

# SEMINAR FOR PROFESSOR SUDIP CHAKRABORTY

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HOSTED BY PROFESSOR BABAK ANASORI



## Professor Sudip Chakraborty

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### ***“Computational Advancement of Sustainable Energy Materials: Connecting a Few Dots”***

**Abstract:** In this talk, I would like to present a three-fold research activity interconnected with a common string “Sustainable Energy”. I will start with a brief introduction of electronic structure calculations based on density functional theory (DFT) formalism and how it could be connected to the computational screening for achieving highly efficient energy materials. The first part would be dedicated to the fundamental mechanism for solar irradiated water splitting in photocatalytic materials. The relevant exploration of novel 2D materials and their applications in such catalytic mechanisms would be elaborated subsequently. The mechanism corresponding to HER and OER under the influence of doping and vacancy defect from DFT based theoretical perspective would be discussed along with our recent high throughput computational investigation of finding efficient HER catalytic materials. The next part would be devoted to the fundamentals and possible implications of Rashba phenomena in non-centrosymmetric structural materials and how it could govern the enhancement of catalytic efficiency, with a case-study of BiCIS Janus monolayer for HER activity. We have recently demonstrated the effect of strain on the overpotential of novel catalytic materials through the tuning of Rashba splitting under the influence of external strain. I will touch upon our extensive work on novel halide perovskites and the corresponding electronic and optical properties under the influence of hydrostatic pressure. I will end my talk with our recent successful endeavor of a pre-intercalation mechanism in Li-ion batteries, which could be further extended for next-generation energy storage materials.

**Biography:** Prof. Sudip Chakraborty is leading the Materials Theory for Energy Scavenging (MATES Lab) group in India’s premier theoretical research Institute, Harish-Chandra Research Institute (HRI) Allahabad (Prayagraj), Department of Atomic Energy, Govt. of India. After completing his Ph.D. at Bhabha Atomic Research Centre (BARC) and the University of Pune, India, he moved to Max Planck Institute for Sustainable Materials, Düsseldorf, Germany, in March 2011 as a Max Planck Postdoctoral Fellow. In February 2013, he joined the Materials Theory Division at Uppsala University, Sweden, as a Förskares (Senior Researcher). Since March 2019, he started leading his group firstly in the Department of Physics of IIT Indore and later on in HRI from May 2021 onwards. He has been awarded the Rising Stars by ACS Materials Au 2021, among 300+ nominations worldwide, while he is the sole recipient from India. He is on the Editorial Board of the Journal of Physical Chemistry A/B/C (ACS), Energy Advances (RSC), Electronic Structure (IOP), Chemistry of Inorganic Materials (Elsevier), and Graphene & 2D Materials (Springer). His works appear in Nature Materials, PNAS, Materials Today, ACS Energy Letters, JACS, ACS Nano, ACS Catalysis, AngewChemie, Advanced Materials, Advanced Functional Materials, Chemistry of Materials, J. Mater. Chem. A, etc. At present, he has 174 International publications with a total 6650 citations and 45 h-index.