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Perovskites

A molecular sieve boosts perovskite stability

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Stand first

A molecular sieve to finely control 2D/3D heterointerface reactions is demonstrated, enabling highly efficient and stable perovskite solar cells.

Perovskite solar cells (PSCs) are a promising technology for renewable energy generation[1], and worldwide research efforts are focussed on surface passivation and interface optimization to increase device efficiency and stability. Beyond traditional '3D' perovskites, low-dimensional perovskites—consisting of a single or few inorganic layers (typically $n < 3$) separated by large organic cations—have recently attracted wide interest for their high structural stability.[2] Used as interfacial layers on top of 3D perovskites, they tune perovskite interfaces, boosting the solar cell stability.[3,4] First developed in 2015, this 2D-modified perovskite interface is now commonly used in PSCs which demonstrate high efficiency and stability.[5] Typically, ammonium-based passivation layers are used and can form in two modes: 1) a heterostructure of low dimensional (2D) perovskite atop the 3D absorber layer, or 2) a molecular cation layer where no 2D perovskite layer is formed. Both approaches provide an increase in the device open circuit voltage (V_{oc}) by their defect passivation effect and an overall increase in the device durability. However, questions remain about whether a single 2D phase is formed, alongside questions on layer homogeneity.[6,7]

Now, writing in *Nature Synthesis*, Zhimin Li[8], Pengfei Guo, Yuanyuan Zhou and co-workers demonstrate an interesting strategy to address this issue by engineering a robust, laminate-structured perovskite heterointerface using a molecular interlayer (molecular sieve) between the 2D and the 3D perovskite layers (Fig. 1). Atomic scale insights are used to link the microstructure with device performance, highlighting the importance of 2D passivator-microstructure uniformity. The strategy enables power conversion efficiencies up to 26% and solar cell lifetimes over 1,000 hours under damp-heat test conditions of 85 °C and 85% relative humidity and maximum-power-point tracking under one-sun illumination. Key to this work is the use of an ultrathin molecular sieve made of [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) which enables both molecular passivation of the 3D perovskite as well the formation of an ultrathin (<10 nm) 2D capping layer of single purity phases (only n=1 and 2). In more detail, an ultrathin PCBM layer is formed on the 3D perovskite surface through simple spin-coating followed by the conventional 2D layer formation, again via spin-coating and thermal annealing at 100 °C (Fig. 1). The modified interface is developed on an inverted pin structure, which is gaining attention over traditional architectures due to its higher efficiency at lower cost and device complexity.

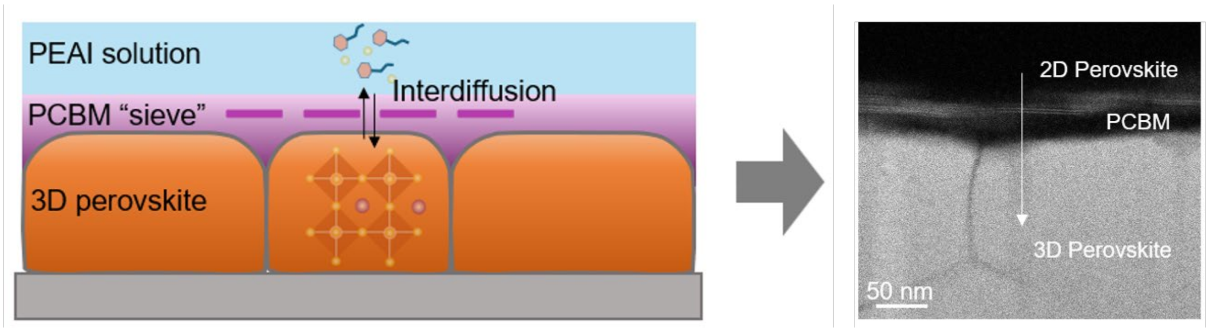

Fig. 1 Overview of the molecular sieve approach for boosting 2D/3D perovskite interface stability. The fullerene derivative PCBM has a multipurpose function, acting as an electron transport layer and mediating ion transport at the 2D/3D heterostructure interface (left). The “sieve” approach enables atomically precise interface control as seen in the cross-sectional high-angle annular dark field scanning transmission electron microscopy image (right). Adapted from Ref. [8]

By conducting high-resolution lattice-resolved scanning transmission electron microscopy Li, Guo, Zhou and co-workers gain interfacial microstructural information (Fig. 1). They find that the heterogeneous uncontrolled process using conventional methods where the 2D molecular salt is dissolved in isopropanol for example followed by spin-coat deposition on the 3D perovskite film leads to discontinuous random 2D perovskite capping with different octahedral-layer numbers (n = 2-5). This disorder is linked with pronounced surface degradation. The molecular sieve presents an unconventional surface passivation route creating a laminate structure which consists of a PCBM interlayer sandwiched between a 2D molecule layer and a 2D perovskite layer. Using this method, the 2D perovskite layer has only n = 1 and 2 phases. Beyond improved microstructure, PCBM also acts as an ion-blocking layer, preventing degradation. The microstructure of the heterointerface containing the molecular sieve remains intact even after long-term stability testing. Moreover, the top 2D layer, with its well aligned energy levels, does not appear to block charge extraction, a common issue for 2D perovskite passivation in pin configuration. Instead, the electron extraction was found to be improved compared to the control device without molecular sieve because of better conduction band alignment.

The method reported by Li, Guo, Zhou and co-workers demonstrates the use of the fullerene derivative PCBM not just as an electron transport layer but also as an ion transport mediator for heterostructure interface control. This strategy addresses the challenges of uncontrolled surface reactions and phase heterogeneity, commonly seen in the conventional 2D passivation method. Future studies should focus on examining and developing the mechanism by which PCBM mediates ion transport and controls the 2D perovskite growth. Molecular dynamic simulations, for example, could model the interactions between PCBM, the ions, and the perovskite surface. Additionally, exploring different molecular interlayers with varying pore sizes and chemical functionalities could lead to better control over the 2D perovskite composition and structure. Finally, while the device stability is impressive, further long-term testing under real-world conditions is necessary to fully assess the potential and scaling up of this approach. As a broader implication, this work effectively connects the observed microstructure to the improved device stability demonstrating the functional relevance of the engineered interface. The laminate-structured passivation opens new avenues for exploring heterointerface design based on the synergistic effect of combining multiple functional layers. This method may also be promising for use in other optoelectronic devices.

Competing interests

The authors declare no competing interests.

Ref.

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