Dopant-Free Hole-Transporting Material with a C_{3h} Symmetrical Truxene Core for Highly Efficient Perovskite Solar Cells

Chuyi Huang (11429007), Weifei Fu, Changzhi Li*, Hongzheng Chen*

E-mail: <u>czli@zju.edu.cn</u>, <u>hzchen@zju.edu.cn</u>



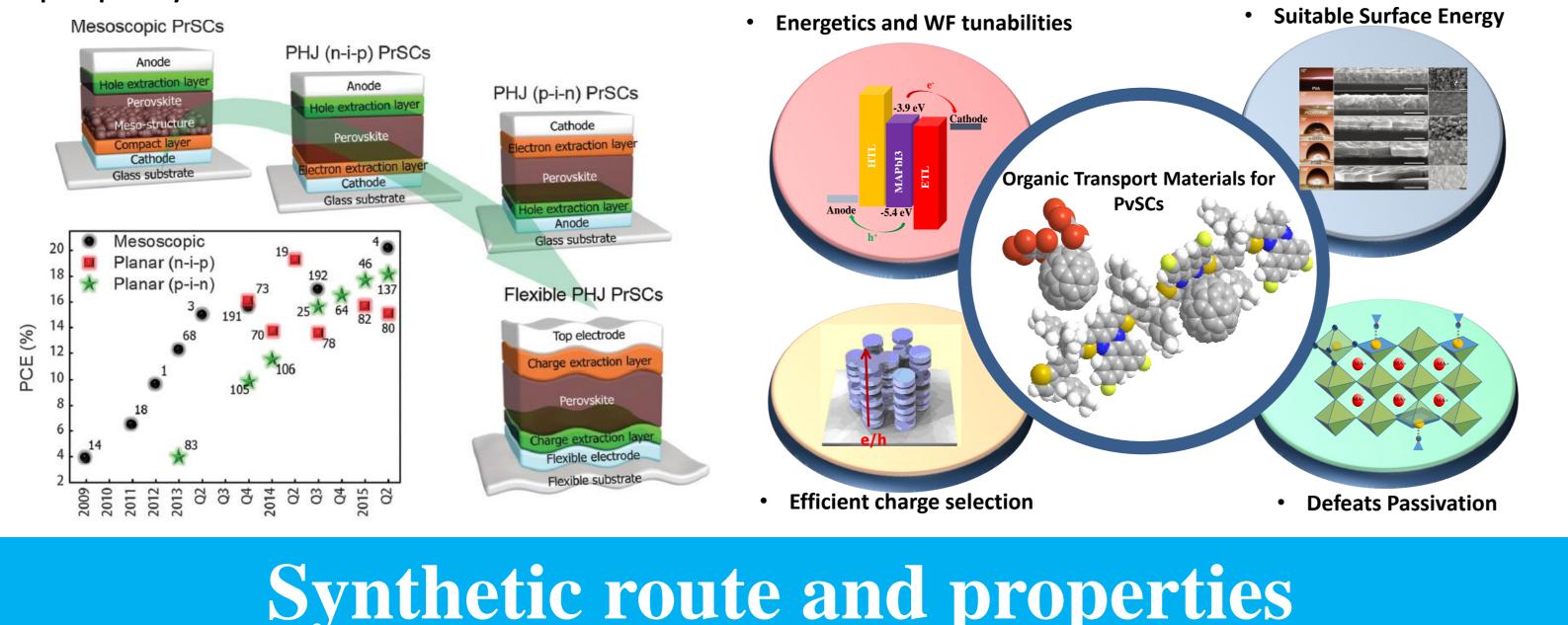
Abstract: Herein we present a new structural design of hole-transporting material, Trux-OMeTAD, which consists of a C3h Truxenecore with arylamine terminals and hexyl side-chains. This planar, rigid, and fully conjugated molecule exhibits excellent hole mobility and desired surface energy to the perovskite uplayer. Perovskite solar cells fabricated using the p-i-n architecture with Trux-OMeTAD as the p-layer, show a high PCE of 18.6% with minimal hysteresis.

