Supporting Information

Thermoelectric Properties of Monolayer GeAsSe and SnSbTe

H.H. Huang[a], Xiaofeng Fan[a,*], David J. Singh[c] and W.T. Zheng[a,b]

a. Key Laboratory of Automobile Materials (Jilin University), Ministry of Education, and College of Materials Science and Engineering, Jilin University, Changchun, 130012, China

b. State Key Laboratory of Automotive Simulation and Control, Jilin University, Changchun 130012, China

c. Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211-7010, USA

*, Correspondence and requests for materials should be addressed,

Email: xffan@jlu.edu.cn (X. Fan)

Tel: +86-159-4301-3494

Figure S1

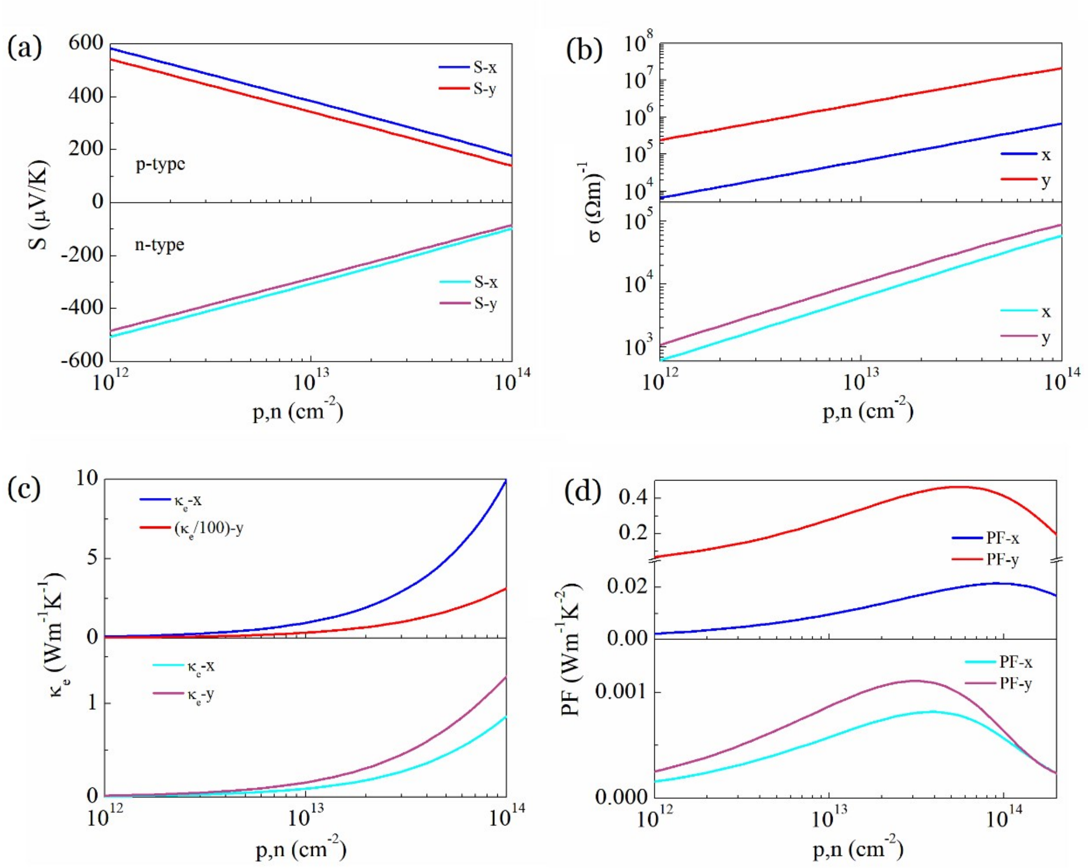

Fig.S1. (a) Calculated the Seebeck coefficient S, (b) the electrical conductivity σ, (c) the electronic thermal conductivity κ_e and (d) power factor (PF) of the monolayer GeAsSe as a function of the carrier concentration along the x and y directions for p-type and n-type doping at 600K.

