Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Colloquium

A Computational Roadmap for Energy Harvesting: Present and Next Generation

Sudip Chakraborty

Uppsala University, Sweden

In this colloquium talk, I would like to present my research activity interconnected with a common string "**Energy**". The fundamental mechanism of hydrogen and oxygen evolution in *photocatalytic materials*, from a theoretical perspective [1] would be explained. The Rational Design based on High-throughput Screening of *Hybrid Perovskite Solar Cells* [2, 3] would be highlighted next. I would conclude by describing our *developed interface* [4] *between Hybrid Eigen-vector Following formalism and DFT* for Transition Pathway prediction with the possible future implications [5, 6].

References:

1. C. Rupp, S. Chakraborty* *et al.*, ACS Appl. Mater. Interfaces, 8, 1536 (2016); *Chem. Mater.* 27, 4930 (2015).
2. S. Chakraborty* *et al.*, *ACS Energy Letters - Perspective,* 2, 837 (2017).
3. A. Banerjee, S. Chakraborty* *et al. J. Mater. Chem. A,* 5, 18561 (2017).
4. I. D. Seymour, S. Chakraborty *et al*, *Chem. Mater.* 27, 5550 (2015).
5. R. Araujo, S. Islam, S. Chakraborty* *et al., J. Mater. Chem. A*, 3, 18564 (2016).
6. W. Teeraphat, P. Barpanda, R. Ahuja, S. Chakraborty*, *J. Mater. Chem. A*, 5, 21726 (2017).

Tuesday, Jan 30th 2018

11:30 AM (Tea/Coffee at 11:00 AM)

Auditorium, TIFR-H