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Energy Spotlight

Stabilization of Perovskite Solar Cells

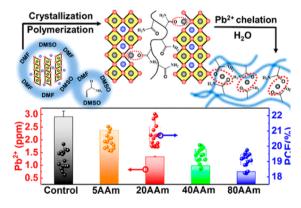
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ong-term operational stability remains a major challenge in the commercialization of perovskite solar cells (PSCs). While the major thrust of recent research effort has been on understanding the degradation mechanism, many new approaches are being explored to improve the performance stability of PSCs. In this issue are four Letters that discuss new strategies to achieve stabilization of PSCs. Editorial Advisory Board members highlight these new advances herein.

MITIGATING THE LEAD LEAKAGE OF HIGH-PERFORMANCE PEROVSKITE SOLAR CELLS VIA IN SITU POLYMERIZED NETWORKS (LETTER)

Benfang Niu, Haotian Wu, Jinglin Yin, Bruce Wang, Gang Wu, Xueqian Kong, Buyi Yan, Jizhong Yao, Chang-Zhi Li*, and Hongzheng Chen

ACS Energy Lett. 2021, 6 (10), 3443–3449 DOI: 10.1021/acsenergylett.1c01487



We can no longer blind ourselves and ignore the harsh reality: the Earth is reacting strongly to even a small increase of greenhouse gases in the atmosphere. In order to stabilize the global temperature and leave a safe living environment for our descendants, we have no choice but to reduce the emission of these gases to restore the Earth's climate balance. More than 120 countries have already announced pledges to achieve net-zero emissions by 2050. To achieve this very important yet formidable goal, developing and deploying clean energy technologies are critical. Solar cells are one kind of these technologies, and indeed, they are considered to be the most important and the largest source of clean energy supply for the future. This calls for urgent, innovative leaps in this sector.

As the most promising, new generation of photovoltaics, PSCs have made great strides in achieving high power conversion efficiencies (PCEs), with the highest value now above 25%. Meanwhile, from the processing point of view, they can be fabricated from solution. These advantages give them promise as a high-efficiency and cost-effective energy solution in the future. Nonetheless, in order to fulfill this vision, several barriers must be overcome. One major barrier blocking their practical implementation is the presence of lead (Pb), a major constituent element in most high-performance PSCs. Ranked in the top 5 on the Substance Priority List by the Agency for Toxic Substances and Disease Registry, Pb poses the highest potential threat to global human health as well as our ecosystems. How can we ensure the leakage of water-dissolved Pb2+ from perovskites to our water system is minimal and below the safety threshold if a solar cell is unexpectedly broken into pieces?

In their pioneering work, Li and co-workers propose and demonstrate an innovative strategy to effectively address this crucial Pb safety issue of PSCs. They used a polymer that can act as a chelating agent for Pb²⁺ ions so as to immobilize them in the polymer network of perovskite-polymer hybrids. Meanwhile, the polymer was selected in such a way that it can act as a beneficial additive to simultaneously enhance the solar cell efficiency. Although it sounds simple, this design principle has never before been reported. To make it work, the authors attempted a one-step direct introduction of the polymer into the perovskite layer, and a two-step in situ polymerization process as well. The latter led to robust polymer networks that could successfully block lead leakage and effect perovskite crystallization to improve the photovoltaic performance. The authors probe and describe in detail the key differences between these two fabrication routes. Furthermore, they demonstrate that this design strategy can be readily scaled up for fabricating perovskite modules. The new findings and insights reported in this work may facilitate the development of PSCs toward the ultimate goal of commercialization and provide a long-term sustainable energy solution. **Dongling Ma**

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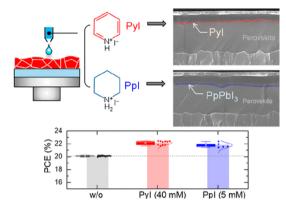
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EFFECT OF CHEMICAL BONDING NATURE OF POST-TREATMENT MATERIALS ON PHOTOVOLTAIC PERFORMANCE OF PEROVSKITE SOLAR CELLS (LETTER)

Jeong-Hyeon Kim, Seul-Gi Kim, and Nam-Gyu Park* ACS Energy Lett. 2021, 6 (10), 3435–3442 DOI: 10.1021/acsenergylett.1c01376



For an efficient photovoltaic process, not only needed are materials providing excellent light-harvesting with an efficient charge transport and low bulk recombination as halide perovskites, but also optimized charge separation at selective contacts is mandatory. Consequently, the reduction of surface recombination is a key aspect for the fabrication of highperformance solar cells. Different passivating systems are currently being extensively tested in PSCs. A deep understanding of how this passivation works and how, in addition, halide perovskite stability can benefit will be a key point in the future development of this technology.

