Dragful electron-phonon transport -- `elphbolt` a year and a half on

Nakib H. Protik & friends

https://github.com/nakib/elphbolt

Unterstützt von / Supported by
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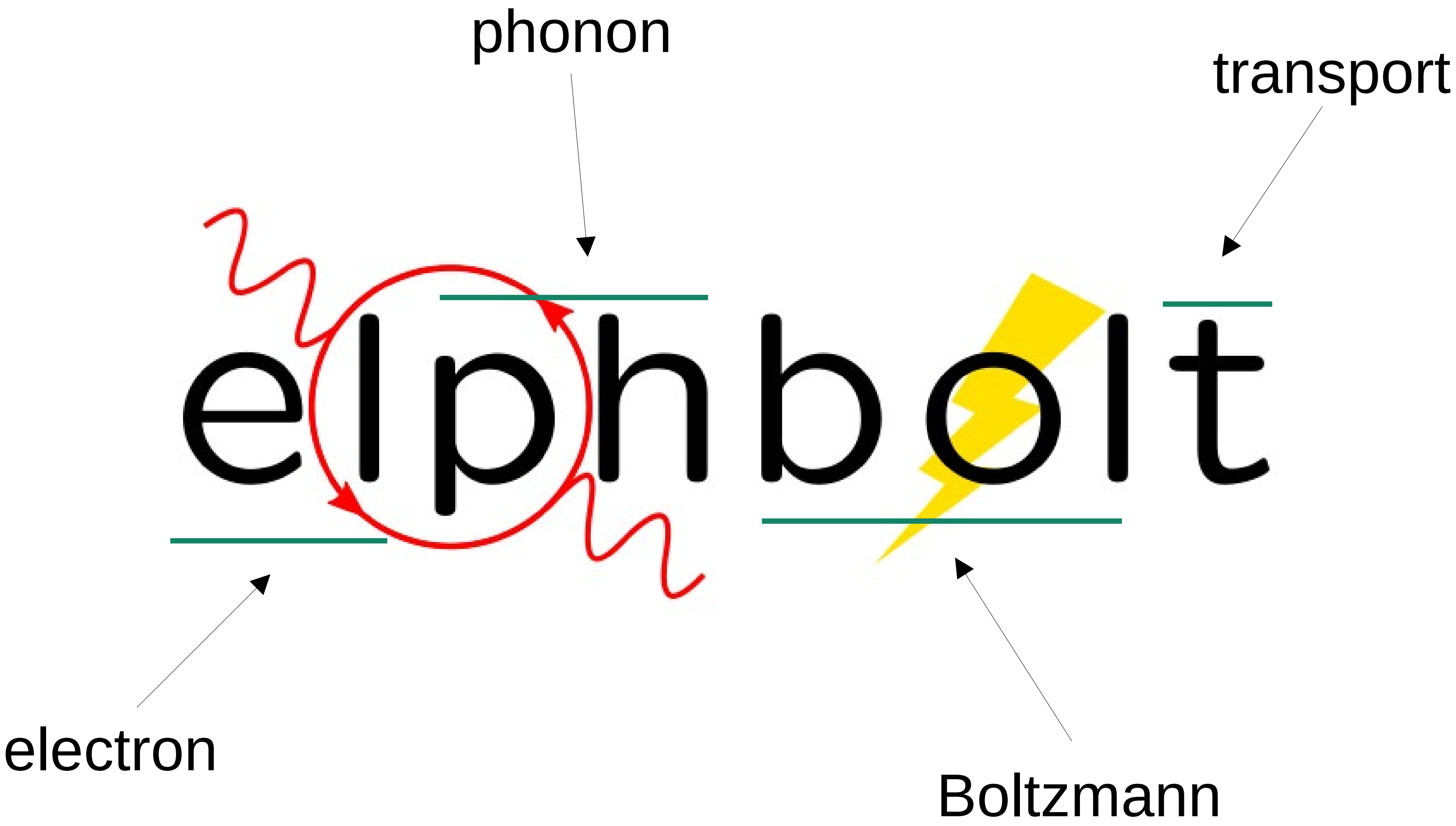

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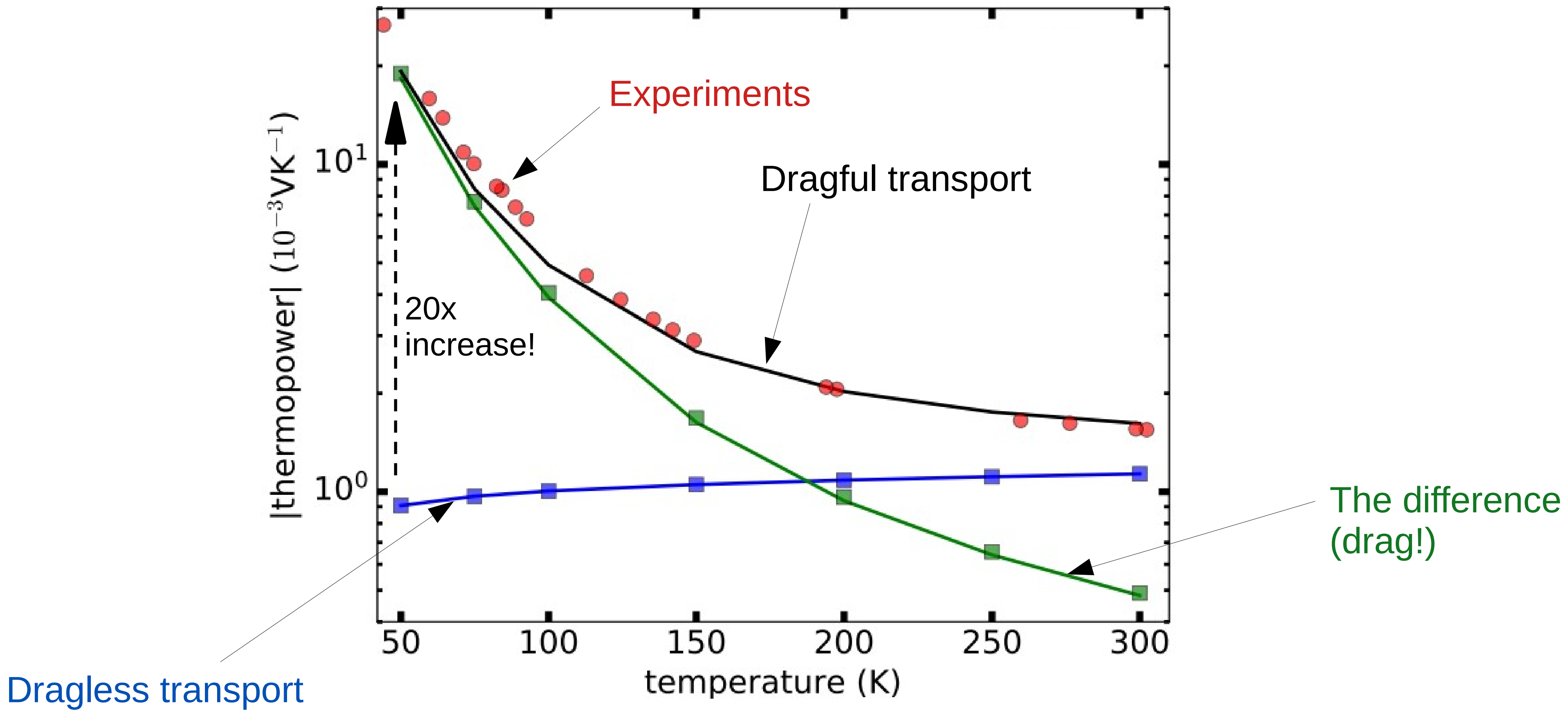
npj Computational Materials 8.1 (2022): 1-9.

Why dragful electron-phonon transport?

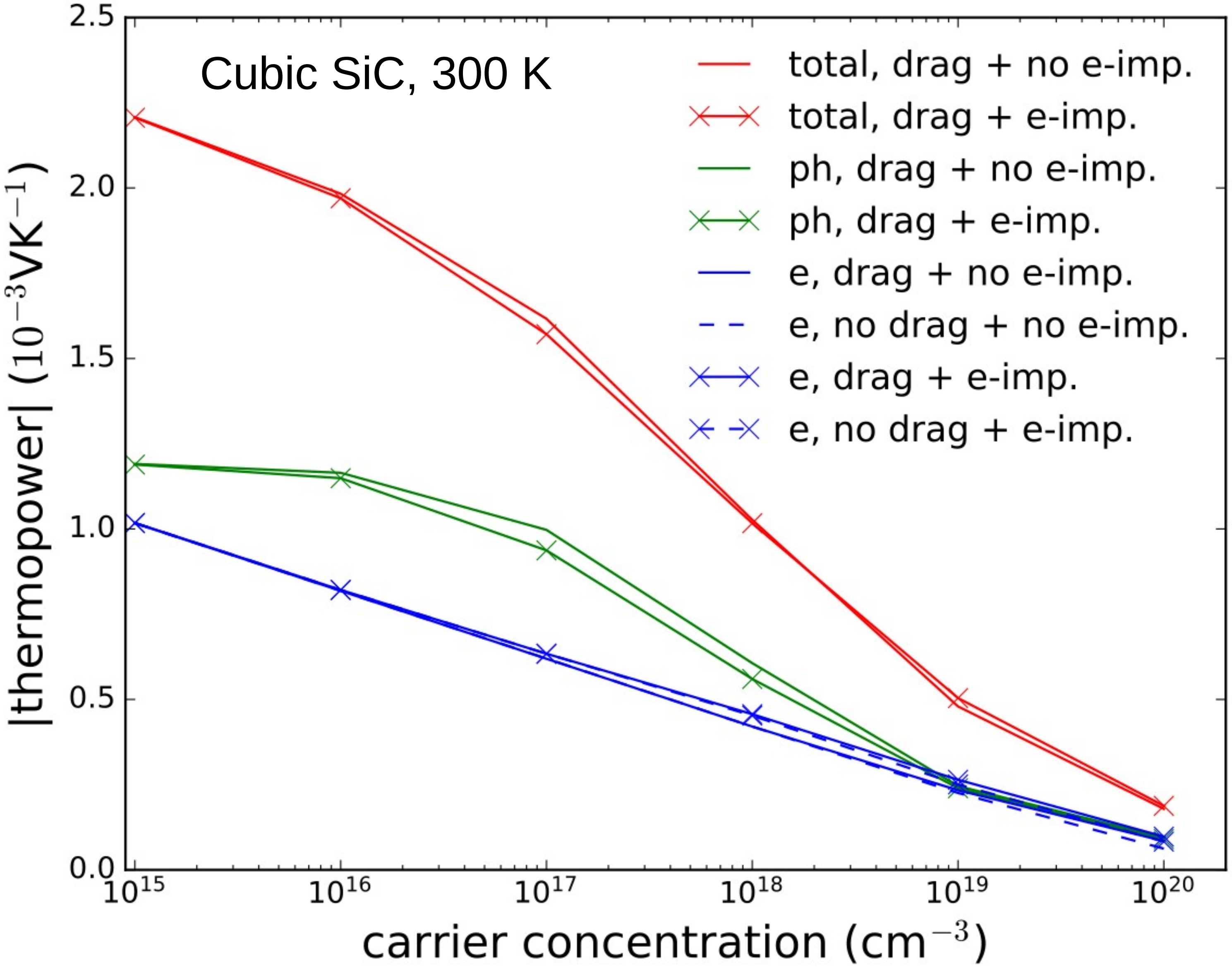
n-type (2.75e14 cm^{-3}) Si



Expt: Geballe & Hull, Phys. Rev. 98, 940 (1955)

Theory: npj Computational Materials 8.1 (2022): 1-9.