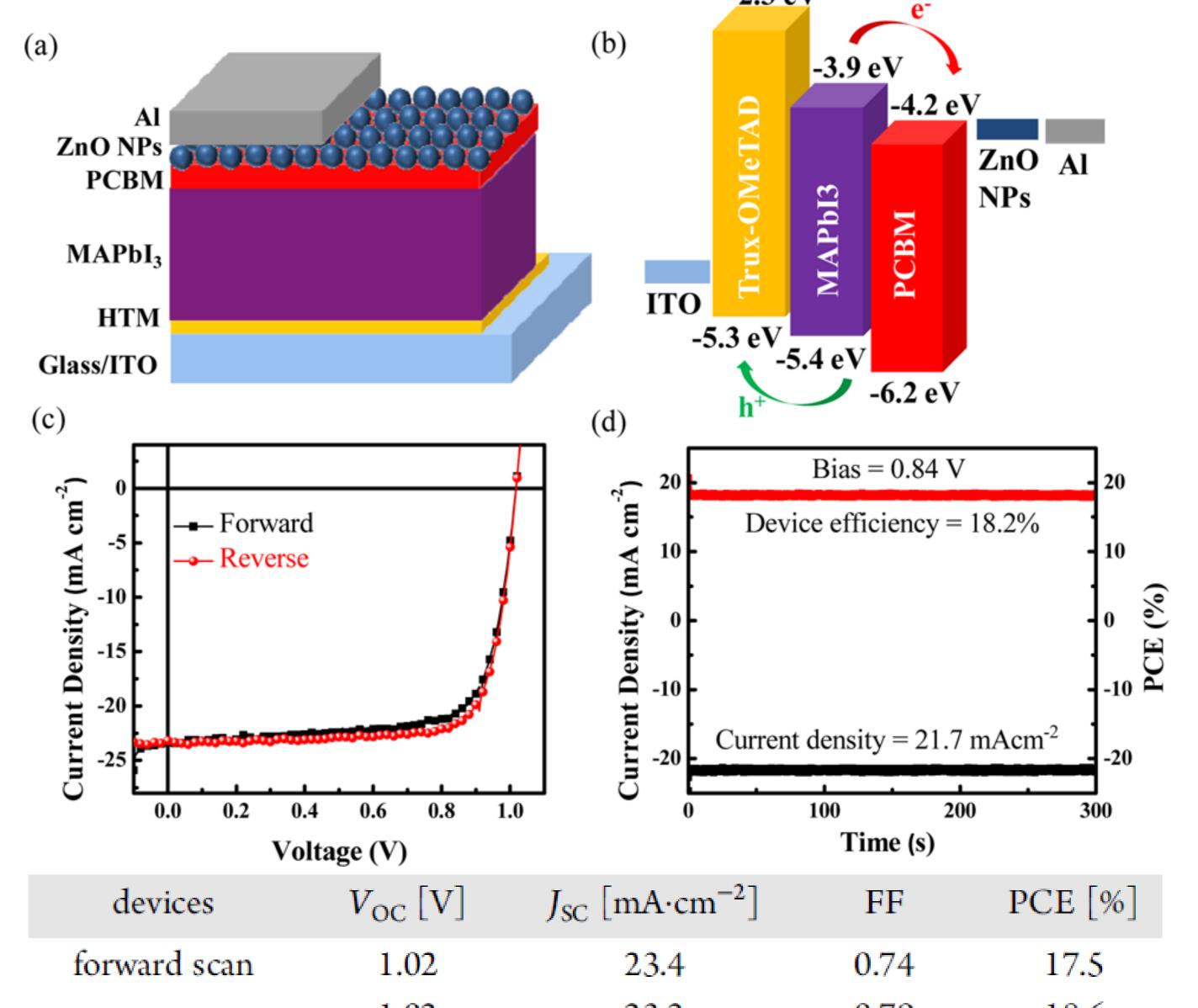
Introduction

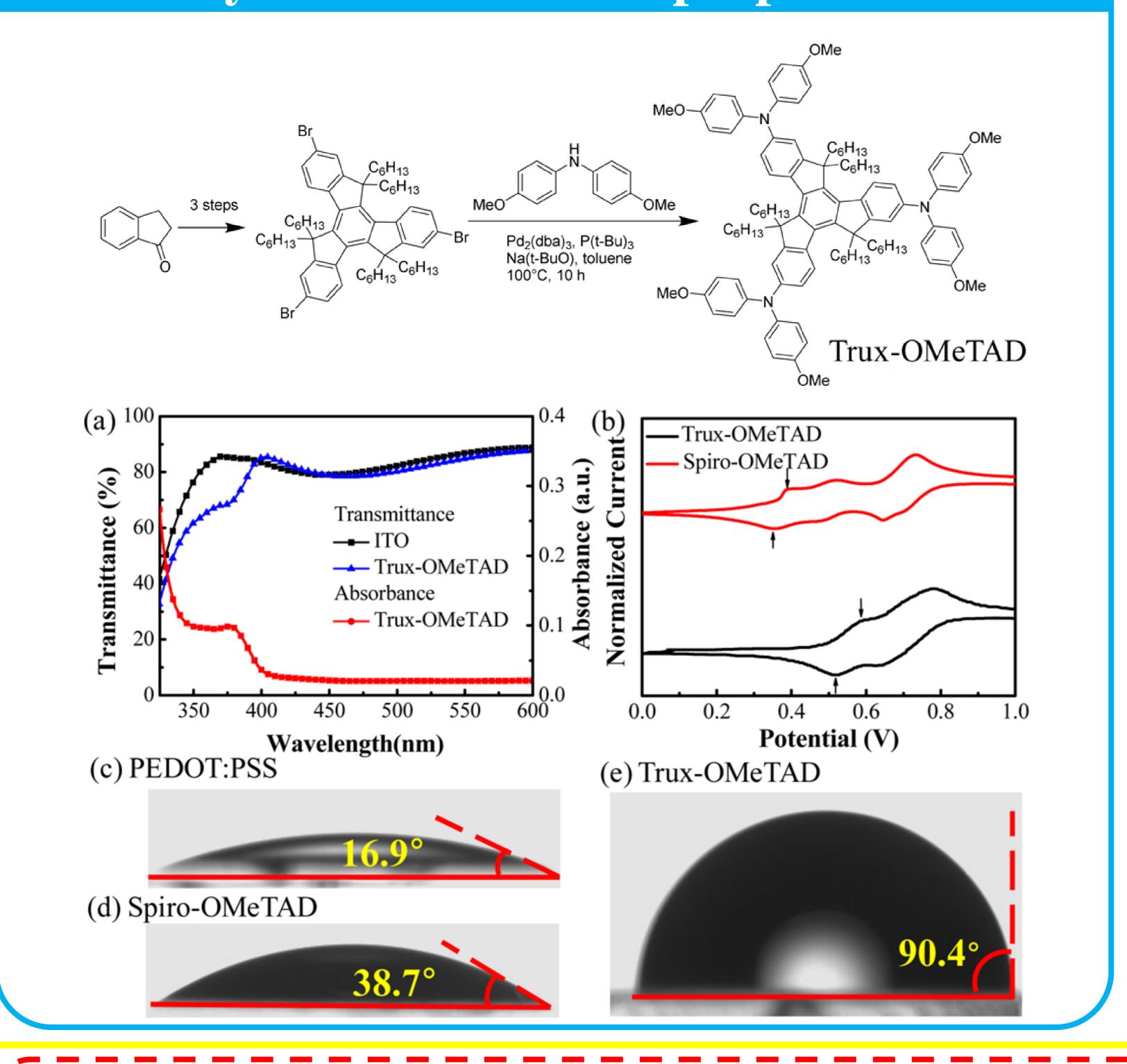
Perovskite solar cells (PvSCs) made with ammonium lead halide, such as $CH_3NH_3PbI_3$

Device structure and performance

have recently gained significant attention due to their capabilities in achieving high power conversion efficiency (PCE) through cost-effective fabrication. The PCE of PvSC has shown exceptionally fast growth rising from 3.8% to 20.1% within only six years. Although significant development of PvSC has been achieved, this is accomplished by very limited number of traditional hole transporting materials (HTMs), such as the frequently used PEDOT:PSS, PTAA and Spiro-OMeTAD, which are subject to the complicate doping protocol, mismatched energy levels, relatively high cost, and limited long-term stability. In this regard, it is highly desirable to develop new HTM for further improving PVSC device efficiency and stability, and probing their structureproperty correlations.

