Theoretical Evaluation of Cu-Sn-S and Cu-Sb-S Based Solar Absorbers for Earth-Abundant Thin-Film Solar Cells\textsuperscript{1} PAWEL ZAWADZKI, HAOWEI PENG, ANDRIY ZAKUTAYEV, STEPHAN LANY, National Renewable Energy Laboratory — Current thin-film solar absorbers such as Cu(In/Ga)Se\textsubscript{2} or CdTe, although remarkably efficient, incorporate limited-supply elements like indium or tellurium. Meeting the cost competitiveness 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\textsubscript{2}SnS\textsubscript{3}, Cu\textsubscript{4}SnS\textsubscript{4}, CuSbS\textsubscript{2} and Cu\textsubscript{3}SbS\textsubscript{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\textsuperscript{-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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