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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<table>
<thead>
<tr>
<th>formula</th>
<th>Energy [eV]</th>
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<tr>
<td>Te-site doping</td>
<td>Ge$<em>{24}$Te$</em>{23}$I</td>
</tr>
<tr>
<td>Interstitial doping of I</td>
<td>Ge$<em>{24}$Te$</em>{24}$I</td>
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Table S1. Formation energy calculation of the Iodine doping at Te-site Ge$_{24}$Te$_{23}$I, and interstitial doping of iodine Ge$_{24}$Te$_{24}$I.

Figure S1. Magnetic field dependence of the Hall resistivity ($\rho_{xy}$) 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 \( \alpha \)- (rhombohedral, open circle) and \( \beta \)- (cubic, 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.
Figure S4. Elemental mapping of GeTe$_{1-x}$I$_x$ (x = 0.05) from energy dispersive X-ray spectroscopy (EDX) images.
Figure S5. Elemental mapping of GeTe$_{1-x}$I$_x$ (x = 0.1) from energy dispersive X-ray spectroscopy (EDX) images.
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).