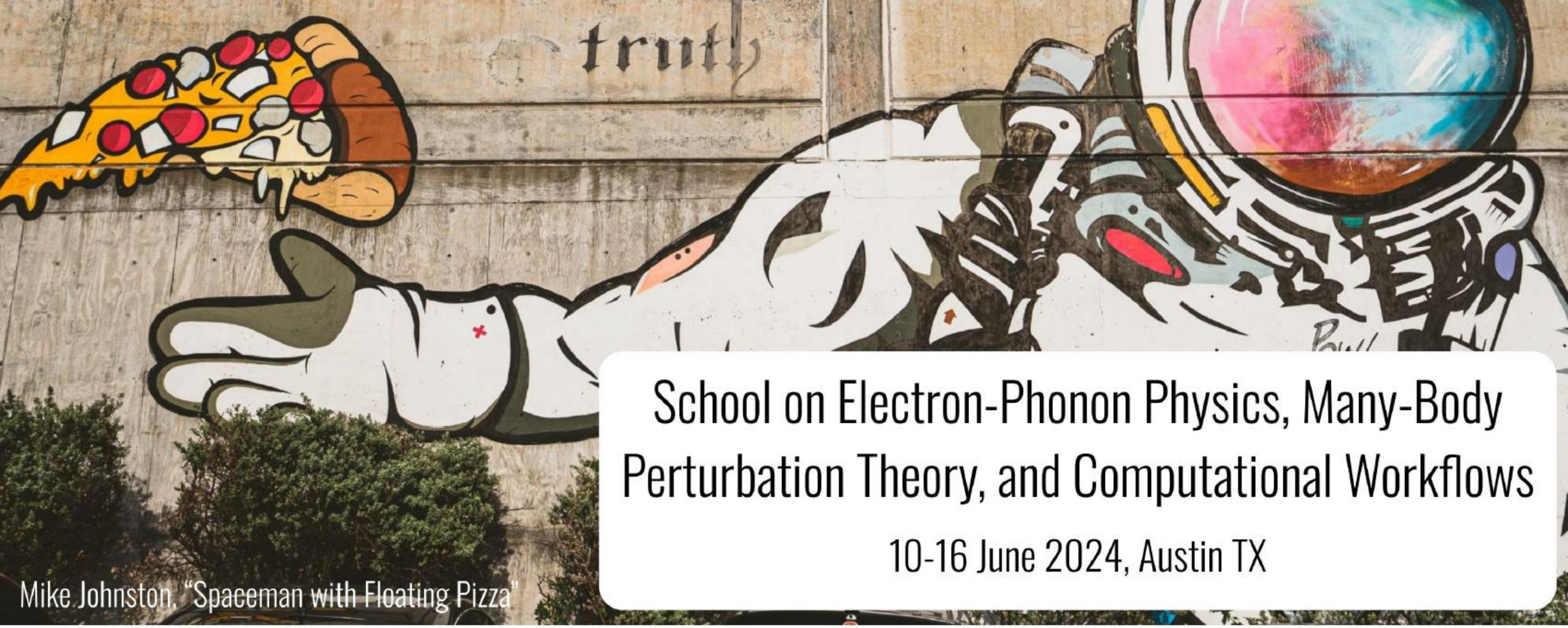


Mike Johnston, "Spaceman with Floating Pizza"

School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

10-16 June 2024, Austin TX

U.S. DEPARTMENT OF ENERGY

NSF

TACC
TEXAS ADVANCED COMPUTING CENTER

ODEN

UCLouvain

Institute of Condensed Matter and Nanosciences

Lecture Sat.4

Wannier function perturbation theory & electron-induced phonon self-energy

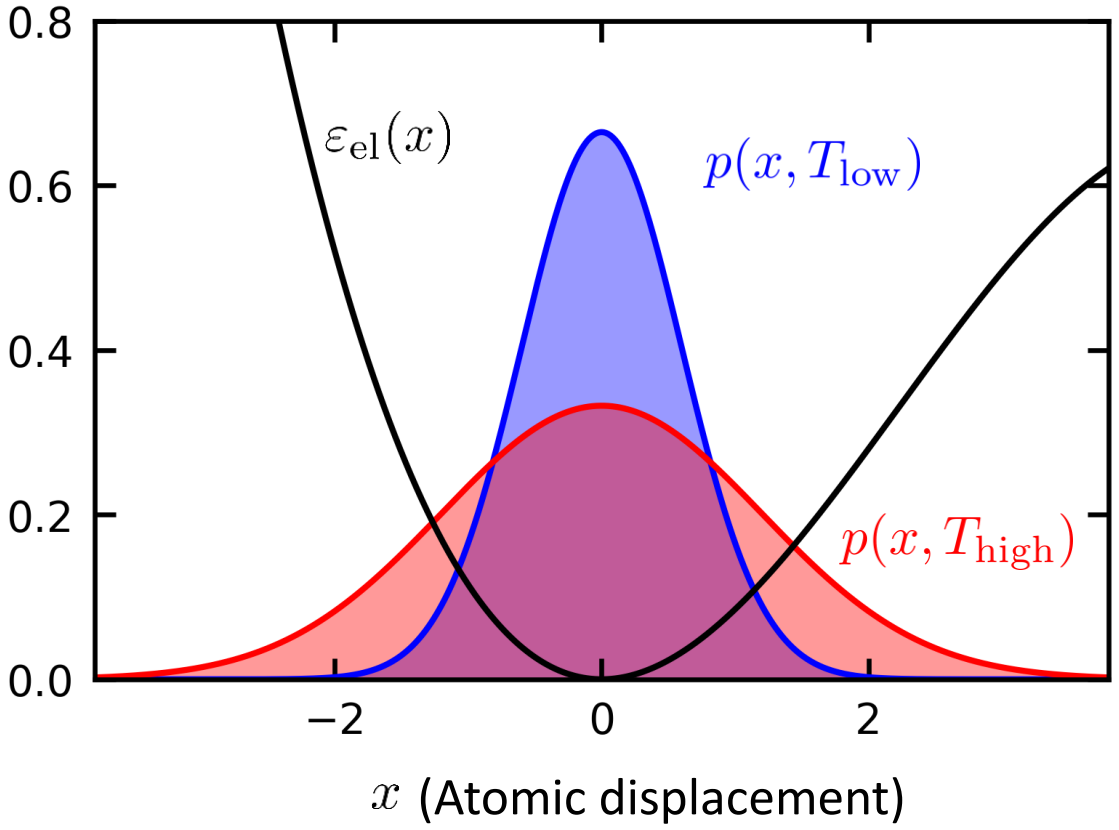
Jae-Mo Lihm

Institute of Condensed Matter and Nanosciences
Université catholique de Louvain, Belgium

Outline

- Phonon-induced electron self-energy: Wannier function perturbation theory
- Electron-induced phonon self-energy: the two-temperature method

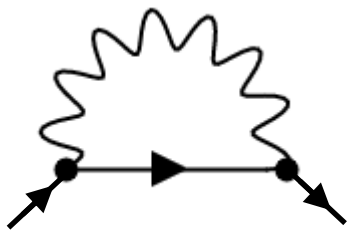
Phonon-induced electron eigenvalue renormalization



$$\Delta\varepsilon_{\mathrm{el}}(T) = \int dx \, [\varepsilon_{\mathrm{el}}(x) - \varepsilon_{\mathrm{el}}(0)] \, p(x, T)$$

Allen-Heine-Cardona theory of band structure renormalization

Σ =



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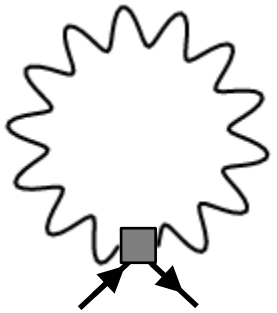


Fan-Migdal self-energy

Debye-Waller self-energy

Second-order perturbation for linear electron-phonon coupling

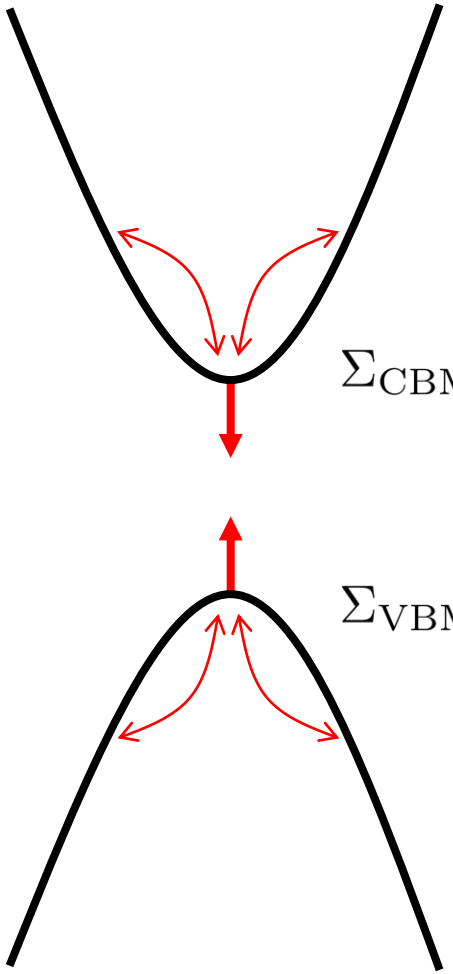
$$\Sigma^{\mathrm{FM}}_{m\mathbf{k}} = \sum_{\mathbf{q}\nu}\sum_{n=1}^{\infty} \frac{\left|\langle\psi_{n\mathbf{k}+\mathbf{q}}|\frac{\partial\hat{V}}{\partial u_{\mathbf{q}\nu}}|\psi_{m\mathbf{k}}\rangle\right|^2}{\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}+\mathbf{q}}}(n_{\mathbf{q}\nu}+\tfrac{1}{2})$$

$$\Sigma^{\mathrm{DW}}_{m\mathbf{k}} = \sum_{\mathbf{q}\nu}\langle\psi_{m\mathbf{k}}|\frac{\partial^2\hat{V}}{\partial u_{-\mathbf{q}\nu}\partial u_{\mathbf{q}\nu}}|\psi_{m\mathbf{k}}\rangle\,(n_{\mathbf{q}\nu}+\tfrac{1}{2})$$

First-order perturbation for quadratic electron-phonon coupling

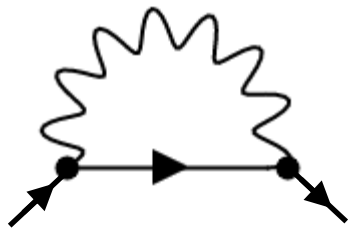
Allen-Heine-Cardona theory of band structure renormalization

- Band gap of semiconductors and insulators are reduced due to the e-ph coupling.