Why dragful electron-phonon transport?



NHP & Kozinsky, Phys. Rev. B 102, 245202 (2020)

Coupled electron-phonon Boltzmann transport

Distribution functions

Fermi-Dirac

Deviation of electron from equilibrium

Electron distribution $$f_{m\mathbf{k}} \approx f^0_{m\mathbf{k}} \left[1 + (1 - f^0_{m\mathbf{k}})\Psi_{m\mathbf{k}}\right]$$

Phonon distribution $$n_{s\mathbf{q}} \approx n^0_{s\mathbf{q}} \left[1 + (1 + n^0_{s\mathbf{q}})\Phi_{s\mathbf{q}}\right]$$

Bose-Einstein

Deviation of phonon from equilibrium

Linear response

Electron response to grad T

Electron response to E

Electron deviation
$$\Psi_{m\mathbf{k}} = -\beta \nabla T \cdot \mathbf{I}_{m\mathbf{k}} - \beta \mathbf{E} \cdot \mathbf{J}_{m\mathbf{k}}$$

Phonon deviation
$$\Phi_{s\mathbf{q}} = -\beta \nabla T \cdot \mathbf{F}_{s\mathbf{q}} - \beta \mathbf{E} \cdot \mathbf{G}_{s\mathbf{q}}$$

Phonon response to grad T

Phonon response to E
(How? Phonons are not charged!)
(Answer: Electron drag!)

Coupled e-ph BTEs (for homogeneous systems at steady state)

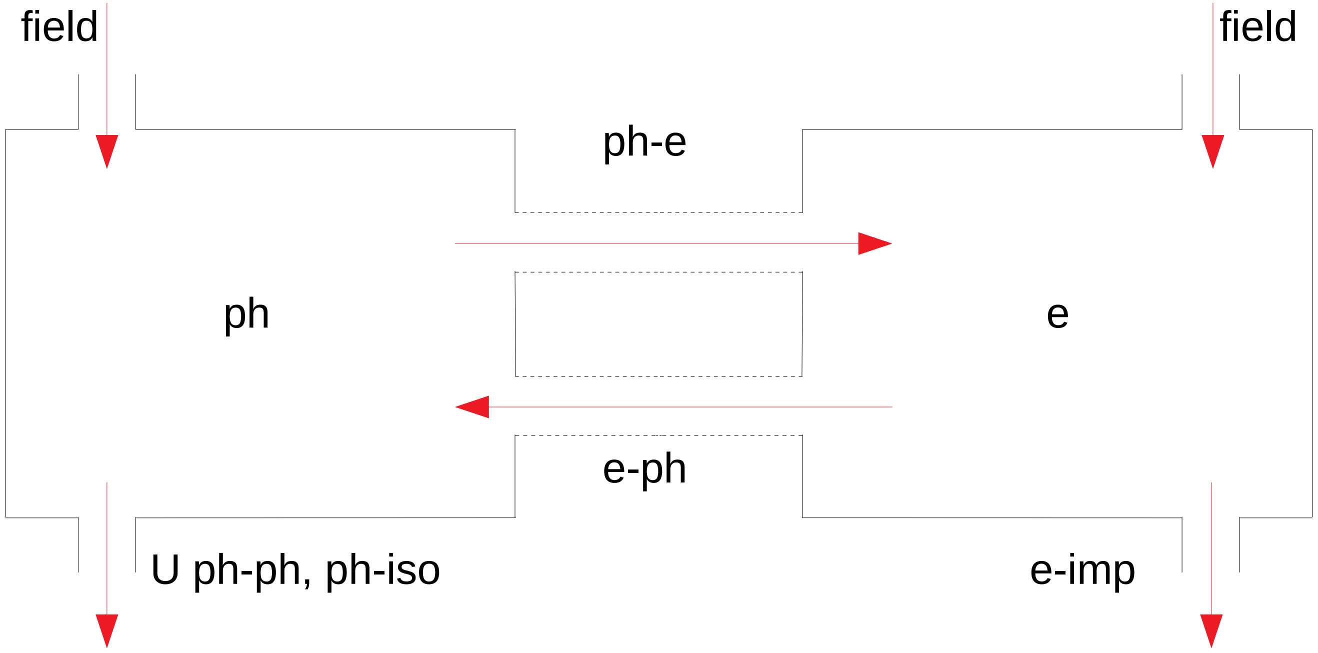
T gradient
- Electron response $$\mathbf{I} = \mathbf{I}^0 + \Delta\mathbf{I}^{\mathrm{S}}[\mathbf{I}] + \Delta\mathbf{I}^{\mathrm{D}}[\mathbf{F}]$$
- Phonon response $$\mathbf{F} = \mathbf{F}^0 + \Delta\mathbf{F}^{\mathrm{S}}[\mathbf{F}] + \Delta\mathbf{F}^{\mathrm{D}}[\mathbf{I}]$$

E field
- Electron response $$\mathbf{J} = \mathbf{J}^0 + \Delta\mathbf{J}^{\mathrm{S}}[\mathbf{J}] + \Delta\mathbf{J}^{\mathrm{D}}[\mathbf{G}]$$
- Phonon response $$\mathbf{G} = \mathbf{G}^0 + \Delta\mathbf{G}^{\mathrm{S}}[\mathbf{G}] + \Delta\mathbf{G}^{\mathrm{D}}[\mathbf{J}]$$

0

Boltzmann

Momentum flow diagram *a la* Herring

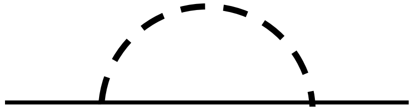


NHP and D. Broido. Phys. Rev. B 101.7 (2020): 075202.

Decoupled BTEs: Relaxation time approximation (RTA)

× **In-scattering correction**

× **Drag**



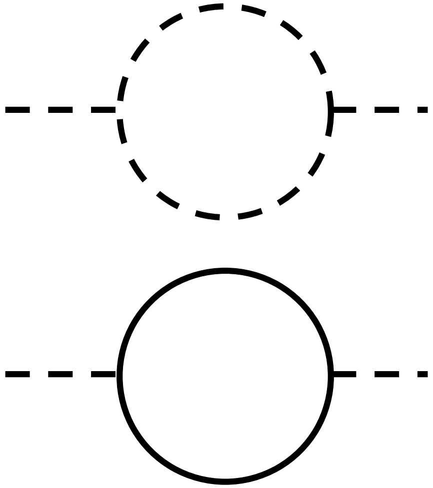
RTA

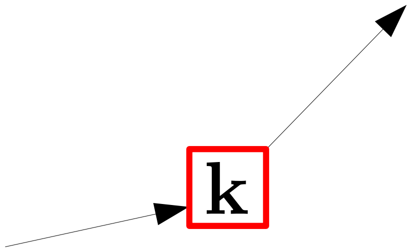
T gradient

Electron response $\mathbf{I} = \mathbf{I}^0$ [redacted]

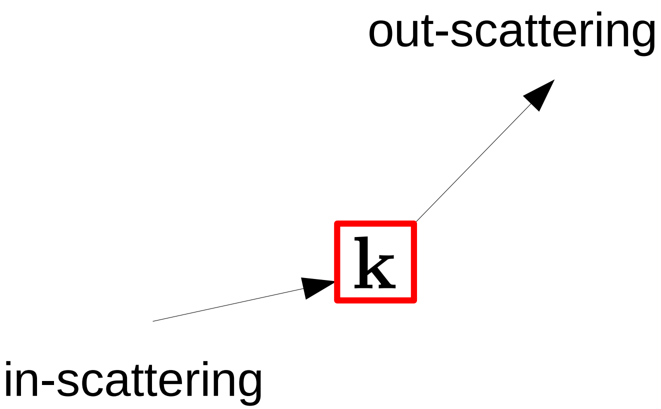
Phonon response $\mathbf{F} = \mathbf{F}^0$ [redacted]

RTA





Decoupled BTEs: full solution



✓ **In-scattering correction**

✕ **Drag**

Decoupled e-BTE (`EPW`, `PERTURBO`, etc.)

T gradient:

- Electron response: $\mathbf{I} = \mathbf{I}^0 + \Delta\mathbf{I}^{\mathrm{S}}[\mathbf{I}]$ [redacted]
- Phonon response: $\mathbf{F} = \mathbf{F}^0 + \Delta\mathbf{F}^{\mathrm{S}}[\mathbf{F}]$ [redacted]

Decoupled ph-BTE (`ShengBTE`, `AlmaBTE`, `phono3py`, etc.)

Coupled e-ph BTEs: full solution – state of the art

- You also get the simpler solutions *en route*!

✓ **In-scattering correction**

✓ **Drag**

elphbolt

Coupled BTEs

T gradient

- Electron response
- Phonon response

$$\mathbf{I} = \mathbf{I}^0 + \Delta\mathbf{I}^{\mathrm{S}}[\mathbf{I}] + \Delta\mathbf{I}^{\mathrm{D}}[\mathbf{F}]$$

$$\mathbf{F} = \mathbf{F}^0 + \Delta\mathbf{F}^{\mathrm{S}}[\mathbf{F}] + \Delta\mathbf{F}^{\mathrm{D}}[\mathbf{I}]$$

