NATIVE DEFECTS AND ALKALI METAL IMPURITIES IN CIGS MATERIALS, FIRST PRINCEPLES CALCULATIONS REVISITED

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During the last years, the research on $Cu(In,Ga)Se_2$ (CIGS) as a promising absorber candidate for low-cost thin-film photovoltaic cells has steadily increased widening our understanding on its basic materials properties and leading to a high efficiency of 21.7 % for the solar cells [1]. Understanding microstructure's evolution during the manufacture and use of solar cells is impossible without knowing the fundamental parameters of its native point defects. Indeed, there exist several recent first-principles studies [2-5] for defect formation energies in $CuInSe_2$ (CIS) and $CuGaSe_2$ (CGS). Their results agree with respect to general trends and orders of magnitudes, but they may differ in some important cases resulting, e.g., in different values for ionization levels within the band gap. A possible reason for the situation could be the use of inappropriate or insufficient computational parameters and post – treatments. We present the results of a detailed systematic study on the influence of computational parameters on the formation energies. Our approach is based on comparing results obtained by different existing corrections for the supercell method and by different electronic-structure calculation schemes (Projector-augmented wave – plane-wave method, All-electron – numerical-atomic-orbitals method).

Another aspect of this presentation is the influence of alkali metal impurities. During the thin film deposition, sodium and potassium diffuse into the CIGS layer [6] and they have also been subjects of several first-principles investigations [7,8]. Inspired by the scatter in the first-principles results for native defects in CIGS materials we have revisited also the formation and migration energies of alkali metals as well as their clustering with other defects. Also we calculated migration barrier for defect in Cu-poor compounds. The migration barriers were determined by the state-of-the-art climbing-image nudged-elastic-band (CI-NEB) method for different types of materials, such as the stoichiometric CIS and the Cu-poor ordered compound.

References:

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