

Supporting Information

Machine learning for predicting ultralow thermal conductivity and high ZT in complex thermoelectric materials

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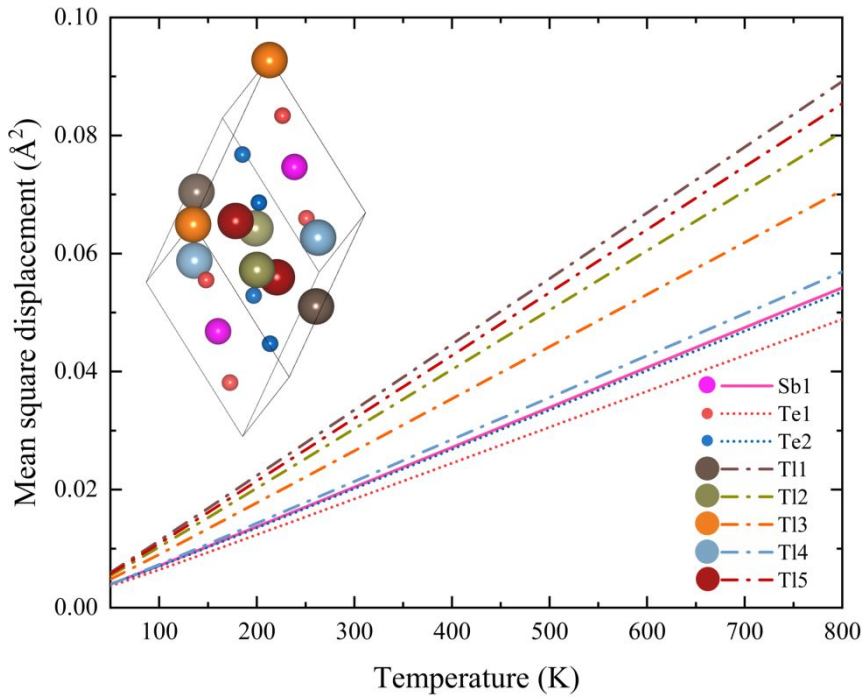


FIG. S1. The mean square atomic displacements (MSDs) with temperature for Tl_9SbTe_6 .

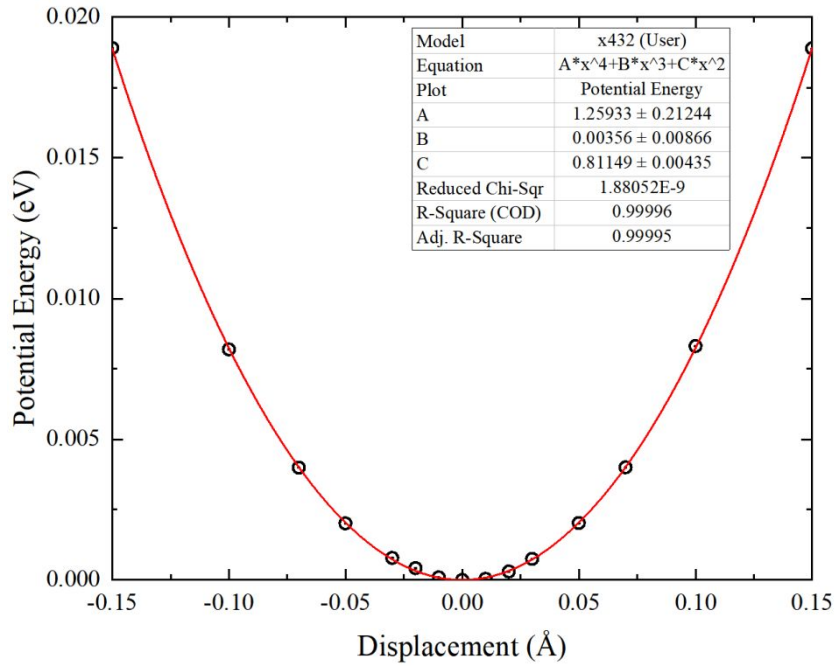


FIG. S2. Anharmonic frozen-phonon potential with quadratic and polynomial fitting. It writes as $y = 1.2593 \times x^4 + 0.0036 \times x^3 + 0.8115 \times x^2$.

