School on Wannier90 v3.0: new features and applications

25-27th March 2020 – Virtual Edition

Electron-phonon coupling and the EPW code

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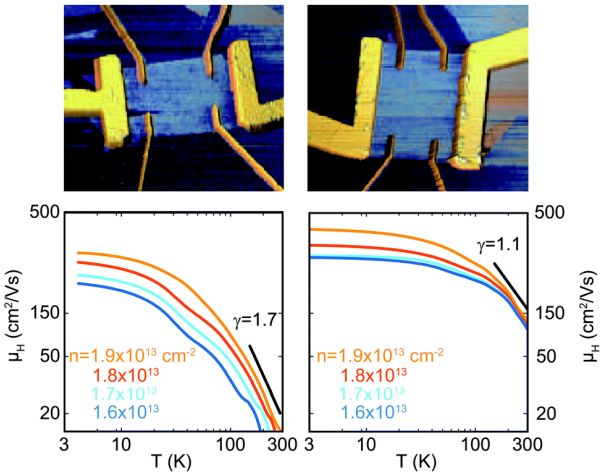
Lecture Summary

- Manifestations of the electron-phonon interaction
- The electron-phonon matrix element
- Brillouin-zone integrals and Wannier interpolation
- Migdal-Eliashberg theory of superconductivity
- Boltzmann transport equation

Why electron-phonon interactions are important?

Some manifestations of electron-phonon interactions

Electron mobility in monolayer and bilayer MoS_2



Nano Lett. 13, 4212 (2013)

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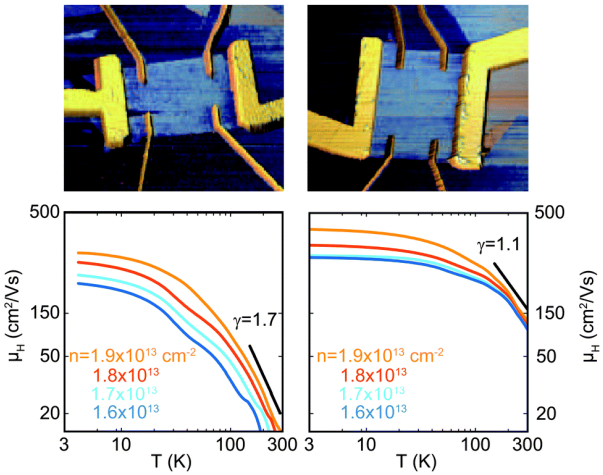

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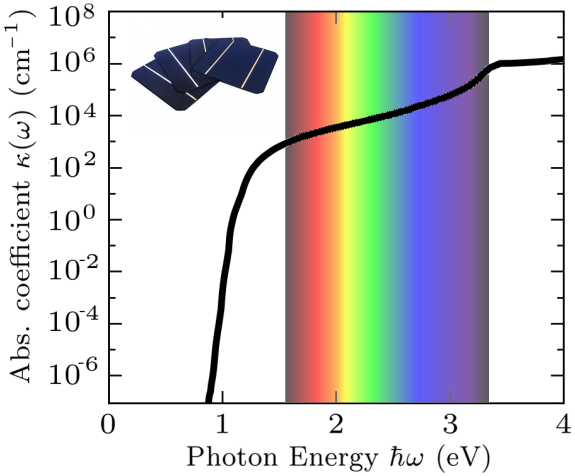
Phonon-assisted optical absorption in silicon



Prog. Photovolt. Res. Appl. 3, 189 (1995)

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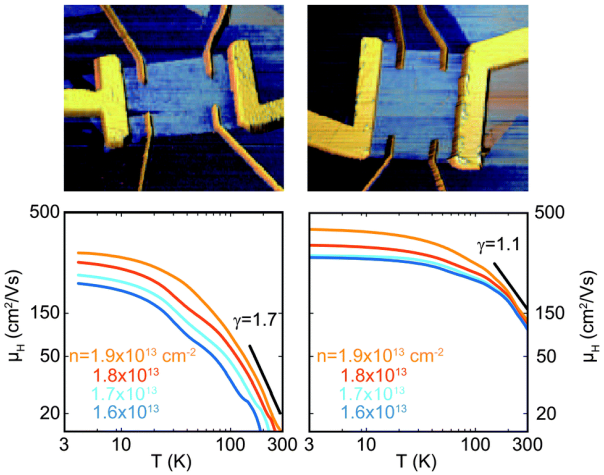

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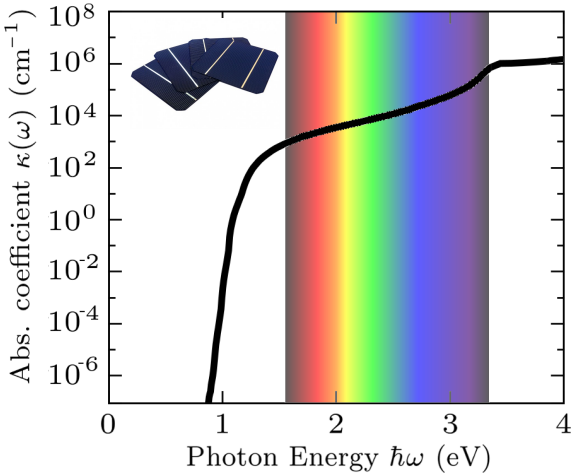

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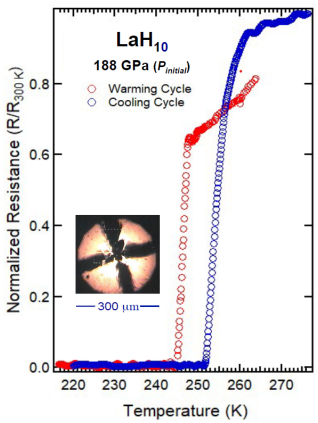
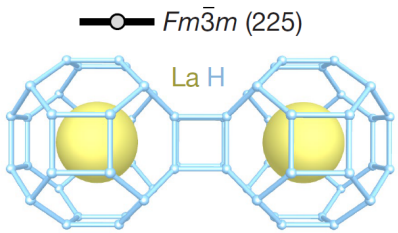
Superconductivity in compressed $LaH_{10\pm x}$





PRL 122, 027001 (2019)

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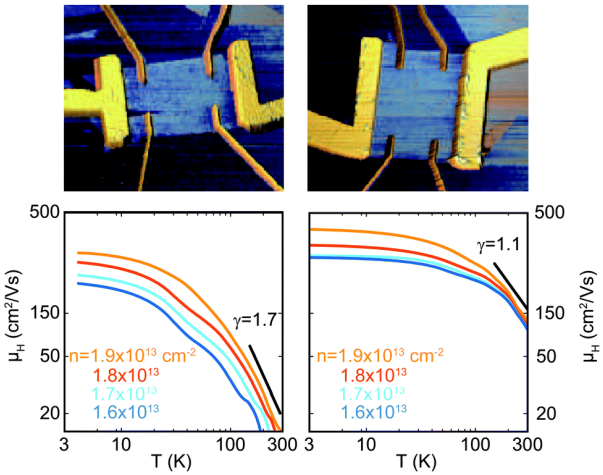

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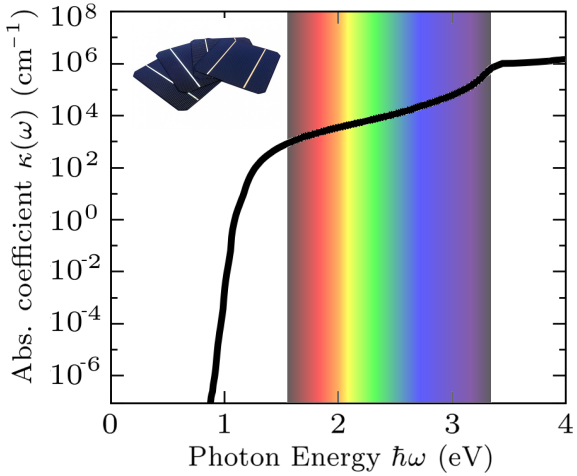

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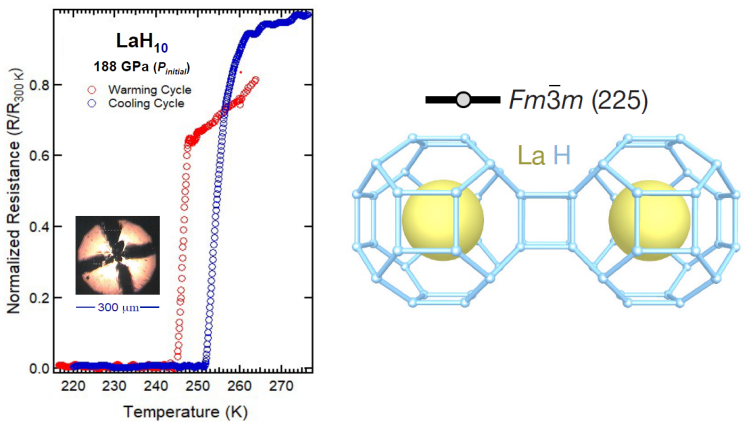

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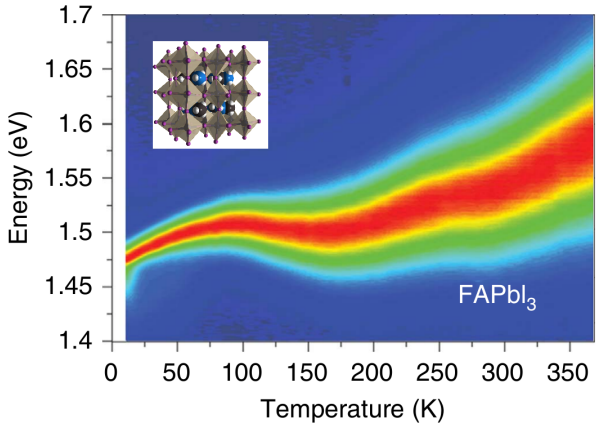
Photoluminescence in hybrid perovskites



Nat. Commun. 7, 11755 (2016)

The electron-phonon matrix element

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$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = \langle u_{m\mathbf{k}+\mathbf{q}} | \Delta_{\mathbf{q}\nu} v_{\mathrm{SCF}} | u_{n\mathbf{k}} \rangle_{\mathrm{uc}}$$

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α Cartesian direction
p Unit cell in the equivalent supercell

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Displacement of a single ion

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Incommensurate modulation

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Brillouin-zone integrals

Example: electron lifetimes in metals, adiabatic approximation

$$\frac{1}{\tau_{n\mathbf{k}}} = 2k_{\mathrm{B}}T\,\frac{2\pi}{\hbar}\sum_{m\nu}\int_{\mathrm{BZ}}\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2}{\hbar\omega_{\mathbf{q}\nu}}\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}})$$

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- A new integral must be evaluated for every $\mathbf{k}$-vector

Wannier interpolation of electron-phonon matrix elements

Wannier functions

$$\mathrm{w}_{mp}(\mathbf{r}) = \frac{1}{N_p} \sum_{n\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_p} U_{nm\mathbf{k}} \, \psi_{n\mathbf{k}}(\mathbf{r})$$

N. Marzari et al., Rev. Mod. Phys. 84, 1419 (2012)

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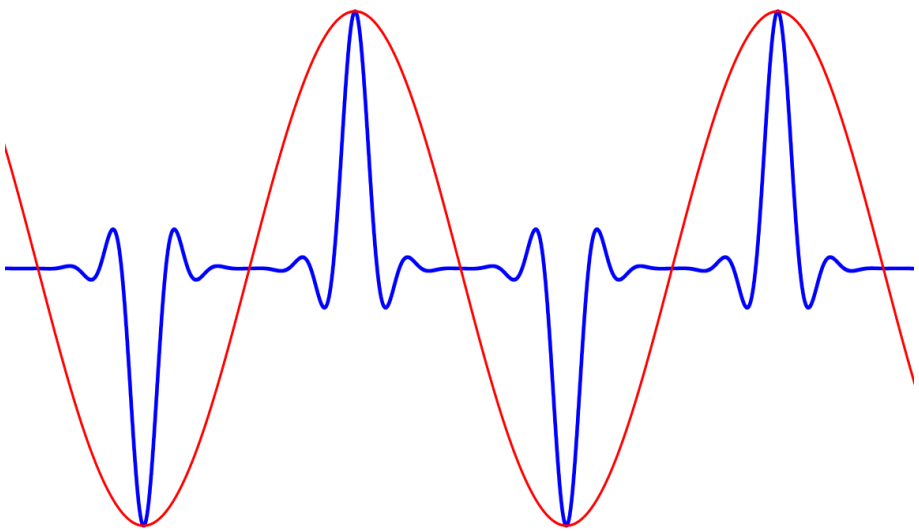

