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

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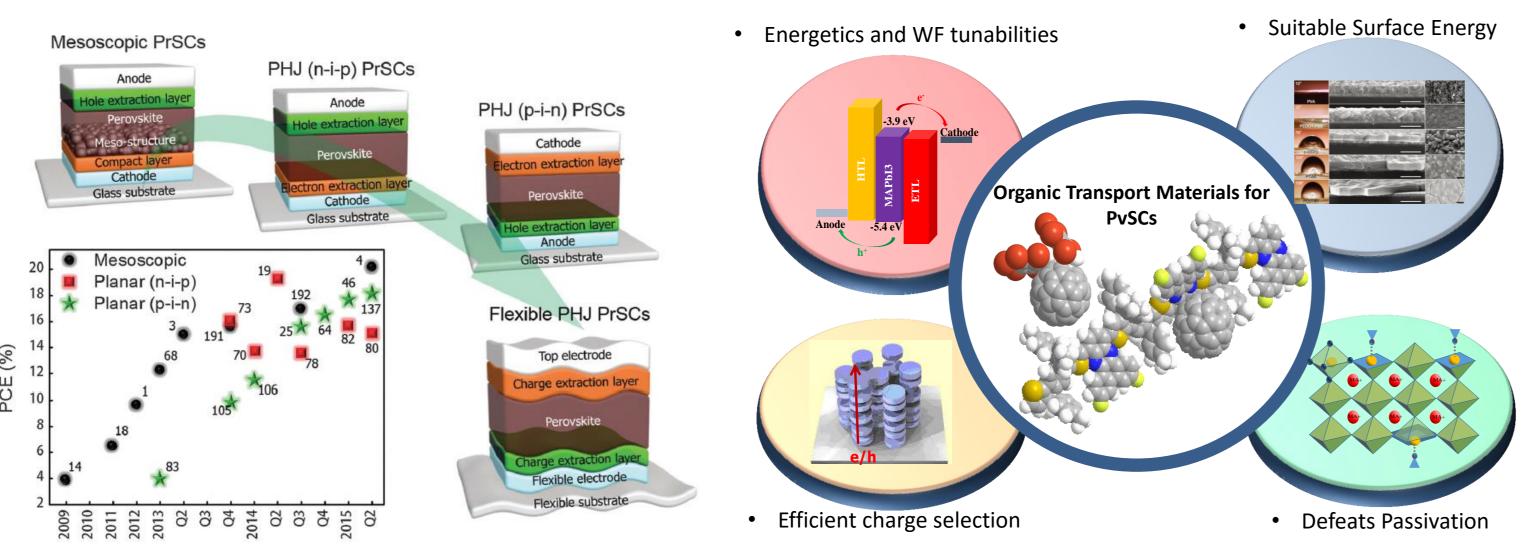


