

RESEARCH HIGHLIGHTS: Perovskites

By **Pabitra K. Nayak**

Perovskite solar cells are at the edge of commercial success. Device efficiency records continue to break at a regular pace, while stability and optimization are progressing rapidly. The first commercial products could reach the market very soon, just a decade since perovskite photovoltaics were first discovered. MRS Bulletin presents coverage of the most recent impactful advances in the burgeoning field of perovskite research.

Formamidinium lead triiodide (FAPbI₃) is the most desirable halide perovskite composition for single-junction solar-cell application owing to its suitable bandgap. However, the perovskite phase, essential for solar-cell applications, is not stable at room temperature. Moreover, previously reported FAPbI₃-based solar-cell parameters have yet to achieve the theoretical limits. Hence improving the electronic quality and stability of FAPbI₃ is vital for further progress of the solar-cell technology based on this material.

Anders Hagfeldt and Michael Grätzel of École Polytechnique Fédérale de Lausanne, Dong Suk Kim of Korea Institute of Energy Research, Jin Young Kim of Ulsan National Institute of Science and Technology, and co-workers have found a simple way to improve the electronic quality of the cubic α -phase of FAPbI₃. They have used an “ion engineering” concept where addition of a pseudo-halide anion, formate (HCOO⁻), suppresses the anion-vacancy defects that are present mostly at the surfaces and grain boundaries. The formate ions

do not replace iodide ions but rather interact with the under-coordinated Pb²⁺ to passivate iodide vacancies. The addition of the pseudo-halide anion also impacts the crystallinity and grain size in the polycrystalline films, which in turn improves the electronic quality. The solar-cell devices with the ion engineered FAPbI₃ as the absorber showed a power-conversion efficiency of 25.6% and long-term operational stability >450 h. The work was published in *Nature* (<https://doi.org/10.1038/s41586-021-03406-5>).

Metal-halide perovskite nanocrystals can show 100% photoluminescence quantum yield, which makes them very attractive for light-emitting applications. The emission color of the nanocrystals can be tuned by changing the nanocrystal composition. Solid-state light-emitting devices with external quantum efficiencies exceeding 20% have been previously demonstrated with pure halide compositions. However, mixed halide systems, which are used for red light emission, have the problem of stability and efficiency due to

the formation of low-bandgap iodide-rich domains.

In work published in *Nature* (<https://doi.org/10.1038/s41586-021-03217-8>), Yasser Hassan and Henry Snaith of the University of Oxford, Cathy Wong of the University of Oregon, Richard Friend of the University of Cambridge, Bo Ram Lee of Pukyong National University, and co-workers have shown that treatment of the mixed-halide perovskite nanocrystals with ligands that can bind with multiple sites can suppress the halide segregation under device operation

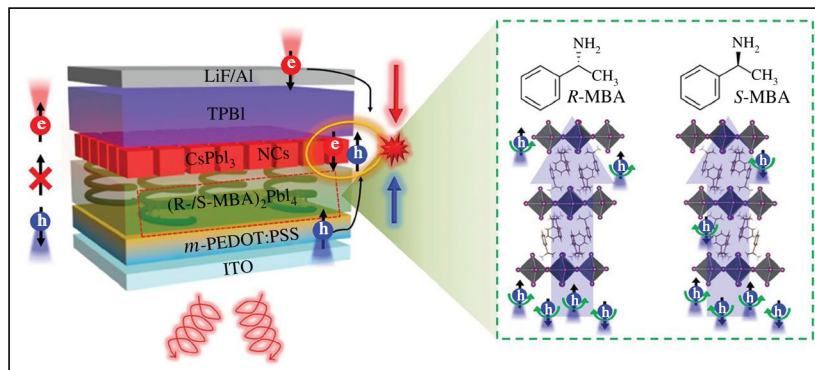
conditions. The researchers have demonstrated color stable red emission (centered at 620 nm) with electroluminescence external quantum efficiency exceeding 20 percent. A “clean” nanocrystal surface was achieved by the removal of lead atoms by the polydentate ligands. Density functional calculations suggest that the interaction of the ligand and the surface suppresses iodine Frenkel defects, which are mainly responsible for the halide segregation and formation of low-bandgap iodide-rich domains.

Pabitra K. Nayak, Tata Institute of Fundamental Research, Hyderabad, India; pabitra.nayak@tifrh.res.in
The author acknowledges support via intramural funding from the Tata Institute of Fundamental Research, Hyderabad.



Control over spin, charge, and light in a spintronic device typically requires the use of both magnetic and electrical fields. In a traditional spin-polarized light-emitting diode (spin-LED), circularly polarized light is emitted from spin-polarized carrier pairs. While the application of an electric field is required to inject the charge carriers, a magnetic field or polarized ferromagnetic contacts are required for the spin-polarization.

Joseph Luther and Matthew Beard of the National Renewable Energy Laboratory, and co-workers have reported in *Science* (<https://doi.org/10.1126/science.abf5291>) that it is possible to achieve polarized electroluminescence at room temperature without the application of a magnetic field or ferromagnetic contacts. The researchers used the chiral-induced spin selectivity (CISS) concept to produce spin-polarized carriers. The CISS layer, which is in a layered organic-inorganic metal-halide



Schematic for the spin-polarized charge injection and circularly polarized electroluminescence in a perovskite spin-polarized light-emitting diode. Image courtesy: *Science*.

hybrid semiconductor framework (see **Figure**), consists of oriented self-assembled small chiral molecules. This layer acts as a spin filter upon the application of the electric field—when electric current is passed through the chiral perovskite, the spin of the transmitting carriers becomes polarized. This architecture obviates the need for a magnetic field or ferromagnetic contacts and produces

$\pm 2.6\%$ circularly polarized electroluminescence at room temperature.

The researchers consider the demonstration of chiral perovskite layers in controlling spin, light, and charge has a wider implication for devices dealing with quantum-based optical computing and information processing, three-dimensional displays, bioencoding, and tomography, for example.

The underpinnings of the superb electronic properties of lead halide perovskites are still not clearly understood. It is thought that the large atomic fluctuations impact the optical and thermal properties in this class of material; however, a clear picture is still missing.

R. Osborn of Argonne National Laboratory, O. Delaire of Duke University, and co-workers used momentum-resolved neutron and x-ray scattering measurements to resolve the structural

and temporal correlations of atomic motions in CsPbBr_3 crystals. These measurements were done as a function of temperature and the results were supported by first-principle simulations. The researchers found a network of diffuse scattering rods that arise from the liquid-like damping of low-energy Br-dominated phonons, which was reproduced in simulations of the anharmonic phonon self-energy. Electronic gap edge states are directly impacted by

the atomic motions, which indicate a link between the soft anharmonic lattice dynamics and optoelectronic properties of this material. In their article published in *Nature Materials* (<https://doi.org/10.1038/s41563-021-00947-y>), the researchers stated that these results provide an understanding of the highly uncommon atomic dynamics of lead halide perovskites, which are relevant for the further optimization of their thermal and optical properties.

#F21MRS



MRS AWARDS

mrs.org/awards

Graduate Student Award Nominations

Nomination Deadline—August 2, 2021