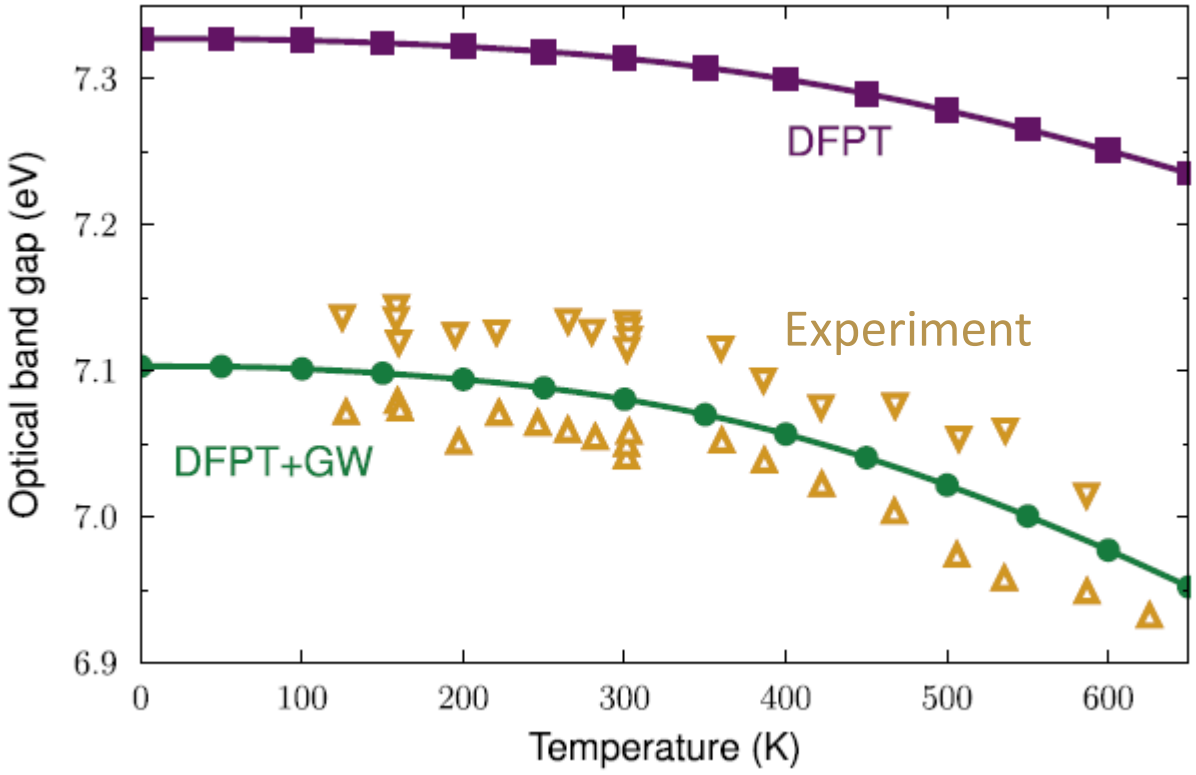


$$\Sigma_{\mathrm{CBM}} \sim \sum_{n \neq \mathrm{CBM}} \frac{\left| \langle n | \frac{\partial \hat{V}}{\partial x} | \mathrm{CBM} \rangle \right|^2}{\varepsilon_{\mathrm{CBM}} - \varepsilon_n} < 0$$

$$\Sigma_{\mathrm{VBM}} \sim \sum_{n \neq \mathrm{VBM}} \frac{\left| \langle n | \frac{\partial \hat{V}}{\partial x} | \mathrm{VBM} \rangle \right|^2}{\varepsilon_{\mathrm{VBM}} - \varepsilon_n} > 0$$



Direct band gap of diamond

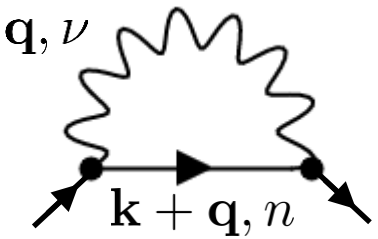


G. Antonius *et al.*, PRL **112**, 215501 (2014)

Inapplicability of the ordinary Wannier function method

Electron-phonon matrix elements

$$\Sigma^{\mathrm{FM}}_{m\mathbf{k}} = \sum_{\pm} \sum_{\mathbf{q},\nu} \sum_{n=1}^{\infty} \frac{\left| \langle \psi_{n\mathbf{k}+\mathbf{q}} | \frac{\partial \hat{V}}{\partial u_{\mathbf{q}\nu}} | \psi_{m\mathbf{k}} \rangle \right|^2}{\varepsilon_{m\mathbf{k}} - (\varepsilon_{n\mathbf{k}+\mathbf{q}} \mp \omega_{\mathbf{q}\nu}) + i0^+} (n_{\mathbf{q}\nu} + \tfrac{1}{2} \pm (f_{n\mathbf{k}+\mathbf{q}} - \tfrac{1}{2}))$$



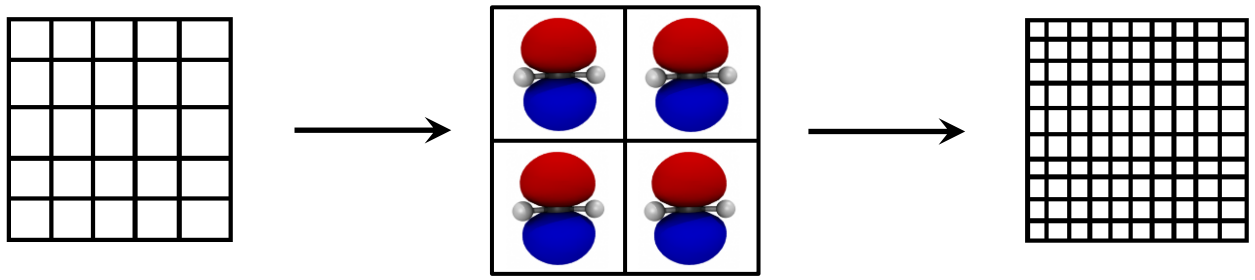
Initial state energy

Intermediate state energy

Phonon and electron occupation factors

Momentum integration: ~100×100×100 grid needed
Solution: use a localized basis set

Sum over states: > 100 bands needed
Wannier function method not applicable



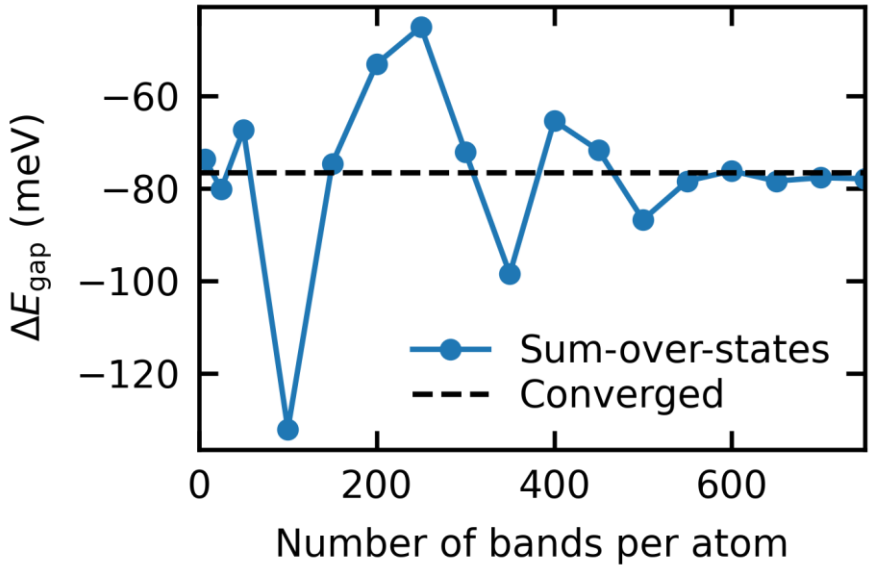
Coarse k/q grid
~10×10×10

Real space
Wannier functions

Dense k/q grid
~100×100×100

WANNIER90 EPW Perturbo Phoebe

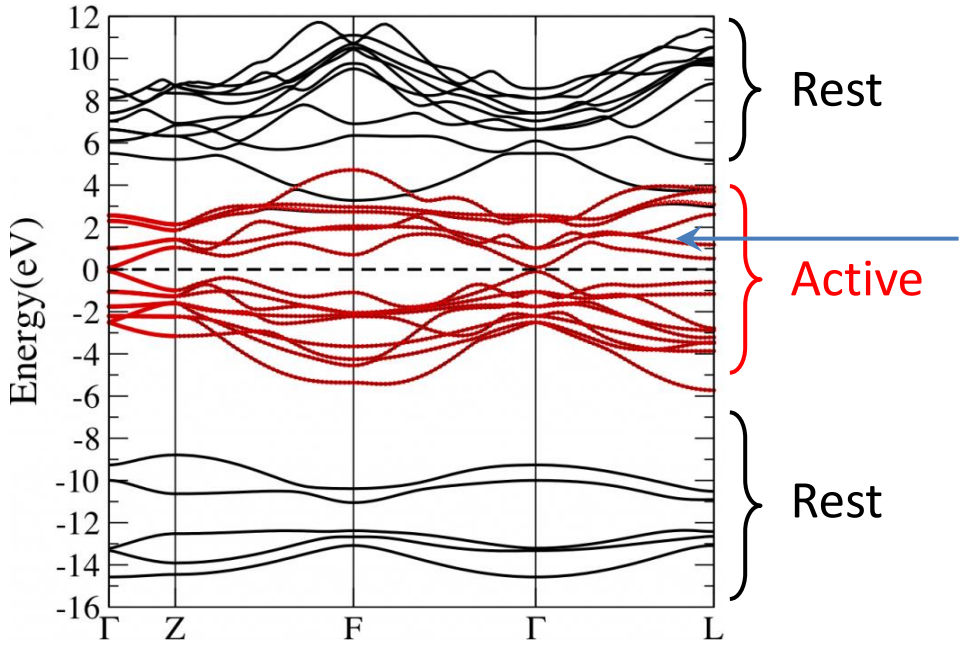
elphbolt EPIq



BAs, zero-point renormalization (T=0)

