Introduction to Transport Properties Calculation of The Thermoelectric Materials

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Section 1

Figure of merit

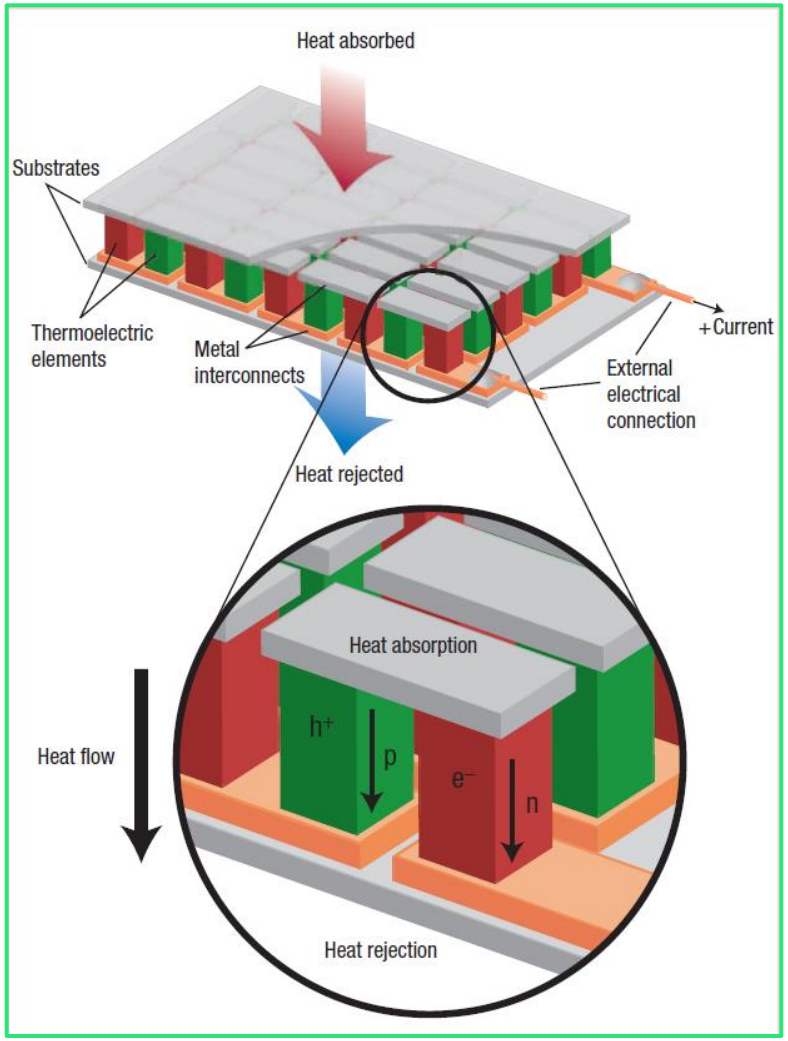
Thermoelectric materials

Definition

Thermoelectric material is a kind of functional material which can achieve conversion between heat and electricity using its internal carrier movement.

Advantage

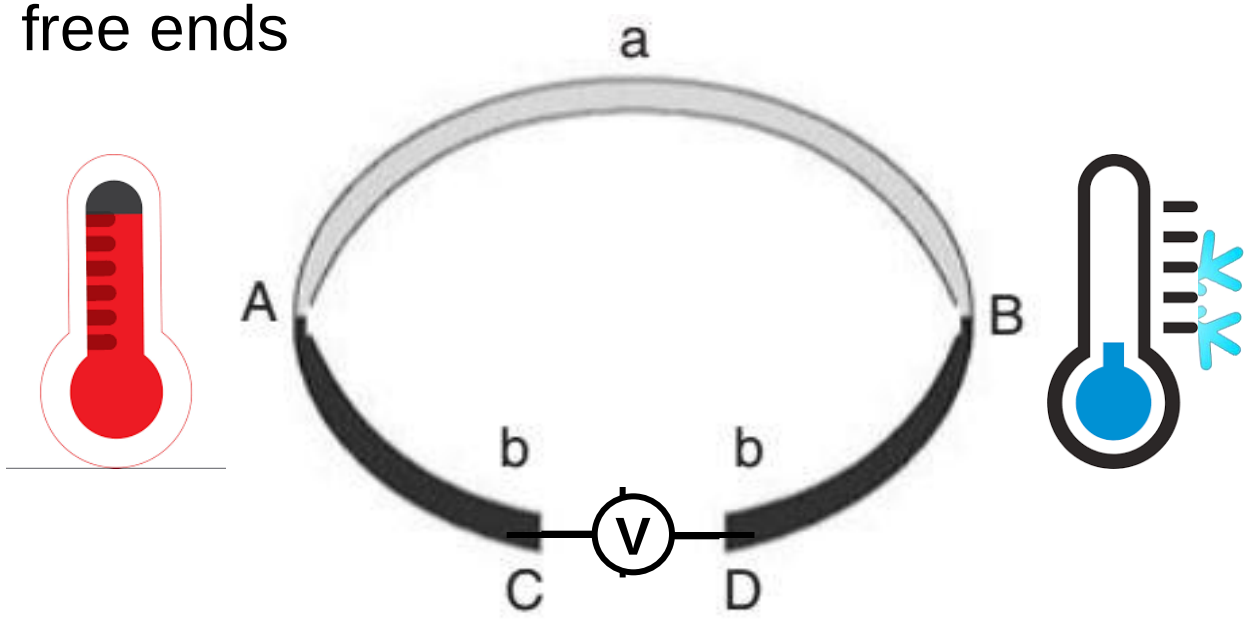
Solid device, no moving part, low noise, reliable performance, size adjustable, ideal for small scale, distributed electric generator.



(Synder & Toberer, *Nature Materials*, 2008)

Thermoelectric effects

a, b: conductors
A, B: joint points
C, D: free ends



Differential Seebeck coefficient:

$$\alpha_{ab} = \frac{V}{\nabla T}$$

Differential Peltier coefficient:

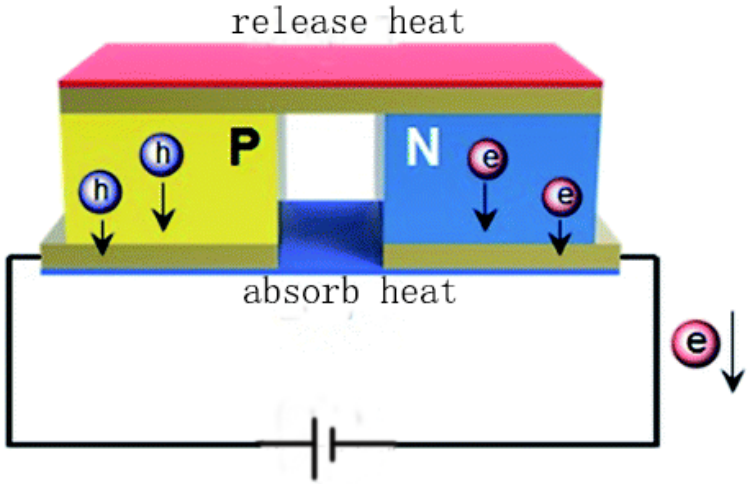
$$\pi_{ab} = \frac{q}{I}$$

Kelvin relationship:

$$\pi_{ab} = \alpha_{ab} T$$

Thermoelectric refrigerator

- Petier effect



the rate of absorption of heat from the source:

$$q_1 = \underbrace{\left(\alpha_p - \alpha_n\right) I T_1}_{\text{Peltier cooling}} - \underbrace{\left(T_2 - T_1\right)\left(K_p + K_n\right)}_{\text{heat conduction}} - \underbrace{I^2\left(R_p + R_n\right)/2}_{\text{Joule heating}}$$

the rate of expenditure of electrical energy:

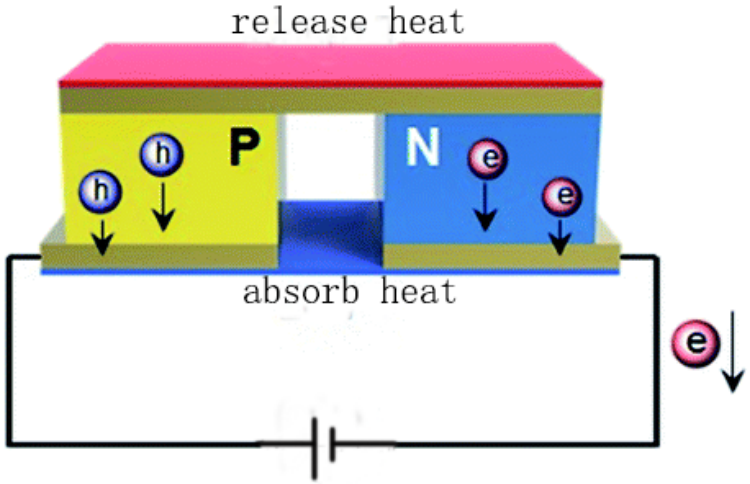
$$w = \underbrace{\left(\alpha_p - \alpha_n\right) I \left(T_2 - T_1\right)}_{\text{rate of working to overcome the thermoelectric voltage}} + \underbrace{I^2\left(R_p + R_n\right)}_{\text{resistive loss}}$$

coefficient of performance $\mathrm{COP} = \dfrac{\text{heat absorbed}}{\text{electrical power input}} = \dfrac{q_1}{w}$

K_p, K_n are the thermal conductance of the branches; R_p, R_n are the electrical resistances of the branches; T_1 is the temperature at the heat source, while T_2 is at the heat sink.

Thermoelectric refrigerator

- Petier effect



L: length
A: cross-sectional area
ρ: electrical conductivity
λ: thermal conductivity

When q_1 is maximized,

$$I_q = \left(\alpha_p - \alpha_n\right) T_1 \Big/ \left(R_p + R_n\right) \qquad \mathrm{COP} = \frac{ZT_1^2/2 - \left(T_2 - T_1\right)}{ZT_2T_1}$$

When COP is maximized,

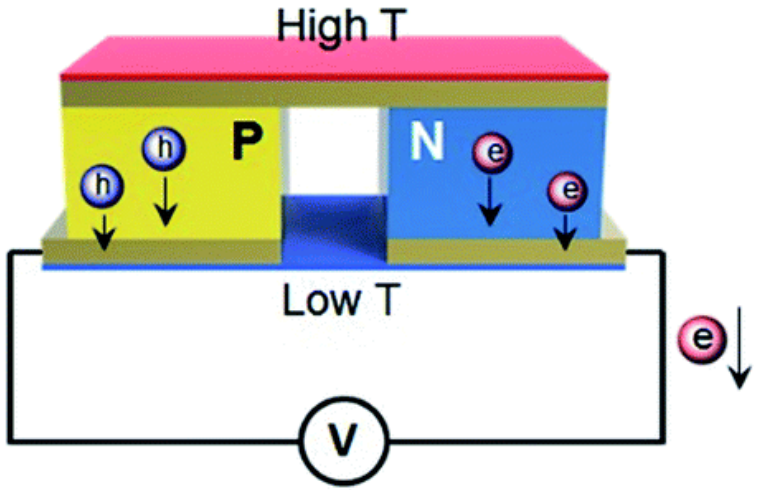
$$I_\phi = \frac{\left(\alpha_p - \alpha_n\right)\left(T_2 - T_1\right)}{\left(R_p + R_n\right)\left\{\left(1+ZT_m\right)^{1/2} - 1\right\}} \qquad \mathrm{COP}_{\max} = \frac{T_1\left\{\left(1+ZT_m\right)^{1/2} - \left(T_2/T_1\right)\right\}}{\left(T_2 - T_1\right)\left\{\left(1+ZT_m\right)^{1/2} + 1\right\}}$$

Here $$Z = \frac{\left(\alpha_p - \alpha_n\right)^2}{\left\{\left(K_p + K_n\right)\left(R_p + R_n\right)\right\}}$$

If $$\frac{L_n A_p}{L_p A_n} = \left(\frac{\rho_p \lambda_n}{\rho_n \lambda_p}\right)^{1/2}$$ then $$Z = \frac{\left(\alpha_p - \alpha_n\right)^2}{\left\{\left(\lambda_p \rho_p\right)^{1/2} + \left(\lambda_n \rho_n\right)^{1/2}\right\}^2}$$

Thermoelectric generator

- Seebeck effect



the power delivered to the load:

$$w = I^2 R_{\mathrm{L}} = \left\{ \frac{\left(\alpha_{\mathrm{p}} - \alpha_{\mathrm{n}}\right)\left(T_1 - T_2\right)}{R_{\mathrm{p}} + R_{\mathrm{n}} + R_{\mathrm{L}}} \right\}^2 R_{\mathrm{L}}$$

the rate of heat flow from the source:

$$q_1 = \underbrace{\left(\alpha_{\mathrm{p}} - \alpha_{\mathrm{n}}\right) I T_1}_{\text{Peltier cooling}} + \underbrace{\left(K_{\mathrm{p}} + K_{\mathrm{n}}\right)\left(T_1 - T_2\right)}_{\text{heat conduction}}$$

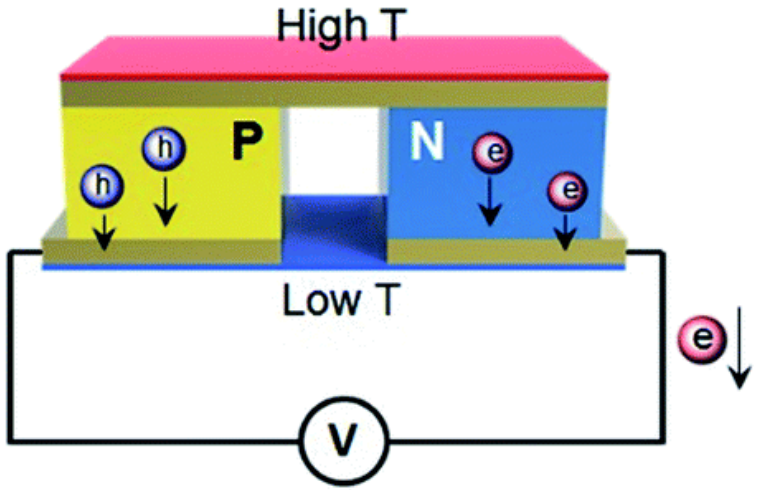
efficiency:

$$\eta = \frac{w}{q_1}$$

K_{p}, K_{n} are the thermal conductance of the branches; R_{p}, R_{n} are the electrical resistances of the branches, R_{L} is the resistance of the load; T_1 is the temperature at the heat source, while T_2 is at the heat sink.

Thermoelectric generator

- Seebeck effect



When *w* is maximized,

$$R_p + R_n = R_L \qquad w_{max} = \frac{\left\{\left(\alpha_p - \alpha_n\right)\left(T_1 - T_2\right)\right\}^2}{4R_L}$$

When η is maximized,

$$\eta = \frac{\left(T_1 - T_2\right)\left(M - 1\right)}{T_1\left(M + T_2/T_1\right)} \qquad M = \frac{R_L}{R_p + R_n} = \left(1 + ZT_m\right)^{1/2}$$

If ZT_m were much greater than 1, *M* would also be very large and the efficiency would approach .(T_1 - T_2)/T_1, which is the value for the Carnot cycle.

Thermoelectric figure of merit

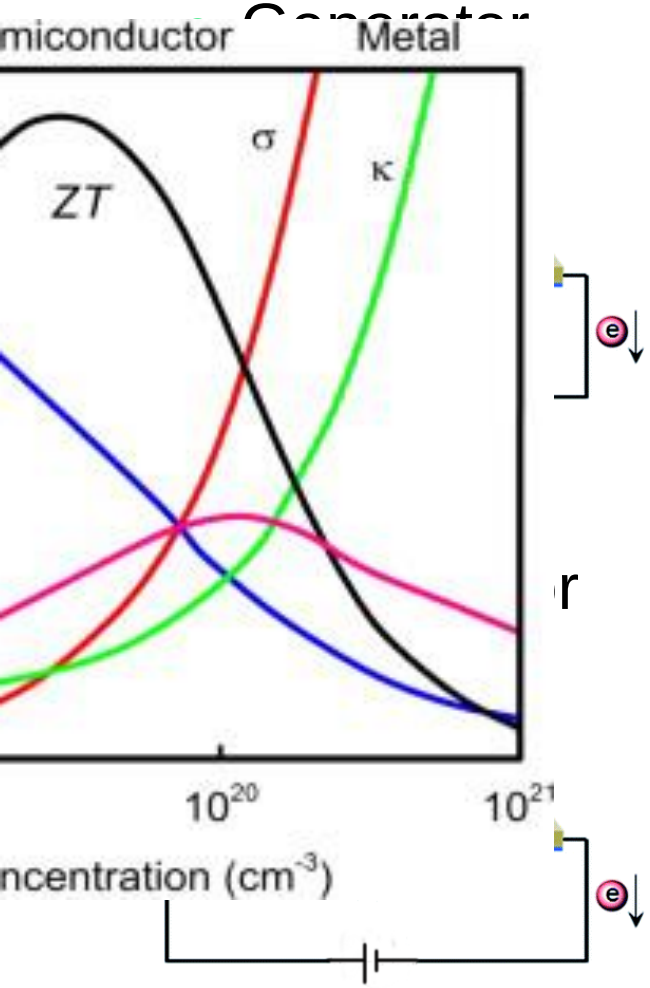


Figure of merit for thermocouple

$$Z = \frac{\left(\alpha_p - \alpha_n\right)^2}{\left\{\left(\lambda_p \rho_p\right)^{1/2} + \left(\lambda_n \rho_n\right)^{1/2}\right\}^2}$$

Figure of merit for a single material $z = \frac{\alpha^2}{\lambda\rho}$

or

$$zT = \frac{\alpha^2 \sigma T}{\kappa_L + \kappa_e}$$

α – Seebeck coefficient,

σ – electrical conductivity,

κ_L – lattice thermal conductivity,

κ_e – electronic thermal conductivity

Reading

[1] Goldsmid, H. Julian. *Introduction to thermoelectricity*. Vol. 121. Berlin: Springer, 2010.

[2] Rowe, David Michael. *Thermoelectrics handbook: macro to nano*. CRC press, 2018.

Section 2

Transport Theory

Electronic transport properties

Drude model (free electron gas model)

Assumption 1: Ignore the interaction between electrons and ionic cores. This is equivalent to treating the ionic system as a uniform positive charge background that keeps the system neutral, also called “jellium model”.

Assumption2: Ignore the interaction among electrons. This is also called “independent electron approximation”.

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\varphi(\boldsymbol{r}) = \varepsilon\varphi(\boldsymbol{r}) \quad \Rightarrow \quad -\frac{\hbar^2}{2m}\nabla^2\varphi(\boldsymbol{r}) = \varepsilon\varphi(\boldsymbol{r})$$

with $\varphi(\boldsymbol{r}) = C\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$

Quasi-classical model

Under the external field (for example, electromagnetic field), In order to discuss transport property of free electrons:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + e\phi\right]\varphi(\boldsymbol{r},t) = \mathrm{i}\hbar\dot{\varphi}(\boldsymbol{r},t)$$

Assumption 1: electrons experience collision. Such a event happens instantaneously. Between two successive collisions, the electrons move in a straight line, following Newton's laws.

Assumption 2: the collision experienced by electrons can be described by relaxation time τ simply. Within dt time, the probability of any electron getting hit is dt/τ.

Only when the particles have large kinetic energy and when the external field changes slowly, the above assumptions are true.

Quasi-classical model

Kinetic equation of electrons:

Assume the average momentum of electrons at t moment is $\boldsymbol{p}(t)$, after dt time, those electrons without getting collision have a contribution to average moment:

$$\boldsymbol{p}(t+\mathrm{d}t)=\left(1-\frac{\mathrm{d}t}{\tau}\right)\left[\boldsymbol{p}(t)+\boldsymbol{F}(t)\mathrm{d}t\right]$$

Under the first-order approximation:

$$\boldsymbol{p}(t+\mathrm{d}t)-\boldsymbol{p}(t)=\boldsymbol{F}(t)\mathrm{d}t-\boldsymbol{p}(t)\frac{\mathrm{d}t}{\tau}$$

$$\frac{\mathrm{d}\boldsymbol{p}(t)}{\mathrm{d}t}=\boldsymbol{F}(t)-\frac{\boldsymbol{p}(t)}{\tau} \quad \text{or} \quad m\frac{\mathrm{d}\boldsymbol{v}(t)}{\mathrm{d}t}=\boldsymbol{F}(t)-m\frac{\boldsymbol{v}(t)}{\tau}$$

Quasi-classical model

$$m\frac{\mathrm{d}\boldsymbol{v}(t)}{\mathrm{d}t} = \boldsymbol{F}(t) - m\frac{\boldsymbol{v}(t)}{\tau}$$

For constant electric field reaching steady state, the electric field force $\boldsymbol{F} = -e\boldsymbol{E}$, and equals to damping force. Thus, the acceleration stops and $\mathrm{d}v(t)/\mathrm{d}t = 0$. The electrons move at a constant velocity:

$$\nu_{\mathrm{d}} = -\frac{e\tau\boldsymbol{E}}{m}$$

The current density: $$\boldsymbol{J} = -ne\boldsymbol{v}_{\mathrm{d}} = \frac{ne^2\tau\boldsymbol{E}}{m}$$

According to Ohm's law: $$\boldsymbol{J} = \sigma\boldsymbol{E}$$

Electrical conductivity: $$\sigma = \frac{ne^2\tau}{m}$$

Quasi-classical model

Classical: average velocity of electrons equals to average velocity of thermal motion

$$v_{\mathrm{th}}^2 = k_{\mathrm{B}} T / m$$

Quasi-classical: average velocity of electrons equals to velocity at fermi surface

$$v_{\mathrm{F}}^2 = 2\varepsilon_{\mathrm{F}} / m$$

Mean free path *l* (the average movement distance between two successive collision of a electron):

$$l = v_{\mathrm{F}} \tau$$

For common metals at room temperature, *τ*~10^-14 s, *l*~10 nm.

