Accepted Manuscript

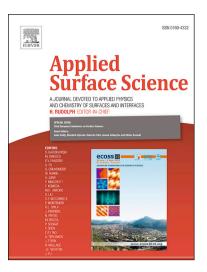
Full Length Article

The nature of the high thermoelectric properties of $CuInX_2$ (X = S, Se and Te): First-principles study

Yang Gui, Lingyun Ye, Chao Jin, Jihua Zhang, Yuanxu Wang

PII:	S0169-4332(18)31887-7
DOI:	https://doi.org/10.1016/j.apsusc.2018.07.013
Reference:	APSUSC 39828
To appear in:	Applied Surface Science

Received Date:19 March 2018Revised Date:20 June 2018Accepted Date:3 July 2018



Please cite this article as: Y. Gui, L. Ye, C. Jin, J. Zhang, Y. Wang, The nature of the high thermoelectric properties of $CuInX_2$ (X = S, Se and Te): First-principles study, *Applied Surface Science* (2018), doi: https://doi.org/10.1016/j.apsusc.2018.07.013

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.

ACCEPTED MANUSCRIPT

The nature of the high thermoelectric properties of CuInX₂ (X = S, Se and Te):

First-principles study

Yang Gui(1), Lingyun Ye(3), Chao Jin(1), Jihua Zhang(2), and Yuanxu Wang(1, 2)*

(1) School of Physics and Electrical Engineering, Anyang Normal University, Anyang Henan,455000 China

(2) Institute for Computational Materials Science, School of Physics and Electronics, Henan University, Kaifeng 475004, China.

(3) Zhengzhou Chenggong University of Finance and Economics

Abstract

CuInX₂ (X = S, Se and Te) are members of Cu-based compounds with diamond-like structures. Their bonding characteristics, electronic structure and thermoelectric properties are studied using first-principles methods and the semiclassical Boltzmann theory. Due to the Cu-3d orbits in CuInX₂, we use the mBJ+U method to obtain the accurate band gap and electronic structures. The analysis of the electronic structure for CuInX₂ indicates that the combination of heavy and light bands near the Fermi level is conductive to achieve high thermoelectric performances. However, few literatures have reported the reason of the combination. Further study on AgGaTe₂, CuGaTe₂, and CuInX₂ (X = S, Se and Te) shows that the stronger interaction between Cu-Te atoms leads to the combination of heavy and light bands in Cu-based compounds. These results provide a valuable theoretical guidance that the introduction of Cu-Te bonding in experimental synthesis is helpful to improve the thermoelectric properties.

Keywords: Cu-based compounds; Seebeck effect; thermoelectric properties;

* Email: wangyx@henu.edu.cn

Download English Version:

https://daneshyari.com/en/article/7832932

Download Persian Version:

https://daneshyari.com/article/7832932

Daneshyari.com