Hybrid Organic-Inorganic Perovskites: Materials and Solar Cells

David Cahen*

With solution-processed, organic-inorganic hybrid lead halide perovskite-based solar cell developments being meteoric over the last few years, how these materials form, how hard or easy it is to decompose them, and how do the solar cells, made with them work, are topics of fundamental interest. Here we will describe our results on these aspects of these materials and cells.
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-1-We have gained insights into their mode of operation from several measurement approaches that are less common among those mostly employed, viz. Electron Beam Induced Current (EBIC), a scanning electron microscopy-based technique, applied to cell cross-sections, Surface photovoltage spectroscopy (SPS) on partial and complete cells, aided by several photoelectron spectroscopic measurements and scanning probe measurements. For thin film, non-mesoporous cells the best model remains that of a solar cell with a low-doped, high electronic quality photovoltaic semiconductor layer between a p- and an n-layer, a less common type of “p-i-n” cell. Under certain conditions, if the cell is very thin, it will become hard to distinguish this readily from a p-n cell, except by way of scanning probe methods. This model alongside the high effective diffusion lengths we measured in working cells, rather than the more common, but indirect approach of optical spectroscopy, explains the remarkably high open circuit voltage ($V_{OC}$) to $E_{gap}$ obtained with these cells.

-2- The reaction to form the material is currently most often performed by reacting a lead halide (e.g., lead iodide, PbI$_2$) with an organic halide salt (e.g. methyl ammonium iodide, CH$_3$NH$_3$I) to form the perovskite (e.g. CH$_3$NH$_3$PbI$_3$). The synthesis method referred to as ‘two step’ involves the reaction of solid-state lead halide with the organic halide salt in solution or vapor phase, and has led to device efficiencies $>15\%$. A major question concerning this reaction process is whether the lead halide reacts with the salt via dissolution of the lead halide crystal and reconstruction into the perovskite structure or
via intercalation of the salt into the lead halide crystal (a topotactic reaction). Using scanning electron microscopy, we have observed the shape and texture changes that PbI$_2$ single crystals undergo upon reaction with CH$_3$NH$_3$I vapor. In support of an intercalation reaction, we observe bending of the PbI$_2$ crystals into a bowl shape, presumably due to the strain induced by the ~2x increase in molar volume upon perovskite formation. Also, preliminary results of a before- and -after study of uniquely identified crystals suggest significant expansion (30%) of the crystal in one dimension. However, the appearance of tightly packed grains over the entire surface of the PbI$_2$ crystals suggests the possibility of dissolution and reconstruction occurring at the surface. Some combination of both processes may be occurring during perovskite formation from CH$_3$NH$_3$I vapor.

-3- The great promise of perovskite-based solar cells is being challenged by its lead content, and its sensitivity to water. We simulate the impact of rain on modules, whose encapsulation has failed, by exposing the MAPbI$_3$ perovskite material and the cell to rain water, and analysing the extent of Pb leaching into the environment. We find that damaged encapsulation will result in complete irreversible decomposition of the absorber layer. Furthermore, due to the moderate solubility of lead iodide in water, with time, a significant amount or even all of the Pb will be solubilized and find its way into the environment. Although eventually the amount of added lead to the environment is small, in comparison to the natural occurrence of lead, for the large-scale scenario we have considered, one must consider the possible implications of implementing lead halide perovskite solar cells for each specific scenario.

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