Dopant-free starlike molecular hole conductor with ordered packing for durable all-inorganic perovskite solar cells Advanced Energy Materials

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All-inorganic n-i-p perovskite solar cells (PSCs) using doped Spiro-OMeTAD as hole transport material (HTM) suffer from photothermal stability due to ionic diffusion and radical-induced degradation by the dopants. In this article, dopant-free starlike molecule (N2, N2-bis(4-(bis(4-methoxyphenyl)amino)phenyl)-N5,N5-bis(4-methoxyphenyl)pyridine-2,5-diamine (BD)) is synthesized to engineer the stacking properties and delivered higher hole mobility than doped Spiro-OMeTAD (3.2 × 10-4 versus 1.76 × 10-4 cm2 V-1 s-1) as dopant-free HTM. Starlike BD HTM has a twisted acceptor unit and strong dipole, forming crystalline and ordered packing film to ensure intramolecular charge transfer and improve mobility. The BD CsPbI3 PSCs deliver the maximum efficiency of 19.19%, which is the highest performance for all-inorganic PSCs based on dopant-free HTMs. Meanwhile, the ordered molecules-packing blocks the migration channel of I- ions to metal electrodes and improves the device stability. BD-based devices maintain more than 93% and 80% of the initial efficiency after 85 °C storage for 35 days and maximum power point (MPP) tracking at 85 °C for 1000 h, respectively.