Abstract

Conjugated materials have emerged as pivotal components in the evolution of next-generation photovoltaic technologies, offering viable, lightweight, and adaptable solutions to address sustainable energy challenges. Organic solar cells (OSCs) and perovskite solar cells (PSCs), in particular, hold immense promise for achieving enhanced energy conversion efficiencies, facilitated by meticulous materials design strategies. This study investigates rational design approaches of numerous series of conjugated materials, specifically designed to serve as acceptors in OSCs and as hole transport materials (HTMs) in PSCs.

Specifically, the design approach revolves around multidirectional fused-ring electron acceptors (FREAs), with benzotrithiophene and benzotripyrrole-based conjugated centers at their core, integrating a range of pi-bridging units and terminal acceptors. Employing quantum modeling techniques such as Density Functional Theory (DFT), the study thoroughly assesses the modulation of optoelectronic properties and photovoltaic performance by atomically fine-tuning the core, bridge, and acceptor units. The results demonstrate enhancements in conjugation, reductions in band gaps, expanded absorption profiles, improved carrier mobilities, and other device-relevant properties, especially when combined with the PM6 donor polymer in OSCs.

Moreover, the study extends to the synthesis of HTMs, incorporating fluorene and benzothiadiazole cores, flanked with indoloquinoxalines having varied electronegative atoms on their periphery. HTMs were successfully synthesized through multi-step organic synthesis, including palladium-catalyzed cross-coupling reactions, and meticulously characterized using spectroscopic techniques. The DFT and SCAPS-1D evaluation of HTMs suggests promising potential for application as HTLs in lead-free PSCs as a potential alternative to the pioneering HTMs.