Supporting Information

High thermoelectric performances of SnSe allotropes

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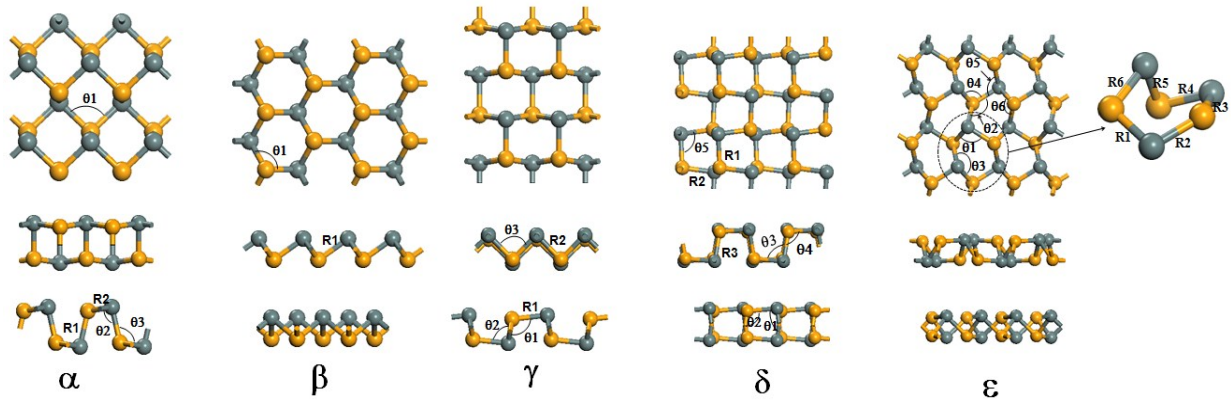

Fig. S1 Schematic structure of bonds and angles for the five optimized SnSe monolayer polymorphs.

Table. S1 The detailed parameters of bonds and angles for the five optimized SnSe monolayer polymorphs.

Phases	R1	R2	R3	R4	R5	R6	θ1	θ2	θ3	θ4	θ5	θ6
α-SnSe	2.60	2.88	-	-	-	-	94.28	104.77	92.80	-	-	-
β- SnSe	2.66	-	-	-	-	-	90.19	-	-	-	-	-
γ- SnSe	3.05	2.62	-	-	-	-	100.78	92.30	90.23	-	-	-
δ- SnSe	2.81	2.79	2.64	-	-	-	102.17	93.30	93.49	103.27	-	-
ε- SnSe	2.69	2.65	2.69	2.69	2.69	2.65	96.13	122.52	101.28	100.95	87.66	79.11