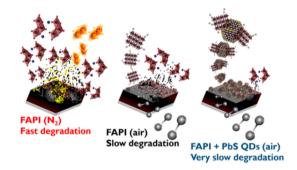
In this line, Park and co-workers present a detailed and systematic analysis of the post-treatment effect on the halide PSC performance considering the post-treatment of the perovskite/hole-selective contact interface with two different molecules, pyridinium iodide (PyI) and piperidinium iodide (PpI). Interestingly, while both molecules present the same geometry and both treatments can improve the performance of the solar cells, optimization with each molecule requires significantly different concentrations, i.e., 40 and 5 mM respectively. As the authors show, this difference has its fundamental in the different character of the heterocyclic rings, with delocalized π electrons for PyI and without a π bond for PpI. One consequence is a stronger dipole moment for Pp⁺ than for Py⁺, which probably benefits the observed formation of PpPbI₃ layered perovskite, hindering the transport at the interface and reducing the performance when treatments with high concentrations of PpI are used. In contrast, for PyI treatment, a similar interlayer thickness is observed, but, in this case, no 2D perovskite was detected taking advantage of the delocalized π electrons for a good charge separation. In addition, no significant degradation was observed in the cells' photoconversion efficiency after 1800 s stabilization when interfacial treatments were used; an improvement was even seen in the case of PyI, in contrast with the 10% decay with respect to the initial value observed for the control sample, stressing also the additional beneficial effect of interfacial treatments on device stability.

The authors present a systematic characterization of films and devices prepared with both treatments and also control devices without any interfacial treatment, allowing readers to understand the way in which the treatment with each molecule should be optimized and the origin of the different optimization parameters in each case. This work is an outstanding example of how molecules with different natures can provide good performance, but their nature has to be understood in order to have its full benefit in the final cell performance. It also can help other groups to design efficient passivating molecules in order to further improve the performance and stability of PSCs. **Iván Mora-Ser**ó

BOOSTING LONG-TERM STABILITY OF PURE FORMAMIDINIUM PEROVSKITE SOLAR CELLS BY AMBIENT AIR ADDITIVE ASSISTED FABRICATION (LETTER)

K. M. Muhammed Salim, Sofia Masi*, Andrés Fabián Gualdrón-Reyes, Rafael S. Sánchez, Eva M. Barea, Marie Kreĉmarová, Juan F. Sánchez-Royo, and Iván Mora-Seró* ACS Energy Lett. 2021, 6 (10), 3511–3521

DOI: 10.1021/acsenergylett.1c01311



Only three materials have surpassed the 25% efficiency barrier for solar cells, i.e., GaAs, Si, and now hybrid perovskites. The unprecedented performance gains of perovskites have raised high hopes toward their industrialization. These high performances were mainly obtained for FAPbI₃ perovskites, which have the most red-shifted bandgap of any hybrid perovskite materials, at close to 1.5 eV (without using Sn). Unfortunately, pure FAPbI₃ exhibits polymorphism at room temperature and therefore shows a photoinactive yellow phase. This is why, in recent years, the stabilization of FAPbI₃ in its photoactive black phase has become a main theme of the research community by using, for example, additives such as Cs, Rb, SCN, or HCOO.

An alternative route to stabilize pure FAPbI₃, without the addition of cations or (pseudo)halides, involves the usage of Lewis acid—base adducts or quantum dots (QDs). However, here one concern is the long-term phase stability, since pure FAPbI₃ perovskites revert to their yellow phase within weeks.

The recent work by Salim, Masi, et al. from the Mora-Seró group at the Institute for Advanced Materials (INAM) in Castellón, Spain, addresses this phase stability challenge by employing a combination of an *N*-methylpyrrolidone adduct and PbS QDs. The authors could show that, when processed in air, the increased presence of Pb–O bonds could mitigate the propagation of the yellow phase. This slows down the degradation to the yellow phase from 21 to 145 days.

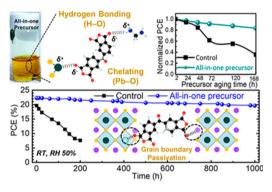
This work shows an important alternative in stabilizing pure $FAPbI_3$ perovskites without elaborate cation/anion additive engineering using instead only adducts and QDs. This potentially simplifies the overall fabrication process, since simpler precursors are used that have a less complicated nucleation process. Hence, this work represents a promising

direction for the future for achieving phase-stable $FAPbI_3$ perovskites. Michael Saliba

ALL-IN-ONE LEWIS BASE FOR ENHANCED PRECURSOR AND DEVICE STABILITY IN HIGHLY EFFICIENT PEROVSKITE SOLAR CELLS (LETTER)

Jun Zhu, Dong Hoe Kim, Ji Dong Kim, Dong Geon Lee, Won Bin Kim, Shi wang Chen, Jun Young Kim, Jae Myeong Lee, Hyemin Lee, Gill Sang Han*, Tae Kyu Ahn*, and Hyun Suk Jung*

ACS Energy Lett. 2021, 6 (10), 3425–3434 DOI: 10.1021/acsenergylett.1c01465



An important first step when considering the performance stability of PSCs is to stabilize the precursor solution. Hyun Suk Jung and co-workers tackle aspects of the stabilization of both precursors and device performance through the introduction of diphthalic anhydride-based Lewis base additives. The Pb²⁺ and FA⁺ cations in the precursor solution and in the perovskite crystals interact with the Lewis base. The precursors solution exhibits excellent stability at 85% ambient storage conditions, and the solar cells retain 90% of their initial efficiency after 1000 h of heating at 80 °C (thermal) or 50% relative humidity atmospheric testing without encapsulation. In addition, the PCE is increased to 22.43% by suppressing the grain boundary defects.

These research efforts demonstrate the importance of stabilization steps introduced from precursor solution to post-treatment of the perovskite films. These developments pave the way for successful commercialization of PSCs in the near future. Lioz Etgar

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Notes

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