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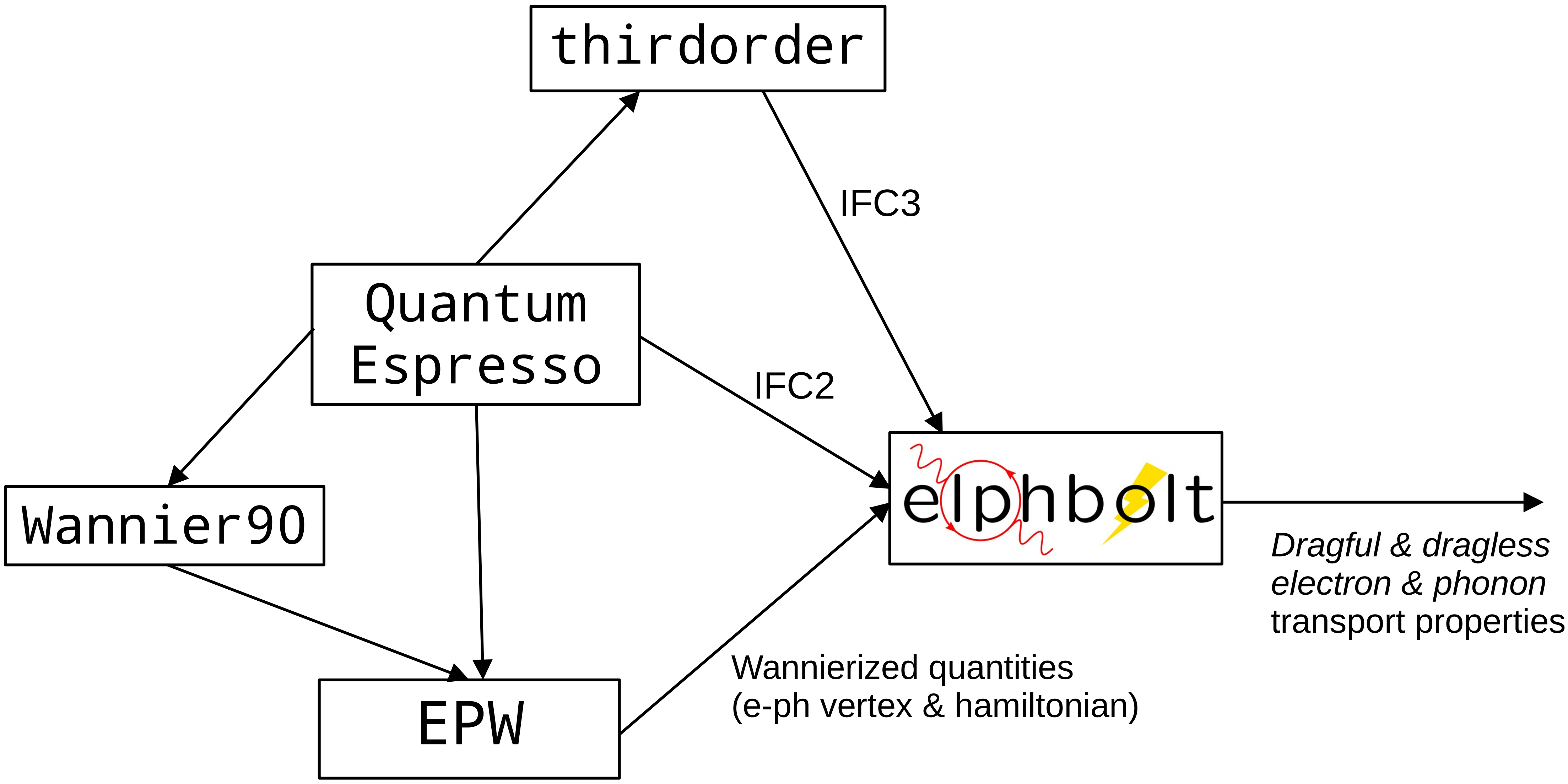
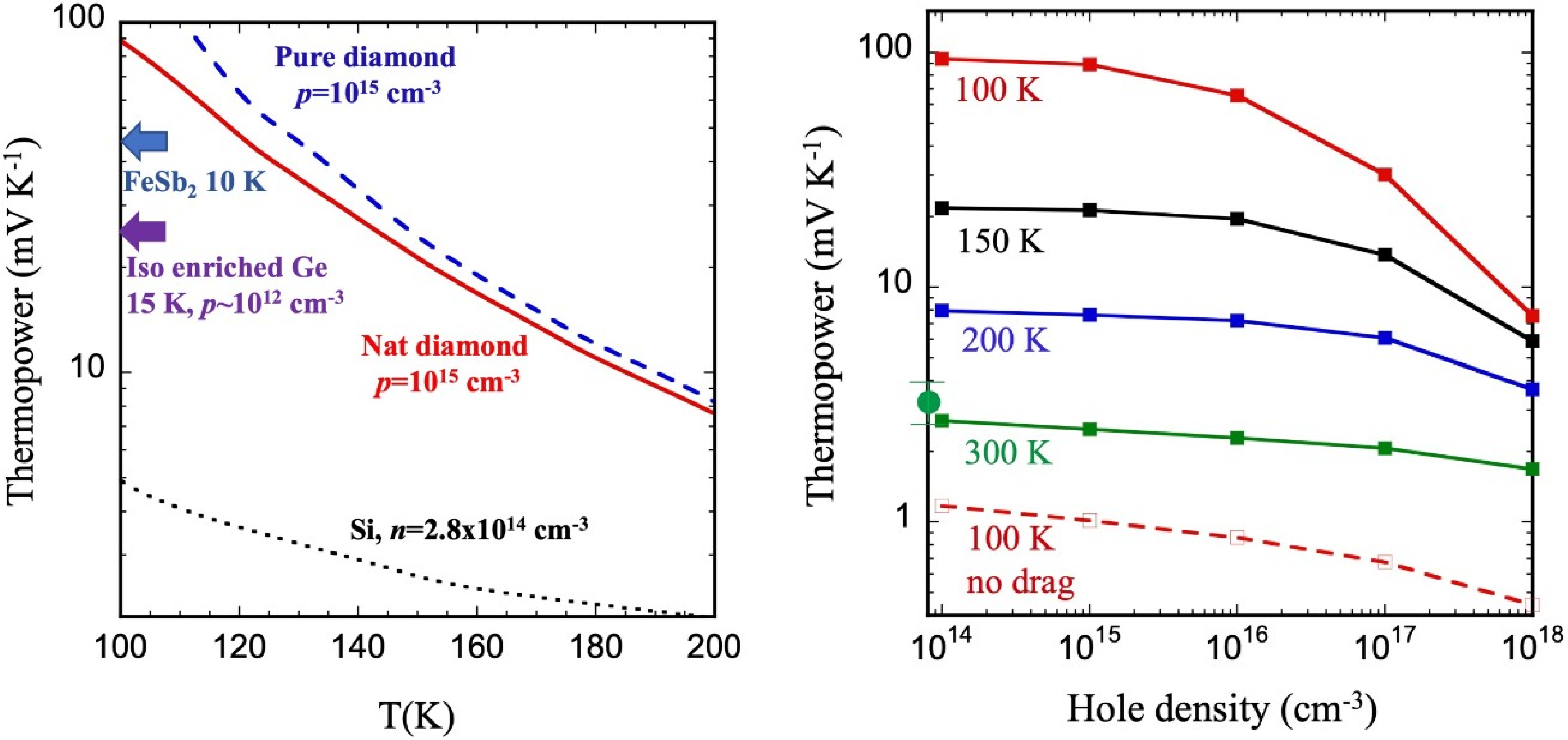
npj Computational Materials 8.1 (2022): 1-9.