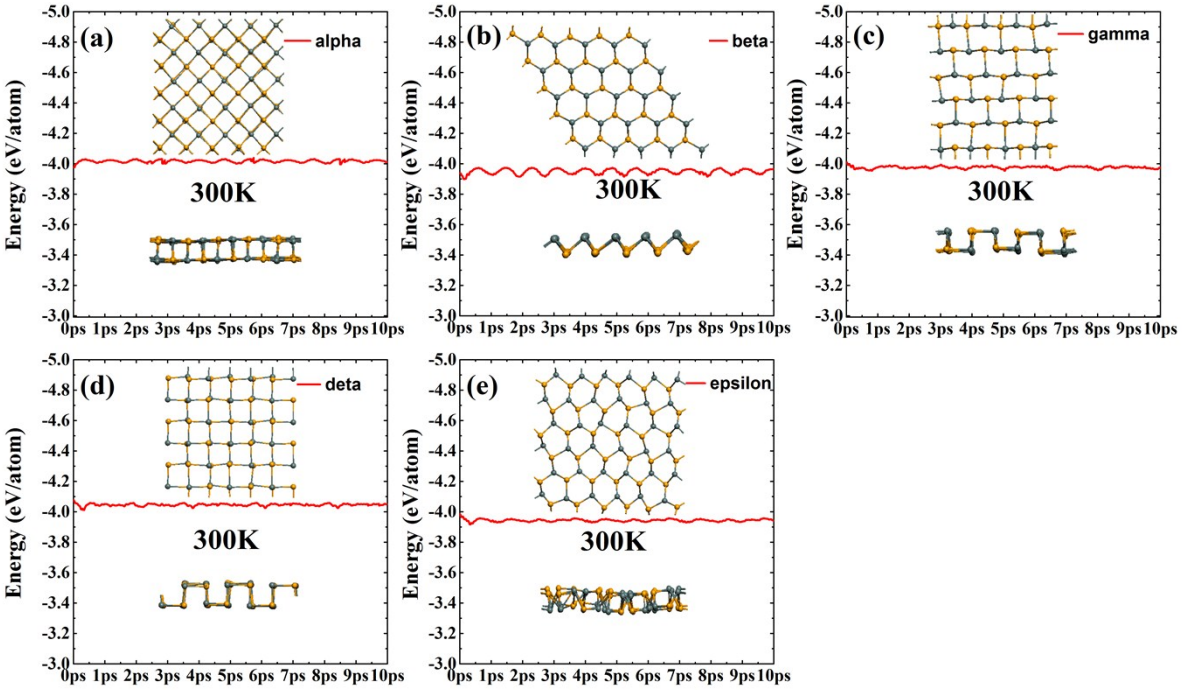

Fig. S2 The evolution of the total potential energy with simulation time of α–SnSe, β–SnSe, γ–SnSe, δ–SnSe and ε–SnSe single-layer during ab initio molecular dynamics simulations and the snapshots of the final atomic configurations at 300K.

Table S2. The calculated elastic constants (C_{ij}), bulk modulus (B), shear modulus (G), density (ρ), volume (V), transverse sound velocity (v_s), longitudinal sound velocity (v_l), , and minimum lattice thermal conductivity (κ_{min}) of α–SnSe, β–SnSe, γ–SnSe, δ–SnSe and ε–SnSe.

Phases	C_{11}(Gpa)	C_{12}(Gpa)	C_{44}(Gpa)	ρ(g/cm^3)	V (Å ^{3})	B(Gpa)	G(Gpa)	V_s(m/s)	V_l(m/s)	κ_{min}
α	20.9	4.42	3.57	6.66	49.31	9.91	5.44	1886	3349	0.175
β	15.7	11.29	5.17	7.52	21.86	12.76	3.98	1861	3965	0.156
γ	34.80	4.31	3.92	7.72	42.50	14.47	8.45	2254	3934	0.219
δ	15.49	5.22	5.20	6.64	99.07	8.64	5.174	2087	3618	0.162
ε	17.43	9.18	7.83	7.55	87.16	11.93	6.35	2222	3982	0.184

Table. S3 The detailed parameters of effective masses at VBM, VBM1, CBM, CBM1 and Seebeck coefficient with the carrier concentration of 5×10^{19} cm^{-3} at 300 K for the five optimized SnSe monolayer polymorphs.

Phases	m*(m0) VBM	m*(m0) CBM	m*(m0) VBM1	m*(m0) CBM1	Seebeck coefficient (μV/K)
α	0.15	0.17	0.17	0.23	66.37
β	1.15	1.10	1.36	0.45	348
γ	1.07	0.11	0.18	0.04	325
δ	0.29	0.71	0.07	0.07	71.32
ε	1.15	0.93	1.68	0.23	265

