Development of π-Conjugated Organic Materials for Optoelectronic Applications: Computational and Experimental Insights

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Abstract:

Conjugated organic materials are widely used in optoelectronic devices because of their tunable electronic properties and solution processability. In this work we study a series of conjugated oligomers and polymers for applications in dye-sensitized solar cells (DSSCs) and bulk heterojunction (BHJ) solar cells [1].

The materials are synthesized by organometallic coupling methods, which afford precise control over molecular structure and conjugation length. Their optoelectronic properties are studied using quantum chemical approaches, mainly Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT) to predict HOMO–LUMO energy levels, absorption spectra, and charge-transfer properties [2–3].

An oligomeric model is used to describe the behavior of polymers and to obtain structure-property relationships. We study the energy level alignment and the electron injection processes for DSSC applications and the donor-acceptor interactions and the exciton dissociation for BHJ systems [4].

These results underscore the fundamental importance of quantum chemical modeling for the prediction and optimization of pi-conjugated materials and support the rational design of efficient organic optoelectronic devices.