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Theoretical Evaluation of Cu-Sn-S and Cu-Sb-S Based Solar Absorbers for Earth-Abundant Thin-Film Solar Cells[1] PAWEL ZAWADZKI, HAOWEI PENG, ANDRIY ZAKUTAYEV, STEPHAN LANY, National Renewable Energy Laboratory — Current thin-film solar absorbers such as $Cu(In/Ga)Se_2$ or CdTe, although remarkably efficient, incorporate limited-supply elements like indium or tellurium. Meeting the cost competiveness criterion necessary for a large-scale deployment of thin-film PV technologies requires development of new earth-abundant solar absorbers. In an effort to accelerate such development we combine first principles theory and high throughput experiments to explore In-free ternary copper chalcogenides. As part of the theoretical evaluation, we study the Cu_2SnS_3, Cu_4SnS_4, $CuSbS_2$ and Cu_3SbS_3 based compounds formed by isovalent alloying on Sn, Sb, and S sites. For this set of materials we predict band-structures and optical absorption coefficients and demonstrate the feasibility of achieving the optimal band gap of 1.3 eV for a single junction cell and a high optical absorption of $\sim 10^4$ cm^{-1} at E_g+0.2 eV. We additionally perform defect studies to elucidate the doping trends within this class of materials.

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