Band structure renormalization from Wannier interpolation

- Step 1: separate the active and rest subspaces



$\varepsilon_{m\mathbf{k}}$

$$m\mathbf{k} \in \text{Active}, \;\; n\mathbf{k}+\mathbf{q} \in \text{Rest}$$
$$|\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}+\mathbf{q}}| \gg \omega_{\mathbf{q}\nu}$$

$$\Sigma^{\text{FM}}_{m\mathbf{k}} = \Sigma^{\text{FM}-\text{Active}}_{m\mathbf{k}} + \Sigma^{\text{FM}-\text{Rest}}_{m\mathbf{k}}$$

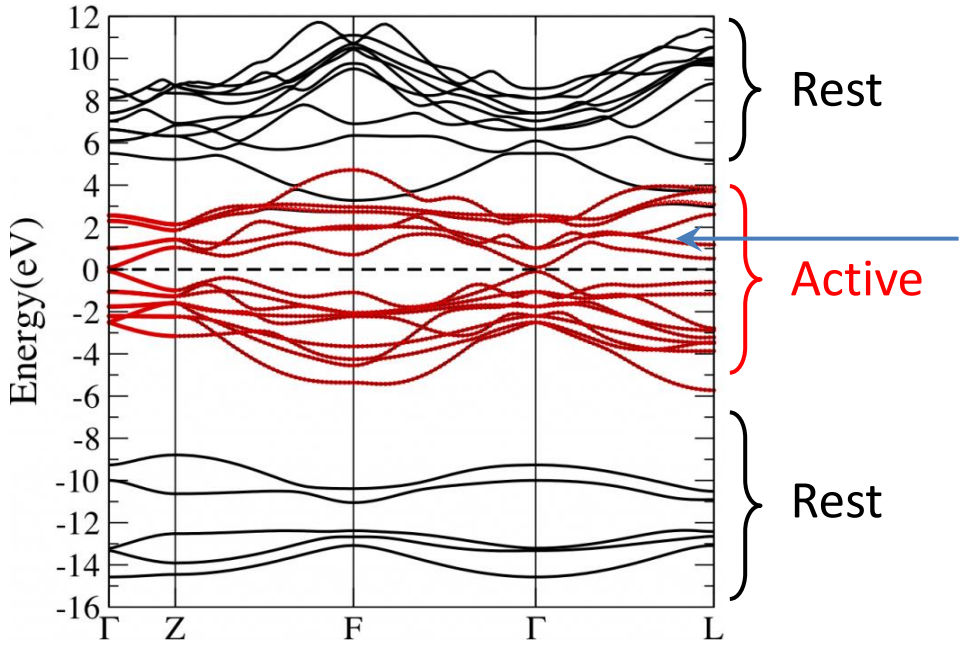
$$\Sigma^{\text{FM}-\text{Active}}_{m\mathbf{k}} = \sum_{\pm} \sum_{\mathbf{q},\nu} \sum_{n}^{\text{A}} \frac{\left| \langle \psi_{n\mathbf{k}+\mathbf{q}} | \frac{\partial \hat{V}}{\partial u_{\mathbf{q}\nu}} | \psi_{m\mathbf{k}} \rangle \right|^2}{\varepsilon_{m\mathbf{k}} - (\varepsilon_{n\mathbf{k}+\mathbf{q}} \mp \omega_{\mathbf{q}\nu}) + i0^+} (n_{\mathbf{q}\nu} + \tfrac{1}{2} \pm (f_{n\mathbf{k}+\mathbf{q}} - \tfrac{1}{2}))$$

$$\Sigma^{\text{FM}-\text{Rest}}_{m\mathbf{k}} = \sum_{\pm} \sum_{\mathbf{q},\nu} \sum_{n}^{\text{R}} \frac{\left| \langle \psi_{n\mathbf{k}+\mathbf{q}} | \frac{\partial \hat{V}}{\partial u_{\mathbf{q}\nu}} | \psi_{m\mathbf{k}} \rangle \right|^2}{\varepsilon_{m\mathbf{k}} - (\varepsilon_{n\mathbf{k}+\mathbf{q}} \mp \omega_{\mathbf{q}\nu}) + i0^+} (n_{\mathbf{q}\nu} + \tfrac{1}{2} \pm (f_{n\mathbf{k}+\mathbf{q}} - \tfrac{1}{2}))$$

S. Poncé *et al.*, J. Chem. Phys. **143**, 102813 (2015)

Band structure renormalization from Wannier interpolation

- Step 1: separate the active and rest subspaces



$\varepsilon_{m\mathbf{k}}$

$$m\mathbf{k} \in \text{Active}, \;\; n\mathbf{k}+\mathbf{q} \in \text{Rest}$$
$$|\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}+\mathbf{q}}| \gg \omega_{\mathbf{q}\nu}$$

$$\Sigma^{\text{FM}}_{m\mathbf{k}} = \Sigma^{\text{FM-Active}}_{m\mathbf{k}} + \Sigma^{\text{FM-Rest}}_{m\mathbf{k}}$$

$$\Sigma^{\text{FM-Active}}_{m\mathbf{k}} = \sum_{\pm} \sum_{\mathbf{q},\nu} \sum_{n}^{\text{A}} \frac{\left| \langle \psi_{n\mathbf{k}+\mathbf{q}} | \frac{\partial \hat{V}}{\partial u_{\mathbf{q}\nu}} | \psi_{m\mathbf{k}} \rangle \right|^2}{\varepsilon_{m\mathbf{k}} - (\varepsilon_{n\mathbf{k}+\mathbf{q}} \mp \omega_{\mathbf{q}\nu}) + i0^+} (n_{\mathbf{q}\nu} + \tfrac{1}{2} \pm (f_{n\mathbf{k}+\mathbf{q}} - \tfrac{1}{2}))$$

$$\Sigma^{\text{FM-Rest}}_{m\mathbf{k}} \approx 2 \sum_{\mathbf{q},\nu} \sum_{n}^{\text{R}} \frac{\left| \langle \psi_{n\mathbf{k}+\mathbf{q}} | \frac{\partial \hat{V}}{\partial u_{\mathbf{q}\nu}} | \psi_{m\mathbf{k}} \rangle \right|^2}{\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}+\mathbf{q}}} (n_{\mathbf{q}\nu} + \tfrac{1}{2})$$

S. Poncé *et al.*, J. Chem. Phys. **143**, 102813 (2015)

Band structure renormalization from Wannier interpolation

- Step 2: rewrite in terms of wavefunction perturbation

$$\Sigma^{\mathrm{FM-Rest}}_{m\mathbf{k}} \approx 2\sum_{\mathbf{q},\nu}\sum_{n}^{\mathrm{R}} \frac{\langle\psi_{m\mathbf{k}}|\frac{\partial\hat{V}}{\partial u_{\mathbf{q}\nu}}|\psi_{n\mathbf{k}+\mathbf{q}}\rangle\langle\psi_{n\mathbf{k}+\mathbf{q}}|\frac{\partial\hat{V}}{\partial u_{\mathbf{q}\nu}}|\psi_{m\mathbf{k}}\rangle}{\varepsilon_{m\mathbf{k}}-\varepsilon_{n\mathbf{k}+\mathbf{q}}}(n_{\mathbf{q}\nu}+\tfrac{1}{2})$$

$$= 2\sum_{\mathbf{q},\nu}\left\langle\psi_{m\mathbf{k}}\middle|\frac{\partial\hat{V}}{\partial u_{\mathbf{q}\nu}}P_{\mathrm{R}}\middle|\frac{\partial\psi_{m\mathbf{k}}}{\partial u_{\mathbf{q}\nu}}\right\rangle(n_{\mathbf{q}\nu}+\tfrac{1}{2})$$

First-order perturbation of wavefunction

$$P_{\mathrm{R}}\left|\frac{\partial\psi_{m\mathbf{k}}}{\partial u_{\mathbf{q}\nu}}\right\rangle = \sum_{n}^{\mathrm{R}}\frac{|\psi_{n\mathbf{k}+\mathbf{q}}\rangle\langle\psi_{n\mathbf{k}+\mathbf{q}}|\frac{\partial\hat{V}}{\partial u_{\mathbf{q}}}|\psi_{m\mathbf{k}}\rangle}{\varepsilon_{m\mathbf{k}}-\varepsilon_{n\mathbf{k}+\mathbf{q}}}$$

Computed by solving the Sternheimer equation (c.f. DFPT lecture by P. Gianozzi)

$$(\varepsilon_{m\mathbf{k}}-\hat{H}_{\mathbf{k}+\mathbf{q}})\left|\frac{\partial\psi_{m\mathbf{k}}}{\partial u_{\mathbf{q}}}\right\rangle = \frac{\partial\hat{V}}{\partial u_{\mathbf{q}}}|\psi_{m\mathbf{k}}\rangle$$

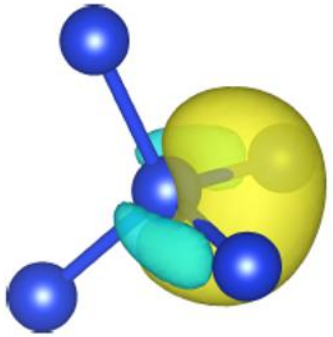
X. Gonze *et al.*, Ann. Phys. **523**, 1, 168 (2011)

Band structure renormalization from Wannier interpolation

- Step 3: transform to a localized basis – Wannier function perturbation theory (WFPT)

$$\Sigma_{m\mathbf{k}}^{\mathrm{FM-Rest}} \approx 2 \sum_{\mathbf{q},\nu} \left\langle \psi_{m\mathbf{k}} \middle| \frac{\partial \hat{V}}{\partial u_{\mathbf{q}\nu}} P_{\mathrm{R}} \middle| \frac{\partial \psi_{m\mathbf{k}}}{\partial u_{\mathbf{q}\nu}} \right\rangle (n_{\mathbf{q}\nu} + \tfrac{1}{2})$$

Wannier functions



?