Figure S2

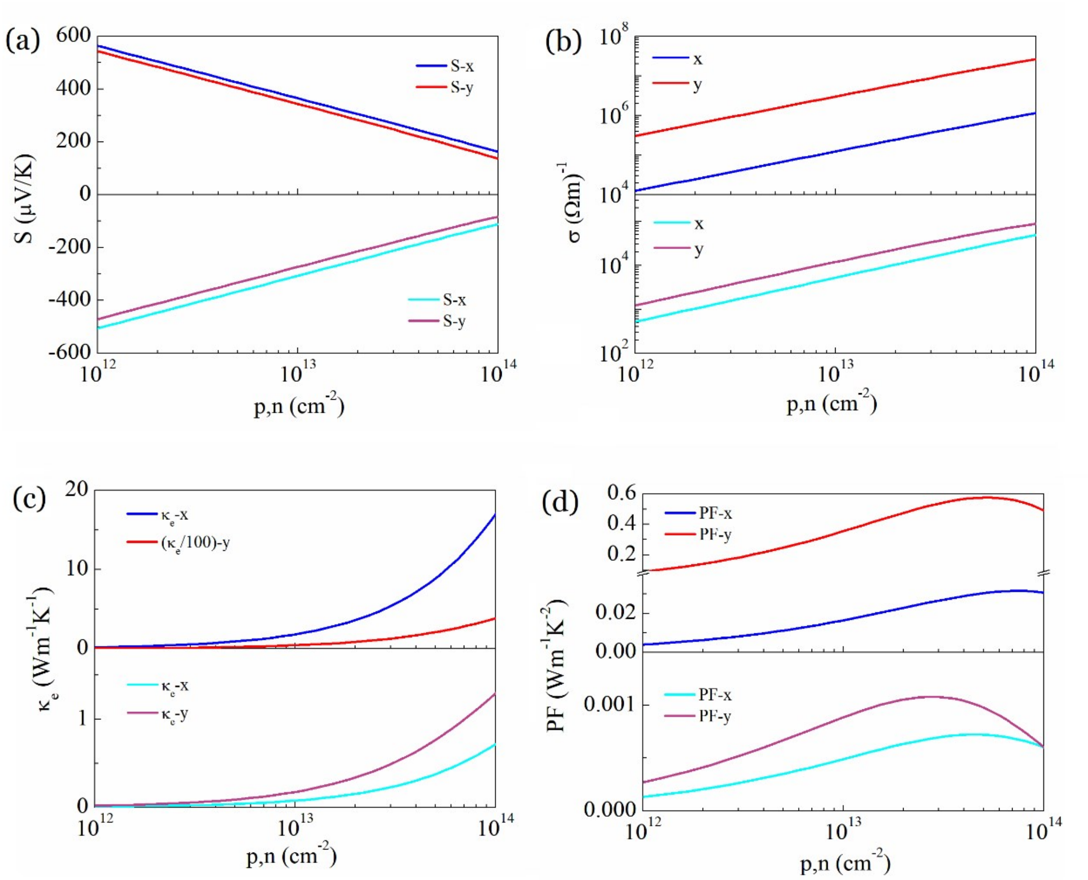

Fig.S2. (a) Calculated the Seebeck coefficient S, (b) the electrical conductivity σ, (c) the electronic thermal conductivity κ_e and (d) power factor (PF) of the monolayer SnSbTe as a function of the carrier concentration along the x and y directions for p-type and n-type doping at 600K.

Figure S3

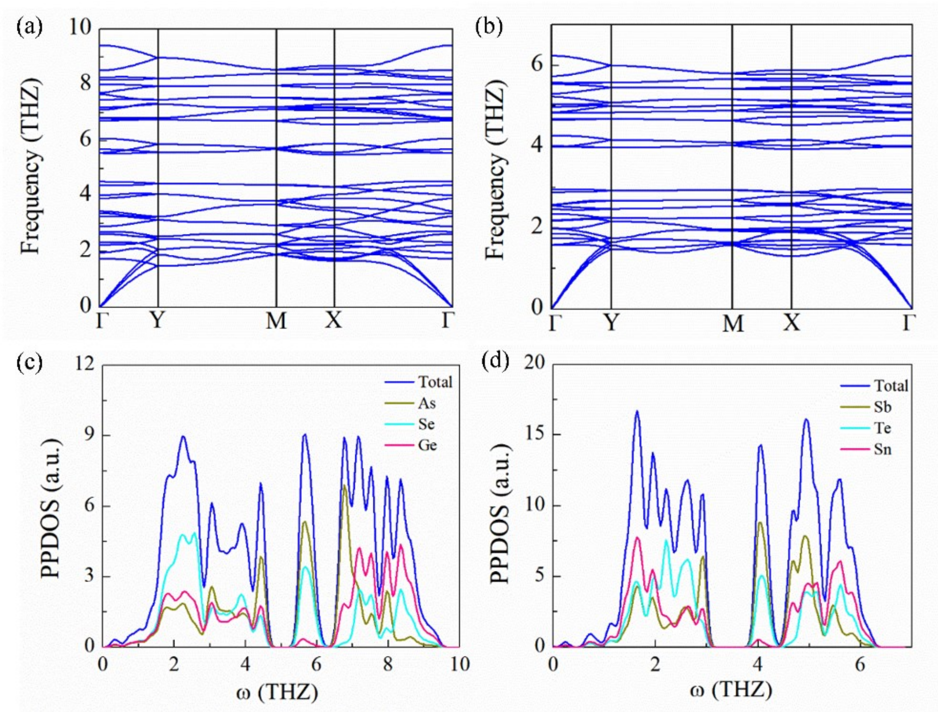

Fig.S3. Phonon spectra and partial phonon density of states (PPDOS) for monolayer (a,c) GeAsSe and (b,d) SnSbTe.

