Supplementary Materials

Strain and Doping in Two-Dimensional SnTe Nanosheets: Implications for Thermoelectric Conversion

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Computational details

The electronic relaxation time of two-dimensional (2D) SnTe was calculated using Quantum Espresso[1] and EPW[2]. The electrical transport properties of 2D SnTe were calculated using BoltzTraP2[3] based on the computed electronic relaxation time. Norm-conserving relativistic pseudopotentials[4, 5] were applied. The kinetic energy cutoff was set to 100 Ry. The convergence criteria for total energy and atomic force were set to 10^{-6} Ry and 10^{-5} Ry/a.u., respectively. A 20×20×1 *k*-mesh was used in the self-consistent calculations and a 10×10×1 *q*-mesh was used in the phonon calculations. For EPW, 20×20×1 *k*-mesh and 10×10×1 *q*-mesh were interpolated to 200×200×1 fine *k*-mesh and 100×100×1 fine *q*-mesh, respectively. A broadening parameter of 10 meV was used in the energy-conserving δ functions.

Table S1. Optimized lattice parameters of the supercells of doped 2D SnTe.

	Sn site		Te site	
	a (Å)	*b* (Å)	*a* (Å)	*b* (Å)
As-doped	18.23	18.29	18.14	18.18
Sb-doped	18.23	18.32	18.16	18.21
Bi-doped	18.26	18.33	18.16	18.23
Br-doped	18.07	18.11	18.26	18.30
I-doped	18.10	18.10	18.31	18.32

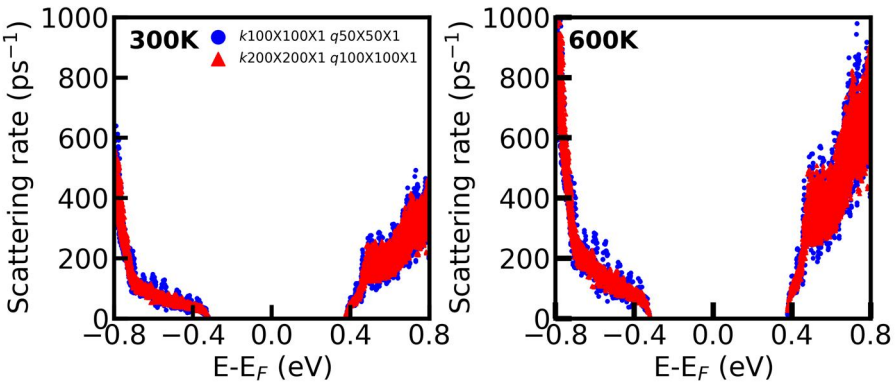

Figure S1. Scattering rate of 2D SnTe at 300 K (left) and 600 K (right) calculated with different *k*-mesh and *q*-mesh densities.