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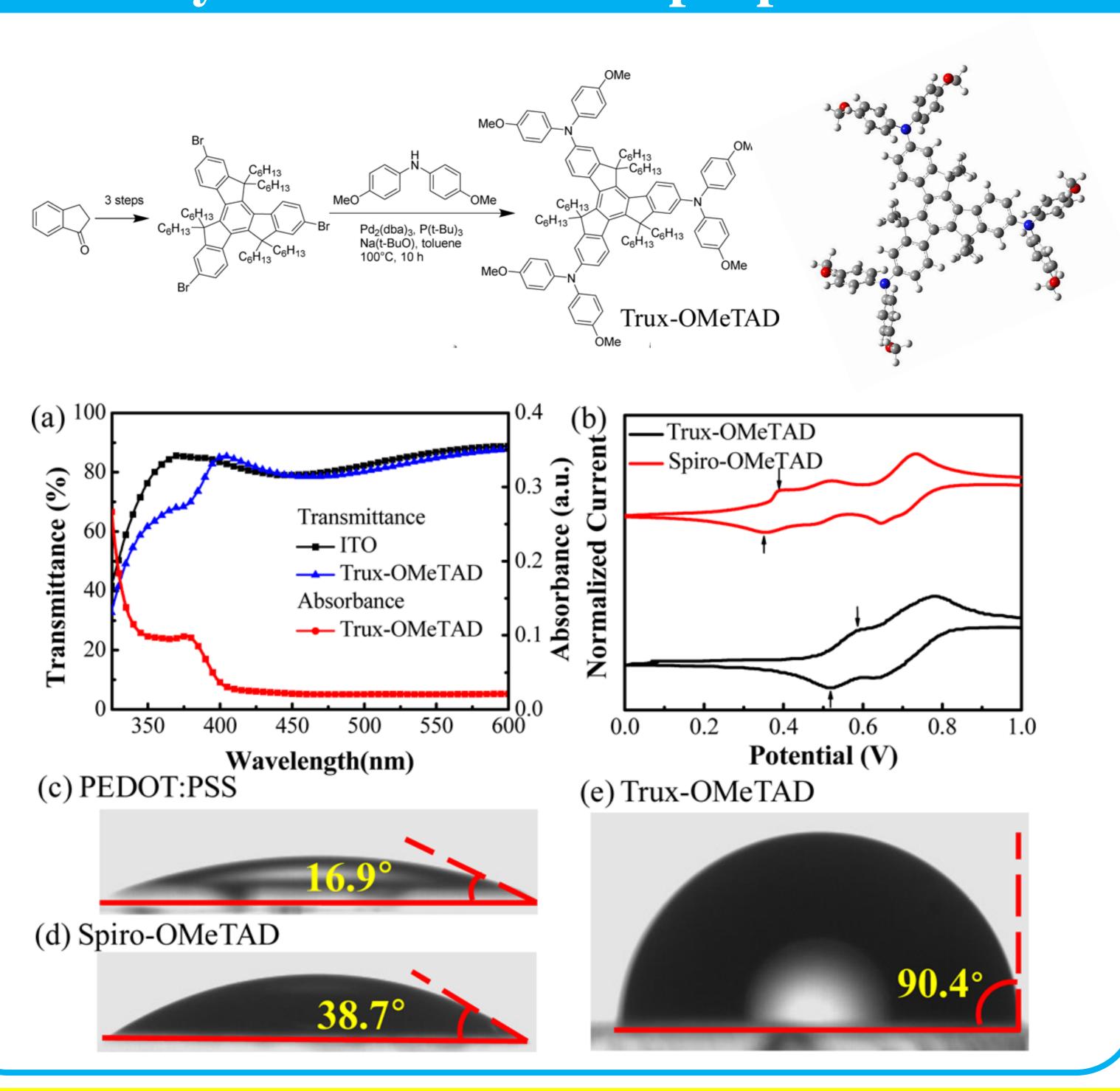
Abstract: Herein we present a new structural design of hole-transporting material, Trux-OMeTAD, which consists of a C3h Truxene-core with arylamine terminals and hexyl side-chains. This planar, rigid, and fully conjugated molecule exhibits excellent hole mobility and desired surface energy to the perovskite 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 made with ammonium lea

Perovskite solar cells (PvSCs) made with ammonium lead halide, such as CH₃NH₃Pbl₃ 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 within recent 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 structure-property correlations.

