Electronic properties of extended defects in solar absorbers

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Thin-film solar absorber materials promise high efficiencies together with low-cost and are actively pursued for next generation solar cell technologies [1]. Although all emerging materials are multicomponent and polycrystalline little is currently known about the role of extended defects and associated point defect segregation [2]. To provide insight into these issues we perform first principles theoretical predictions of the electronic properties of highly stable extended defects in several next generation solar absorber materials. These include 111 twin boundaries in pure formamidinium lead iodide (FAPI); a mixed ion lead halide perovskite containing formamidinium, Cs, I and Br; and a 1/2[110](001) anti-site boundary (ASB) in $Cu_2ZnSnSe_4$ (CZTSe).

We find the 111 twin boundary in pure FAPI is extremely stable but introduces no electron or hole trapping states and presents relatively small barriers (< 100 meV) to transport of electrons and holes, suggesting they are relatively benign for solar cell performance [3]. However, in the mixed ion perovskite twin boundaries serve as a nucleation site for formation of an I- and Cs-rich secondary phase. The reduced band gap in this segregated phase leads to hole trapping and is likely to enhance electron-hole recombination and lead to reduced open circuit voltage in solar cell devices. The 1/2[110](001) ASB in CZTSe is also highly stable but like pure FAPI does not present a recombination site or current blocking layer, so that photovoltaic device performance is not significantly degraded [4]. Altogether, these results provide atomistic insight into the properties of stable extended defects in solar absorbers and highlight the role they can play as nucleation sites for seconda ry phases which can be extremely detrimental to solar cell performance.

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