

## **Beyond Perovskite Solar Absorbers: Exploring Alternative Structures for Lead Free Materials**

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Halide perovskite solar absorbers have been intensively researched for the past decade. They have shown a number of exceptional properties: high absorption coefficient, a small and tuneable band gap, ambipolar charge transport with exceptional diffusion lengths and very high tolerance for defects, solution processability and so on. However, drawbacks remain, namely poor stability and toxicity of many of the most successful compositions. Whilst the oxide perovskites are well known to be able to accommodate a large number of different combinations of elements, in fact there is only a small number of compositions that can successfully form halide perovskites. Therefore, from a chemist's point of view, there is little that can be done to improve on the existing materials.

By moving away from the perovskite structure, it is possible to have a much wider selection of elements. In this talk I will describe our results on the fundamental structural and chemical properties of two categories of perovskite-like materials. Firstly, A<sub>2</sub>BX<sub>6</sub> materials, which are very similar to perovskites but with half of the B site cations removed in an face centred cubic fashion. We have studied mixed anion A<sub>2</sub>BX<sub>6</sub> compounds and identify a new kind of structural distortion that occurs in these materials that allows these materials to remain crystallographically cubic over wide composition ranges. Additionally, we show a very large band bowing driven by symmetry breaking at the B site. We show that anion distribution can be measured easily using Raman spectroscopy, and some anion order is present in iodide containing compounds.

Secondly, we have studied A<sub>3</sub>B<sub>2</sub>X<sub>9</sub> compounds, which can adopt either a layered structure, with 2-dimensions B<sub>2</sub>X<sub>9</sub> sheets, or a dimer structure, with isolated B<sub>2</sub>X<sub>9</sub> units. The layered structure is preferred for charge transport, but can only be achieved by adding a large amount of bromide, which makes the band gap much wider, and unsuitable for most PV applications. We have found that alloying two metals on the B site, as well as two anions on the X site, enables control of the structure and band gap simultaneously.

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