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DEFECT ENERGETICS IN PROTOTYPE SOLAR CELL MATERIAL $CuInSe_2$

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Abstract:

There is a strong effort to find optimal materials for solar cells. A candidate is $Cu(In,Ga)Se_2$ (CIGS) that has a very high efficiency. There are several studies on this material, but still many of its basic material properties remain unexplained, like the atomistic structure of defects and their influence on the characteristics of CIGS [1].

We have performed electronic-structure calculations [2] using density functional theory to describe the CIGS material. In this contribution we concentrate on the material $CuInSe_2$ and in particular the intrinsic vacancies. This materials has been used to produce photovoltaic modules [3]. We have used the HSE06 [4] screened, hybrid exchange-correlation functional that replaces 25 % of the GGA exchange by the Hartree-Fock exchange energy. This improves in particularly the description of the band gap.

Our results show that there are no ionisation levels in the band gap of $CuInSe_2$ due to copper or indium vacancies, but the selenium vacancy has a deep acceptor level $\varepsilon(0/2-)$. The copper vacancy has a low formation energy, as generally believed from experiments.

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