Supplementary Information for

Engineering electronic band structure and thermoelectric performance of GeTe via lattice structure manipulation from first-principles

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S.1 RESULTS AND DISCUSSIONS

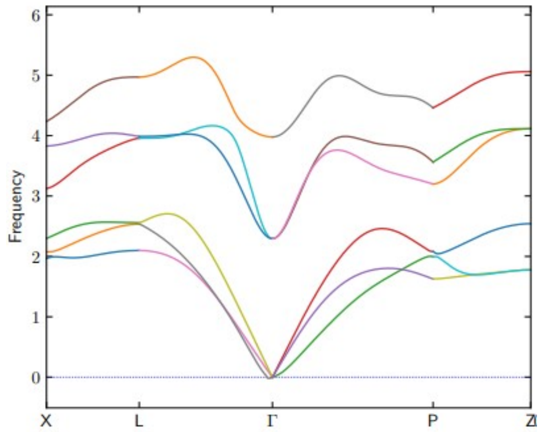
S.1.1 Crystal-structure modification influences the electronic structure

TABLE.S1 lists the first-principles calculation results. It contains the values of band gap(Eg) and band convergence($\Delta E_{L\Sigma}$) influenced by crystal-structure modification

TABLE.S1. Influence of various crystal structure on the band gap(Eg) and band convergence($\Delta E_{L\Sigma}$)

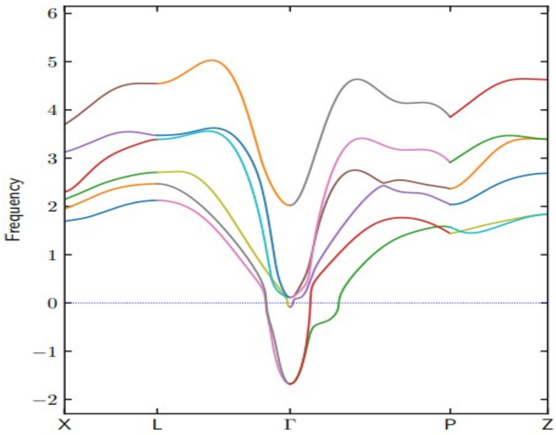
		c-Eg (eV)	c-$\Delta E_{L\Sigma}$(eV)	r-Eg (eV)	r-$\Delta E_{L\Sigma}$(eV)
interaxial angle(°)	57	0.051	0.217	0.379	0.297
	58	0.011	0.239	0.471	0.218
	59	0.112	0.152	0.552	0.143
	60	0.238	0.061	0.599	0.071
lattice parameter(Å)	4.2	0.112	0.073	0.151	0.277
	4.25	0.229	0.062	0.247	0.266
	4.3	0.335	0.050	0.337	0.249
	4.35	0.428	0.037	0.419	0.237
	4.4	0.508	0.023	0.491	0.227
reciprocal displacement	0.47	0.439	0.553	0.455	0.230
	0.48	0.386	0.292	0.374	0.203
	0.49	0.339	0.063	0.065	0.171
	0.5	0.238	0.061	-0.131	0.143

(a)



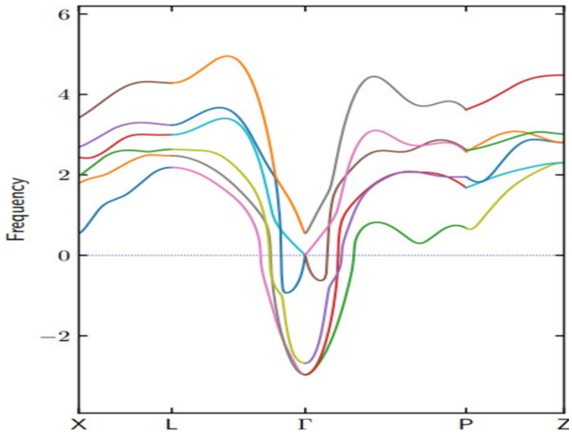
Te(0.47,0.47,0.47)

