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

Internal Webinar

Mechanistic Understanding of turn-on Fluorescence and Structural Disorder-Dependent Raman Responses through First-Principles Simulations and Machine Learning

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In this presentation, I will present two research projects that employ first-principles simulations and machine learning to investigate structure–property relationships in molecular and materials systems. The first project focuses on elucidating the fluorescence turn-on mechanism of the boronic acid-based extracellular matrix imaging probe. Using density functional theory (DFT), ab initio molecular dynamics (AIMD), time-dependent DFT (TDDFT), and Franck–Condon/Franck–Condon–Herzberg–Teller (FC/FCHT) analyses, we have demonstrated that the probe predominantly exists in a single water-bound configuration under physiological conditions. The calculations reveal that fluorescence quenching arises from the combined effects of photo-induced electron transfer (PET) and non-radiative internal conversion, whereas sugar binding suppresses both pathways, leading to the experimentally observed fluorescence enhancement. The second project investigates the correlation between Raman responses and structural disorder in graphene oxide using an autoencoder-based machine learning framework. By learning latent representations of displacement-vector distributions associated with Raman-active normal modes, the model establishes quantitative relationships between microscopic structural disorder and Raman spectral features. Together, these studies illustrate the potential of combining first-principles simulations and machine learning to gain fundamental insights into complex structure–property relationships in molecular and materials systems.

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11:30 Hrs