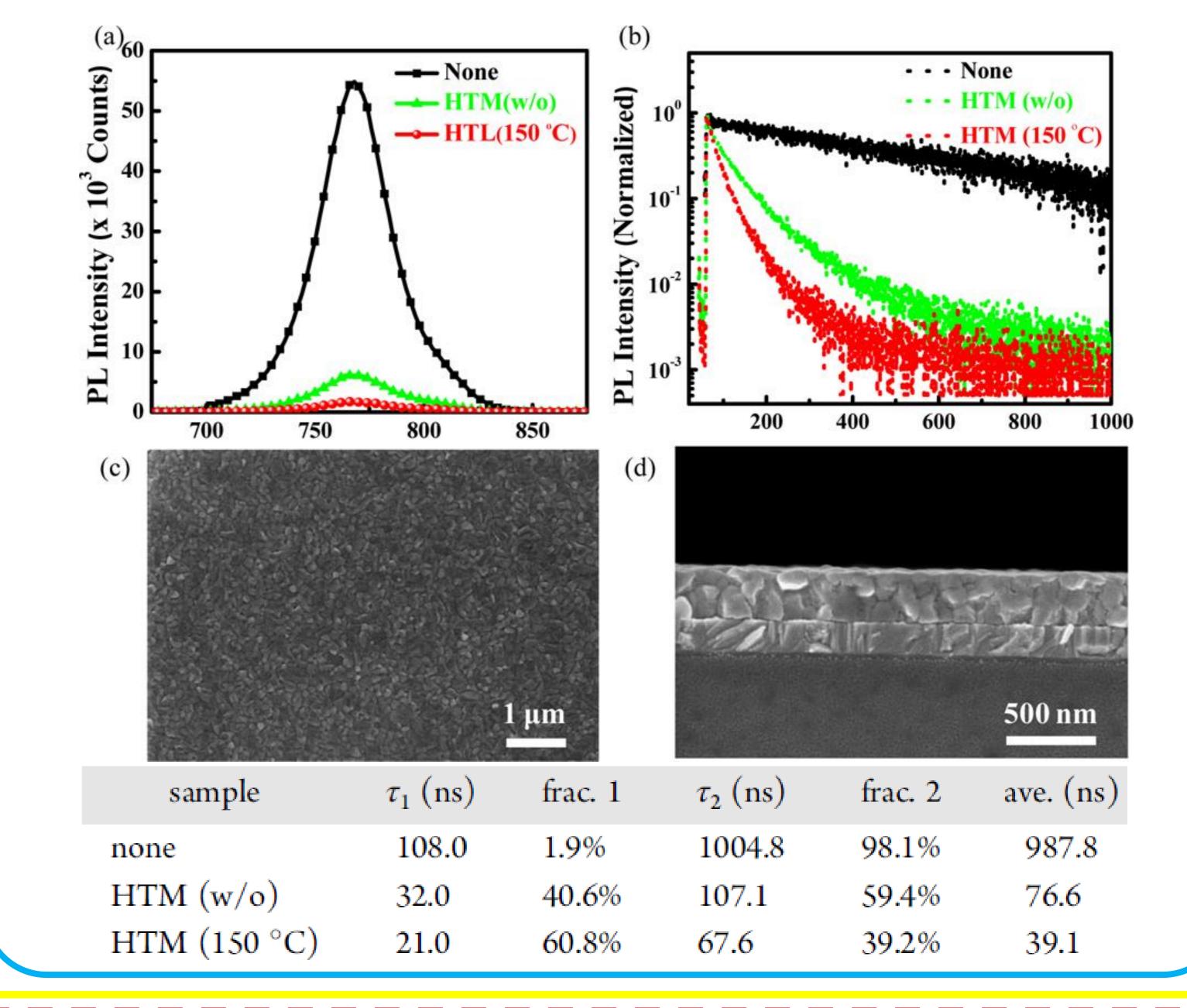


Synthetic route and properties



Device structure and performance (a) -3.9 eV -4.2 eV ZnO NPs ZnO Al **PCBM NPs** MAPbI₃ ITO HTM -5.3 eV -5.4 eV Glass/ITO -6.2 eV (c) Bias = 0.84 VDevice efficiency = 18.2% Forward Reverse Current density = 21.7 mAcm^{-2} Time (s) Voltage (V) $V_{\rm OC}\left[{ m V}\right]$ PCE [%] FF devices $J_{\rm SC}$ [mA·cm⁻²] forward scan 17.5 1.02 0.74 23.4 1.02 18.6 reverse scan

PL lifetime and perovskite morphology



Conclusions: A novel HTM was developed by introducing arylamine and aliphatic side-chains onto the C_{3h} 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.

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