

Accepted Manuscript

First-principles Calculation of Structural, Electronic, and Optical Properties of Wurtzite-stannite $\text{Cu}_2\text{MgSi}(\text{S}_x\text{Se}_{1-x})_4$ Alloys

Dan Li, Furi Ling

PII: S2210-271X(15)00430-2

DOI: <http://dx.doi.org/10.1016/j.comptc.2015.10.024>

Reference: COMPTC 1971

To appear in: *Computational & Theoretical Chemistry*

Received Date: 5 August 2015

Revised Date: 30 September 2015

Accepted Date: 22 October 2015



Please cite this article as: D. Li, F. Ling, First-principles Calculation of Structural, Electronic, and Optical Properties of Wurtzite-stannite $\text{Cu}_2\text{MgSi}(\text{S}_x\text{Se}_{1-x})_4$ Alloys, *Computational & Theoretical Chemistry* (2015), doi: <http://dx.doi.org/10.1016/j.comptc.2015.10.024>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

First-principles Calculation of Structural, Electronic, and Optical Properties of Wurtzite-stannite $\text{Cu}_2\text{MgSi}(\text{S}_x\text{Se}_{1-x})_4$ Alloys

Dan Li ^{a,*}, Furi Ling ^b

^a School of Physics and Electronics Information, Hubei University of Education,
Wuhan 430205, China

^b School of Optical and Electronic Information, Huazhong University of Science and
Technology, Wuhan 430074, China

Abstract

The structural, electronic, and optical properties of wurtzite-stannite $\text{Cu}_2\text{MgSi}(\text{S}_x\text{Se}_{1-x})_4$ alloys have been calculated based on Heyd-Scuseria-Ernzerhof (HSE) screened hybrid functional. The calculated band gap bowing parameter is 0.164 eV which may be a good reference for future research. According to the calculations of the density of states, we find that the peaks in the conduction band have a tendency of shifting to the lower energy as S concentration decreases. Furthermore, the dielectric function, reflectivity, and absorption coefficient are presented and discussed in detail. The spectra of dielectric function shift to lower energy region with the decrease of the S concentration. The static dielectric constants increase with the decrease of S mole fraction. And the strength of absorption peaks almost decrease. The absorption edge and the peak in the reflectivity have a tendency of shifting to lower energy.

* Corresponding author. Tel./fax: +86 27 87793023. 1
E-mail address: 417218520@qq.com (D. Li).

Download English Version:

<https://daneshyari.com/en/article/5393104>

Download Persian Version:

<https://daneshyari.com/article/5393104>

[Daneshyari.com](https://daneshyari.com)