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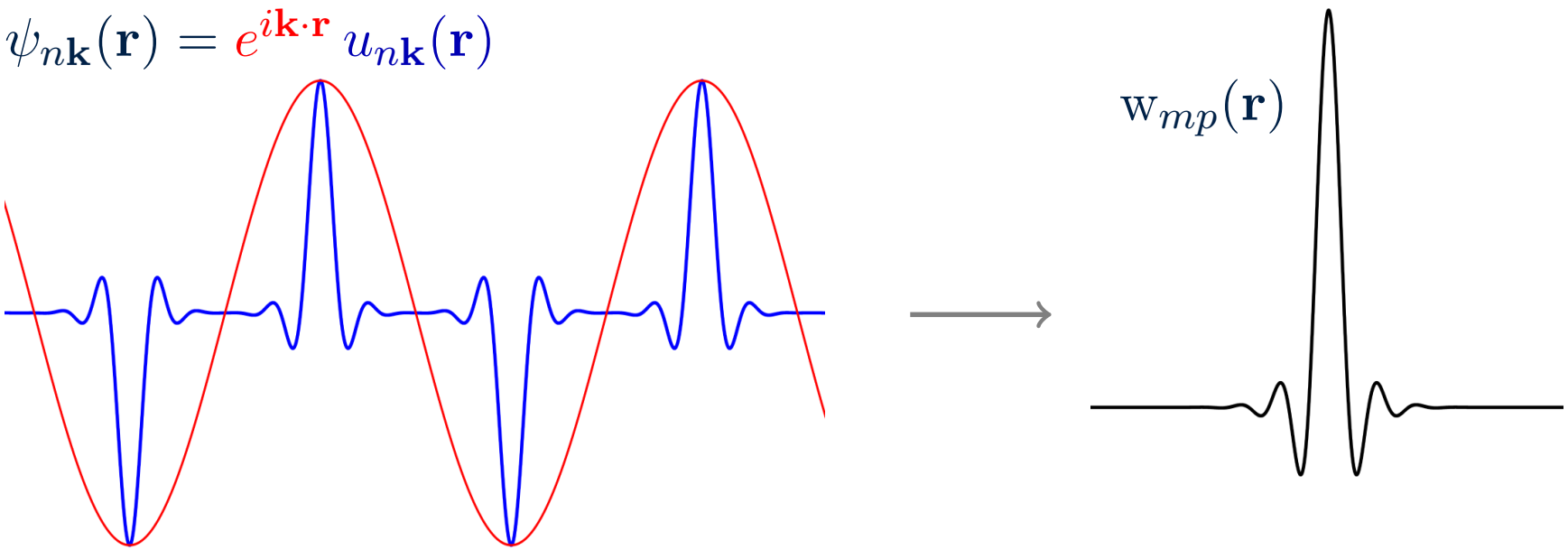

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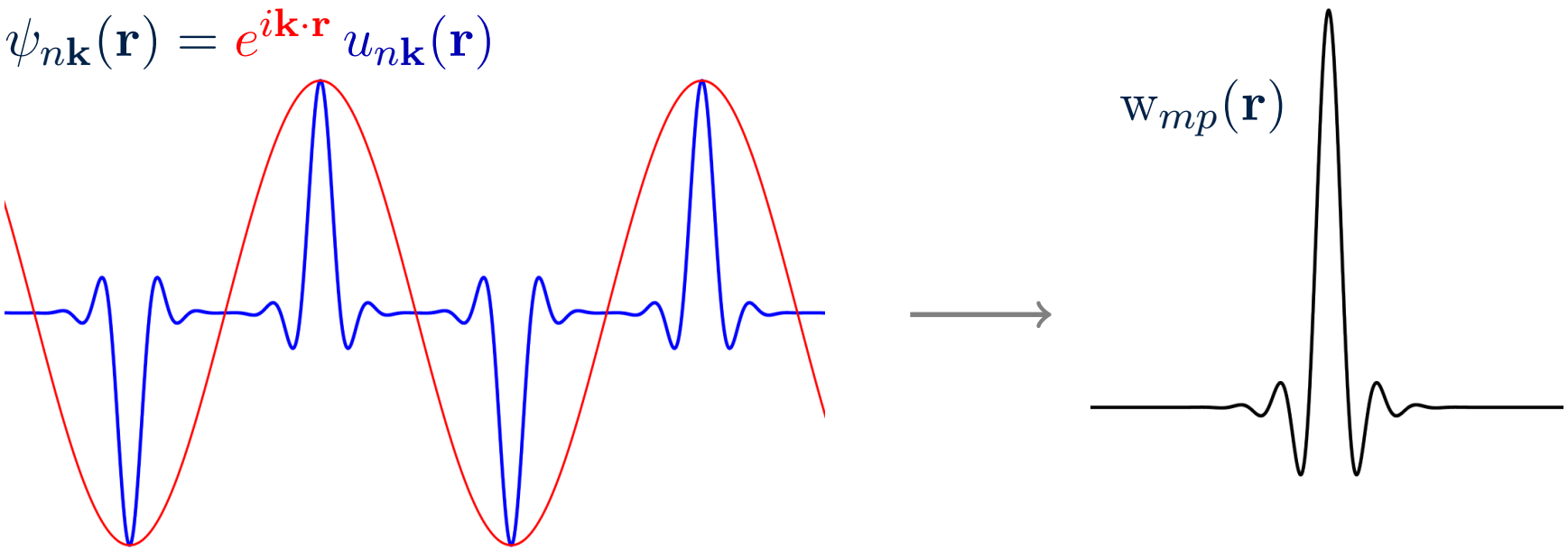

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Wannier interpolation of electron-phonon matrix elements

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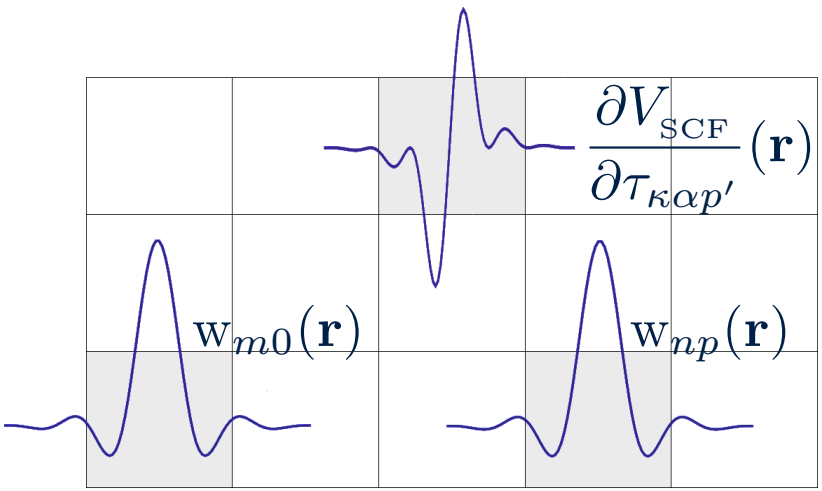

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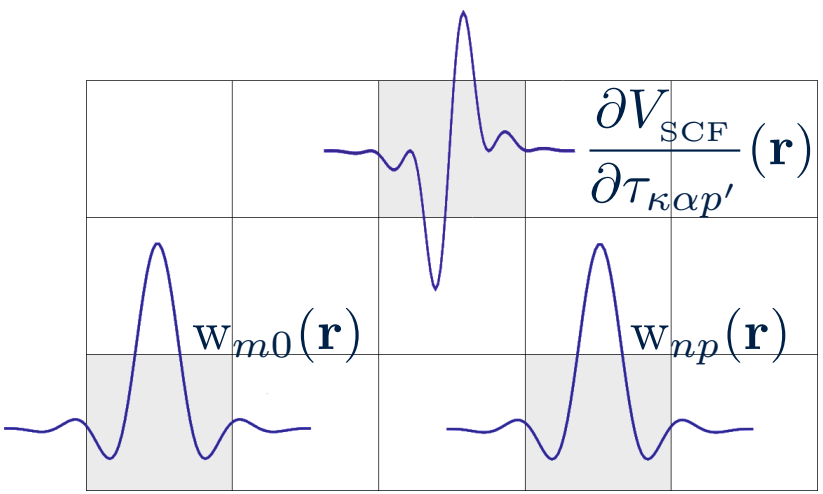
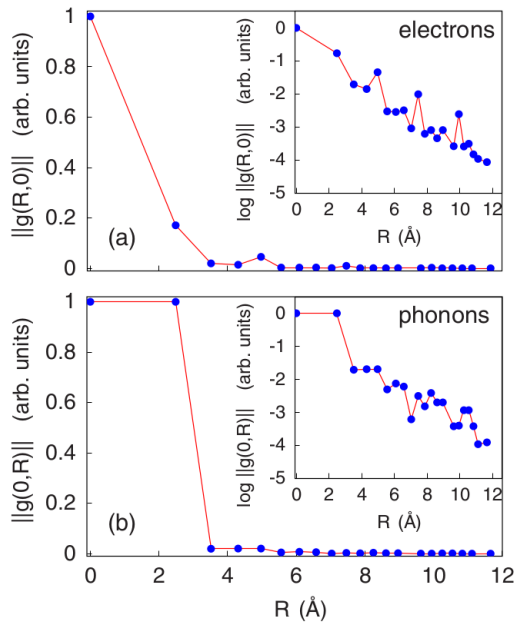
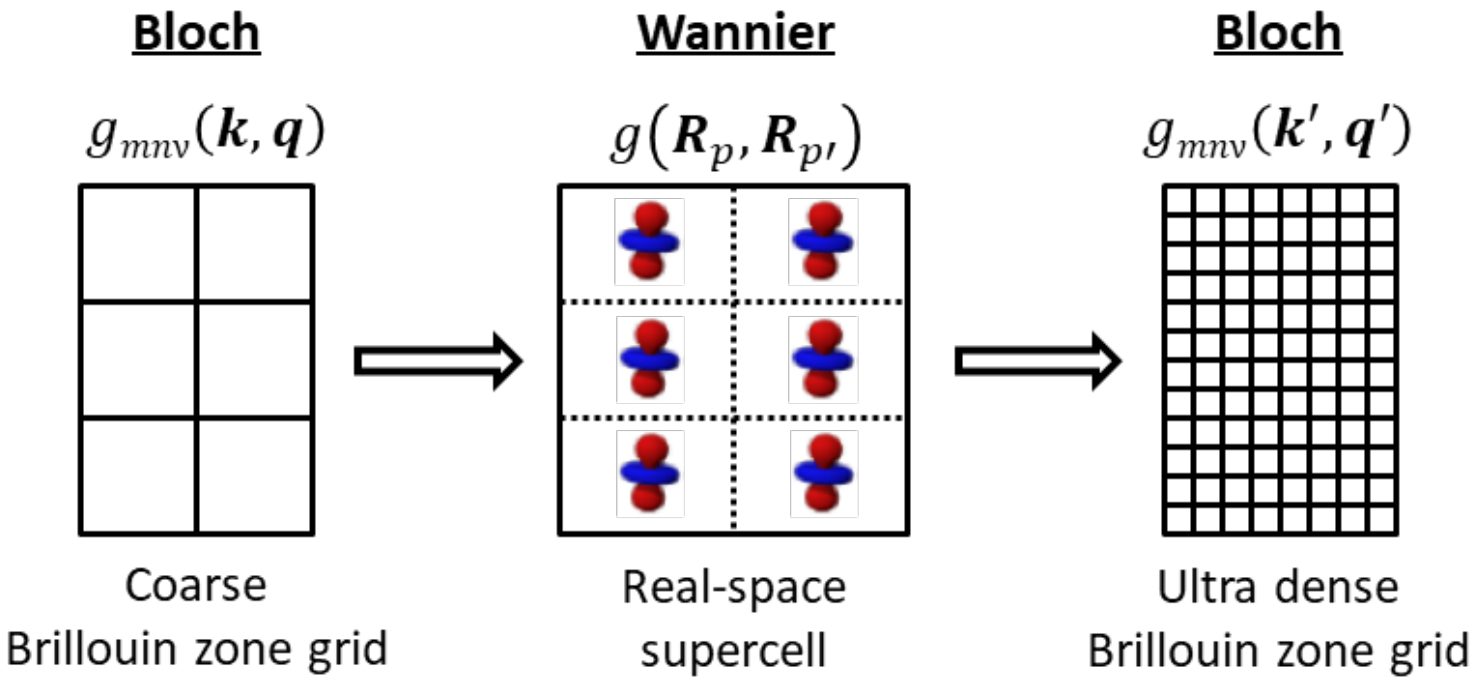




Figures from Giustino et al, Phys. Rev. B 76, 165108 (2007)

EPW software



Electron-phonon Wannier (`EPW`) is a free GPL Fortran software, part of `Qunatum-Espresso`, that relies on maximally localized Wannier functions (MLWF) to interpolate electron-phonon matrix elements on ultra dense momentum grids.

