Supporting Information

The role of electronegativity on the thermoelectric performance of GeTe - I-V-VI₂ solid solutions

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1. Single parabolic band (SPB) model

The following equations are used to estimate the effective mass:\(^1\):

\[ s = -\frac{k_B}{e} \left( \frac{5}{2} + \lambda \right) \frac{F_3}{\frac{3}{2} + \lambda} (\eta) \left( \frac{3}{2} + \lambda \right) F_1 \left( \frac{3}{2} + \lambda \right) \eta \]

(1)

\[ n_H = -\frac{4\pi(2m^*_d k_B T)^2 F_1(\eta)}{\hbar^3 r_H} \]

(2)

\[ r_H = \frac{3}{2} F_1(\eta) \left( \frac{3}{2} + \lambda \right) \frac{F_1}{\frac{3}{2} + \lambda} (\eta)^2 \]

(3)

\[ F_i(\eta) = \int_0^{\infty} x^i \frac{1}{1 + \exp[\eta(x - \eta)]} dx \]

(4)
where \( \eta = \frac{E_F}{k_B T} \) is the reduced Fermi level, \( x \) is the reduced carrier energy, \( F(x) \) is the Fermi-Dirac integral, \( \tau_H \) is the Hall factor, \( m^*_d \) is the density of states (DOS) effective mass, \( h \) is the Planck constant, and \( \lambda \) is the scattering factor which depends on the energy dependence of the carrier relaxation time \( \tau \) via \( \tau = \tau_0 \xi^\lambda \). When the acoustic phonon scattering or alloy scattering is dominant, \( \lambda = -1/2 \).

2. B factor \& \( zT \)

\( \beta \) is defined by the relation:

\[
\beta = \left( \frac{\kappa}{e^2} \frac{\mu T}{\lambda L} \right)
\]

(5)

where \( \kappa \) is the Boltzmann constant, \( \lambda L \) is the lattice thermal conductivity, \( \sigma_0 \) is a quantity termed as transport coefficient that depends on the carrier mobility and the effective mass according to:

\[
\sigma_{eo} = 2e\mu \left( \frac{2\pi m^*_d}{\hbar^2} \right)^{3/2}
\]

(6)

where \( \mu \) is the carrier mobility, \( m^*_d \) is the density of states (DOS) effective mass, \( h \) is the Planck constant.

To see how the definition of \( \beta \) is justified, we can now separate the \( \eta \)-dependent terms from \( zT \):

\[
zT = \frac{S^2 \sigma T}{\lambda_L + \lambda_e} = \frac{S^2}{\lambda_L/\sigma T + L}
\]

\[
= \frac{S^2(\eta)}{\lambda_L / T \sigma_{eo} \cdot \ln(1 + e^\eta) + L(\eta)}
\]
\[ S^2(\eta) = \frac{(k_B/\eta)^2}{\beta \cdot \ln(1 + e^\beta_x)} + L(\eta) \]

where \( \beta \) combines all the \( \eta \)-independent material parameters, giving the definition of the dimensionless material quality factor in Eq.5. The natural unit of the Lorenz number \( (k_B/\eta)^2 \) was multiplied in the term containing \( 1/\beta \) to make \( \beta \) dimensionless for convenience.

**References**


**Figure S1.** (a-b) The magnified area of the powder X-ray diffraction pattern of (GeTe)	extsubscript{1-x}(NaPnTe	extsubscript{2})	extsubscript{x} and (GeTe)	extsubscript{1-x}(CuPnTe	extsubscript{2})	extsubscript{x} in the angles(2\theta) from 29° to 31°. (c-d) The lattice constants (c-axis) of (GeTe)	extsubscript{1-x}(NaPnTe	extsubscript{2})	extsubscript{x} and (GeTe)	extsubscript{1-x}(CuPnTe	extsubscript{2})	extsubscript{x}.

**Figure S2.** The comparison of the thermal and electrical performance data of (GeTe)	extsubscript{0.98}(NaBiTe	extsubscript{2})	extsubscript{0.02} after hot pressing (powder was consolidated to a disk by a direct-current-induced hot pressing at about 873 K for 40 min and under the pressure of ~50 MPa) and direct cutting.

**Figure S3.** SEM image of fresh fracture surface morphology of (GeTe)	extsubscript{0.98}(NaBiTe	extsubscript{2})	extsubscript{0.02} after (a) direct cutting and (b) hot pressing.