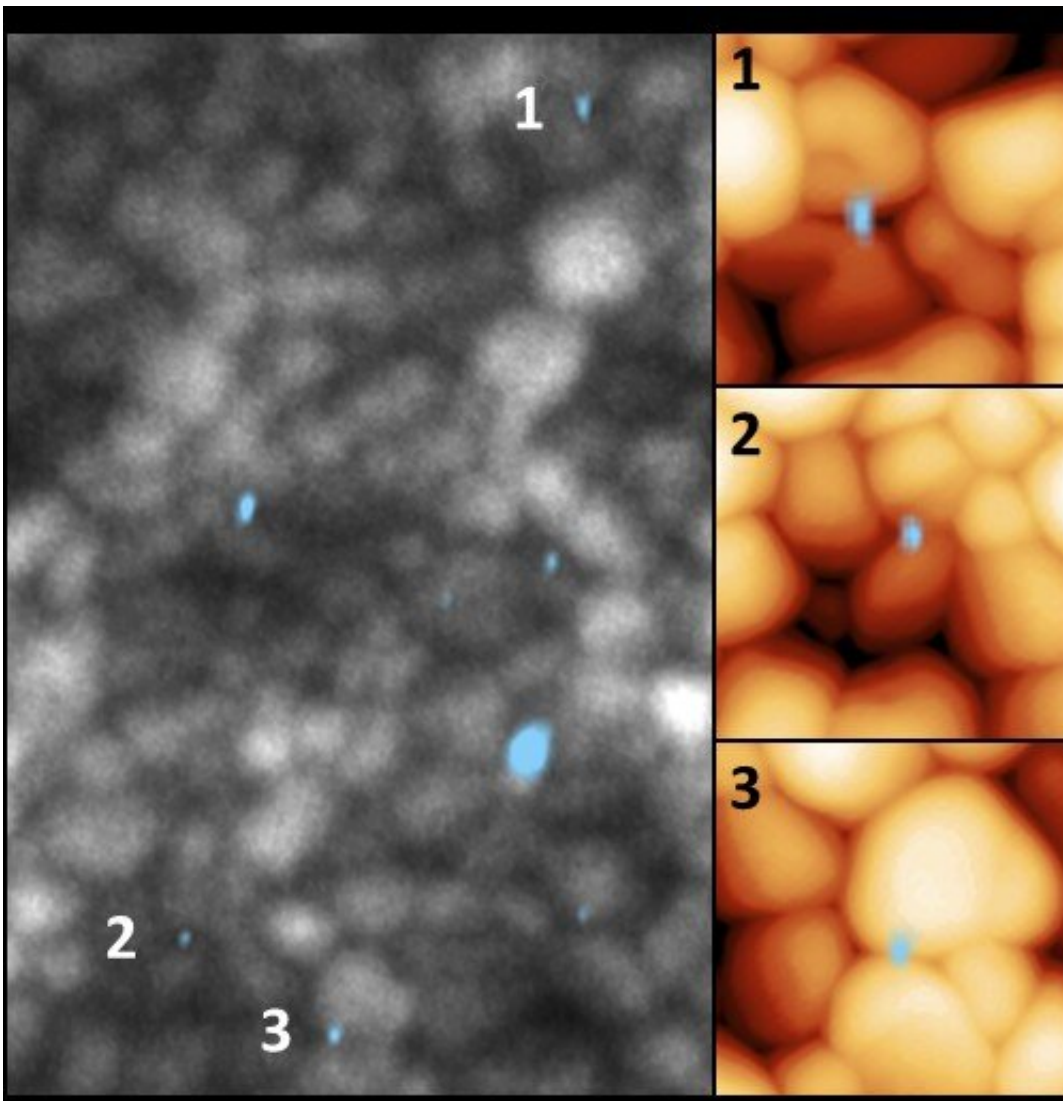


Scientists pinpoint origin of defects that sap potential of next gen solar tech

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The trap clusters (light blue) were found to exist at the boundaries between certain grains. Credit: OIST

In the last decade, perovskites—a diverse range of materials with a specific crystal structure—have emerged as promising alternatives to silicon solar cells, as they are cheaper and greener to manufacture, while achieving a comparable level of efficiency.

However, perovskites still show significant performance losses and instabilities, particularly in the specific materials that promise the highest ultimate efficiency. Most research to date has focused on ways to remove these losses, but their actual physical causes remain unknown.

Now, in a paper published today in *Nature*, researchers from Dr. Sam Stranks's group at Cambridge University's Department of Chemical Engineering and Biotechnology and Cavendish Laboratory, and Professor Keshav Dani's Femtosecond Spectroscopy Unit at OIST in Japan, identify the source of the problem. Their discovery could streamline efforts to increase the efficiency of perovskites, bringing them closer to mass-market production.

