

# Thermoelectricity: From Atoms to Systems

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Week 2: Thermoelectric Transport Parameters

Lecture 2.7: **Using full band dispersions (ex. of  $\text{Bi}_2\text{Te}_3$ )**  
**Bonus Lecture**

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## Why use full band dispersions of materials?

- 1) Extract meaningful and reliable parameters.
- 2) Predict the properties of new materials, where little or no experimental data is available.

# Bonus lecture: outline

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Work through an example of how to extract the TE properties using full band dispersions (case of  $\text{Bi}_2\text{Te}_3$ ).

- 1) Review of TE equations
- 2) Number of modes (electron & phonon)
- 3) Electronic TE properties (electrical conductivity, Seebeck, electronic thermal conductivity)
- 4) Lattice thermal conductivity

# review: TE equations

electrical current:

$$E_x = \rho J_x + S \frac{dT}{dx}$$

heat current:

$$J_{Qx} = \pi J_x - (\kappa_e + \kappa_L) \frac{dT}{dx}$$

Differential lattice thermal conductivity

$$\kappa_L = \int_0^{+\infty} \kappa'_L(\hbar\omega) d(\hbar\omega)$$

**Phonons**

$$\sigma = \int_{-\infty}^{+\infty} \sigma'(E) dE \quad \rho = \frac{1}{\sigma}$$

Differential electrical conductivity

$$S = \frac{-\frac{1}{qT} \int_{-\infty}^{+\infty} (E - E_F) \sigma'(E) dE}{\int_{-\infty}^{+\infty} \sigma'(E) dE} \quad \pi = TS$$

$$\kappa_0 = \frac{1}{q^2 T} \int_{-\infty}^{+\infty} (E - E_F)^2 \sigma'(E) dE$$

$$\kappa_e = \kappa_0 - T \sigma S^2$$

**Electrons**

# review: differential conductivity

## Boltzmann approach

$$\sigma'(E) = q^2 \Sigma_{\text{el}}(E) \left[ -\frac{\partial f}{\partial E} \right] \quad \kappa'_L(\hbar\omega) = \frac{(\hbar\omega)^2}{T} \Sigma_{\text{ph}}(\hbar\omega) \left[ -\frac{\partial n}{\partial(\hbar\omega)} \right]$$

Transport distribution

$$\Sigma(E) = \frac{1}{\Omega} \sum_{\vec{k}} \left[ v_x(\vec{k}) \right]^2 \tau(\vec{k}) \delta(E - E_{\vec{k}}) \longrightarrow \Sigma(E) = \frac{1}{h} M(E) \lambda(E)$$

Transport distribution has clear physical interpretation, the product of:

- ✓ Number of modes (*depends only on dispersion, easy to extract*).
- ✓ Mean-free-path for backscattering (*depends on scattering physics and dispersion*).

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# number of modes: definition

$$M_{3D}(E) = \frac{1}{A} \sum_{\vec{k}_{\perp}, n^+} \Theta(E - E_{\vec{k}_{\perp}})$$

Number of conducting channels per cross sectional area  $A$ , units:  $\text{m}^{-2}$

Sum over k-points  
in the plane  
perpendicular to  
transport

Sum over all bands  
or branches with  
positive velocity

Heaviside function: If the  
band has a state at energy  $E$ ,  
assign one mode

- ✓ Number of modes is easy to calculate !
- ✓ “Band counting” is an efficient approach to extract  $M(E)$ .

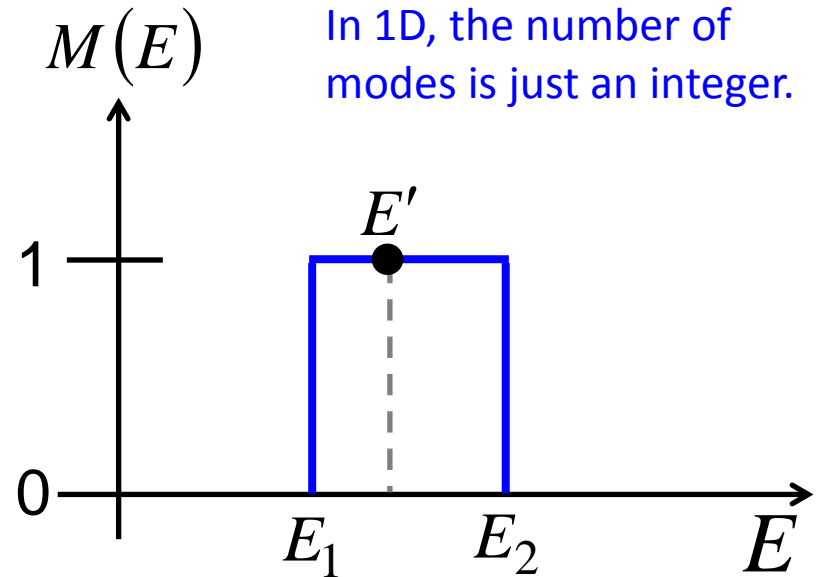
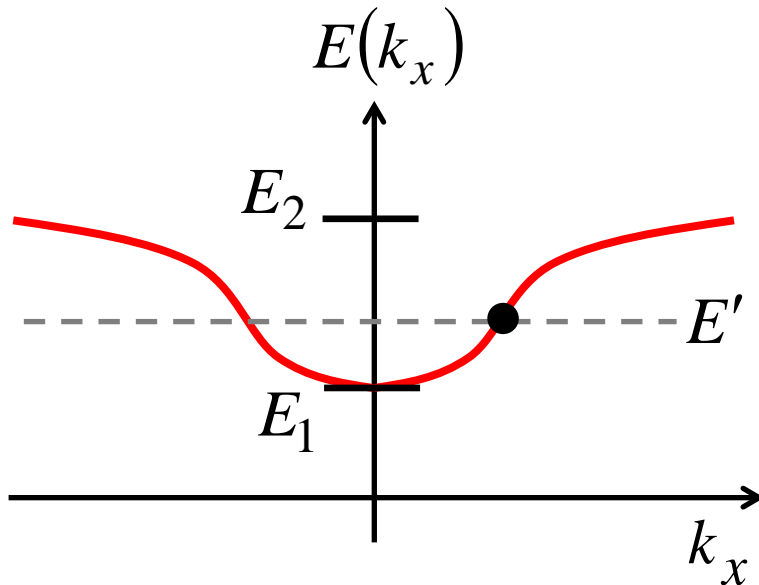
*Demonstrate approach with two simple examples  
(1D and 2D cases)*



# number of modes: 1D example

$$M_{1D}(E) = \sum_{n^+} \Theta(E - E_0)$$

Transport along x, no periodicity  
along y and z, units:  $m^{-d+1} = m^0$



In 1D, the number of  
modes is just an integer.

