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End-capped engineering of Quinoxaline core-based non-fullerene acceptor materials with improved power conversion efficiency

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Abstract

Improving the light-harvesting efficiency and boosting open circuit voltage are crucial challenges for enhancing the efficiency of organic solar cells. This work introduces seven new molecules (SA1-SA7) to upgrade the optoelectronic and photovoltaic properties of Q-C-F molecule-based solar cells. All recently designed molecules have the same alkyl-substituted Quinoxaline core and CPDT donor but vary in the end-capped acceptor subunits. All the investigated molecules have revealed superior properties than the model (R) by having absorbance ranging from 681 nm to 782 nm in the gaseous medium while 726nm–861 nm in chloroform solvent, with the lowest band gap ranging from 1.91 to 2.19eV SA1 molecule demonstrated the highest λ_{max} (861 nm) in chloroform solvent and the lowest band gap (1.91 eV). SA2 molecule has manifested highest dipole moment (4.5089 D), lower exciton binding energy in gaseous (0.33eV) and chloroform solvent (0.47eV), and lower charge mobility of hole (0.0077693) and electron (0.0042470). At the same time, SA7 showed the highest open circuit voltage (1.56eV) and fill factor (0.9166) due to solid electron-pulling acceptor moieties. From these supportive outcomes, it is inferred that our computationally investigated molecules may be promising candidates to be used in advanced versions of OSCs in the upcoming period.