Semi-classical model

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) \right] \varphi(\boldsymbol{r}) = \varepsilon\varphi(\boldsymbol{r})$$

With periodic potential approximation: $V(\boldsymbol{r}+\boldsymbol{R}_n) = V(\boldsymbol{r})$

According to Bloch theorem: $\varphi(\boldsymbol{r}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} u_{\boldsymbol{k}}(\boldsymbol{r})$ and $u_{\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{R}_n) = u_{\boldsymbol{k}}(\boldsymbol{r})$

Semi-classical model: each electron has determinate location ***r***, wave vector ***k*** and band index *n*. For a specified $\varepsilon_n(\boldsymbol{k})$, under the external fields, ***r***, ***k*** and *n* vary with time by following the rules:

1. Band index *n* is constant, ignoring the probability of electronic transition;
2. The velocity of electron: $\dot{\boldsymbol{r}} = \boldsymbol{v}_n(\boldsymbol{k}) = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon_n(\boldsymbol{k})$
3. The variation of ***k*** with time: $\hbar\dot{\boldsymbol{k}} = -e\left[\boldsymbol{E}(\boldsymbol{r},t) + \boldsymbol{v}_n(\boldsymbol{k}) \times \boldsymbol{B}(\boldsymbol{r},t) \right]$

Semi-classical model

1 Full occupied bands don't contribute to the current density $\boldsymbol{J}$.

Each electron in the band has a contribution of $-e\boldsymbol{v}(\boldsymbol{k})$ to $\boldsymbol{J}$, then the total contribution from all electrons is

$$\boldsymbol{J} = -e\int_{\text{occ}} \boldsymbol{v}(\boldsymbol{k})\frac{\mathrm{d}\boldsymbol{k}}{4\pi^3} \qquad \text{with} \qquad \boldsymbol{v}_n(\boldsymbol{k}) = -\boldsymbol{v}_n(-\boldsymbol{k})$$

Thus, the contribution from *k* state and *–k* state electrons just cancels each other out.

2 Partial occupied bands and the origin of hole.

$$\boldsymbol{J} + (-e)\int_{\text{unocc}} \boldsymbol{v}(\boldsymbol{k})\frac{\mathrm{d}\boldsymbol{k}}{4\pi^3} = 0 \quad \Rightarrow \quad \boldsymbol{J} = e\int_{\text{unocc}} \boldsymbol{v}(\boldsymbol{k})\frac{\mathrm{d}\boldsymbol{k}}{4\pi^3}$$

Boltzmann equation

In thermal equilibrium condition, the electrons' distribution follows Fermi-Dirac distribution function f_0

$$f_0\left(\varepsilon_{\boldsymbol{k}}\right)=\frac{1}{\mathrm{e}^{\left(\varepsilon_{\boldsymbol{k}}-\mu\right)/k_{\mathrm{B}}T}+1}$$

When external fields exist, and involving collision, the distribution deviates from f_0, the nonequilibrium distribution function $f(\boldsymbol{r},\boldsymbol{k},t)$

$$f\left(\boldsymbol{r},\boldsymbol{k},t\right)=f\left(\boldsymbol{r}-\dot{\boldsymbol{r}}\mathrm{d}t,\boldsymbol{k}-\dot{\boldsymbol{k}}\mathrm{d}t,t-\mathrm{d}t\right)+\left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}}\mathrm{d}t \quad \Rightarrow \quad \frac{\partial f}{\partial t}+\dot{\boldsymbol{r}}\bullet\frac{\partial f}{\partial \boldsymbol{r}}+\dot{\boldsymbol{k}}\bullet\frac{\partial f}{\partial \boldsymbol{k}}=\left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}}$$

In the steady state, $\partial f/\partial t=0$,

$$\underbrace{\dot{\boldsymbol{r}}\bullet\frac{\partial f}{\partial \boldsymbol{r}}+\dot{\boldsymbol{k}}\bullet\frac{\partial f}{\partial \boldsymbol{k}}}_{\text{drift term}}=\underbrace{\left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}}}_{\text{collision term}}$$

Boltzmann equation

The nonequilibrium function *f* just has a small deviation from f_0

$$f = f_0 + f_1$$

The relaxation time approximation

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{f - f_0}{\tau} = -\frac{f_1}{\tau}$$

For a situation with electrical field, magnetic field and collision,

$$\dot{\boldsymbol{r}} \bullet \frac{\partial f_0}{\partial \boldsymbol{r}} - \frac{e\boldsymbol{E}}{\hbar} \bullet \frac{\partial f_0}{\partial \boldsymbol{k}} = -\frac{f_1}{\tau} + \frac{e}{\hbar}\left(\boldsymbol{v}_{\boldsymbol{k}} \times \boldsymbol{B}\right) \bullet \frac{\partial f_1}{\partial \boldsymbol{k}}$$

A simple case, only constant electrical field.

$$-\frac{e\boldsymbol{E}}{\hbar} \bullet \frac{\partial f_0}{\partial \boldsymbol{k}} = -\frac{f_1}{\tau} \qquad \text{or} \qquad f_1 = \frac{e\tau \boldsymbol{E}}{\hbar} \bullet \frac{\partial f_0}{\partial \boldsymbol{k}}$$

Boltzmann equation

Current density $\boldsymbol{J}$:

$$\boldsymbol{J} = -\frac{1}{4\pi^3}\int e\boldsymbol{v}_{\boldsymbol{k}} f \mathrm{d}\boldsymbol{k} = -\frac{1}{4\pi^3}\int e\boldsymbol{v}_{\boldsymbol{k}} \left(f_0 + f_1\right)\mathrm{d}\boldsymbol{k}$$

Since

$$\int e\boldsymbol{v}_{\boldsymbol{k}} f_0 \mathrm{d}\boldsymbol{k} \equiv 0$$

Then

$$\boldsymbol{J} = -\frac{1}{4\pi^3}\int e\boldsymbol{v}_{\boldsymbol{k}} f_1 \mathrm{d}\boldsymbol{k} = -\frac{1}{4\pi^3}\int e\boldsymbol{v}_{\boldsymbol{k}} \frac{e\tau \boldsymbol{E}}{\hbar}\frac{\partial f_0}{\partial \boldsymbol{k}}\mathrm{d}\boldsymbol{k} = \boldsymbol{\sigma}\bullet\boldsymbol{E}$$

Define transport distribution function

$$\sigma_{\alpha\beta}\left(\varepsilon\right) = \frac{e^2}{N_{\boldsymbol{k}}\Omega}\sum_{n,\boldsymbol{k}}\tau_{n,\boldsymbol{k}}\nu_{\alpha}\left(n,\boldsymbol{k}\right)\nu_{\beta}\left(n,\boldsymbol{k}\right)\delta\left(\varepsilon-\varepsilon_{n,\boldsymbol{k}}\right)$$

Generalized transport coefficients

$$L^{(\lambda)}\left(\mu;T\right) = \int \sigma\left(\varepsilon\right)\left(\varepsilon-\mu\right)^{\lambda}\left(-\frac{\partial f_0\left(\varepsilon;\mu,T\right)}{\partial\varepsilon}\right)\mathrm{d}\varepsilon$$

$$\sigma = L^{(0)} \qquad S = \frac{1}{eT}\frac{L^{(1)}}{L^{(0)}} \qquad \kappa_e = \frac{1}{e^2T}\left[\frac{\left(L^{(1)}\right)^2}{L^{(0)}} - L^{(2)}\right]$$

Relaxation time

Relaxation time :

$$\tau_{n,\boldsymbol{k}} = \Gamma_{n\boldsymbol{k}}^{-1} \qquad \Gamma_{n\boldsymbol{k}}^{-1} = \frac{1}{N_{\boldsymbol{q}}} \sum_{m,\nu\boldsymbol{q}} W_{n\boldsymbol{k},m\boldsymbol{k}+\boldsymbol{q}}^{\nu\boldsymbol{q}}$$

$$W_{n\boldsymbol{k},m\boldsymbol{k}+\boldsymbol{q}}^{\nu\boldsymbol{q}} = \frac{2\pi}{\hbar} \left| g_{mn\nu}(\boldsymbol{k},\boldsymbol{q}) \right|^2 \times [\delta\left(\varepsilon_{n\boldsymbol{k}} - \hbar\omega_{\nu\boldsymbol{q}} - \varepsilon_{m\boldsymbol{k}+\boldsymbol{q}}\right)\left(1 + N_{\nu\boldsymbol{q}}^0 - f_{m\boldsymbol{k}+\boldsymbol{q}}^0\right) + \delta\left(\varepsilon_{n\boldsymbol{k}} + \hbar\omega_{\nu\boldsymbol{q}} - \varepsilon_{m\boldsymbol{k}+\boldsymbol{q}}\right)\left(N_{\nu\boldsymbol{q}}^0 - f_{m\boldsymbol{k}+\boldsymbol{q}}^0\right)]$$

Here $N_{\boldsymbol{q}}$ is the number of $\boldsymbol{q}$-points and $g_{mn\nu}(\boldsymbol{k},\boldsymbol{q})$ are the e-ph matrix elements quantifying the probability amplitude for an electron to scatter from an initial state $|n\boldsymbol{k}\rangle$ to the final state $|m\boldsymbol{k}+\boldsymbol{q}\rangle$, by emitting or absorbing a phonon with wavevector $\boldsymbol{q}$ and mode index ν; $N_{\nu\boldsymbol{q}}^0$ are equilibrium Bose-Einstein phonon distribution functions.

Software

Table 1 The commonly used software for calculating electronic transport properties

	Complexity	link
AICON	Low	https://github.com/Baijianlu/AICON2.git
BoltzTrap2	Normal	https://gitlab.com/sousaw/BoltzTraP2
BoltzWann	Normal	https://doi.org/10.1016/j.cpc.2013.09.015
EPA	A bit high	https://doi.org/10.1002/aenm.201800246
EPIC STAR	A bit high	https://doi.org/10.1038/s41524-020-0316-7
AMSET	A bit high	https://github.com/hackingmaterials/amset
PERTURBO	High	https://perturbo-code.github.io/
elphbolt	High	https://github.com/nakib/elphbolt

Lattice thermal conductivity

In the presence of a temperature gradient ∇T, the phonon distribution function f deviates from f_0 (Bose–Einstein distribution), and this deviation can be obtained from the BTE. In the steady state, the rate of change in the distribution must vanish,

$$\frac{\mathrm{d}f_\lambda}{\mathrm{d}t} = \frac{\partial f_\lambda}{\partial t}\Big|_{\text{diffusion}} + \frac{\partial f_\lambda}{\partial t}\Big|_{\text{scattering}} = 0 \qquad \text{and} \qquad \frac{\partial f_\lambda}{\partial t}\Big|_{\text{diffusion}} = -\nabla T \cdot v_\lambda \frac{\partial f_\lambda}{\partial T}$$

where λ comprises both a phonon branch index n and a wave vector $\boldsymbol{q}$, $\boldsymbol{v}_\lambda$ is the group velocity of phonon mode λ.

Usually, the norm of ∇T is small enough that f_λ can be expanded to first order in ∇T

$$f_\lambda = f_0 + g_\lambda$$

g_λ can be chosen to be

$$g_\lambda = -\boldsymbol{F}_\lambda \cdot \nabla T \frac{\mathrm{d}f_0}{\mathrm{d}T}$$

Lattice thermal conductivity

Consider only two- and three-phonon processes, the BTE can be written as

$$\boldsymbol{F}_\lambda = \tau_\lambda^0 \left(\boldsymbol{v}_\lambda + \boldsymbol{\Delta}_\lambda \right)$$

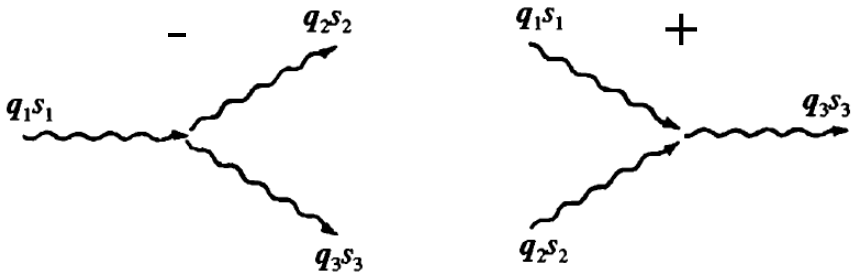
with

$$\frac{1}{\tau_\lambda^0} = \frac{1}{N} \left(\sum_{\lambda\lambda'}^{+} \Gamma^{+}_{\lambda\lambda'\lambda''} + \sum_{\lambda\lambda'}^{-} \frac{1}{2} \Gamma^{-}_{\lambda\lambda'\lambda''} \right)$$

$$\Gamma^{+}_{\lambda\lambda'\lambda''} = \frac{\hbar\pi}{4} \frac{f_0' - f_0''}{\omega_\lambda \omega_{\lambda'} \omega_{\lambda''}} \left| V^{+}_{\lambda\lambda'\lambda''} \right|^2 \delta\left(\omega_\lambda + \omega_{\lambda'} - \omega_{\lambda''} \right)$$

$$\Gamma^{-}_{\lambda\lambda'\lambda''} = \frac{\hbar\pi}{4} \frac{f_0' + f_0'' + 1}{\omega_\lambda \omega_{\lambda'} \omega_{\lambda''}} \left| V^{-}_{\lambda\lambda'\lambda''} \right|^2 \delta\left(\omega_\lambda - \omega_{\lambda'} - \omega_{\lambda''} \right)$$

$$V^{-}_{\lambda\lambda'\lambda''} \sim \sum_{ijk} \sum_{\alpha\beta\gamma} \Phi^{\alpha\beta\gamma}_{ijk}$$



Here $\omega\lambda$ is the angular frequency, N is the number of $\boldsymbol{q}$ points in the Brillouin zone, f_0' stands for $f_0(\omega_{\lambda'})$, $\Gamma^{+}_{\lambda\lambda'\lambda''}$ corresponds to absorption processes ($\omega_\lambda + \omega_{\lambda'} = \omega_{\lambda''}$) while $\Gamma^{-}_{\lambda\lambda'\lambda''}$ corresponds to emission processes ($\omega_\lambda = \omega_{\lambda'} + \omega_{\lambda''}$)

Finally,

$$\kappa_{\mathrm{L}}^{\alpha\beta} = \frac{1}{k_{\mathrm{B}} T^2 N_{\boldsymbol{q}} \Omega} \sum_\lambda f_0 \left(f_0 + 1 \right) \left(\hbar\omega_\lambda \right)^2 v_\lambda^\alpha F_\lambda^\beta$$

Software

Table 2 The commonly used software for calculating lattice thermal conductivity

	Characteristics	link
AICON	Debye-Callaway model, fast	https://github.com/Baijianlu/AICON2.git
ShengBTE	Iteratively solving BTE starting from RTA, slow	https://www.shengbte.org/
Phono3py	RTA, slow	http://phonopy.github.io/phono3py/
AFLOW-AAPL	Iteratively solving BTE starting from RTA, making use of symmetry to reduce the number of static calculation for IFC, a bit slow	http://www.aflow.org/
LAMMPS	nonequilibrium molecular dynamics or Green-Kubo method, require high-quality interatomic potential, slow	https://www.lammps.org/

Assignment

Assignment 1:

Ziman, John M. *Electrons and phonons: the theory of transport phenomena in solids*. Oxford university press, 2001.

Assignment 2:

Download and install AICON, BoltzTrap2 and ShengBTE, run their examples, familiarize yourself with the process of calculating transport properties.

Section 3

Introduction of AICON

Electronic transport properties

Electronic relaxation time, according to Matthiessen's rule:

$$\frac{1}{\tau} = \frac{1}{\tau_{aco}} + \frac{1}{\tau_{opt}} + \frac{1}{\tau_{imp}} + \frac{1}{\tau_{BD}} + \ldots$$

Electronic transport properties

- acoustic phonon scattering

τ_{aco} can be described by deformation potential theory proposed by Bardeen [2]

- Isotropic crystal
- Elastic scattering
- Nondegenerate → Degenerate
- Energy band is parabolic → Nonparabolicity
- Effective mass of carrier equals to mass of electron (constant energy surface is sphere) → Ellipsoidal constant energy surface

[2] Bardeen J, Shockley W., Physical review, 1950, 80(1): 72.

Electronic transport properties

Modified Kane band model within the framework of **k-p** theory, [3]

The energy dispersion law

$$\frac{\hbar^2 k_\perp^2}{m_{\perp 0}^*} + \frac{\hbar^2 k_\parallel^2}{2m_{\parallel 0}^*} = \xi\left(1 + \frac{\xi}{\xi_g}\right)$$

The energy dependency of effective mass

$$m_i^* = m_{i0}^*\left(1 + \frac{2\xi}{\xi_g}\right) = m_{i0}^*\left(1 + 2\beta z\right)$$

The density of states

$$\rho = \frac{2^{1/2} m_d^{3/2}}{\pi^2 \hbar^3} \xi^{1/2}\left(1 + \frac{\xi}{\xi_g}\right)^{1/2}\left(1 + \frac{2\xi}{\xi_g}\right) \quad \text{with} \quad m_d^* = N^{2/3}\left(m_\parallel^* m_\perp^{*2}\right)^{1/3}$$

[3] Y. I. Ravich, *et al*., Semiconducting Lead Chalcogenides, Plenum Press, New York, 1970

Electronic transport properties

Formula for electron-acoustic phonon scattering:

$$\frac{1}{\tau_{\text{aco}}(z)} = \mathrm{C}\left|M\right|^2 \rho = \frac{\pi k_0 T \rho(z) E_1^{\,2}}{\hbar c_l N}\left[1 - \frac{8\beta\left(z+\beta z^2\right)}{3\left(1+2\beta z\right)^2}\right]$$

Here,

$$z = \frac{\xi}{k_B T} \qquad \beta = \frac{k_B T}{\xi_g}$$

The factor in bracket as function of two quantities z and β describes the energy dependence of the squared coupling matrix element.

Electronic transport properties

- polar optical phonon scattering

$$\frac{1}{\tau_{\mathrm{opt}}(z)} = \frac{2^{1/2} k_0 T e^2 m_{d1}^{*1/2} \left(\varepsilon_\infty^{-1} - \varepsilon_0^{-1}\right)}{\hbar^2 \left(z k_0 T\right)^{1/2}} \frac{1+2\beta z}{\left(1+\beta z\right)^{1/2}}$$
$$\times \left\{ \left[1 - \delta \ln\left(1+\frac{1}{\delta}\right) \right] - \frac{2\beta\left(z+\beta z^2\right)}{\left(1+2\beta z\right)^2} \left[1 - 2\delta + 2\delta^2 \ln\left(1+\frac{1}{\delta}\right) \right] \right\}$$

The factor in braces describes the energy dependence of the squared matrix element and screening effect (δ).