（b）



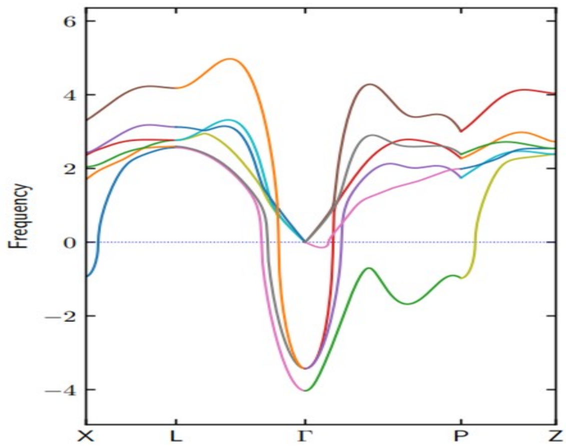
Te(0.48,0.48,0.48)

(c)



Te(0.49,0.49,0.49)

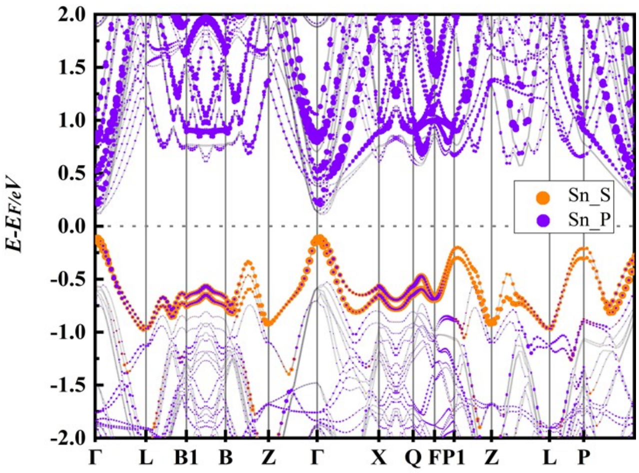
(d)



Te(0.50,0.50,0.50)

Figure S1 The calculated phonon dispersion with the increase of reciprocal displacement.

. (a)



$Ge_7Sn_1Te_8$

Figure S2 Pband Structure of GeTe doped with Sn.

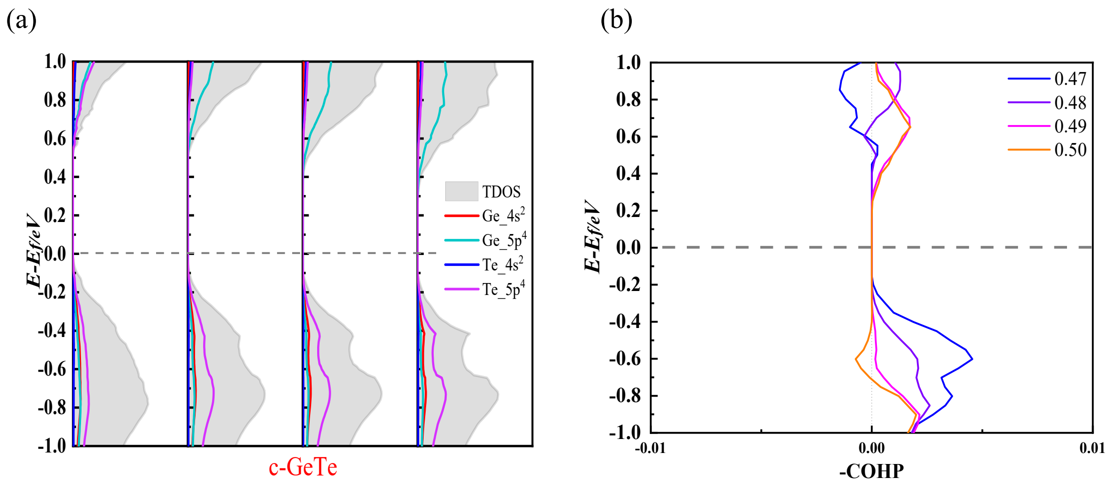


Figure S3 The calculated electronic structure (a)DOS and PDOS, (b) -COHP of c-GeTe with the increase of reciprocal displacement.

