Study reveals a way to enhance the efficiency of perovskite solar cells

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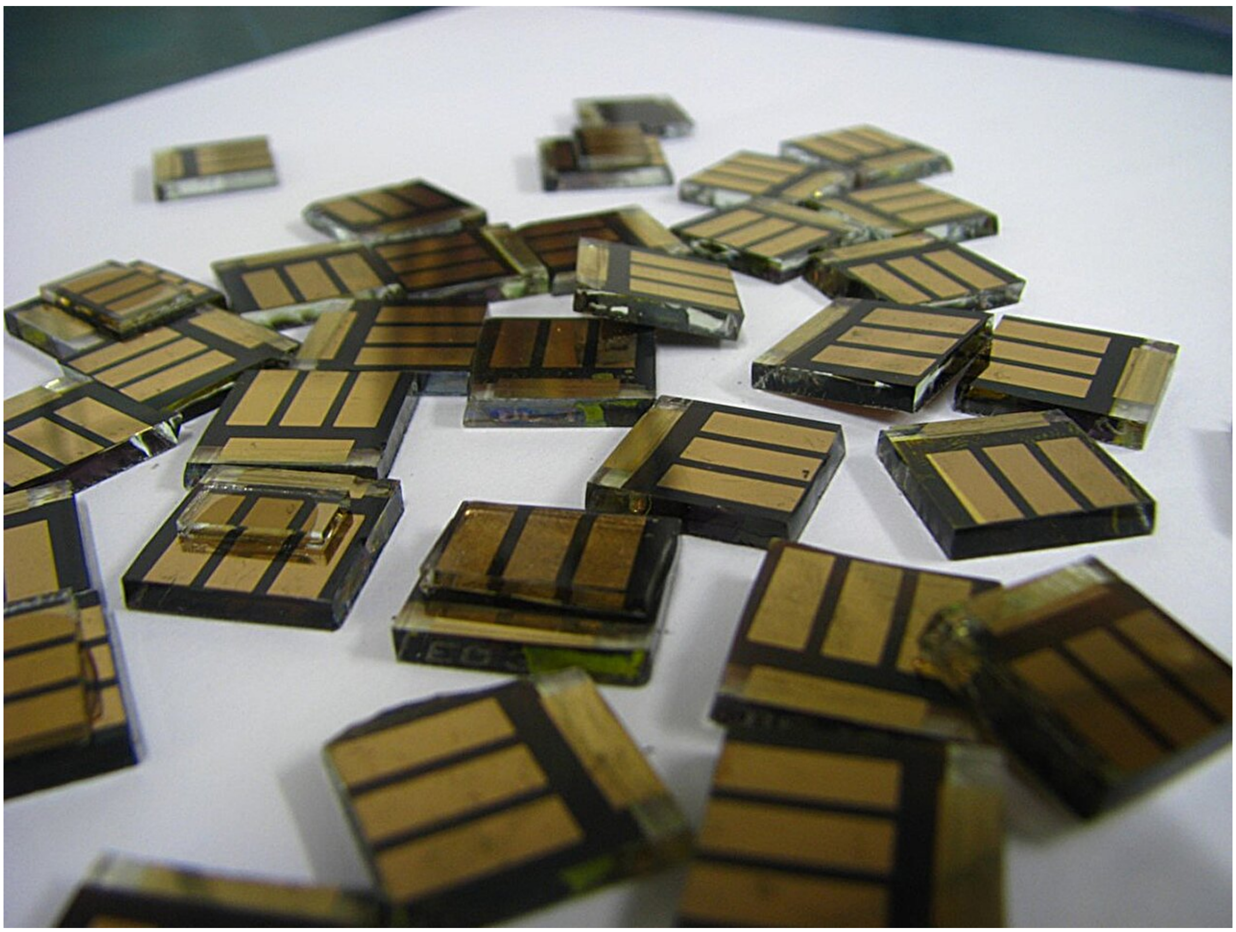

