The route towards high efficiency kesterite solar cells by selective doping and alloying

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Cu$_2$ZnSn(S,Se)$_4$ (CZTSSe) is currently considered one of the most relevant emerging thin film photovoltaic technology based on earth abundant elements. Nevertheless, and in spite of the impressive progresses achieved in the last years, this technology still exhibit a large voltage deficit, remarkably higher than those obtained in commercial thin film technologies like CdTe and Cu(In,Ga)Se$_2$. This can be related to different origins, all of them linked to the complex structure and off-stoichiometric composition of these materials, including secondary phases formation, Cu/Zn disorder, Sn volatility and multivalence, macro and micro inhomogeneities, etc.; which usually degrades the electrical and transport charge properties of kesterites. Attempts to solve this very relevant issue includes doping and alloying strategies, which have been revealed as the most promising ways to reduce the current voltage deficit.

In this talk, the most relevant doping and alloying strategies reported in the literature will be presented. In particular, the effect of different doping elements (Li, Na, K, Rb, Cs, Ge, Sb, Bi, etc.) will be analyzed, including their impact onto the optoelectronic properties of solar cell devices. Additionally, different strategies for kesterite alloying by cation substitution will be reviewed, in particular the substitution of Cu by Ag, Zn by Ba, Cd or Mg, and Sn by Ge or Si. Their potential for the solution of the different problems identified in kesterites such as Cu/Zn disorder, Sn multivalence, Sn volatility etc., will be discussed, in regards of their effect onto the solar cell devices properties. The application of these alloying elements for the formation of graded band-gap concepts in kesterites, as well as the most promising strategies to be followed in the future for the improvement of the conversion efficiency through the reduction of the voltage deficit will be deeply analyzed.