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

Seminar

Computational investigations of chemical shifts in core electron binding energies of organic molecules

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X-ray Photoelectron Spectroscopy (XPS) relies on state-based distinction of molecules through characteristic binding energies of core electrons. Theoretical validation of XPS requires *ab initio* simulation, but currently available methods are either computationally expensive or suffer from numerical instabilities, making it challenging to identify optimal approaches for theoretical prediction. We highlight current methods through systematic benchmarks and create robust, automated high-throughput workflows to generate a computational dataset. This data is used to train lightweight machine learning models that can predict XPS for small organic molecules, overcoming computational challenges faced by traditional methods. In the second part of the talk, we will discuss XPS of solvated molecules and evaluate the role of implicit and explicit solvent description.

Thursday, Jul 10th 2025

11:30 Hrs (Tea / Coffee 11:15 Hrs)

Auditorium, TIFRH