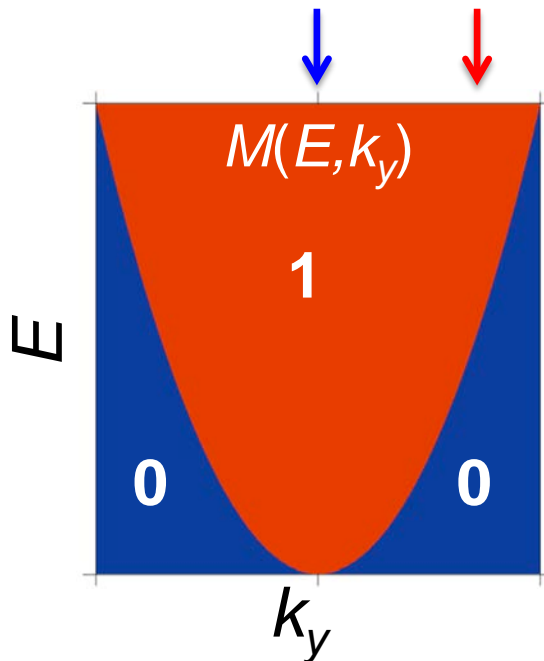
Reference: Jeong, Kim, Luisier, Datta, Lundstrom, J. Appl. Phys. **107**, 023707 (2010).



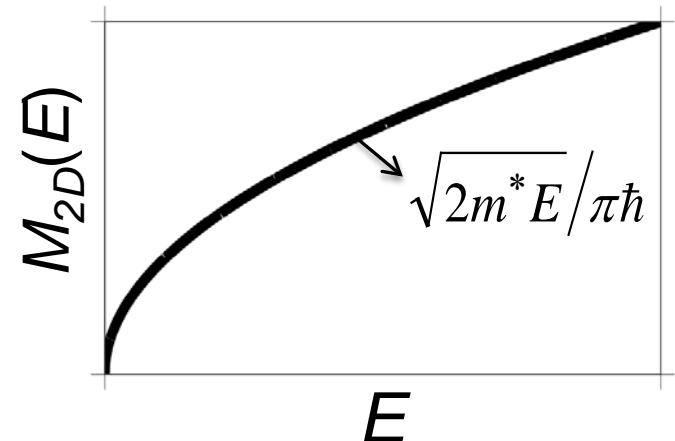
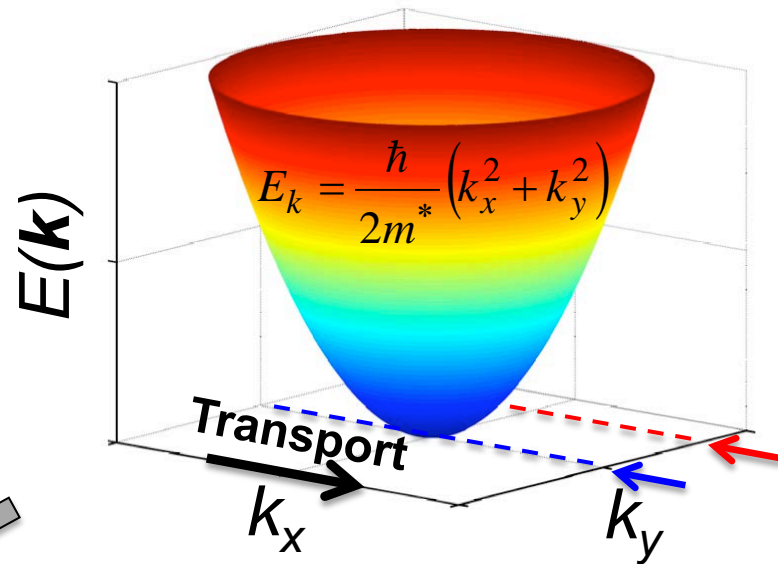
# number of modes: 2D example

$$M_{2D}(E) = \frac{1}{2\pi} \int \sum_{n^+} \Theta(E - E_{k_y}) dk_y$$

Transport along x, periodicity  
along y, units:  $m^{-d+1} = m^{-1}$



(Same as 1D  
example, but  
for each  $k_y$ .)