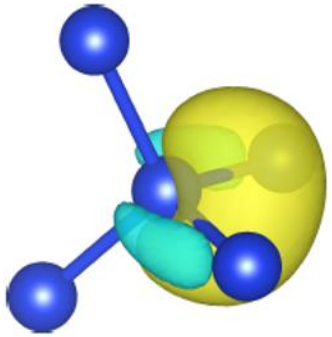
J.-M. Lihm and C.-H. Park, PRX **11**, 041053 (2021)

Band structure renormalization from Wannier interpolation

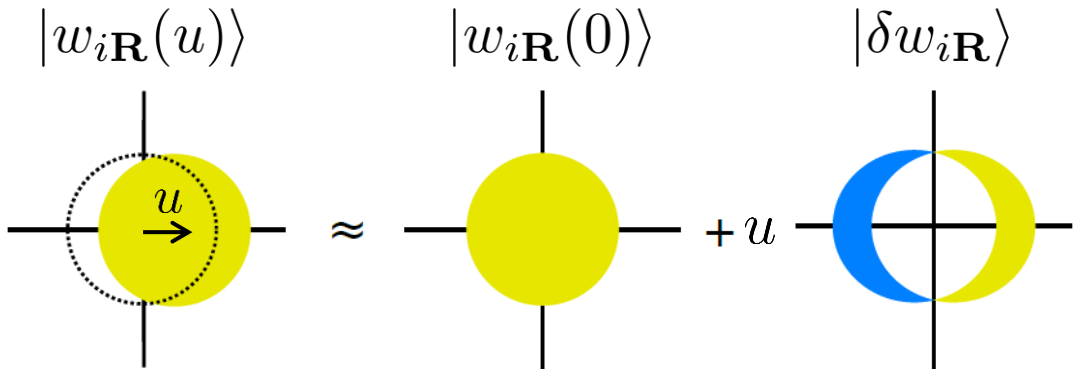
- Step 3: transform to a localized basis – Wannier function perturbation theory (WFPT)

$$\Sigma^{\mathrm{FM-Rest}}_{m\mathbf{k}} \approx 2\sum_{\mathbf{q},\nu} \left\langle \psi_{m\mathbf{k}} \middle| \frac{\partial \hat{V}}{\partial u_{\mathbf{q}\nu}} P_{\mathrm{R}} \middle| \frac{\partial \psi_{m\mathbf{k}}}{\partial u_{\mathbf{q}\nu}} \right\rangle (n_{\mathbf{q}\nu} + \tfrac{1}{2})$$

Wannier functions



Wannier function perturbations



$$|\delta w_{i\mathbf{R}}\rangle = \lim_{u\to 0} \frac{|w_{i\mathbf{R}}(u)\rangle - |w_{i\mathbf{R}}(0)\rangle}{u}$$

Define $|w_{i\mathbf{R}}(u)\rangle$ using $|w_{i\mathbf{R}}(0)\rangle$ as the initial guess without further localization.

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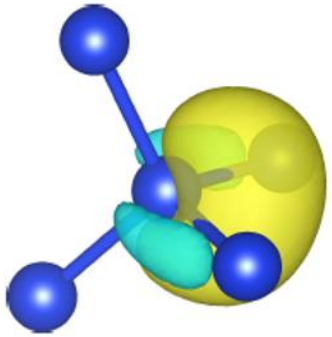
Band structure renormalization from Wannier interpolation

- Step 3: transform to a localized basis – Wannier function perturbation theory (WFPT)

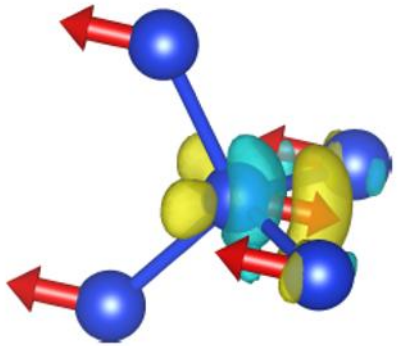
$$\Sigma^{\mathrm{FM-Rest}}_{m\mathbf{k}} \approx 2\sum_{\mathbf{q},\nu} \left\langle \psi_{m\mathbf{k}} \middle| \frac{\partial \hat{V}}{\partial u_{\mathbf{q}\nu}} P_{\mathrm{R}} \middle| \frac{\partial \psi_{m\mathbf{k}}}{\partial u_{\mathbf{q}\nu}} \right\rangle (n_{\mathbf{q}\nu} + \tfrac{1}{2})$$

Wannier functions



$$|w_{i\mathbf{R}}\rangle = \sum_{\mathbf{k}} |\psi_{m\mathbf{k}}\rangle\, U_{mi,\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}}$$

Wannier function perturbations



$$|\delta_{\mathbf{q}\nu} w_{i\mathbf{R}}\rangle = \sum_{\mathbf{k}} (\hat{\mathbb{1}} - \hat{P}_{\mathrm{W}}) \left| \frac{\partial \psi_{m\mathbf{k}}}{\partial u_{\mathbf{q}\nu}} \right\rangle U_{mi,\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}}$$

$$S_{ij\mathbf{R};\mathbf{q}\nu} = \langle w_{i\mathbf{0}} | \frac{\partial \hat{V}}{\partial u_{\mathbf{q}\nu}} | \delta_{\mathbf{q}\nu} w_{j\mathbf{R}} \rangle$$

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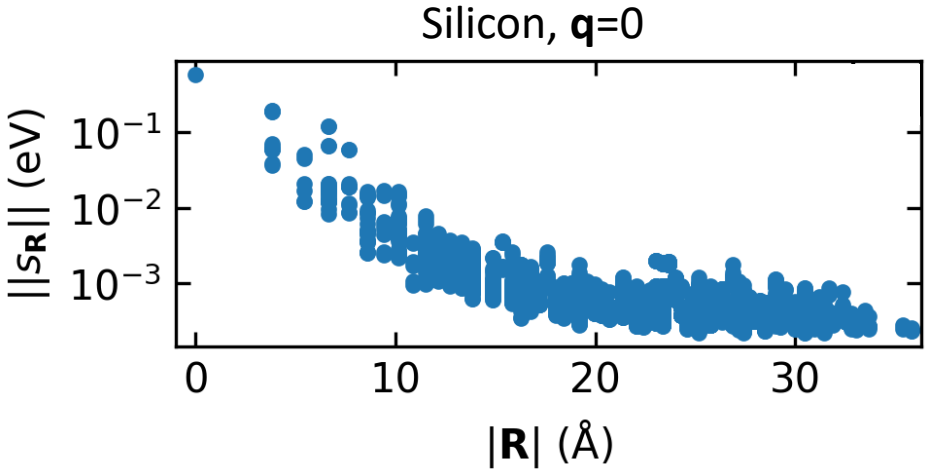
Band structure renormalization from Wannier interpolation

- Step 3: transform to a localized basis – Wannier function perturbation theory (WFPT)

$$\Sigma^{\mathrm{FM-Rest}}_{m\mathbf{k}} \approx 2\sum_{\mathbf{q},\nu} \left\langle \psi_{m\mathbf{k}} \middle| \frac{\partial \hat{V}}{\partial u_{\mathbf{q}\nu}} P_{\mathrm{R}} \middle| \frac{\partial \psi_{m\mathbf{k}}}{\partial u_{\mathbf{q}\nu}} \right\rangle (n_{\mathbf{q}\nu} + \tfrac{1}{2})$$

$$= 2\sum_{\mathbf{q},\nu}\sum_{ij\mathbf{R}} U^{\dagger}_{mi;\mathbf{k}} S_{ij\mathbf{R};\mathbf{q}\nu} U_{jm;\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} (n_{\mathbf{q}\nu} + \tfrac{1}{2})$$

$$S_{ij\mathbf{R};\mathbf{q}\nu} = \langle w_{i\mathbf{0}} | \frac{\partial \hat{V}}{\partial u_{\mathbf{q}\nu}} | \delta_{\mathbf{q}\nu} w_{j\mathbf{R}} \rangle$$



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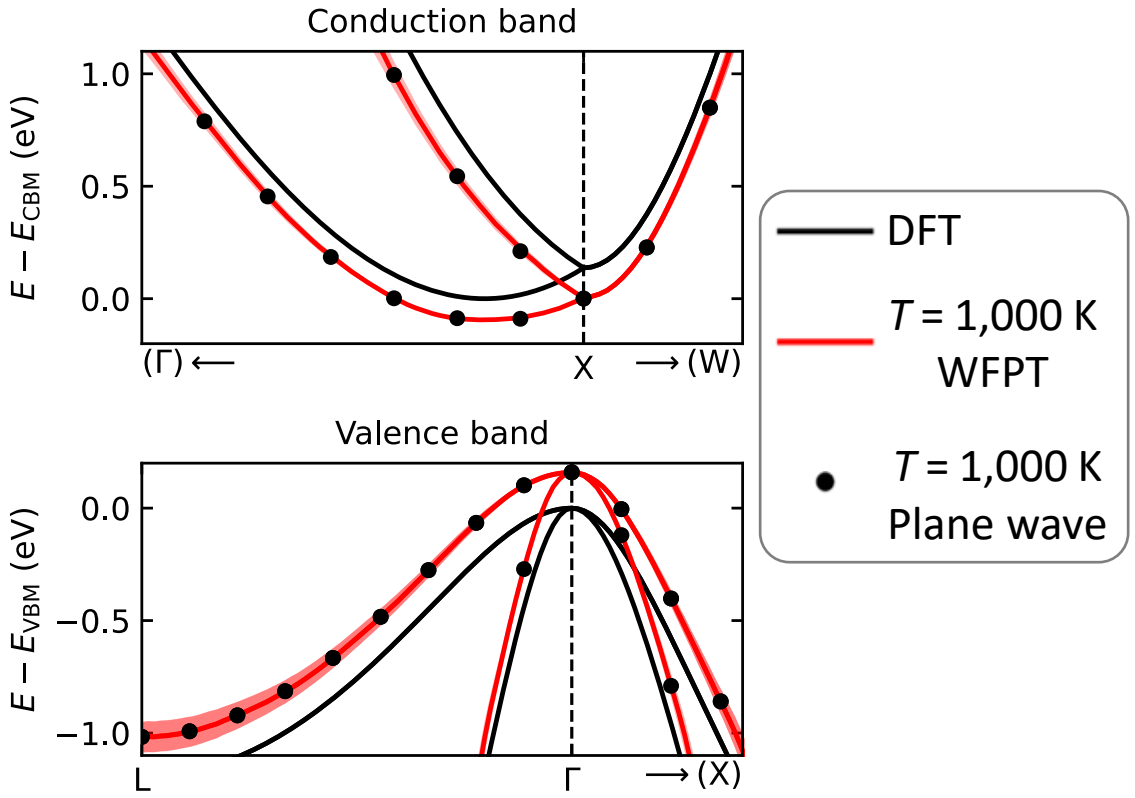
WFPT application: band structure renormalization

- WFPT gives ~1,000× speedup in the calculation of the phonon-induced electron self-energy.

