Tailoring Electronic Structure and Charge Transport properties for Efficient Third Generation Solar Cells

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Abstract:

Third-generation solar cells, particularly organic solar cells (OSCs), have garnered significant interest due to their lightweight, flexible, and cost-effective nature, along with their compatibility with solution-based fabrication techniques. This study explores five newly designed small molecule-based donors (SMDs) characterized by an A–D–A structure: CTPT, CTPS, CTQTD, CTQT, and CTQDT. Utilizing density functional theory (DFT) simulations, we investigate the electronic and charge-transport properties, absorption profiles, stability, and energy loss characteristics of these engineered SMDs in comparison to a reference SMD, PCz(DPP)2. Our findings reveal that the new SMDs exhibit low bandgaps (1.73 to 2.25 eV), reduced energy losses (0.24 to 0.81 eV), and enhanced light-harvesting efficiencies (0.0450 to 0.8095), with significant absorption extending into the near-infrared region. The engineered SMDs also demonstrate superior solubility and lower exciton binding energies, alongside comparable stability to the reference SMD. Detailed analyses indicate effective electron transfer, reduced recombination losses, and enhanced charge transport properties, with hole hopping rates ranging from 3.023×10^{13} to 7.172×10^{14} s^{-1}. These promising results suggest that these tailored SMDs could substantially improve the efficiency and performance of OSCs, paving the way for advancements in solar energy technology.

Keywords:

Small molecule-based donors; Bi-functional acceptors; Organic solar cells; DFT and TD-DFT calculations.