Study: Chemical nature of defects that cause trap states in metal halide perovskite solar cells

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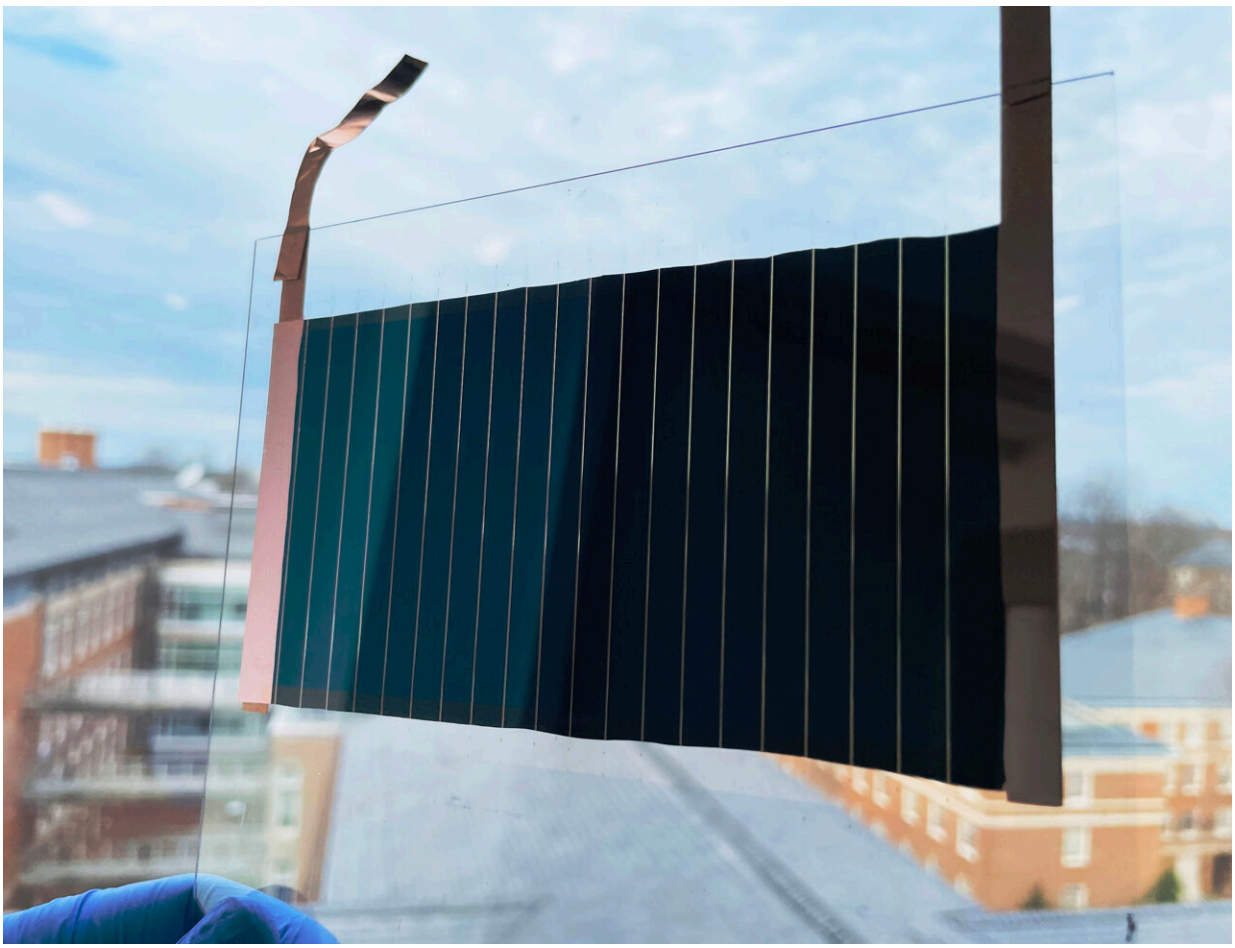

Credit: Zhenyi Ni.

In recent years, engineers worldwide have been working to create alternative and sustainable energy solutions, such as solar cells. Solar cells made of perovskites, a class of semiconductors with a characteristic structure and advantageous properties, are among the most promising solar technologies, as they have recently hit record-high efficiencies of around 25.5%.

