Abstract Submitted
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First principles simulations of $Cu_2ZnSnS_xO_{4-x}$ alloys[1] CHAOCHAO DUN, N.A.W. HOLZWARTH, YUAN LI, WENXIAO HUANG, DAVID CARROLL, Wake Forest University — Crystalline Cu_2ZnSnS_4 (CZTS) has been well studied for its photovoltaic properties. This paper reports a systematic computational study of CZTS alloys with oxygen substituting for S in the form $Cu_2ZnSnS_xO_{4-x}$ in order to understand their stability and structural forms. The calculations find the heat formation of Cu_2ZnSnO_4 (CZTO) to be 4.7 eV lower than that of CZTS, a result which is consistent with the general observation that CZTS is very reactive when exposed to air. Interestingly, the results find that CZTS is stable with respect to its decomposition products; the calculated enthalpy for CZTS $\rightarrow$ Cu_2S + ZnS + SnS_2 is ΔH_{cal}= +0.6 eV. However, for CZTO the corresponding decomposition is predicted to be exothermic; the calculated enthalpy for CZTO $\rightarrow$ Cu_2O + ZnO + SnO_2 is ΔH_{cal}= -1.7 eV. The simulations of S/O alloys show that there are preferred structures for the O configurations. For example, for alloys with $x = 2$, the energy difference between the lowest and highest energy O arrangements is 0.25 eV/formula unit.

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Chaochao Dun
Wake Forest University

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