Electronic transport properties

- ionized impurity scattering in highly degenerate samples

$$\frac{1}{\tau_{\mathrm{imp}}} = \frac{2e^4 N m_{d1}^* \left(1 + 2\zeta / \xi_g\right) \Phi\left(\delta_0\right)}{3\pi\varepsilon_0^2 \hbar^3}$$

Here $\Phi(\delta)$ describes the screen effect from carriers:

$$\Phi\left(\delta_0\right) = \ln\left(1 + \delta_0^{-1}\right) - \left(1 + \delta_0\right)^{-1}$$

Electronic transport properties

The key parameters involved in scattering rate, which need to be calculate by first-principles method:

- ❑ Effective mass
- ❑ Elastic constant
- ❑ Band gap
- ❑ Band degeneracy
- ❑ Deformation potential constant
- ❑ Dielectric constant

Lattice thermal conductivity

Debye-Callaway model

The original Callaway model based on four assumptions:

- only acoustic phonons account for lattice thermal conductivity
- the crystal vibration spectrum is isotropic and dispersion-free
- four scattering mechanisms are considered, including point impurities (isotopes disorder), normal three-phonon processes, Umklapp processes and boundary scattering
- phonon scattering processes can be represented by frequency-dependent relaxation times

Lattice thermal conductivity

According to Morelli[4]

$$\kappa = \kappa_{LA} + 2\kappa_{TA}$$

$$\kappa_i = \kappa_{i1} + \kappa_{i2} \quad i \text{ denoting } LA, TA$$

$$\kappa_{i1} = \frac{1}{3} C_i T^3 \int_0^{\theta_i/T} \frac{\tau_C^i(x)\, x^4 e^x}{\left(e^x - 1\right)^2} dx \qquad \kappa_{i2} = \frac{1}{3} C_i T^3 \frac{\left[\int_0^{\theta_i/T} \frac{\tau_C^i(x)\, x^4 e^x}{\left(e^x - 1\right)^2} dx\right]^2}{\int_0^{\theta_i/T} \frac{\tau_C^i(x)\, x^4 e^x}{\tau_N^i(x)\, \tau_R^i(x) \left(e^x - 1\right)^2} dx}$$

$$C_i = k_B^4 / 2\pi^2 \hbar^3 \nu_i \qquad x = \hbar\omega / k_B T \qquad \left(\tau_C^i\right)^{-1} = \left(\tau_N^i\right)^{-1} + \left(\tau_R^i\right)^{-1} \qquad \left(\tau_R^i\right)^{-1} = \left(\tau_U^i\right)^{-1} + \left(\tau_I^i\right)^{-1} + \left(\tau_B^i\right)^{-1}$$

$$\left[\tau_N^L(x)\right]^{-1} = \frac{k_B^3 \gamma_L^2 V}{M \hbar^2 \nu_L^5} \left(\frac{k_B}{\hbar}\right)^2 x^2 T^5 \qquad \left[\tau_N^T(x)\right]^{-1} = \frac{k_B^4 \gamma_T^2 V}{M \hbar^3 \nu_T^5} \left(\frac{k_B}{\hbar}\right) x T^5 \qquad \left[\tau_U^i(x)\right]^{-1} = \frac{\hbar \gamma_i^2}{M \nu_i^2 \theta_i} \left(\frac{k_B}{\hbar}\right)^2 x^2 T^3 e^{-\theta_i/3T}$$

[4] Morelli, D. T., J. P. Heremans, and G. A. Slack. *Physical Review B* **66**.19 (2002): 195304.

Lattice thermal conductivity

Contribution from optical phonons can be important, for example, at high temperature, or compounds with complex structure.

$$\kappa = \kappa_{\mathrm{LA}} + \kappa_{\mathrm{TA}} + \kappa_{\mathrm{TA'}} + \kappa_{\mathrm{O}}$$

with

$$\kappa_{\mathrm{O}} = \frac{1}{3} C_V \nu^2 \tau = \frac{1}{3}(3p-3)\frac{N}{V} k_{\mathrm{B}} f_{\mathrm{E}}\left(\frac{\Theta_E}{T}\right) \nu_{\mathrm{O}}^2 \tau_C^{\mathrm{O}} \left[1 + \frac{\tau_R^{\mathrm{O}}}{\tau_N^{\mathrm{O}}} \right]$$

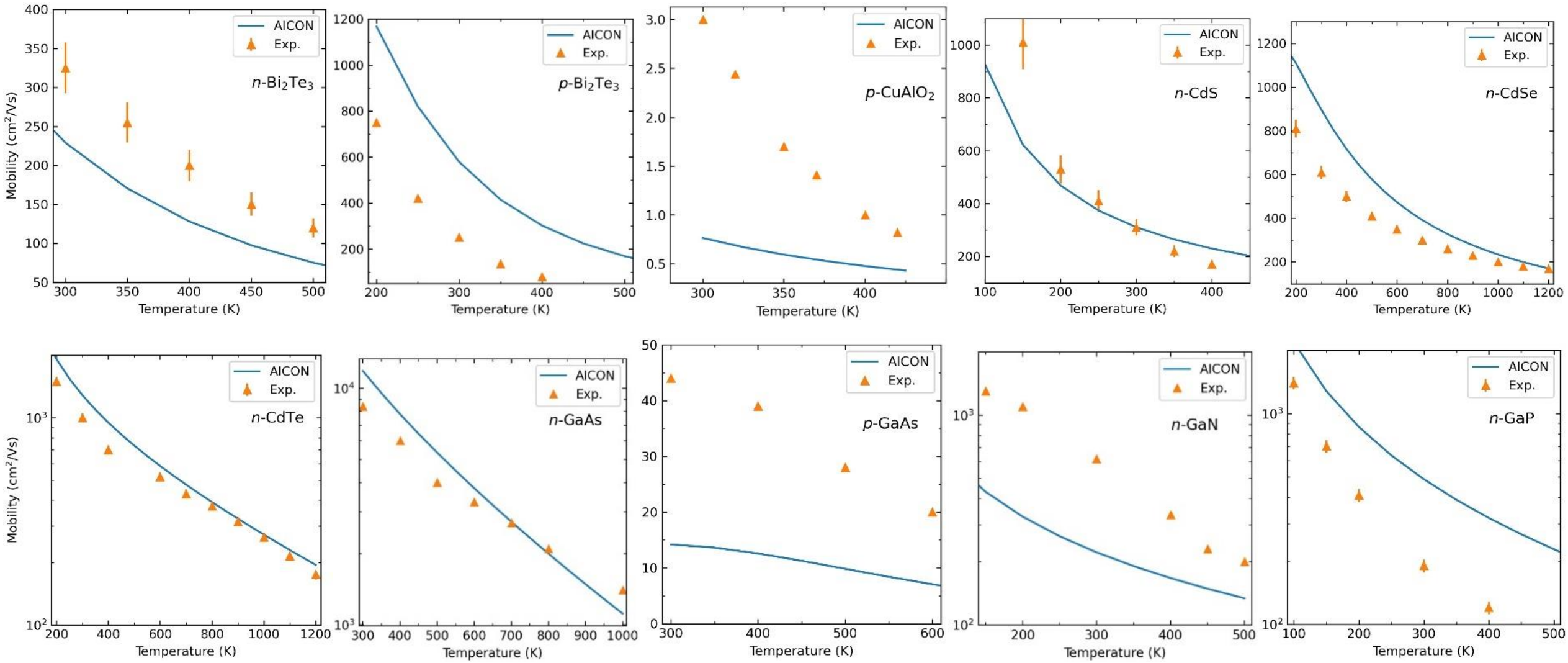
$$f_{\mathrm{E}}(x) = x^2 \frac{e^x}{\left(e^x - 1\right)^2}$$

Model test

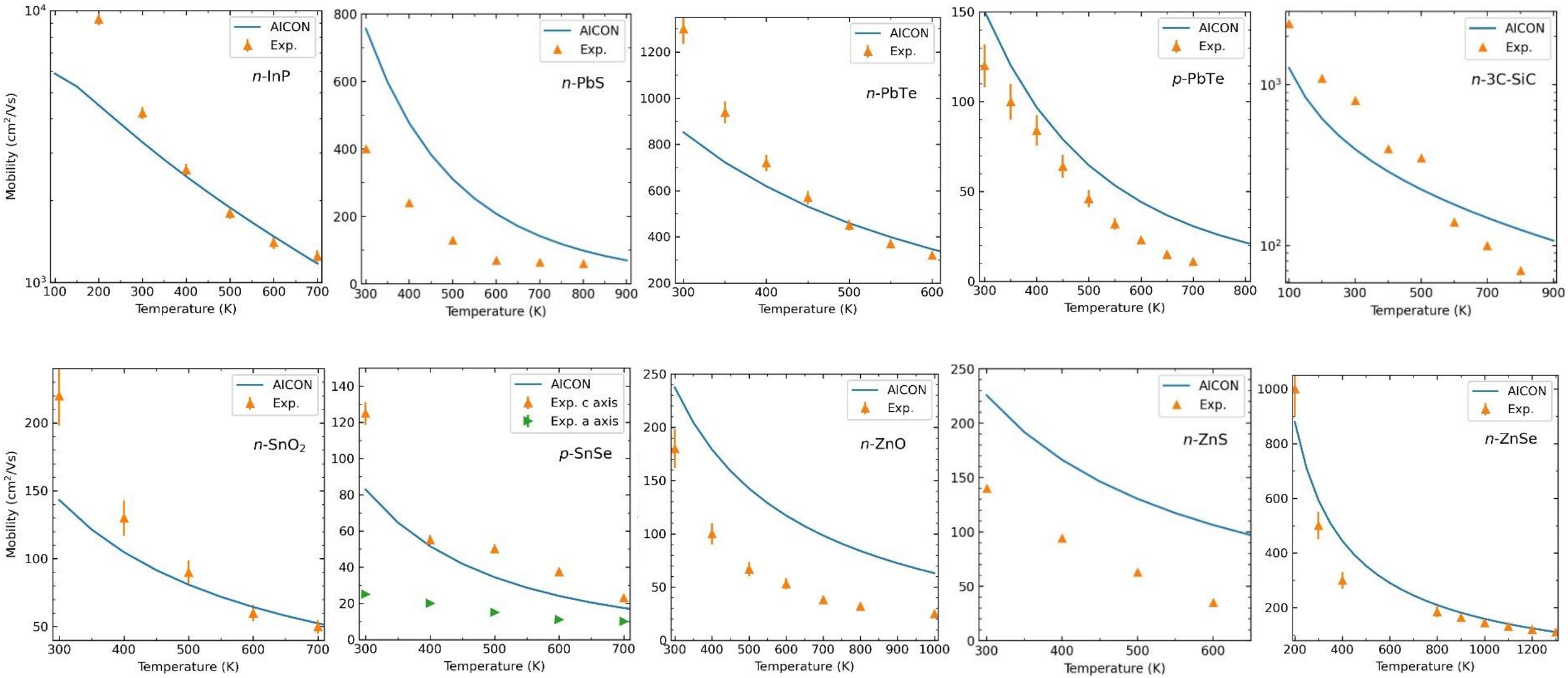
Mobility test

Materials	Doping	*T* (K)	*n* (cm^{-3})	Materials	Doping	*T* (K)	*n* (cm^{-3})
$CuAlO_2$	p-type	300-430	1.3×10^{17}	PbTe	n-type	300-600	1.8×10^{19}
CdS	n-type	100-400	5.0×10^{15}	PbTe	p-type	300-800	1.4×10^{20}
CdSe	n-type	200-1200	1.0×10^{17}	SiC	n-type	100-900	4.0×10^{15}
CdTe	n-type	200-1200	1.0×10^{15}	SnO_2	n-type	300-700	1.0×10^{17}
GaAs	n-type	300-1000	3.0×10^{13}	SnSe	p-type	300-900	3.3×10^{17}
GaAs	p-type	300-600	6.4×10^{19}	ZnO	n-type	300-1000	8.2×10^{16}
GaN	n-type	150-500	3.0×10^{16}	ZnS	n-type	300-650	1.0×10^{16}
GaP	n-type	100-500	3.0×10^{16}	ZnSe	n-type	200-1300	1.0×10^{15}
InP	n-type	100-700	1.5×10^{16}	Bi_2Te_3	n-type	300-500	3.3×10^{19}
PbS	n-type	300-900	3.6×10^{17}	Bi_2Te_3	p-type	200-500	1.1×10^{19}

Model test


AICON
Exp.
n-Bi2Te3
p-Bi2Te3
p-CuAlO2
n-CdS
n-CdSe
n-CdTe
n-GaAs
p-GaAs
n-GaN
n-GaP
Mobility (cm²/Vs)
Temperature (K)

Model test

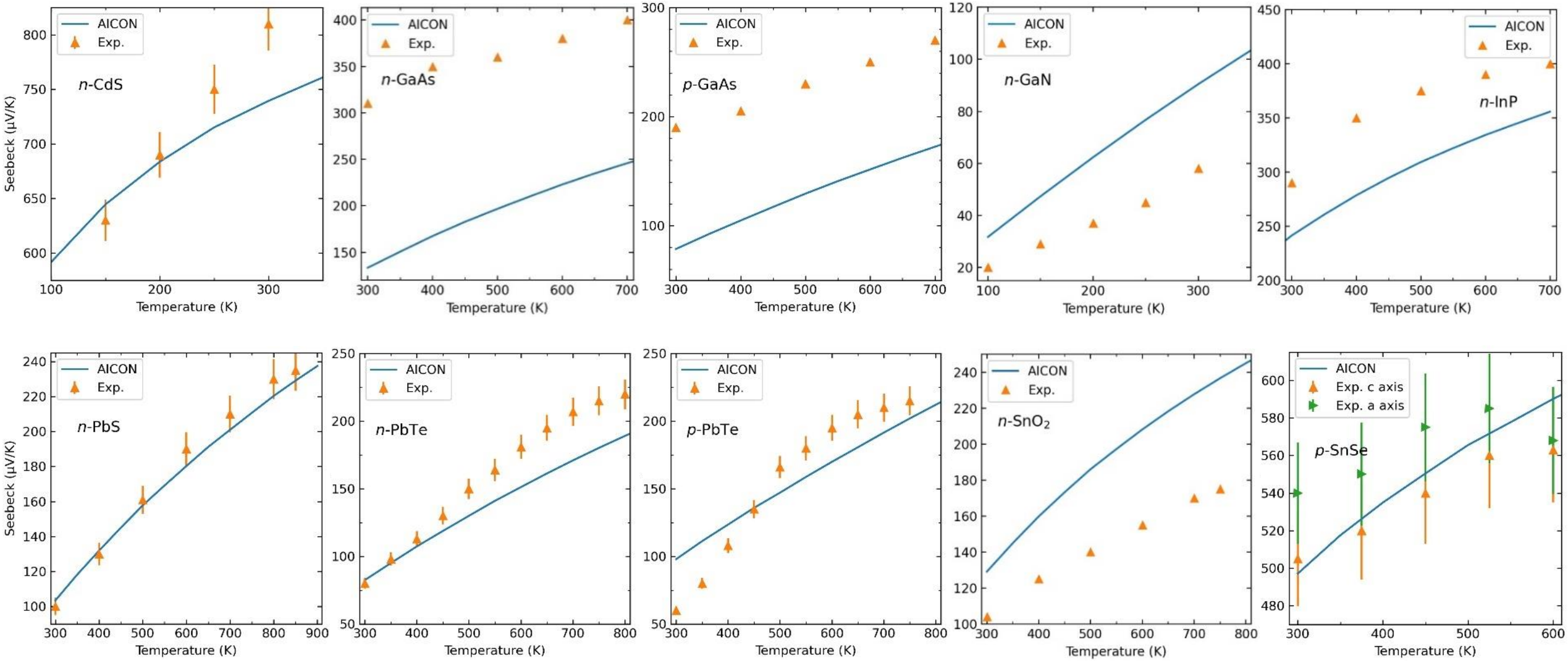

Mobility (cm²/Vs)
Temperature (K)
AICON
Exp.
n-InP
n-PbS
n-PbTe
p-PbTe
n-3C-SiC
n-SnO2
Exp. c axis
Exp. a axis
p-SnSe
n-ZnO
n-ZnS
n-ZnSe

Model test

Seebeck coefficient test

Materials	Doping	*T* (K)	*n* (cm^{-3})
CdS	n-type	100-300	2.8×10^{15}
GaAs	n-type	400-750	3.5×10^{17}
GaAs	p-type	300-700	6.4×10^{19}
GaN	n-type	100-300	1.3×10^{19}
InP	n-type	150-700	2.1×10^{17}
PbS	n-type	300-800	2.5×10^{19}
PbTe	n-type	300-800	1.8×10^{19}
PbTe	p-type	300-800	1.4×10^{20}
SnO_2	n-type	300-800	8.2×10^{18}
SnSe	p-type	300-900	3.3×10^{17}
ZnO	n-type	200-1000	5.2×10^{17}

Model test


AICON
Exp.
n-CdS
n-GaAs
p-GaAs
n-GaN
n-InP
n-PbS
n-PbTe
p-PbTe
n-SnO2
p-SnSe
Exp. c axis
Exp. a axis
Seebeck (μV/K)
Temperature (K)

Model test

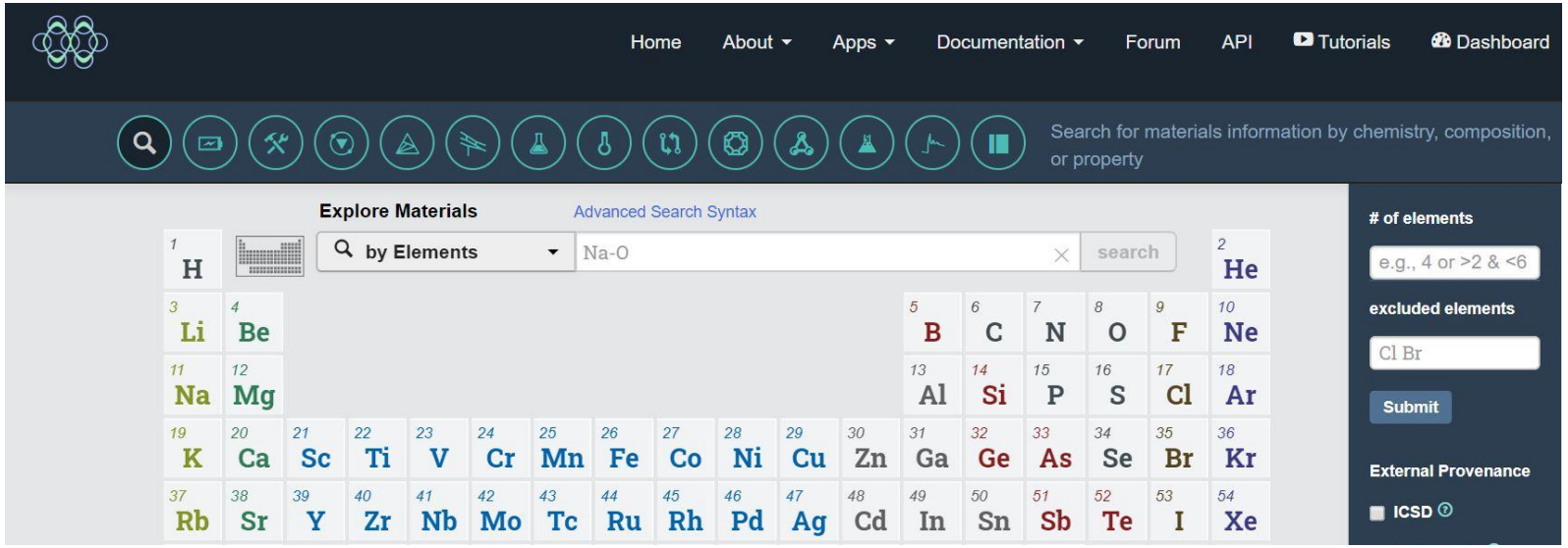
Calculated and experimental lattice thermal conductivity of testing compounds at 300 K
unit: $W \cdot m^{-1} \cdot K^{-1}$

Formula	κ_{exp}	κ_{cal}	Formula	κ_{exp}	κ_{cal}
C(Dia)	2200	2325.41	NaI	1.8	1.92
Si	141	135.83	PbS	2.9	2.69
AgCl	1	0.57	RbBr	3.8	1.55
BaO	2.3	4.27	RbI	2.3	0.99
CaO	27	29.79	SrO	12	14.98
KBr	3.4	2.41	CdF_2	4.3	2.25
KCl	7.1	2.42	$SrCl_2$	2.3	2.84
KI	2.6	1.29	Mg_2Si	12.14	13.47
LiF	17.6	16.48	Mg_2Ge	15.7	20.47
LiH	15	33.28	Mg_2Sn	11.1	9.67
MgO	60	65.42	CaF_2	9.76	7.21
NaBr	2.8	2.02	CeO_2	10.8	7.98
NaCl	7.1	4.04	ZnO	37.5	18.76
NaF	16.5	12.97			

Application

Objects: Chalcogenides

Database: Materials Project



Standards:

Elements	Band gap	E_above_convexhull	Symmetry
S, Se, Te anions	$0 < \mathcal{E}g < 1.2$ eV	<= 0.1 eV	Cubic (Tetragonal, Orthorhombic, Hexagonal, …)