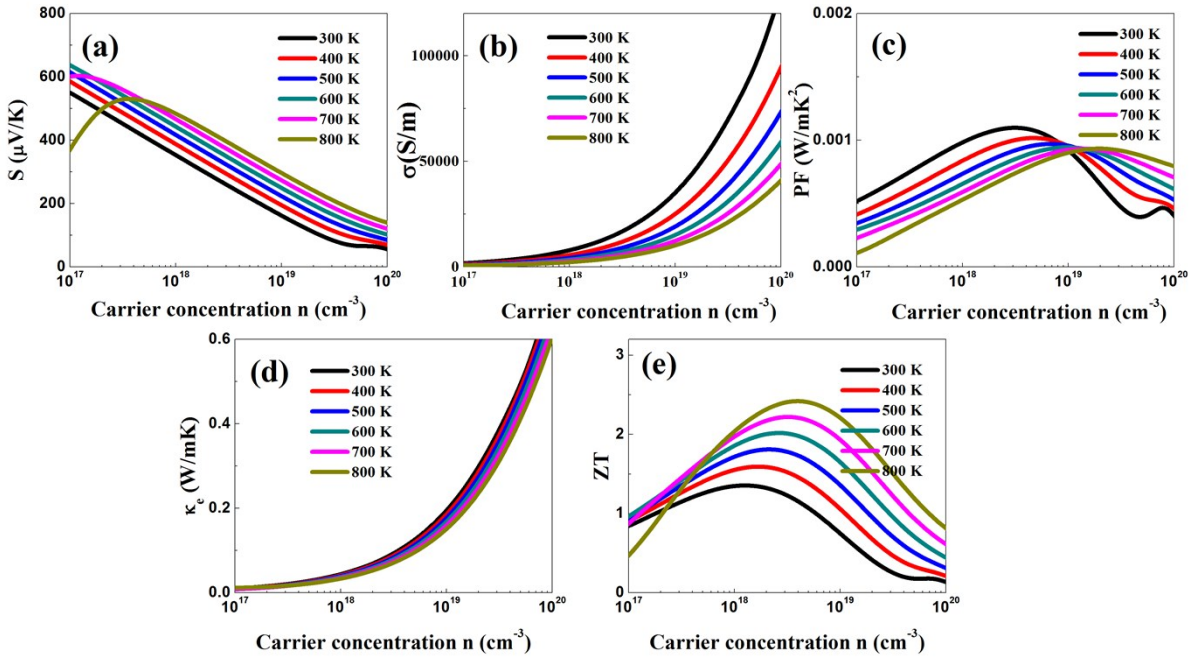

Fig. S3 Thermoelectric properties as a function of temperature from 300K to 800K for hole-doped SnSe crystals. (a) Electrical conductivity. (b) Seebeck coefficient. (c)Power factor (PF). (d) Total thermal conductivity. (e) ZT values for α–SnSe.

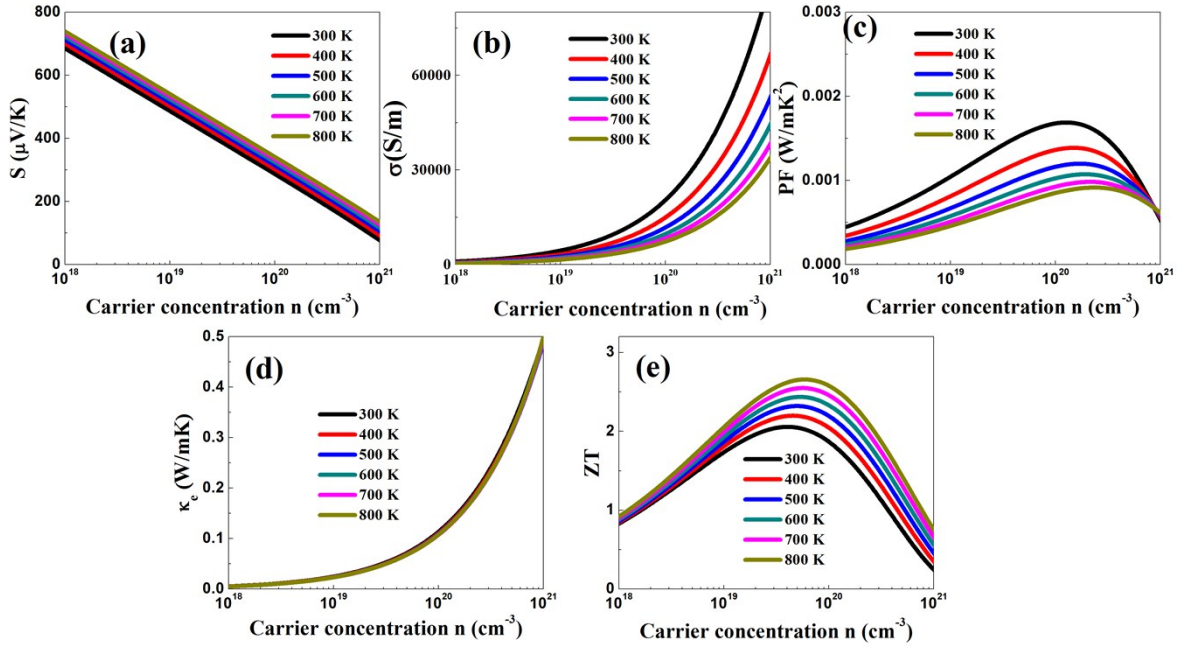

Fig. S4 Thermoelectric properties as a function of temperature from 300K to 800K for hole-doped SnSe crystals. (a) Electrical conductivity. (b) Seebeck coefficient. (c)Power factor (PF). (d) Total thermal conductivity. (e) ZT values for β–SnSe.

