First-principles calculations on stability of absorber-buffer interface in CIGS-based thin filmsolar cells

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Introduction
In$_2$S$_3$ as alternative for CdS buffer layer in Cu(In, Ga) (S, Se)$_2$ (CIGS)-base thin film solar cells has gained a lot of scientific attention in recent years. When indium sulfide is deposited on CIGS, it forms an intermixed absorber-buffer interface involving a high concentration of Cu and Na. So the question is whether the CIGS-In$_2$S$_3$ interface is stable or we would expect to have Na containing and Cu containing secondary phases at the interface region. There are two theoretical ways of addressing this question: Defect thermodynamics calculations and direct interface calculations. To unveil the driving force of Na and Cu formation in In$_2$S$_3$, we compared the formation energy of these dopants in buffer and absorber layers.

Methods
For studying the defect thermodynamics, we have used an exchange potential with 25% contribution of Hartree-Fock exchange. For direct interface calculations, however, with systems containing around one thousand atoms a hybrid functional cannot be used. Therefore, the interface calculations were performed using the PBE functional, in which the atoms were allowed to relax until the Hellmann-Feynman forces acting on them became less than 0.05 eV/Å. To construct the interface we have used a periodic slab model, in which the slab is...
repeated in the direction perpendicular to the interface (z-axis), and each slab is separated from its periodic images by a vacuum gap of 16 Å. Since constituents of both chalcopyrite and spinel-like structure at this orientation relationship form layered crystal structure consisting of alternative anion and cation planes, four different interface termination layers have been considered across the interface. Note that these termination layers are fundamentally different, representing differently electronically compensated interfaces.

**Results**

According to our calculations both, Na and Cu, would preferably occupy the interstitial vacancy in In$_2$S$_3$. The very high solubility of Na and Cu in In$_2$S$_3$ represents their massive driving force for the occurrence of side reactions leading to the formation of interfacial phases.

To get a first impression from direct interface calculations, we used CuInSe$_2$(112)-In$_2$S$_3$(103) interface orientation. The results obtained from geometry optimization indicate structural distortions and massive structural relaxations as shown in the Figure. As the next step, we have modified the interface to get a junction between the CuInSe$_2$ absorber layer and Cu-containing and Na-containing buffer layers. These results reveal that both Na and Cu containing indium sulfides form more stable interfaces with the absorber layer than pure In$_2$S$_3$.

**Publications**


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