Application

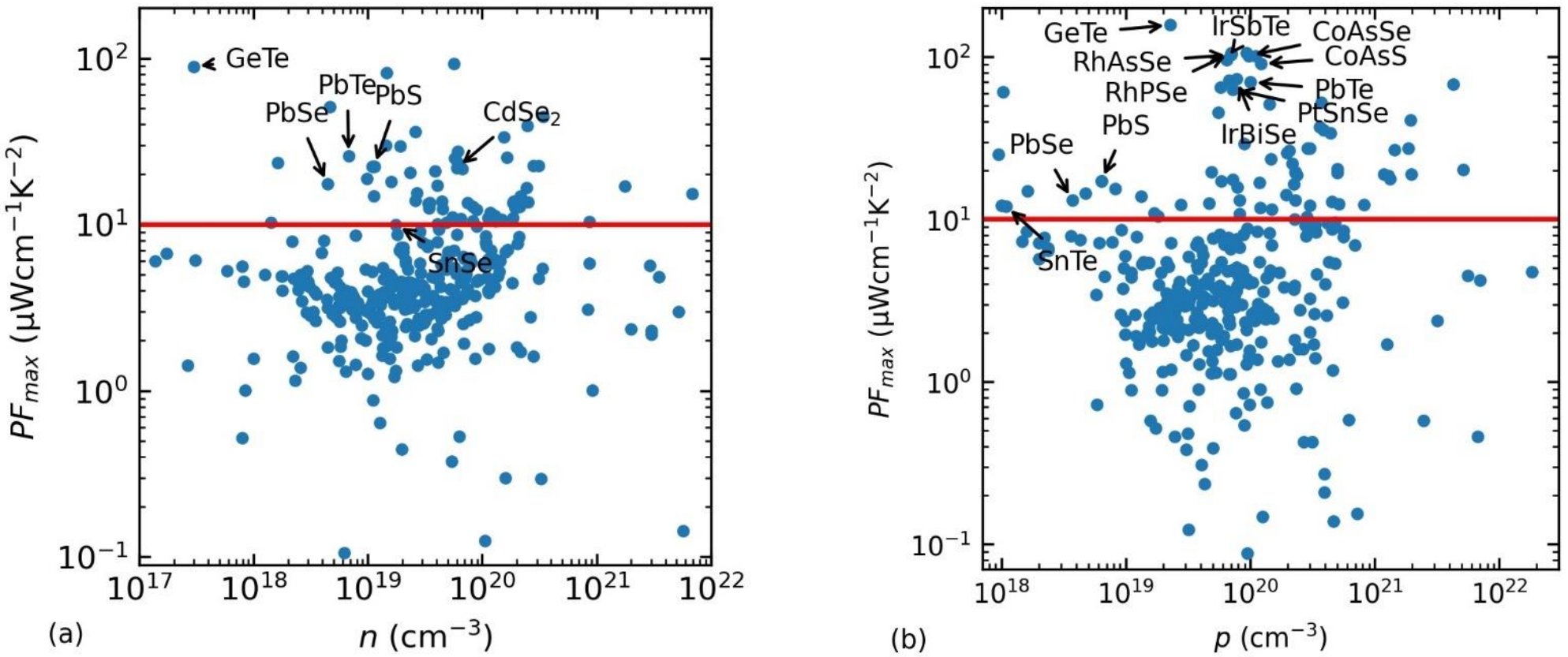
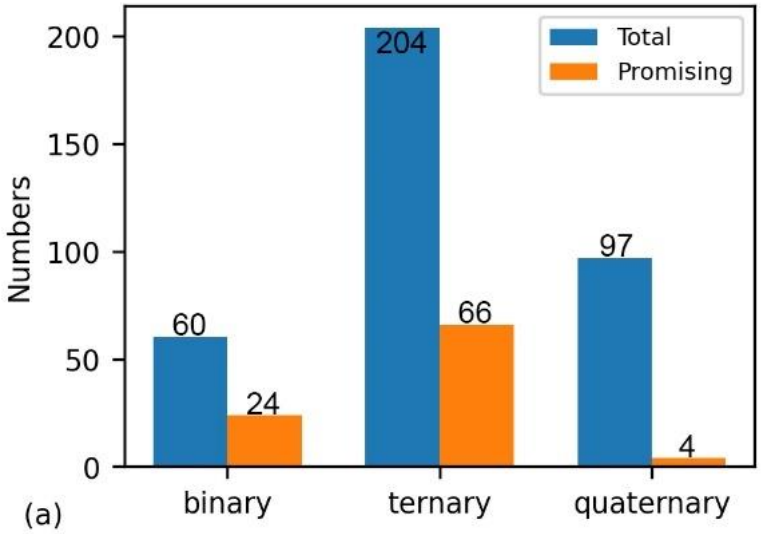
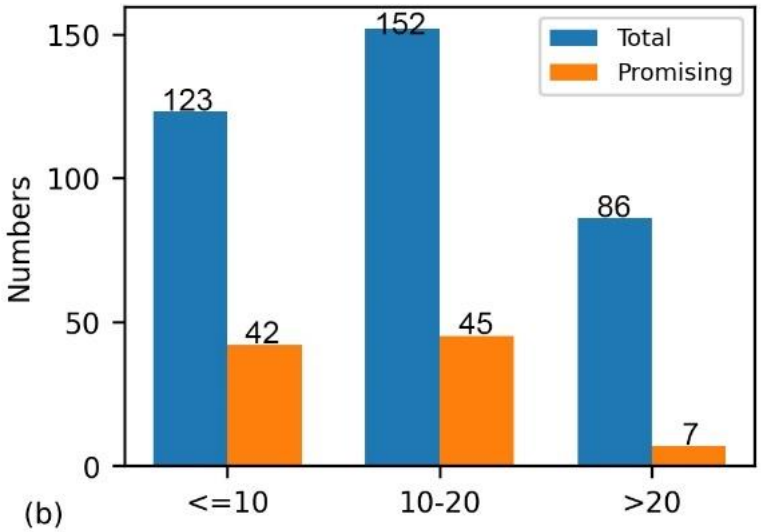


Figure 1. Maximum power factor as a function of the corresponding carrier concentration for the studied compounds in the temperature range from 300 K to 1000 K.

Statistical data





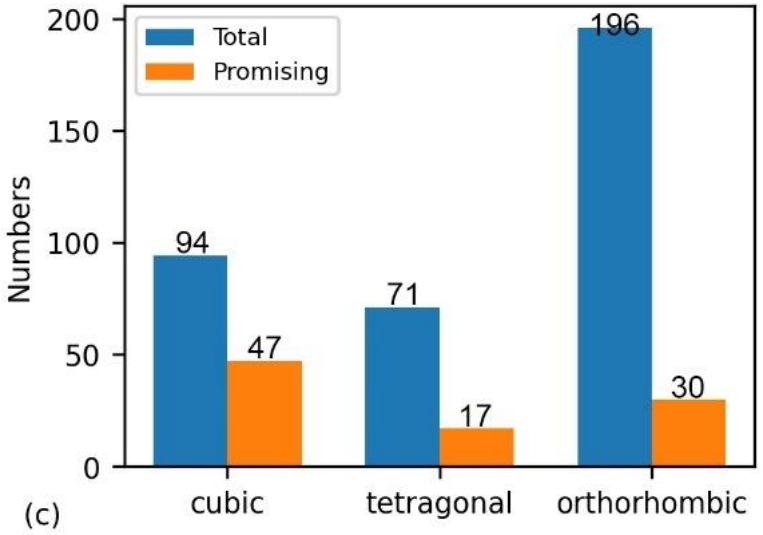


Figure 2. The number of calculated compounds in different classifications: (a) by the number of chemical elements in the composition; (b) by the number of atoms in the primitive cell; (c) by the crystal system.

Good index

m_d^* and m_c^* enter into every formulas related with electronic transport properties

$$\frac{1}{m_c^*} = \frac{1}{3}\left(\frac{1}{m_{\parallel}^*} + 2\frac{1}{m_{\perp}^*}\right)$$

$$m_d^* = N^{2/3}\left(m_{\parallel}^* m_{\perp}^{*2}\right)^{1/3}$$

$$\mu = \frac{e\langle\tau\rangle}{m_c^*}$$

$$n = \frac{\left(2m_{d_0}^* k_B T\right)^{3/2}}{3\pi^2\hbar^3}\int_0^{\infty}\left(-\frac{\partial f}{\partial z}\right)\left(z+\beta z^2\right)^{3/2}\mathrm{d}z$$

$$\alpha \approx \frac{2\pi^{2/3}k_B^2 T m_d^*}{3^{5/3} e n^{2/3}\hbar^2}\left(r+3/2\right)$$

Good index

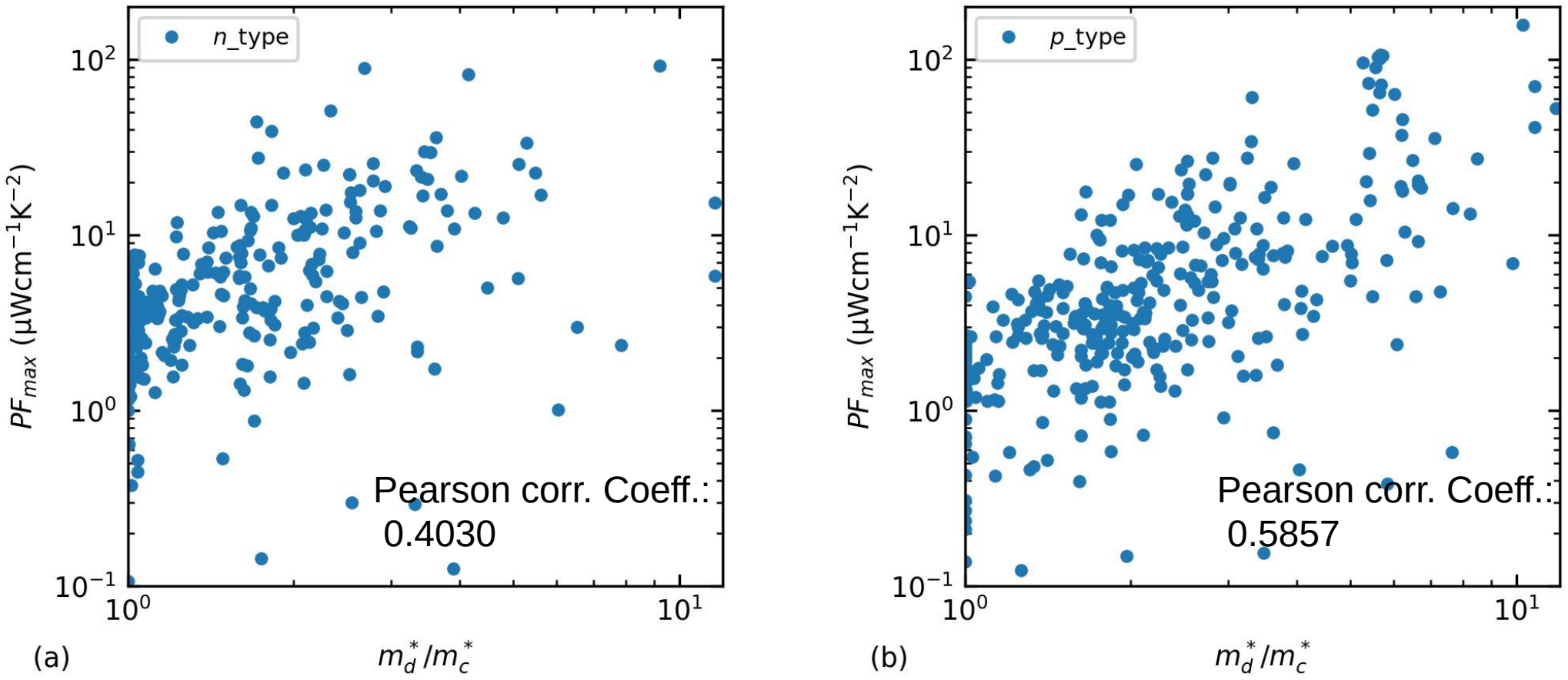


Figure 4. Maximum power factor versus m_d^*/m_c^* for the studied compounds

Good index

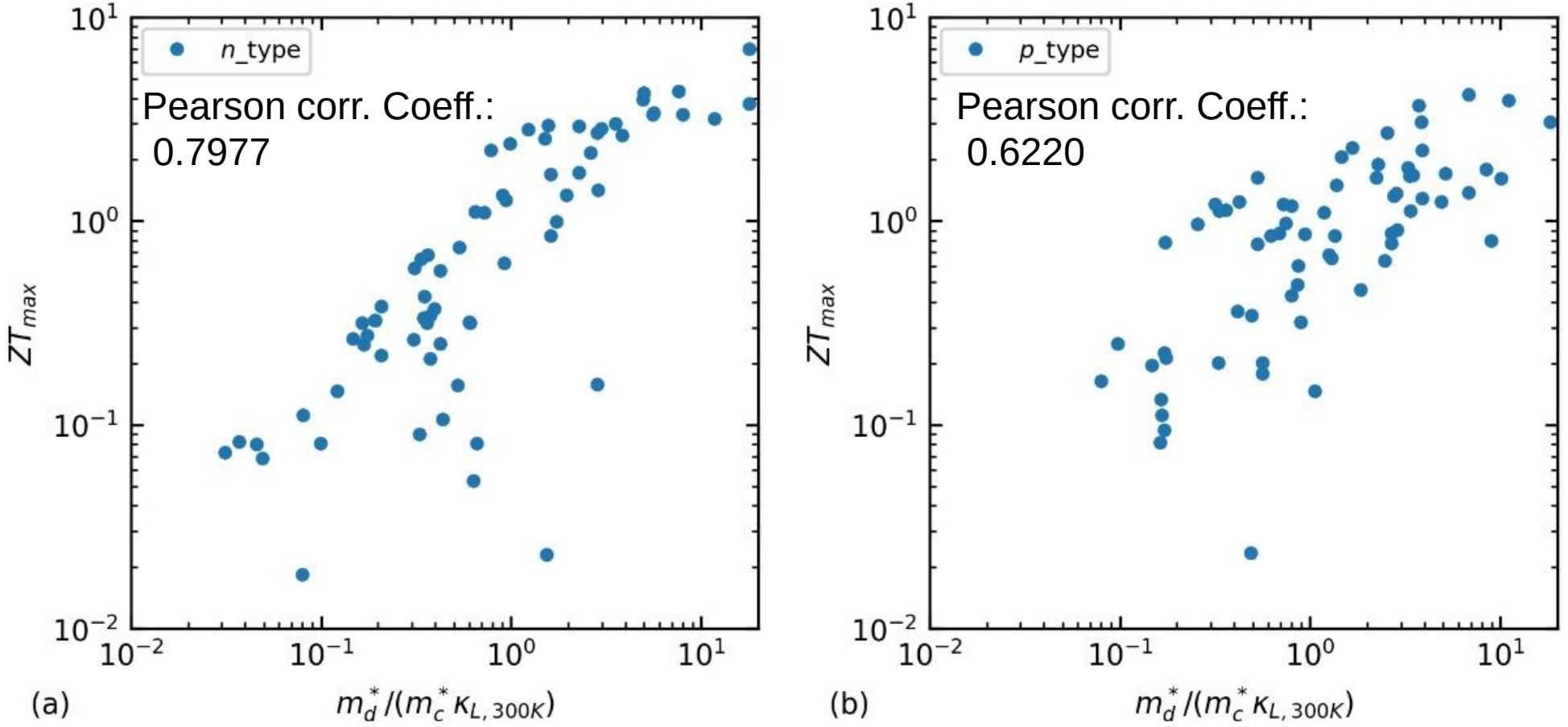
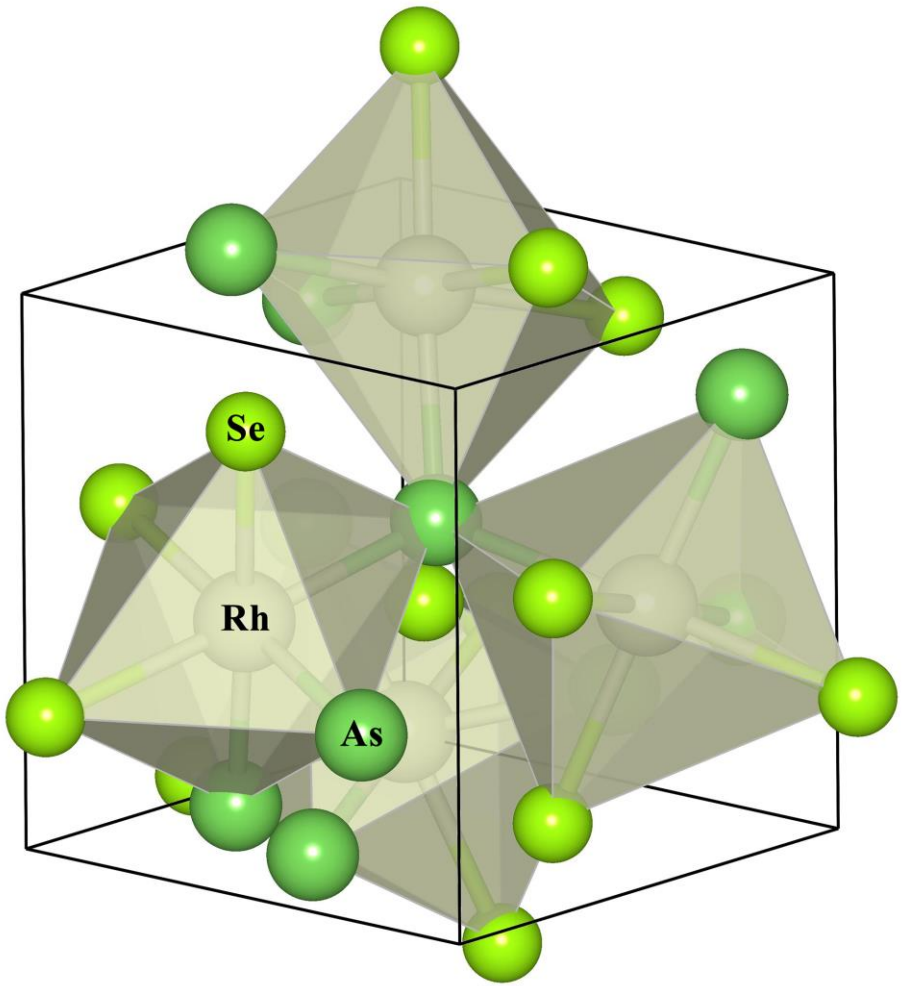


Figure 5. Maximum figure of merit versus $m_d^*/(m_c^* \kappa_{L,300K})$ for the studied compounds

$X_4Y_4Z_4$ (X=VIII B; Y=IV A, V A; Z=VI A)



Compounds with this chemical formula, including RhAsSe, RhSbTe, IrSbTe, IrBiSe, IrBiTe, RhBiSe, RhBiTe, CoAsS, CoAsSe, CoPS, CoPSe, RhPSe, CoSbS, PtSnSe, and PtGeTe. These compounds have the same structure (space group $P2_13$) and they belong to the pyrite structure type. They are found to be good p-type thermoelectric materials due to their large power factor.