Silicon band structure renormalization



Computational cost for 379 *k* points (cpu*hour)

Calculation	Plane waves	WFPT
DFT	300	300
Wannierization	-	600
Electron-phonon	4,451,800*	2,900
Total	4,452,100*	3,800

* Estimated from a smaller calculation

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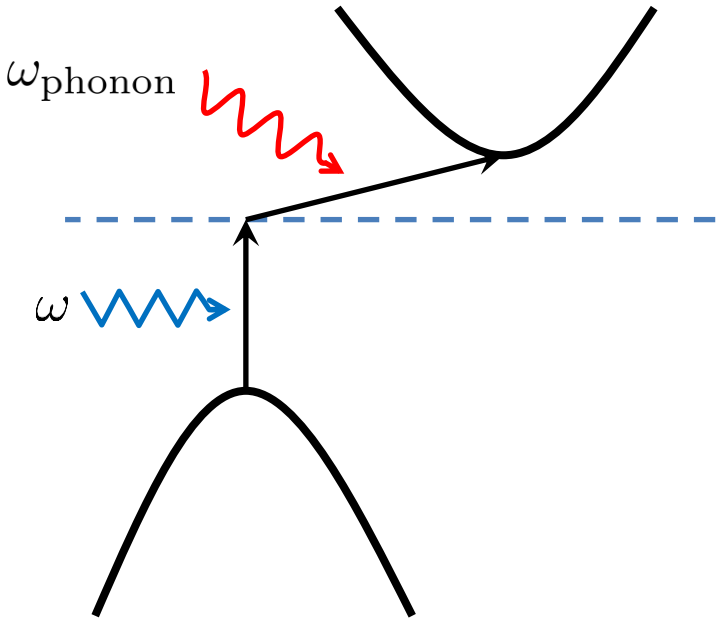
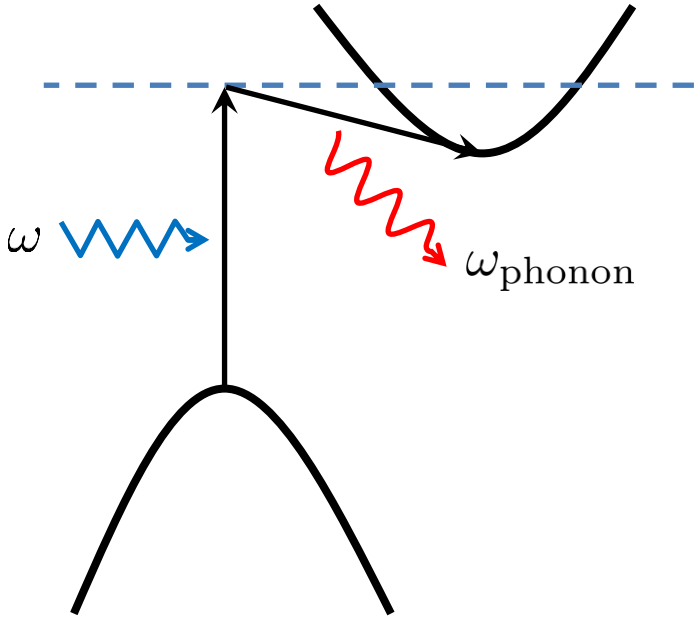
WFPT application: indirect optical absorption of silicon

Phonon absorption
(Only at high temperatures)

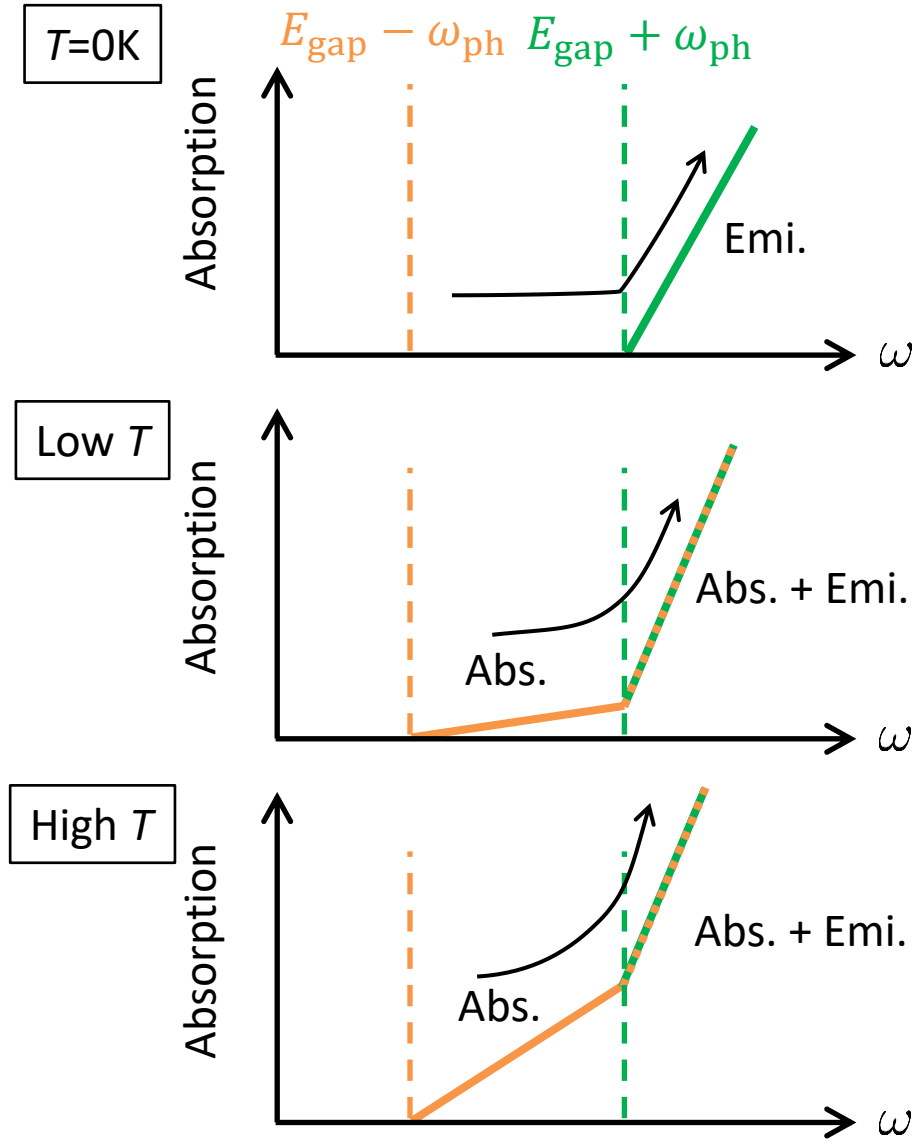


$\propto n_{\mathrm{phonon}}$

Phonon emission
(At all temperatures)



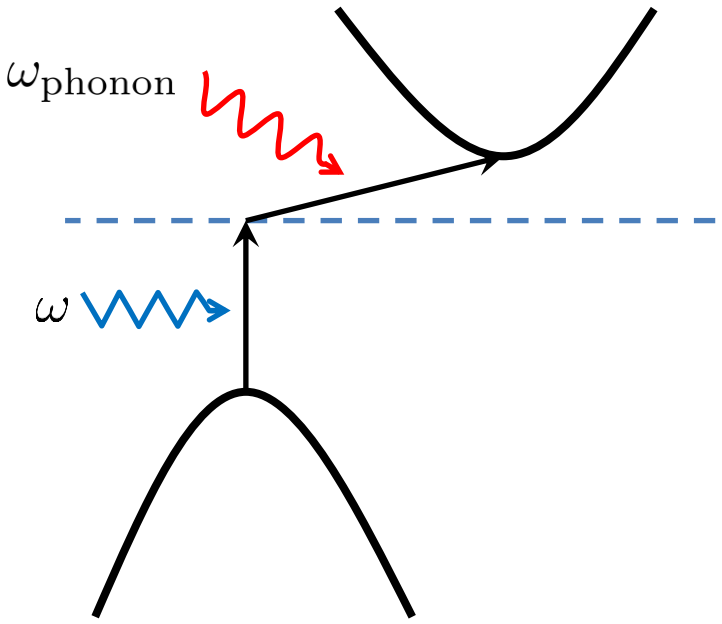
$\propto n_{\mathrm{phonon}} + 1$



F. Bassani and G. P. Parravicini, *Electronic States and Optical Transitions in Solids*, Pergamon Press (1975)
E. Kioupakis *et al.*, PRB **81**, 241201 (2010)

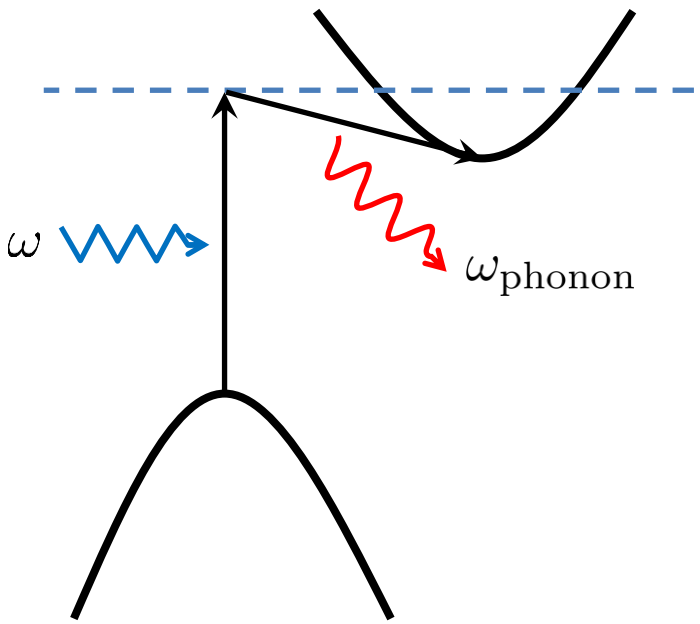
WFPT application: indirect optical absorption of silicon

Phonon absorption
(Only at high temperatures)

