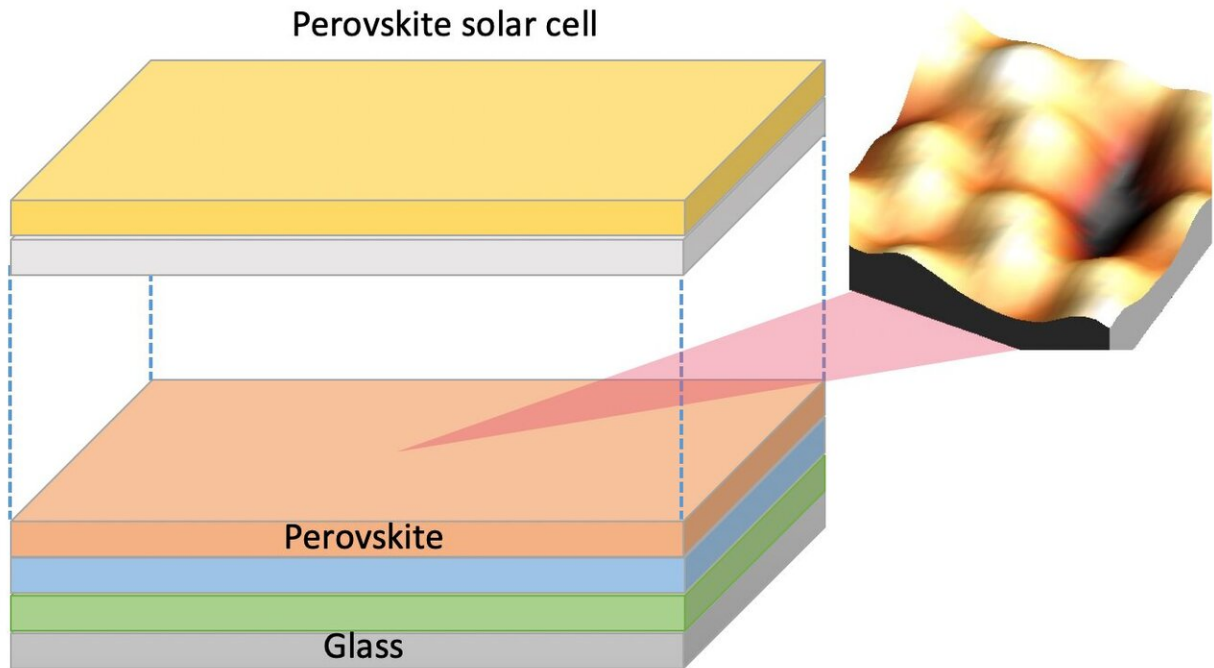


Scratching the surface of perovskites

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OIST's Energy Materials and Surface Science Unit studies perovskite solar cells, which are formed by layering perovskite compounds on top of other materials like glass. Credit: Okinawa Institute of Science and Technology

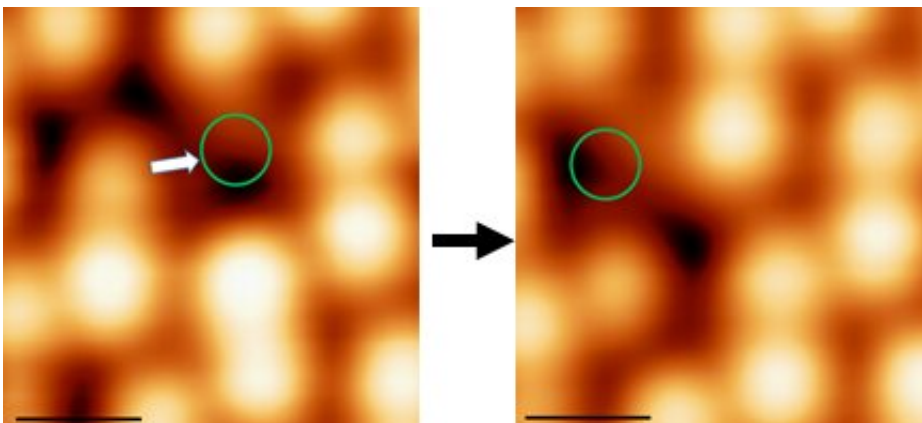
Versatile compounds called perovskites are valued for their application in next generation solar energy technologies. Despite their efficiency and relative cheapness, perovskite devices have yet to be perfected; they often contain atomic-level structural defects.

Professor Yabing Qi and his team in the Energy Materials and Surface Sciences Unit at OIST, in collaboration with researchers at the University of Pittsburgh, U.S., have, for the first time, characterized the structural defects that prompt the movement of ions, destabilizing the perovskite materials. The researchers' findings, published in *ACS Nano*, may inform future engineering approaches to optimize perovskite solar cells.

"For a long time, scientists have known structural defects exist, but didn't understand their precise chemical nature," said Collin Stecker, an OIST Ph.D. student and the first author of the study. "Our study delves into fundamental characteristics of perovskite materials to help device engineers further improve them."

Surface-level issues

Perovskite compounds share a unique structure that makes them useful in electronics, engineering, and photovoltaics. They are exceptional at absorbing light, as well as generating and transporting [charge carriers](#) responsible for current in semiconductor materials. Sandwiching perovskite materials between other functional layers forms perovskite solar cells. However, defects in the perovskite layer can disrupt charge transfer between the perovskite and adjacent layers of the cell, hindering the device's overall performance and stability.



This image of a perovskite surface shows the shifting of ions across the surface, and the vacancies causing these movements. Credit: Okinawa Institute of Science and Technology

To understand the electronic and dynamic properties of these perovskite defects, the OIST researchers used a method called scanning tunneling microscopy to take high-resolution images of the movements of individual ions on the perovskite surfaces.

Upon analyzing these images, Stecker and his colleagues noticed groups of vacant spaces across the surfaces where atoms were missing. In addition, they saw that pairs of Br⁻ (bromide) ions on the perovskite surfaces were shifting and changing direction. The researchers' collaborators at the University of Pittsburgh performed a series of theoretical calculations to model the pathways these ions took, supporting these experimental observations.

The OIST scientists concluded that the surface vacancies were likely causing these ions to move across the [perovskite materials](#). Understanding this mechanism of ion movement may later help scientists and engineers mitigate the structural and functional consequences of these defects.

The researchers acknowledged that, although perovskites are promising alternatives to the widely used silicon, the technology needs to be refined before it's commercialized.

"These [perovskite](#) surfaces are much more dynamic than we previously anticipated," said Stecker. "Now, with these new findings, we hope engineers can better account for the effect of defects and their motion in order to improve devices."

More information: Collin Stecker et al. Surface Defect Dynamics in Organic–Inorganic Hybrid Perovskites: From Mechanism to Interfacial Properties, *ACS Nano* (2019). [DOI: 10.1021/acsnano.9b06585](https://doi.org/10.1021/acsnano.9b06585)

Provided by Okinawa Institute of Science and Technology

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