A strategy to stabilize 3D/2D perovskite heterostructures for solar cells

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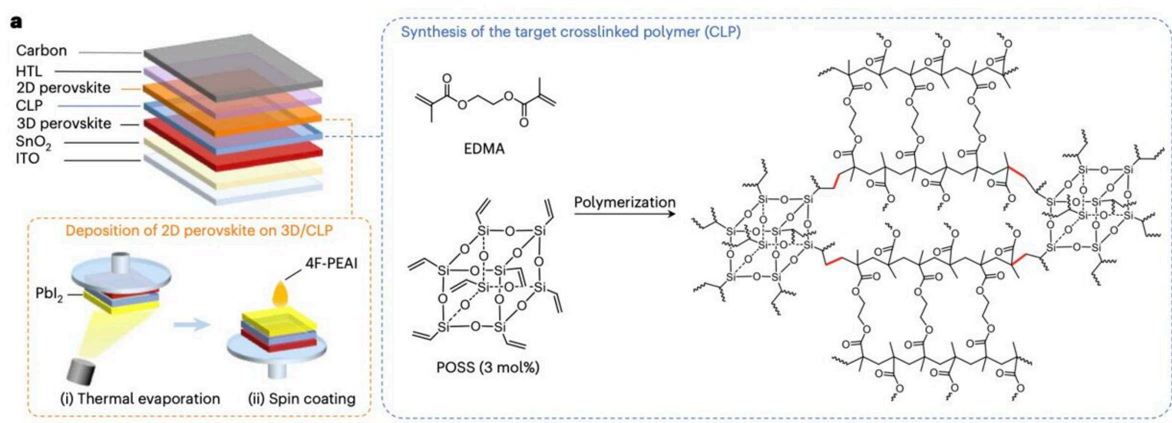

Schematic of the device structure, the deposition of the 2D perovskite layer and the molecular structures and synthesis process of POSS, EDMA and the CLP. Credit: Luo et al

Hybrid perovskite solar cells (PSCs) made of organic and inorganic materials are highly promising energy solutions that could help to reduce carbon emissions worldwide. In recent years, these cells' power-conversion efficiencies (PCEs) have improved significantly, ultimately exceeding 25%.

A key milestone in the fabrication of efficient PSCs was the use of 2D and quasi-2D modified 3D perovskite heterostructures (i.e., structures comprised of 3D and 2D perovskite materials). These structures have several advantageous qualities, for instance they enable the passivation of defects and a favorable band alignment, which in turn improves the cells' open-change voltage and fill factor.

3D/2D heterostructures are typically created by spin coating an organic cation salt solution on top of a 3D perovskite material and forming a thin 2D perovskite layer on its surface. This process, however, can facilitate the subsequent degradation of the heterostructures in some conditions, due to the diffusion of ions between the 2D perovskite surface and underlying bulk 3D perovskite.

Researchers at Huazhong University of Science and Technology, Wuhan University of Technology and University of Toronto recently introduced a new approach for fabricating more stable 3D/2D heterostructures, preventing their degradation. Their approach, introduced in a paper published in *Nature Energy*, entails the introduction of an additional layer between the structures; 3D and 2D perovskite layers.

"The ionic diffusion between the surface 2D and bulk 3D perovskites leads to the degradation of the 3D/2D perovskite heterostructures and limits the long-term stability of PSCs," Long Luo, Haipeng Zeng and their colleagues wrote in their paper. "We incorporate a cross-linked polymer (CLP) on the top of a 3D perovskite layer and then deposit a 2D perovskite layer via a vapor-assisted two-step process to form a 3D/CLP/2D perovskite heterostructure."

Essentially, Luo, Zeng and their colleagues proposed introducing an interlayer between 3D bulk perovskites and 2D surface perovskites in 3D/2D heterostructures. This interlayer is made of a cross-linked polymer (CLP) that can inhibit ion diffusion without impacting the charge transport between the 3D and 2D perovskite layers.

"Photoluminescence spectra and thickness-profiled elemental analysis indicate that the CLP stabilizes the heterostructure by inhibiting the diffusion of cations (formamidinium, FA^+ and 4-fluorophenylethylammonium, $4F\text{-}PEA^+$) between the 2D and 3D perovskites," Luo and his colleagues explained in their paper.

To test the effectiveness of their updated 3D/2D heterostructure design, the researchers used it to create a series of small-area solar cells, as well as mini solar modules. These cells and modules attained remarkable results, as they appeared significantly more stable than perovskite-based cells and modules with conventional 3D/2D heterostructure designs.

"For devices based on carbon electrodes, we report small-area devices with an efficiency of 21.2% and mini-modules with an efficiency of 19.6%," Luo and his colleagues wrote in their paper. "Devices retain 90% of initial performance after 4,390 hours operation under maximum power point tracking and one-sun illumination at elevated temperatures."

In the future, the new design introduced by Luo and his colleagues could help to stabilize solar cells based on 3D/2D perovskite heterostructures, without affecting their efficiencies. In addition, their study could inspire other teams to devise similar approaches that introduce an interlayer between 3D and 2D perovskite layers to prevent degradation caused by ionic diffusion.

More information: Long Luo et al, Stabilization of 3D/2D perovskite heterostructures via inhibition of ion diffusion by cross-linked polymers for solar cells with improved performance, *Nature Energy* (2023). DOI: 10.1038/s41560-023-01205-y