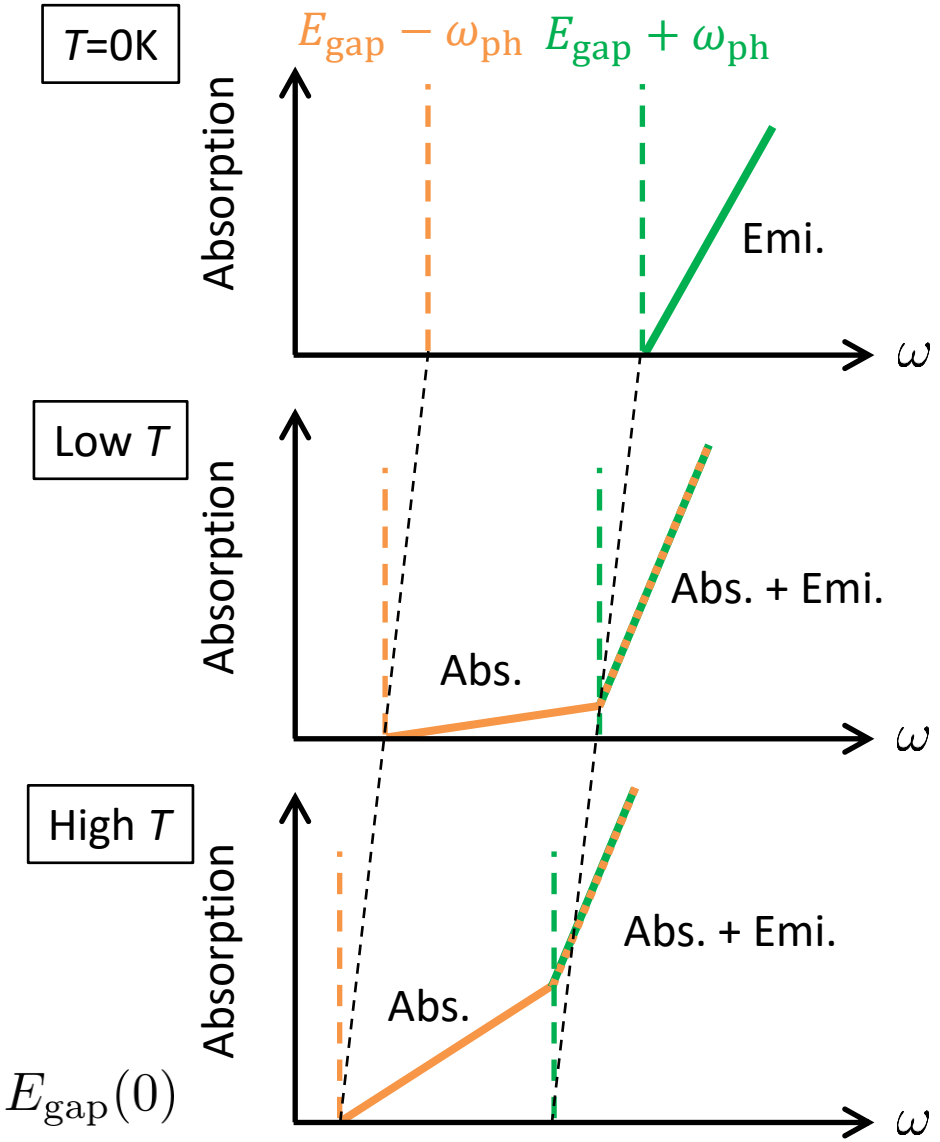


$\propto n_{\text{phonon}}$

Phonon emission
(At all temperatures)



$\propto n_{\text{phonon}} + 1$



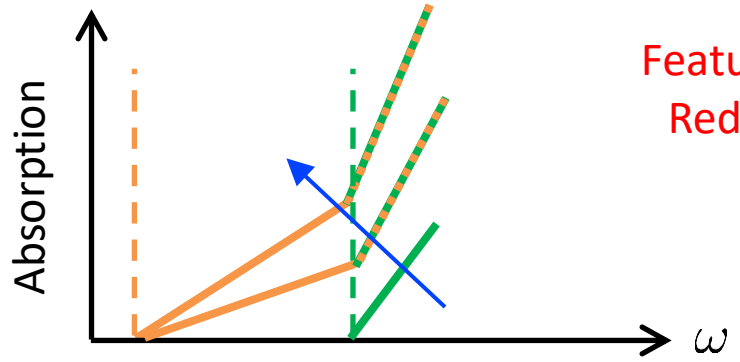
$$E_{\text{gap}}(T) < E_{\text{gap}}(0)$$

F. Bassani and G. P. Parravicini, *Electronic States and Optical Transitions in Solids*, Pergamon Press (1975)

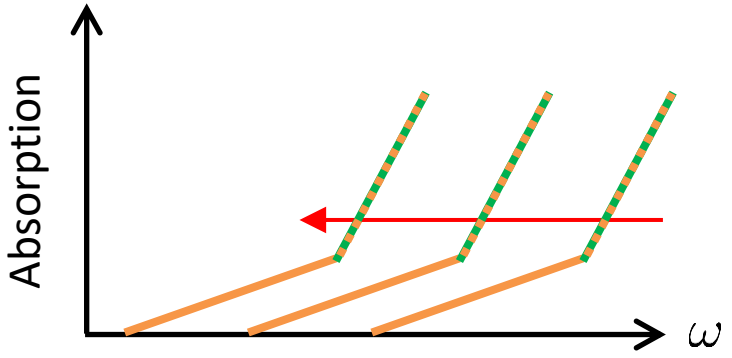
E. Kioupakis *et al.*, PRB **81**, 241201 (2010)

WFPT application: indirect optical absorption of silicon

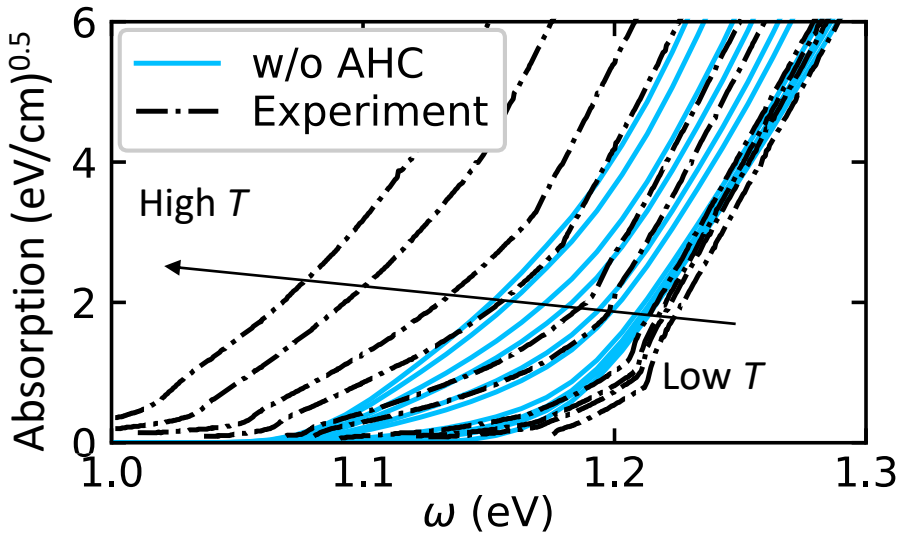
Feature (1)
Smoother kink



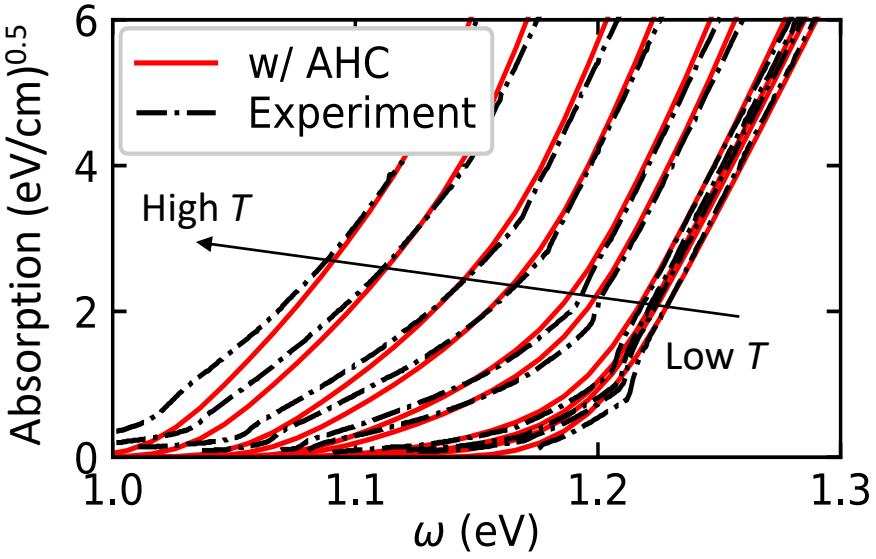
Feature (2)
Redshift



Without band structure renormalization



With band structure renormalization computed using WFPT



J.-M. Lihm and C.-H. Park, PRX **11**, 041053 (2021). Experiment: G. G. Macfarlane *et al.*, Phys. Rev. **111**, 1245 (1958)

Frequency-dependent self-energy and spectral functions

$$\Sigma_{m\mathbf{k}}(\omega) = \Sigma_{m\mathbf{k}}^{\mathrm{FM-Active}}(\omega) + \Sigma_{m\mathbf{k}}^{\mathrm{FM-Rest}} + \Sigma_{m\mathbf{k}}^{\mathrm{DW}}$$

$$\Sigma_{m\mathbf{k}}^{\mathrm{FM-Active}}(\omega) = \sum_{\pm} \sum_{\mathbf{q},\nu} \sum_{n}^{\mathrm{A}} \frac{\left| \langle \psi_{n\mathbf{k}+\mathbf{q}} | \frac{\partial \hat{V}}{\partial u_{\mathbf{q}\nu}} | \psi_{m\mathbf{k}} \rangle \right|^2}{\omega - (\varepsilon_{n\mathbf{k}+\mathbf{q}} \mp \omega_{\mathbf{q}\nu}) + i0^+} (n_{\mathbf{q}\nu} + \tfrac{1}{2} \pm (f_{n\mathbf{k}+\mathbf{q}} - \tfrac{1}{2}))$$

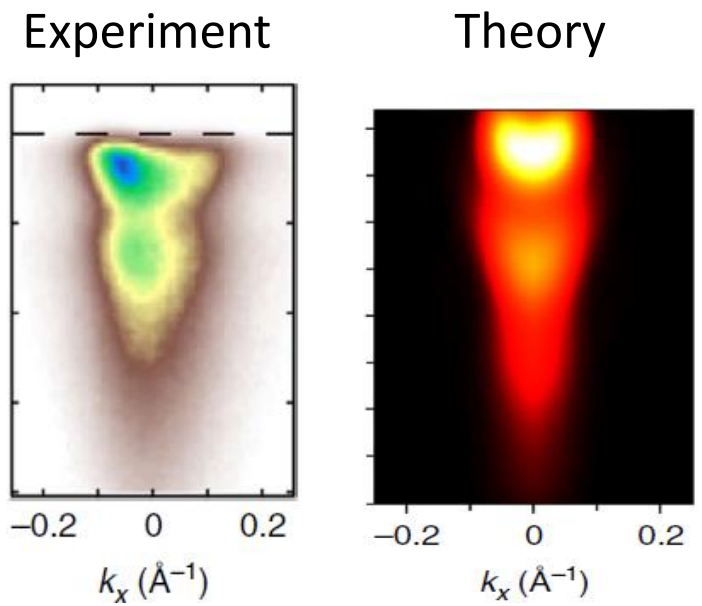
$$A_{m\mathbf{k}}(\omega) = -\frac{1}{\pi} \mathrm{Im} \frac{1}{\omega - \varepsilon_{m\mathbf{k}} - \Sigma_{m\mathbf{k}}(\omega)}$$