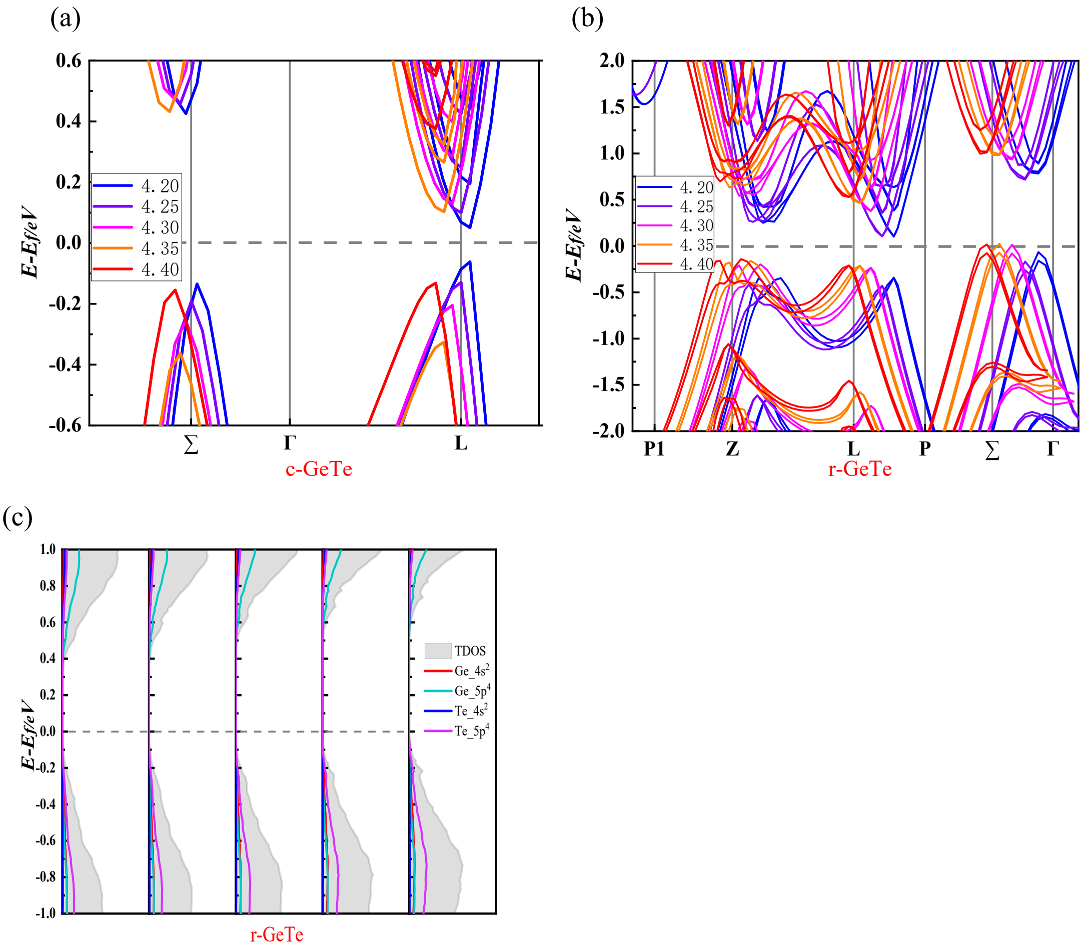


Figure S4 The enlarged view of the valence bands(VBs) near the L point and Σ point of (a)c-GeTe and (b)r-GeTe. The calculated electronic structure DOS and (c)PDOS of r-GeTe with the increase of lattice parameters.

