

Colloquium

Homogeneous and Interfacial Proton Coupled Electron Transfer Reactions

Soumya Ghosh

University College London, UK

Proton coupled electron transfer (PCET) reactions are integral part of several catalytic processes, e.g. reduction of dioxygen to water, oxidation of water to dioxygen, carbon dioxide reduction, reduction of dinitrogen to ammonia, that are crucial for energy storage, fuel cell research and several biological 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. 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. The role of p-hydroquinone as electron proton transfer mediator is explored in details. 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.

Monday, Feb 5th 2018

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

Auditorium, TIFR-H