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Molecular Engineering of Conjugated Polymers for Efficient Hole Transport and Defect Passivation in Perovskite Solar Cells

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Organic-inorganic hybrid perovskite solar cells represent an exceptional candidate for next-generation photovoltaic technology. However, the presence of surface defects in perovskite crystals limits the performance as well as the stability of perovskite solar cells. We have employed a series of carbazole and benzothiadiazole (BT) based donor-acceptor copolymers, which have different lengths of alkoxy side-chains grafted on the BT unit, as the dopant-free hole transport materials (HTMs) for perovskite solar cells. We demonstrate that although these side-chains can reduce the π - π stacking structural order of these copolymers to affect the hole transport properties, the methoxy unit introduces a desired defect passivation effect. Compared to the Spiro-OMeTAD-based device, the copolymer with methoxy side-chains on the BT unit (namely PCDTBT1) as the HTM achieved superior power conversion efficiency and stability due to efficient hole transport and the suppression of trap-induced degradation, whilst the copolymer with octyloxy side-chains on the BT unit (namely PCDTBT8) as the HTM lead to poor performance and stability.

Graphical abstract:

A series of carbazole and benzothiadiazole (BT) based copolymers have been employed as the dopant-free hole transport materials (HTMs) for perovskite solar cells. The side-chains of these HTM can reduce the π - π stacking structural order but can also introduce desired defect passivation effect.

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