Perovskite materials are much more tolerant of defects in their structure than silicon [solar cells](#), and previous research carried out by Stranks's group found that to a certain extent, some heterogeneity in their composition actually improves their performance as solar cells and light-emitters.

However, the current limitation of [perovskite](#) materials is the presence of a "deep trap" caused by a certain type of defect, or minor blemish, in the material. These are areas in the material where energised [charge carriers](#) can get stuck and recombine, losing their energy to heat, rather than converting it into useful electricity or light. This undesirable recombination process can have a significant impact on the efficiency and stability of solar panels and LEDs.

Until now, very little was known about the cause of these traps, in part

because they appear to behave rather differently to traps in traditional solar cell materials.

In 2015, Dr. Stranks and colleagues published a Science paper looking at the luminescence of perovskites, which reveals how good they are at absorbing or emitting light. "We found that the material was very heterogeneous; you had quite large regions that were bright and luminescent, and other regions that were really dark," says Stranks. "These dark regions correspond to power losses in solar cells or LEDs. But what was causing the power loss was always a mystery, especially because perovskites are otherwise so defect-tolerant."

Due to limitations of standard imaging techniques, the group couldn't tell if the darker areas were caused by one, large trap site, or many smaller traps, making it difficult to establish why they were forming only in certain regions.

Later on in 2017, Professor Keshav Dani's group at OIST published a paper in *Nature Nanotechnology*, where they made a movie of how electrons behave in semiconductors after absorbing light. "You can learn a lot from being able to see how charges move in a material or device after shining light. For example, you can see where they might be getting trapped," says Dani. "However, these charges are hard to visualize as they move very fast—on the timescale of a millionth of a billionth of a second; and over very short distances—on the length scale of a billionth of a metre."

On hearing of Dani's work, Dr. Stranks reached out to see if they could work together to address the problem visualising the dark regions in perovskites.

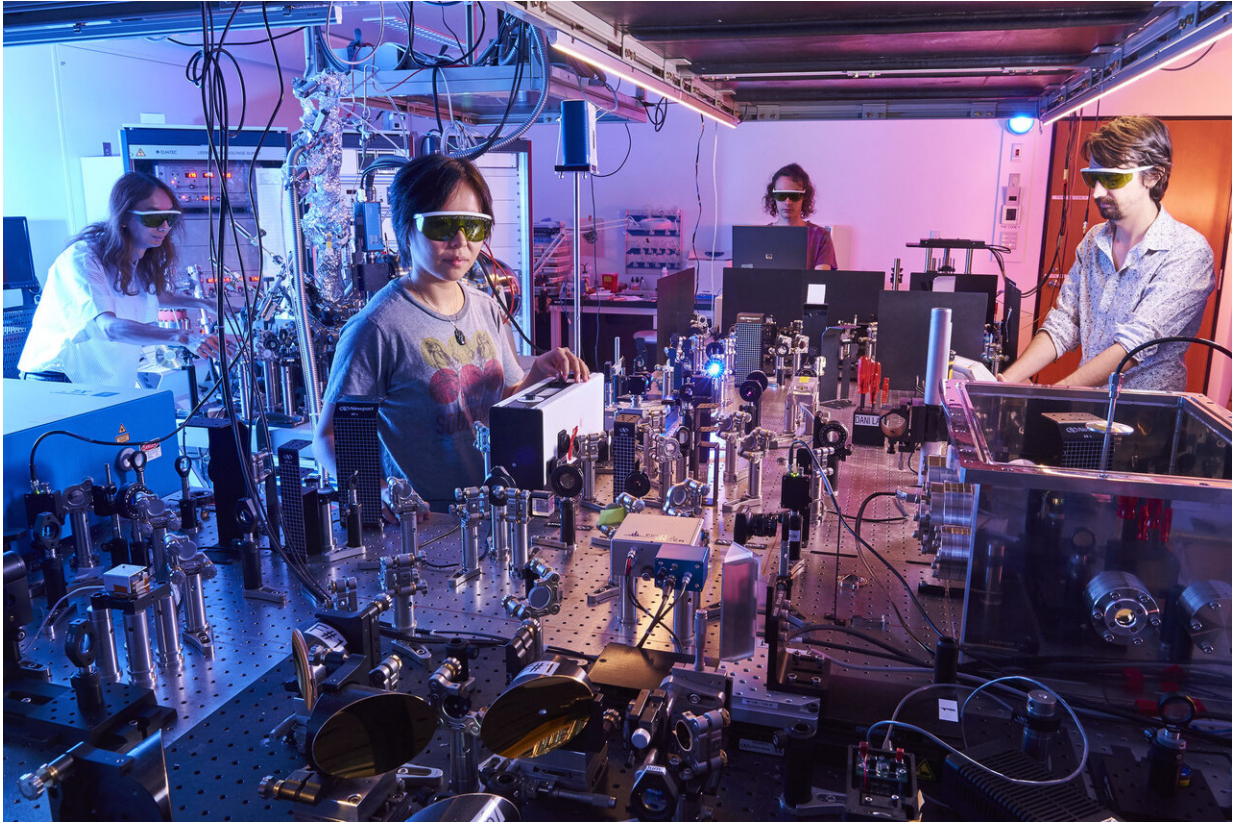
The team at OIST used a technique called photoemission electron microscopy (PEEM) for the first time on perovskites, where they probed