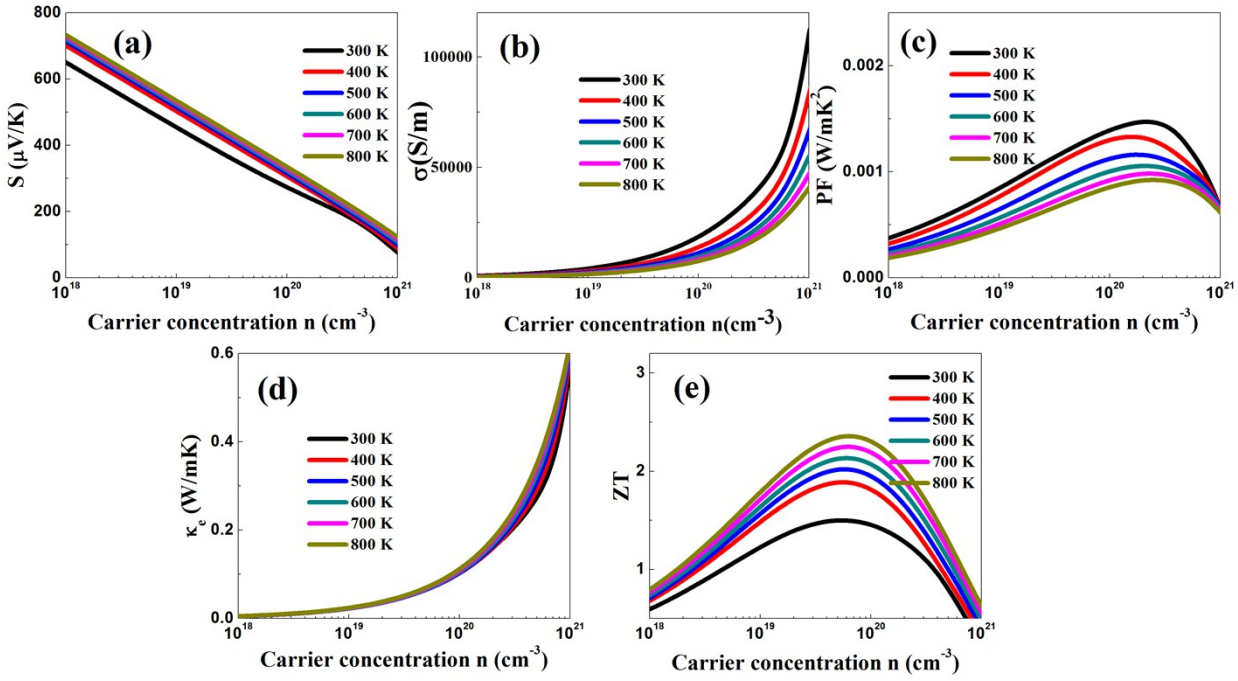

Fig. S5 Thermoelectric properties as a function of temperature from 300K to 800K for hole-doped SnSe crystals. (a) Electrical conductivity. (b) Seebeck coefficient. (c)Power factor (PF). (d) Total thermal conductivity. (e) ZT values for γ–SnSe.

