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

Internal Seminar

Machine Learning and Density Functional Theory Assisted Design of Metal Halide Perovskite Solar Cell Materials for Sustainable Energy Solutions

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The rising global energy demand calls for innovative materials to drive sustainable and efficient solar technologies. My research focuses on the computational design of metal halide perovskites by integrating density functional theory (DFT) with machine learning (ML) techniques. Thereby, in the first project, I investigate lead-free double halide perovskites, combining high-level DFT calculations with ML models to predict accurate bandgaps, analyse key structure–property relationships, and perform band alignment for device viability. Moving forward to my second project, I have focused on Ruddlesden–Popper perovskites, where I employ ML-guided feature analysis and HOMO–LUMO alignment strategies to systematically tune organic spacer cations and enhance vertical charge transport. Additionally, the presentation includes findings from my PhD work on impurity-doped quantum dots, where we investigated noise-driven modifications of their electronic and optical properties under external fields. In conclusion, I aim to extend computational and ML techniques towards the development of efficient, scalable energy materials for real-world applications.

Friday, Jun 20th 2025

15:00 Hrs

CR-4, TIFRH