Prediction of Frontier Orbitals and Excitons in Conjugated Molecules for Organic Photovoltaics Using Computational Models

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Organic photovoltaics can offer environmentally and cost-friendly alternatives to inorganic photovoltaics due to their lightweight nature, flexibility, and low production cost. The active layer of organic photovoltaics blends electron acceptors and donor materials, comprising organic semiconducting small molecules and conjugated polymers. The optoelectronic properties of organic photovoltaics, including light absorption, exciton dissociation, intramolecular, and intermolecular charge transfer, depend on the energetics of the frontier molecular orbitals within the constituent organic molecules. The modularity in the molecular design of recently developed non-fullerene acceptors allows for a tunable molecular structure and has propelled the power conversion efficiency of organic photovoltaics to exceed 19%. A typical chemical design strategy for optimizing an organic semiconductor involves taking the conjugated aromatic units that form the molecular backbone and introducing systematic variations to isolate and study the effects of substituents on molecular orbitals. In this study, we propose a novel computational model based on the tight-binding approach. This model combines theoretical principles with simulations to compute the frontier orbitals and excitons within π-conjugated molecules, including non-fullerene acceptors. Our model contributes not only to the advancement of computational techniques for deducing structure-property relationships but also holds promise for enhancing the overall efficiency of organic photovoltaic devices through the rapid screening of thousands of candidate molecules, thereby shaping a more targeted experimental synthesis approach.