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

Seminar

First-Principles Study of Fifth-Generation Light Emitters: Energy Levels and Molecular Design

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This talk is based on my doctoral thesis work on inverted singlet-triplet gap systems for next-generation organic light-emitting diodes (OLEDs). Fifth-generation OLEDs have recently attracted attention due to their ability to exhibit delayed fluorescence without thermal activation. This behavior is associated with a rare violation of Hund's rule leading to an inverted (negative) singlet-triplet energy gap. In this talk, I will present a systematic investigation of such systems, focusing on the interplay between computational methodology and structure-property relationships. I will show that small organic molecules do not exhibit genuine Hund's rule violations, and that widely used approaches such as DFT and double-hybrid DFT can yield false positives, whereas higher-level wavefunction-based methods predict the sign of the gap accurately. I also studied the choice of computational methods for both geometry optimization and excited-state calculations, aiming to balance accuracy with computational cost, and examined this in terms of the bias-variance tradeoff between different levels of theory. I will further demonstrate how molecular structure governs excited-state energetics, using azaphenalenes as a model system where symmetry lowering and geometric relaxation remove apparent inversions. Building on this, I explored larger chemical spaces and discovered new classes of molecules, including B,N-substituted non-planar systems, that genuinely show inverted gaps under stringent criteria. Through this work, I aim to highlight how careful choice of methods and a clear understanding of structure are both essential for identifying realistic candidates for next-generation OLED applications.

Monday, Jul 13th 2026

10:30 Hrs (Tea / Coffee 10:15 Hrs)

Auditorium, TIFRH