Supplementary Information

Chemical potential tuning and anharmonic lattice effect on the enhancement of thermoelectric performance in GeTe_{1-x}I_x compounds

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	formula	Energy [eV]
Te-site doping	Ge ₂₄ Te ₂₃ I	1.25
Interstitial doping of I	Ge ₂₄ Te ₂₄ I	0.28

Table S1. Formation energy calculation of the lodine doping at Te-site $Ge_{24}Te_{23}I$, and interstitial doping of lodine $Ge_{24}Te_{24}I$.



Figure S1. Magnetic field dependence of the Hall resistivity (ρ_{xy}) for GeTe_{1-x}I_x (x = 0.0, 0.01, 0.05, 0.1, 0.15 and 0.2) compounds at 300K.



Figure S2. Seebeck coefficient with chemical potential at various temperature, as indicated of the α - (rhombohedral, open circle) and β - (cuibic, colored lines) phases.



Figure S3. Temperature derivative of Seebeck coefficient as function of temperature for $GeTe_{1-x}I_x$ (x = 0.0, 0.01, 0.05, 0.1, 0.15 and 0.2) compounds.



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Element	At. No.	Mass [%]	Mass Norm. [%]	Atom [%]	abs. error [%] (3 sigma)
Ge	32	33.52	34.36	47.92	3.20
Te	52	63.32	64.91	51.50	5.60
I.	53	0.71	0.72	0.58	0.20
		97.55	100.00	100.00	

Figure S4. Elemental mapping of $GeTe_{1-x}I_x$ (x = 0.05) from energy dispersive X-ray spectroscopy (EDX) images.



	2.2			
Te-La	HV: 20 kM WD: 8.3 mm		-	10 µm

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Element	At. No.	Mass [%]	Mass Norm. [%]	Atom [%]	abs. error [%] (3 sigma)
Ge	32	36.02	35.48	49.14	3.43
Те	52	64.25	63.30	49.89	5.71
I.	53	1.24	1.22	0.97	0.27
		101.51	100.00	100.00	

Figure S5. Elemental mapping of $GeTe_{1-x}I_x$ (x = 0.1) from energy dispersive X-ray spectroscopy (EDX) images.





Map

Element	At. No.	Mass [%]	Mass Norm. [%]	Atom [%]	abs. error [%] (3 sigma)
Ge	32	33.57	36.05	49.77	3.20
Te	52	57.34	61.59	48.38	5.08
L	53	2.19	2.35	1.86	0.34
		93.10	100.00	100.00	

Figure S6. Elemental mapping of $GeTe_{1-x}I_x$ (x = 0.2) from energy dispersive X-ray spectroscopy (EDX) images.



Figure S7. Temperature-dependent specific heat $C_p(T)$ of $GeTe_{1-x}I_x$ (x = 0.0, 0.01, 0.05, 0.1, 0.15 and 0.2) compounds from 2K to 200K.



Figure S8. Temperature-dependent electrical resistivity $\rho(T)$, Seebeck coefficient S(T), and power factor of the GeTe_{1-x}I_x (x = 0.0, 0.01, 0.05, 0.1, 0.15, and 0.2) compounds. After measuring samples (named as 1st), the same samples were re-measured from room temperature to high temperature (named as 2nd).