elphbolt v1 workflow

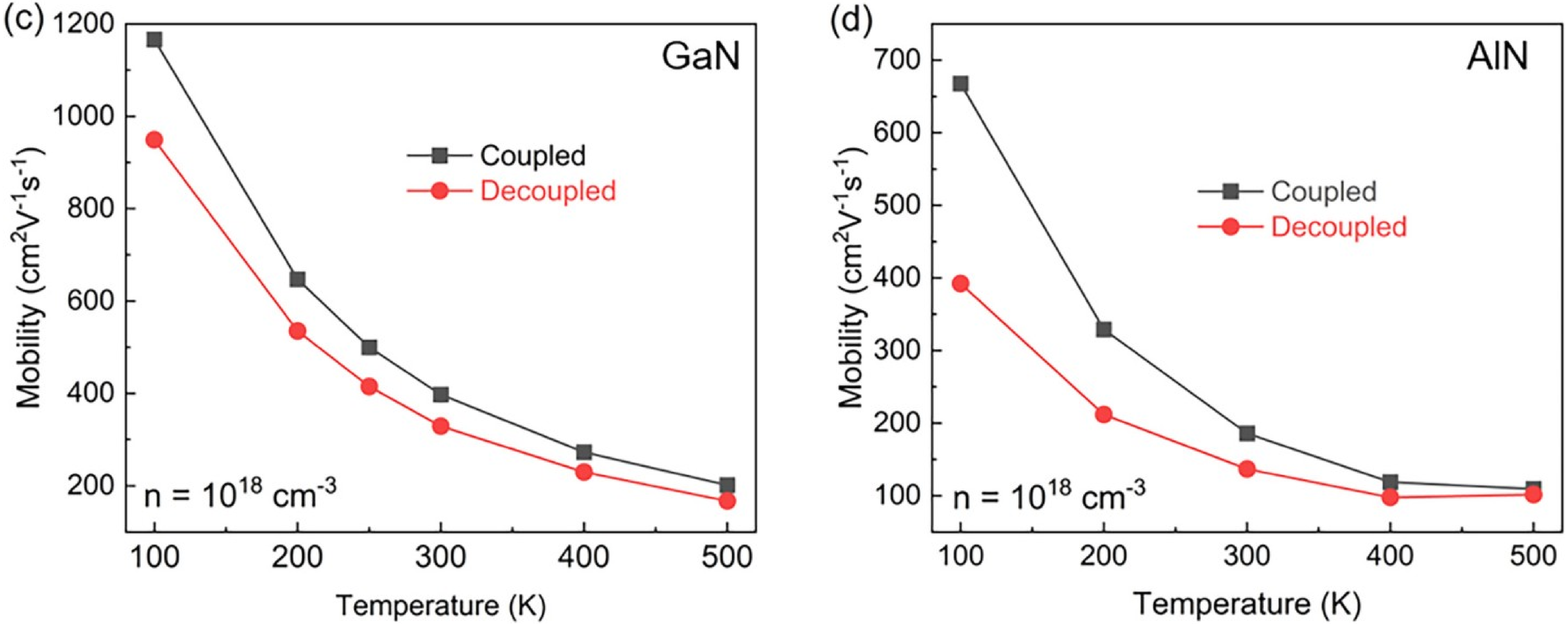


Colossal low T drag in diamond



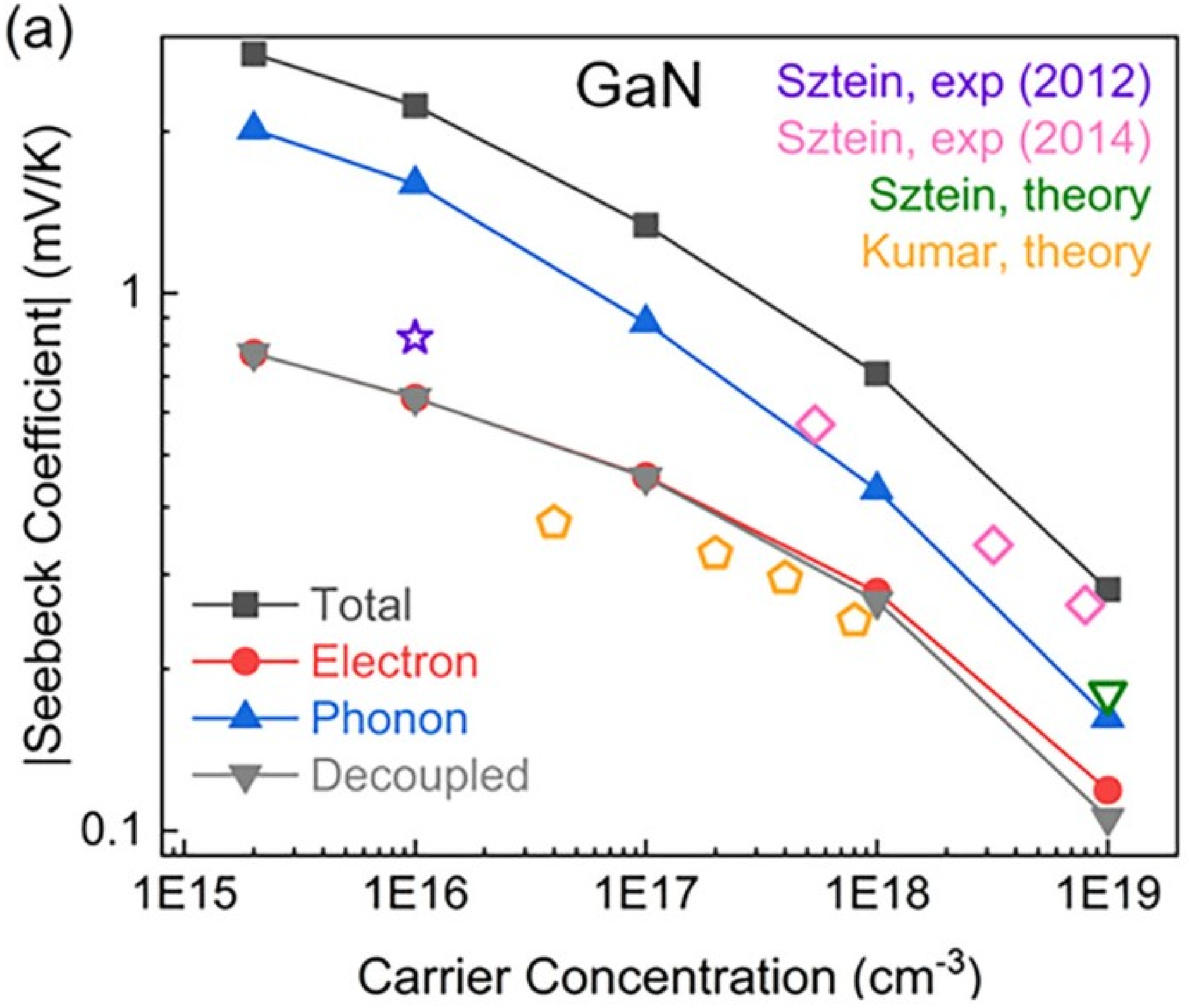
C. Li, et al. Mat. Tod. Phys. 27, 100740, 2022.

Drag effect in GaN and AlN mobility

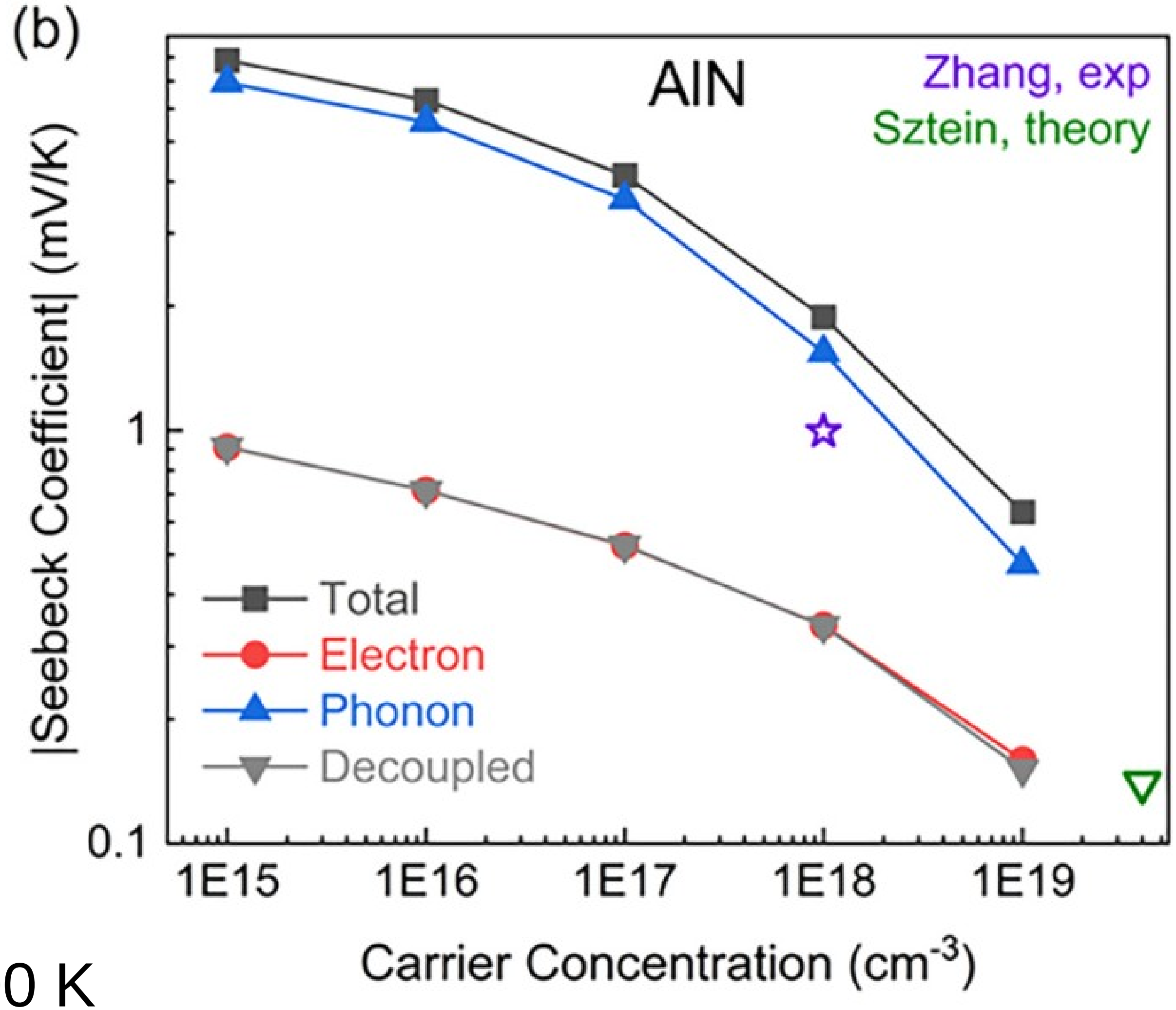


Quan et al. Phys. Rev. B. 107, 245202, 2023.

Drag effect in GaN and AlN thermopower



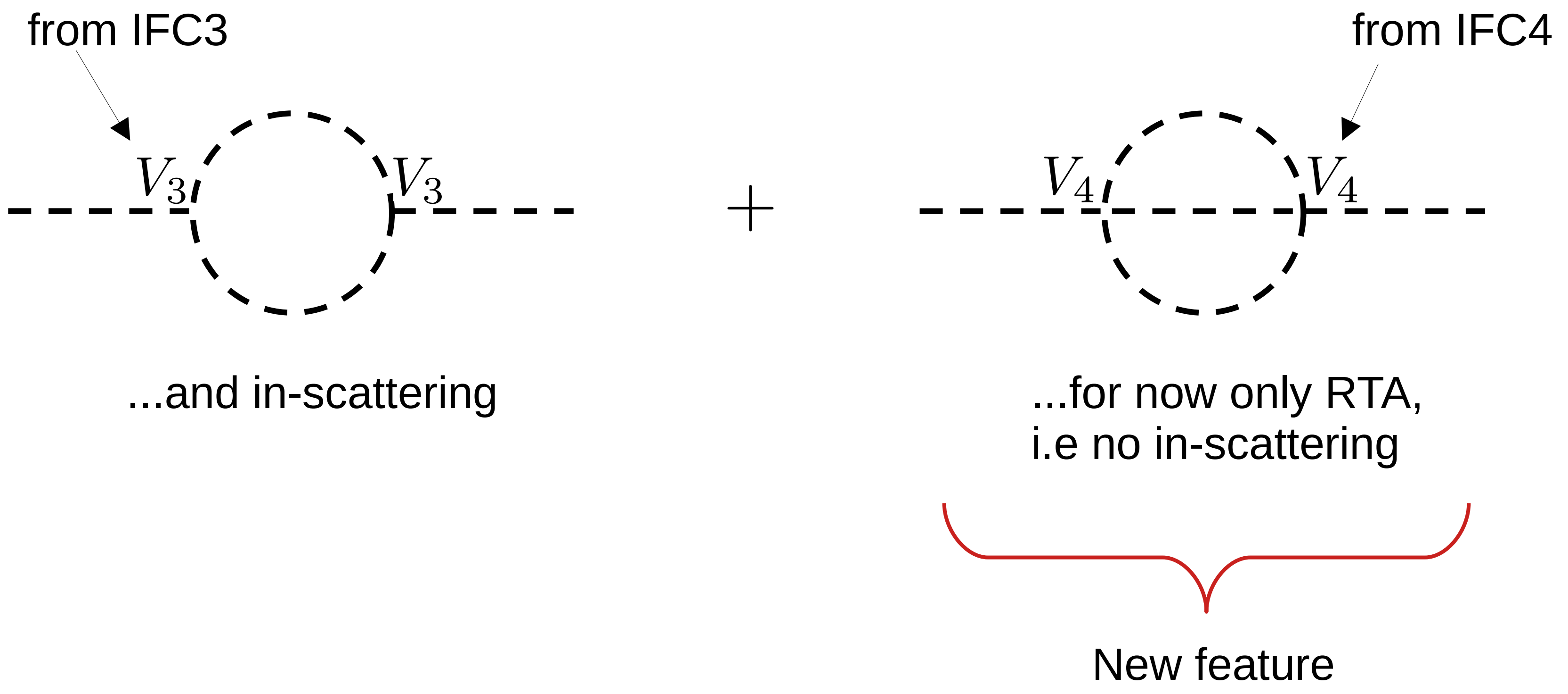
300 K



Quan et al. Phys. Rev. B. 107, 245202, 2023.