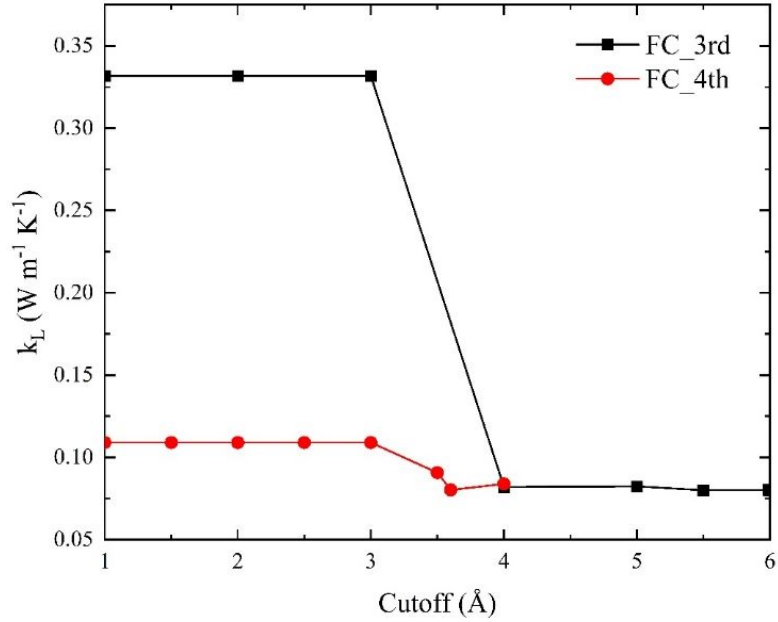


FIG. S3. The lattice thermal conductivity as a function of cutoff distances with interatomic third-order and fourth-order force constants.

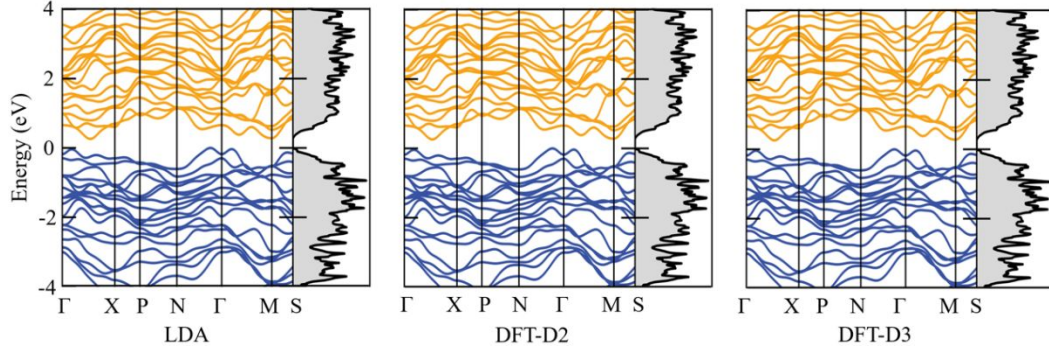


FIG. S4. The electronic band gap with different computational functionals.

