Impact of Ge incorporation on the opto-electronic properties and the physics of deep defects in kesterites

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Abstract

To boost the efficiency of kesterite-based solar cells, cationic substitution has been widely investigated. Specifically, a growing interest has developed for the Germanium which leads an improvement of the solar cell V_{OC} value, considered as the weak characteristic of kesterite material for PV applications. To obtain a comprehensive view of the relevance of Ge substitution in the Sn-based kesterite, using an *ab initio* approach, we studied the opto-electronic properties as well as the physical behaviour of points defects in Sn- and Ge-based kesterites. Controlling the nature of defects appears as a crucial requirement for an optimal tuning of the physical properties of kesterite absorber layers.

First, we highlight the high absorption coefficients (10^4 cm^{-1}) and the band gap values of 1.32 and 1.89 eV obtained respectively for the Sn- and Ge-based compounds. Then, using an improved version of the Shockley-Queisser model allowing a fine tuning of the recombination rate, we highlight the possible efficiency improvement of both CZTS and CZGS based solar cells while promoting their use as top cell for tandem approach.

Additionally, to gather a full picture of the impact of Ge incorporation in kesterite, we explored in detail the physical behaviour of point defects following both Ge doping and alloying of the Sn-based material. In both CZTS and CZGS, we highlight the net Cu/Zn disorder as well as the intrinsic p-type conductivity. More significantly for PV applications, we report on recombination centres that reduce the performances of kesterite-based solar cells. Upon Ge incorporation, in the both the Sn-based (doped) and the Ge-based (alloyed) kesterite, we observe a reduction of the lattice distortion following the formation of the Ge_{Zn} substitutional defect that leads, in comparison to its Sn_{Zn} parent, to a reduction of its carrier capture cross section, which we report as a possible explanation for the experimentally reported V_{OC} enhancement.

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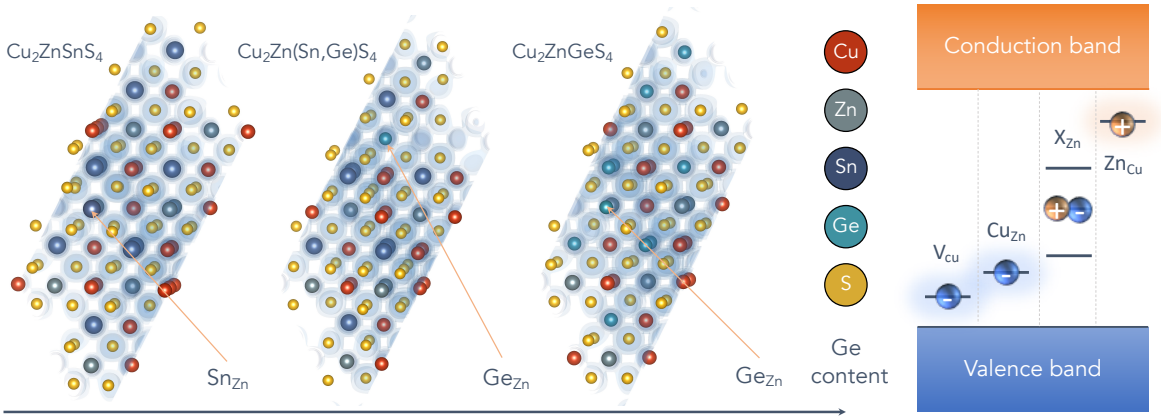
Ratz, Thomas, et al. "Opto-electronic properties and solar cell efficiency modelling of Cu_2ZnXS_4 (X= Sn, Ge, Si) kesterites." *Journal of Physics: Energy* 3.3 (2021): 035005.
Ratz, Thomas, et al. "Relevance of Ge incorporation to control the physical behaviour of point defects in kesterite." *Journal of Materials Chemistry A* 10.8 (2022): 4355-4365.



Graphical abstract