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**Abundant defects and defect clusters in kesterite $Cu_2ZnSnS_4$ and $Cu_2ZnSnSe_4$**[1] SHIYOU CHEN, East China Normal University, and Lawrence Berkeley National Lab, LIN-WANG WANG, Lawrence Berkeley National Lab, ARON WALSH, University of Bath, XIN-GAO GONG, Fudan Univerisity, SU-HUAI WEI, National Renewable Energy Lab — $Cu_2ZnSnS_4$ and $Cu_2ZnSnSe_4$ are drawing intensive attention as the light-absorber materials in thin-film solar cells. A large variety of intrinsic defects can be formed in these quaternary semiconductors, which have important influence on their optical and electrical properties, and hence their photovoltaic performance. We will present our first-principles calculation study on a series of intrinsic defects and defect clusters in $Cu_2ZnSnS_4$ and $Cu_2ZnSnSe_4$, and discuss: (i) strong phase-competition between the kesterites and the coexisting secondary compounds; (ii) the dominant $Cu_{Zn}$ antisites and Cu vacancies which determine the intrinsic p-type conductivity, and their dependence on the elemental ratios; (iii) the high population of charge-compensated defect clusters (like $V_{Cu}$+$Zn_{Cu}$ and $2Cu_{Zn}$+$Sn_{Zn}$) and their contribution to non-stoichiometry ; (iv) the deep-level defects which act as recombination centers. Based on the calculation, we will explain the experimental observation that Cu poor and Zn rich conditions give the highest solar cell efficiency, as well as suggesting an efficiency limitation in $Cu_2ZnSn(S,Se)_4$ cells with high S composition.

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