Tata Institute of Fundamental Research
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Seminar

Homogeneous and Interfacial Proton Coupled Electron Transfer and Charge Transfer Reactions

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Proton coupled electron transfer (PCET) reactions are integral part of several catalytic processes that are crucial for energy storage, fuel cell research and several biological processes. On the other hand, excited state charge transfer reactions are at the heart of many photoinduced processes. In this presentation, I will discuss (i) computational investigations of role of PCET reaction in the mechanism of oxygen reduction reaction by a Co-salophen complex in the presence of p-hydroquinone as a co-catalyst, (ii) computational study of PCET reaction between ZnO nanocrystal and an organic radical (iii) new theoretical methods to calculate solvent reorganization energies for electron transfer and PCET reactions in electrochemical systems, and (iv) implementation of a novel method to incorporate nuclear quantum effects in charge transfer dynamics. In the first part of the talk we will see that my calculations along with substantial experimental studies provide ample evidence for reduction of dioxygen to a coordinated hydrogen peroxide intermediate, which is subsequently reduced to water. In the second part of the presentation I will show how to estimate rate constant for PCET between photoreduced ZnO nanocrystal and TEMPO. We will further explore the role of proton diffusion inside the ZnO nanocrystal coupled to PCET reaction at the surface to explain the experimental studies of reaction dynamics of the PCET reaction mentioned above at longer timescales. For reactions that involve a substantial redistribution of charge density in a polar environment, it is important to estimate the energy penalty involved in rearranging the solvent dipoles in order to estimate rate constant for the charge transfer process. In the third part of this talk I will describe a new method for calculating this important parameter, solvent reorganization energy, in the context of electrochemical electron transfer and PCET reactions. In the final part of this talk I will introduce my ongoing research on incorporating nuclear quantum effects in charge transfer dynamics within the framework of ring polymer surface hopping algorithm.

Tuesday, Feb 6th 2018

04:00 PM (Tea/Coffee at 03:30 PM)

Seminar Hall, TIFR-H