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

Internal Webinar

Theoretical Design Principles for Enhanced Hydrogen Storage in Porous Materials Using Molecular Modelling and Monte Carlo Simulations

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My research employs density functional theory (DFT) and grand canonical Monte Carlo (GCMC) simulations to investigate hydrogen storage in metal-organic frameworks (MOFs) and covalent organic frameworks (COFs). Motivated by the U.S. Department of Energy (DOE) targets for practical H_2 storage in vehicles, the work focuses on designing porous materials with optimal binding enthalpies (7-20 kJ/mol) and high storage capacities under realistic conditions. DFT provides atomic-level insights into H_2-metal interactions, while GCMC predicts gravimetric and volumetric uptakes. The results reveal promising binding strengths and capacities that guide rational material design for sustainable energy applications.

Monday, Jan 12th 2026

11:30 Hrs