Supporting Information

Bi_8Se_9: Effective Reduction of Bipolar Diffusion via Increasing Band Gap

Rui Wang, Fei Jia, Xuan Li, Ling Chen, and Li-Ming Wu**

Beijing Key Laboratory of Energy Conversion and Storage Materials, College of Chemistry, Beijing Normal University, Beijing 100875, People's Republic of China

Supporting Information

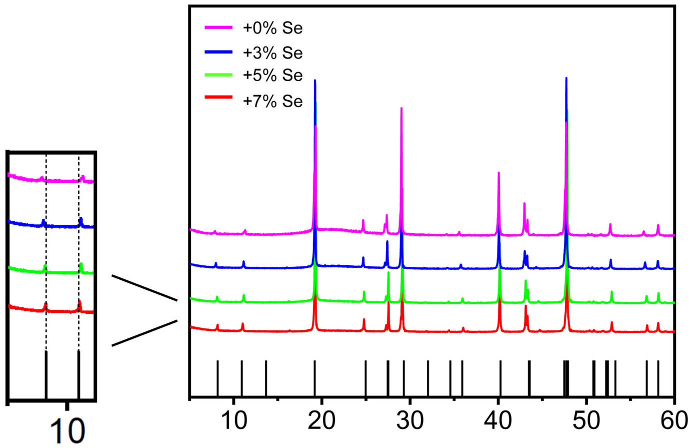

Figure S1. Powder XRD patterns of Bi_8Se_9 of different excessive Se.

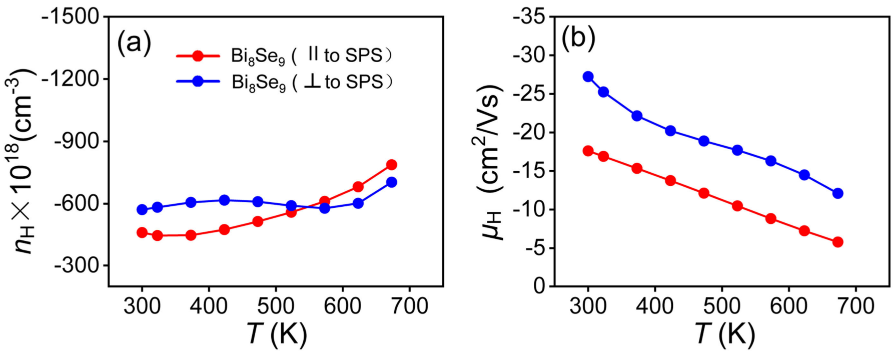

Figure S2. Temperature dependent (a) the Hall carrier concentration (n_H), (b) the Hall carrier mobility (μ_H) of $Bi_8Se_{9\parallel SPS}$ and $Bi_8Se_{9\perp SPS}$.

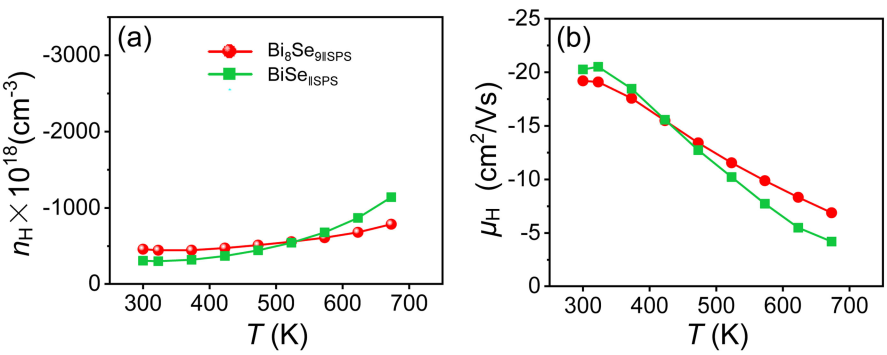

Figure S3. Temperature dependent (a) the Hall carrier concentration (n_H), (b) the Hall carrier mobility (μ_H) of $Bi_8Se_{9\parallel SPS}$ and $BiSe_{\parallel SPS}$.