$X_4Y_4Z_4$ (X=VIII B; Y=IV A, V A; Z=VI A)

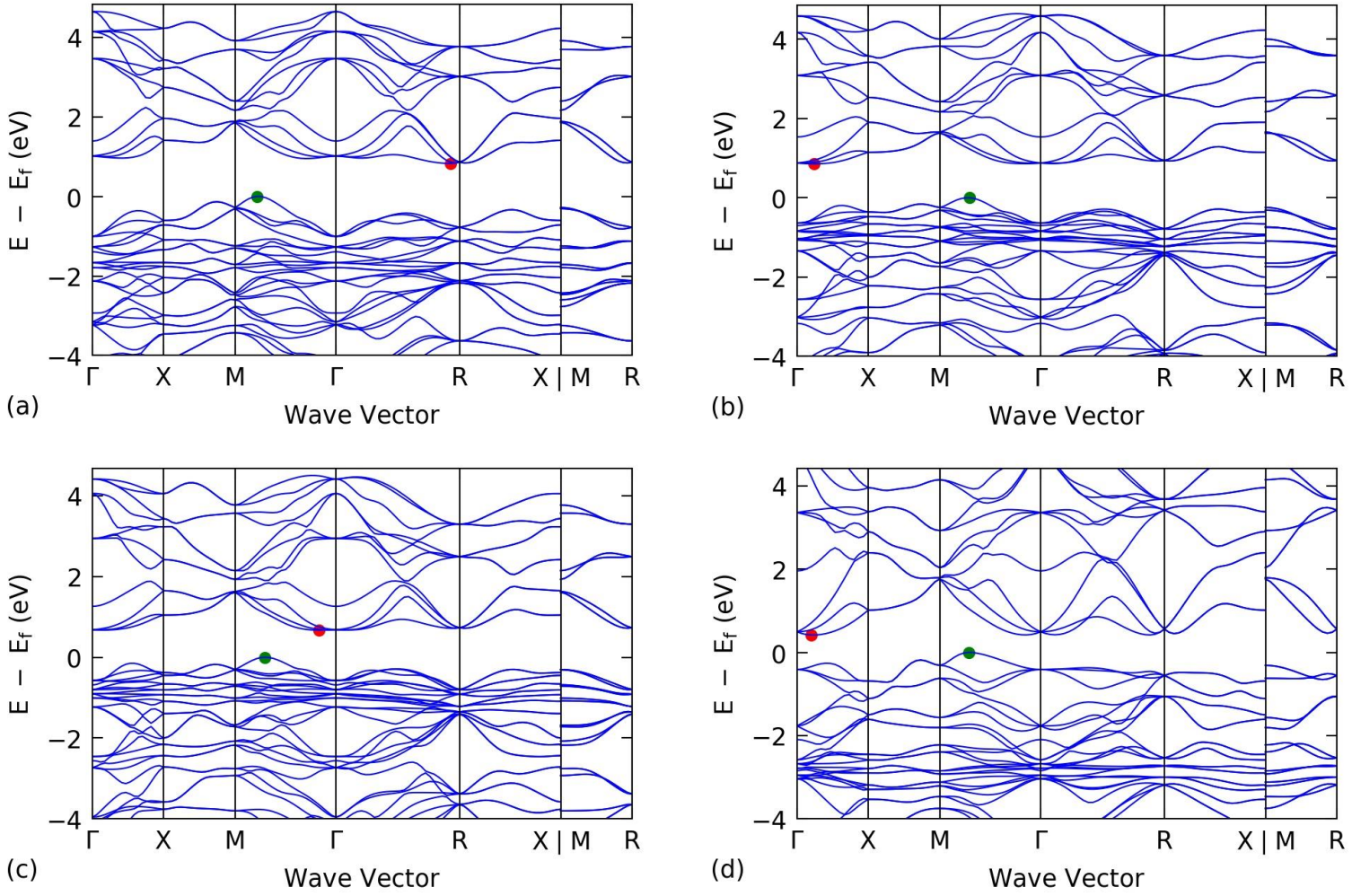


Figure 6. Band structures of (a) RhAsSe, (b) CoAsS, (c) CoAsSe, and (d) PtSnSe

$X_4Y_4Z_4$ (X=VIII B; Y=IV A, V A; Z=VI A)

Table 1. Key parameters for p-type transport

	m_c^* (m_e)	m_d^* (m_e)	Ξ (eV)	N	E_g (eV)	c (GPa)	ε_∞	ε_0
CoAsS	0.5128	2.8524	13.58	12	0.85	139.60	24.79	31.91
CoAsSe	0.4413	2.4915	12.45	12	0.67	121.86	28.29	36.55
CoPS	0.4862	2.7459	14.49	12	1.14	164.48	21.40	27.02
CoPSe	0.4349	2.4668	13.50	12	0.84	142.05	24.88	31.81
CoSbS	0.5315	2.9145	14.93	12	0.55	105.20	28.54	38.17
RhPSe	0.3805	2.1787	13.94	12	1.11	126.03	19.99	24.02
RhAsSe	0.3712	2.0853	12.97	12	0.83	109.46	22.04	27.08
RhBiSe	0.3545	1.9159	13.25	12	0.13	74.64	34.54	44.90
RhBiTe	0.2798	1.5197	13.67	12	0.07	69.88	41.99	53.79
RhSbTe	0.2929	1.6533	14.66	12	0.37	84.43	28.13	36.32
IrBiSe	0.3601	1.9450	12.94	12	0.38	90.84	25.90	34.50
IrBiTe	0.3152	1.7895	13.33	12	0.33	87.55	28.69	38.23
IrSbTe	0.3045	1.8577	14.20	12	0.70	102.02	20.93	27.82
PtSnSe	0.3206	1.9248	13.67	12	0.42	73.29	27.61	36.34
PtGeTe	0.2307	1.4327	15.46	12	0.17	84.80	33.18	41.78

$X_4Y_4Z_4$ (X=VIII B; Y=IV A, V A; Z=VI A)

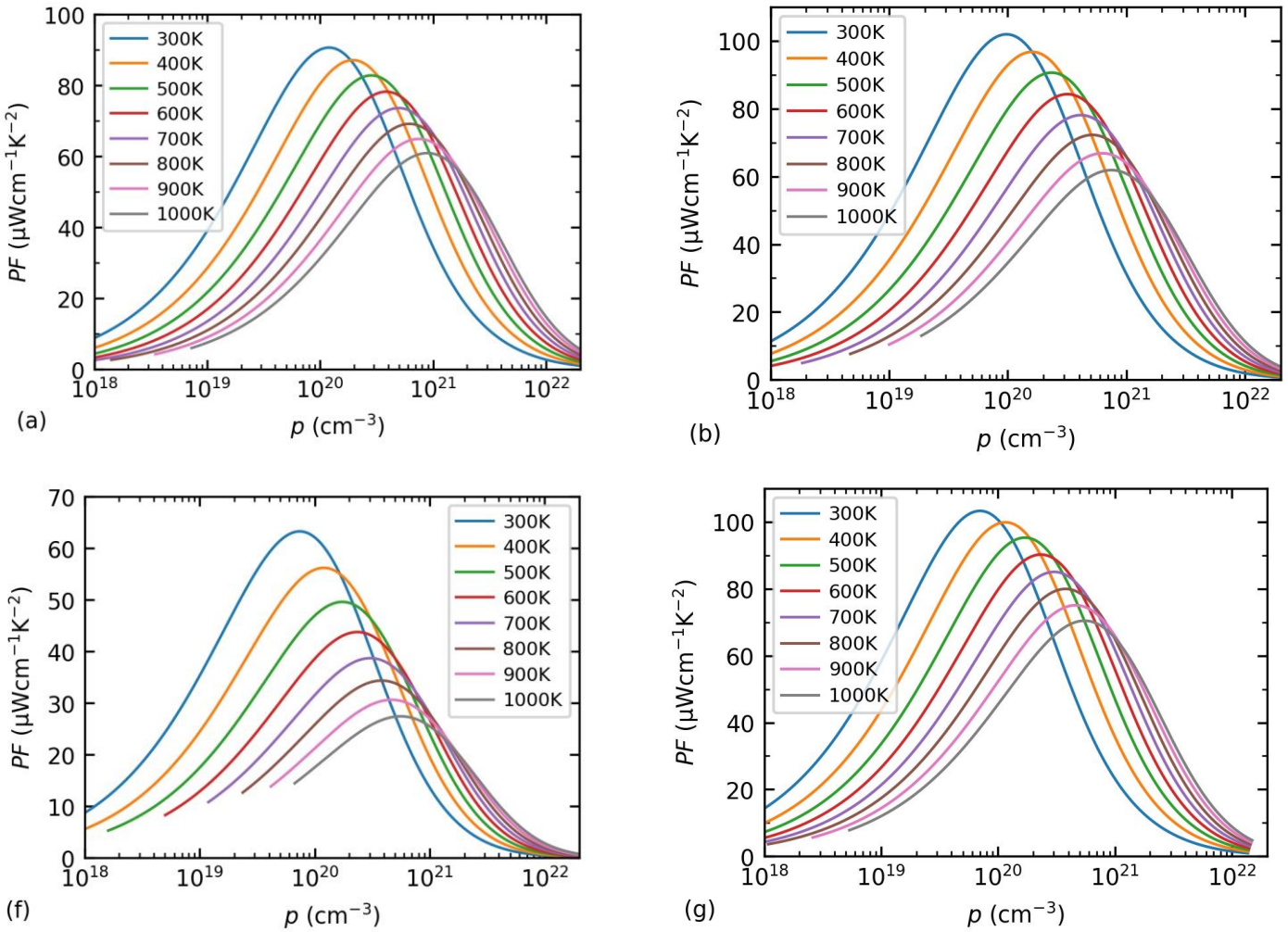


Figure 7. Power factor of (a) CoAsS, (b) CoAsSe, (f) PtSnSe, and (g) RhAsSe.

$X_4Y_4Z_4$ (X=VIII B; Y=IV A, V A; Z=VI A)

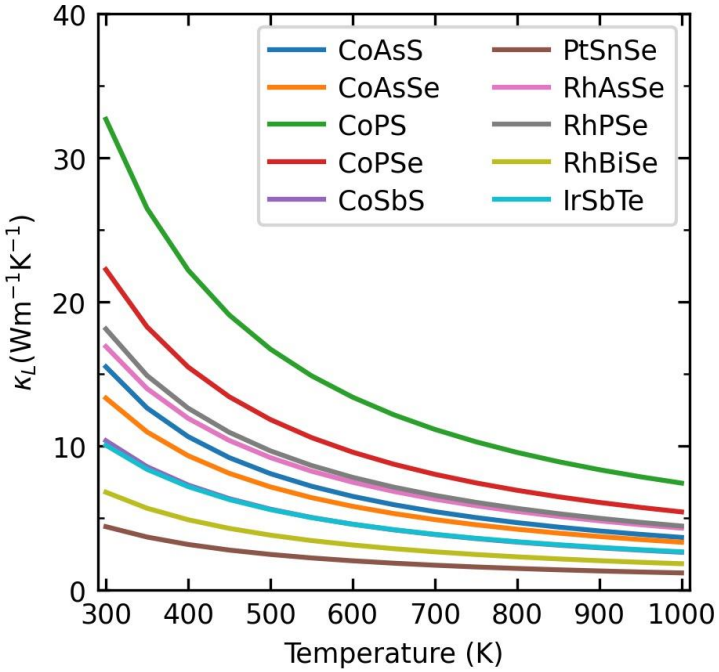


Figure 8. Lattice thermal conductivity

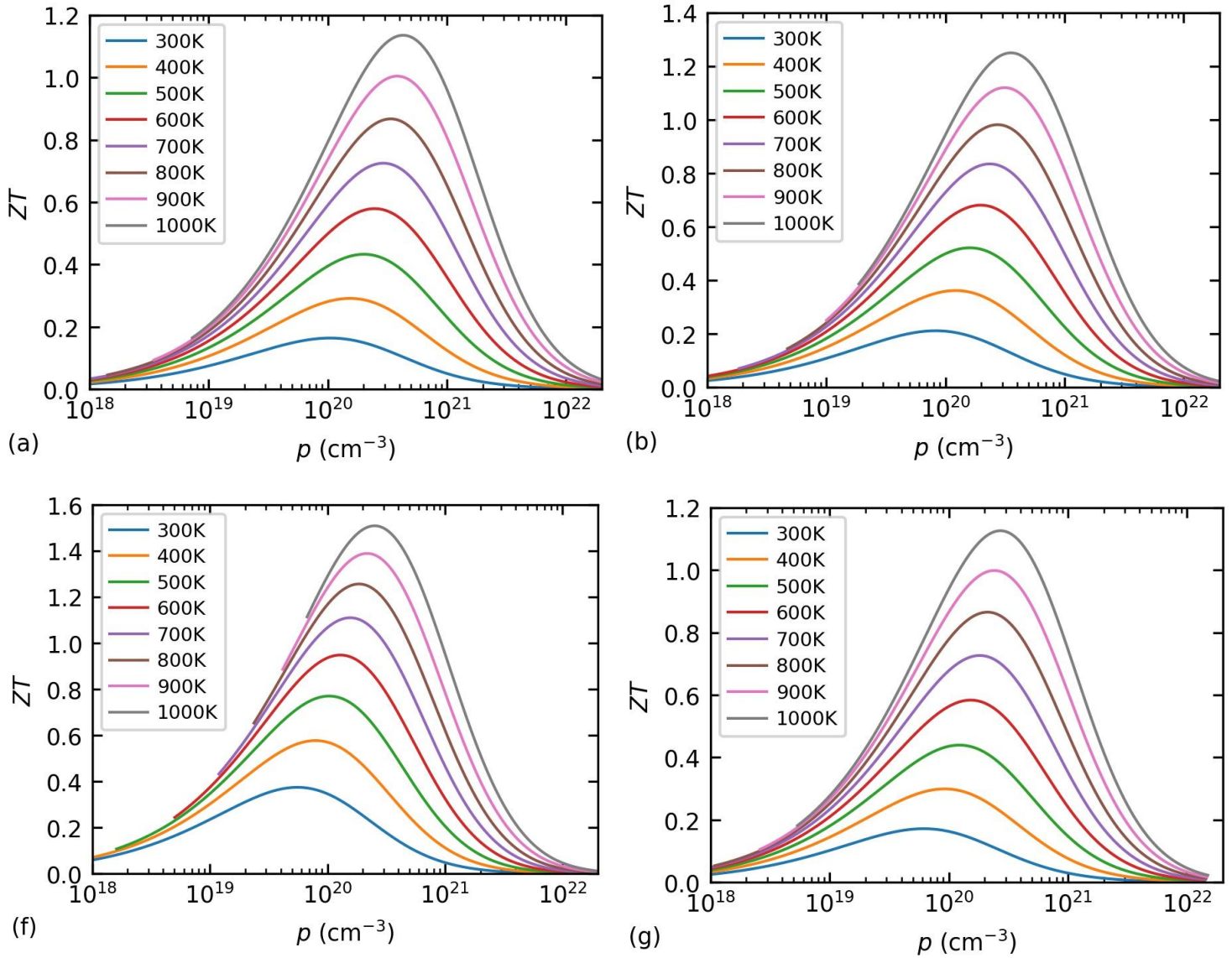
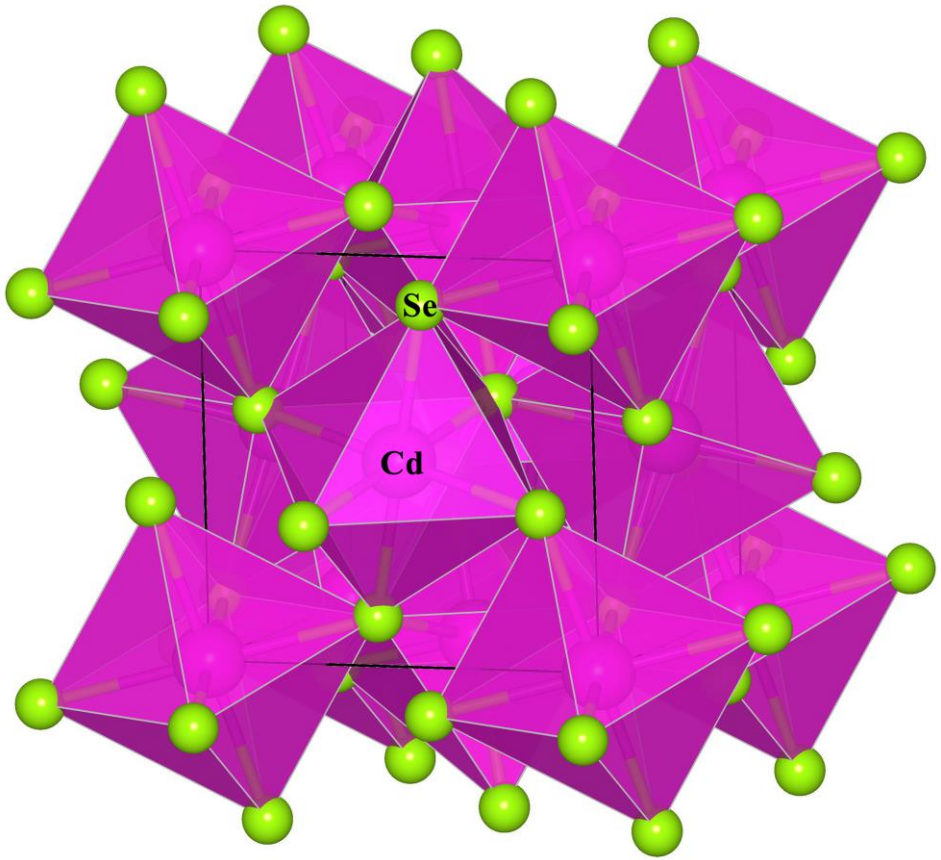


Figure 9. Figure of merit (a) CoAsS, (b) CoAsSe, (f) PtSnSe, and (g) RhAsSe.

$CdSe_2$



The structure of $CdSe_2$ has a space group *Pa*-3 (pyrite type structure). Cd atoms occupy the corner and each of them forming an octahedron with six Se atoms around. Different octahedrons are connected by one Se atom. This compound is found to be a promising n-type thermoelectric material

$CdSe_2$

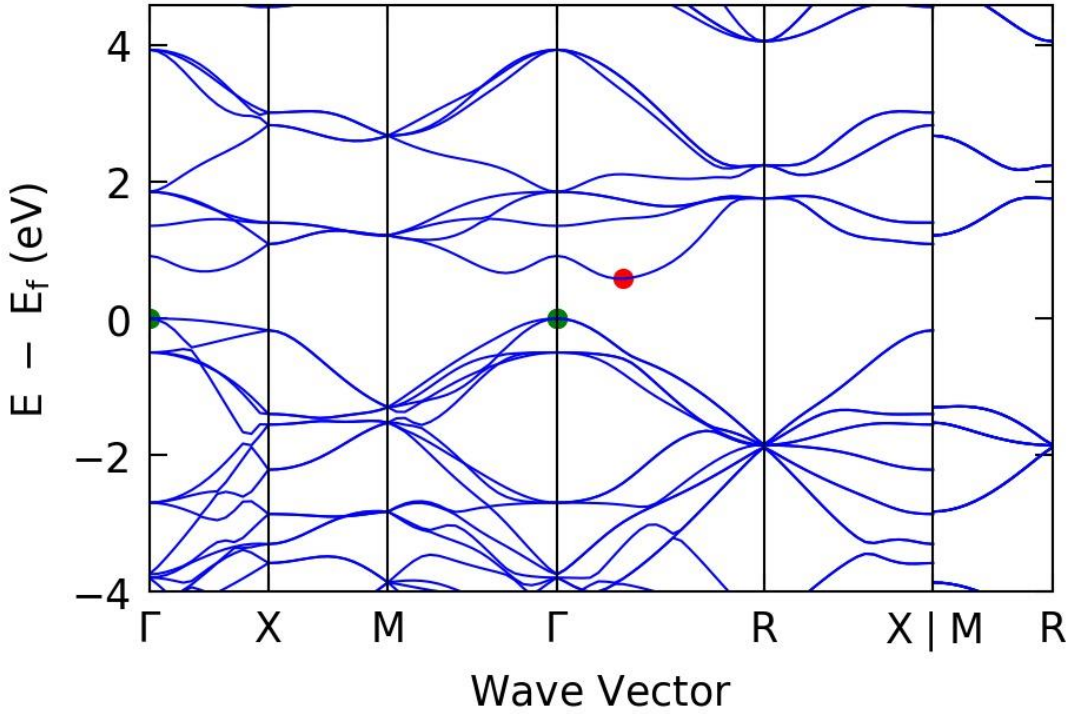
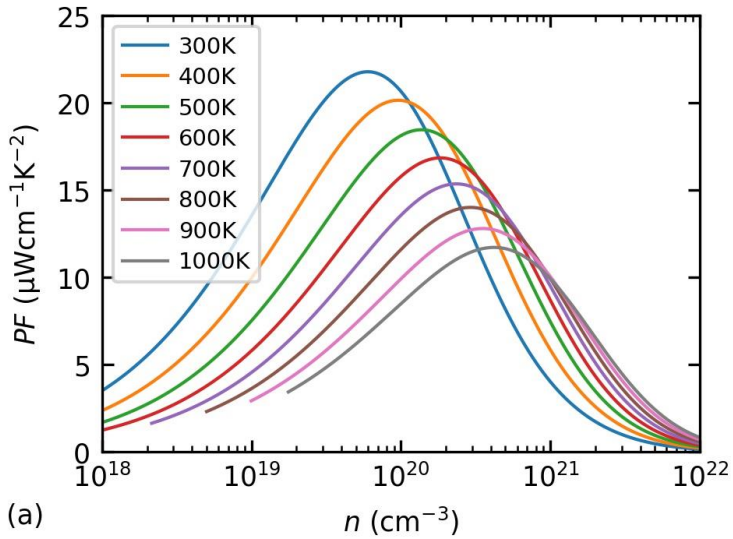


