Disorder on the nanoscale may be responsible for solar-cell efficiency

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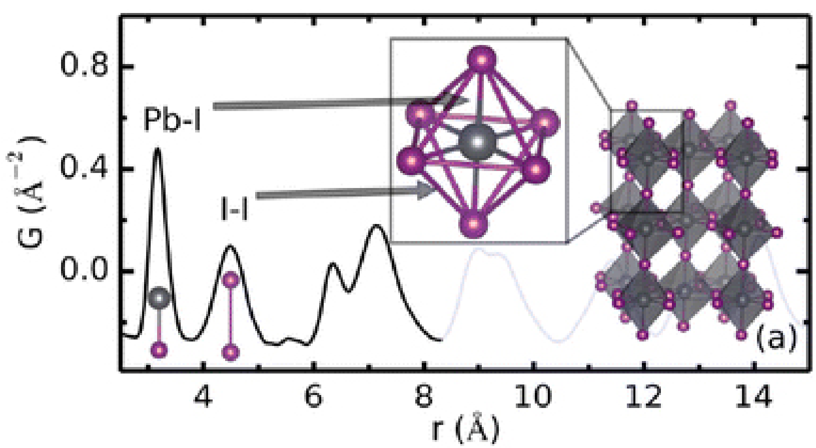

Methylammonium lead iodide perovskite

(Phys.org) —In the past few years, perovskite solar cells have made large leaps forward in efficiency, recently achieving energy conversion with up to 16 percent efficiency. These simple and promising devices are easy enough to make and are made up of earth abundant materials, but little work has been done to explore their atomic makeup.

Researchers at Brookhaven National Laboratory and Columbia University used high-energy x-rays at the National Synchrotron Light Source (NSLS) to characterize the structure of methylammonium lead iodide (MAPbI3) in titanium oxide – the active material in high-performance perovskite solar cells. Their results are reported in a paper published online in *Nano Letters* on November 22, 2013,

Photoluminescent properties of these materials are thought to depend sensitively on the degree of structural order and defects. To characterize the structure, the researchers used beamline X17A at NSLS to study samples of the MAPbI3. Atomic pair distribution function analysis of x-ray diffraction data revealed that 30 percent of the material forms a tetragonal perovskite phase, while 70 percent exists in a disordered state. The presence of disordered material correlates with strong changes in the photoluminescence and absorbance spectra.

This disordered structure has been undetected by conventional x-ray diffraction techniques used in previous studies. "This nanostructure is expected to have a significant impact on the optoelectronic properties and device performance of the perovskites," said Simon Billinge, coauthor on the paper and a physicist with a joint appointment at Brookhaven National Laboratory and Columbia University.

For example, the absorption of this composite material, made of both ordered and disordered states, is blue shifted by about 50 meV compared to the bulk perovskite crystalline structure. They also found that disordered MAPbI3 is photoluminescent, while the crystalline material is not.

This new understanding of the structure of these materials will lead to better deposition and processing methods that may increase the performance and efficiency of future solar cells.

The high-energy x-ray atomic pair distribution function analysis performed in this paper will be applied to a wide range of even more challenging problems at the higher brightness XPD-2 beamline (PDF) at NSLS-II.

More information: "Structure of Methylammonium Lead Iodide Within Mesoporous Titanium Dioxide: Active Material in High-Performance Perovskite Solar Cells." Joshua J. Choi, Xiaohao Yang, Zachariah M. Norman, Simon J. L. Billinge, and Jonathan S. Owen. *Nano Letters* 2014 14 (1), 127-133. [DOI: 10.1021/nl403514x](https://dx.doi.org/10.1021/nl403514x)

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