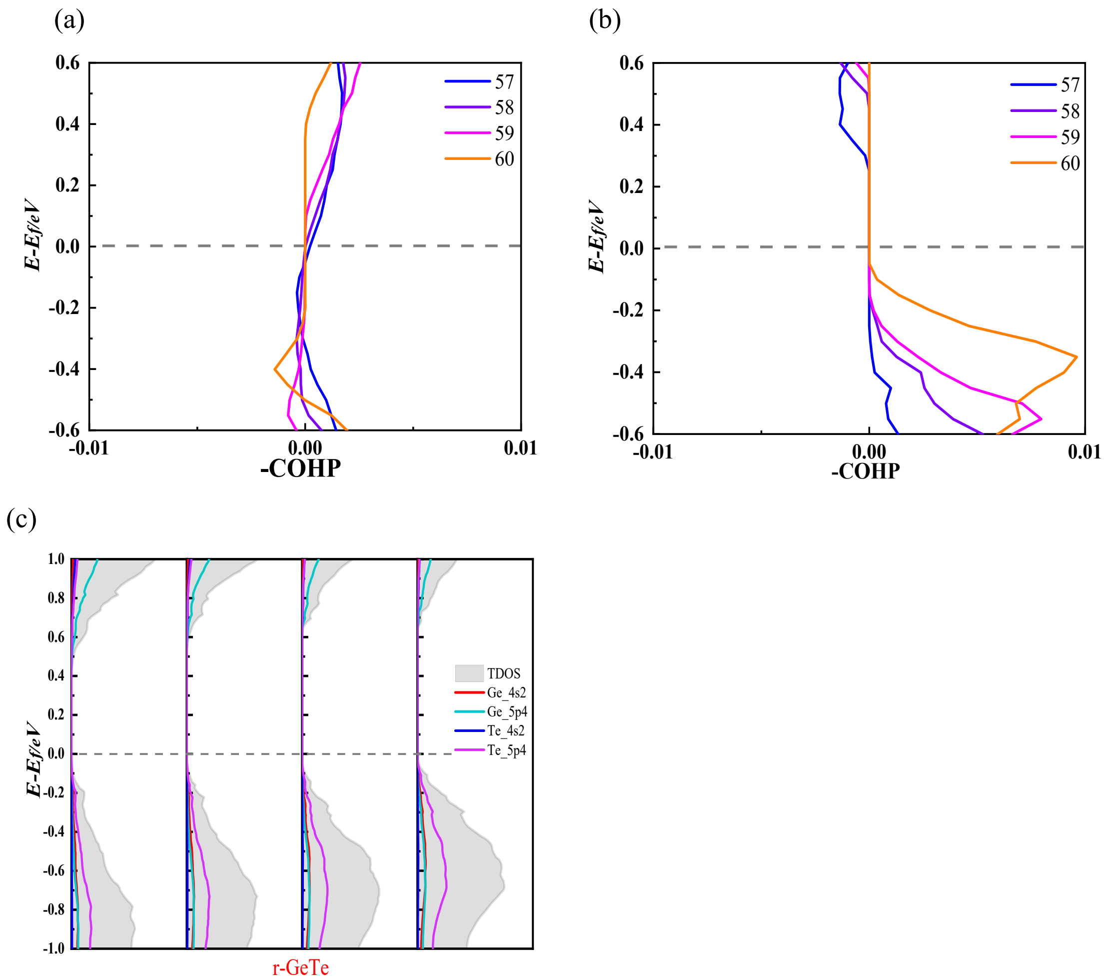


Figure S5 The calculated electronic structure -COHP of (a)c-GeTe and (b)r-GeTe, (c)DOS and PDOS of r-GeTe with the increase of interaxial angle.

S.1.2 Crystal-structure modification influences the TE properties of GeTe using semiclassical Boltzmann theory