the material with ultraviolet light and built up an image based on how the emitted electrons scattered.

When they looked at the material, they found that the dark regions contained traps, around 10-100 nanometers in length, which were clusters of smaller atomic-sized trap sites. These trap clusters were spread unevenly throughout the perovskite material, explaining the heterogeneous luminescence seen in Stranks's earlier research.

Intriguingly, when the researchers overlaid images of the trap sites onto images that showed the crystal grains of the perovskite material, they found that the trap clusters only formed at specific places, at the boundaries between certain grains.

To understand why this only occurred at certain grain boundaries, the groups worked together with Professor Paul Midgley's team from Cambridge University's Department of Materials Science and Metallurgy using a technique called scanning electron diffraction to create detailed images of the perovskite crystal structure. The project team made use of the electron microscopy setup at the ePSIC facility at the Diamond Light Source Synchrotron, which has specialized equipment for imaging beam-sensitive materials, like perovskites.



Researchers from the OIST Femtosecond Spectroscopy Unit conduct experiments in the laser lab. Credit: OIST/Togo

"Because these materials are very beam-sensitive, typical techniques that you would use to probe local crystal structure on these length scales will quite quickly change the material as you're looking at it, which can make interpreting the data very difficult" explains Tiarnan Doherty, a Ph.D. student in Stranks's group and co-lead author of the study. "Instead, we were able to use very low exposure doses and therefore prevent damage.

"From the work at OIST, we knew where the trap clusters were located, and at ePSIC, we scanned around those same areas to see the local structure. We were then able to quickly pinpoint unexpected variations

in the crystal structure around the trap clusters."

The group discovered that the trap clusters only formed at junctions where an area of the material with slightly distorted structure met an area with pristine structure.

"In perovskites, we have these regular mosaic grains of material and most of the grains are nice and pristine—the structure we would expect," says Stranks. "But every now and again, you get a grain that's slightly distorted and the chemistry of that grain is inhomogeneous. What was really interesting and which initially confused us, was that it's not the distorted grain that's the trap but where that grain meets a pristine grain; it's at that junction that the traps cluster."

With this understanding of the nature of the traps, the team at OIST also used the custom-built PEEM instrumentation to visualize the dynamics of the charge carrier trapping process happening in the perovskite material. "This was possible as one of the unique features of our PEEM setup is that it can image ultrafast processes—as short as femtoseconds," explains Andrew Winchester, a Ph.D. student in Prof. Dani's Unit, and co-lead author of this study. "We found that the trapping process was dominated by charge carriers diffusing to the trap clusters."

These discoveries represent a major breakthrough in the quest to bring perovskites to the solar energy market.

"We still don't know exactly why the traps are clustering there, but we now know that they do form there, and seemingly only there," says Stranks. "That's exciting because it means we now know what to target to bring up the performances of perovskites. We need to target those inhomogeneous phases or get rid of these junctions in some way."

"The fact that charge carriers must first diffuse to the [traps](#) could also

suggest other strategies to improve these devices," says Dani. "Maybe we could alter or control the arrangement of the trap clusters, without necessarily changing their average number, such that charge carriers are less likely to reach these defect sites."

The teams' research focused on one particular perovskite structure. The scientists will now be investigating whether the cause of these trapping clusters is universal across other perovskite materials.

"Most of the progress in device performance has been trial and error and so far, this has been quite an inefficient process," says Stranks. "To date, it really hasn't been driven by knowing a specific cause and systematically targeting that. This is one of the first breakthroughs that will help us to use the fundamental science to engineer more efficient devices."

More information: Performance-limiting nanoscale trap clusters at grain junctions in halide perovskites, *Nature* (2020). [DOI: 10.1038/s41586-020-2184-1](https://doi.org/10.1038/s41586-020-2184-1) , [nature.com/articles/s41586-020-2184-1](https://www.nature.com/articles/s41586-020-2184-1)

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