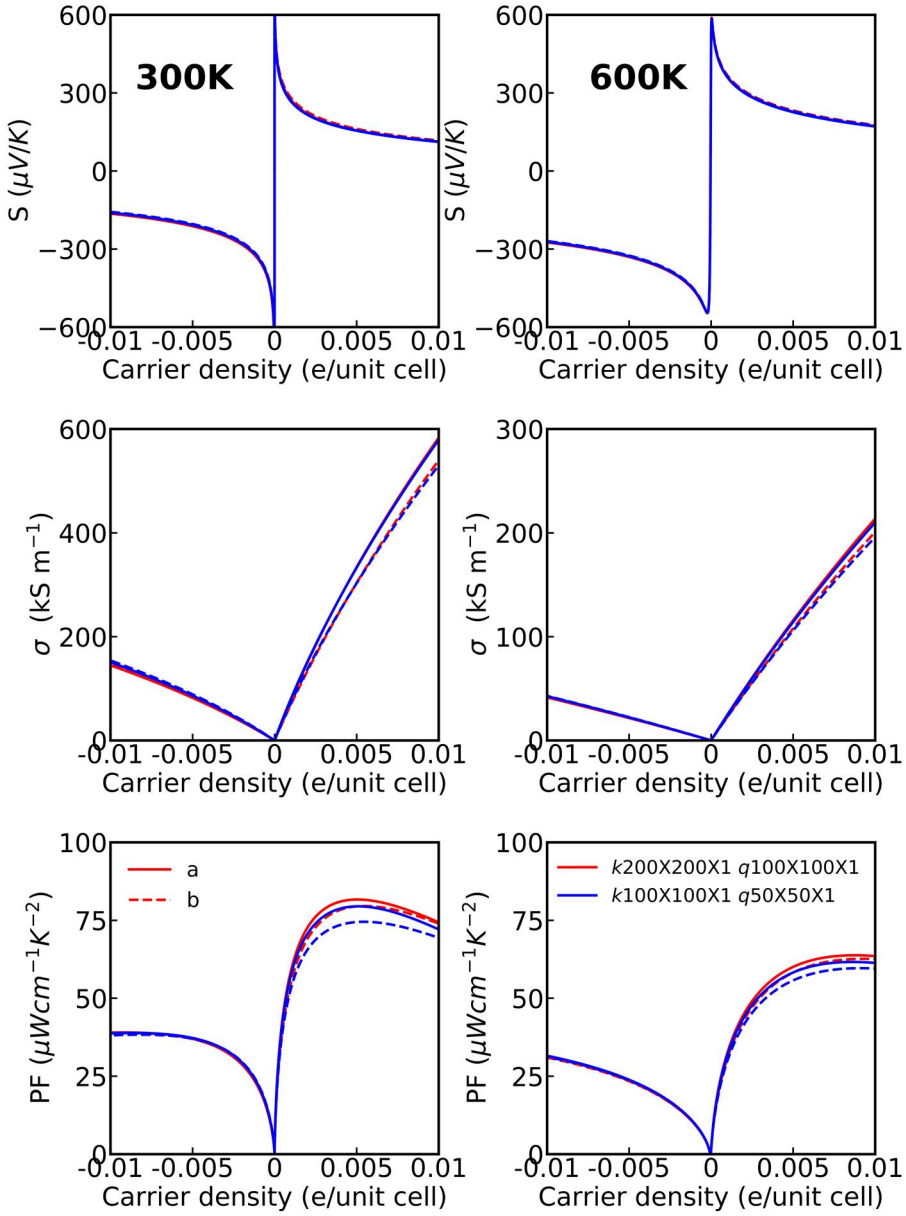

Figure S2. Seebeck coefficients (top), electrical conductivities (middle) and power factors (bottom) of 2D SnTe along *a* (solid curves) and *b* (dashed curves) directions at 300 K (left) and 600 K (right) calculated with different *k*-mesh and *q*-mesh densities.

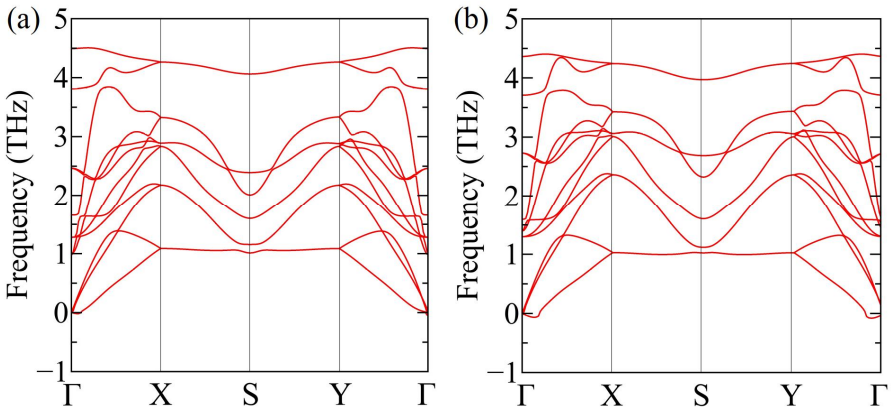

Figure S3. Phonon dispersions of 2D SnTe under different equibiaxial compressive stresses: (a) $|\Delta a/a_0|$ = 1.23% and (b) $|\Delta a/a_0|$ = 2.35%. Negative values represent imaginary phonon frequencies.

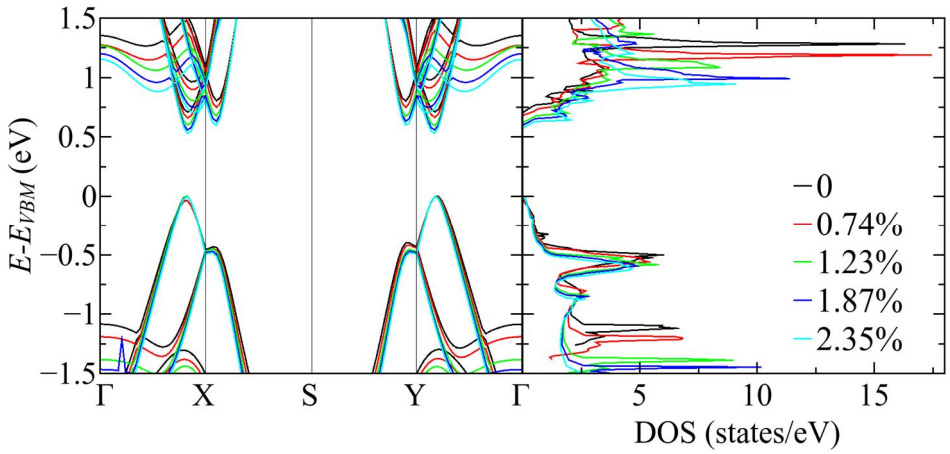

Figure S4. Band structures and density of states of 2D SnTe under different equibiaxial compressive stresses (the values of $|\Delta a/a_0|$ are given in the figure). The valence band maximum is shifted to 0 eV.

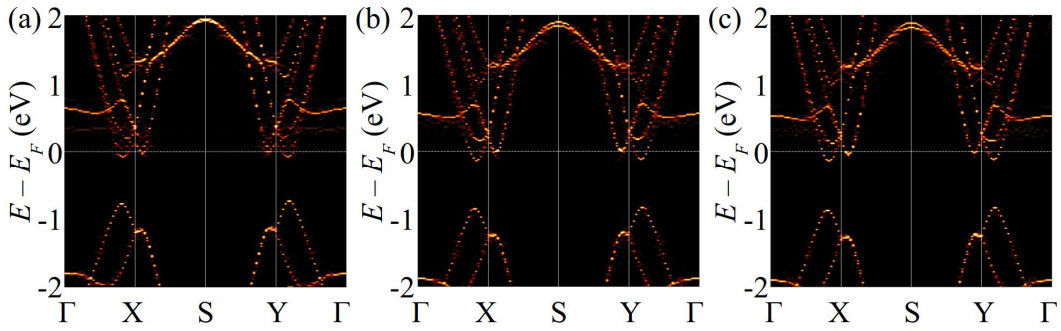

Figure S5. Effective band structures of (a) Bi-doped (Sn site), (b) Br-doped (Te site), and (c) I-doped (Te site) 2D SnTe. Fermi level is located at 0 eV.

References

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