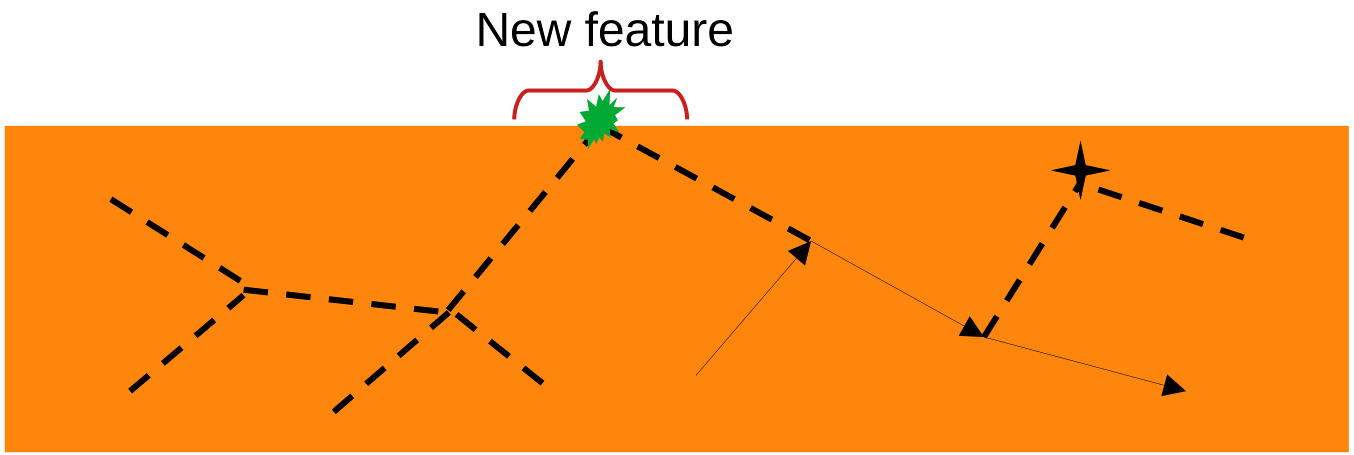
New features

4ph scattering



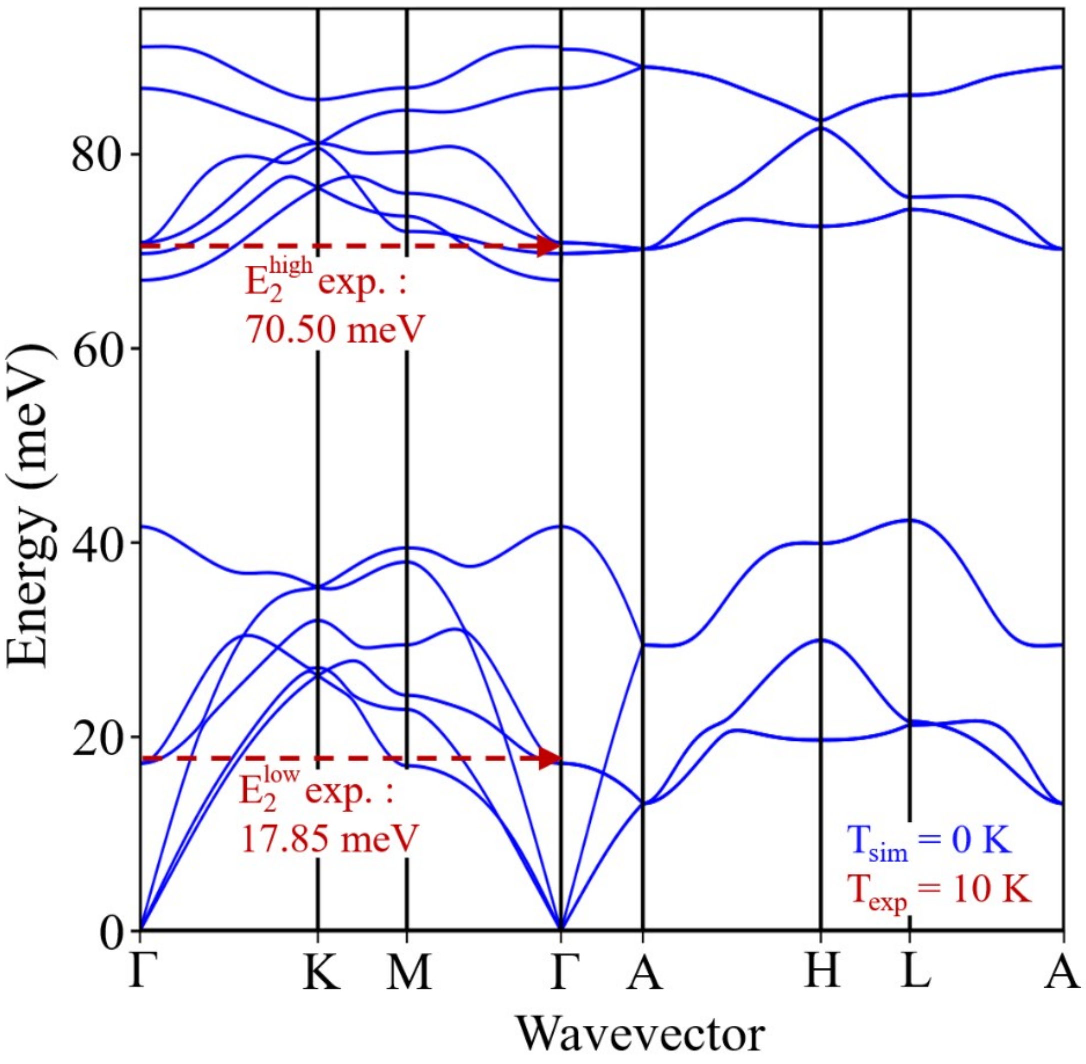
- Calculate 4ph scattering rates using `FourPhonon` on a relatively coarse **q**-mesh
- Interpolate to ultrafine transport **q**-mesh in `elphbolt`
- In-scattering terms of 4ph interaction ignored at the moment
- In future will compute 4ph vertices within `elphbolt`

Ph-thin-film boundary scattering

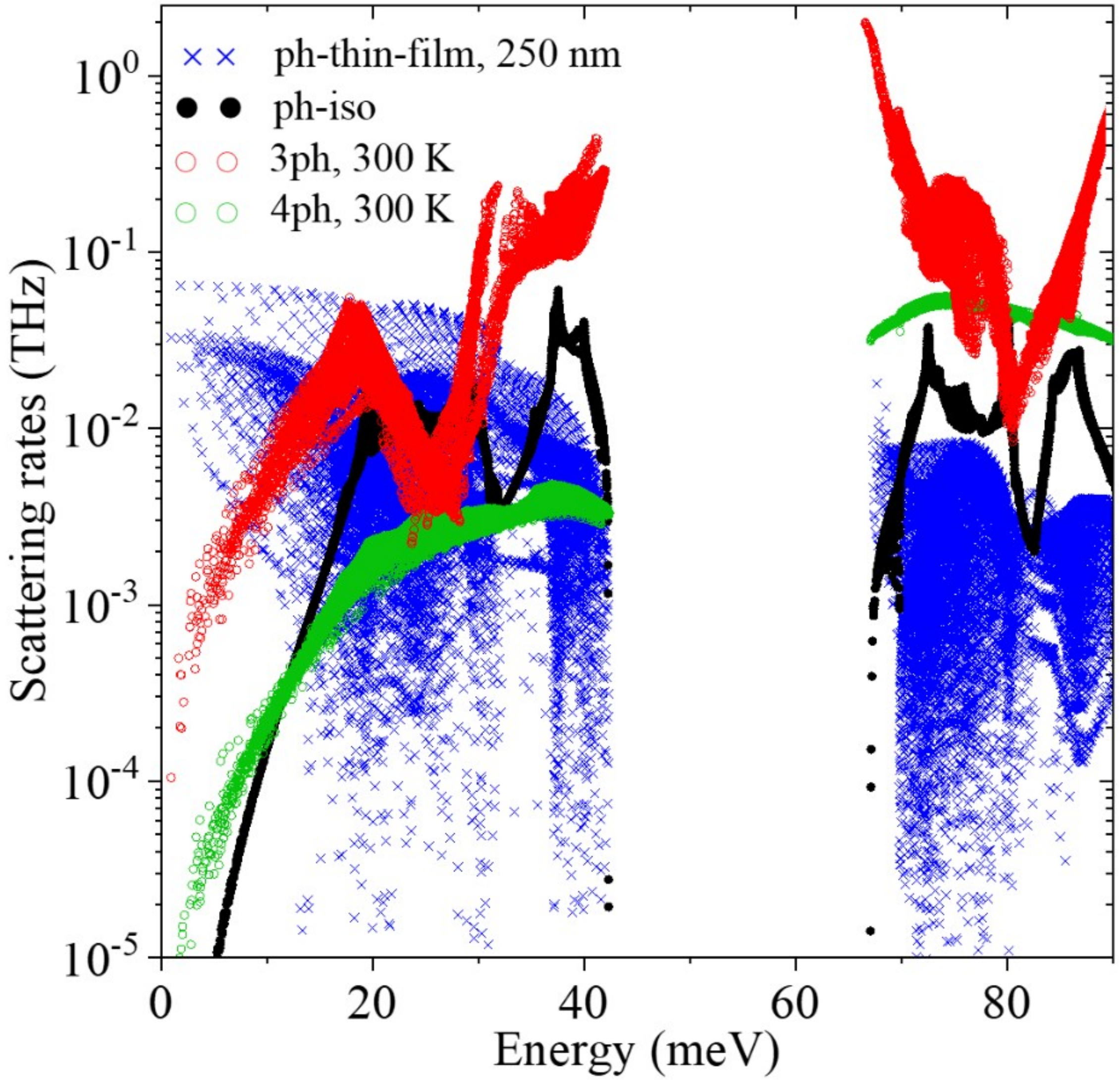


- Cross-plane scattering from Fuchs-Sondheimer theory
  - Full expression
  - Ballistic limit
  - No in-scattering correction at the moment

