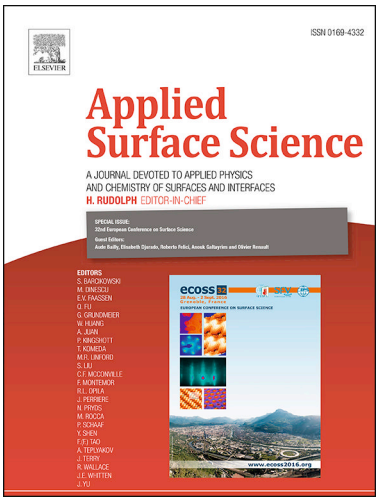

Full Length Article

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 2018
Revised Date: 20 June 2018
Accepted 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

The nature of the high thermoelectric properties of $CuInX_2$ (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

$CuInX_2$ (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 $CuInX_2$, we use the mBJ+U method to obtain the accurate band gap and electronic structures. The analysis of the electronic structure for $CuInX_2$ 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 $AgGaTe_2$, $CuGaTe_2$, and $CuInX_2$ (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