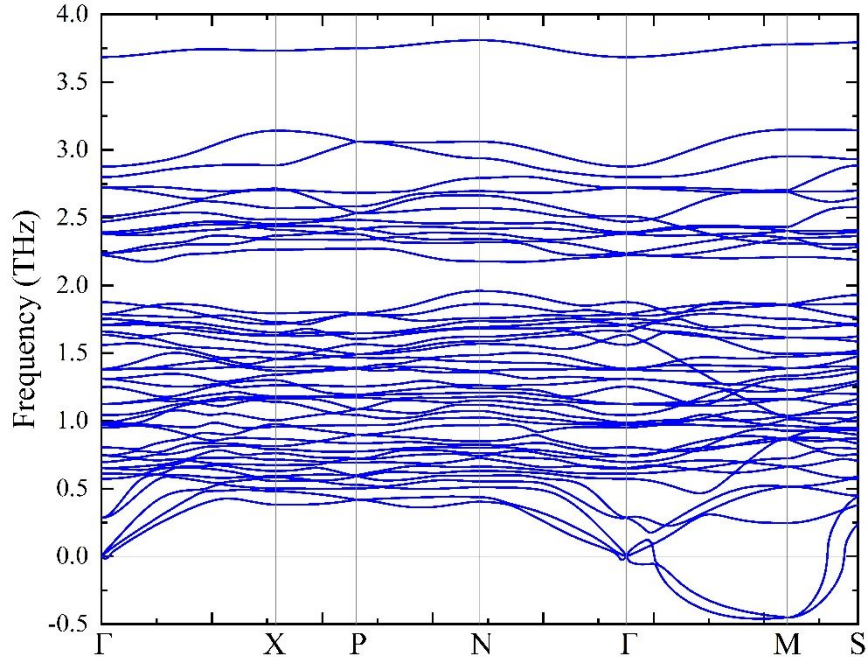


FIG. S5. Phonon dispersion of Ti9SbTe6 calculated by DFT using PBE functionals.

Table S1. The calculated lattice constants using different functionals.

	a=b (Å)	c (Å)	V (Å ³)	Difference (%)		
				a=b	c	V
EXP	8.8298	13.0126	1014.532			
PBE_JAP ^[15]	8.9724	13.5146	1087.979	1.614986	3.857799	7.239464
PBE	8.9665	13.7248	1103.448	1.548166	5.473157	8.764237
LDA	8.6293	12.7693	950.8636	-2.27072	-1.86973	-6.27566

Crystal structure

1.0

8.6292883350027196	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.6292883350027196	0.0000000000000000
0.0000000000000000	0.0000000000000000	12.7693421744020377

Sb Te Tl

2 12 18

Direct

0.0000000000000000	0.0000000000000000	0.4925074820904819
0.5000000000000000	0.5000000000000000	0.9925074820904819
0.5000000000000000	0.5000000000000000	0.2324471203967869
0.1496558830371512	0.3268119126970722	0.4925075660583969
0.6731880873029278	0.1496558830371512	0.4925075660583969
0.0000000000000000	0.0000000000000000	0.2525674930863173
0.3268119126970722	0.8503441169628488	0.4925075660583969
0.8503441169628488	0.6731880873029278	0.4925075660583969
0.0000000000000000	0.0000000000000000	0.7324471203967868
0.6496558830371512	0.8268119126970722	0.9925075660583969
0.1731880873029277	0.6496558830371512	0.9925075660583969
0.5000000000000000	0.5000000000000000	0.7525674930863173
0.8268119126970722	0.3503441169628490	0.9925075660583969
0.3503441169628490	0.1731880873029277	0.9925075660583969
0.8605435682760887	0.6525161389068509	0.1534484841752498
0.1525159611646714	0.6394565687184035	0.3315675802827766
0.5000000000000000	0.5000000000000000	0.4925085723607120
0.8474840388353286	0.3605434312815965	0.3315675802827766
0.1394564317239113	0.3474838610931491	0.1534484841752498
0.6525161389068509	0.1394564317239113	0.1534484841752498
0.3605434312815965	0.1525159611646714	0.3315675802827766
0.6394565687184035	0.8474840388353286	0.3315675802827766
0.3474838610931491	0.8605435682760887	0.1534484841752498
0.3605435682760887	0.1525161389068508	0.6534484841752498
0.6525159611646714	0.1394565687184035	0.8315675802827766
0.0000000000000000	0.0000000000000000	0.9925085723607120
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0.6394564317239113	0.8474838610931491	0.6534484841752498
0.1525161389068508	0.6394564317239113	0.6534484841752498
0.8605434312815965	0.6525159611646714	0.8315675802827766
0.1394565687184035	0.3474840388353286	0.8315675802827766
0.8474838610931491	0.3605435682760887	0.6534484841752498