

Abstract Submitted
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A theoretical study on the pure-phase stability of complex solar absorber materials¹ MUHAMMAD N. HUDA, CEDRIC L. MAYFIELD, PRANAB SARKER, Department of Physics, University of Texas, Arlington — To make solar energy competitive with fossil fuels, sustainable and cost effective solar absorber materials are needed. In this regards, we are particularly interested in multi-cation oxide/sulfide materials as they present flexible pathways to tune their electronic and optical properties. Once a material is selected, the primary challenge is to predict whether the material or the material with preferred doping can be synthesized as pure-phase in thermodynamic equilibrium conditions. We will present density functional theory (DFT) studies on two such examples for solar absorber materials: (i) $\text{Cu}_2\text{ZnSnS}(\text{Se})$ (CZTS) and (ii) $\text{Bi}_2\text{Ti}_2\text{O}_7$ (BTO). We'll first show from the chemical potential landscape analysis that the formation of stoichiometric CZTS is practically impossible under thermodynamic equilibrium condition. Our study justifies the experimental growth conditions of CZTS (Zn rich and Cu-poor) for higher solar-to-current conversion efficiency. Growth condition for p-type CZTS and suitable reaction pathways will be presented. In the second example, a recent experiment showed that a transition metal such as Fe inclusion can enhanced photo-current of bismuth titanate ($\text{Bi}_2\text{Ti}_2\text{O}_7$) up to an impurity concentration of ~1%. Beyond this impurity concentration the photocurrent decreased due to the formation of Fe_2O_3 phase. Our theoretical study predicted the doping configurations and suitable chemical potential ranges to avoid formation of the Fe_2O_3 phase in Fe- doped BTO in order to increase the photo-current.

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