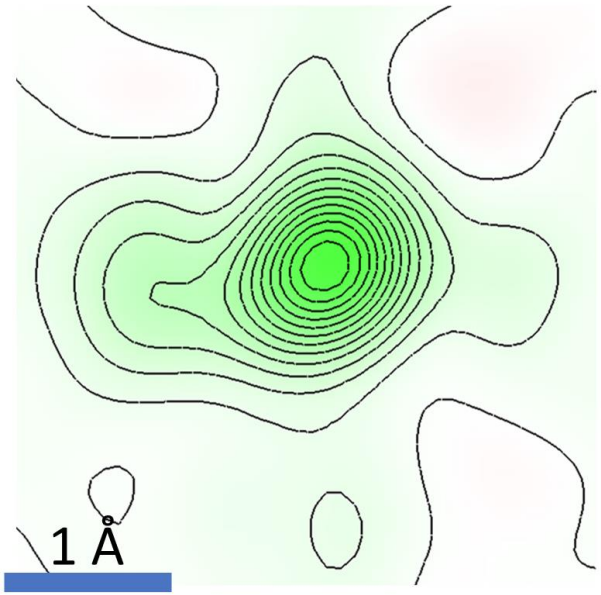
Scientists Resolve Origin of Perovskite Instability



The room temperature Cs electron density shows strong elongation – a signature of rattling.

Scientific Achievement

Scientists have demystified the reason for the instability of the halide perovskite $CsPbI_3$.

Significance and Impact

Halide perovskites such as $CsPbI_3$ have the potential for creating highly efficient solar cells; this work shows that the source of their thermodynamic instability is the cesium atom, suggesting new methods for engineering stable $CsPbI_3$-based solar cells.

Research Details

- Single-crystal X-ray diffraction and X-ray pair distribution function measurements characterized the perovskite $CsPbI_3$ between 100 and 295 K.
- Measurements used the PDF beamline at NSLS-II.
- Analysis showed that the cesium (Cs) atom "rattles" in its iodine atom cage, causing the instability.
- The limitations of tolerance factor arguments in predicting perovskite stability were revealed.

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