Example: ARPES spectra of anatase TiO2

Using cumulant expansion

F. Aryasetiawan *et al.*, PRL **77**, 2268 (1996)

S. Story *et al.*, PRB **90**, 195135 (2014)



C. Verdi *et al.*, Nat. Commun. **8**, 15769 (2017)

- Phonon-induced electron self-energy: Wannier function perturbation theory

- Electron-induced phonon self-energy: the two-temperature method

Phonon self-energy

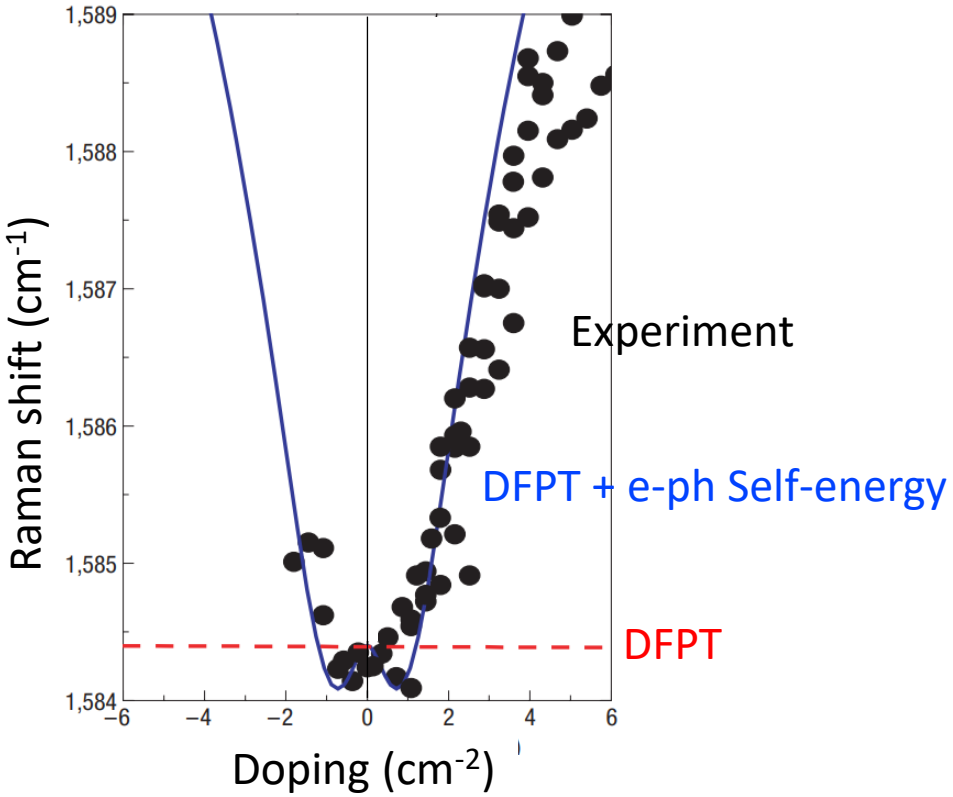
- Frequency-dependent dynamical matrix

$$D_{\mu\nu}(\mathbf{q},\omega) = \omega^2_{\mathbf{q}\nu}\delta_{\mu\nu} + \Delta\Pi_{\mu\nu}(\mathbf{q},\omega)$$

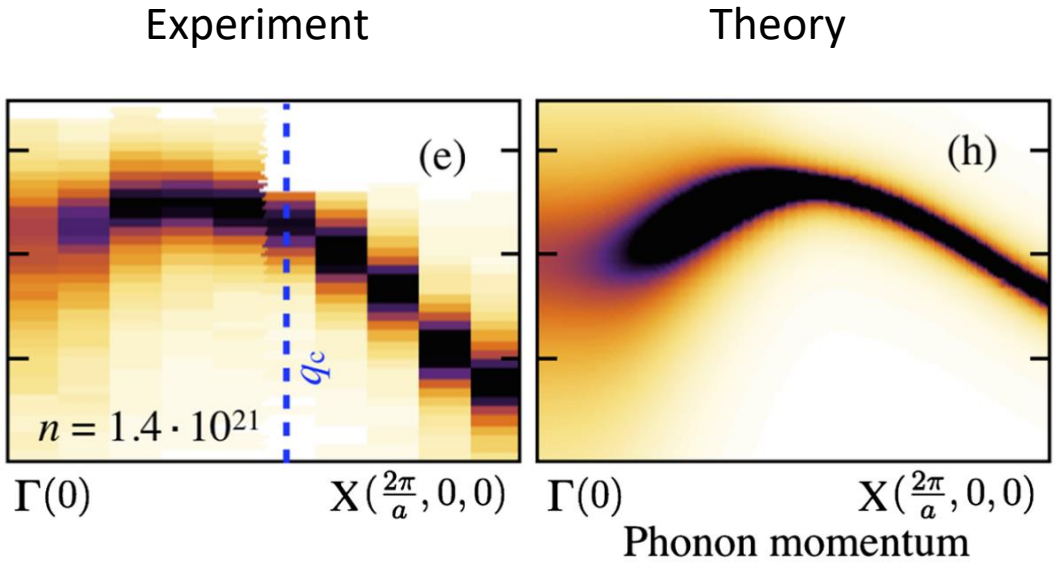
- Phonon spectral function

$$A(\mathbf{q},\omega) = -\frac{2\omega}{\pi}\,\mathrm{Im}\,\mathrm{Tr}\left[(\omega+i\eta)^2\delta_{\mu\nu} - D_{\mu\nu}(\mathbf{q},\omega)\right]^{-1}$$

Raman spectroscopy of doped graphene



Inelastic X-ray scattering of doped diamond



Other probes: neutron scattering, electron energy loss spectroscopy (EELS), infrared spectroscopy, …

S. Pisana *et al.*, Nat. Mater. **6**, 198 (2007), F. Caruso et al., PRL **119**, 017001 (2017)

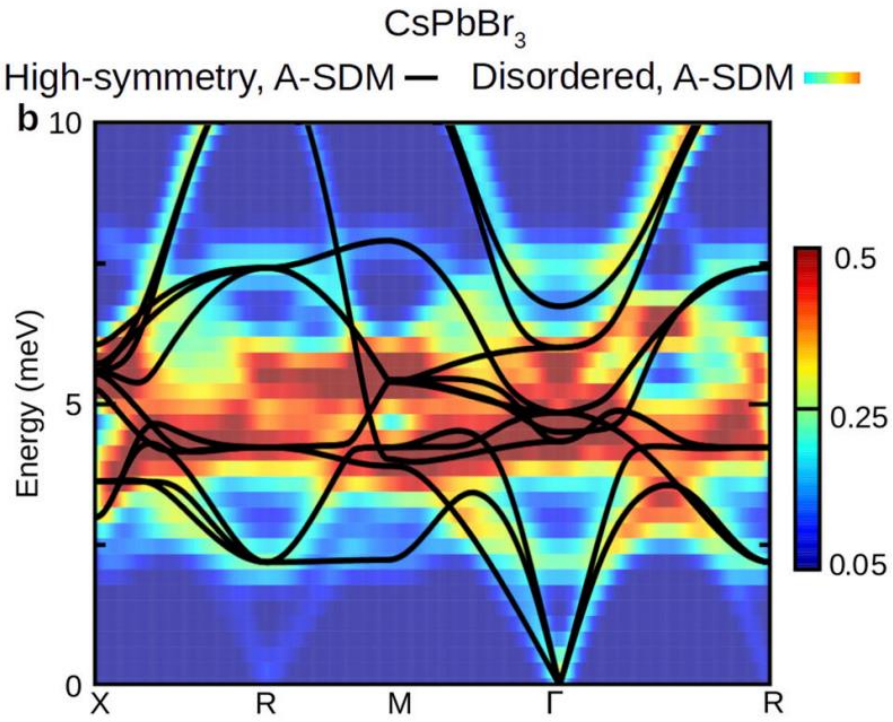
Contributions to phonon self-energy

1. Electron-phonon interaction
   - Doped semiconductors, metals.

2. Phonon-phonon interaction
   - Anharmonic materials, high temperature.

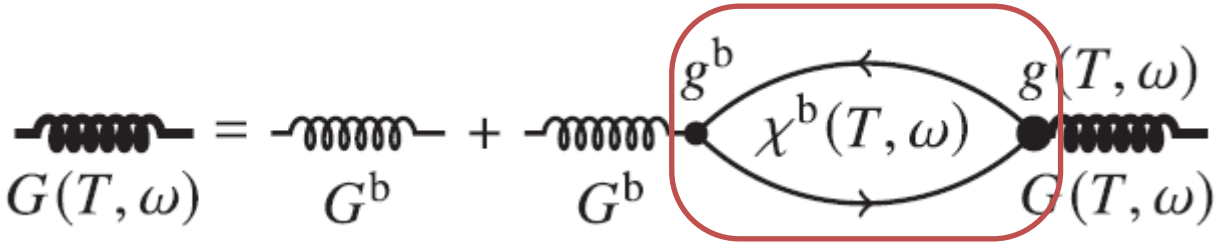
3. Disorder
   - Polymorphous structure, isotope mass disorder, …

TDEP



M. Zacharias *et al.*, npj Comput. Mater. **9**, 153 (2023)

Phonon self-energy from electron-phonon coupling



$$\Pi_{\mu\nu}(\mathbf{q},\omega;T) = \frac{1}{N_k}\sum_{mn\mathbf{kq}} [g^{\mathrm{b}}_{mn\mu}(\mathbf{k},\mathbf{q})]^* \frac{f_{n\mathbf{k}}(T) - f_{m\mathbf{k+q}}(T)}{\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k+q}} + \omega + i\eta} g_{mn\nu}(\mathbf{k},\mathbf{q},\omega;T)$$

J. Berges et al., PRX **13**, 041009 (2023)

Phonon self-energy: the “two temperatures” method

- In DFPT, we compute the phonon frequencies using a high temperature and ω = 0.
- In EPW, we want to compute the phonon dispersion at a low temperature and ω ≠ 0.
- We compute the self-energy at the two temperatures and take their difference.

$$\Delta\Pi_{\mu\nu}(\mathbf{q},\omega) = \frac{1}{N_k}\sum_{mn\mathbf{k}} \Delta\chi^0_{mn\mathbf{kq}}(\omega)[g_{mn\mu}(\mathbf{k},\mathbf{q})]^* g_{mn\nu}(\mathbf{k},\mathbf{q})$$

: Accurate up to $O(\Delta\chi^0)$

$$\Delta\chi^0_{mn\mathbf{kq}}(\omega; T^{\text{high}} \to T^{\text{low}}) = \chi^{0,\,\text{EPW}}_{mn\mathbf{kq}}(\omega; T^{\text{low}}) - \chi^{0,\,\text{DFPT}}_{mn\mathbf{kq}}(0; T^{\text{high}})$$

$$\chi^0_{mn\mathbf{kq}}(\omega; T) = \frac{f_{n\mathbf{k}}(T) - f_{m\mathbf{k+q}}(T)}{\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k+q}} + \omega + i\eta}$$

M. Calandra et al., PRB **82**, 165111 (2010), J. Berges et al., PRX **13**, 041009 (2023)

Summary

- Phonon-induced electron self-energy
  - Wannier function perturbation theory enables an efficient and accurate calculation of the electron self-energy using EPW.
  - The theory can be used to simulate ARPES experiments.

