What's so special about metal halide perovskites?

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We* scrutinized some of the apparent inconsistencies in these remarkable optoelectronic materials, such as high lifetimes *cum* modest mobilities, low temperature preparation *cum* low defect density, apparently flexible inorganic lattice *cum* very sharp diffraction peaks.[1]

To start understanding these property combinations one first needs realize that the halide perovskites, HaPs *should be compared much more with inorganic than with organic semi-conductors* and that *concepts from organic photovoltaic (PV) or dye-sensitized solar cells are often inapplicable*. This is reflected in the similarities that we find between $CsPbBr_3$ and $CH_3NH_3PbBr_3$.[2]

In addition statements like they are "GaAs on the cheap", while true in some aspects, also cannot be defended as a general truth. An important factor is that electron-lattice coupling mechanisms are active at room temperature, and very likely dominate carrier scattering,[1] which connects to the materials' elasto-mechanical properties.[3]

Another issue, often invoked to explain hysteresis in the current-voltage characteristics of PV cells, and to rationalize the remarkably low recombination rate of photogenerated carriers (and, thus, high V_{OC}/E_G) in esp. the methyl-ammonium and formamidinium Pb(II) tri-iodide and the methyl-ammonium or Cs Pb(II) tri-iodide, is ferroelectricity. However, direct evidence for bulk ferroelectricity, with voltage-induced reversible switching is absent or tenuous. Thus, the obvious thing is …. to look for it, which is what we (with the Lubomirsky, Ehre andMeirzadeh) did, using the periodic temperature change (Chynoweth) technique to see if methylammonium lead bromide ($MAPbBr_3$) is pyroelectric. We chose as the first material to try the bromide HaP, rather than the iodide, to avoid complications due to phase transitions. We find that $MAPbBr_3$ is non-polar, and, thus, cannot be ferroelectric. Whenever signs for polarity were detected, they could be shown to be due to trapped charges, likely at the interface between the metal electrode and the $MAPbBr_3$ semiconductor. Thus, ferroelectric effects cannot affect steady-state performance of $MAPbBr_3$ solar cells. To further check this we measured second harmonic generation signals in $MAPbBr_3$, $MAPbI_3$ and $CsPbBr_3$ and found a clear signal for the $MAPbI_3$, but not for the other two. This shows that the iodide is non-centrosymmetric, a first condition for ferroelectricity. Experiments to test it for pyroelectricity are in progress.

If time permits I will present results on

- understanding the cause(s) for the current-voltage hysteresis (with U of Oxford);
- stability of HaPs esp. under conditions often used for their characterization with electro-magnetic radiation, electron and ion beams, with some emphasis on Cs vs. other HaPs;
- changes in their properties as function of ambient environment and the implications for their electronic transport behavior.[4]

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