Hole-Transporting Materials for Perovskite Solar Cells. A Theoretical insight into Chemical Design and Charge Transport

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Hole-transporting materials (HTMs) are a crucial component in obtaining high photoelectric conversion efficiencies (PCEs) in perovskite-based solar cells (PSCs). They play the important roles of extracting the photogenerated holes, formed within the perovskite film, and transporting them to the electrodes. Among the wide number of chemical structures proposed as HTMs for PSCs, small organic molecules have received special attention with spiro-OMeTAD as a reference. In this communication, we first focus on how the donor ability and hole reorganization energy change with the chemical structure of the HTM. π-Extended, sulfur-rich compounds, such as the anthracene-tetrathiophene ATT-OMe system displayed in Figure 1a, that have been used as HTMs in PSCs achieving remarkable PCEs, are theoretically described.[1] Second, we investigate a series of HTMs based on fused polyheteroaromatic molecules incorporating 7-azaindole terminal moieties bearing hydrogen-bond donor and hydrogen-bond acceptor sites (Figure 1b). The 7-azaindole units induce the hydrogen-bond self-assembly of the conjugated molecules thus increasing the supramolecular ordering in the HTM layer. The effects of this ordering on the charrier transport in the HTM semiconducting layer are theoretically discussed.[2] Third, we briefly present a multi-level theoretical approach based on DFT calculations and molecular dynamics and Kinect Monte Carlo simulations to estimate the carrier mobility in HTMs with different molecular structure such as spiro-OMeTAD and IDIDF in both crystal and amorphous phases.[3]

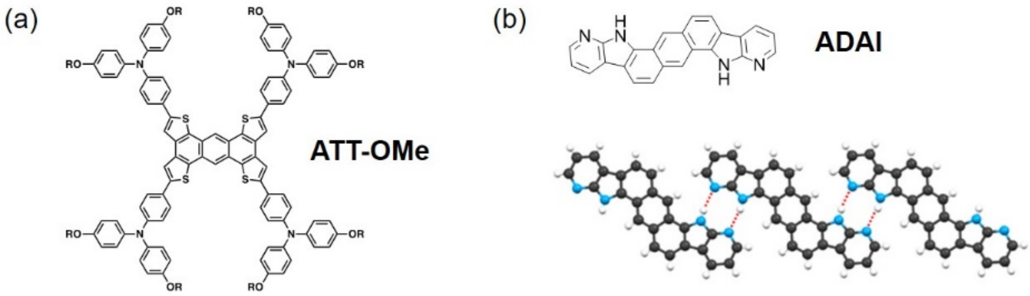

Figure 1. Structure of the sulfur-rich ATT-OMe (a) and the H-bond-promoting ADAI (b) HTM molecules.

References

[1] I. Zimmermann *et al.*, *ACS Appl. Mater. Interfac.* **2017**, 7, 1601674.
[2] P. Gómez *et al.*, *J. Mater. Chem. C* **2021**, *13*, 10819-10829.
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