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Multivalency of Sn in Cu_2ZnSnS_4[1] KOUSHIK BISWAS, STEPHAN LANY, ALEX ZUNGER, National Renewable Energy Laboratory — The highly efficient ternary chalcopyrites such as $2(CuInSe_2) = Cu_2In_2Se_4$ can be replaced as absorber materials in photovoltaic cells by Cu_2ZnSnS_4 (band gap $\sim$ 1.5 eV) in order to avoid the costly element In. Yet, the question remains whether a Fermi-level pinning defect can form spontaneously in these quaternary materials just as the In_{Cu} intrinsic *DX* centers in $CuInSe_2$ [1]. Here we study theoretically the deep gap levels introduced by the Sn_{Cu} and Sn_{Zn} defects in Cu_2ZnSnS_4. We find that these originate from the multi-valency of Sn, which can change into a +II oxidation state instead of the normal +IV state. Such a transition can even occur for Sn on its native site. Thus, we compare to the respective defect behavior in the kesterite $Cu_2ZnGeSe_4$, which has a similar band gap, but a less pronounced multi-valency of the respective IV-valent element Ge.

[1] S. Lany and A. Zunger, Phys. Rev. Lett. 100, 016401 (2008).

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