Using 4PTSC as a multifunctional additive greatly improves crystal growth in tin-halide perovskites, reducing the number of defects that typically hamper efficiency. Moreover, thanks to the chemical properties of this compound, oxidation and moisture infiltration are minimized, which boosts the durability of the material. Credit: University of Oxford Press Office. https://openverse.org/image/279011b5-abb4-47c9-9e28-e5b002d50b7a

Solar energy is one of humanity's best bets against the ongoing energy crises and climate change. With solar panels becoming an attractive energy solution, both in open fields and on rooftops in urban areas, scientists are diligently working to advance existing photovoltaic technologies and achieve new heights in sustainability. While many types of photovoltaic materials are being studied, perovskites are undoubtedly among the most promising due to their potential for low-cost production and higher efficiency.

In particular, tin halide perovskites (Sn-HPs) serve as powerful alternatives to the exceptionally high-performing lead (Pb)-based perovskites. Given that Sn is significantly less toxic to the environment than Pb, research into Sn-HPs is a worthwhile endeavor. Unfortunately, perovskite solar cells (PSCs) made from Sn-HPs still face several challenges that need to be addressed.

Specifically, the rapid and disordered crystallization during production leads to the formation of defects in the crystal structure of the perovskite layer, which hampers conversion efficiency. Additionally, Sn-HPs suffer from low stability and high sensitivity to moisture and ambient conditions, limiting the overall lifetime of PSCs made from them.

Now, however, a research team from Korea may have found an elegant and efficient solution to these issues. Their study was recently published in *Advanced Energy Materials* and was led by Associate Professor Dong-Won Kang from Chung-Ang University. In this study, the team revealed that introducing 4-Phenylthiosemicarbazide (4PTSC) as an additive during the production of Sn-HPs can boost the performance of PSCs.

Through extensive analyses and experimental comparisons between regular Sn-HP PSCs and those containing the proposed additive, the researchers showcased the multiple functionalities of 4PTSC as an additive.

"We purposely chose a multifunctional molecule that acts as a coordination complex and a reducing agent, passivates defect formation, and improves stability," explains Kang. But what does this mean?

Since 4PTSC functions as a coordinating ligand, it can effectively regulate the process of crystal growth. On the one hand, the π-conjugated phenyl ring in the 4PTSC molecule promotes preferred crystal growth orientation, minimizing the formation of defects. Interestingly, 4PTSC also passivates any defects that do form through the chemical coordination of 4PTSC and SnI_2.

In turn, this shields the perovskite surface and prevents uncoordinated Sn^{2+} and halide ions from participating in unwanted reactions. What's more, the $–NH_2$ nucleophilic sites in 4PTSC further hinder SnI_2 oxidation and ion migration, improving the stability of the PSCs.

Thanks to this powerful additive, the researchers were able to produce PSCs with unprecedented performance. "The 4PTSC-modified devices achieved a peak efficiency of 12.22% with an enhanced open-circuit voltage of 0.94 V and exhibited superior long-term stability, retaining almost 100% of the initial power conversion efficiency, even after 500 h and about 80% after 1200 h in ambient conditions without any encapsulation. This is different from the marked degradation observed in control devices within the first 300 h," highlights Kang.

Given that Sn-HPs are relatively inexpensive to manufacture and demonstrate good performance and great durability, the findings of this study could pave the way to more accessible and long-lasting solar panels . In turn, this can help in making energy cheaper for the general population while staying in line with current sustainability goals.

"Addressing the key challenges of Sn-HPs and significantly improving their performance aligns with our goal of contributing to developing efficient and sustainable renewable energy solutions, thereby advancing green technologies and promoting a sustainable future," concludes Kang.

More information: Padmini Pandey et al, 4-Phenylthiosemicarbazide Molecular Additive Engineering for Wide-Bandgap Sn Halide Perovskite Solar Cells with a Record Efficiency Over 12.2%, *Advanced Energy Materials* (2024). DOI: 10.1002/aenm.202401188

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