Quantum Chemical Design of Near-Infrared Sensitive Fused Ring Electron Acceptors Containing Selenopheneas π-bridge for High-Performance Organic Solar Cells

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Abstract

End-capped acceptor modification of fused-ring electron acceptors (FREAs) is an attractive strategy to boost the optoelectronic and photovoltaic properties of the materials. FREAsare proved beneficial due to their tremendous applications in organic solar cells (OSCs). Among fused-ring electronic species, small fullerene-free FREAs have already been drawn more attention due to their near-infrared sensitivity and constantly increasing efficiencies. Therefore, we have designed six new FREAs (K1-K6) having selenophene as π-bridge in between the central alkylated indaceno[1,2-b:5,6b]dithiophene (IDT) unit after the incorporations of various end-capped acceptors on to the recently synthesized IDT2SeC2C4-4F molecule. Structural-property relationship, photophysical and photovoltaic properties of newly designed molecules are studied with the help of density functional theory (DFT) and time-dependent-density functional theory (TD-DFT). Certain critical specifications like frontier molecular orbital (FMOs) alignment, the density of states (DOS), absorption maxima, excitation energy, binding energy (B.E) along with transition density matrix (TDM), and the specifically estimated re-organizational energy values of electron and hole and the open circuit voltages of newly designed molecules are computed and compared with reference molecule. Generally, a red-shifting absorption behavior of FREAs is considered the most important reason for their high efficiencies in OSCs. Our novel designed molecules exhibit redshift in the absorption spectrum. Similarly, low excitation and binding energies of designed molecules offer improved power conversion efficiencies (PCE) with the highest possible charge photo-current density (Jsc) in OSCs devices. Furthermore, the study of the PTB7-Th/K1 complex is also done in order to examine charge transfer between within complex. By introducing the efficient end-capped acceptor moieties in reference molecule, enhancement in charge mobilities is noted. The large open-circuit voltage, low reorganizational energies, narrower HOMO-LUMO energy gap, lower binding and excitation energies, and highly red-shifting in absorption phenomenon indicates an efficient designing of molecules that could be best fitted for high-efficiency OSCs. Finally, theorized molecules are much superior related to their photovoltaic and electronic properties and thus are recommended to experimentalists for their synthesis and out-looking future developments of highly efficient solar cell devices.

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