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

Seminar

Energy Materials: Atomic-scale Insights from ab initio modelling

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On a global scale, clean energy generation and its efficient use are important aspects to meet rising energy demands with sustainability. However, complex and interdependent structure-property-performance relations strongly limit the directed search and discovery of efficient materials for targeted energy applications. To tackle these challenges, we apply cutting-edge computational simulations that are invaluable for understanding and manipulating the functionalities and performances of a wide range of energy materials. In this talk, first I will discuss the details of charge carrier dynamics and structural stability of metal halide perovskites that are leading contenders for next-generation optoelectronic devices. Using non-adiabatic molecular dynamics, I will illustrate the complex influences of dynamic structures on the excited-state carrier dynamics that strongly impact the optoelectronic performances of these materials. Following that, my talk will focus on defect formations and their impact on the functional properties of materials. I will discuss our findings on the substantial influences of surface defects on the optoelectronics of semiconductor materials. The defect-assisted ion migration and its suppression through compositional engineering will also be explored through examples. I will conclude the talk with the overview of our current effort to use data-driven approaches to accelerate the designing and optimisation of energy materials.

Tuesday, Jul 25th 2023

4:00 PM (Tea / Coffee 03.45 PM)

Auditorium, TIFR-H