# number of modes: effect of dimensionality

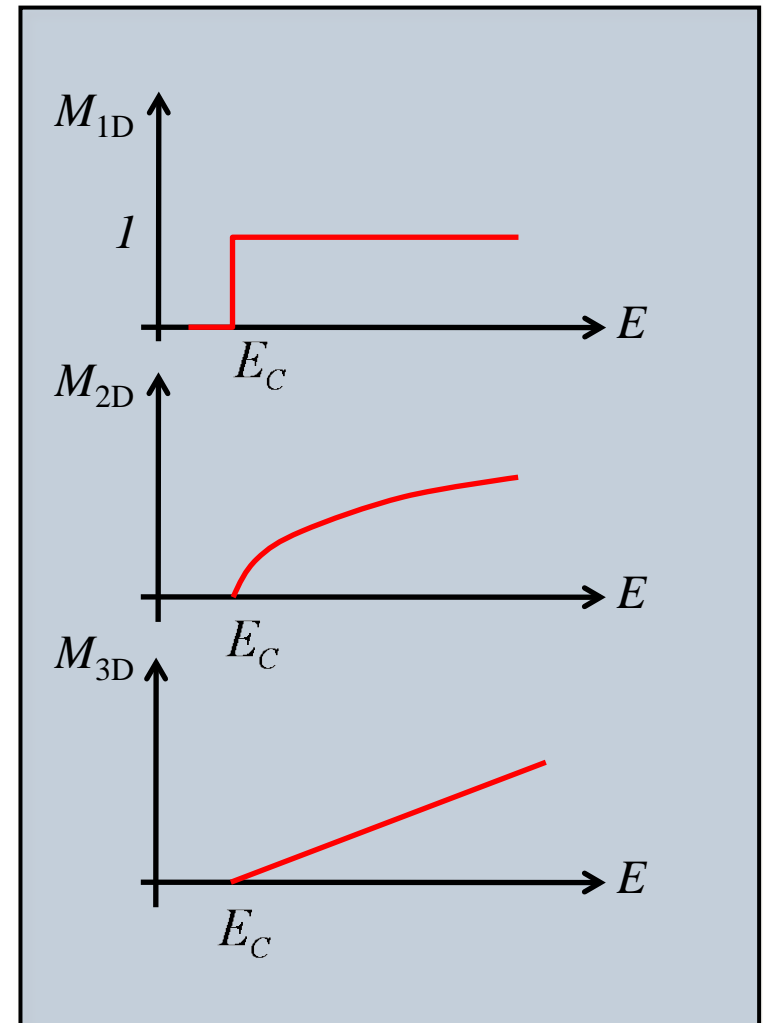
## Parabolic bands

$$M(E) = M_{1D}(E) = \Theta(E - E_C)$$

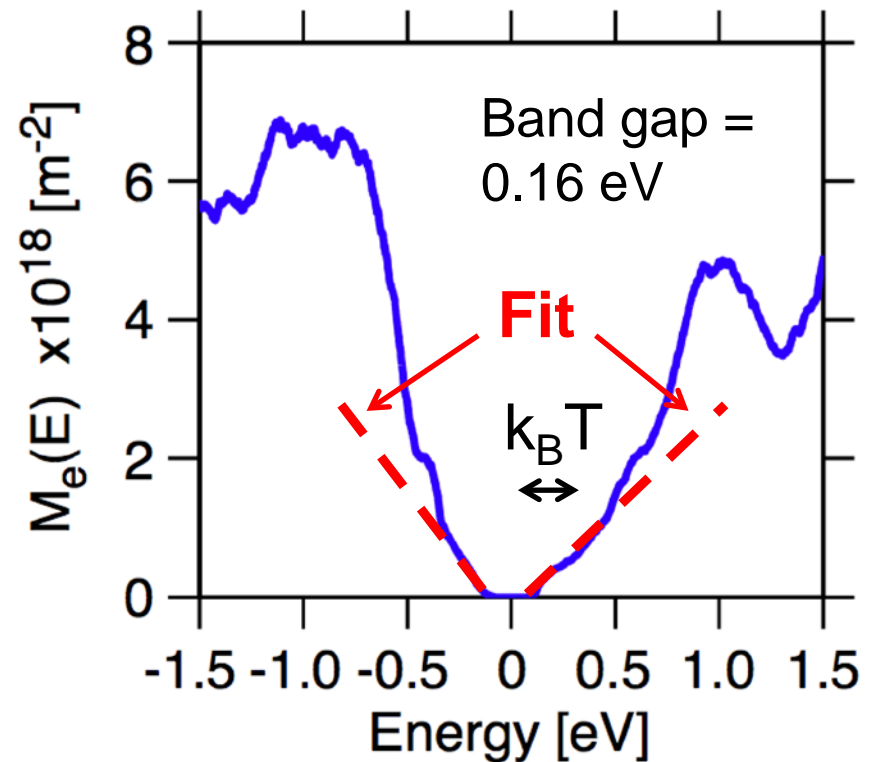
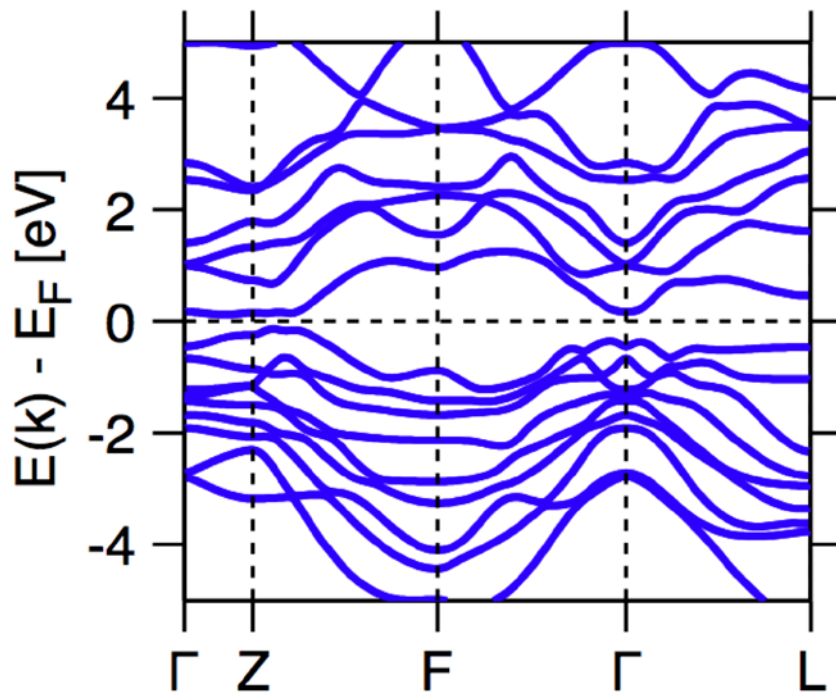
$$M(E) = W M_{2D}(E) = W \frac{\sqrt{2m^*(E - E_C)}}{\pi \hbar}$$