Thermal conductivity in wGaN thin-films

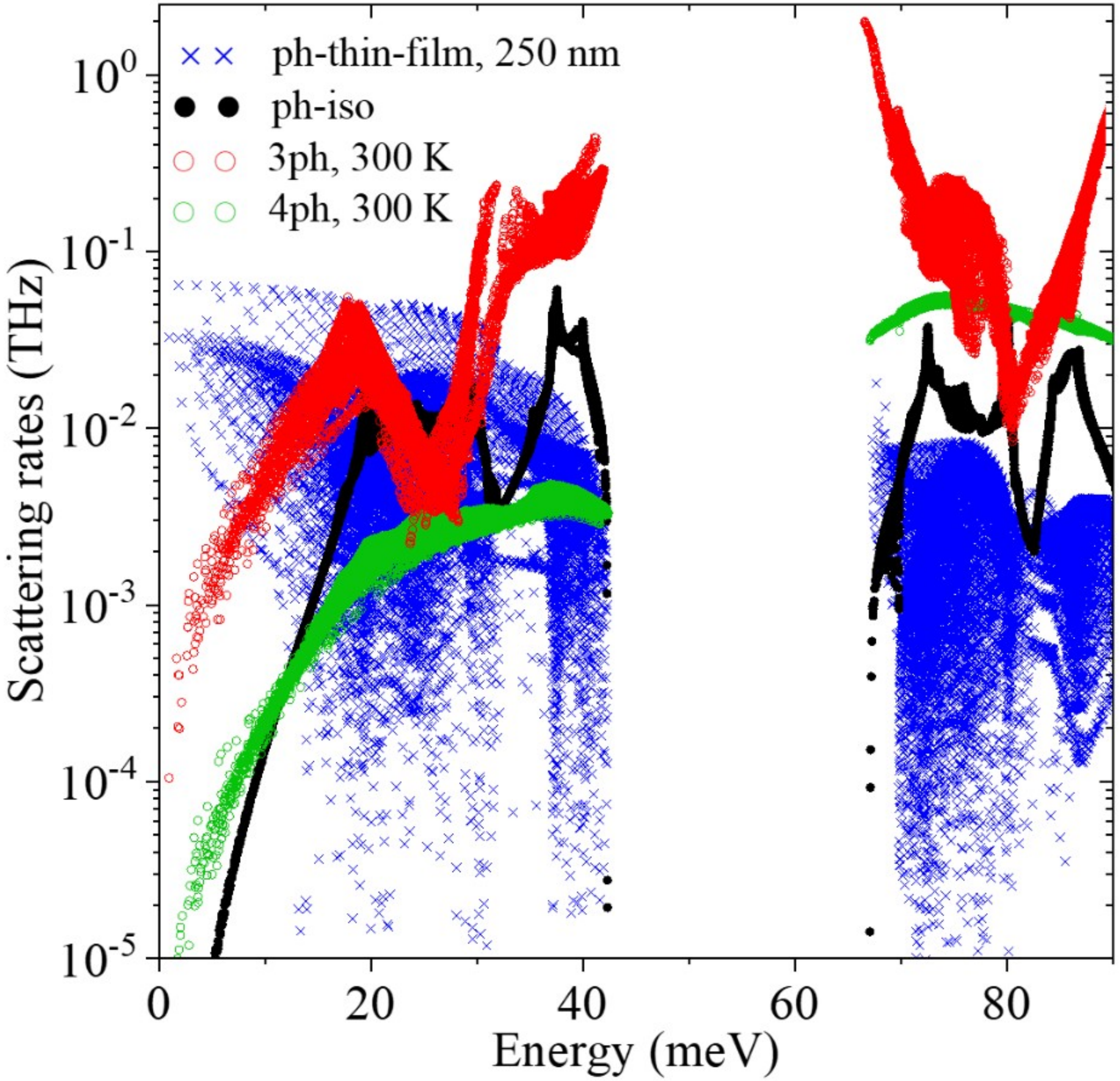


300K

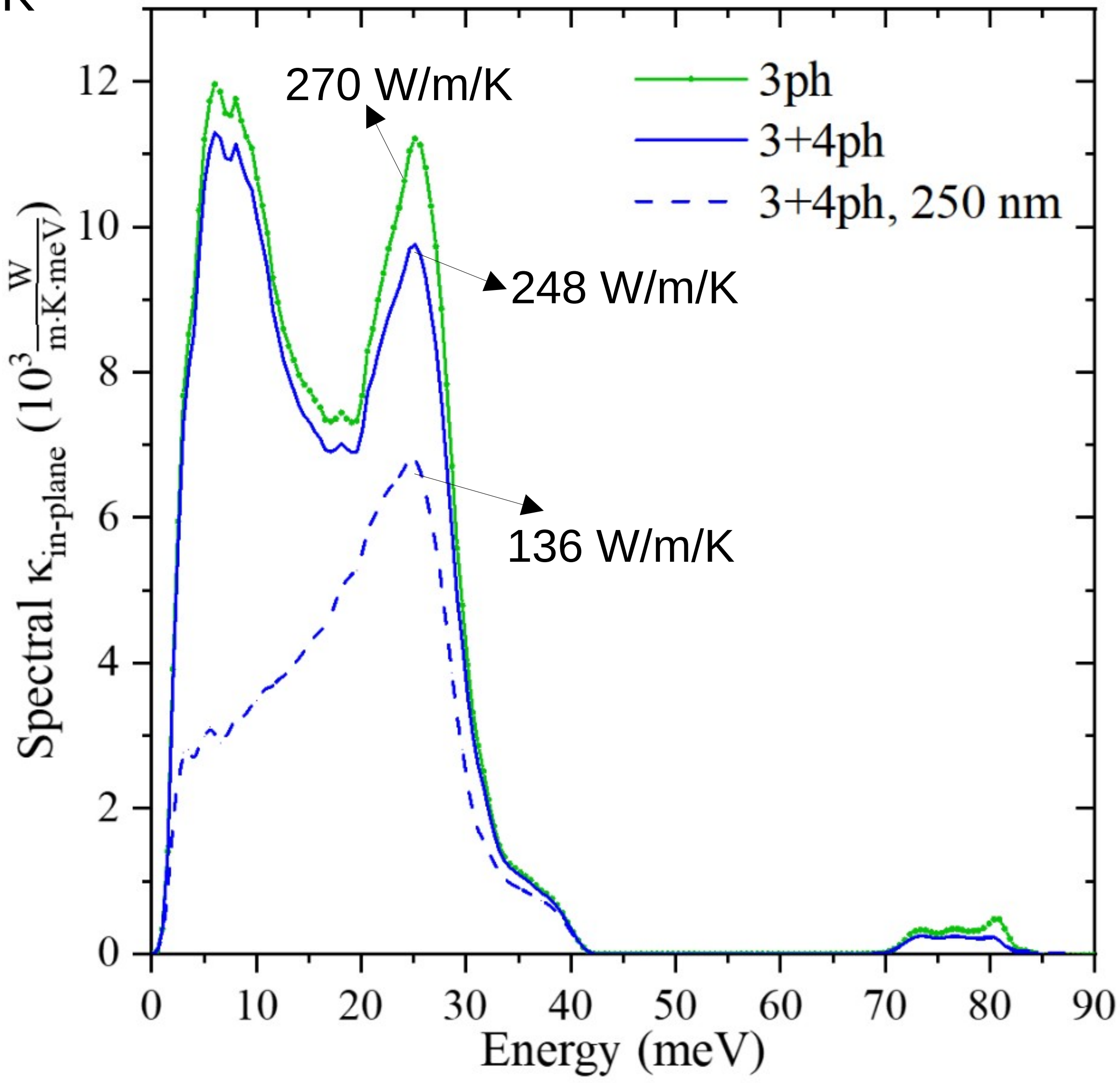


Elhajhasan et al. ArXiv:2306.16980 (2023)

Thermal conductivity in wGaN thin-films

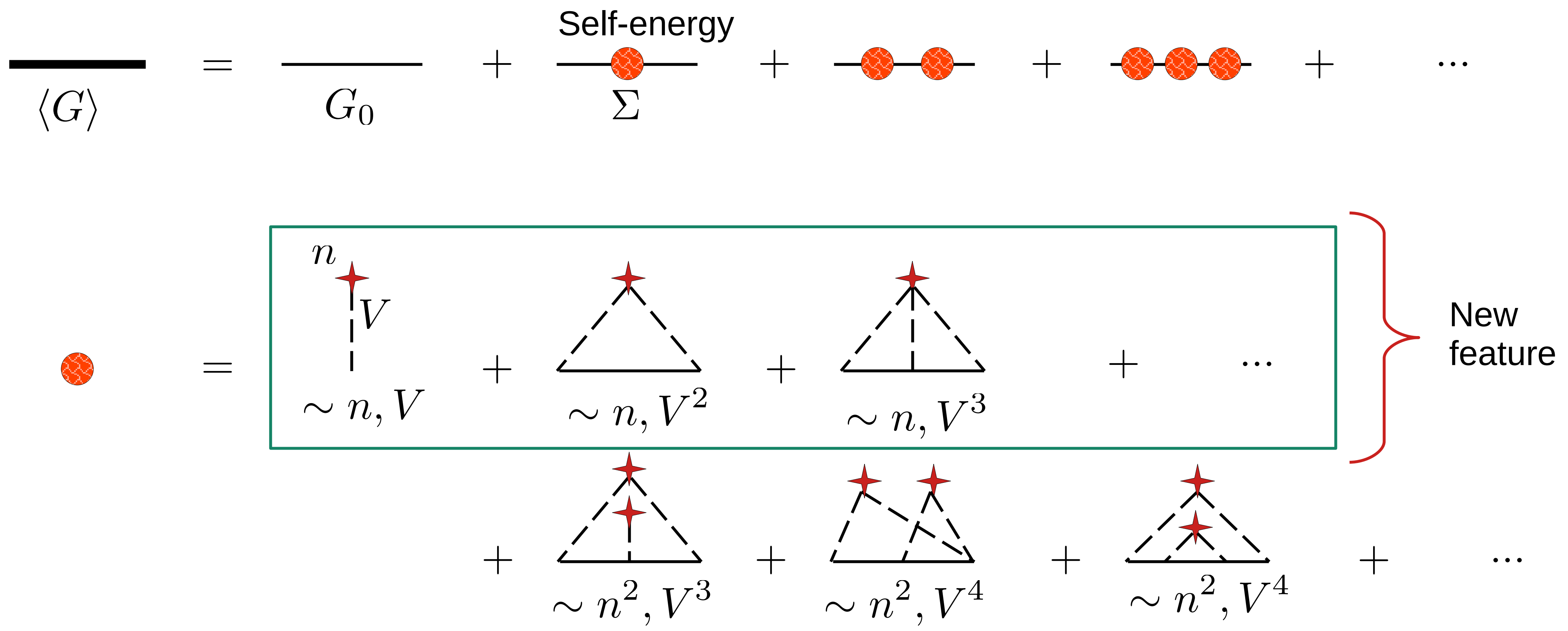


300K



Elhajhasan et al. ArXiv:2306.16980 (2023)

