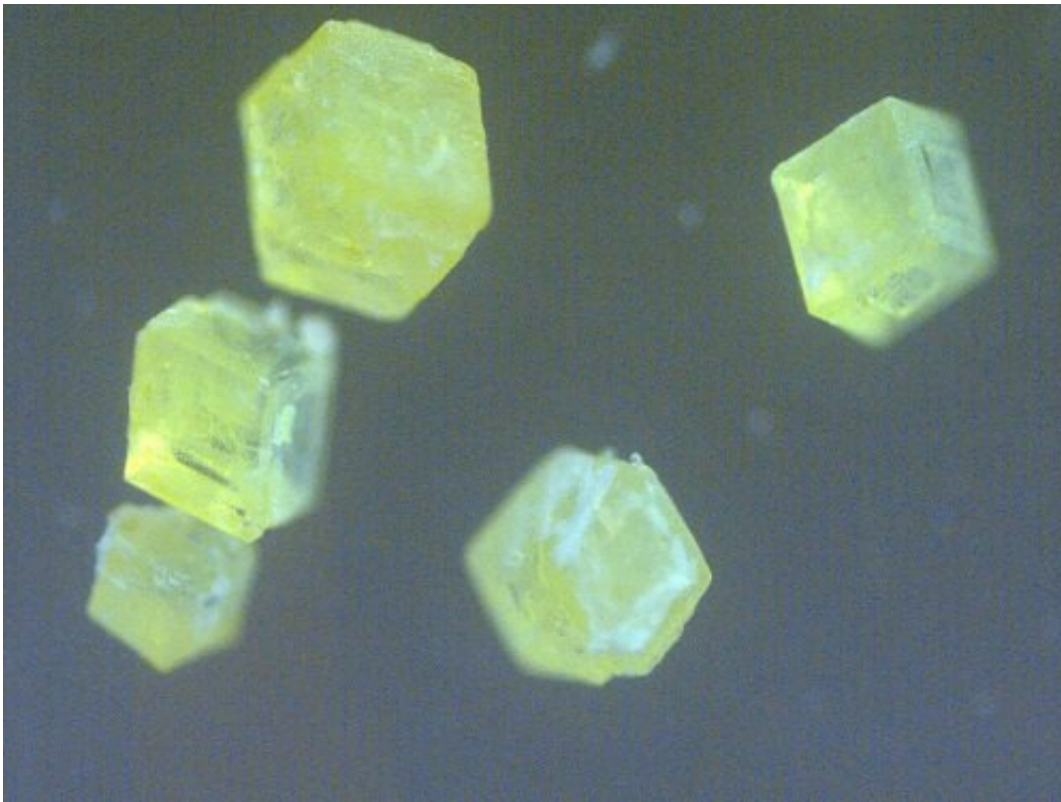


# Missing atoms in a forgotten crystal bring luminescence

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The perovskite has a strong green fluorescence. Credit: © 2017 De Bastiani

A little-studied member of the perovskite family of materials could find use in a range of electronic devices, after researchers at KAUST discovered the secret of its strong photoluminescence.

Perovskites are a wide group of materials that are known to have

remarkable optical and electronic properties. Perovskites with the general formula  $ABX_3$ , and particularly the [perovskite](#) methylammonium lead trihalide, have attracted almost all the research attention thanks to their great promise as low-cost, high-efficiency solar cell materials.

Other members of the perovskite family and perovskite derivatives are also worthy research subjects, says Michele De Bastiani, a postdoctoral researcher in Osman Bakr's group at KAUST.

De Bastiani and his colleagues have been testing  $Cs_4PbBr_6$ , a perovskite of the  $A_4BX_6$  branch of the family. This material is noted for its strong [photoluminescence](#)—the ability to absorb light at one wavelength and re-emit it at another.

The material's potential applications include color-converting coatings on LED light bulbs, lasers and photodetectors. But to be able to fine-tune the material's optoelectric properties for each application, researchers need to solve the mystery of why the perovskite photoluminesces so strongly.

"We investigated the structural and optoelectronic properties of  $Cs_4PbBr_6$  to understand the origin of its photoluminescence," De Bastiani says. Subjecting the material to a barrage of tests, the team discovered that when a  $Cs_4PbBr_6$  crystal was heated to  $180^\circ\text{C}$ , its photoluminescence was irreversibly destroyed.

Photoluminescence is a two-step process; absorption of light generates a pair of quasi-particles called excitons within the perovskite, which must recombine to re-emit the light. Using temperature-dependent X-ray diffraction to track structural changes to the material as heat was applied, the team discovered that at  $180^\circ\text{C}$ ,  $CsPbBr_3$  nanocrystals form within the mineral.

The heat-induced structural rearrangements that create these nanocrystals also swallow natural defects in the original crystal where bromine atoms were missing, the researchers concluded. These bromine vacancies act as traps for passing excitons. Confined in these traps, the excitons are much more likely to recombine and emit light.

"Now that we have this fundamental understanding, our next step is to move on to potential applications," De Bastiani says. "The unique photoluminescence manifested by Cs<sub>4</sub>PbBr<sub>6</sub> makes these perovskites compelling [materials](#) for electroluminescence devices, lasers and [light](#) converters."

Meanwhile, many other little-explored members of the perovskite family with interesting properties are waiting to be revealed, De Bastiani adds. "One example is CsPb<sub>2</sub>Br<sub>5</sub>, a single crystal we recently synthesized for the first time with unseen [optoelectronic properties](#)."

**More information:** Michele De Bastiani et al, Inside Perovskites: Quantum Luminescence from Bulk Cs<sub>4</sub>PbBr<sub>6</sub> Single Crystals, *Chemistry of Materials* (2017). [DOI: 10.1021/acs.chemmater.7b02415](https://doi.org/10.1021/acs.chemmater.7b02415)

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