$$M(E) = A M_{3D}(E) = A \frac{m^*(E - E_C)}{2\pi \hbar^2}$$

$$E(\vec{k}) = E_C + \hbar^2 k^2 / 2m^*$$

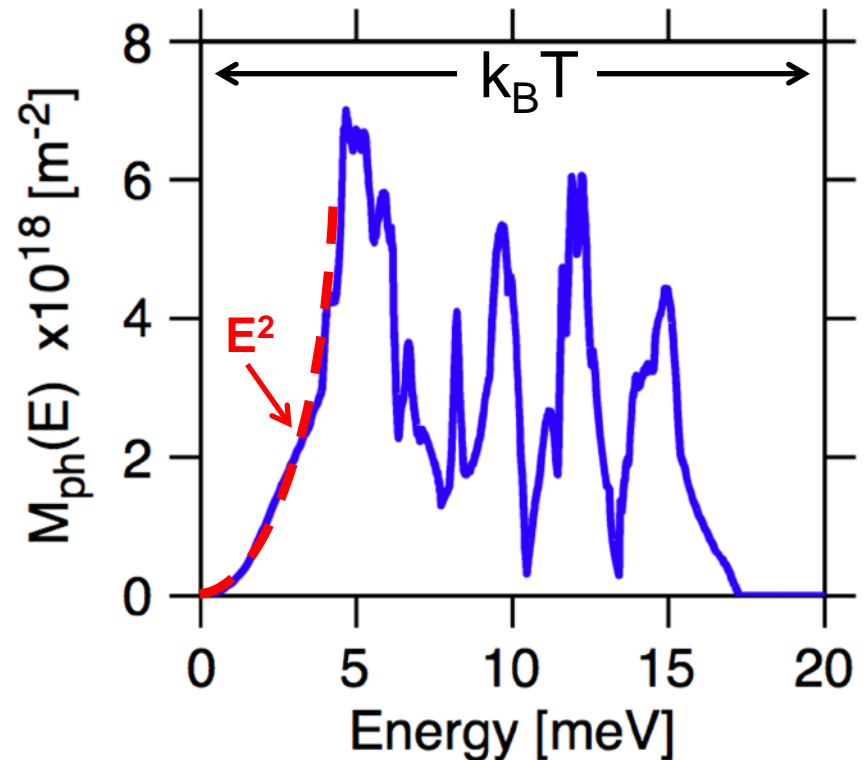
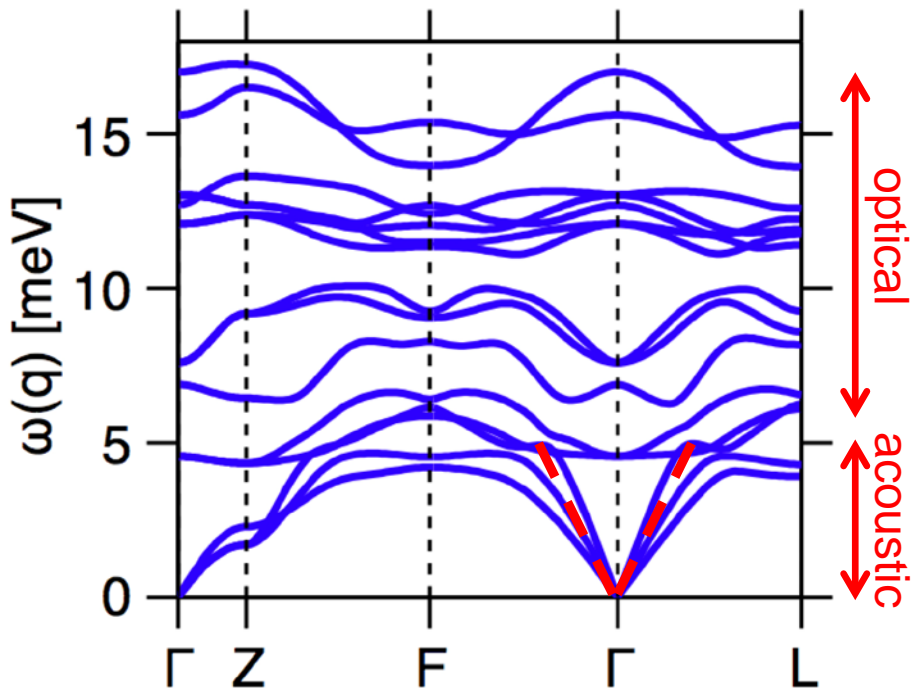


## number of modes: $\text{Bi}_2\text{Te}_3$ (electron)



- Complicated band structure.
- Not well represented by the parabolic band approximation.
- Roughly fit by a straight line near band edges (i.e. parabolic band approx.).
- Surprising given the non-parabolic  $E(k)$ .
- Only small fraction of modes are thermally active.

## number of modes: $\text{Bi}_2\text{Te}_3$ (phonon)



- Complicated band structure.
- Not well represented by simple dispersion model.
- At low energy, modes fit well with quadratic function (i.e. Debye model).
- At room temperature all modes are thermally active.

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Work through an example of how to extract the TE properties using full band dispersions (case of  $\text{Bi}_2\text{Te}_3$ ).

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- 4) Lattice thermal conductivity

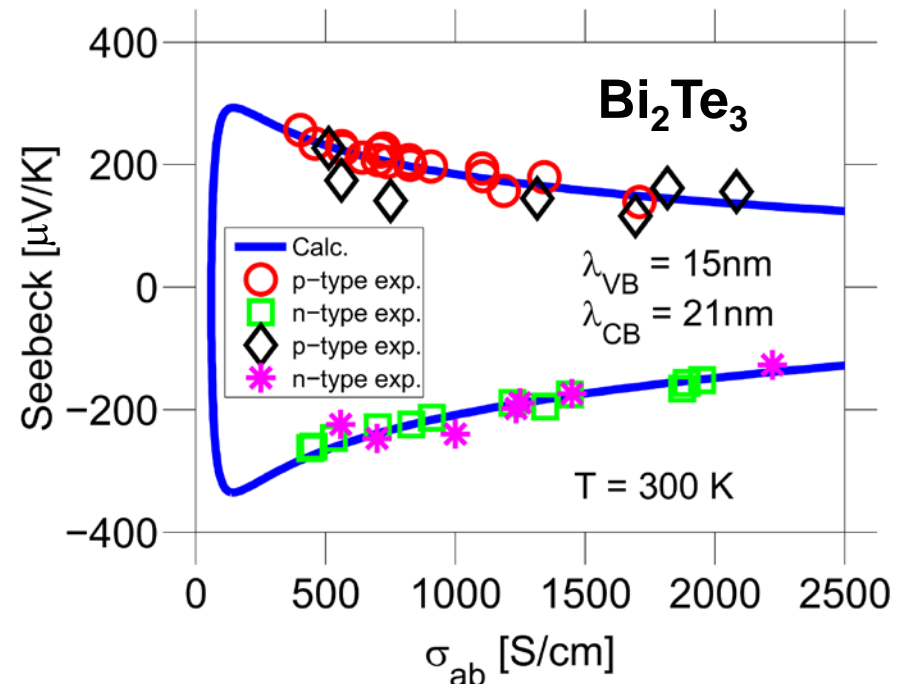
# electronic TE properties

$$\sigma'(E) = \frac{2q^2}{h} M_{\text{el}}(E) \lambda_{\text{el}}(E) \left[ -\frac{\partial f}{\partial E} \right]$$

Central quantity to calculate the electronic TE coefficients

Mean-free-path for backscattering

- A constant MFP is reasonable in many cases (exact when assuming parabolic bands and electron-phonon scattering\*).
- Calibrate MFP to experimental data:  $\longrightarrow$
- Can calculate MFP, but can be difficult.