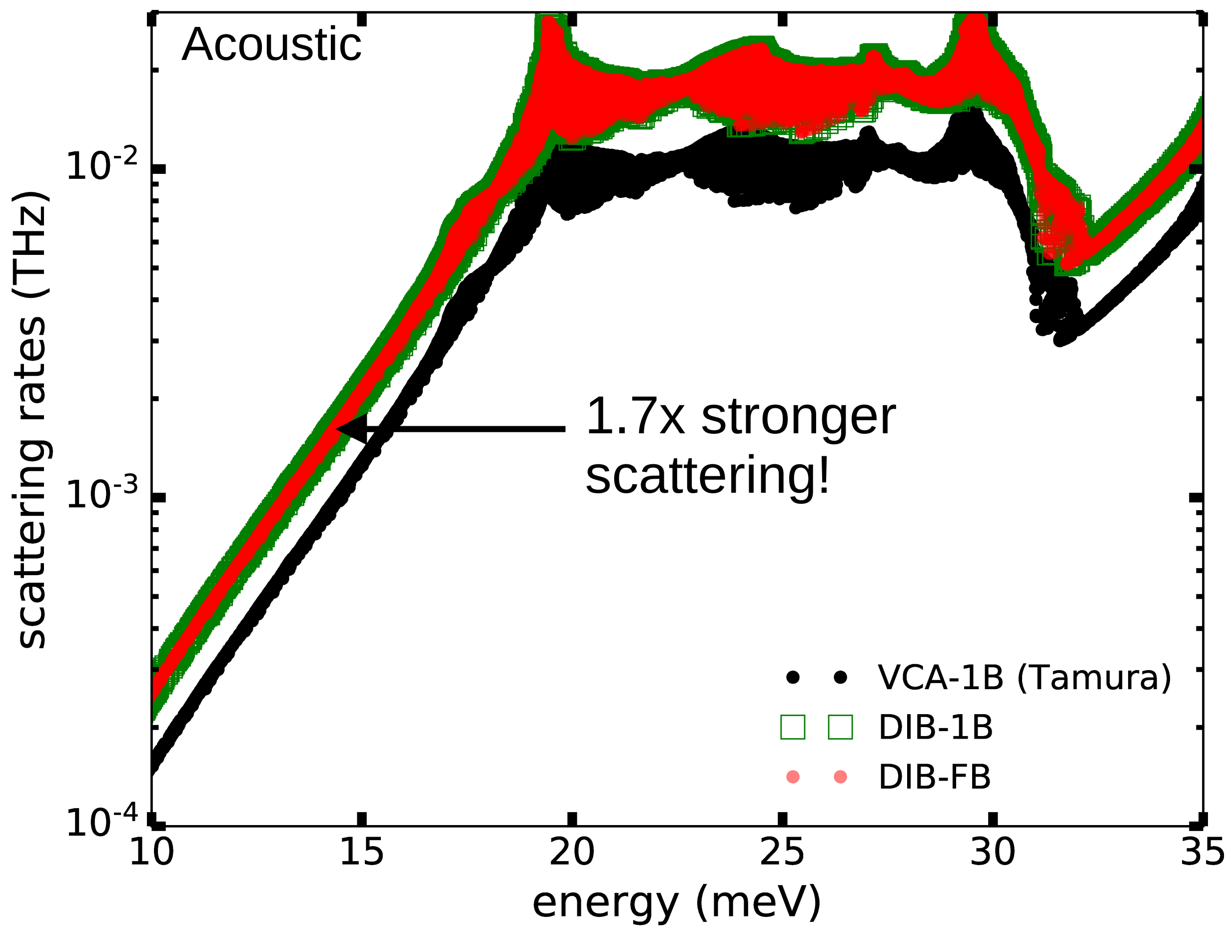
ph-point defect scattering

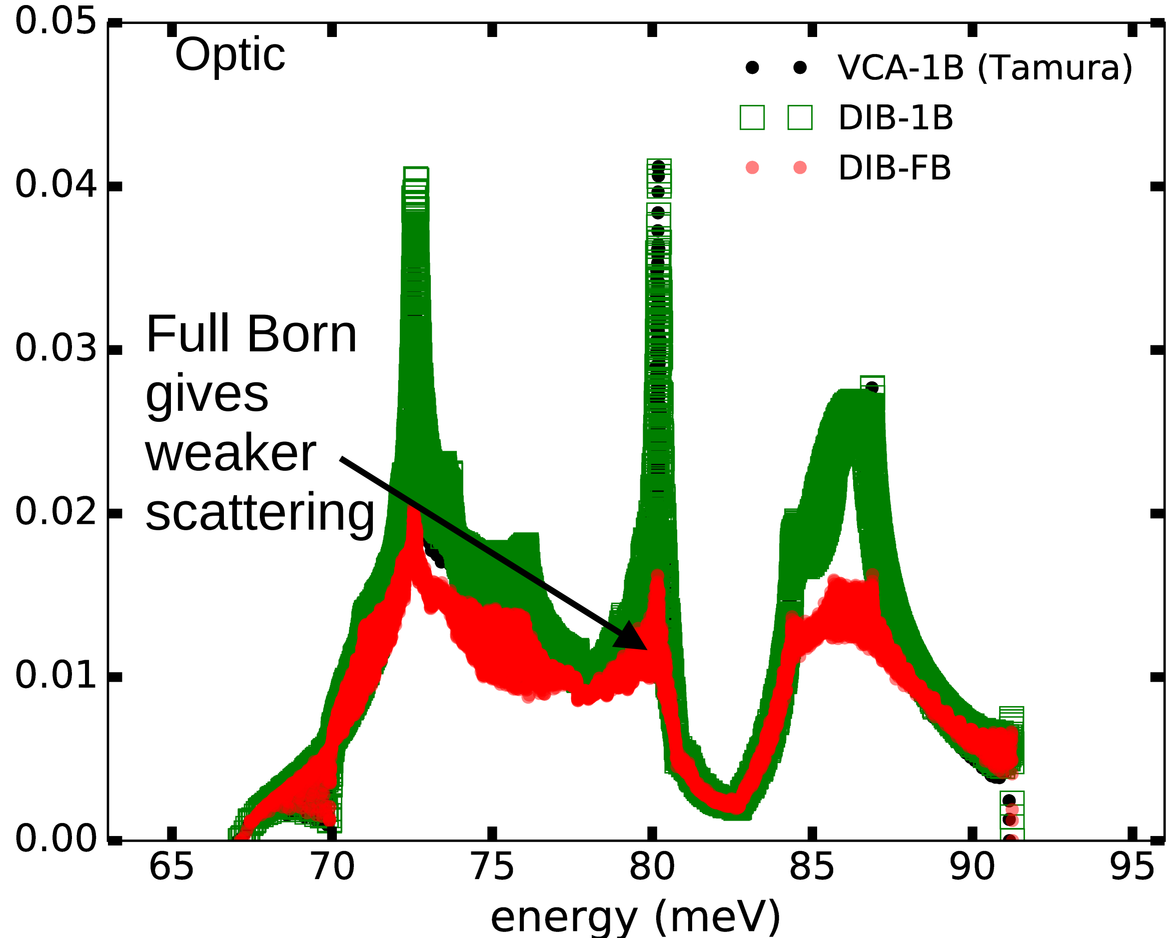


- Low doping resum -- full Born approximation
- Green’s function based
  - Reusable methodology for 1d/2d and el-defect scattering

Beyond Tamura model of ph-isotope scattering in wGaN

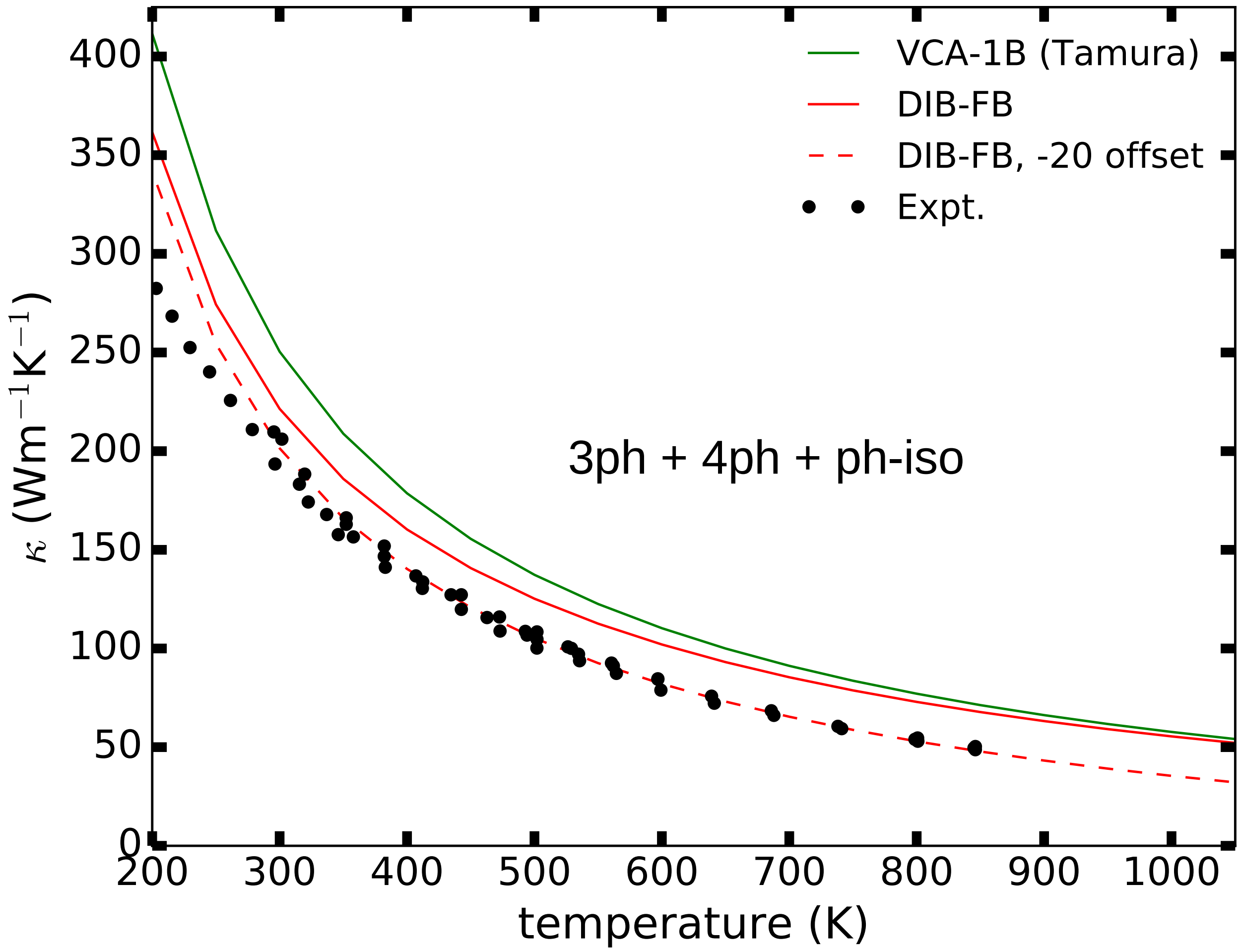
- VCA (virtual crystal approximation)
  - All isotopes are substitutions on top of VCA ground state
- DIB (dominant isotope background)
  - Minority isotopes are substitutions on top of majority isotope ground state





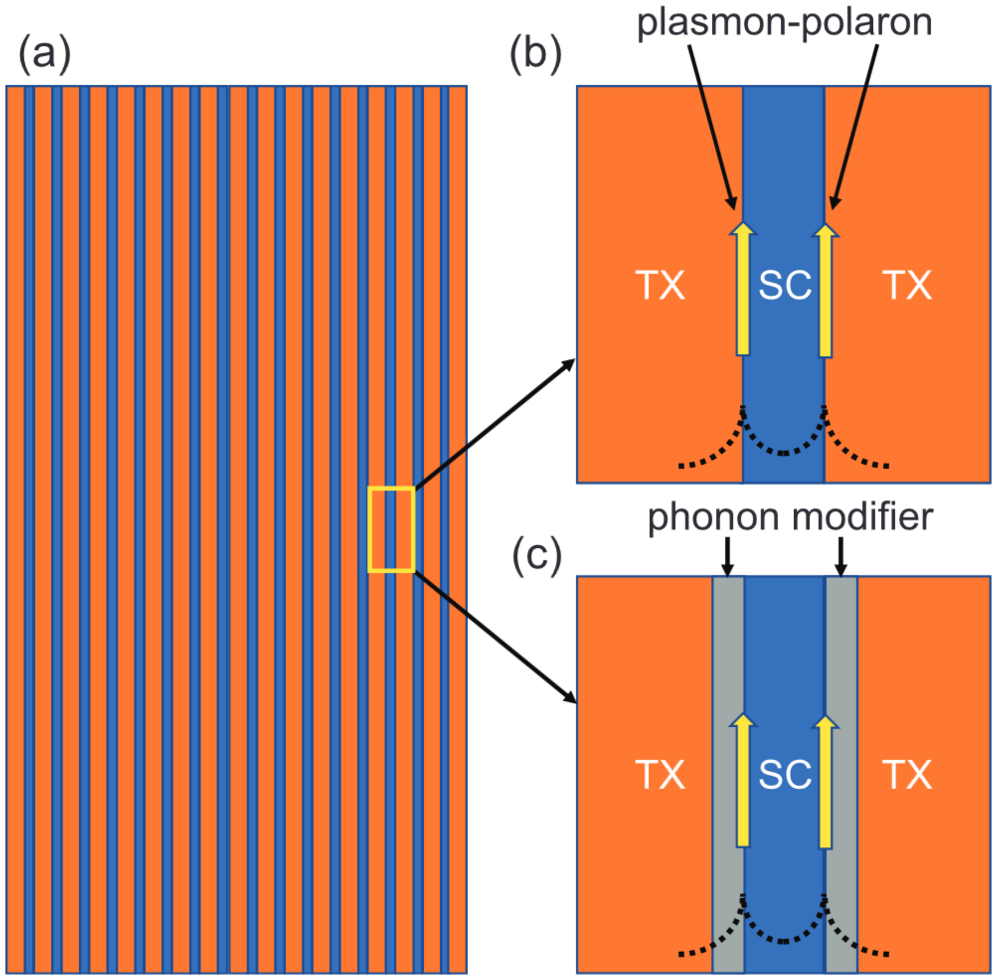
Beyond Tamura model of ph-isotope scattering in wGaN

