Theoretical designing of novel quad-rotor-shaped non-fullerene acceptor materials with proficient photovoltaic characteristics for organic solar cells

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Abstract

Small molecules non fullerene acceptors (NFAs) especially fused ring electrons accepters (FREAs) are the potential agents of revolution in organic photovoltaic devices. Fused ring core based organic solar cells (OSCs) have been revealed high power conversion efficiency; however, they still need further modification due to their low electron mobility. To make better FREAs with better electron mobility and enhanced optoelectronic properties, designing of accepter molecules through variation of end-capped units is considered a useful strategy now a day. Herein, an effort has been made to design and propose eight novel quad-rotor shaped fused ring core electron accepters (QRFR-1-QRFR-8) through modulating the four end-capped units of recently synthesized BFTT-TN molecule having quad–rotor structure., Employing DFT and TDDFT, optoelectronic properties of newly proposed accepter molecules have been determined through frontier molecular orbitals (FMO) analysis, density of states (DOS) analysis, transition density matrix (TDM), analysis of charge transfer and compared with reference molecule (BFTT-TN as QRFR).All the tailored molecules (QRFR-1-QRFR-8) disclose reduction in energy gap and intensive absorption near IR region than reference QRFR after end-capped engineering. The highest value of open circuit voltage (Voc) with respect to HOMOPM6–LUMOacceptor is found in QRFR-6 (1.66 V) than reference QRFR (1.63V) and comparable to reference QRFR in QRFR-8 molecule. Binding energies values of all designed molecules are found to be better and comparable with QRFR molecule. The reorganization energies of electron (λe) are found to be smaller than reference QRFR in all molecules except QRFR-5 molecule. The hole reorganization energies of QRFR-4, QRFR-8 QRFR-1, QRFR-2 are found to be less than QRFR. While λh of QRFR 6, QRFR-7, QRFR-3 and QRFR-5 are found to be higher than QRFR. The proposed quad-rotor shaped novel molecules have proficient hole and electron transfer mobilities and can serve as best candidate when blended with PM6 film. This study not only enlighten the researchers to use end-capped group modification as successful strategy for designing new quad-rotor shaped materials, but also provide novel materials to experimentalist for synthesis and their potential usage in future photovoltaic application of organic solar cell.

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