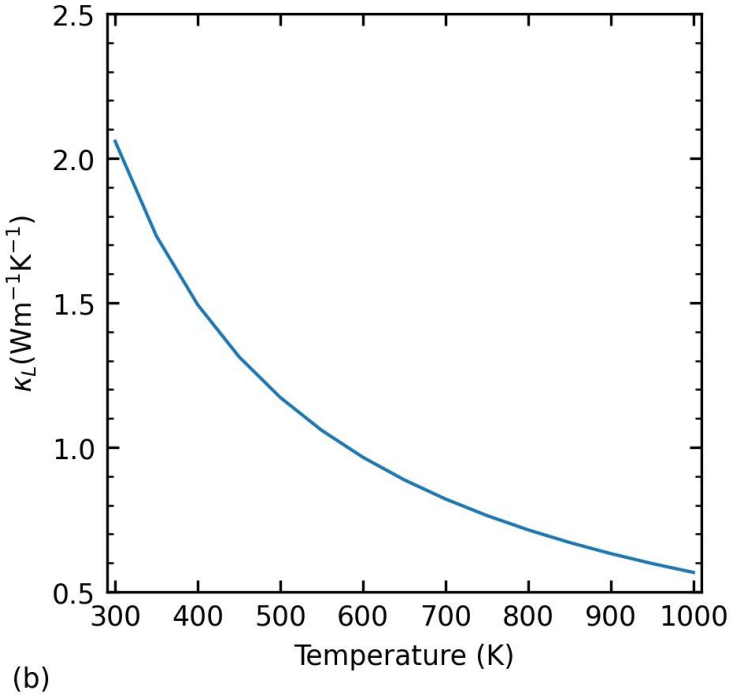
Figure 10. Band structures of $CdSe_2$

Table 2. Key parameters for n-type transport

	m_c^* (m_e)	m_d^* (m_e)	Ξ (eV)	N	E_g (eV)	c (GPa)	ε_∞	ε_0
$CdSe_2$	0.41	1.64	10.19	8	0.58	23.96	11.41	19.90

$CdSe_2$





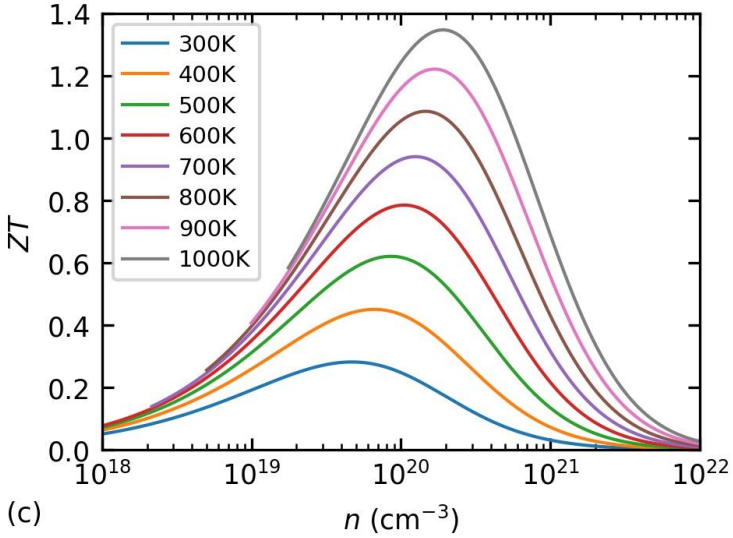
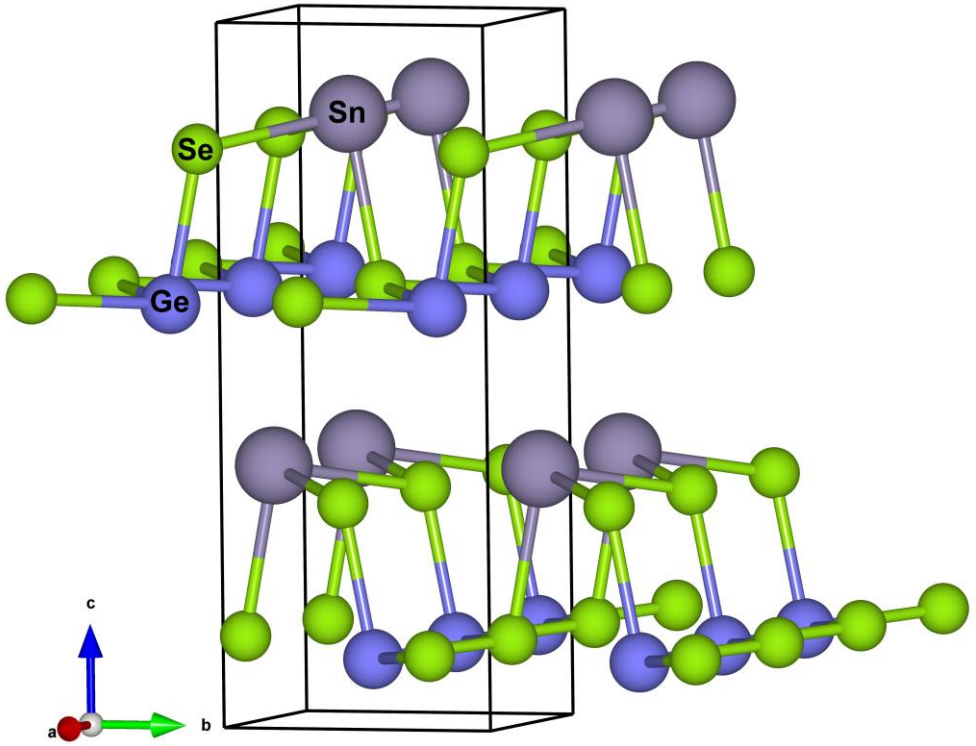


Figure 11. Thermoelectric properties of $CdSe_2$.

SnSe-like compounds

Pnma-type



Compounds belong to this group include $Sn_2Ge_2Se_4$, $Ge_4Se_2S_2$, Ge_4Se_4, $Sn_2Pb_2S_4$, Ge_4Te_4. . The unit cell contains eight atoms (four IVA atoms, four VIA atoms). The IVA and VIA atoms are combined with strong heteropolar bonds to form the crystalline layers. The adjacent layers along *c*-axis are weakly bonded by a combination of van der Waals forces and electrostatic attractions.

SnSe-like compounds

Pnma-type

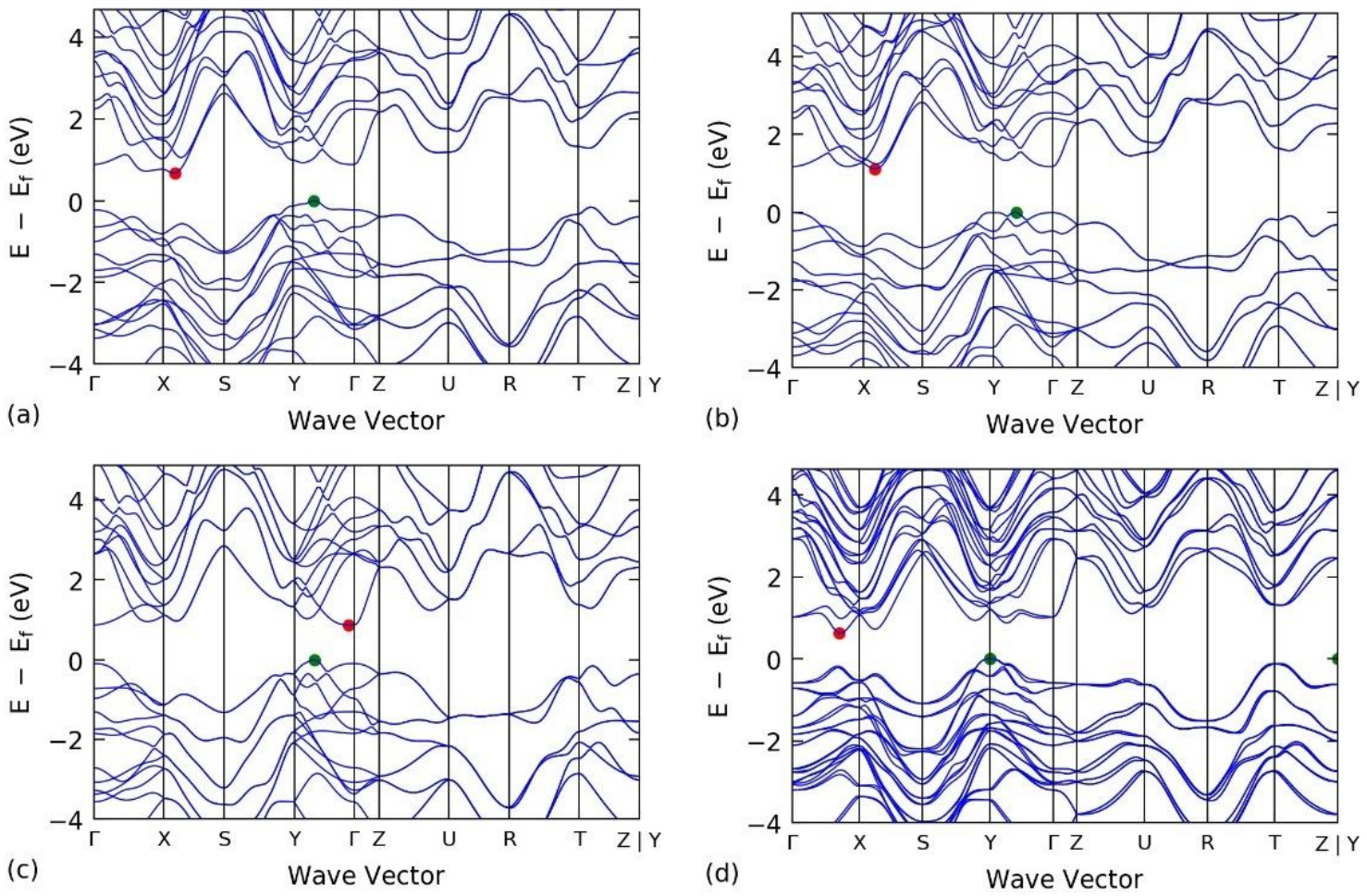


Figure 12. Band structures of (a) $Sn_2Ge_2Se_4$, (b) $Ge_4Se_2S_2$, (c) Ge_4Se_4 and (d) $Sn_2Pb_2S_4$.

SnSe-like compounds

Pnma-type

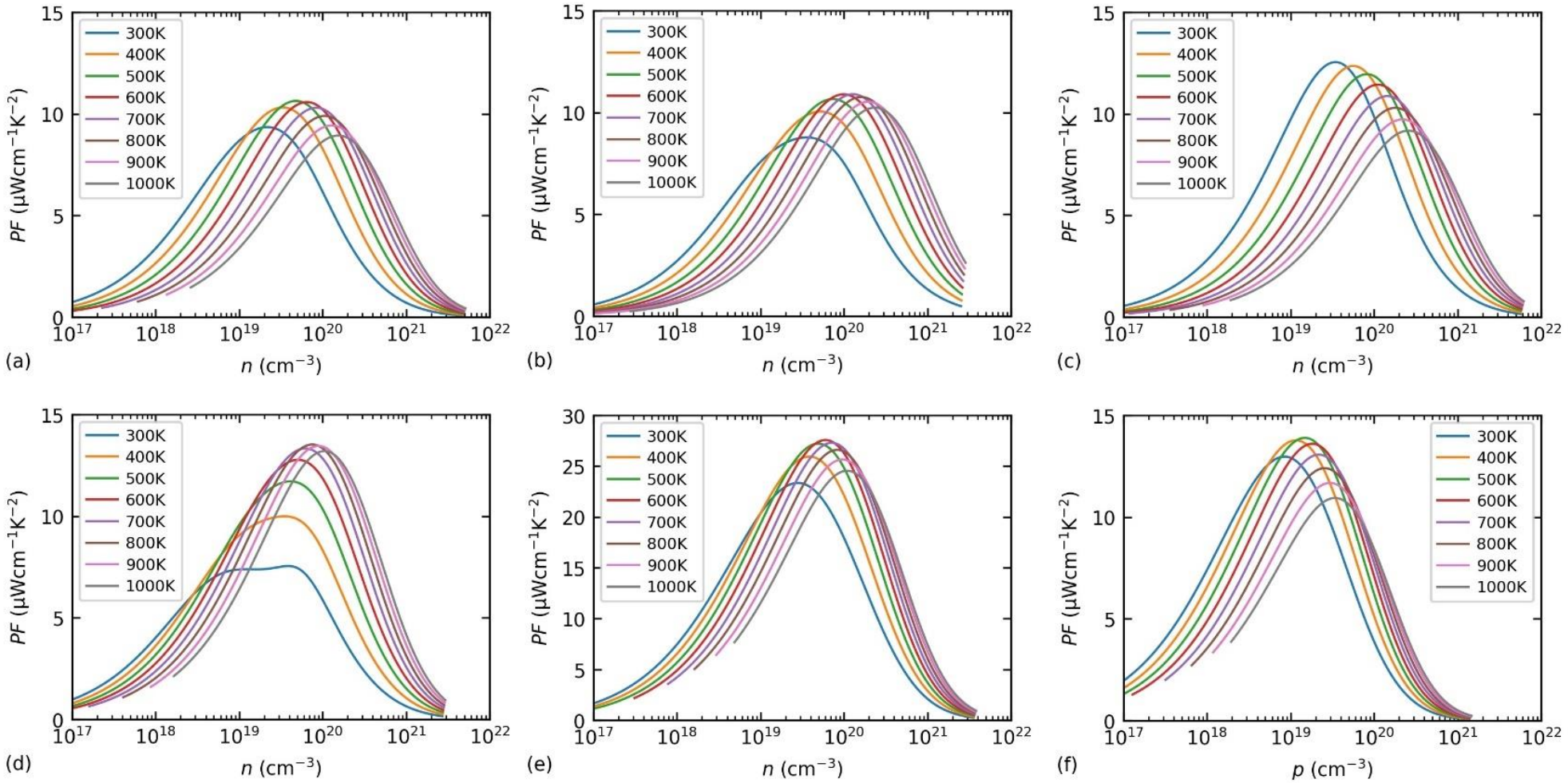


Figure 13. Power factor of (a) $Sn_2Ge_2Se_4$, (b) $Ge_4Se_2S_2$, (c) Ge_4Se_4, (d) $Sn_2Pb_2S_4$, (e)(f) Ge_4Te_4.

SnSe-like compounds

Pnma-type

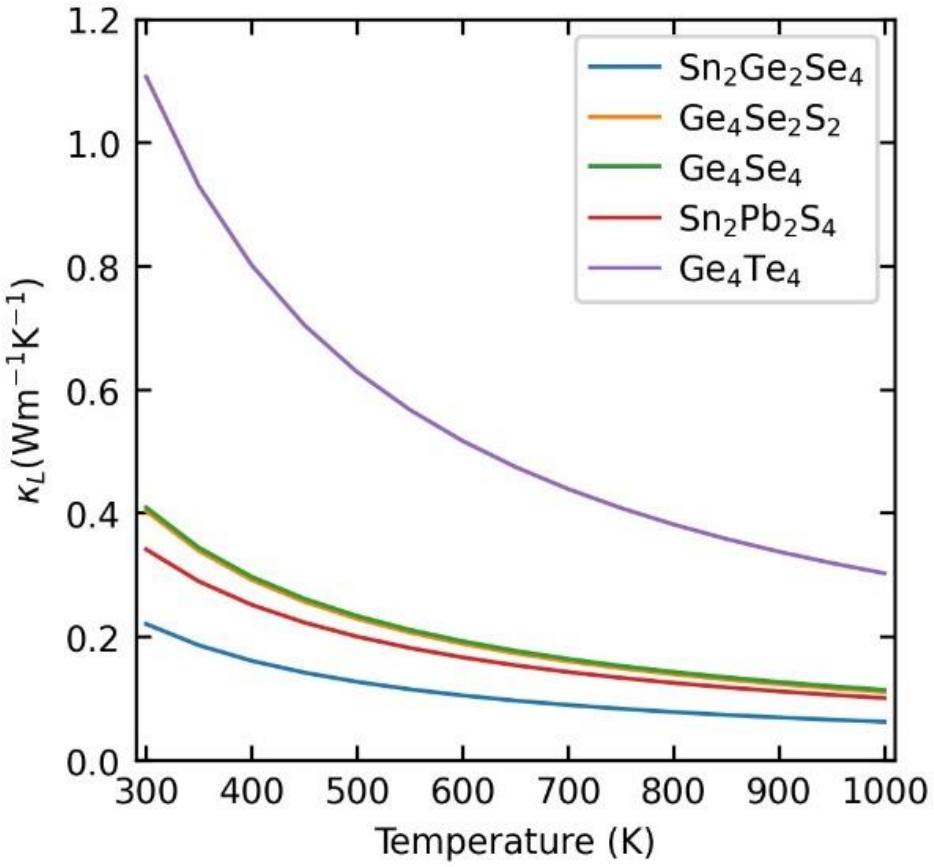


Figure 14. Lattice thermal conductivity

Table 3. Phonon velocity *v* and Grüneisen parameter *γ*

	v_{TA}	$v_{TA'}$	v_{LA}	γ_{TA}	$\gamma_{TA'}$	γ_{LA}
$Sn_2Ge_2Se_4$	1552.21	2333.82	3085.96	5.23	3.97	3.75
$Ge_4Se_2S_2$	2478.90	2024.00	3231.27	5.17	3.39	3.01
Ge_4Se_4	3618.81	1646.25	3019.41	5.08	4.01	2.48
$Sn_2Pb_2S_4$	1453.16	2057.29	2863.01	4.66	2.87	2.76
Ge_4Te_4	1718.25	2694.27	3481.99	3.64	2.78	2.39

SnSe-like compounds

Pnma-type

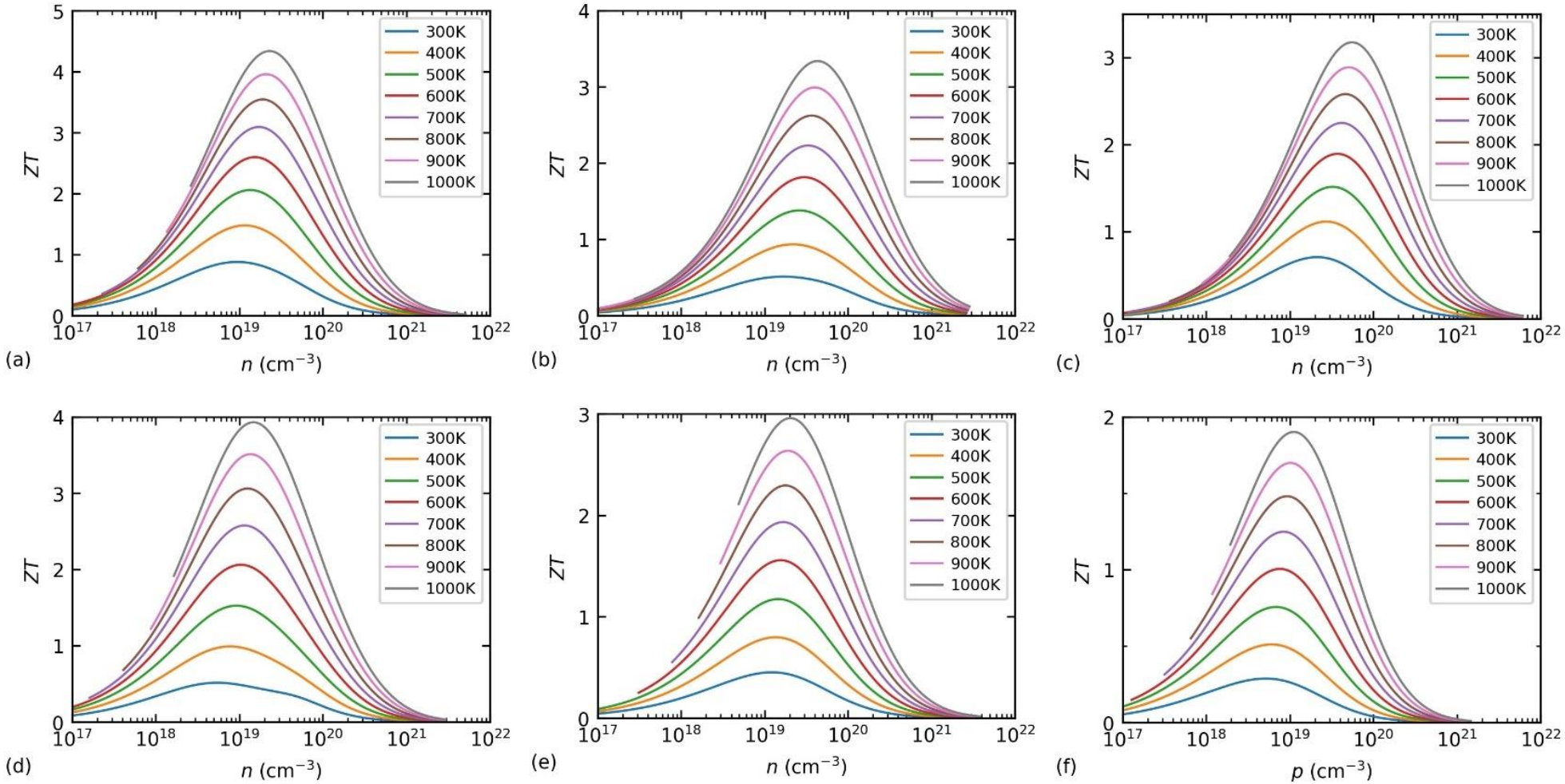
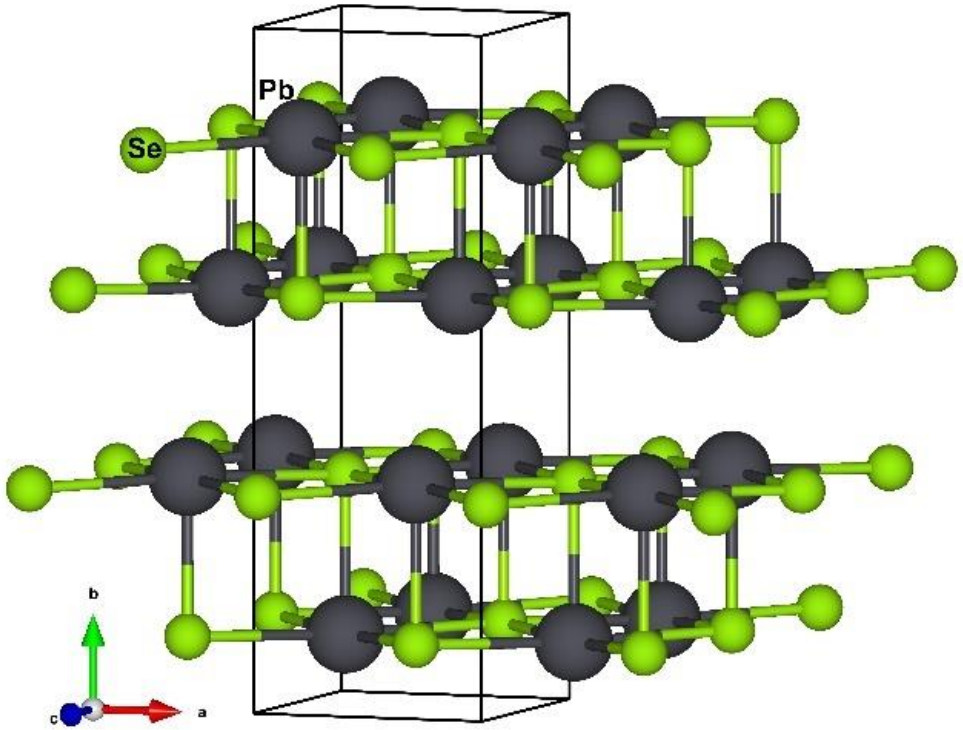


Figure 15. Figure of merit of (a) $Sn_2Ge_2Se_4$, (b) $Ge_4Se_2S_2$, (c) Ge_4Se_4, (d) $Sn_2Pb_2S_4$, (e)(f) Ge_4Te_4.

