Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Internal Webinar

Computational Modelling of Molecular Electrocatalysts for Hydrogen Production using Transition metal based Polypyridyl ligands

Murugesan Pannerselvam

Loyola College, Chennai

To battle-out the consequences of having obliviously exploited non-renewable resources for over a century now and deal with the exponentially increasing energy demand, environmentally benign production of hydrogen fuels by molecular electrocatalysts under transition metal based Polypyridyl complexes have emerged as a propitious choice. The state-of-the-art DFT methods were used to study the hydrogen evolution reaction (HER) mechanism by pentapyridyl and bipyridyl based transition metal complexes (Co, Fe, Ni, Rh and Ir) using transition state modelling. The energetics of hydrogen evolution is further studied by calculating the respective reduction potential and pKa values. The present study is aiming to shed light on the proper chemical insights on understanding their reaction mechanism, catalytic activity and efficiency of the HER catalysts through potential energy surface modelling. Overall my doctoral studies provide a brief outline about the hydrogen production activity of available transition metal molecular electrocatalysts, highlighting the necessity of developing novel molecular electrocatalysts and pinpoint the importance of understanding their mechanistic aspects through quantum chemical calculations.

References:

1. Panneerselvam,M.; Jaccob, M. Inorg. Chem. 2018, 57, 8116–8127.
2. King, A. E.; Surendranath, Y.; Piro, N. A.; Bigi, J. P.; Long, J. R.; Chang, C. J. Chem. Sci. 2013, 4, 1578–1587.

Wednesday, Aug 11th 2021

3:00 PM