- DIB theory better than VCA theory at low Ts
- DIB theory better at high Ts
- Beyond T > 1000 K, ph-iso scattering unimportant



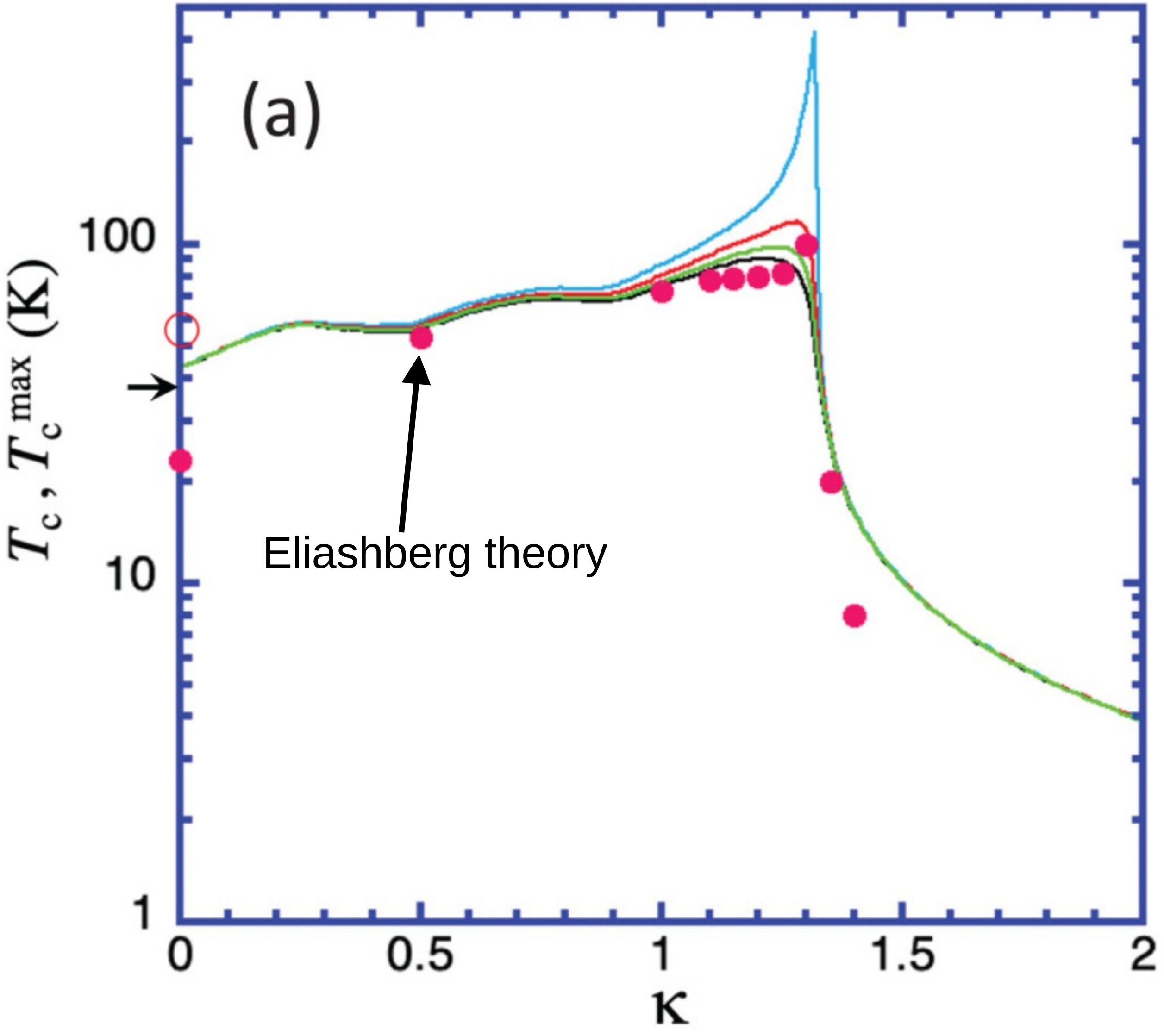
Expt. data from Zheng et al. Phys. Rev. Mat. 3, 014601 (2019)

Phonon-mediated superconductivity – `superconda` sister app



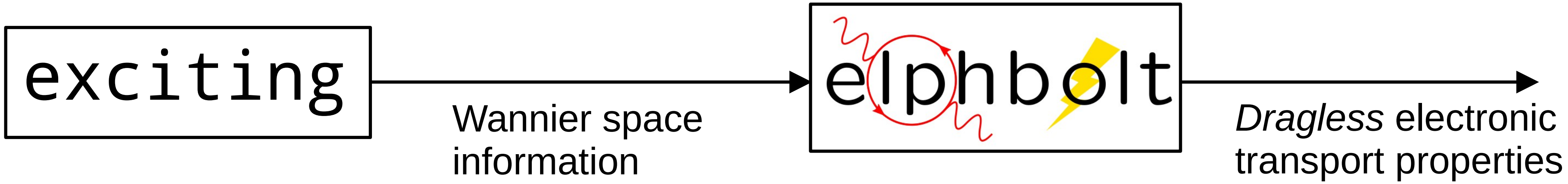
Topological insulator-superconductor superlattice

$$\alpha^2 F(\omega) \rightarrow \frac{\alpha^2 F(\omega)}{|\epsilon_{\rm sup}(\omega)|^2}$$



Kempa et al. Phys. Rev. B. 107, 184518 (2023)

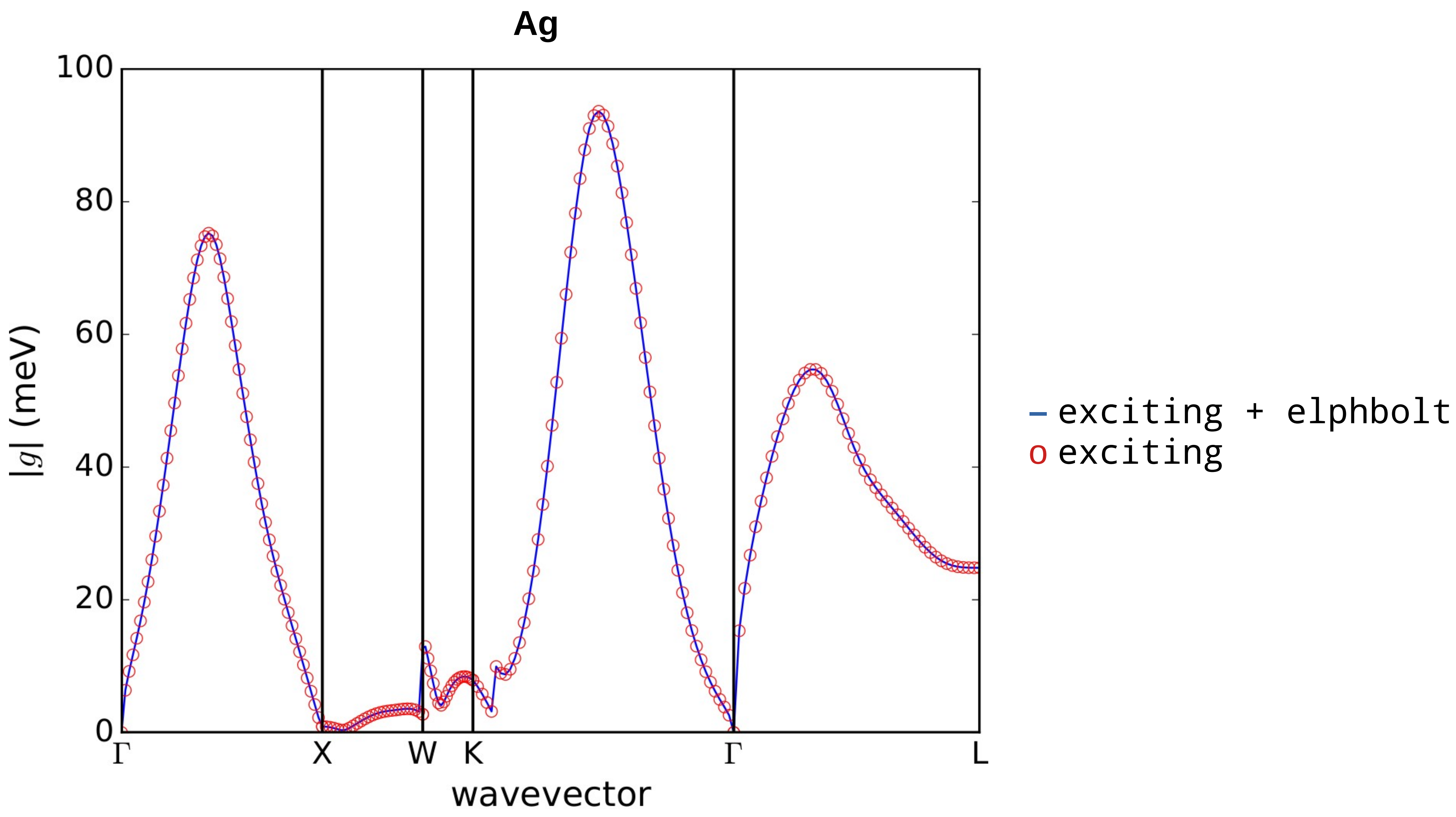
exciting + elphbolt workflow



- Convenient and fast Wannierization in `exciting` [*]
- DFPT feature
  - phonons
  - electron-phonon coupling (stay tuned...)
- Dragless transport via `elphbolt` at the moment
- Dragful transport planned for future
- Superconductivity via `superconda`

[*] Tillack, Gulans, & Draxl, Phys. Rev. B. 101, 235102 (2020)

exciting + elphbolt interface



exciting Wannier data from Sebastian Tillack & Marten Pretorius

Electron-phonon drag in nanowires and nanoribbons

- Attend Marti’s talk!

Acknowledgment

- HU
  - Claudia Draxl
  - Sebastian Tillack
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