The electron-phonon interaction in polar materials

The electron-phonon matrix element in polar materials

- Wannier interpolation in the presence of Fröhlich interactions

  In polar materials, $g_{mn,\nu}(\mathbf{k},\mathbf{q})$ diverges as $1/|\mathbf{q}|$ for $|\mathbf{q}| \to \mathbf{0}$
  Split the electron-phonon matrix elements into a short- ($\mathcal{S}$) and a long-range ($\mathcal{L}$) contribution:

$$g(\mathbf{k},\mathbf{q}) = g^{\mathcal{S}}(\mathbf{k},\mathbf{q}) + g^{\mathcal{L}}(\mathbf{k},\mathbf{q})$$

Verdi and Giustino, Phys. Rev. Lett. 115, 176401 (2015)

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$$g^{\mathcal{L}}(\mathbf{k},\mathbf{q}) = i\frac{4\pi}{\Omega}\frac{e^2}{4\pi\varepsilon_0}\sum_{\kappa}\left(\frac{\hbar}{2N_p M_\kappa\,\omega_{\mathbf{q}}}\right)^{\frac{1}{2}} \times$$

$$\sum_{\mathbf{G}\neq-\mathbf{q}} \frac{(\mathbf{q}+\mathbf{G})\cdot\mathbf{Z}^*_\kappa\cdot\mathbf{e}_\kappa(\mathbf{q})}{(\mathbf{q}+\mathbf{G})\cdot\boldsymbol{\epsilon}^\infty\cdot(\mathbf{q}+\mathbf{G})}\langle\psi_{\mathbf{k}+\mathbf{q}}|e^{i(\mathbf{q}+\mathbf{G})\cdot(\mathbf{r}-\boldsymbol{\tau}_\kappa)}|\psi_{\mathbf{k}}\rangle_{\mathrm{sc}}$$

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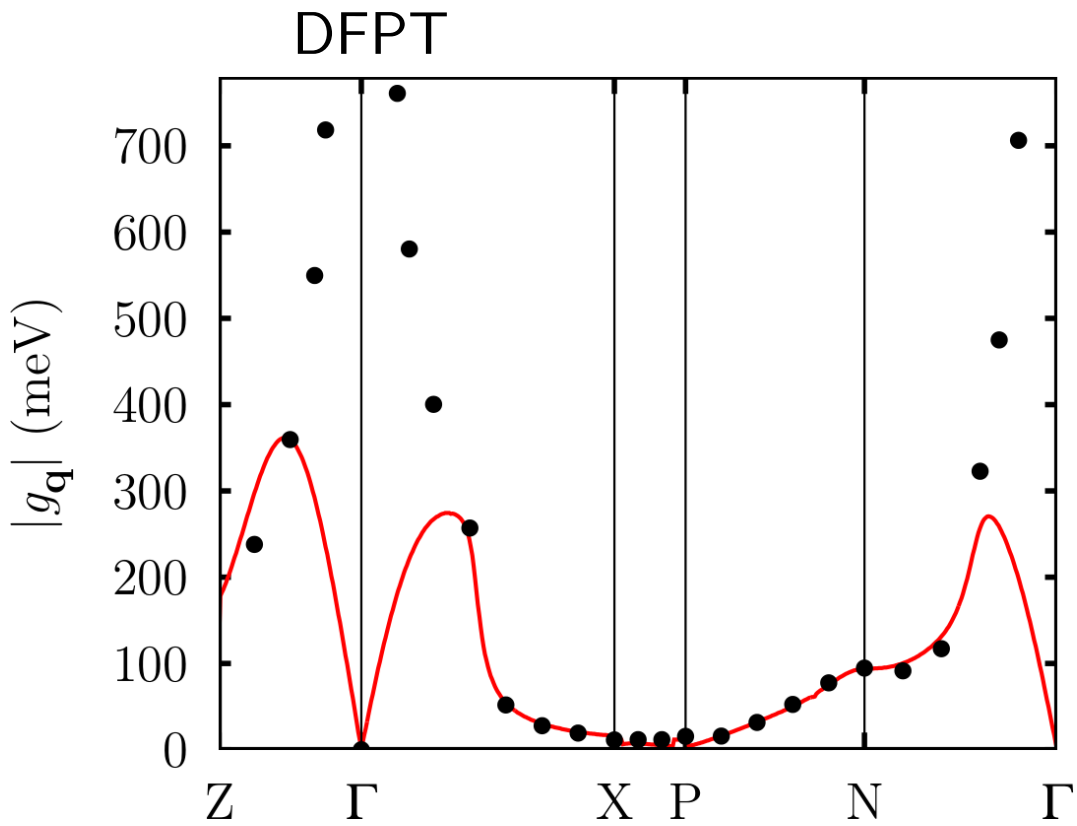

EPW without Fröhlich long-range

Figure from Verdi and Giustino, Phys. Rev. Lett. 115, 176401 (2015)

The electron-phonon matrix element in polar materials

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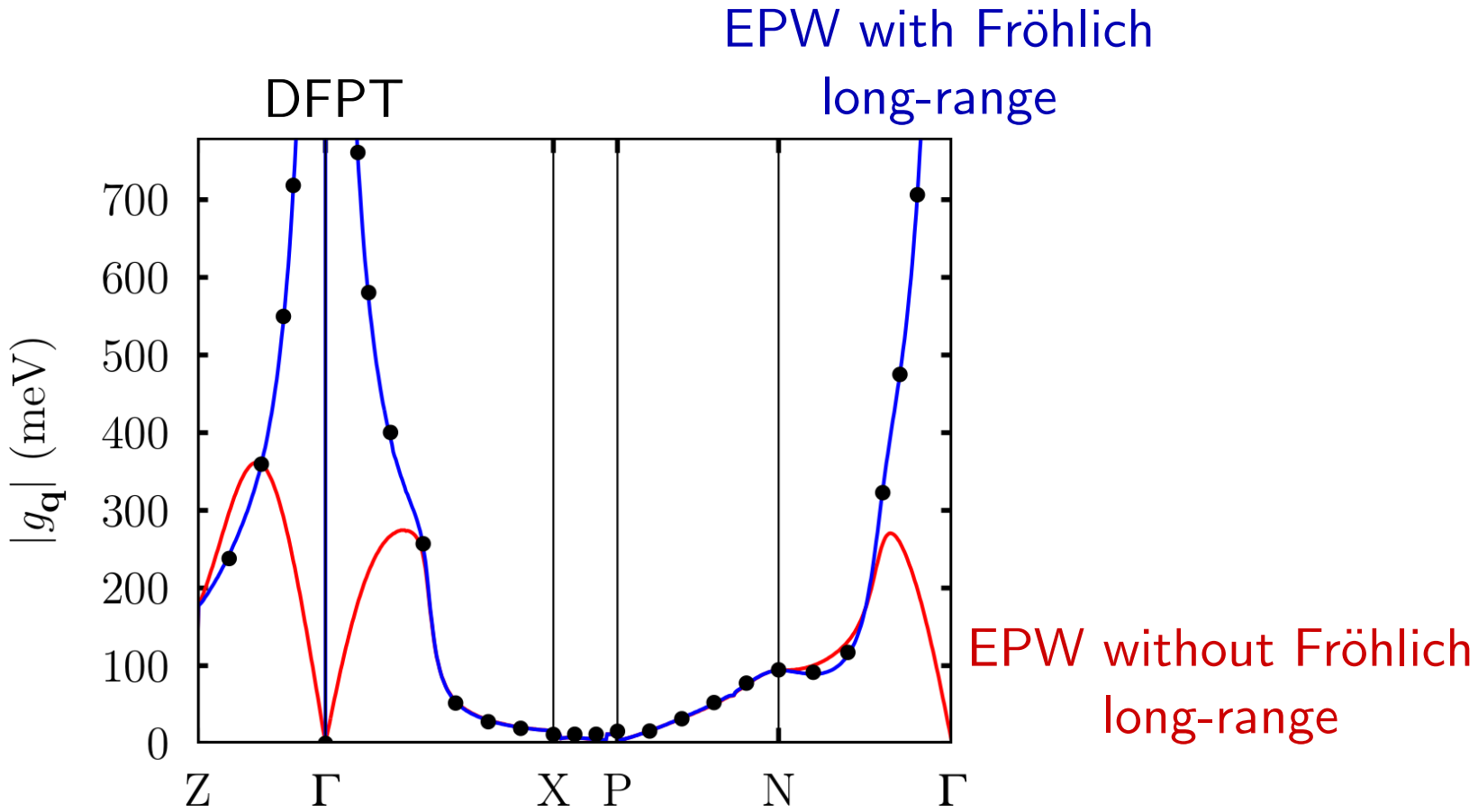

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Phonon-mediated superconductivity

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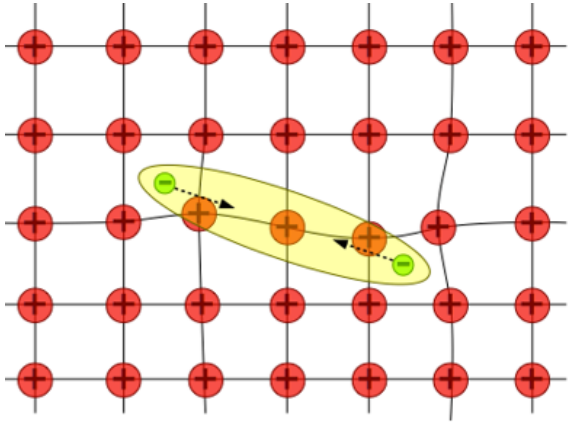

electron Cooper pairs in a lattice

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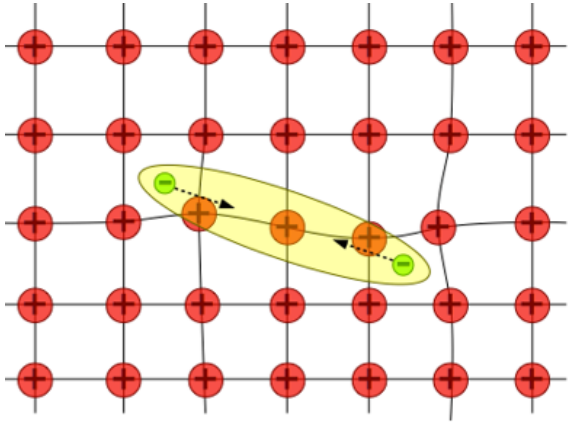

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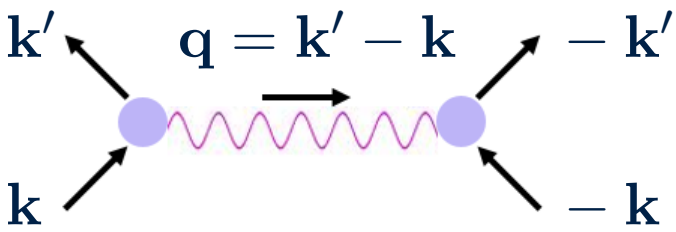
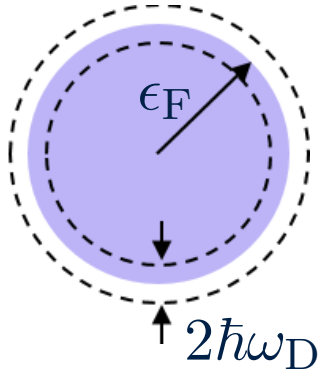
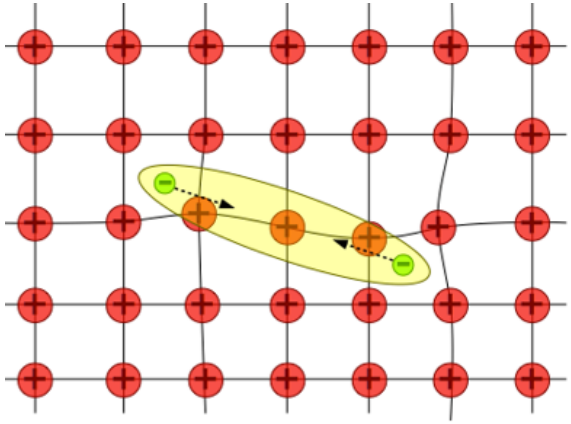