SnSe-like compounds

Cmcm-type



Compounds belong to this group include Pb_4Se_4, Pb_4S_4. The unit cell contains eight atoms and adopts a double-layered structure. Different from the α-phase structure, within each layer of β-phase, one IVA (or VIA) atom is instead bonded to five neighboring VIA (or IVA) atoms in a less distorted structure. The adjacent layers along *b*-axis are weakly bonded by a combination of van der Waals forces and electrostatic attractions.

SnSe-like compounds

Cmcm-type

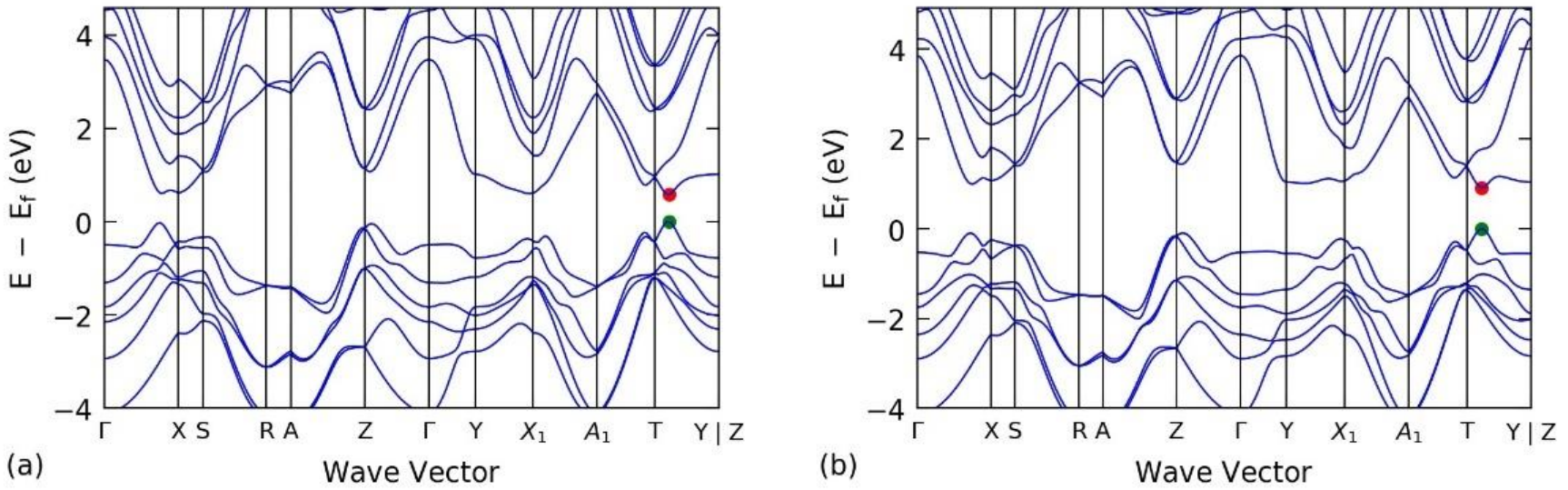


Figure 16. Band structures of (a) Pb_4Se_4, (b) Pb_4S_4.

SnSe-like compounds

Cmcm-type

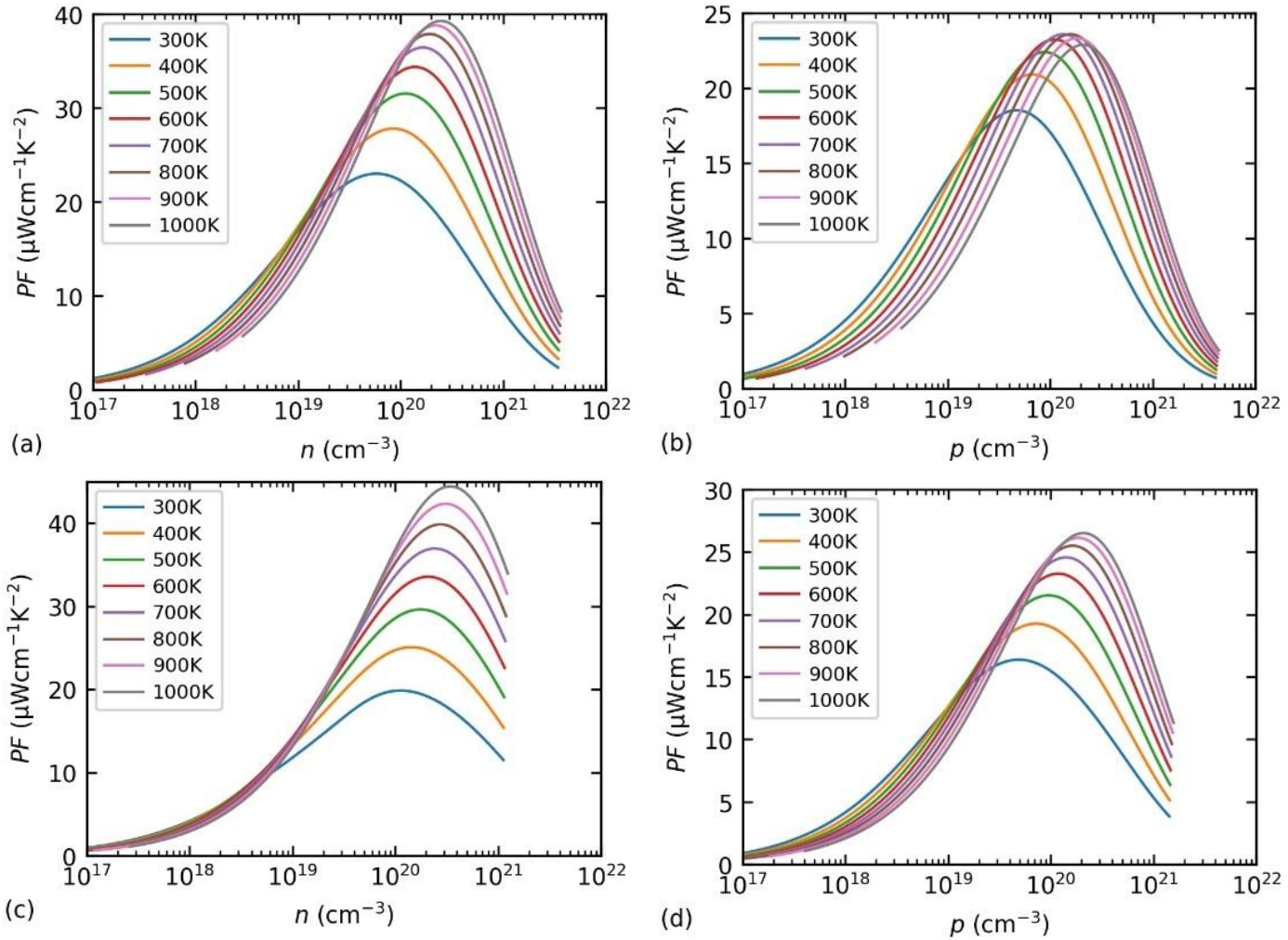


Figure 17. Power factor of (a)(b) Pb_4Se_4, (c)(d) Pb_4S_4.

SnSe-like compounds

Cmcm-type

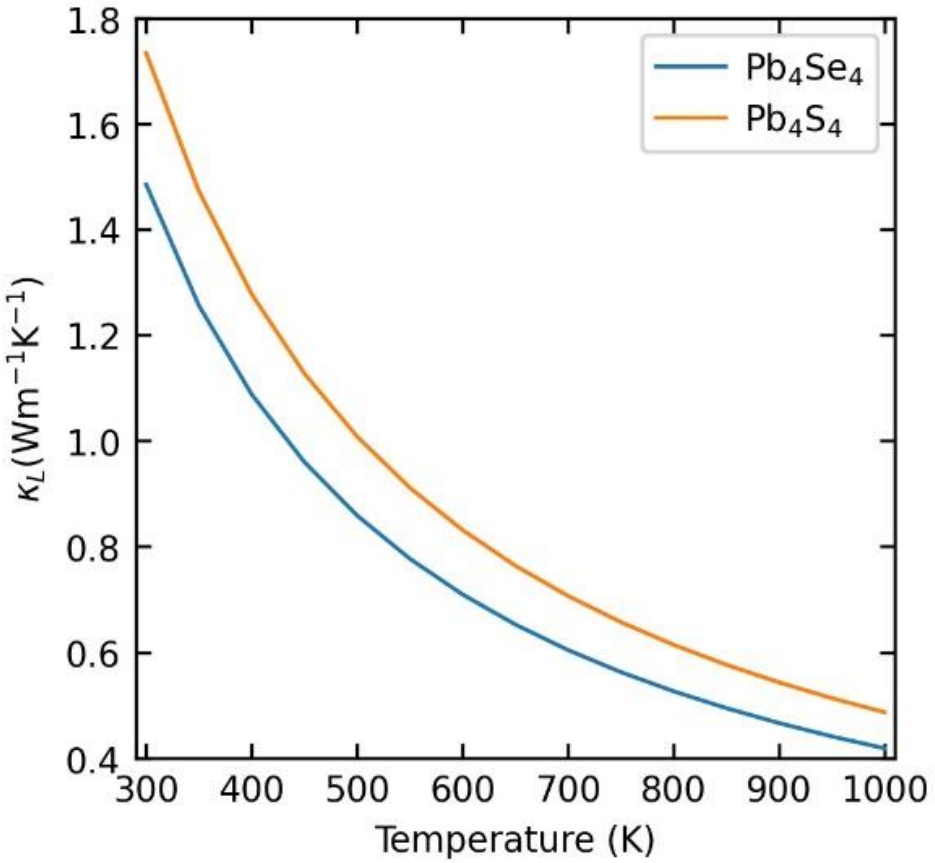


Figure 18. Lattice thermal conductivity

Table 4 Phonon velocity *v* and Grüneisen parameter *γ*

	v_{TA}	$v_{TA'}$	v_{LA}	γ_{TA}	$\gamma_{TA'}$	γ_{LA}
Pb_4Se_4	1045.73	1986.53	2537.70	4.85	2.26	1.34
Pb_4S_4	896.77	1909.94	2736.21	6.89	2.91	1.79

SnSe-like compounds

Cmcm-type

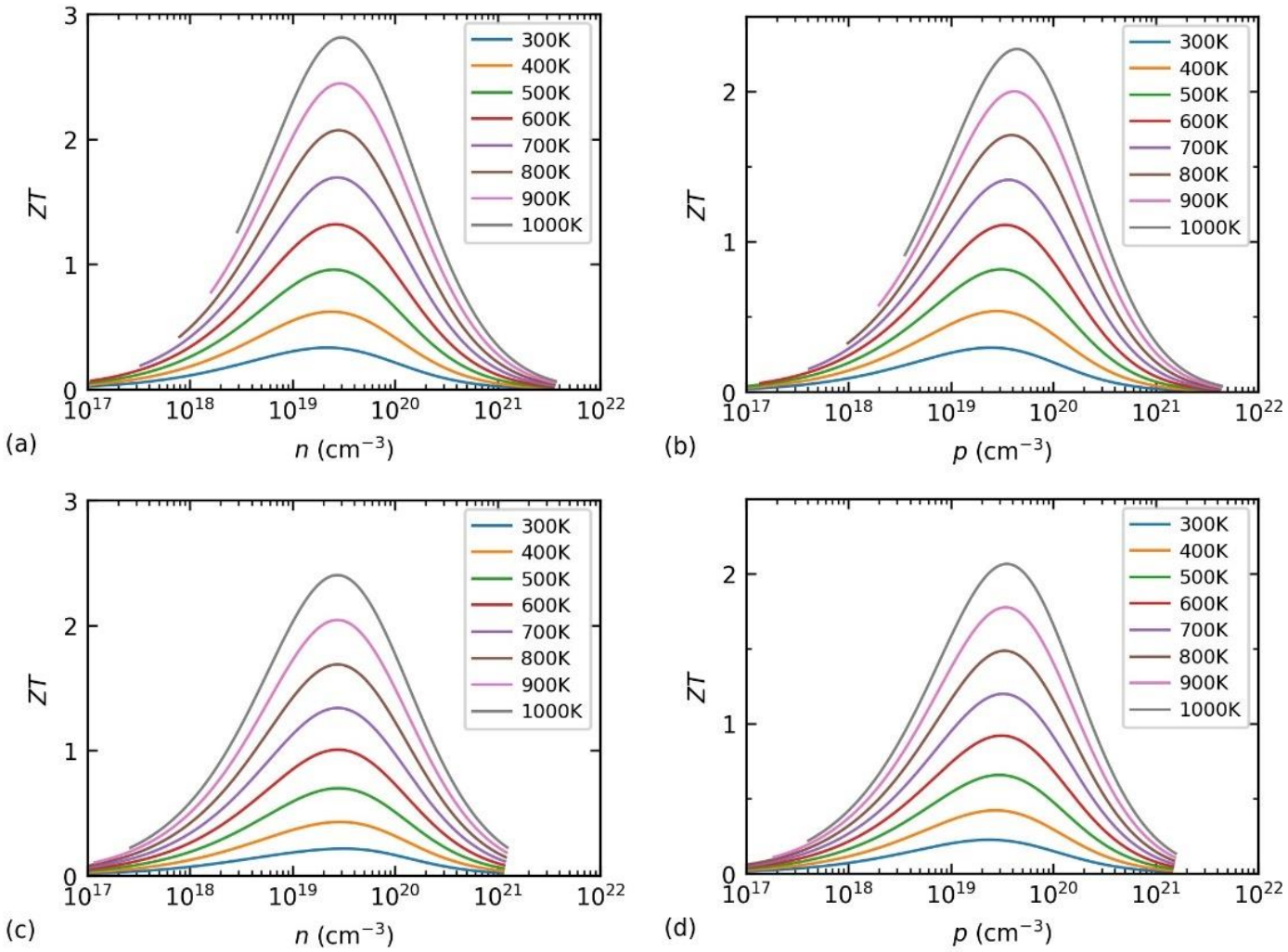


Figure 19. Figure of merit of (a)(b) Pb_4Se_4, (c)(d) Pb_4S_4.

Reading

[1] Tao Fan, Artem R. Oganov. "AICON: A program for calculating thermal conductivity quickly and accurately." *Computer Physics Communications* 251 (2020): 107074.

[2] Tao Fan, Artem R. Oganov. "AICON2: A program for calculating transport properties quickly and accurately." *Computer Physics Communications* 266 (2021): 108027.

[3] Tao Fan, Artem R. Oganov. "Discovery of high performance thermoelectric chalcogenides through first-principles high-throughput screening." *Journal of Materials Chemistry C* 9.38 (2021): 13226–13235.

Section 4

AICON Workshop

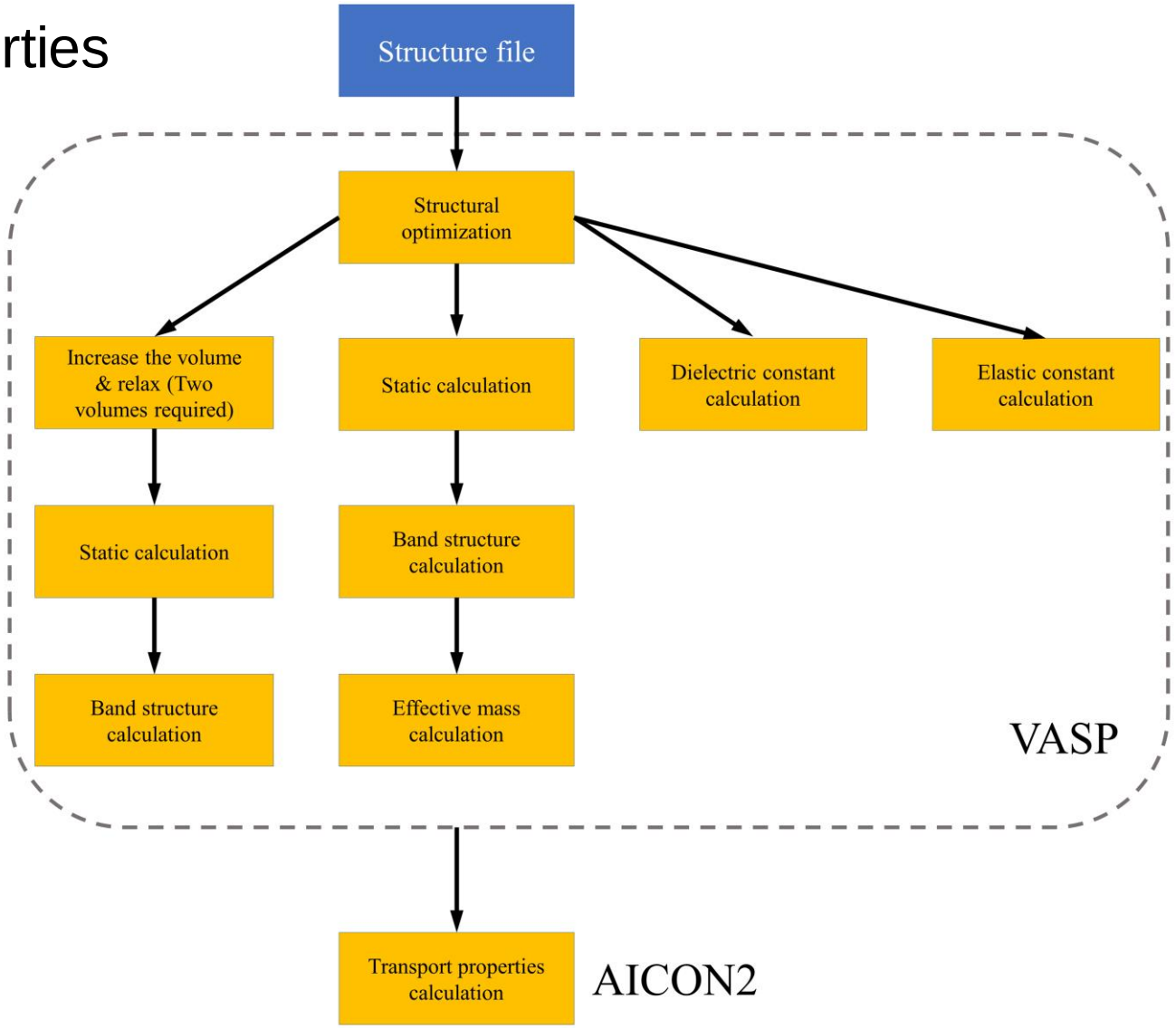
Installation

https://github.com/Baijianlu/AICON2.git

From pip: pip install AICON
From source package: python setup.py install

Workflow

Electronic transport properties



Workflow

equi	folder of equilibrium structure's band structure
0.5per	folder of 0.1% larger structure's band structure
1.0per	folder of 0.2% larger structure's band structure
CBM	folder of conduction band minimum calculation
VBM	folder of valence band maximum calculation
VSB	folder of second valence band calculation
dielect	folder of dielectric constant calculation
elastic	folder of elastic constant calculation

Commands

```
(base) [taofan@headnode conductivity]$ AICON -h
usage: AICON [-h] [--elec] [--phon] [-m MODE]
             [-t TEMPERATURE [TEMPERATURE ...]] [--tmax TMAX] [--tmin TMIN]
             [--tstep TSTEP] [-d DOPE [DOPE ...]] [--dope_max DOPE_MAX]
             [--dope_min DOPE_MIN] [--dope_step DOPE_STEP] [--highpath]
             [--noSB] [--scale]

AICON command-line-tool

optional arguments:
  -h, --help            show this help message and exit
  --elec                Calculate electrical conductivity
  --phon                Calculate lattice thermal conductivity
  -m MODE, --mode MODE  mode for electrical conductivity calculation, either
                        standard or doping
  -t TEMPERATURE [TEMPERATURE ...], --temperature TEMPERATURE [TEMPERATURE ...]
                        Specified temperature
  --tmax TMAX           Maximum calculated temperature
  --tmin TMIN           Minimum calculated temperature
  --tstep TSTEP         Calculated temperature step
  -d DOPE [DOPE ...], --dope DOPE [DOPE ...]
                        Specified carrier concentration
  --dope_max DOPE_MAX   Maximum calculated carrier concentration
  --dope_min DOPE_MIN   Minimum calculated carrier concentration
  --dope_step DOPE_STEP
                        Calculated concentration step
  --highpath            Obtain high-symmetry path
  --noSB                Disable second band calculation
  --scale               If multiply a scaling factor with Kappa
```

Commands

--mode (-m) “standard” or “doping”

standard	doping
➢ Properties as a function of temperature and chemical potential ➢ Chemical potential starts from the middle of the gap and till the 1 eV above with a step of 2 meV	➢ Properties as a function of temperature and doping concentration.

