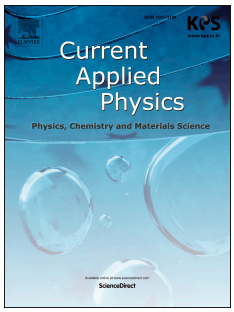
Accepted Manuscript



Prediction on the physical properties of $CuInS_2$ with various anion positions

Yiming Ren, Yonghong Hu, Haibo Zeng, Li Xue

PII: S1567-1739(18)30005-1

DOI: 10.1016/j.cap.2018.01.005

Reference: CAP 4659

To appear in: *Current Applied Physics*

Received Date: 15 October 2017

Revised Date: 8 January 2018

Accepted Date: 9 January 2018

Please cite this article as: Y. Ren, Y. Hu, H. Zeng, L. Xue, Prediction on the physical properties of $CuInS_2$ with various anion positions, *Current Applied Physics* (2018), doi: 10.1016/j.cap.2018.01.005.

Prediction on the physical properties of $CuInS_2$ with various anion positions

Yiming Ren[1], Yonghong Hu[1], Haibo Zeng[2] and Li Xue[1+]

1 School of Electronic and Information Engineering, Hubei University of Science and Technology, Xianning 437100, PR China

2 Institute of Optoelectronics & Nanomaterials, College of Materials Science and Engineering, Nanjing University of Science and Technology, Nanjing 210094, PR China

Abstract: The effects of various anion displacements (*u*) on electronic structures, elastic constants, Debye temperature and the minimum thermal conductivity of $CuInS_2$ are studied by first-principles calculation. The lattice constant couples with the anion displacement, however, they are not consistent with the relation proposed by Abrahams and Bernstein. When the anion displacement varies from 0.2 to 0.3, the Cu-S bond length is elongated, while the In-S bond length is shortened, which cause the increase of band gap with anion displacement. The anisotropies of sound velocities and lattice thermal conductivities are also discussed. The results imply that the lattice thermal conductivity along [110] direction is the smallest and decreases with *u*. These research findings shed light on improving the thermoelectric properties by manipulating *u* and the direction of propagation.

Keywords: $CuInS_2$, electronic structures, elastic properties, first principles

[+]Corresponding author Tel: +86 715 8342263

E-mail address: xueli0610@163.com