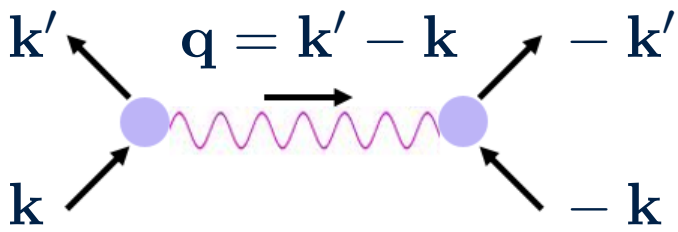


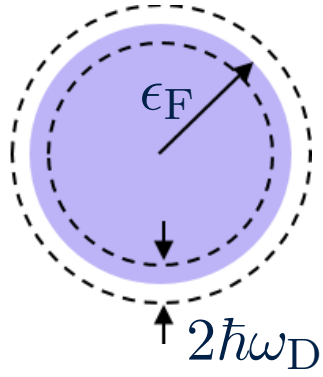
exchange of virtual phonons produces an attraction for electrons close to Fermi level

Phonon-mediated superconductivity



electron Cooper pairs in a lattice





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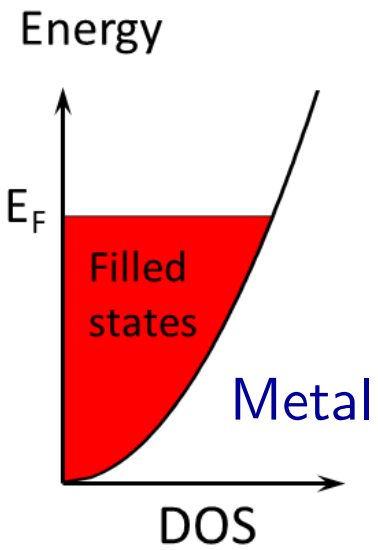
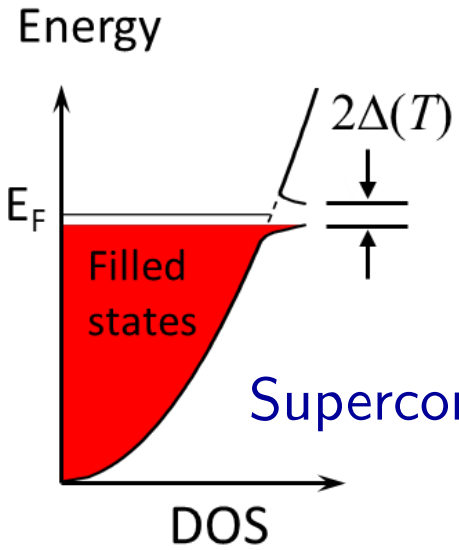
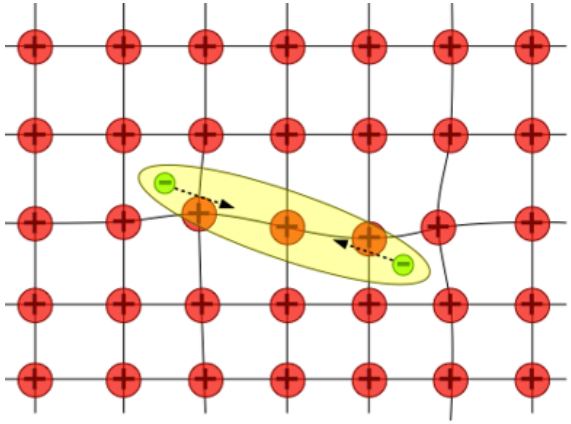


Metal



Superconductor

Phonon-mediated superconductivity



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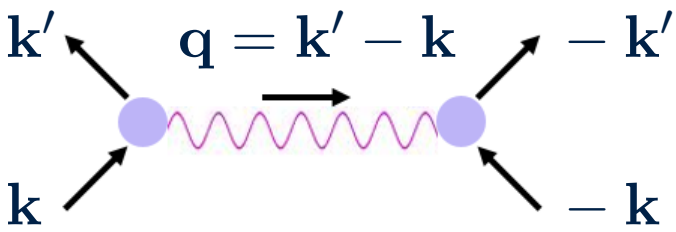

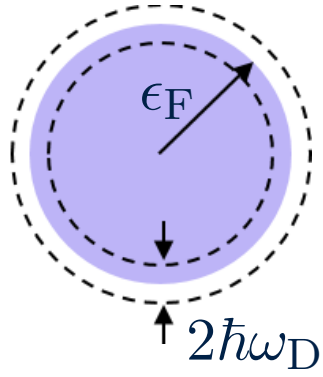

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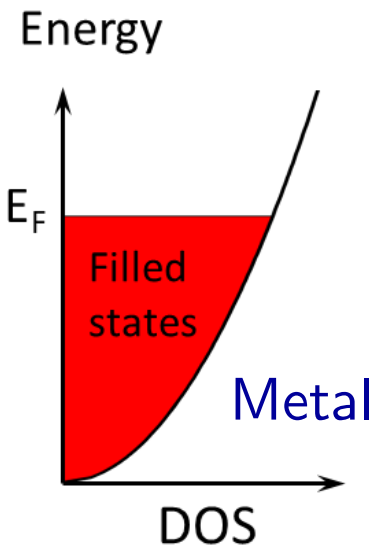

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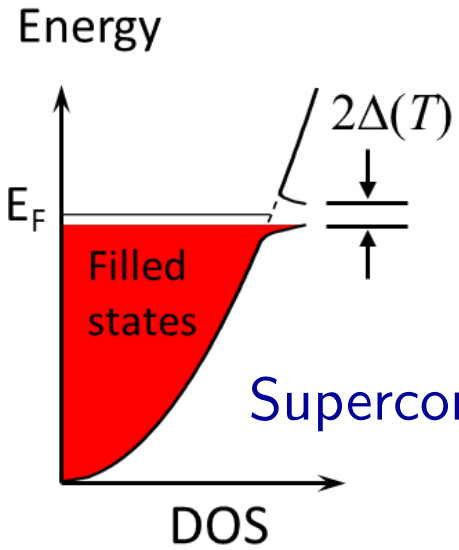
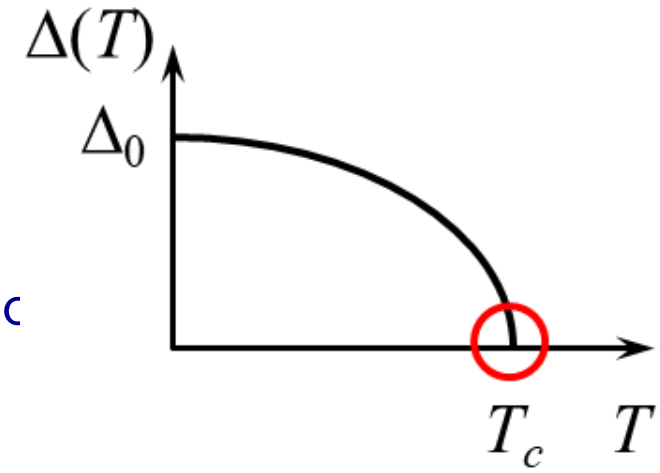


Superconduc



Migdal-Eliashberg theory

paring self-energy

dressed phonon propagator

screened Coulomb interaction

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = g_{nm\nu}(\mathbf{q},\mathbf{k})\, D_{\mathbf{q}\nu}(i\omega_j - i\omega_{j'})\, \hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\, g_{mn\nu}(\mathbf{k},\mathbf{q}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'})\, \hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})$$

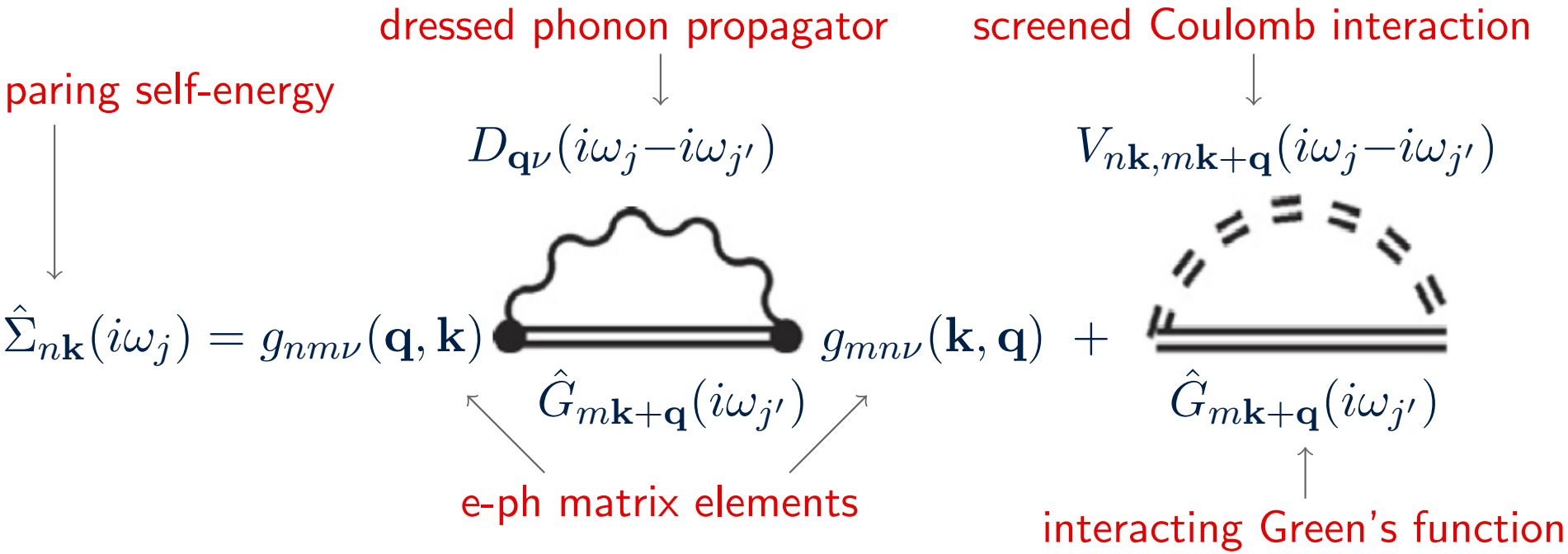
e-ph matrix elements

interacting Green's function

Allen and Mitrović, Solid State Phys. 37, 1 (1982);

Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Migdal-Eliashberg theory



Migdal's theorem

Only the leading terms in Feynman diagram of the self-energy are included.

The neglected terms are of the order of $(m_{\mathrm{e}}/M)^{1/2} \propto \omega_{\mathrm{D}}/\epsilon_{\mathrm{F}}$.

