Multiscale Simulations for Organic Semiconductors in Optoelectronic Applications

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Organic semiconductors underpin a wide range of optoelectronic technologies, including organic light-emitting diodes (OLEDs), organic photovoltaics (OPVs), and photocatalysts. Realizing high device performance hinges on identifying materials with application-specific properties, yet conventional trial-and-error discovery is costly and slow. Predictive models that estimate key properties prior to synthesis and characterization can accelerate this process, and computer simulations offer a powerful route.

Early, molecule-centric screens based on quantum-mechanical methods—most commonly density-functional theory (DFT) in the gas phase—enable rapid estimation of frontier orbital energies and other descriptors and can be coupled to high-throughput workflows. However, such isolated-molecule calculations neglect solid-state packing and interfacial effects that critically govern optical excitations, charge transport, and reactivity. To close this gap, multiscale simulation protocols that integrate DFT, molecular dynamics, and kinetic Monte Carlo are needed to connect molecular structure to mesoscale morphology and device-level function.

In this talk, I will present high-throughput screening for rapid candidate identification and multiscale strategies that uncover structure–property–performance relationships in OLEDs, OPVs, and HER photocatalysts, highlighting opportunities and current limits in predictive materials discovery.