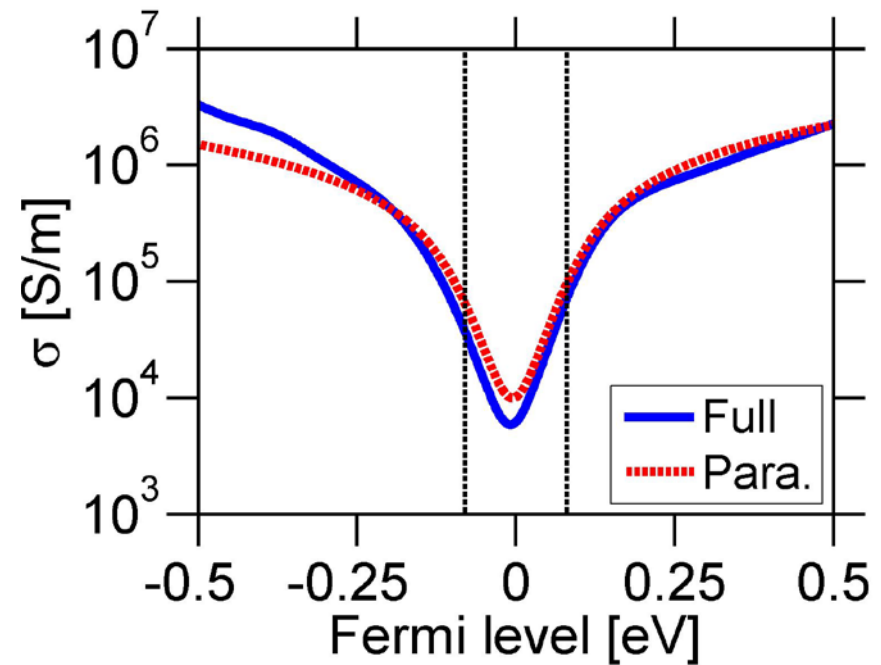
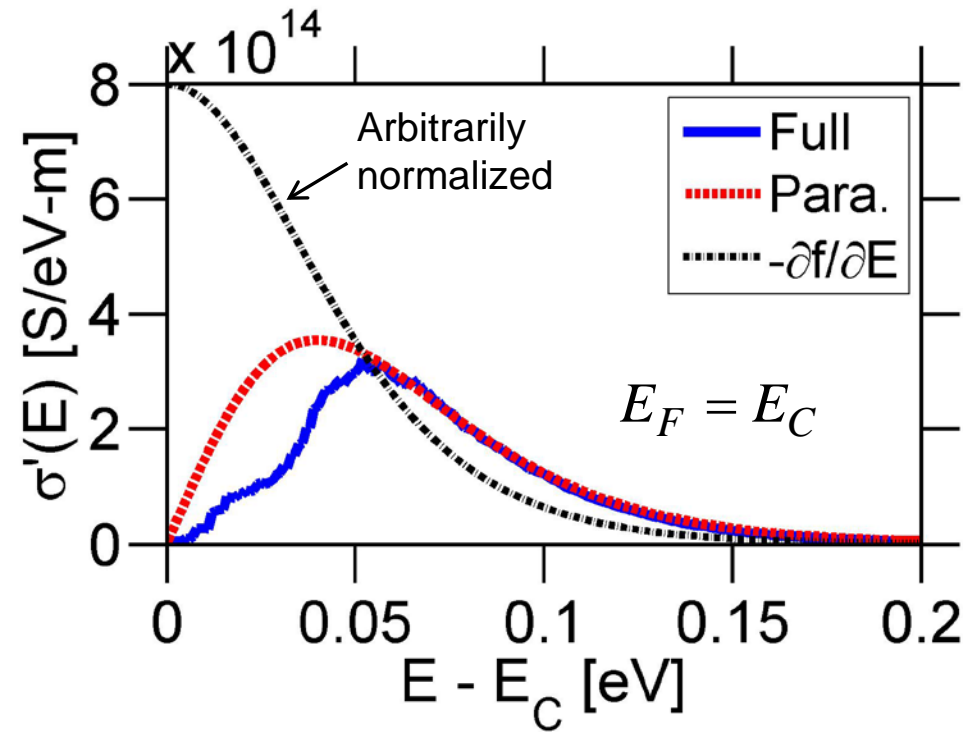


\*Mark Lundstrom, *Fundamentals of Carrier Transport*, Cambridge University Press, 2000.

# electronic TE properties: *conductivity*

$$\sigma'(E) = \frac{2q^2}{h} M_{\text{el}}(E) \lambda_{\text{el}}(E) \left[ -\frac{\partial f}{\partial E} \right]$$

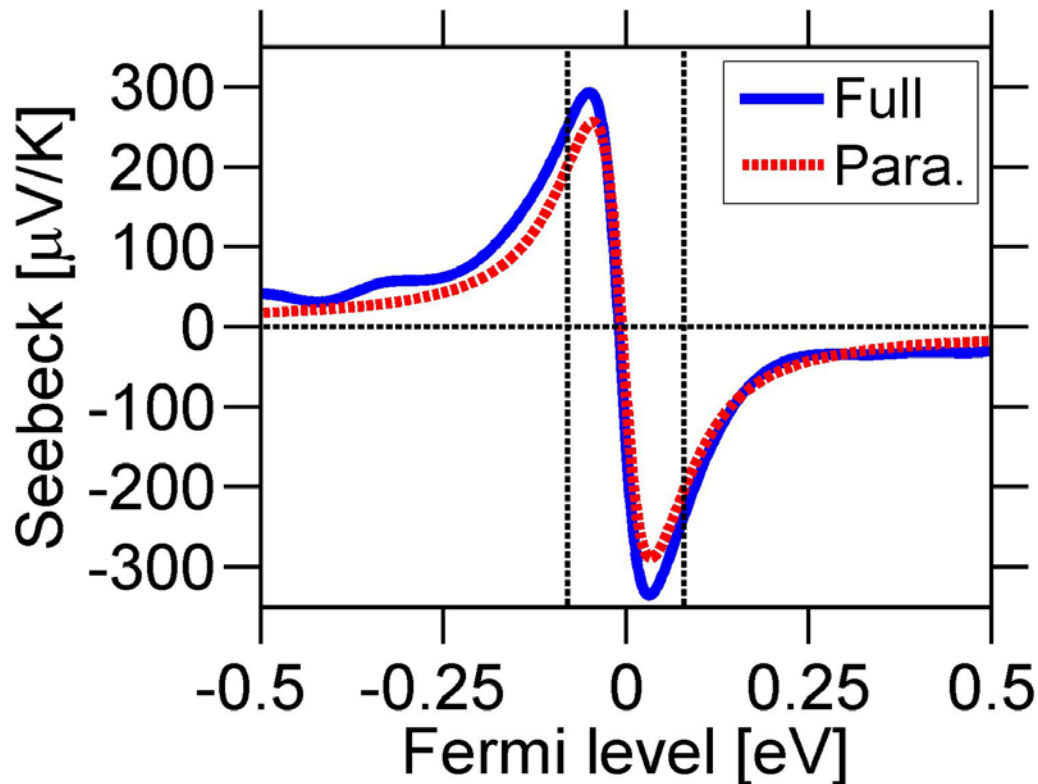
$$\sigma = \int_{-\infty}^{+\infty} \sigma'(E) dE$$