Allen and Mitrović, Solid State Phys. 37, 1 (1982);

Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Anisotropic Migdal-Eliashberg equations

$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{\pi T}{\omega_j N_\mathrm{F}} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_\mathrm{BZ}} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}}$$

mass renormalization function

$$\times \lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_\mathrm{F})$$

$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{N_\mathrm{F}} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_\mathrm{BZ}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}}$$

superconducting gap function

$$\times \left[\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - \mu_\mathrm{c}^*\right] \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_\mathrm{F})$$

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superconducting gap function

$$\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j) = N_\mathrm{F} \sum_\nu \int_0^\infty d\omega \frac{2\omega}{\omega_j^2 + \omega^2} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \delta(\omega - \omega_{\mathbf{q}\nu})$$

anisotropic e-ph coupling strength

Anisotropic Migdal-Eliashberg equations

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anisotropic e-ph coupling strength

$i\omega_j = i(2j+1)\pi T$ (j integer) are Matsubara frequencies

Anisotropic Migdal-Eliashberg equations

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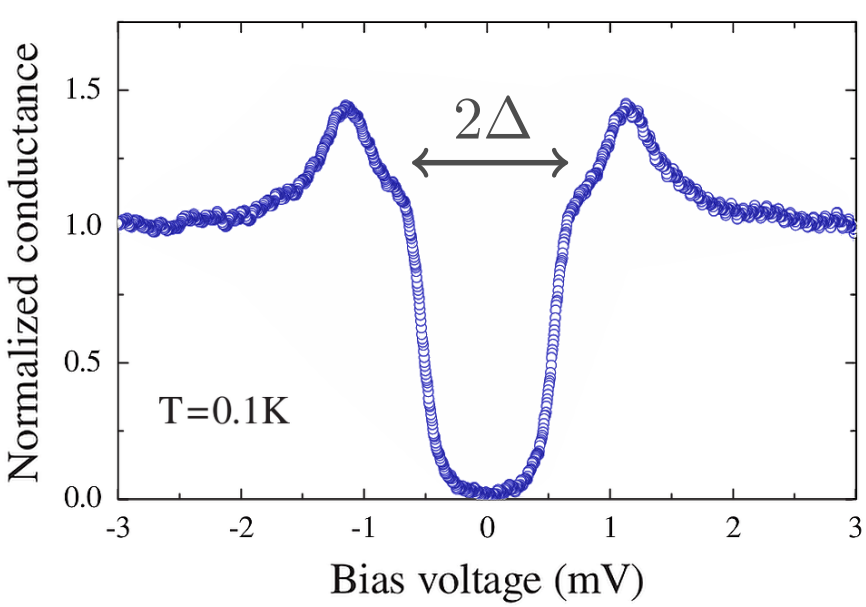
- The equations must be evaluated on dense electron $\mathbf{k}$- and phonon $\mathbf{q}$-meshes to properly describe anisotropic effects
- The sum over Matsubara frequencies must be truncated (typically set to four to ten times the largest phonon energy)
- $Z_{n\mathbf{k}}$ and $\Delta_{n\mathbf{k}}$ are only meaningful for $n\mathbf{k}$ at or near the Fermi surface

Superconductivity in 2H-NbS_2

Scanning tunneling spectra of 2H-NbS_2



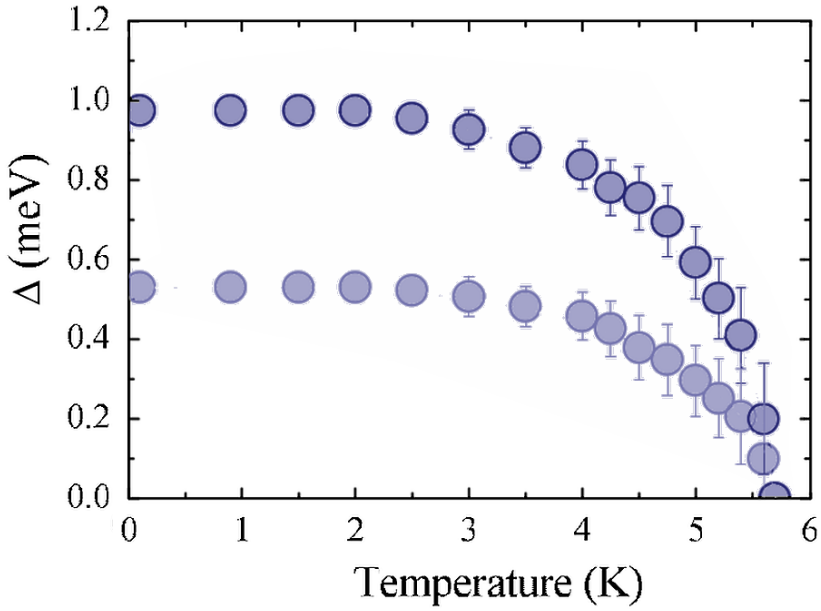


Figure from Guillamón et al, Phys. Rev. Lett. 101, 166407 (2008)

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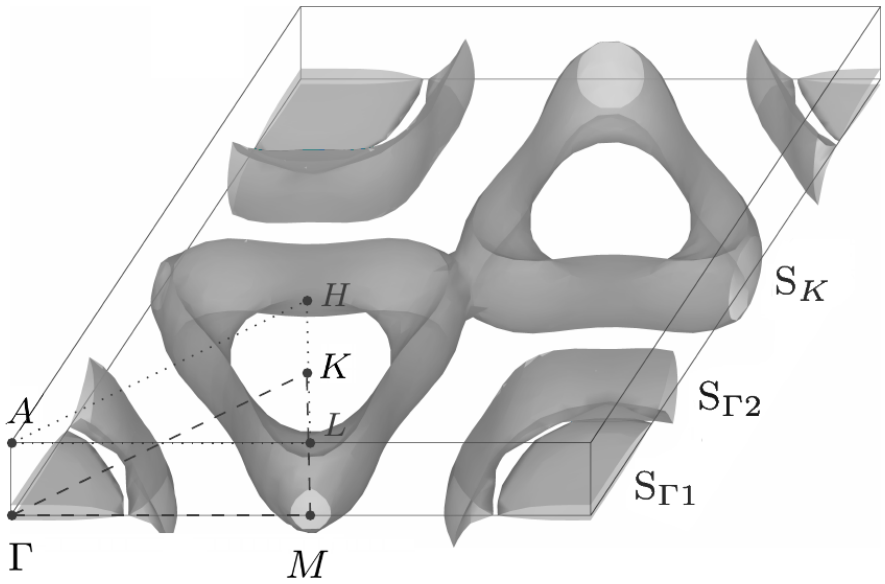

Heil, Poncé, Lambert, Schlipf, Margine, and Giustino, Phys. Rev. Lett., 119, 087003 (2017)

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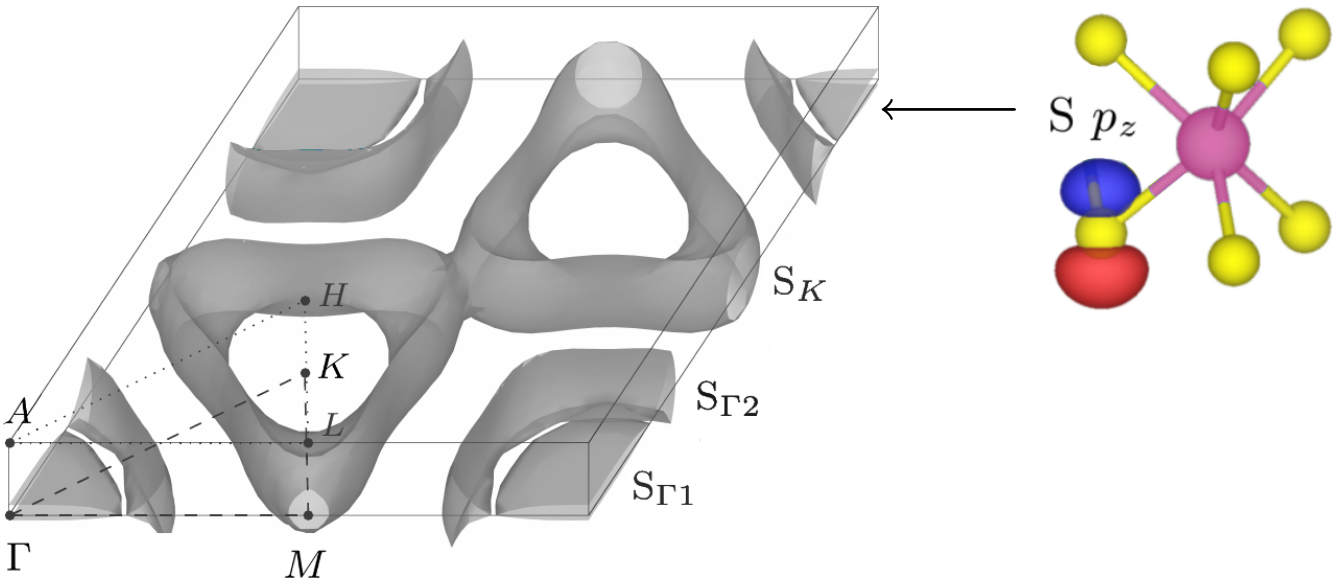

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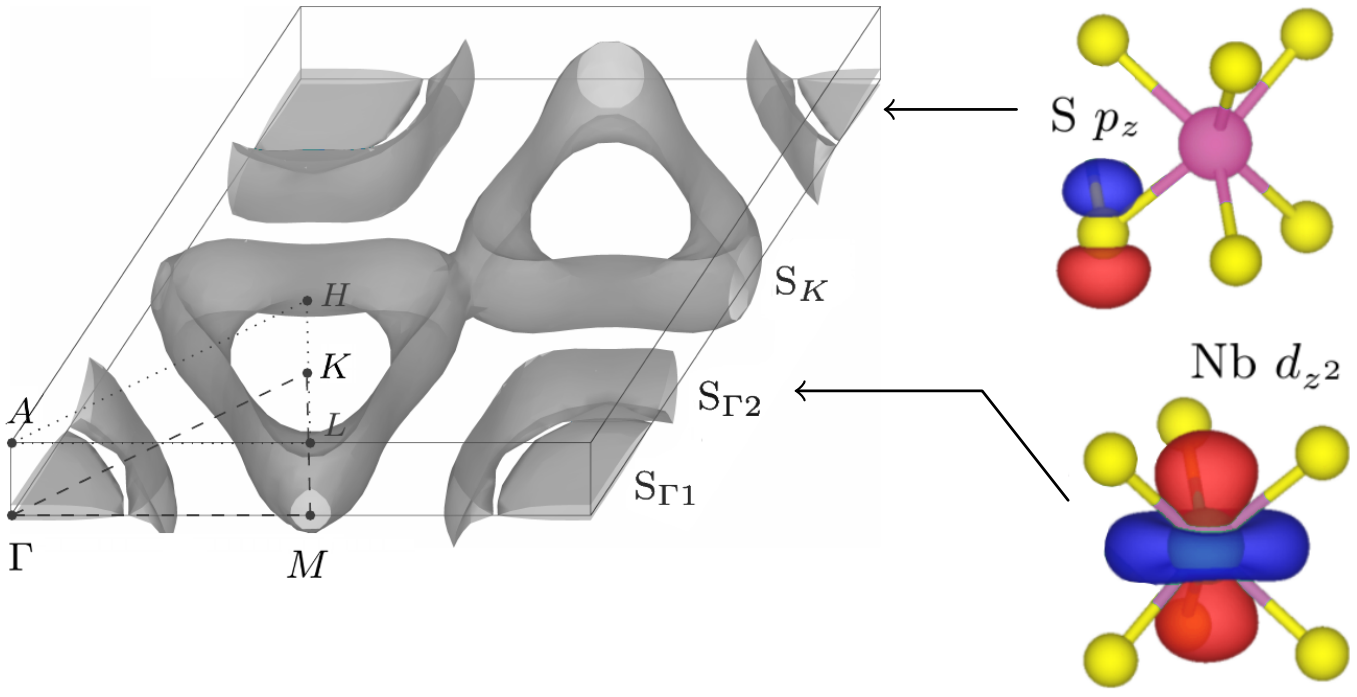

