Self-healing crystal voids in double perovskite nanocrystal

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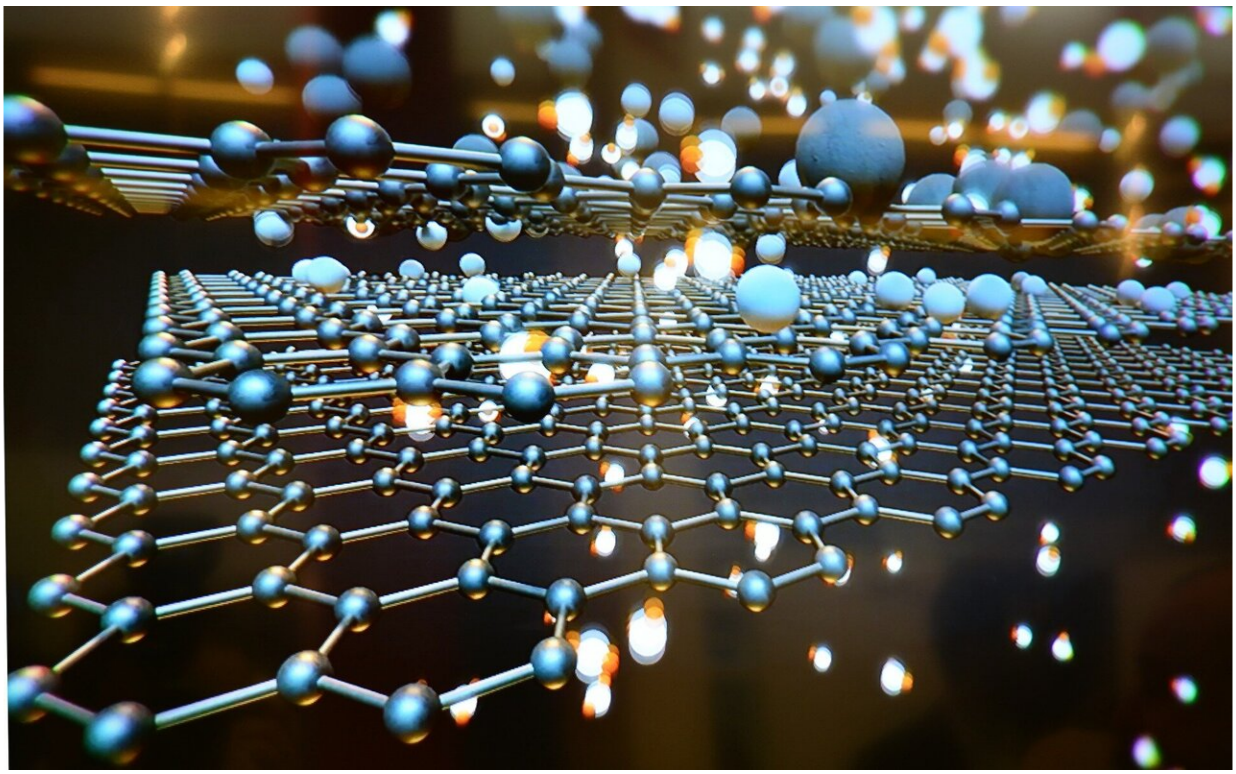

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From the Terminator to Spiderman's suit, self-repairing robots and devices abound in sci-fi movies. In reality, though, wear and tear reduce the effectiveness of electronic devices until they need to be replaced. What is the cracked screen of your mobile phone healing itself overnight, or the solar panels providing energy to satellites continually repairing the damage caused by micro-meteorites?

The field of self-repairing materials is rapidly expanding, and what used to be science fiction might soon become reality, thanks to Technion—Israel Institute of Technology scientists who developed eco-friendly nanocrystal semiconductors capable of self-healing. Their findings, recently published in *Advanced Functional Materials*, describe the process, in which a group of materials called double perovskites display self-healing properties after being damaged by the radiation of an electron beam. The perovskites, first discovered in 1839, have recently garnered scientists' attention due to unique electro-optical characteristics that make them highly efficient in energy conversion, despite inexpensive production. A special effort has been put into the use of lead-based perovskites in highly efficient solar cells.

The Technion research group of Professor Yehonadav Bekenstein from the Faculty of Material Sciences and Engineering and the Solid-State Institute at the Technion is searching for green alternatives to the toxic lead and engineering lead-free perovskites. The team specializes in the synthesis of nano-scale crystals of new materials. By controlling the crystals' composition, shape, and size, they change the material's physical properties.

Nanocrystals are the smallest material particles that remain naturally stable. Their size makes certain properties more pronounced and enables research approaches that would be impossible on larger crystals, such as imaging using electron microscopy to see how atoms in the materials move. This was, in fact, the method that enabled the discovery of self-repair in the lead-free perovskites.

The perovskite nanoparticles were produced in Prof. Bekenstein's lab using a short, simple process that involves heating the material to 100°C for a few minutes. When Ph.D. students Sasha Khalfin and Noam Veber examined the particles using a transmission electron microscope, they discovered the exciting phenomenon. The high voltage electron beam used by this type of microscope caused faults and holes in the nanocrystals. The researchers were then able to explore how these holes interact with the material surrounding them and move and transform within it.

They saw that the holes moved freely within the nanocrystal, but avoided its edges. The researchers developed a code that analyzed dozens of videos made using the electron microscope to understand the movement dynamics within the crystal. They found that holes formed on the surface of the nanoparticles, and then moved to energetically stable areas inside. The reason for the holes' movement inwards was hypothesized to be organic molecules coating the nanocrystals' surface. Once these organic molecules were removed, the group discovered the crystal spontaneously ejected the holes to the surface and out, returning to its original pristine structure—in other words, the crustal repaired itself.

This discovery is an important step towards understanding the processes that enable perovskite nanoparticles to heal themselves, and paves the way to their incorporation in solar panels and other electronic devices.

More information: Sasha Khalfin et al, Self-Healing of Crystal Voids in Double Perovskite Nanocrystals Is Related to Surface Passivation, *Advanced Functional Materials* (2021). DOI: 10.1002/adfm.202110421

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