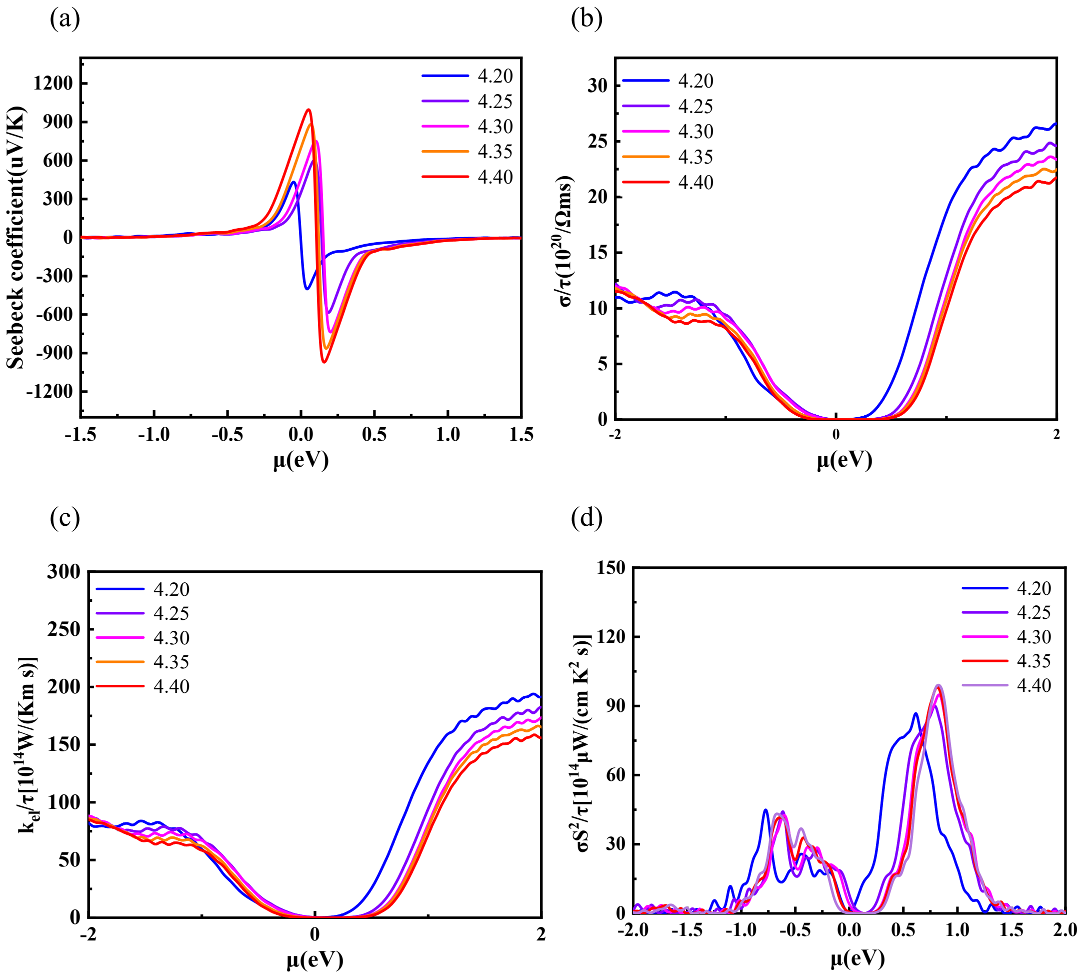


Figure S6 Dependences of (a) Seebeck coefficient, (b) electrical conductivity, (c) thermal conductivity, and (d) power factor by scaling them with τ of r-GeTe on the chemical potential at various lattice parameters at 300 K.