- Electron-induced phonon self-energy
  - EPW can compute phonon self-energy and spectral function induced by electron-phonon coupling.
  - The two-temperature method is an accurate approximation to the dynamical, low-*T* self-energy.

References

- Allen-Heine-Cardona theory
  - P. B. Allen *et al*., J. Phys. C **9**, 2305 (1976), PRB **23**, 1495 (1981), PRB **27**, 4760 (1983)
  - F. Giustino, Rev. Mod. Phys. **89**, 015003 (2017)

- Debye-Waller self-energy
  - X. Gonze *et al*., Ann. Phys. **523**, 1, 168 (2011), J.-M. Lihm and C.-H. Park, PRB **101**, 121102 (2020)

- Wannier function perturbation theory
  - J.-M. Lihm and C.-H. Park, PRX **11**, 041053 (2021)

- Electron-induced phonon self-energy
  - M. Calandra *et al*., PRB **82**, 165111 (2010), J. Berges *et al*., PRX **13**, 041009 (2023)

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Institute of Condensed Matter and Nanosciences

Tutorial Sat.5

Wannier function perturbation theory & electron-induced phonon self-energy

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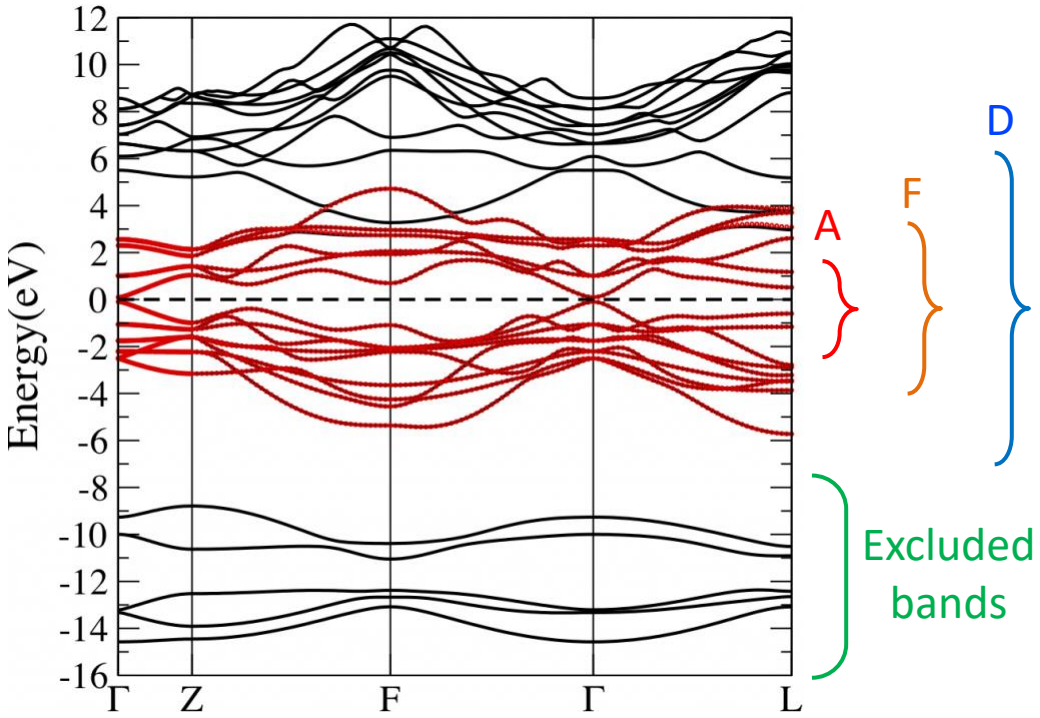
Wannier function perturbation theory: three windows



Window arguments for WFPT

The three windows should follow the following relation:

Active space ⊂ Frozen ⊂ Disentanglement

1. Active space window (AHC window): `ahc_win_min, _max`
This window should contain all states you want to compute the self-energy.

2. Frozen window (inner window): `dis_froz_min, _max`

3. Disentanglement window (outer window): `dis_win_min, _max`

Number of bands argument for WFPT

- ahc_nbnd: The number of bands in the disentanglement (outer) window (NOT the number of Wannier functions)
- ahc_nbndskip: The number of low-energy bands excluded from Wannierization

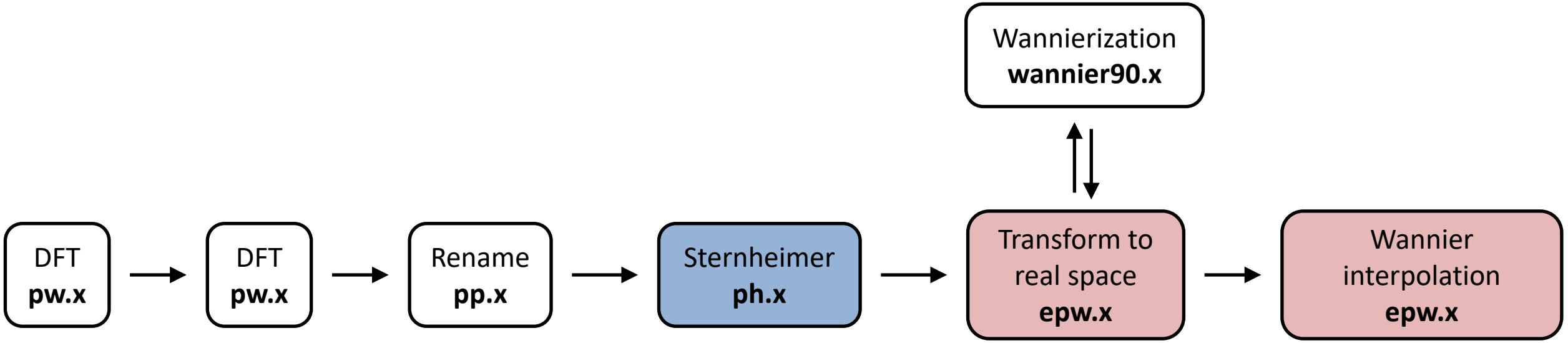
Example) 5 semicore bands to exclude, 10 valence/conduction bands Wannierized into 8 Wannier functions

`nscf.in:` nbnd = 15

`ahc.in:` ahc_nbndskip = 5; ahc_nbnd = 10

`epw.in:` ahc_nbndskip = 5; ahc_nbnd = 10; bands_skipped = 'exclude_bands = 1:5'; nbndep = 8

Electron self-energy: Workflow for Wannier function perturbation theory



New input parameters for **ph.x**

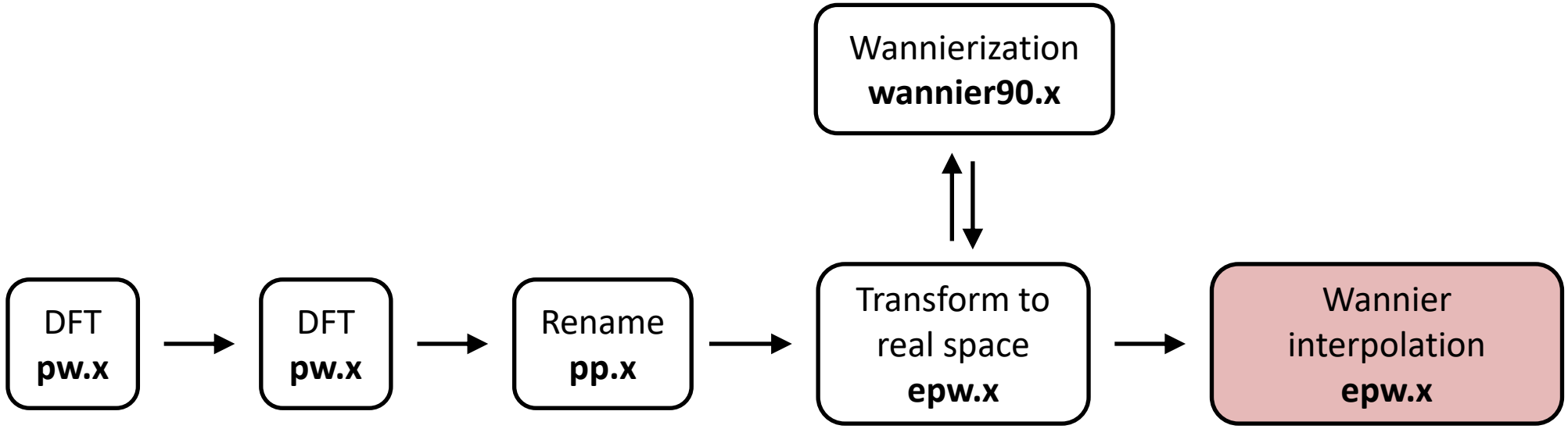
```
electron_phonon = 'ahc'
trans = .false.
ahc_nbnd = 8
ahc_dir = './save/ahc_dir/'
```

New input parameters for **epw.x**

```
! --- For WFPT ---
lwfpt = .true.
ahc_nbnd = 8
ahc_win_max = 23.0
ahc_win_min = -100.0
```

```
! --- For electron self-energy ---
elecselfen = .true.
filkf = './kpt.txt'
nqf1 = 10
nqf2 = 10
nqf3 = 10
degaussw = 0.02 ! eV
temps = 0.0 ! Kelvin
```

Phonon spectral function workflow



New input parameters for **epw.x**

```
! --- For phonon spectral function ---
specfun_ph = .true.
filqf = './qpt.txt'
nkf1 = 10
nkf2 = 10
nkf3 = 10
```

```
wmin_specfun = 0.00 ! eV
wmax_specfun = 0.12 ! eV
nw_specfun = 200
degaussw = 0.05 ! eV
temps = 300.0 3157.75 ! Kelvin (0.02 Ry = 3157.75 K)
```