COMPUTATIONAL CHEMISTRY BI-WEEKLY SEMINAR SERIES

TOPIC: Catalyzed Reduction of Carbon Dioxide to Methanol in 3 Hydride/Proton Transfer Steps

SPEAKER: Prof. James T. Hynes
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TIME: 10:30-11:30, May 11, 2015

VENUE: Room 152, Geography Building, 3663 Zhongshan Road North, Shanghai (中山北路校区，地理楼 152 室)

ABSTRACT OF THE TALK

Conversion of carbon dioxide to fuels enabling a closed-carbon cycle powered by recyclable energy has the potential to dramatically impact the energy and environmental fields, and accordingly has received very considerable experimental and theoretical attention. In this talk, we will describe quantum chemical calculations---ultimately inspired by the Bocarsly group’s experimental discovery of the efficient catalytic reduction of CO2 to CH3OH by pyridine---to discover a (largely) homogeneous pathway for this reaction in aqueous solution. This pathway involves the production of the hydride donor 1,2-dihydropyridine PyH2, a 2H+/2e- transfer product of pyridine (Py), which acts as a powerful recyclable organo-hydride that reduces CO2 to CH3OH via three hydride and proton transfer (HTPT) steps. The molecular level coupled (or uncoupled) character of these steps, as well as the driving force for them, will be discussed.

BIOGRAPHY

Prof. Hynes received his Ph.D. from Princeton University and was an NIH Postdoctoral Fellow at MIT. His research interests include the theory of dynamics of chemical reactions and related solvation, vibrational and reorientational dynamics in solution, at atmospheric and other interfaces, in enzymes and other biomolecules, and in catalysis related to solar energy. Among other awards and honors, Prof. Hynes has held Sloan and Guggenheim Fellowships, is a Fellow of the American Chemical and the American Physical Societies, an ISI Highly Cited Researcher, and has received the Hirschfelder Prize in Theoretical Chemistry and the ACS Hildebrand Award. He is a member of the American Academy of Arts and Sciences and the National Academy of Science.