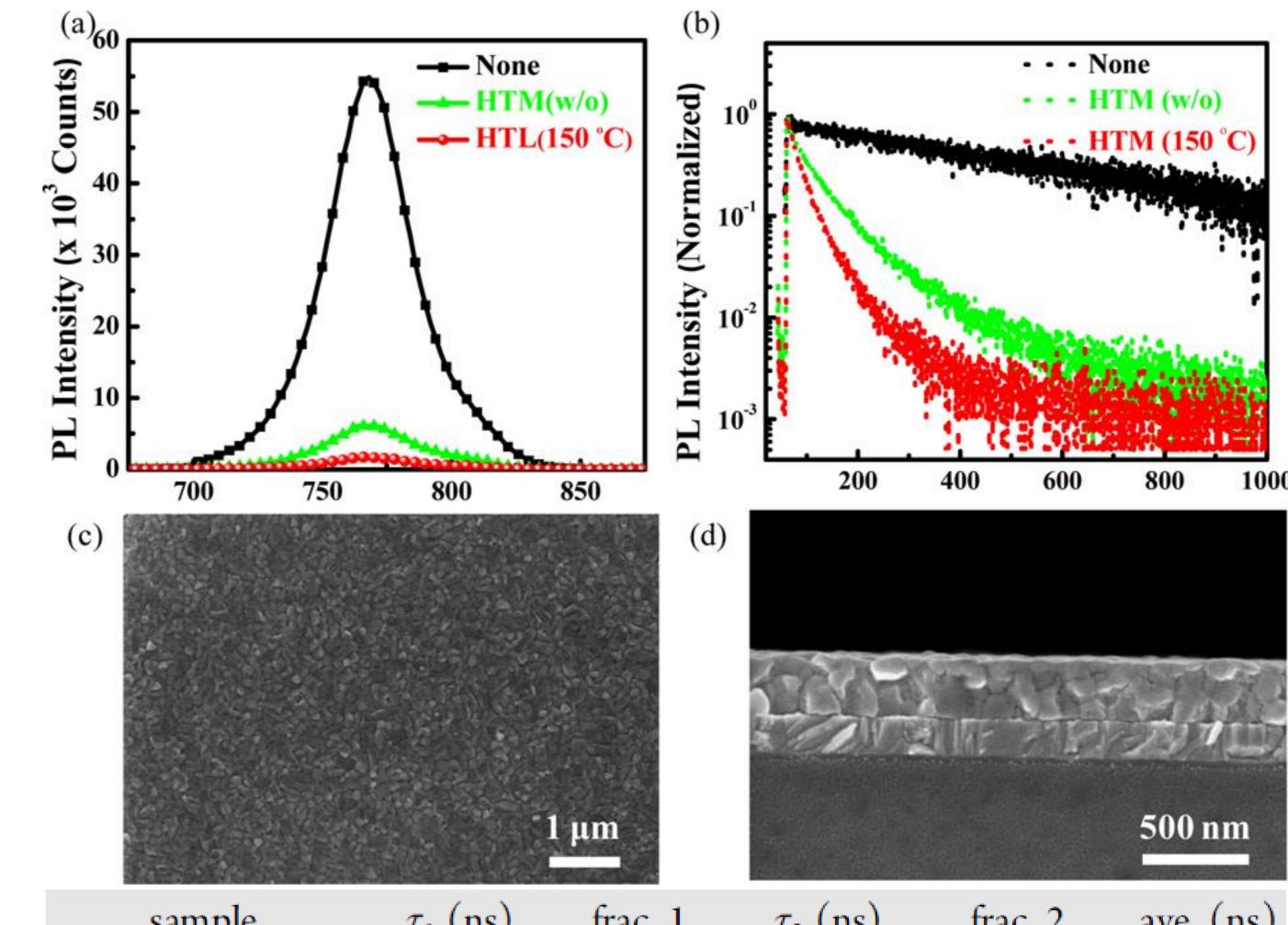






reverse scan	1.02	23.2	0.79	18.6	
--------------	------	------	------	------	--

PL lifetime and perovskite morphology



sample	t_1 (IIS)	11ac. 1	t_2 (IIS)	11 dC. 2	ave. (IIS)	
none	108.0	1.9%	1004.8	98.1%	987.8	
HTM (w/o)	32.0	40.6%	107.1	59.4%	76.6	
HTM (150 °C)	21.0	60.8%	67.6	39.2%	39.1	

Conclusions: A novel HTM was developed by introducing triarylamine and aliphatic side-chains onto the C3h Truxene-core to successfully demonstrate its application for highly efficient and stable PVSCs. A PCE as high as 18.6% was achieved from devices fabricated through a simple solution process. The planar and fully conjugated C_{3h} HTM result in excellent hole mobility and proper surface energy for the perovskite layer cast atop to facilitate more efficient hole extraction for achieving high-performance PVSCs.

References:

[1] Kim, H.; Lim, K.-G.; Lee, T.-W. *Energy Environ. Sci.* **2016**, *12*, 12–30.

[2] Bi, C.; Wang, Q.; Shao, Y.; Yuan, Y.; Xiao, Z.; Huang, J. Nat. Commun. 2015, 6, 7747.

[3] deQuilettes, D. W.; Vorpahl, S. M.; Stranks, S. D.; Nagaoka, H.; Eperon, G. E.; Ziffer, M. E.; Snaith, H. J.; Ginger, D. S. Science 2015, 348, 683.

[4] Huang, C. Y., Fu, W. F., Li, C.Z., Zhang, Z. Q., Qiu, W. M., Shi, M. M., Heremans, P., Jen, A. K. Y., Chen, H. Z. J. Am. Chem. Soc. 2016, 138, 2528-2531.