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## Stabilize lead-free perovskite solar cells



(Left) Molecular structure of perovskite (blue) with zinc-based coating (green). (Right) The FP process the researchers used to coat the perovskite with a zinc-based coating. Credit: NTU Singapore.

Solar cells made from perovskite, a material capable of capturing sunlight and converting it to electricity, have great potential to replace silicon solar cells.

Despite being superior in performance, efficient and cheaper to produce, perovskite Solar cells have not yet been produced commercially for the consumer market.

Perovskites decompose when they react with moisture and oxygen or when they are exposed to light, heat or are used for a long period of time, leading to concerns that small amounts of lead. Toxic heavy metals present in perovskite solar cells can pollute the environment when the solar cells are damaged or discarded.

Lead comes from both the perovskite material and the compound used to make the components of perovskite solar cells, known as coatings.

Now, research by scientists from Nanyang Technological University, Singapore (NTU Singapore) and the Institute of Materials Research and Engineering (IMRE) under the Agency for Science, Technology and Research (A\*STAR) in Singapore has provided capping of materials based on non-toxic metals being used in the production of perovskite solar cells.

Their research, published in *Nature Energy* in February 2023 and led by Professor Sum Tze Chien, Director of the Institute for Advanced Study at NTU and Associate Dean (Research) of NTU's School of Science, and Professor Lam Yeng Ming, Chair of NTU's Materials Science and Engineering may join perovskite solar cells one step closer to market. Perovskite solar cells are made of several layers of materials, including a light-collecting perovskite layer and a coating. A coating is applied over the perovskite layer to protect the solar cell from environmental stresses such as temperature and humidity, while increasing the battery's performance.



To make the zinc-based coating, the researchers dissolved the chemicals and coated the solution on the perovskite layer in the glove box. The glove box protects the perovskite from oxygen and moisture in the environment before it is coated. Credit: NTU Singapore.

To make sure that the coating is compatible with the underlying perovskite layer, researchers often use a method called the half-precursor (HP) method to fabricate the coating. One of the first chemical precursors deposited on the perovskite layer provides another precursor. Through a process known as cation exchange reaction, the deposited precursors then react with the lead ions present in the underlying perovskite layer to form the lead-based chemical compound that makes up the coating.

Due to the HP method, lead is also present in the protective cap. A method that allows the use of non-toxic metals in coatings would be a game changer for perovskite solar cells.

To make perovskite solar cells more environmentally friendly, NTU scientists devised a method, known as the full precursor solution (FP) method, to synthesize a coating that does not contain lead.

Using the FP method, the scientists coated perovskite with a solution containing metal halide salts a compound made up of metals and elements including chlorine, fluorine, and iodine—and commonly known phenethylammonium iodide (PEAI) Apply to perovskite to improve the performance of perovskite solar cells. PEAI contains ammonium, a positively charged ion containing nitrogen and hydrogen, which is essential for chemical reactions.

## **Guided zinc-based compounds**

The researchers found that a zinc-based compound PEA<sub>2</sub>ZnX<sub>4</sub> synthesized by this method was the most effective covering material among the other materials tested.

Unlike the HP method, it is not necessary to draw lead ions from the underlying perovskite layer to form this protective coating when using the FP method. This paves the way for the use of non-toxic metals in coatings.

According to the researchers, the FP process is also more efficient than the HP method in making coatings because the chemicals in the solution can react with each other directly on the surface of the perovskite.



The researchers used a vacuum evaporation system to synthesize the remaining layers of perovskite solar cells, a method commonly used to make perovskite solar cells. Credit: NTU Singapore.

Fabrication of PEA<sub>2</sub>ZnX<sub>4</sub> coated solar cells, the researchers first dissolved the zinc halide and PEAI salts in a solvent called acetonitrile, which is commonly used for industrial applications. They then placed the solution on a rapidly rotating layer of perovskite that was attached to a conductive glass substrate to form a thin and uniform layer—a process known as spin coating.

The coated perovskite is heated at 100°C for 10 min to bond the coating to the surface of the perovskite. The researchers then used a process called vacuum evaporation, in which the material is heated in a vacuum chamber to create vapors deposited on the coated perovskite, to synthesize the other layers of the battery. perovskite sun.

Using the FP method, the scientists created a 1-inch x 1-inch prototype solar cell coated with a zincbased compound. The scientists examined the zinc-based coating using electron microscopy and spectroscopy and found that it did not affect the electrical properties of the underlying perovskite layer. The coating also helps to mask surface defects of the perovskite layer and improve its light-gathering ability.

The researchers say their method contributes to efforts to make perovskite solar cells more environmentally friendly. For example, this method could be used in conjunction with the lead-free perovskite material currently being explored to develop solar cells that do not release toxic metals when removed.

This method also opens up the possibility of fabricating the composition of the coating to improve the performance of perovskite solar cells.

"One of the biggest disadvantages of using perovskite solar cells is their impact on the environment. By allowing the use of zinc and other non-toxic metals in the coating, our innovation has the potential to solve a major obstacle preventing widespread use of perovskite solar cells," said Dr. Ye Senyun, a researcher from NTU's School of Mathematical and Physical Sciences, one of the researchers. The main study of the study said.

Co-author Dr Rao Haixia, a research fellow from NTU's School of Materials Science and Engineering, said: "Since our method does not require extraction lead ions from perovskite, this allows the possibility of using a variety of materials to increase the stability and efficiency of perovskite solar cells."

The researchers found that the built solar cells are just as efficient at converting sunlight into energy as conventional perovskite solar cells. In experiments with simulated sunlight, the solar cell was able to convert 24.1% of the light captured into electricity, which is close to the highest efficiency achieved by perovskite solar cells to date. For comparison, the highest certified light conversion efficiency of silicon solar cells is 25.2%.



(Left) Diagram showing the different layers of a perovskite solar cell coated with a zinc-coated material made by the researchers. (Right) The green dotted rectangle represents the active region of a perovskite solar cell that captures sunlight and converts it into electricity. Credit: NTU Singapore.

"The coating is a key component of perovskite solar cells. This new approach to coating design is a major milestone in the design of perovskite solar cells with enhanced properties," said Professor Michael. Grätzel, Director of the Photonics and Interfaces Laboratory at the École Polytechnique Fédérale de Lausanne in Switzerland, who was not involved in the study.

The prototype also exhibited good reproducibility, with an average light conversion rate of nearly 23% across the 103 cells tested. It has a long lifespan, maintaining more than 90% of its light-to-electricity conversion capacity for more than 1,000 hours at full capacity.

The performance of the device is also more stable at high temperatures than devices without coating.

"By expanding the library of materials that can be used, our findings open up new opportunities to develop superior materials for coatings, for efficient perovskite solar cells," said Professor Sum. and more stable". "This lead-free protective capping method could also be extended to other applications such as perovskite light-emitting devices, lasers and detectors."

Professor Lam added: "As fossil fuels are rapidly depleting, we need to harness renewable energy sources such as solar energy even better. Perovskite solar cells are environmentally friendly and stable. could be the answer, and this innovation has the potential to accelerate the adoption of perovskite on a broader scale than solar cells for solar energy harvesting."

Scientists are working on replicating the method for full-size fabrication solar battery. They are also in the process of filing a patent with NTUitive, the innovation and enterprise arm of NTU Singapore.

Details of the study can be found in *Nature Energy*.

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