

## Enhanced Stability of PbS Quantum Dot Solar Cells Using Novel Molecular Hole Transport Layers

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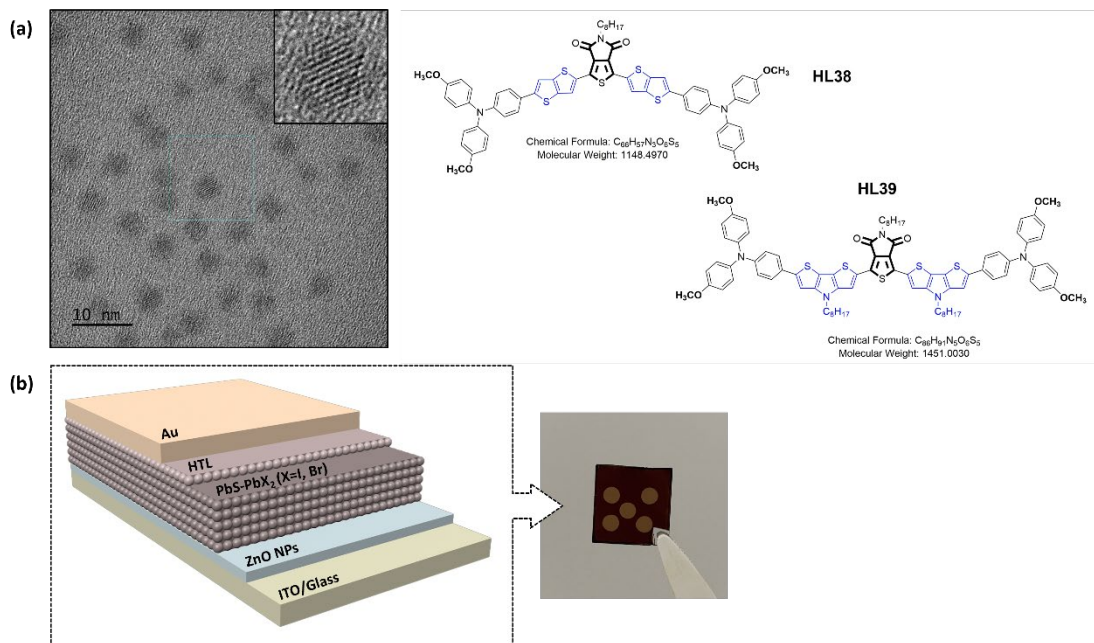
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**Abstract:** Solution-processed semiconducting nanomaterials, such as colloidal quantum dots (QDs), are increasingly being recognized for their potential in next-generation photovoltaic devices due to their tunable optical properties and cost-effective fabrication methods. Among these, PbS QDs have gained attention due to their tunable bandgap and their broad absorption spectrum from the visible to the near-infrared spectrum. However, a significant challenge remains: the instability of PbS QD solar cells (QDSCs), particularly when exposed to environmental factors such as oxygen and moisture. In particular, the commonly used 1,2-ethylenedithiol (EDT) treatment in the PbS QD hole transport layer (HTL) renders them vulnerable to oxidation. In previous studies, this EDT-treated PbS QD HTL has been pointed out as the culprit for the performance degradation over time for PbS QDSCs. In addition, the aggressive EDT treatments can lead to damages and defects of the other layers underneath the HTL.

To address the stability issue due to the EDT-treated HTL, this study investigated the impact of a series of new organic HTLs on both the efficiency and the stability of PbS QDSCs. These new HTLs investigated here are based on thieno-thiophene derivatives, D- $\pi$ -A- $\pi$ -D small molecules, containing thieno[3,4-c]pyrrole-4,6(5H)-dione as central acceptor unit, triphenylamine derivatives as the donor moieties together with different conjugated  $\pi$ -spacers (namely HL38 and HL39). They exhibit suitable HOMO and LUMO levels with potentials to replace the conventional EDT-treated PbS HTL. Functional solar cells are fabricated and characterized. In terms of stability, by maximum power point (MPP) tracking in ambient humid air (RH = 40%-50%) under continuous AM1.5G 1-sun illumination, we compared the stability of unencapsulated PbS QD solar cells with their HTLs being PbS-EDT (the reference condition), HL38, and HL39. After 8 hours of testing, the power conversion efficiency (PCE) of the unencapsulated PbS-EDT device decreased to 58% of its initial value, whereas devices with HL38 and HL39 exhibited improved stability, retaining 75% and 77% of their initial PCE, respectively. These results highlight organic HTLs, such as HL38 and HL39, can be viable HTL choices alternatives to EDT-treated PbS HTLs for better stability.



**Fig. 1.** (a) TEM image of PbS QDs and molecular structures of HL38 and HL39. (b) Schematic device structure and photograph of PbS QDSCs.