Electronic Supplementary Material (ESI) for RSC Advances.

Improved thermoelectric performance of $CuGaTe_2$ with convergence of band valleys:A first-principles study

Jueming Yang, Yuli Yan, Yuan Xu Wang* and Gui Yang

Institute for Computational Materials Science,

School of Physics and Electronics, Henan University,

Kaifeng 475004, People's Republic of China

*Electronic address: wangyx@henu.edu.cn

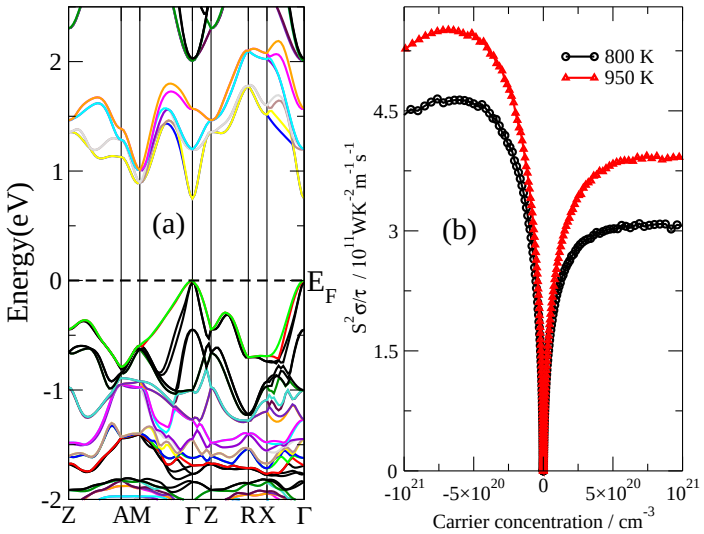

FIG. 1: (a) The energy band of $CuGaTe_2$. Top of the valence band is set to zero; (b) power factors with respect to relaxation time, $\frac{S^2\sigma}{\tau}$ (unit in 10^{11} $WK^{-2}m^{-1}s^{-1}$).

The structure of $CuGaTe_2$ was optimized using the Vienna *ab initio* simulation package (VASP) based on density functional theory (DFT) with the exchange-correlation potential Perdew-Burke-Ernzerhof (PBE) with generalized-gradient approximation (GGA). The optimized lattice parameters by PBE are $a = 6.103$ Å, $c = 12.186$ Å, respectively. Then, self-consistent calculation are carried out with TB-mBJ exchange-correlation potential as implemented in the WIEN2k package and transport properties are calculated. Fig. S1(a) displayed the energy band gap is 0.75 eV. The power factors with respect to relaxation time at 800 and 950 K are shown in Fig. S1(b). We find n-type $CuGaTe_2$ also displaying better thermoelectric properties than the p-type $CuGaTe_2$ with the direct gap electronic structure because the M and Gamma points near CBM can also be regarded as nearly converged.

FIGURE CAPTIONS

Fig. S1. (a) The energy band of $CuGaTe_2$. Top of the valence band is set to zero; (b) power factors with respect to relaxation time, $\frac{S^2\sigma}{\tau}$ (unit in $10^{11}WK^{-2}m^{-1}s^{-1}$).