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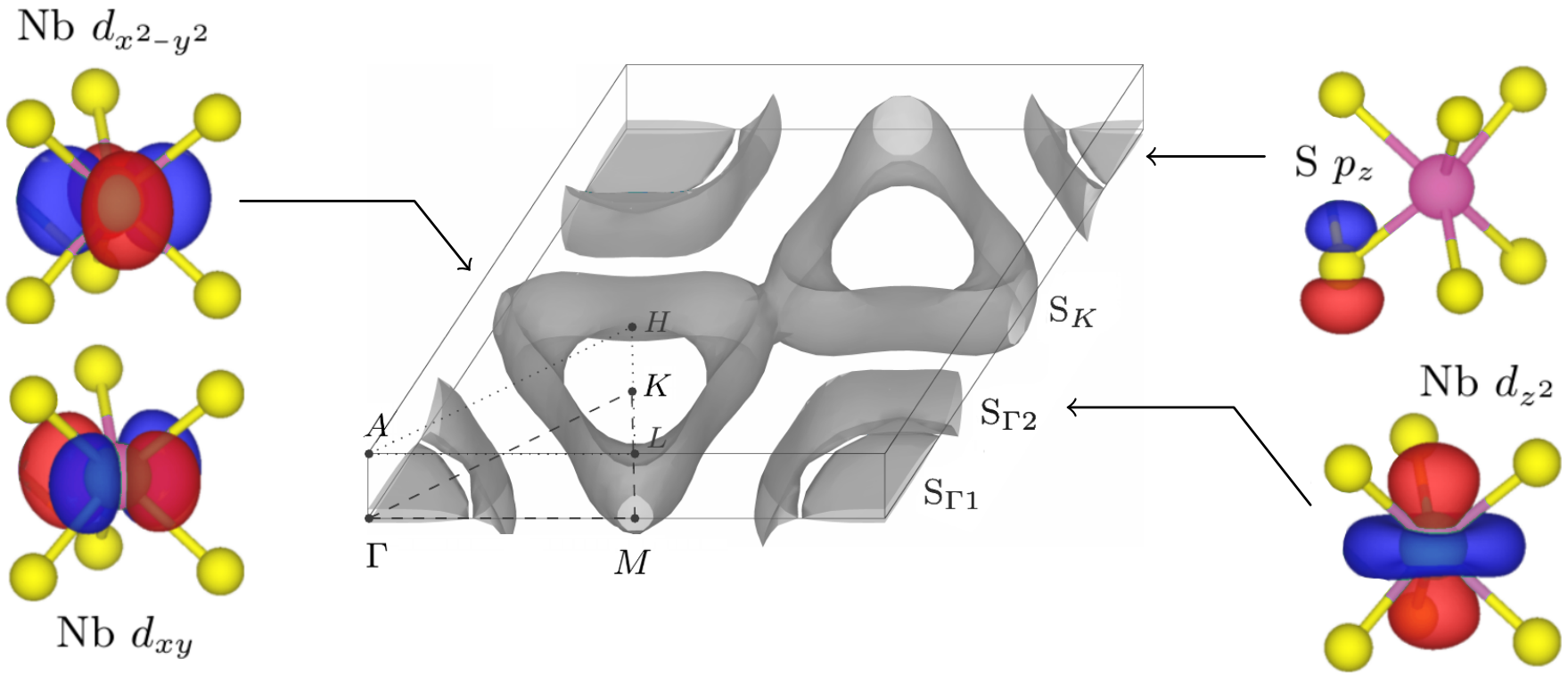

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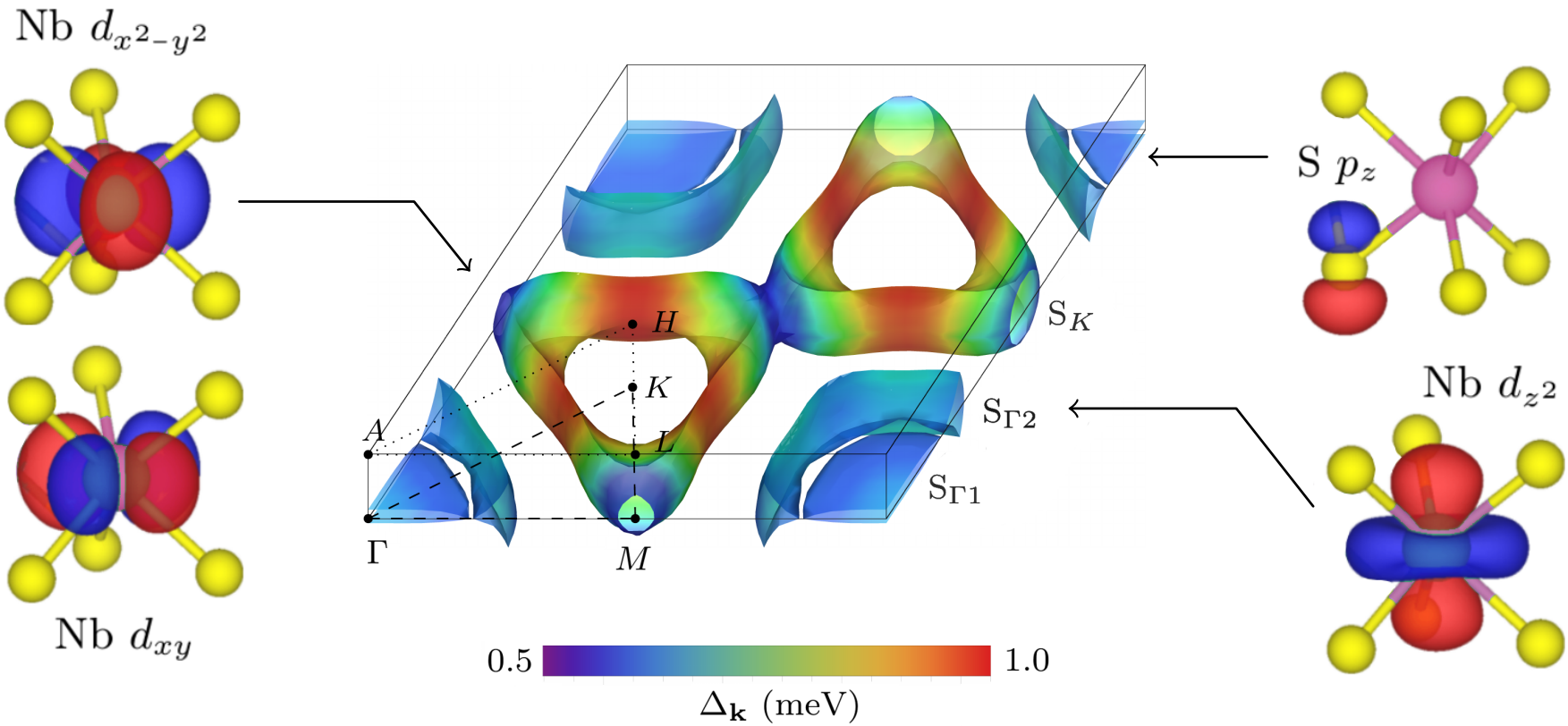

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Superconductivity in 2H-NbS_2

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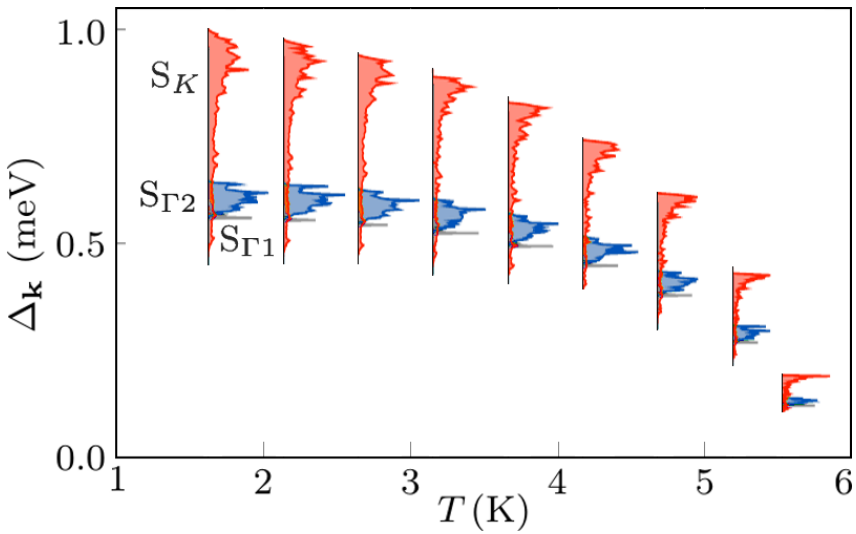

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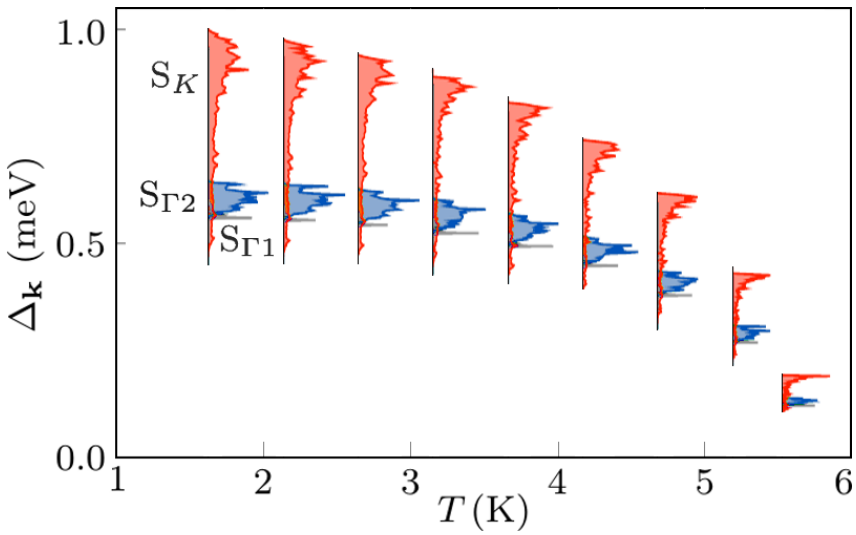

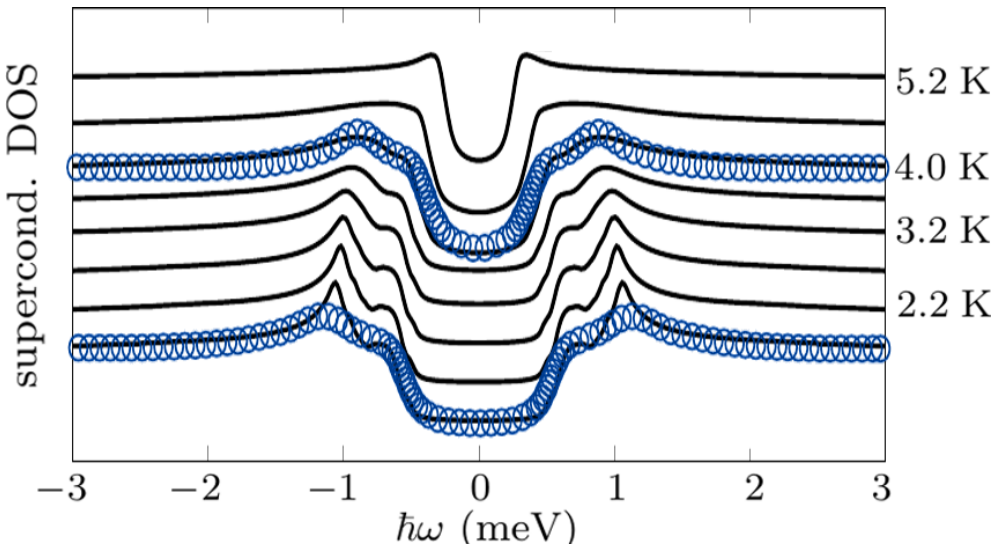

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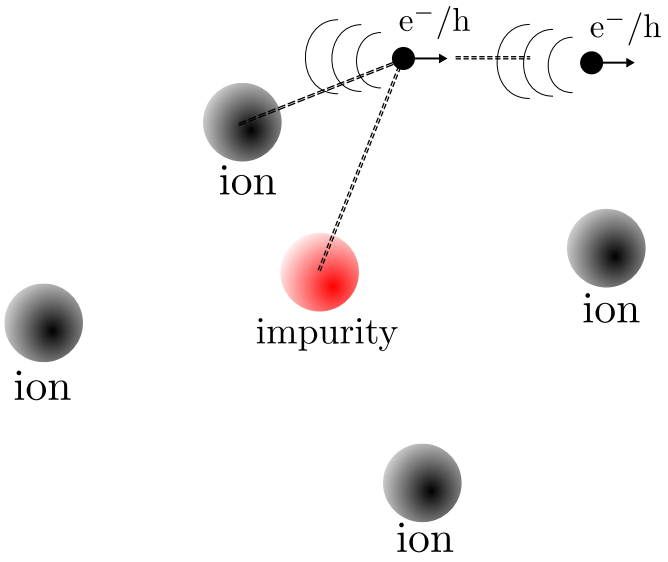
Phonon-limited carrier transport

Carrier transport



- Lattice scattering
- Impurity scattering
- Ionized impurity scattering

Electric current and mobility

- The steady-state electric current $\mathbf{J}$ is related to the driving electric field $\mathbf{E}$ via the mobility tensors $\boldsymbol{\mu}$ as:

$$J_\alpha = e\,(n_\mathrm{e}\,\mu_{\mathrm{e},\alpha\beta} + n_\mathrm{h}\,\mu_{\mathrm{h},\alpha\beta})E_\beta = -e\,\Omega^{-1}\sum_n \Omega_\mathrm{BZ}^{-1}\int d\mathbf{k}\, f_{n\mathbf{k}}\, v_{n\mathbf{k},\alpha}$$

where $v_{n\mathbf{k},\alpha} = \hbar^{-1}\partial\varepsilon_{n\mathbf{k}}/\partial k_\alpha$ is the band velocity.

