Rational Design of Cyclopenta Dithiophene-bridged Hole Transport Materials for High Efficient and Stable Perovskite Solar Cells

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A series of small-molecule-based hole-transporting materials (HTMs) featuring a 4H-cyclopenta[2,1-b:3,4-b']dithiophene as the central core with triphenylamine- and carbazole-based side groups were synthesized and evaluated for efficient perovskite solar cells (PSCs) applications. The effect of the chemical structure of the HTMs and the photovoltaic performance were studied through investigation of the different combinations of the central π-bridge moieties. In this respect, the Photoluminescence, Time-Resolved Photoluminescence, energy level and hole mobility are systematically investigated, revealing the significantly influence of the central core planarity and packing structure on their photovoltaic performance. The optimized device based on CT3 exhibited a PCE (power conversion efficiency) of 16.97% with a device architecture of FTO/TiO\textsubscript{2}/CH\textsubscript{3}NH\textsubscript{3}PbI\textsubscript{3}/HTM/MoO\textsubscript{3}/Ag, which was found that cell fabricated based on state-of-the-art spiro-OMeTAD (17.50%) as HTM. Moreover, stability assessment showed a similar stability for CPDT-based HTMs as compared with spiro-OMeTAD over 1300 hours, indicating that the devices with CPDT-based HTMs have good long-term stability.