**$\text{Bi}_2\text{Te}_3$**

# electronic TE properties: *Seebeck*

$$S = -\frac{1}{qT} \int_{-\infty}^{+\infty} (E - E_F) \sigma'(E) dE \bigg/ \int_{-\infty}^{+\infty} \sigma'(E) dE$$

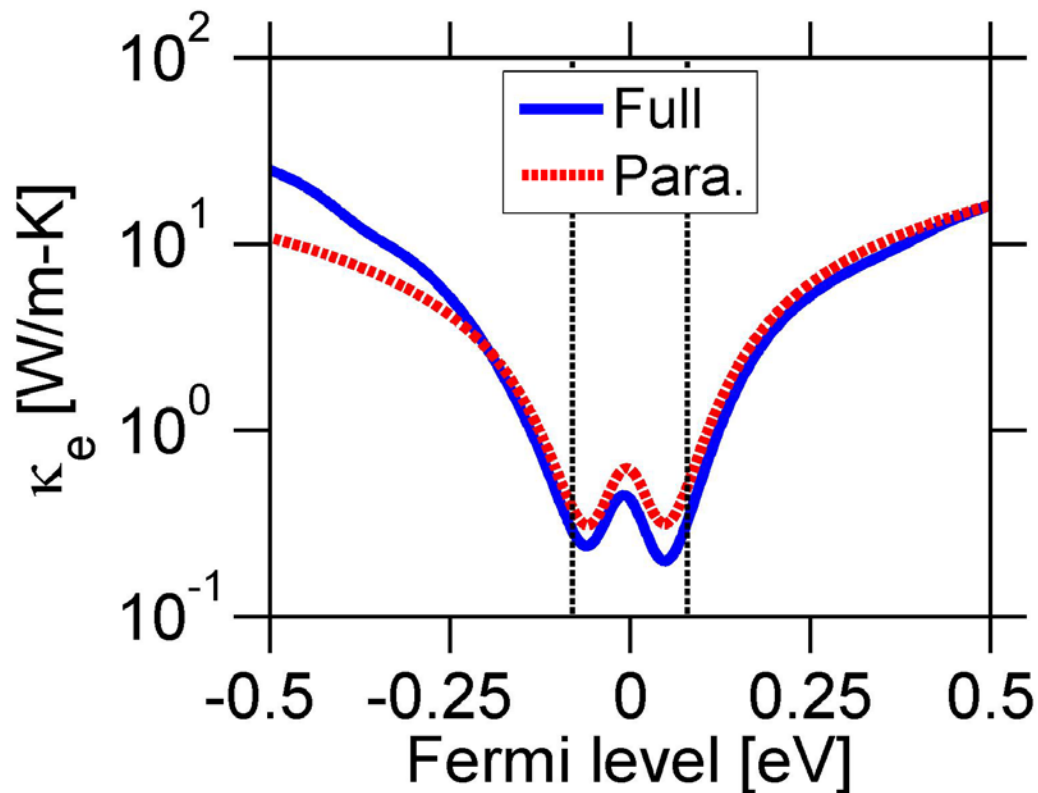


**$\text{Bi}_2\text{Te}_3$**



# electronic TE properties: *thermal conductivity*

$$\kappa_e = \frac{1}{q^2 T} \int_{-\infty}^{+\infty} (E - E_F)^2 \sigma'(E) dE - T \sigma S^2$$



**Bi<sub>2</sub>Te<sub>3</sub>**

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# Bonus lecture: outline

$$\kappa'_L(\hbar\omega) = \frac{(\hbar\omega)^2}{hT} M_{\text{ph}}(\hbar\omega) \lambda_{\text{ph}}(\hbar\omega) \left[ -\frac{\partial n}{\partial(\hbar\omega)} \right] \quad \kappa_L = \int_0^\infty \kappa'_L(\hbar\omega) d(\hbar\omega)$$

Mean-free-path for backscattering

- Typical scattering mechanisms for phonons\*:
  - ✓ Umklapp scattering (phonon-phonon)
  - ✓ Boundary scattering
  - ✓ Defect scattering
- Calibrate MFP to experimental data (next slide).
- Calculate MFP, but can be difficult.

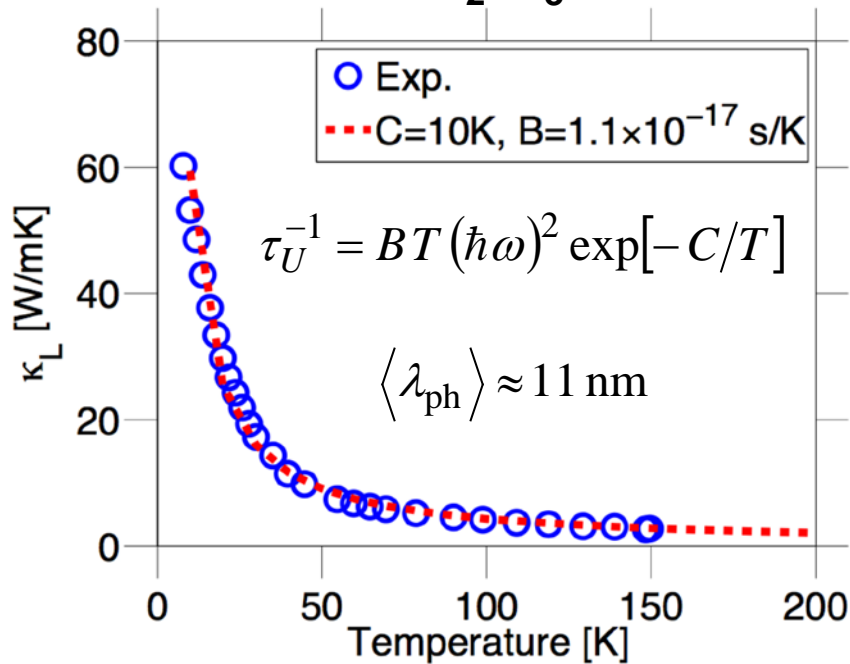
$$\lambda = 2 \frac{\langle v_x^2 \rangle}{\langle |v_x| \rangle} \tau$$
$$\tau^{-1} = \tau_1^{-1} + \tau_2^{-1} + \dots$$

\*Jeong, Datta, Lundstrom, J. Appl. Phys. **109**, 073718 (2011).

