

Effective design of benzoselenadiazole core D-A-A small molecule for bulk heterojunction organic solar cells via alkyl bithiophene and 3,5-bis(trifluoromethyl)benzene terminal unit

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A new asymmetric D-A-A type small organic chromophore named 4-(3,5-bis(trifluoromethyl)phenyl)-7-(5'-hexyl-[2,2'-bithiophen]-5-yl)benzo[c][1,2,5]selenadiazole (RT-BSe-F) based on central benzoselenadiazole (BSe) core was successfully synthesized by coupling reaction. Strong electron affinity of 3,5-bis(trifluoromethyl)benzene acceptor unit significantly tune the electrochemical features with aligned HOMO and LUMO energy level of -5.33 and -3.31 eV. Fluorination enables the fast charge transfer owing to high mobility of RT-BSe-F and tempts absorption and photoluminescence behavior thus permit the better spectral overlap with solar spectrum. Bulk heterojunction (BHJ) organic devices fabricated with RT-BSe-F:PC₆₀BM (1:2, w/w) achieved a high power conversion efficiency (PCE) of ~3.75% accredited to high J_{sc} of ~ 12.56 mA cm⁻², V_{oc} of ~0.71 V and FF of ~0.42.