- We need to find the occupation function $f_{n\mathbf{k}}$ which reduces to the Fermi-Dirac distribution $f^0_{n\mathbf{k}}$ in the absence of the electric field

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- We need to find the occupation function $f_{n\mathbf{k}}$ which reduces to the Fermi-Dirac distribution $f^0_{n\mathbf{k}}$ in the absence of the electric field

- The mobility is defined as:

$$\mu_{\mathrm{e},\alpha\beta} = \frac{\sigma_{\alpha\beta}}{n_e} = \frac{1}{n_e}\frac{\partial J_\alpha}{\partial E_\beta} = -\sum_{n\in\mathrm{CB}}\int d\mathbf{k}\; v_{n\mathbf{k},\alpha}\,\partial_{E_\beta} f_{n\mathbf{k}} \Big/ \sum_{n\in\mathrm{CB}}\int d\mathbf{k}\, f^0_{n\mathbf{k}}$$

- We need to evaluate the linear response of the distribution function $f_{n\mathbf{k}}$ to the electric field $\mathbf{E}$.

Boltzmann transport equation

$$\left.\frac{\partial f_{n\mathbf{k}}(T)}{\partial t}\right|_{\text{scatt}} = (-e)\mathbf{E}\cdot\frac{\partial f_{n\mathbf{k}}(T)}{\partial \mathbf{k}}$$

S. Poncé, W. Li, S. Reichardt, and F. Giustino, Rep. Prog. Phys. 83, 036501 (2020)

Boltzmann transport equation

$$\left.\frac{\partial f_{n\mathbf{k}}(T)}{\partial t}\right|_{\text{scatt}} = (-e)\mathbf{E} \cdot \frac{\partial f_{n\mathbf{k}}(T)}{\partial \mathbf{k}}$$

The right-hand side is the collisionless term of Boltzmann's equation for a uniform and constant electric field, in the absence of temperature gradients and magnetic fields

S. Poncé, W. Li, S. Reichardt, and F. Giustino, Rep. Prog. Phys. 83, 036501 (2020)

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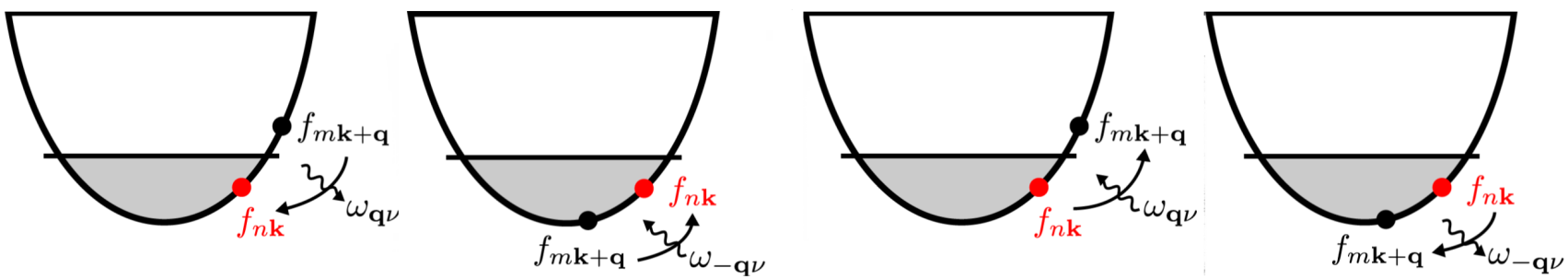
The right-hand side is the collisionless term of Boltzmann's equation for a uniform and constant electric field, in the absence of temperature gradients and magnetic fields

This left-hand side is the modification of the distribution function arising from electron-phonon scattering in and out of the state $|n\mathbf{k}\rangle$, via emission or absorption of phonons with frequency $\omega_{\mathbf{q}\nu}$



S. Poncé, W. Li, S. Reichardt, and F. Giustino, Rep. Prog. Phys. 83, 036501 (2020)

Linearized Boltzmann transport equation

We expend $f_{n\mathbf{k}}$ into $f_{n\mathbf{k}} = f^0_{n\mathbf{k}} + \mathcal{O}(\mathbf{E})$ for small $\mathbf{E}$ and keep only the linear term in $\mathbf{E}$ to get

$$(-e)\mathbf{E}\cdot\frac{\partial f_{n\mathbf{k}}(T)}{\partial \mathbf{k}} = (-e)\mathbf{E}\cdot\mathbf{v}_{n\mathbf{k}}\frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}}$$

$$\begin{aligned}\frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}}\mathbf{v}_{n\mathbf{k}}\cdot(-e)\mathbf{E} = \frac{2\pi}{\hbar}\sum_{m\nu}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \\ \times\Big\{(1-f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}\nu})(1+n_{\mathbf{q}\nu}) \\ +(1-f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu} \\ -f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}\nu})(1+n_{\mathbf{q}\nu}) \\ -f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu}\Big\}\end{aligned}$$

Linearized Boltzmann transport equation

We take the derivatives of the Boltzmann equation with respect to $\mathbf{E}$ to obtain the iterative Botlzmann transport equation (IBTE):

$$\begin{aligned}\partial_{E_\beta} f_{n\mathbf{k}} = & e\frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} v_{n\mathbf{k},\beta}\tau^0_{n\mathbf{k}} + \frac{2\pi\tau^0_{n\mathbf{k}}}{\hbar}\sum_{m\nu}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \\ & \times\Big[(1+n_{\mathbf{q}\nu}-f^0_{n\mathbf{k}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}\nu}) \\ & \quad +(n_{\mathbf{q}\nu}+f^0_{n\mathbf{k}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}\nu})\Big]\ \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}\end{aligned}$$

having defined the relaxation time:

$$\begin{aligned}\frac{1}{\tau^0_{n\mathbf{k}}} = & \frac{2\pi}{\hbar}\sum_{m\nu}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\,|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \\ & \times\Big[(1-f^0_{m\mathbf{k}+\mathbf{q}}+n_{\mathbf{q}\nu})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}\nu}) \\ & \quad +(f^0_{m\mathbf{k}+\mathbf{q}}+n_{\mathbf{q}\nu})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}\nu})\Big]\end{aligned}$$

Self-energy relaxation time approximation (SERTA)

We can approximate IBTE by neglecting $\partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}$

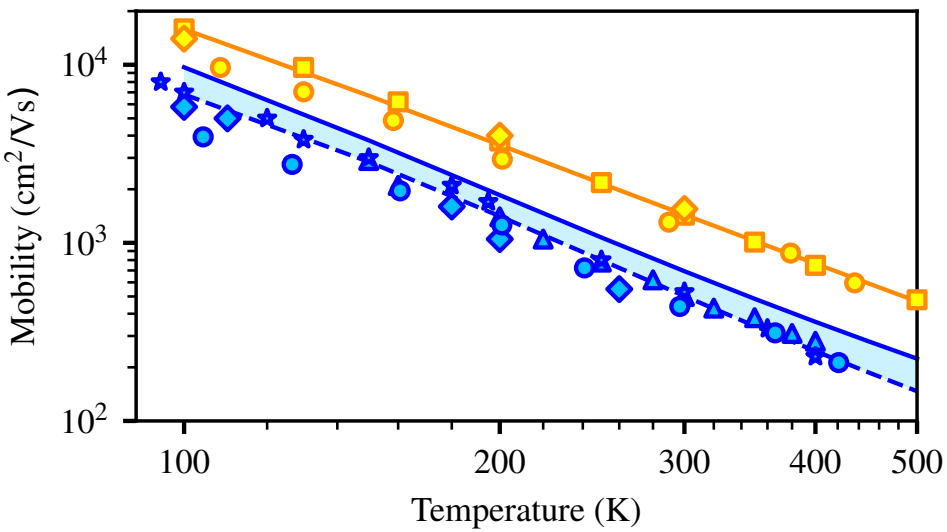
$$\partial_{E_\beta} f_{n\mathbf{k}} = e \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} v_{n\mathbf{k},\beta} \tau^0_{n\mathbf{k}}$$

The intrinsic electron mobility is therefore:

$$\begin{aligned}
\mu_{\mathrm{e},\alpha\beta} &= -\sum_{n\in\mathrm{CB}} \int d\mathbf{k}\; v_{n\mathbf{k},\alpha}\, \partial_{E_\beta} f_{n\mathbf{k}} \Big/ \sum_{n\in\mathrm{CB}} \int d\mathbf{k}\, f^0_{n\mathbf{k}} \\
&= \frac{-e}{n_\mathrm{e}\,\Omega} \sum_{n\in\mathrm{CB}} \int \frac{d\mathbf{k}}{\Omega_\mathrm{BZ}}\; \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} v_{n\mathbf{k},\alpha}\, v_{n\mathbf{k},\beta}\, \tau^0_{n\mathbf{k}}
\end{aligned}$$

Intrinsic carrier mobility in Si

Electron and hole mobility in silicon (EPW)



Poncé, Margine, and Giustino, Phys. Rev. B 97, 121201(R) (2018)

Intrinsic carrier mobility in Si

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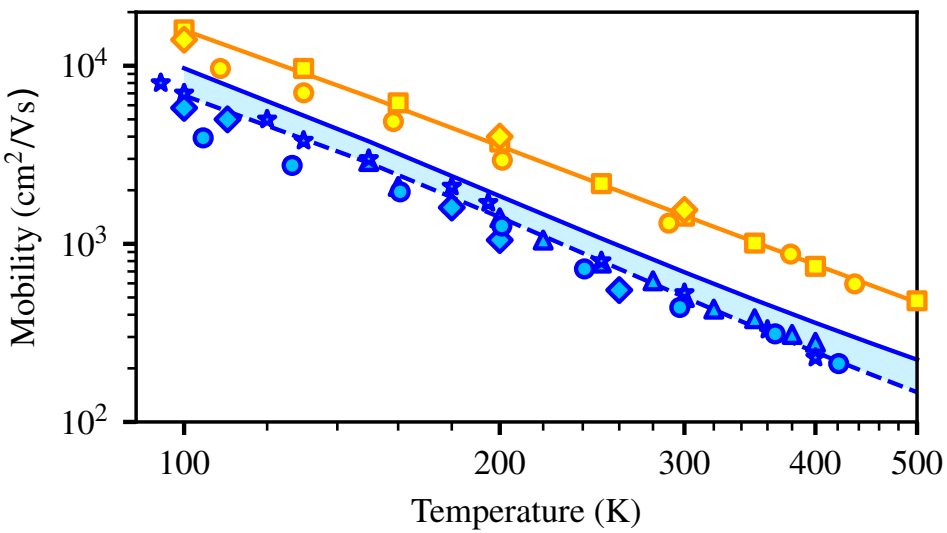
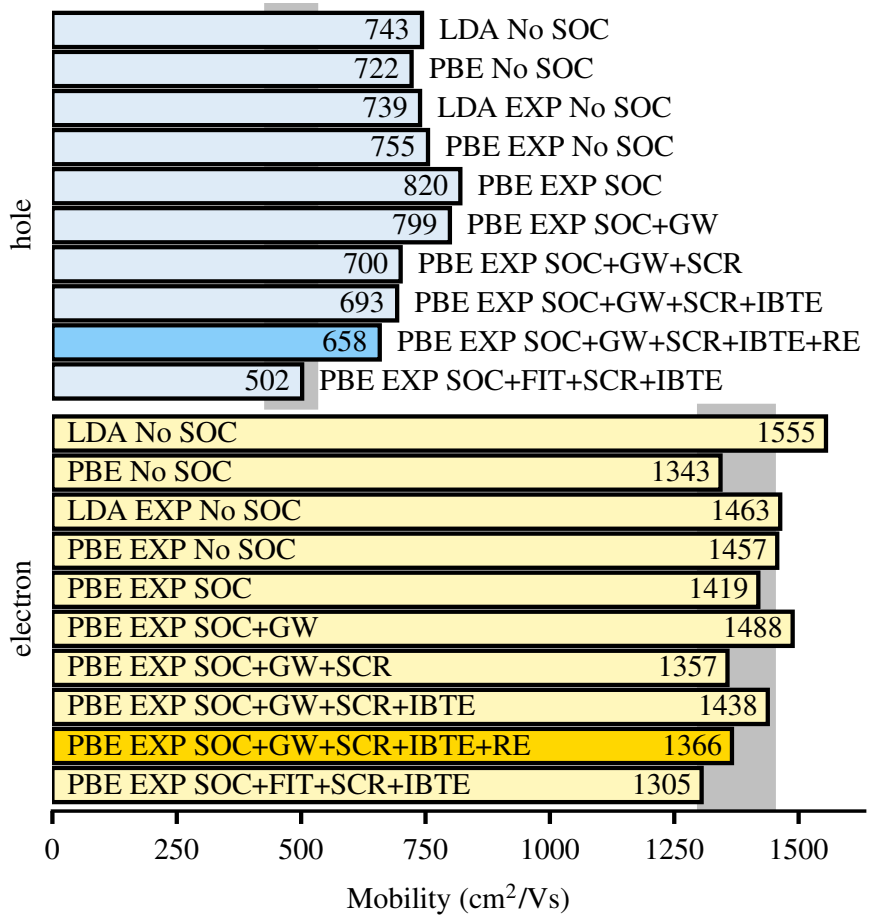
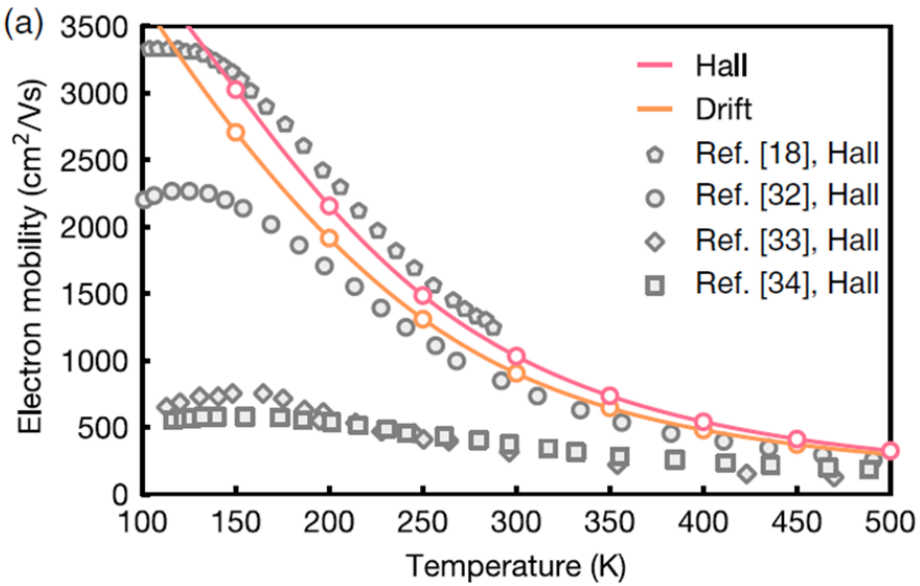


