PRESS RELEASE

GIST Researchers Develop New Defect Passivation Strategy for Perovskite Solar Cells

New defect passivation strategy for improved power conversion efficiency and stability of perovskite solar cells

Polycrystalline formamidinium lead iodide (FAPbI₃), widely used for making perovskitebased solar cells due to its superior optoelectronic properties, suffers from defects in its crystalline structure. Researchers from the Gwangju Institute of Science and Technology (GIST) introduced hexagonal polytype perovskite (6H) into the cubic polytype (3C) FAPbI₃ to reduce these defects, which led to improved power conversion efficiency and operational stability of perovskite solar cells, when compared with their existing counterparts.



Image title: Improving power conversion efficiency and stability of perovskite solar cells with defect engineering Image caption: Scientists introduced hexagonal polytype perovskite (6H) into cubic polytype (3C) FAPbI₃, so-called α -phase and engineered its defects. This defect passivation led to improvement in power conversion efficiency and operational stability of perovskite solar cells.

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Solar energy is a promising way of reducing our dependence on fossil-fuel-based energy resources and opt for cleaner energy forms. Over the years, solar cells that can harness this renewable energy have undergone significant progress.

Metal-halide perovskite has gained significant attention as a promising light-absorbing material for solar cells due to their exceptional optoelectronic properties which enable them to efficiently generate energy from sunlight.

A popular choice of material for building high power conversion efficiency (PCE) perovskite solar cells (PSCs) is polycrystalline formamidinium lead iodide (FAPbI₃) owing to its narrow energy band gap. Despite their superior optoelectronic properties and versatility, polycrystalline perovskites like FAPbI₃ often suffer from defects (imperfections) in their crystal structure which are harmful to the structural stability and carrier dynamics, ultimately affecting their energy conversion abilities.

To fill this gap, a team of researchers led by Professor Hobeom Kim from the Gwangju Institute of Science and Technology (GIST) has developed a new defect passivation strategy, a process to significantly reduce defects and improve PCE and stability of perovskite solar cells. In their recent study published on 04 July 2024 in <u>Nature Communications</u>, the team reported introducing hexagonal polytype (6H) [different structural forms with the same composition] perovskite into the cubic polytype (3C) FAPbI₃, which led to a remarkable increase in their PCE when compared to their counterparts.

But why use 6H perovskite polytype? "A typical approach so far has been to introduce an external chemical reagent to deal with the defect problem. However, bringing in external reagents could directly impact the crystalline quality of the perovskite during crystal growth, so our work does not rely on such stabilizers. Instead, we employ a chemically identical polytype of perovskite, 6H polytype containing a corner-sharing component that effectively suppresses the formation of defects in perovskite," explains Prof. Kim.

The researchers incorporated 6H perovskite into FAPbI₃, by using excess of lead iodide and methylammonium chloride, thereby creating a component that intervened with the dominant defect site (halide vacancies, V_1^+) of α -phase cubic polytype (3C) FAPbI₃. They found that the 6H phase improved the structural integrity and carrier dynamics of FAPbI₃. This led to an ultralong carrier lifetime of greater than 18 microseconds, PSCs with PCEs of 24.13% and a module with PCEs of 21.92% (certified power conversion efficiency of 21.44%) with long-term operational stability.

The researchers suggested that the 3C/6H hetero-polytypic perovskite design might be the closest to the ideal configuration of a polycrystalline perovskite film. The study demonstrated how engineering defects in perovskite can accelerate the development of advanced PSCs for personal and commercial uses, such as in rooftop solar panels, wearable electronics, and portable chargers.

"Perovskite solar cells offer a transformative solution for achieving carbon neutrality and addressing global warming. Their efficiency, versatility, and reduced environmental impact make them an essential component in the transition to a sustainable future," concluded Prof. Kim.

Reference

| Title of original | Shallow-level defect passivation by 6H perovskite polytype for highly |
|-------------------|---|
| paper: | efficient and stable perovskite solar cells |
| Journal: | Nature Communications |
| DOI: | <u>10.1038/s41467-024-50016-6</u> |

About the Institute

The Gwangju Institute of Science and Technology (GIST) was founded in 1993 by the Korean government as a research-oriented graduate school to help ensure Korea's continued economic growth and prosperity by developing advanced science and technology with an emphasis on collaboration with the international community. Since that time, GIST has pioneered a highly regarded undergraduate science curriculum in 2010 that has become a model for other science universities in Korea. To learn more about GIST and its exciting opportunities for researchers and students alike, please visit: http://www.gist.ac.kr/

About the author

Professor Hobeom Kim is currently an Assistant Professor at the School of Materials Science and Engineering in Gwangju Institute of Science and Technology (GIST). His group focuses on the development of optoelectronic semiconductor materials and their applications for nextgeneration LEDs, solar cells, and neuromorphic devices. Prior to joining GIST, he received his Ph.D in Materials Science and Engineering from Pohang University of Science and Technology (POSTECH), South Korea in 2017 and performed research as a postdoc in École Polytechnique Fédérale de Lausanne (EPFL), Switzerland from 2018 to 2022.

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