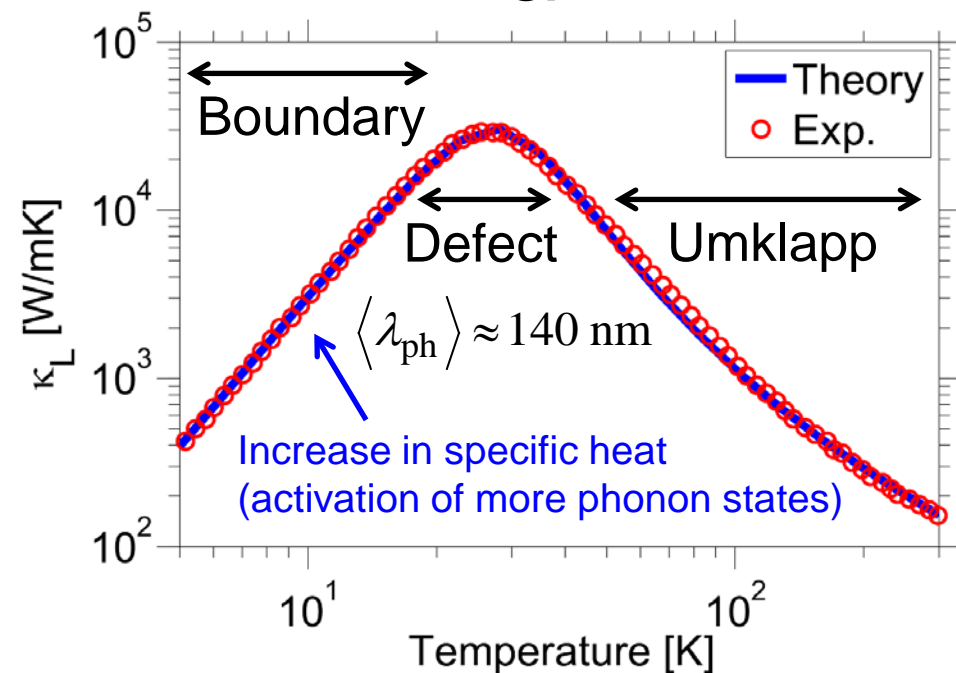
# lattice thermal conductivity: *calibrate MFP*

$$\kappa'_L(\hbar\omega) = \frac{(\hbar\omega)^2}{hT} M_{\text{ph}}(\hbar\omega) \lambda_{\text{ph}}(\hbar\omega) \left[ -\frac{\partial n}{\partial(\hbar\omega)} \right] \quad \kappa_L = \int_0^\infty \kappa'_L(\hbar\omega) d(\hbar\omega)$$

**Bi<sub>2</sub>Te<sub>3</sub>**



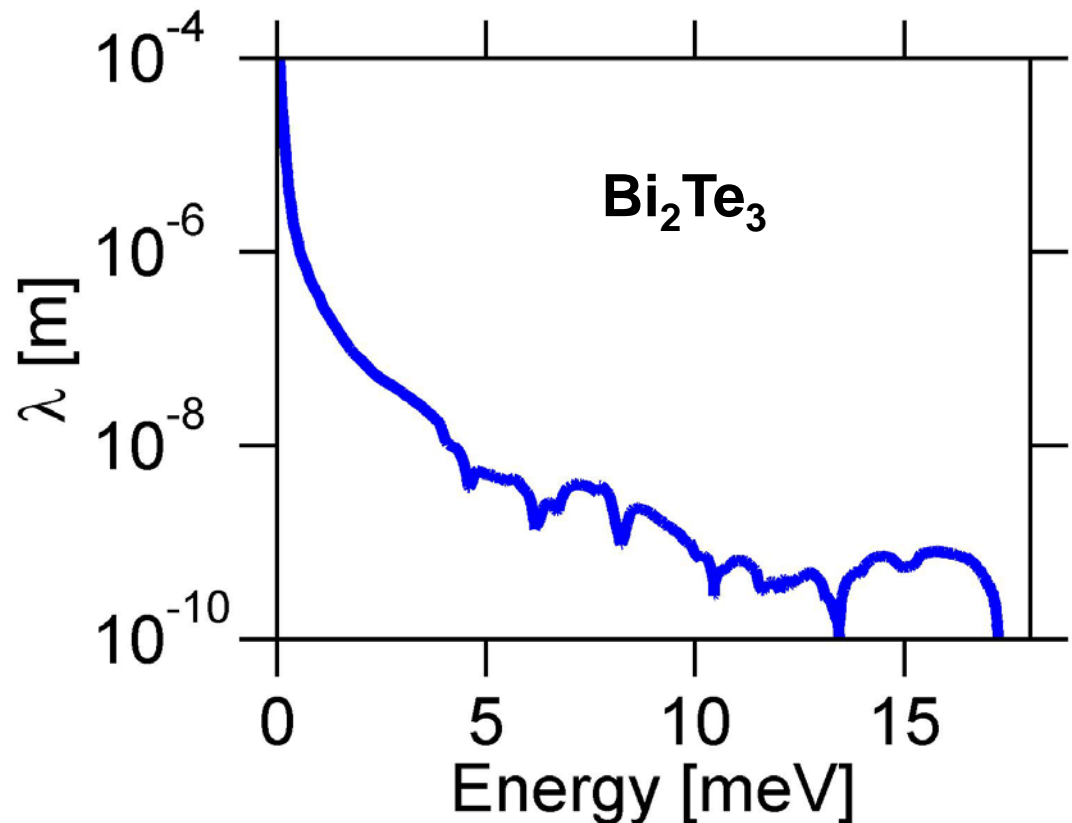
**Si**



# lattice thermal conductivity: *energy-dep. MFP*

$$\kappa'_L(\hbar\omega) = \frac{(\hbar\omega)^2}{hT} M_{\text{ph}}(\hbar\omega) \lambda_{\text{ph}}(\hbar\omega) \left[ -\frac{\partial n}{\partial(\hbar\omega)} \right] \quad \kappa_L = \int_0^\infty \kappa'_L(\hbar\omega) d(\hbar\omega)$$

- The MFP of phonons can vary by many orders of magnitude.
- In stark contrast to the case of electrons, where the MFP is well approximated by a constant.



