Physical Chemistry of Hybrid Perovskite Solar Cells

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Hybrid perovskite solar cells have provided a step change in photovoltaics research. They combine the key advantages of all emerging photovoltaic technologies, including: inorganic thin-film photovoltaics (high efficiency); organic photovoltaics (ease of deposition and diversity of materials) and dye-sensitized solar cells (chemical versatility and architecture). For this reason, they have attracted a large community of researchers working at the interface of chemistry, physics and engineering.

These materials have not been an overnight success, but are the result of four decades of research effort and progress. In brief, the synthesis and characterization of methylammonium lead iodide was first reported in 1978 by D. Weber¹. The chemical diversity of these materials was explored extensively in the 1990s, with reports of organic-inorganic perovskites with variable composition and dimensionality². The first perovskite-sensitised solar cell was published in 2009 by T. Miyasaka,³ with reports of high-efficiency solid-state perovskite solar cells appearing from 2012⁴⁻⁷.

The past five years have seen a significant increase in light-to-electricity conversion efficiency, with the champion perovskite solar cells now on par with well-established inorganic photovoltaic technologies (e.g. CdTe)⁸. There is now a chance to step back and probe deeper into the physical chemistry and chemical physics of hybrid halide perovskite materials and solar cells. There exist a large number of fundamental challenges in the field and many opportunities for physical scientists, including:

- Hysteresis – how to limit time-dependent current-voltage behavior;
- Charge transport – what is the dominant scattering mechanism;
- Charge recombination – why is electron-hole recombination so slow;
- Ionic conductivity – what is the role in working devices;
- Dynamic disorder – connecting vibrations / rotations to optoelectronic properties;
- Chemical stability – protection from oxygen and water;
- Ferroelectricity – does lattice polarization play a role in high performance devices;
- Surfaces and interfaces – understanding how crystals terminate;
- Band gap engineering – avoiding photoinstability of alloys;
- Beyond 3D – exploring the performance of lower dimensional perovskites;
- Pb-free – maintain high performance with lead-free materials.

Several of these issues are touched upon in the **X** contributions found in this special issue. Solving them requires reliable and quantitative data, and the collaboration between theory, simulation and experiment. It is worth recalling the situation in the dye-sensitised solar cell community where despite over 1000 research publications per year, the photovoltaic

efficiencies became stagnant. As summarized by L. M. Peter in his 2011 review⁹ just before the emergence of perovskite solar cells: “we do not need just more research; we need *better focused* research.”.

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