydrogen atom transfers [1]. The principles of PCET have been developed mostly with molecular systems, including the thermochemical and kinetic importance of the proton and electron. PCET is also a central reaction at solid/solution interfaces, from electrodes to colloidal nanoparticles, including metallic and semiconducting surfaces. Molecular PCET principles provide the foundation for understanding such interfacial reactions but additional complexities arise, such as free energies of reaction that are a function of the extent of surface coverage. After a short introduction with molecular reactivity, PCET reactions of iridium dioxide and tungsten trioxide nanoparticles will be presented and analyzed. The presentation will show that Coordination Chemistry approaches are highly applicable and valuable to the important area of interfacial chemistry.

---

[1] "Free Energies of Proton-Coupled Electron Transfer Reagents and Their Applications" Agarwal, R.G., Coste, S.C., Groff, B.D., Heuer, A.M., Noh, H., Parada, G.A., Wise, C.F., Nichols, E.M., Warren, J.J., and Mayer, J.M. *Chem. Rev.* **2022**, *122*, 1-49

[2] "Colloidal Hexagonal Tungsten Oxide Nanorods: Synthesis, Characterization, and Proton-Coupled Electron Transfer" Gibson, N.J., Parada, G.A., Mercado, B.Q., and Mayer, J.M. *Inorg. Chem.* **2026**, *65*, 2659-2668.