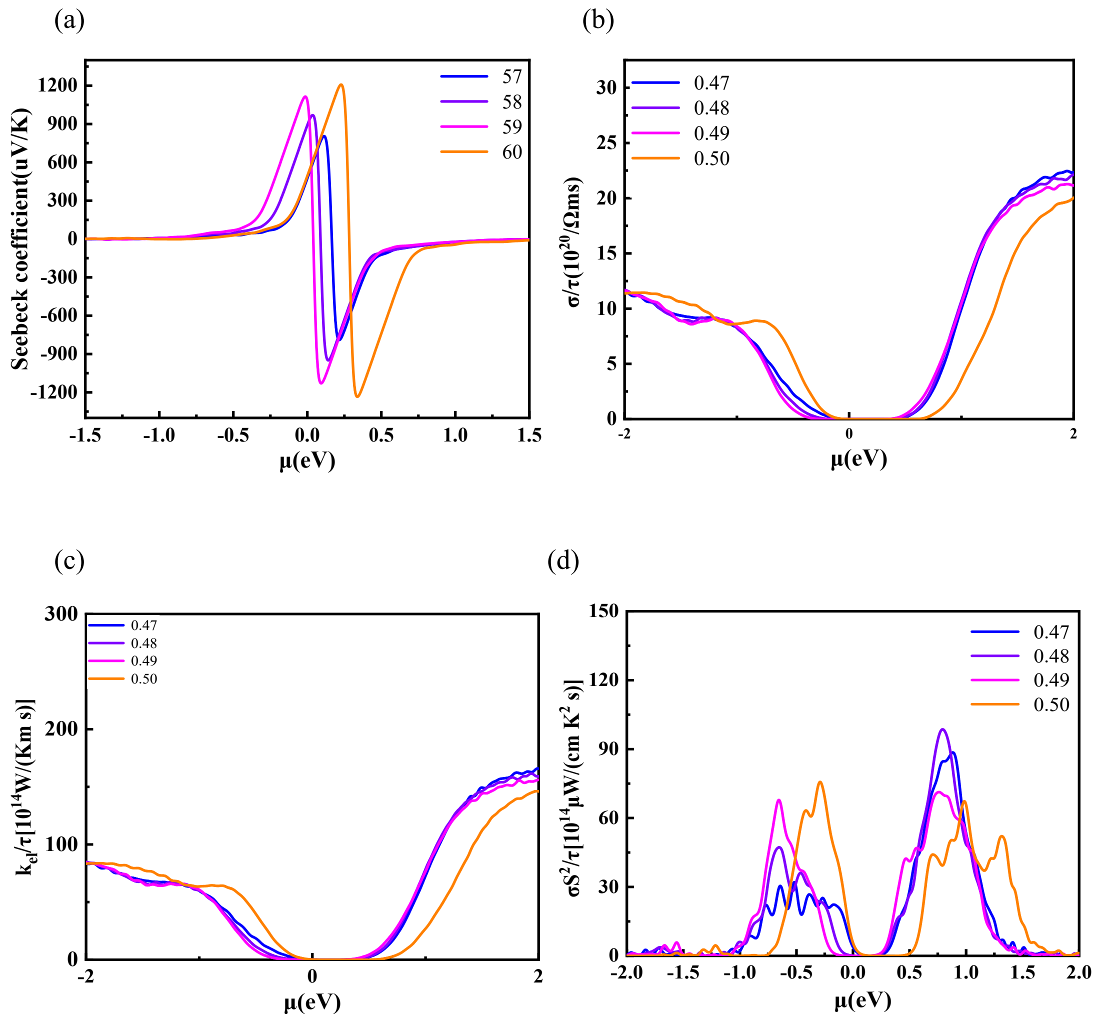


Figure S7 Dependences of (a) Seebeck coefficient, (b) electrical conductivity, (c) thermal conductivity, and (d) power factor by scaling them with τ r-GeTe on the chemical potential at various interaxial angle at 300 K.

TABLE.S2 lists the first-principles calculation results for thermoelectric parameters. It contains the maximum values of thermoelectric parameters of GeTe by scaling them with τ at 300K

TABLE.S2. Influence of varying lattice structures on the maximum value of thermoelectric parameters of GeTe by scaling them with τ at 300K

		r-GeTe S (μV/K)	r-GeTe PF(×10^{14}μW/cm K^2s)	c-GeTe S (μV/K)	c-GeTe PF(×10^{14}μW/cm K^2s)
interaxial angle (°)	57	805.4	88.5	82.1	263.4
	58	969.4	98.5	109	319
	59	1129	71.3	234.8	445.8
	60	1232.8	67.3	389.5	530.5
lattice parameter (Å)	4.2	432.4	86.7	-311	482
	4.25	602	90	-391.5	531.9
	4.3	751.8	94.8	-466.9	578.4
	4.35	882.6	98.1	-532.6	624
	4.4	996.5	99.1	-584	661.2
reciprocal displacement	0.47	951	105	446	285.6
	0.48	794.2	113.98	465.2	473.6
	0.49	358.9	99.4	443	541.6
	0.5	171.7	116.8	398	536