Figure S4

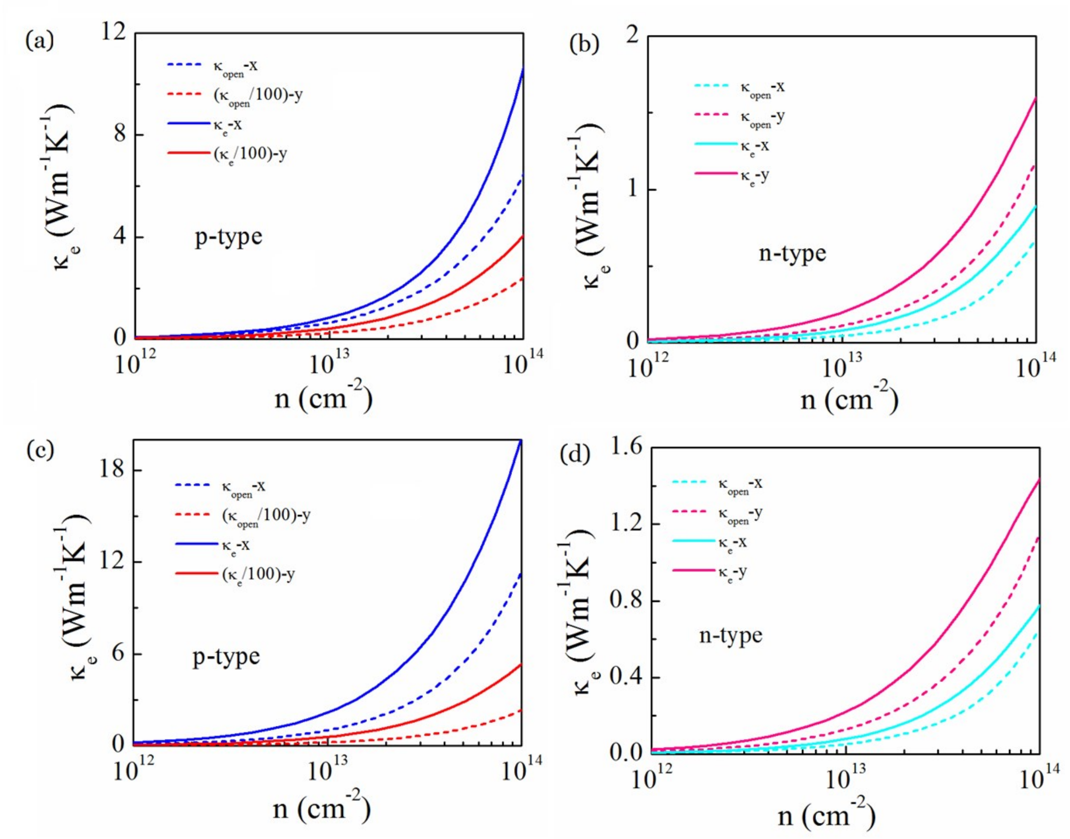

Fig.S4. Electronic thermal conductivity of (a, b) GeAsSe and (c, d) SnSbTe at 300K. The full lines and dotted lines are for the results with constant Lorenz number and corrected thermal conductivity from BoltzTraP, respectively.

The Grüneisen parameter is defined by the relation between phonon frequency and change of volume with the formula,

$$\gamma_i = -\frac{V}{\omega_i}\frac{\partial \omega_i}{\partial V}\ , \quad (1)$$

where V and ω_i are the volume and phonon frequency, respectively. In long-wave limit, the relation between ω_i and sound velocity υ_i is $\omega_i=\upsilon_i q$, where q is wave vector, while the sound velocity is related to bulk modulus *B* and shear modulus *G*. With the model proposed by Jia *et al.*[1], the averaged acoustic Grüneisen parameter γ_e is related with the *B* and *G* and expressed as,

$$\begin{aligned} \gamma_e &= \sqrt{\left[\left(\gamma_L^e\right)^2 + 2\left(\gamma_S^e\right)^2\right]\Big/3} \\ \gamma_L^e &= -\frac{1}{2}\frac{V}{B+\frac{4G}{3}}\frac{\partial\left(B+\frac{4G}{3}\right)}{\partial V} - 1/6 \\ \gamma_S^e &= -\frac{1}{2}\frac{V}{G}\frac{\partial G}{\partial V} - 1/6 \end{aligned} \quad . \quad (2)$$

By changing the volume, we can obtain the change of B and G and thus get the averaged acoustic Grüneisen parameter γ_e.

References

1. Jia, T.; Chen, G.; Zhang, Y., Lattice thermal conductivity evaluated using elastic properties. *Phys. Rev. B* **2017,** *95* (15), 155206.