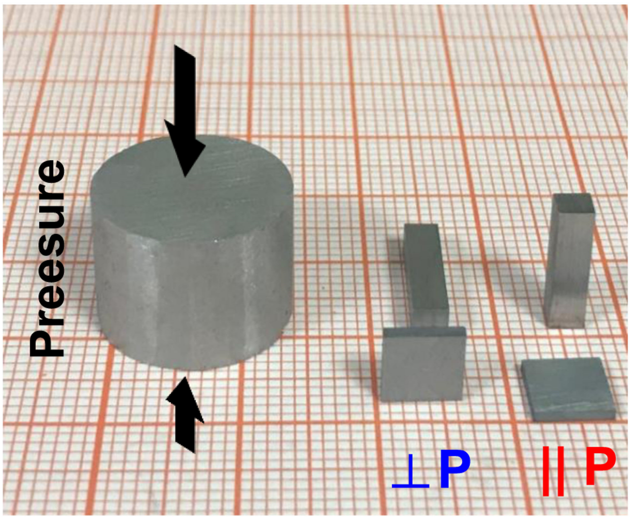

Figure S4. Samples cut from the SPS ingot along the parallel to (//) or perpendicular to (⊥) the SPSing pressure direction.

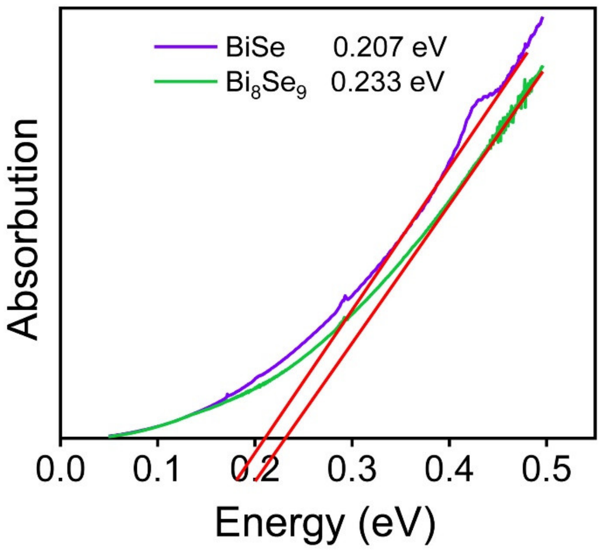

Figure S5. The optical band gaps of Bi_8Se_9 and BiSe measured by the Fourier transform infrared spectroscopy.

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Table S1 Relevant formulas and parameters applied in theoretical calculation of lattice thermal conductivity.

parameters	Bi_8Se_9		BiSe	Formulas[1-3]
A	3.1×10^{-6}			
N	17		12	$\kappa_l = A\frac{\overline{M}\Theta_D^3 V^{1/3}}{\gamma^2 N^{2/3} T}$
V (Å^3)	28.53		21.08	
$\overline{M}$ (g/mol)	140.11		143.97	
longitudinal sound velocity, v_{ls} (ms^{-1})	$2626_{\parallel}$	$2897_{\perp}$	$2714_{\parallel}$	$v_{ds} = (\frac{1}{3}v_{ls}^{-3} + \frac{2}{3}v_{ts}^{-3})^{-1/3}$
transversal sound velocity, v_{ts} (ms^{-1})	$1574_{\parallel}$	$1736_{\perp}$	$1583_{\parallel}$	
Θ_D (K)	$107.94_{\parallel}$	$119.13_{\perp}$	$107.86_{\parallel}$	$\Theta_D = \frac{\hbar}{k_B}\frac{2}{\pi}v_{ds}(\frac{6\pi^2}{VN})^{1/3}$
γ	$1.36_{\parallel}$	$1.37_{\perp}$	$1.46_{\parallel}$	$\gamma = \frac{3}{2}\left(\frac{3(\frac{v_{ls}}{v_{ts}})^2 - 4}{(\frac{v_{ls}}{v_{ts}})^2 + 2}\right)$

References

(1) Li, J.; Zheng, S. Q.; Fang, T.; Yue, L.; Zhang, S.; Lu, G. W. Computational Prediction of a High *ZT* of n-Type Mg_3Sb_2-Based Compounds with Isotropic Thermoelectric Conduction Performance. *Phys. Chem. Chem. Phys.* **2018**, *20*, 7686–7693.

(2) Slack, G. A. Nonmetallic Crystals with High Thermal Conductivity. *J. Phys. Chem. Solids* **1973**, *34*, 321–335.

(3) Chen, Z. W.; Zhang, X. Y.; Lin, S. Q.; Chen, L. D.; Pei, Y. Z. Rationalizing Phonon Dispersion for Lattice Thermal Conductivity of Solids. *Natl. Sci. Rev.* **2018**, 5, 888–894.