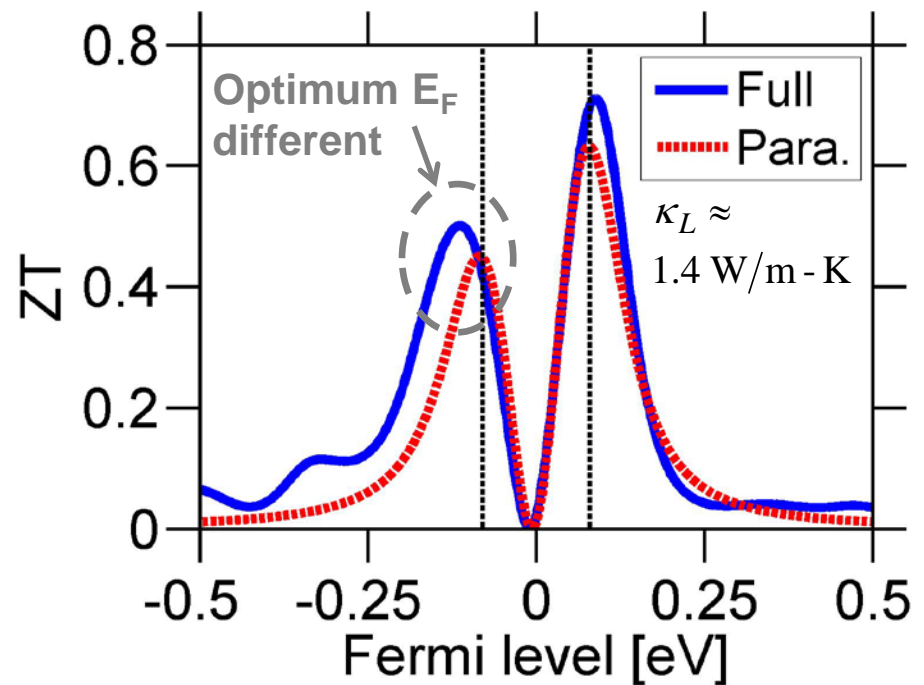
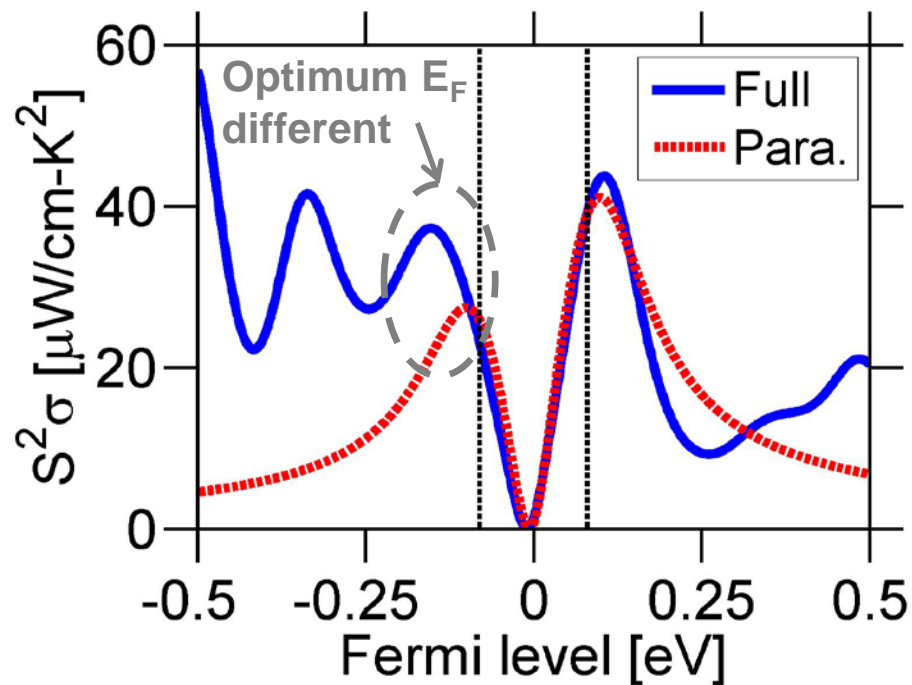
# TE performance of $\text{Bi}_2\text{Te}_3$

Combine electronic and lattice TE properties to determine TE performance metrics:

Power factor ( $S^2\sigma$ )

Features not present with simple model !

Figure of merit,  $ZT = S^2\sigma T / (\kappa_e + \kappa_L)$



# summary: TE properties from full band approach

- Full dispersion-based TE calculations, for electrons and phonons, are particularly useful for
  - ✓ Provide meaningful / accurate physical parameters
  - ✓ Studying / predicting the properties of novel material systems
- Within the Landauer approach, which readily spans ballistic-to-diffusive transport regimes, one needs two things:
  - ✓ **Number of modes:** easy to calculate from general dispersion using the “band counting” method.
  - ✓ **Mean-free-path (MFP) for backscattering:** can calibrate to exp. using phenomenological expressions (easy) or calculate from first principles (difficult).
- Realistic descriptions of TE materials are not always well represented by simple band dispersions. Valuable skill to calculate and predict the TE properties of materials with complex electronic states.

# summary: TE properties from full band approach

**LanTraP** tool available online  
on *nanoHUB*:

[nanohub.org/resources/lantrap](http://nanohub.org/resources/lantrap)

The screenshot shows the nanoHUB.org website. The header includes the nanoHUB.org logo, the text "an INCO project", and "ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY". There are 114 New Messages from Jesse Maassen. The navigation bar includes Home, Resources, Members, Explore, nanoHUB-U, Partners, About, and Support. Below the navigation bar, there is a breadcrumb trail: Home > Groups > NEEDS: Nano-Engineered Electronic Device Simulation Node > Resources > Tools > LanTraP > About. The main content area features the LanTraP logo, the text "By Kyle Conrad<sup>1</sup>, Jesse Maassen<sup>1</sup>, Mark Lundstrom<sup>1</sup>", and "1. Purdue University". A description states: "This tool calculates the distribution of modes, the electronic thermoelectric transport coefficients, and the lattice thermal transport properties from band structure information." There is a "Launch Tool" button and version information: "Version 1.0 - published on 18 Sep 2013", "doi:10.4231/D3FB4WM2X cite this", and "This tool is closed source." A link to "View All Supporting Documents" is also present. Below the main content, there is a tabbed interface with tabs for About, Usage, Citations, Questions, Reviews, Wishlist, Versions, and Supporting Docs. The Usage tab is selected, showing a preview of the tool's interface.

The screenshot shows the LanTraP tool interface with the "TE Options" tab selected. The interface includes a "Load Data" button, a "Modes Options" button, and a "Simulate" button. The "TE Options" section contains the following fields:

- Particle: Electron
- Temperature (K): 300K
- Transport type: Quasi-Ballistic
- Electron Options
  - Ef min (eV): -0.5eV
  - delta Ef (eV): 0.001eV
  - Ef Max (eV): 0.5eV
- Diffusive transport options
  - MFP CB (nm): 10
  - CB scattering parameter: 0
  - Conduction Band Minimum: 0eV
  - MFP VB (nm): 10
  - VB scattering parameter: 0
  - Valence Band Maximum: -1eV
  - Conductor Length (nm): 10

