Surface engineering of charge transport in inverted perovskite solar cells with azulene derivatives

Dimitris Tsikritzis[1,3], Nikolaos Tzoganakis[1], Boxu Feng[2], Michalis Loizos[1], Miron Krassas[1], Xiaodong Zhuang[2] and Emmanuel Kymakis[1,3]

[1]*Department of Electrical & Computer Engineering, Hellenic Mediterranean University (HMU), Heraklion 71410, Crete, Greece.*
[2]*Meso-Entropy Matter lab, State Key Laboratory of Metal Matrix Composites Shangai Key Laboratory of Electrical Insulation and Thermal gaining, School of Chemistry and Chemical Engineering, Frontiers Science Center for Transformative Molecules, Shanghai Jiao Tong University, Shanghai 200240, P. R. China*
[3]*Institute of Emerging Technologies (i-EMERGE) of HMU Research Center, Heraklion 71410, Crete, Greece*

Perovskite solar cells (PSCs) have reshaped the thin-film photovoltaic technology owning to their exceptional high power conversion efficiency (PCE) in conjunction with their low-cost and facile production[1]. The inverted PSCs although exhibit lower PCEs compared to normal ones, they show negligible hysteresis, better stability, and prolonged lifetime. In this work, novel azulene derivatives, namely Az-4TPA and biAz-4TPA, were synthesized and incorporated in inverted PCEs. The energy levels of the new molecules favour the hole charge extraction and by forming a thin biAz-4TPA/PTAA bilayer, the optimized devices reached a PCE up to 18.48% due to the improved energy level alignment at the hole extraction side of the device. Moreover, the devices incorporated the biAz-4TPA/PTAA bilayer show improved stability. We demonstrate a simple method for reducing the dependence for PTAA in inverted devices by using ultrathin PTAA films between a novel azulene derivative and perovskite layers. The optimal PTAA concentration of 0.75 mg mL^{-1} corresponds to more than 62% less PTAA used for the fabrication of the device, while delivering higher PCE and stability. The results show that the hydrophobic substrate is essential for perovskite growth in inverted PSCs and the potential new HTLs must conform with this, or interface engineering is needed to modify the wettability of the surface. Finally, we show that azulene derivates have the potential to be used as HTLs for PSCs and their functionalization and molecular tuning is expected to deliver improved devices.

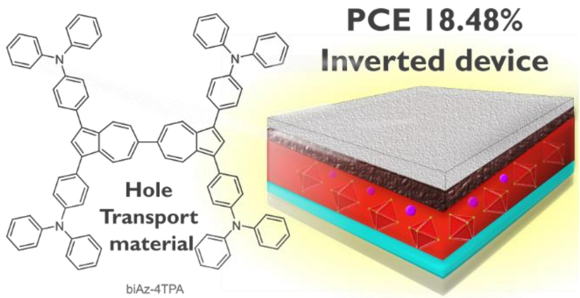

Figure 1: A novel π-conjugated azulene molecule was used as efficient Hole Transport Layer in inverted perovskite solar cells delivering PCE up to 18.48%.

References

1. Jeong, J. *et al.* Pseudo-halide anion engineering for α-FAPbI3 perovskite solar cells. *Nature* **592**, 381–385 (2021).