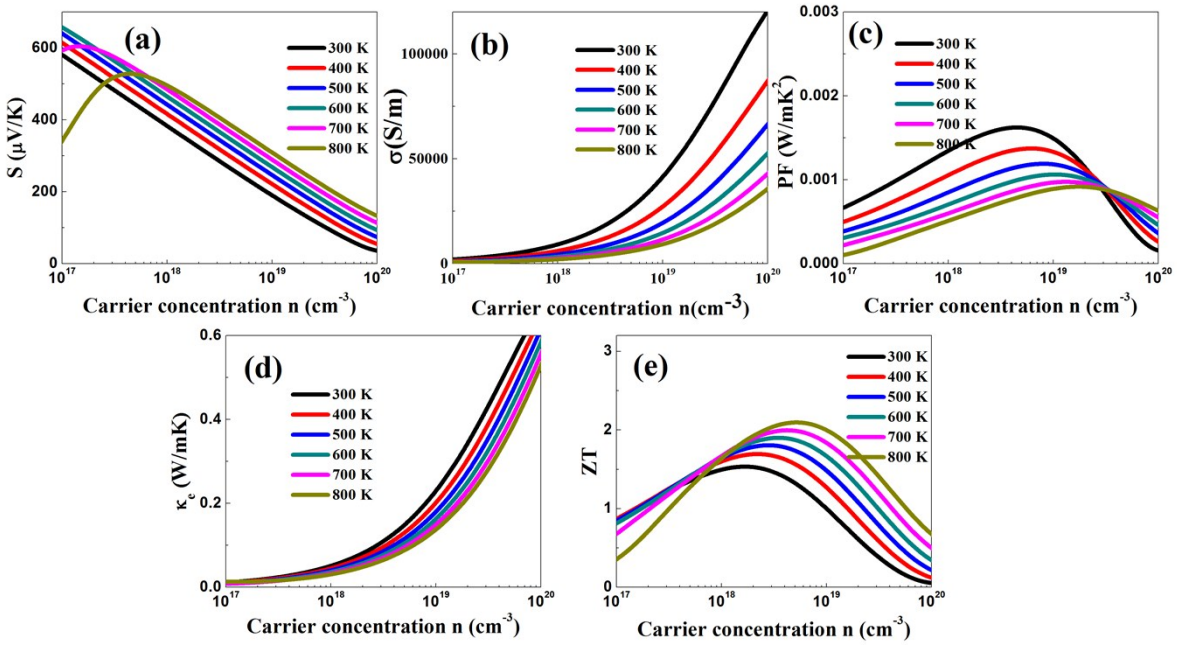

Fig. S6 Thermoelectric properties as a function of temperature from 300K to 800K for hole-doped SnSe crystals. (a) Electrical conductivity. (b) Seebeck coefficient. (c)Power factor (PF). (d) Total thermal conductivity. (e) ZT values for δ–SnSe.

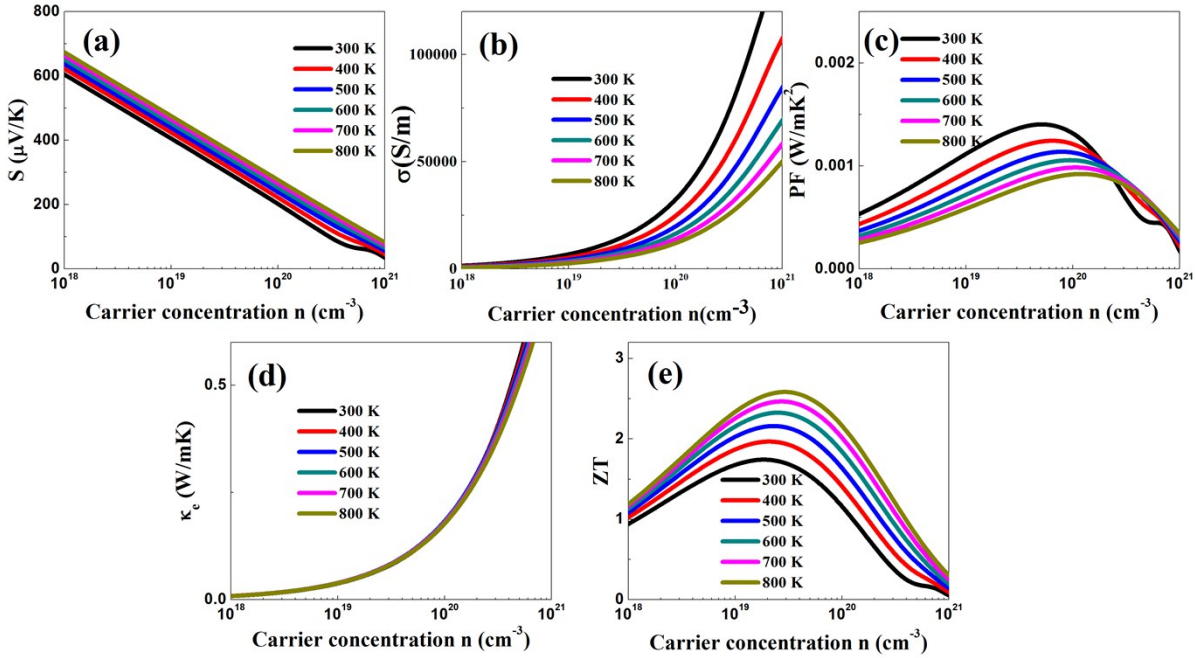

Fig. S7 Thermoelectric properties as a function of temperature from 300K to 800K for hole-doped SnSe crystals. (a) Electrical conductivity. (b) Seebeck coefficient. (c)Power factor (PF). (d) Total thermal conductivity. (e) ZT values for ε–SnSe.

Crystal Coordinate Lists:

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_symmetry_cell_setting            orthorhombic
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  -x,y,z
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  -x+y,-x,z
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  x,x-y,z
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3. gamma.cif

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  x+1/2,-y,z+1/2
  -x,y,z
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  x+1/2,-y,z
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_atom_site_occupancy
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Sn1    Se1     2.644   4_655 S
Se1    Sn1     2.819   2_664 S
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Se1    Sn1     2.644   4_654 S
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5. epsilon.cif

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Se1    Se    0.86529   0.45994   0.84600   0.01267  Uiso   1.00
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Se1    Sn1     2.687   1_556 S
Se1    Sn1     2.693   2_765 S
Se1    Sn1     2.648   4_655 S
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