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Effects of point defects on thermal-mechanical properties of BiCuOTe: a first-principles study

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Figure S1. Total energy of unit-cell of BiCuOTe under different (a) cut-off energies and (b) k-point samplings.

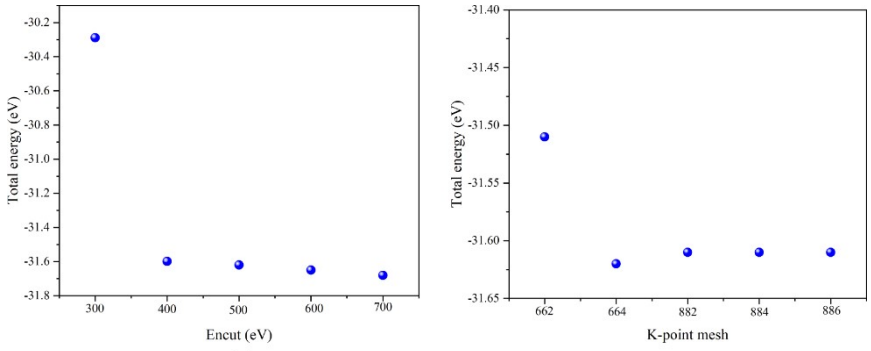

Figure S1

Table S1. The internal energy of Bi, Cu, Te and BiCuOTe obtained from DFT calculations.

	Total energy (eV)	Potential energy (eV/atom)
Bi	-15.43	-3.86
Cu	-16.40	-4.10
Te	-9.47	-3.16
BiCuOTe	-31.62	-

Table S2. The Gibbs free energy (G) of O_2, H_2 and H_2O. E: Total energy obtained from DFT calculations. Δ G: the correction to Gibbs free energy.

	Pressure (bar)	Temperature (K)	E (eV)	Δ G (eV)	G (eV)
O_2 (g)	1	298.15	-	-	-9.91
H_2 (g)	1	298.15	-6.76	-0.045	-6.80
H_2O (l)	0.035	298.15	-14.22	-0.001	-14.22