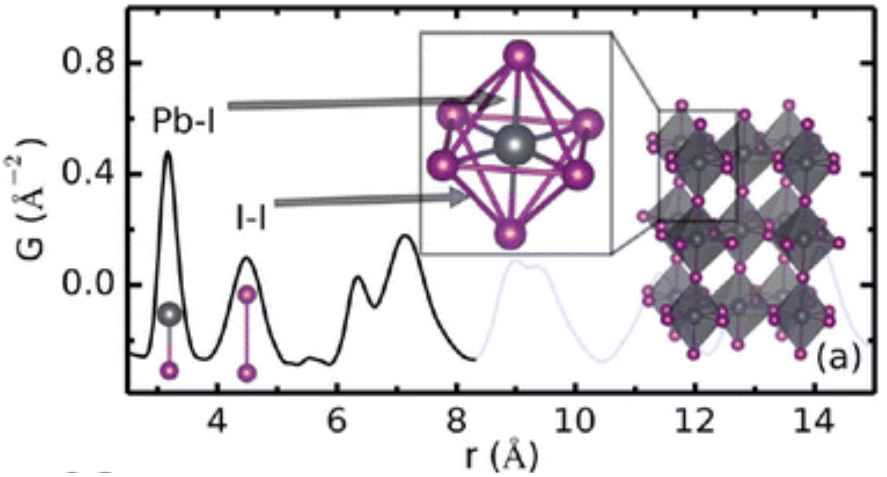
Disorder on the nanoscale may be responsible for solar cell efficiency

Scientific Achievement

The first characterization of the structure of methylammonium lead iodide in mesoporous titanium oxide – the active material in high-performance perovskite solar cells.

Significance and Impact

Photoluminescent properties of these active materials in perovskite solar cells are thought to depend sensitively on the degree of structural order and defects. Understanding how they are structured will lead to better deposition and processing methods that can increase the performance and efficiency of the device.



Atomic pair distribution function of bulk methylammonium lead iodide perovskite. The first peak corresponds to the nearest neighbor distance (Pb–I), the second peak the shortest I–I distance, and so on.

Research Details

- X-ray powder diffraction done at beamline X17A at NSLS yielded the nanostructure and bond length information, and confirmed that crystallites of $MAPbI_3$ form a tetragonal perovskite phase in about 30% of the material, while nearly 70% of the material exists in a significantly disordered state.
- The mesoporous titanium oxide support controls the nanostructure of the material by confining grains to the dimensions of the pores (2-50 nm), affecting the optoelectronic properties and device performance. For example, defects in the nanostructure may be responsible for a noticeable blue shift.

J. J. Choi, X. Yang, Z. Norman, S. Billinge, J. Owen. *Nanoletters* (2013) *14* (1), 127–133 Work was performed at Brookhaven National Laboratory