Example

“standard” mode

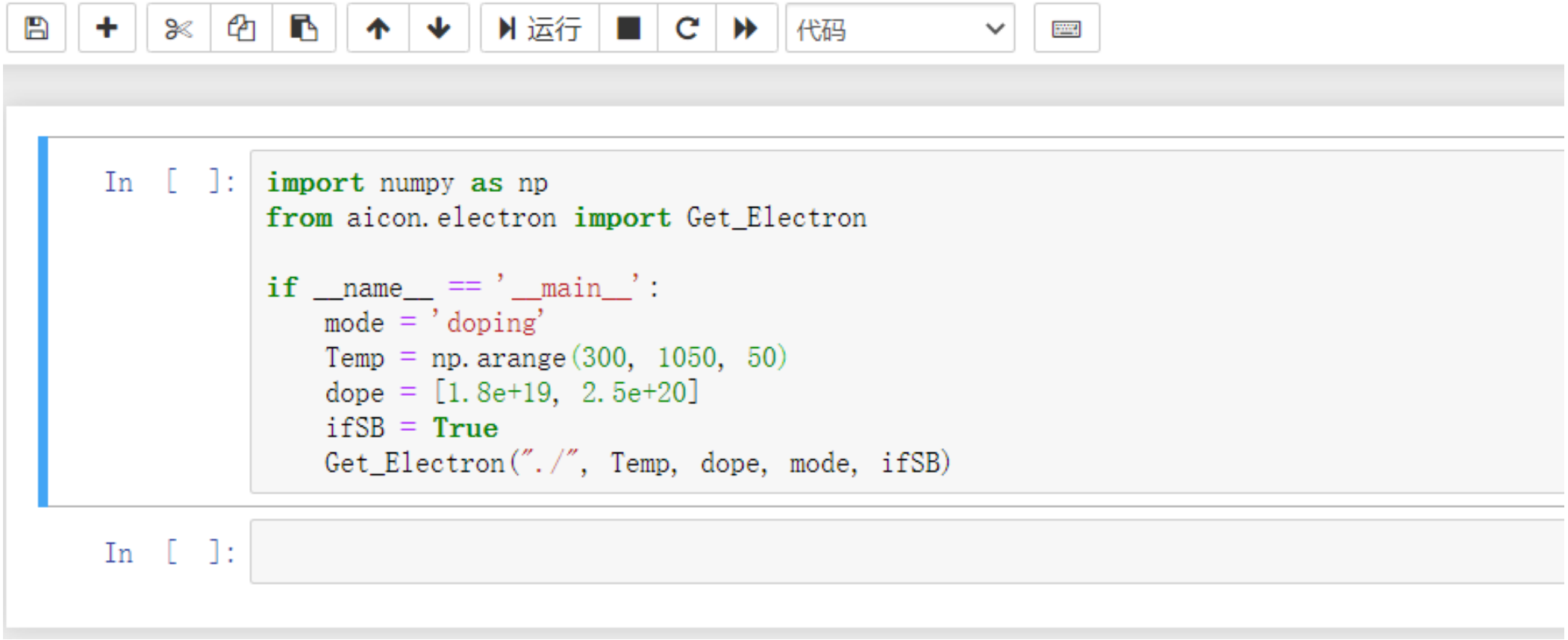
AICON --elec -m standard --tmin 300 --tmax 1000 --tstep 100

“doping” mode

AICON --elec -m doping --tmin 300 --tmax 1000 --tstep 100 -d 1e+18 1e+19

Example

Call AICON from python script



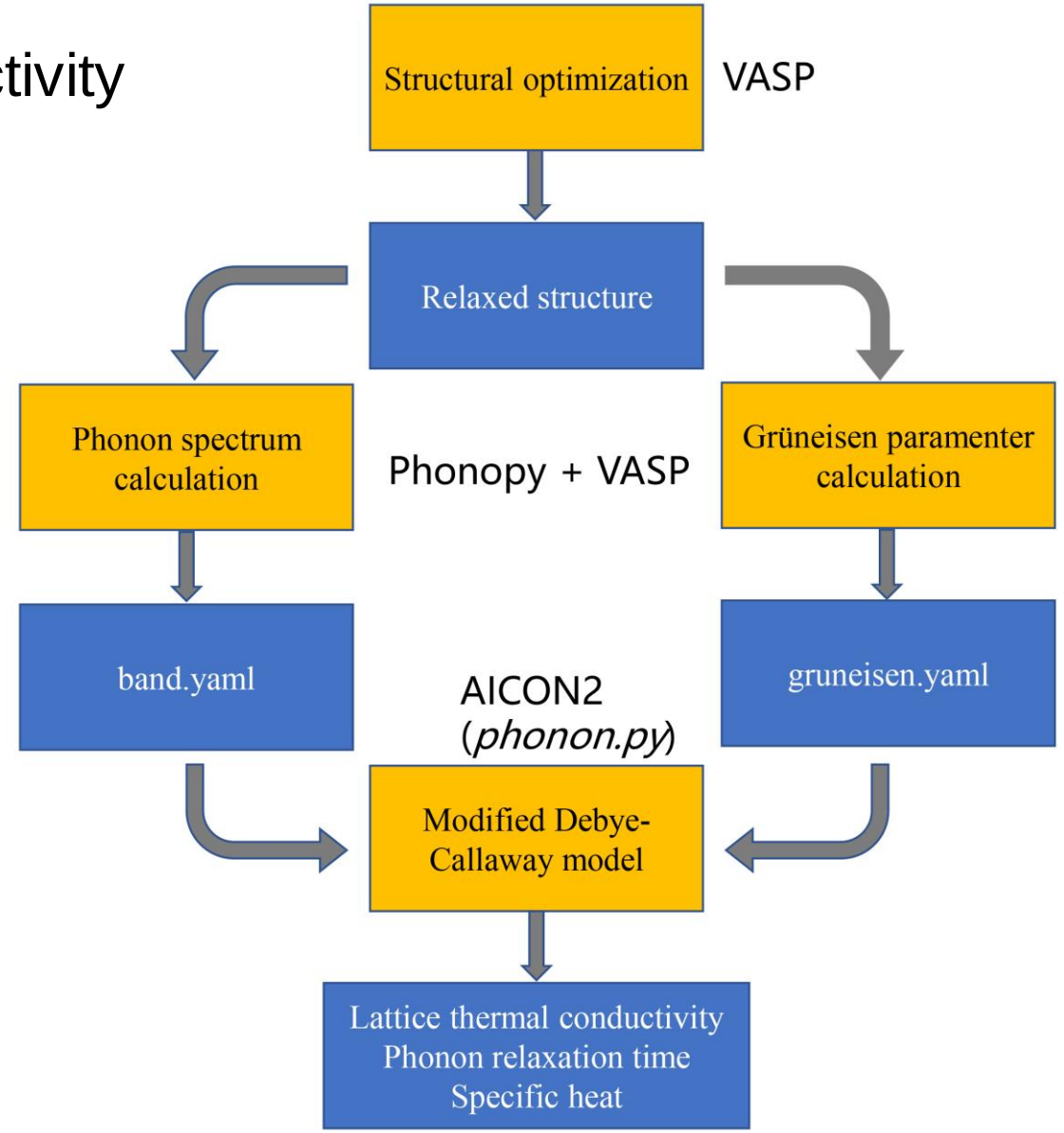
Example

```
(base) [t.fan@arkuda1 launcher_2020-07-10-15-55-29-784099]$ ls
0.5per          CBM       elastic  FW_offline.json                    jobscript   TVB.xlsx  VSB
1.0per          CBM.xlsx  equi     FW_ping.json                       log         VBM       VSB.xlsx
aiconforele.py  dielect   FW.json  FW--TePb-electrical_conductivity  Parameters  VBM.xlsx
(base) [t.fan@arkuda1 launcher_2020-07-10-15-55-29-784099]$
```

- transport properties's data are stored as a pandas.DataFrame object and it could be saved as any file format pandas supports.

Workflow

Lattice thermal conductivity



Example

Step1: get high-symmetry path

AICON --phon --highpath

Step 2: calculate lattice thermal conductivity

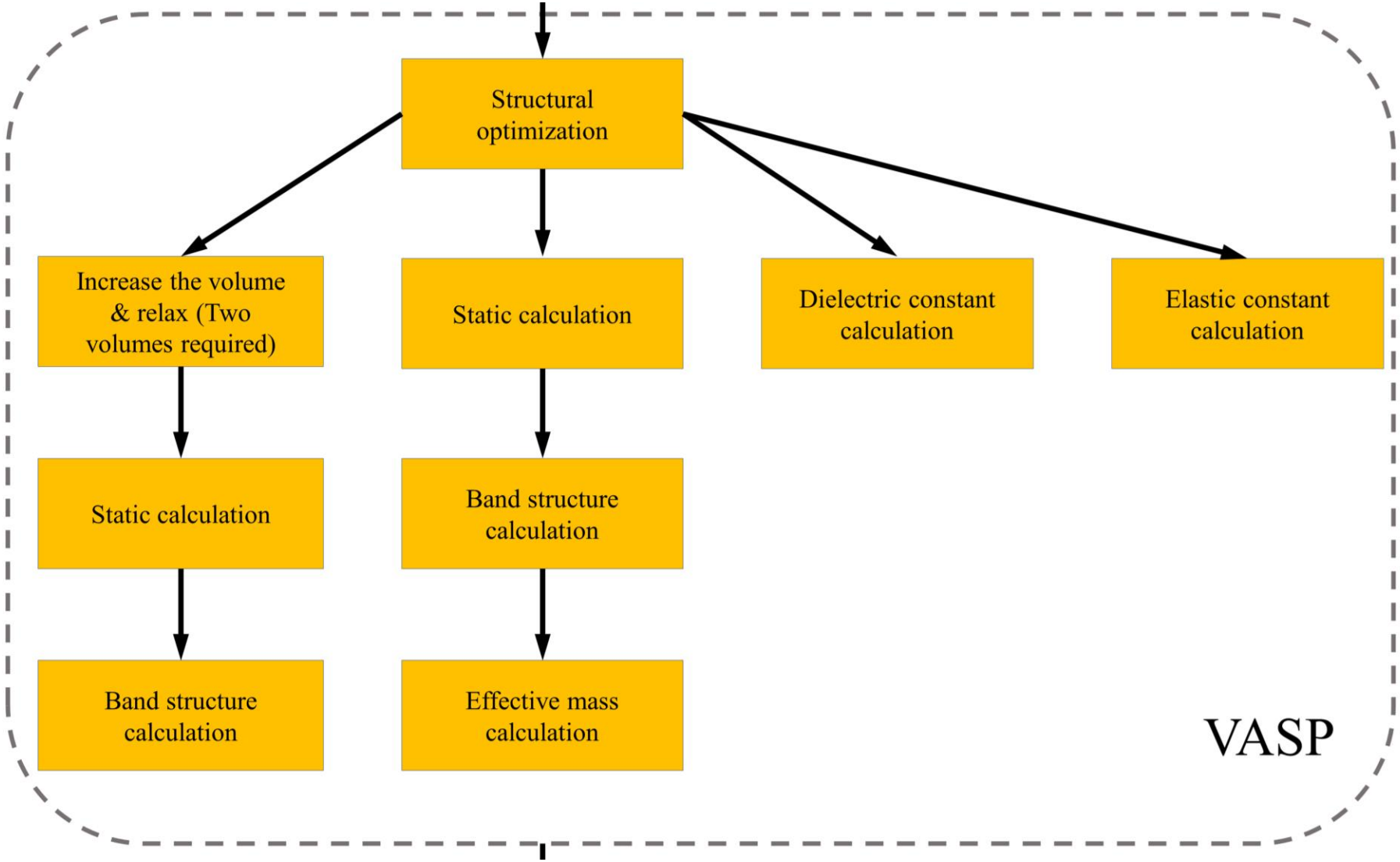
AICON --phon --tmin 300 --tmax 1000 --tstep 50

Example

```
(base) [t.fan@arkuda1 gruneisen]$ ls
band.yaml  gruneisen.yaml  grunsi  jobscript  Kappa.xlsx  minus  orig  plus  POSCAR
(base) [t.fan@arkuda1 gruneisen]$
```

- transport properties's data are stored as a pandas.DataFrame object and it could be saved as any file format pandas supports.

Automatic calculation



Section 5

BoltzTrap2 Workshop

BoltzTraP2

“BoltzTraP2 is a modern implementation of the smoothed Fourier interpolation algorithm for electronic bands that formed the base of the original BoltzTraP code, One of the most typical uses is the calculation of thermoelectric transport coefficients as functions of temperature and chemical potential in the rigid-band picture.”

Homepage: https://gitlab.com/sousaw/BoltzTraP2
Related papers: https://doi.org/10.1016/j.cpc.2006.03.007 and
https://doi.org/10.1016/j.cpc.2018.05.010

BoltzTraP2

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View Journal | View Issue

Cite this: *J. Mater. Chem. C*, 2016, 4, 4414

Understanding thermoelectric properties from high-throughput calculations: trends, insights, and comparisons with experiment†

Wei Chen,[ab] Jan-Hendrik Pöhls,[c] Geoffroy Hautier,[d] Danny Broberg,[e] Saurabh Bajaj,[af] Umut Aydemir,[fg] Zachary M. Gibbs,[f] Hong Zhu,[h] Mark Asta,[e] G. Jeffrey Snyder,[fg] Bryce Meredig,[i] Mary Anne White,[c] Kristin Persson[ae] and Anubhav Jain*[a]

https://contribs.materialsproject.org/projects/carrier_transport

Installation

Prerequisites:

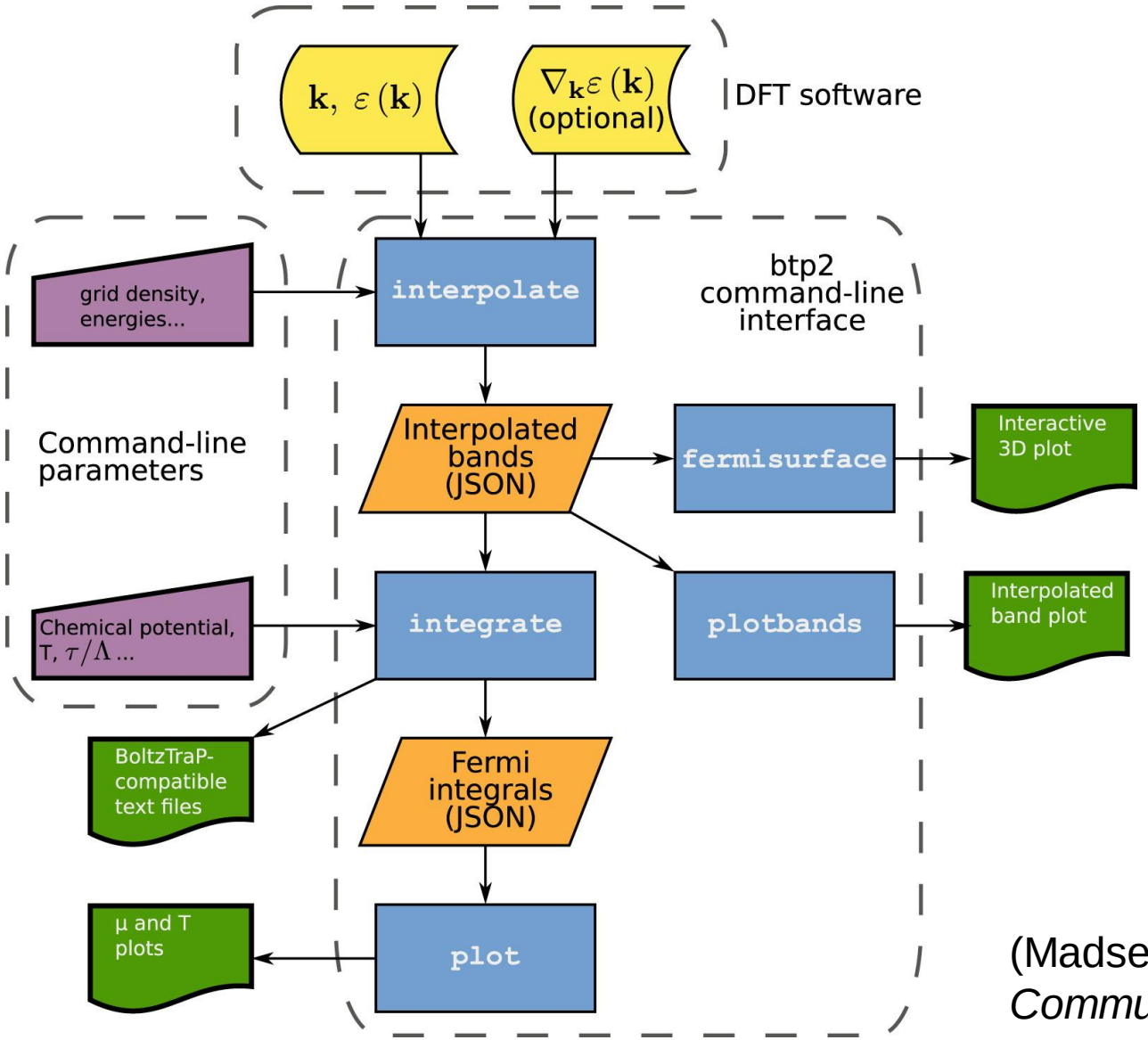
Required: NumPy, SciPy, matplotlib, spglib, NetCDF4 and ASE

Optional: pyFFTW, VTK, colorama

Compile and install:

From pip: pip install BoltzTraP2
From source package: python setup.py install

Workflow



(Madsen et al, *Computer Physics Communications*, 2018)

Commands

1. Getting help

btp2 -h

btp2 interpolate -h

2. Interpolating the band energies

Input: vasprun.xml, IBZKPT

btp2 -vv interpolate -o PbTe.bt2 -e -0.4 -E 0.4 -m 10 ${PBS_O_WORKDIR}

Output: xxx.bt2

Commands

3. Computing the transport coefficients

Input: xxx.bt2

btp2 -vv integrate -p PbTe PbTe.bt2 300:1000:50

Output: xxx.btj, xxx.condtens, xxx.halltens, and xxx.trace

column	1	2	3	4	5	6	7	8	9	10
quantity	μ	T	N	$n(\mu)$	S	σ/τ	R_H	κ^0	c	χ
unit	Ry	K	e/uc	e/uc	V/K	$1/(\Omega$ m s)	m^3/C	W/(m K s)	J/(mol K)	m^3/mol

Example

Show: Call BoltzTraP2 from python script

Thanks