ABSTRACT

The field of organic photovoltaics (OPVs) has experienced a transformative shift with the ascendancy of non-fullerene acceptors (NFAs). These materials offer remarkable tunability in their electronic and optical properties, and have enabled the development of organic solar cells (OSCs) with power conversion efficiencies (PCEs) exceeding 21%. The emergence of non-fullerene acceptors (NFAs) has significantly advanced the field of organic solar cells (OSCs), driving power conversion efficiencies (PCEs) to record levels and paving the way for their potential application in real-world scenarios. The computational tools have developed as an indispensable technology in increasing the optimization and discovery of new materials. In this study, we have designed six no-fused electron acceptors for used in solar cells. The replacement of core and bridges in Y6 has been take place using Density Functional Theory (DFT). This modification results in efficient charge transfer and improve overall efficiency of acceptor materials. The created materials have bandgap in very precise range of 2 to 2.14 eV, which seems to be very efficient that they absorb near IR region and exhibit good mobility. The high Light-Harvesting Efficiency (LHE) of upto 1.00 indicates the high absorption wavelength. The analysis of all acceptor molecules provides valuable insights into structure property relations for the creation of next generation acceptor material used in organic photovoltaics.