3D chemistry boosts perovskite efficiency to 23.9%

November 11 2021

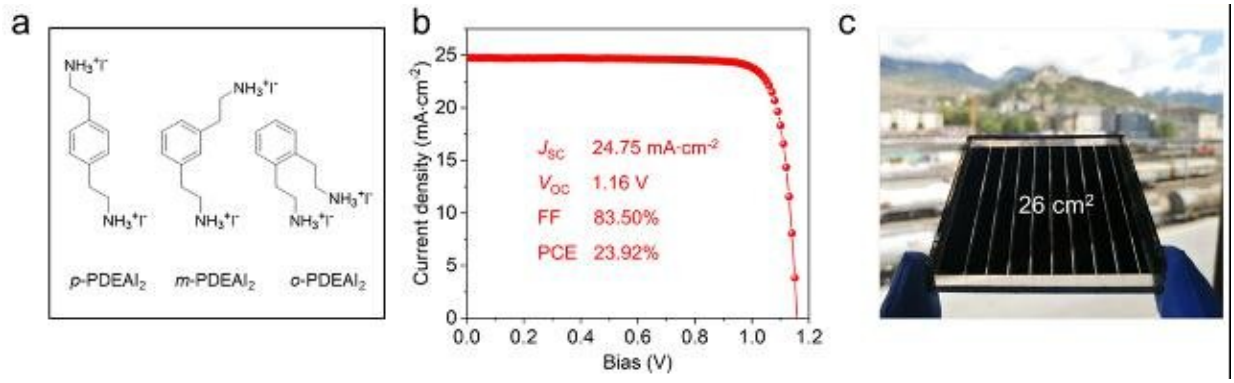

Fig. 1 a The structures of the $PDEAI_2$ isomers. b J-V characteristics of the champion device with o-$PDEAI_2$. c Photograph of the fabricated perovskite solar module. Credit: MK Nazeeruddin

An international collaboration led by EPFL chemical engineers has overcome a problem in the manufacturing of perovskites that reduces their efficiency as solar panels. The approach produced perovskite solar panels with an efficiency of 23.9 percent and operational stability longer than 1000 hours.

Perovskites are hybrid compounds made from metal halides and organic constituents, and show great potential in a range of applications, e.g. LED lights, lasers, and photodetectors. However, their major contribution is in solar cells, where they are poised to overtake the

market and replace their silicon counterparts.

Among the leading candidates for highly efficient and stable solar cells are lead iodide perovskites, which show excellent light-harvesting capabilities. However, their efficiency depends greatly on their manufacturing, and a key factor is removing defects from their light-harvesting surface.

Passivation and perovskite efficiency

The way this is typically done is with a method called "passivation," which coats the surface of perovskite films with chemicals (alkylammonium halides) to make them more resistant and stable. The process adds a two-dimensional perovskite layer on top of the primary perovskite light absorber, which improves the stability of the device.

The problem is that passivation actually backfires by forming so-called "in-plane" perovskite layers that don't "move" electrical charge as well, especially under heat. This is an obvious disadvantage for scaling up and commercializing potential solar panels.

3D chemistry to the rescue

In a new study, scientists led by Mohammad Nazeeruddin at EPFL's School of Basic Sciences, have found a way to solve the problem by treating them with different isomers of an iodide used to make perovskites. In chemistry, isomers are compounds that have the same molecular formulas but their atoms are arranged differently in three-dimensional space.

The scientists studied the minimum energy required to form two-dimensional perovskites from different isomers of the iodide $PDEAI_2$

(phenylenediethylammonium). The isomers were designed for what the researchers call "tailored defect passivation," meaning that their passivation effect on perovskites was very well characterized in advance.

The approach turned out to be very effective in staving off the negative effects of passivation on perovskite efficiency. Specifically, the most effective $PDEAI_2$ isomer was also the most "sterically hindered," a term that refers to a slowing of chemical reactivity simply because of the compound's molecular bulk. In fact, steric hindrance is often used to prevent or minimize unwanted reactions.

The perovskite solar cells produced with this method showed an efficiency of 23.9 percent with operational stability beyond 1000 hours. The work also achieved a record efficiency of 21.4 percent for perovskite modules with an active area of 26 cm^2.

More information: Cheng Liu et al, Tuning structural isomers of phenylenediammonium to afford efficient and stable perovskite solar cells and modules, *Nature Communications* (2021). DOI: 10.1038/s41467-021-26754-2

Provided by Ecole Polytechnique Federale de Lausanne