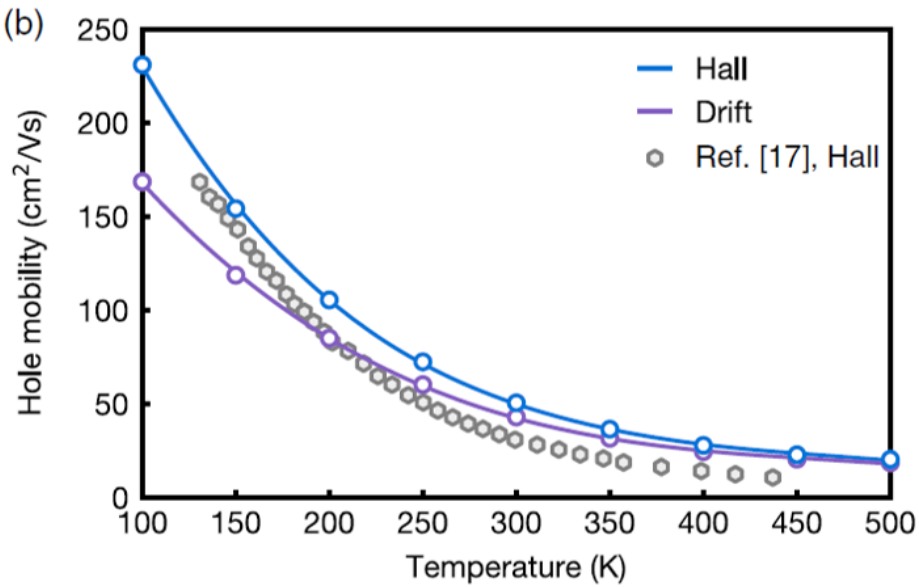


Poncé, Margine, and Giustino, Phys. Rev. B 97, 121201(R) (2018)

Intrinsic carrier mobility in GaN

Electron and hole mobility in GaN (EPW)

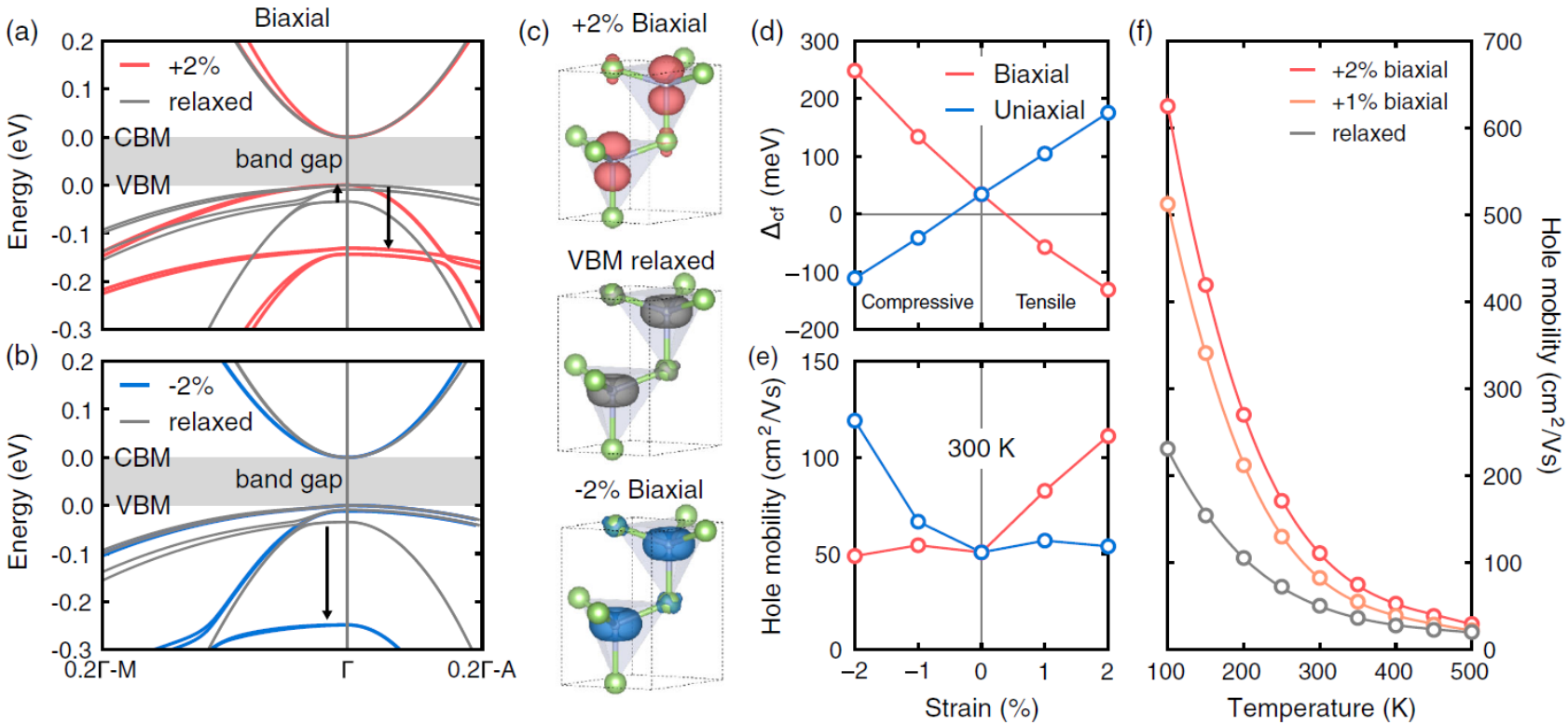




Poncé, Jena, and Giustino, Phys. Rev. Lett. 123, 096602 (2019)

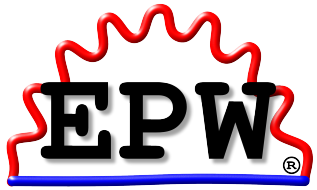
Route to high mobility in GaN

Crystal-field engineering of band structure and mobility in GaN



Poncé, Jena, and Giustino, Phys. Rev. Lett. 123, 096602 (2019)

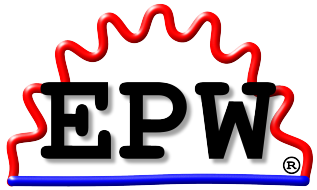
EPW capabilities



- electron and phonon linewidths, scattering rates, and lifetimes
- electron and phonon spectral functions
- electron-phonon vertex in the presence of Fröhlich interactions (polar materials)
- electron-phonon coupling strength
- phonon-limited optical absorption
- anisotropic superconducting properties
- electronic transport properties (mobility and resistivity)

Poncé, Margine, Verdi, and Giustino, Comput. Phys. Commun. 209, 116 (2016)

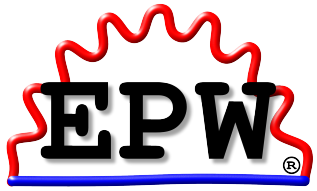
EPW specs



Features:

- Supports LDA/GGA functionals
- Supports NC and US pseudopotentials
- Supports spin-orbit coupling
- Supports time-reversal symmetry
- Polar divergence correctly interpolated
- Integrated into QE and rely on `Wannier90`
- MPI parallelization
- Has a test-farm for stability and portability of the code

EPW outlook



- mobility at finite magnetic field
- e-ph interactions in 2D materials
- high-throughput e-ph computations with AiiDA
- parallelization over G-vectors
- spin-transport
- fully ab initio Migdal-Eliashberg approach for superconductivity

http://epw.org.uk

https://gitlab.com/QEF/q-e

Acknowledgments

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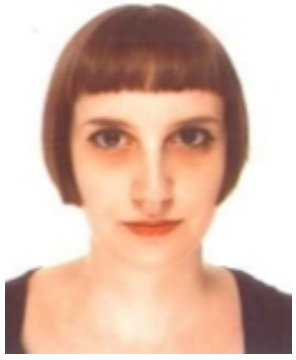

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The Leverhulme Trust

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References methodology

- F. Giustino, M. L. Cohen, and S. G. Louie, Phys. Rev. B 76, 165108 (2007) [link]
- E. R. Margine and F. Giustino, Phys. Rev. B 87, 024505 (2013) [link]
- C. Verdi and F. Giustino, Phys. Rev. Lett. 115 (17), 176401 (2015) [link]
- F. Giustino, Rev. Mod. Phys. 89, 015003 (2017) [link]
- S. Poncé, E. R. Margine, and F. Giustino, Phys. Rev. B 97, 121201(R) (2018) [link]
- S. Poncé, W. Li, S. Reichardt, and F. Giustino, Rep. Prog. Phys. 83, 036501 (2020) [link]
- S. Baroni, S. de Gironcoli, A. Dal Corso, P. Giannozzi, Rev. Mod. Phys. 73, 515 (2001) [link]
- N. Marzari, A. A. Mostofi, J. R. Yates, I. Souza, D. Vanderbilt, Rev. Mod. Phys. 84, 1419 (2012) [link]

References software

- S. Poncé, E. R. Margine, C. Verdi, and F. Giustino, Comput. Phys. Commun. 209, 116 (2016) [link]
- P. Giannozzi et al., J.Phys.:Condens.Matter 29, 465901 (2017) [link]
- G. Pizzi et al., J. Phys.: Condens. Matter 32, 165902 (2020) [link]

References applications

- C. Heil, S. Poncé, H. Lambert, M. Schlipf, E. R. Margine, and F. Giustino, Phys. Rev. Lett., 119, 087003 (2017) [link]
- M. Gao, Q.-Z. Li, X.-W. Yan, and J. Wang, Phys. Rev. B 95, 024505 (2017) [link]
- F. Zheng and J. Feng, Phys. Rev. B 99, 161119(R) (2019) [link]
- T.-H. Liu, J. Zhou, B. Liao, D. J. Singh, and G. Chen, Phys. Rev. B 95, 075206 (2017) [link]
- S. Poncé, D. Jena, and F. Giustino, Phys. Rev. Lett. 123, 096602 (2019) [link]
- M. Schlipf, S. Poncé, and F. Giustino, Phys. Rev. Lett. 121, 086402 (2018) [link]