Hessisches Kompetenzzentrum
für Hochleistungsrechnen

First-Principles Calculations on Stability of Absorber-Buffer Interface in CIGS-Based Thin Filmsolar Cells

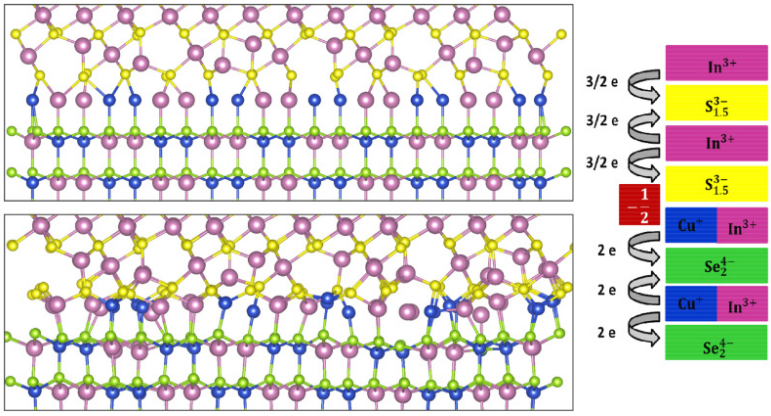

Figure 1: The $CuInSe_2$(112)-In_2S_3(103) interface with a cation terminated layer on the absorber side and anion terminated layer on the buffer side. The top panel shows the interface before atomic optimization and the bottom panel corresponds to the same interface after atomic optimization.

Introduction

In_2S_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 scientifc 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_2S_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_2S_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),

Project Manager
Dr. Elaheh Ghorbani

Principal Investigator
Prof. Dr. rer. nat. Karsten Albe

Project Term
2016 - 2020

Project Areas
Materials Science, Molecular Chemistry

Clusters
Lichtenberg Cluster Darmstadt

Software
VASP

Institute
Fachgebiet Materialmodellierung

University
Technische Universität Darmstadt

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 cationplanes, 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_2S_3. The very high solubility of Na and Cu in In_2S_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_2S_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_2S_3.

Publications

[1] Ghorbani, E.; Albe, K.: "Intrinsic point defects in β-In2S3 studied by means of hybrid density-functional theory.", J. Appl. Phys., 123, 53-60, (2018) https://doi.org/10.1063/1.5020376

[2] Ghorbani, E.; Albe, K.: "Influence of Cu and Na incorporation on the thermodynamic stability and electronic properties of β-In2S3.", J. Mater. Chem.C, 6, 7226-7231, (2018) https://doi.org/10.1039/c8tc01341a

[3] Ghorbani, E.; Albe, K.: "Role of oxygen and chlorine impurities in β-In2S3: A first-principles study.", Phys. Rev. B, 98, 205201(1-8), (2018) https://doi.org/10.1103/PhysRevB.98.205201

[4] Ghorbani, E.; Erhart, P.; Albe, K.: "Energy level alignment of Cu(In,Ga)(S,Se)2 absorber compounds with In2S3, NaIn5S8, and CuIn5S8 Cd-free buffer materials", Phys. Rev. Materials, 3, 075401-1, (2019) https://doi.org/10.1103/PhysRevMaterials.3.075401

Last Update: 2022-04-25 17:47