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Tuning the optoelectronic properties of selenophene-diketopyrrolopyrrole-based non-fullerene acceptor to obtain efficient organic solar cells through end-capped modification

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Abstract

With the goal of developing a high-performance organic solar cell, nine molecules of A_2-D-A_1-D-A_2 type are originated in the current investigation. The optoelectronic properties of all the proposed compounds are examined by employing the DFT approach and the B3LYP functional with a 6-31G (d, p) basis set. By substituting the terminal moieties of reference molecule with newly proposed acceptor groups, several optoelectronic and photovoltaic characteristics of OSCs have been studied, which are improved to a significant level when compared with reference molecule, i.e., absorption properties, excitation energy, exciton binding energy, band gap, oscillator strength, electrostatic potential, light-harvesting efficiency, transition density matrix, open-circuit voltage, fill factor, density of states and interaction coefficient. All the newly developed molecules (**P1–P9**) have improved λ_{max}, small band gap, high oscillator strengths, and low excitation energies compared to the reference molecule. Among all the studied compounds, **P9** possesses the least binding energy (0.24eV), **P8** has high interaction coefficient (0.70842), **P3** has improved electron mobility due to the least electron reorganization energy (λ_e=0.009182eV), and **P5** illustrates high light-harvesting efficiency (0.7180). **P8** and **P9** displayed better V_{oc} results (1.32eV and 1.33eV, respectively) and FF (0.9049 and 0.9055, respectively). Likewise, the phenomenon of charge transfer in the PTB7-Th/P1 blend seems to be a marvelous attempt to introduce them in organic photovoltaics. Consequently, the outcomes of these parameters demonstrate that adding new acceptors to reference molecule is substantial for the breakthrough development of organic solar cells (OSCs).