Despite their huge potential and their advantageous qualities, perovskites and other semiconductors can be adversely affected by what are known as 'trap states.' These are states that cause charge carriers (i.e., electrons and holes) to be trapped inside a material.

Trap states caused by structural defects can affect both the efficiency and stability of perovskite solar cells. More specifically, these states can capture light-generated charge carriers, leading to electrical energy losses.

Researchers at University of North Carolina and University of Toledo have recently carried out a study that closely examined the evolution of trap state-related defects during the degradation of metal halide perovskite solar cells. Their paper, published in *Nature Energy*, offers new valuable insight that could help to significantly improve the performance of perovskite-based solar technologies.

"Trap states are like holes in a highway, depending on how shallow or deep they are, they will either slow a car down or trap it completely," Jinsong Huang, one of the researchers who carried out the study, told TechXplore. "Determining how to further reduce trap states in the current star photovoltaic product (i.e., perovskite solar cells) is an important and challenging task. In our previous work, we solved one big problem, which was finding out where the trap states are and how deep they are in perovskite solar cells, pointing out what should be addressed to further reduce the trap states."

As part of their new study, Huang and his colleagues built on their previous work to address a further interesting research question. Their objective was to better understand the chemical nature of trap states that limit the efficiency and stability of metal halide perovskite solar cells. This would in turn allow them to devise strategies or solar cells designs that can reduce the presence of trap states and thus minimize their adverse effects.

"In perovskite solar cells, trap states are caused by defects, which are usually the result of some imperfect crystal structures in perovskite materials," Zhenyi Ni, another researcher who conducted the study, said. "The good thing is that defects in perovskites that cause trap states are commonly electrically charged, which means they can move under external electric fields. Keeping this in mind, we were able to trigger the movement of defects in perovskite solar cells by applying continuous reverse or forward biases and measure their spatial distributions with a capacitance measurement technique: drive-level capacitance profiling (DLCP)."

Using DLCP, a technique typically used to study amorphous and polycrystalline materials, the researchers were able to determine how defects in perovskite solar cells moved when specific electrical fields were applied to them. This then allowed them to gather information about the charge states of these defects (i.e., whether they are positive or negative) and ultimately unveil their chemical nature.

"The degradation of metal halide perovskite solar cells is closely related to the evolution of defects in perovskites," Huang explained. "Where the defects start to generate represents the location that the degradation of the solar cells starts, just like a piece of bread, for example, always begins to rot where mold starts to grow."

When they started conducting their study, Huang and his colleagues were

aware that defects in perovskites evolve over time, yet the exact degradation mechanisms associated with this evolution was poorly understood. To find out more about these mechanisms, they had to closely examine how defects changed or evolved during the degradation of perovskite solar cells.

"To do this, we used DLCP, as we know that it can help to create a profile of both the energetic and spatial distributions of trap states in perovskite solar cells, thus allowing us to track the defect generation and movement in perovskite solar cells during degradations," Huang said. "Knowing where different species of defects start to generate and how their density change allowed us to determine how the perovskite solar cell degrades under reverse bias and illumination."

The recent study by this team of researchers could have important implications for the development of solar technologies based on perovskites. Most notably, Huang and his colleagues were able to solve a long-standing challenge in the development of perovskite solar cells, namely gaining a better understanding of the chemical nature of defects causing trap states.

Their paper delineates the types of defects that are more detrimental to the performance of metal halide perovskite solar cells and should thus be addressed beforehand to reduce the density of trap states. In the future, these results could inform the development of effective strategies to reduce the impact of defects and increase both the efficiency and stability of this promising class of solar cells.

"Perovskite solar cells have a great potential for further bringing down the cost of solar power, while improving the efficiency and stability of perovskite solar cells is still the most important direction," Huang said. "Now any further improvement of the efficiency and stability of perovskite solar cells has to rely on the reducing defects in perovskites to

minimize any unwanted energy losses and our discovery points out the direction for future research."

More information: Zhenyi Ni et al, Evolution of defects during the degradation of metal halide perovskite solar cells under reverse bias and illumination, *Nature Energy* (2021). DOI: 10.1038/s41560-021-00949-9