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Dynamic disorder and defects in halide perovskite solar cells

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Perovskites are the wonder compounds of materials science, with examples of magnets, ferroelectrics, superconductors, ion conductors, and most recently, high-efficiency solar cells. This talk will address some of the chemical and physical properties that make halide perovskites unique. After six years of intensive research, there has been a number of breakthroughs in understanding, but challenges and opportunities remain.

To understand the success of methylammonium lead iodide photovoltaics, we have been applying materials theory and simulation across multiple length scales [1-5]. These organic-inorganic semiconductors satisfy the optoelectronic criteria for an active photovoltaic layer, i.e. spectral response in the visible range combined with light electron and hole effective masses. In addition, these systems are structurally and compositionally flexible with large dielectric constants, and the ability to alloy on each of the lattice sites.

I will discuss issues ranging from disorder associated with molecular vibrations and rotations within the inorganic network, to microscopic polarisation arising from correlations in cell dipole orientations. The temporal behaviour of hybrid perovskites has recently been validated through a combination of neutron scattering, time-resolved vibrational spectroscopy, and kinetic measurements of the current-voltage response. The implications for non-radiative electron-hole recombination and new models for the cooling of hot carriers in operating solar cells will be discussed.

This research has been supported a University Research Fellowship from the Royal Society and the European Research Council (grant no. 277757).

1. “Atomistic origins of high-performance in hybrid halide perovskite solar cells” Nano Letters, 14, 2584 (2014)
2. “Self-regulation mechanism for charged point defects in hybrid halide perovskites” Angewandte Chemie Int. Ed. 54, 1791 (2015)
3. “Role of microstructure in the electron–hole interaction of hybrid lead halide perovskites” Nature Photonics 9, 695 (2015)
4. "Direct observation of dynamic symmetry breaking above room temperature in methylammonium lead iodide perovskite" ACS Energy Lett. 1, 880 (2016)
5. "Slow cooling of hot polarons in halide perovskite solar cells" ACS Energy Letters 2, 2647 (2017)

Biography:

Aron Walsh is Professor of Materials Design at Imperial College London. He was awarded his Ph.D in chemistry from Trinity College Dublin (Ireland), completed a postdoctoral position at the National Renewable Energy Laboratory (USA), and held a Marie Curie fellowship at University College London. He began his independent research career at the University of Bath and held a Royal Society University Research Fellowship in the Department of Chemistry. His research combines technique development and applications at the interface between solid-state chemistry and physics. In 2015 he was awarded the EU-40 prize from the Materials Research Society for his work on the theory of solar energy materials. Group website: http://www.imperial.ac.uk/people/a.walsh