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

# Internal Seminar

## Computational Modelling of Nanomaterials for Energy Storage Applications

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The transition towards renewable energy resources has become essential as the rapid increase in population, exhaustion of fossil fuel reserves and global warming emphasizes the need for energy storage devices that are not only efficient and affordable but also environmentally safe. Addressing this challenge, our research focuses on computational modelling to design and evaluate novel materials for next-generation energy storage systems. In this context, we present density functional theory (DFT) investigations into advanced cathode and anode materials for metal-ion batteries, along with potential candidates for hydrogen storage. The first part of the talk highlights the electrochemical properties of bare and halogen-doped $X_{12}Y_{12}$ nanocages, and structurally tuned covalent organic frameworks (COFs) for sodium-ion battery applications. The second part explores the gravimetric capacity and structural properties of metal-decorated boron nanosheets ($B_n$; n = 3–14, 20), graphitic carbon nitride nanosheets, and perovskite-based systems for efficient hydrogen storage. The key aspects of some of these findings will be presented.

***Thursday, May 29th 2025***

***11:30 Hrs***

***CR-4, TIFRH***