Wannier 2022 Summer School

16-20 May 2022 - An ICTP Hybrid Meeting

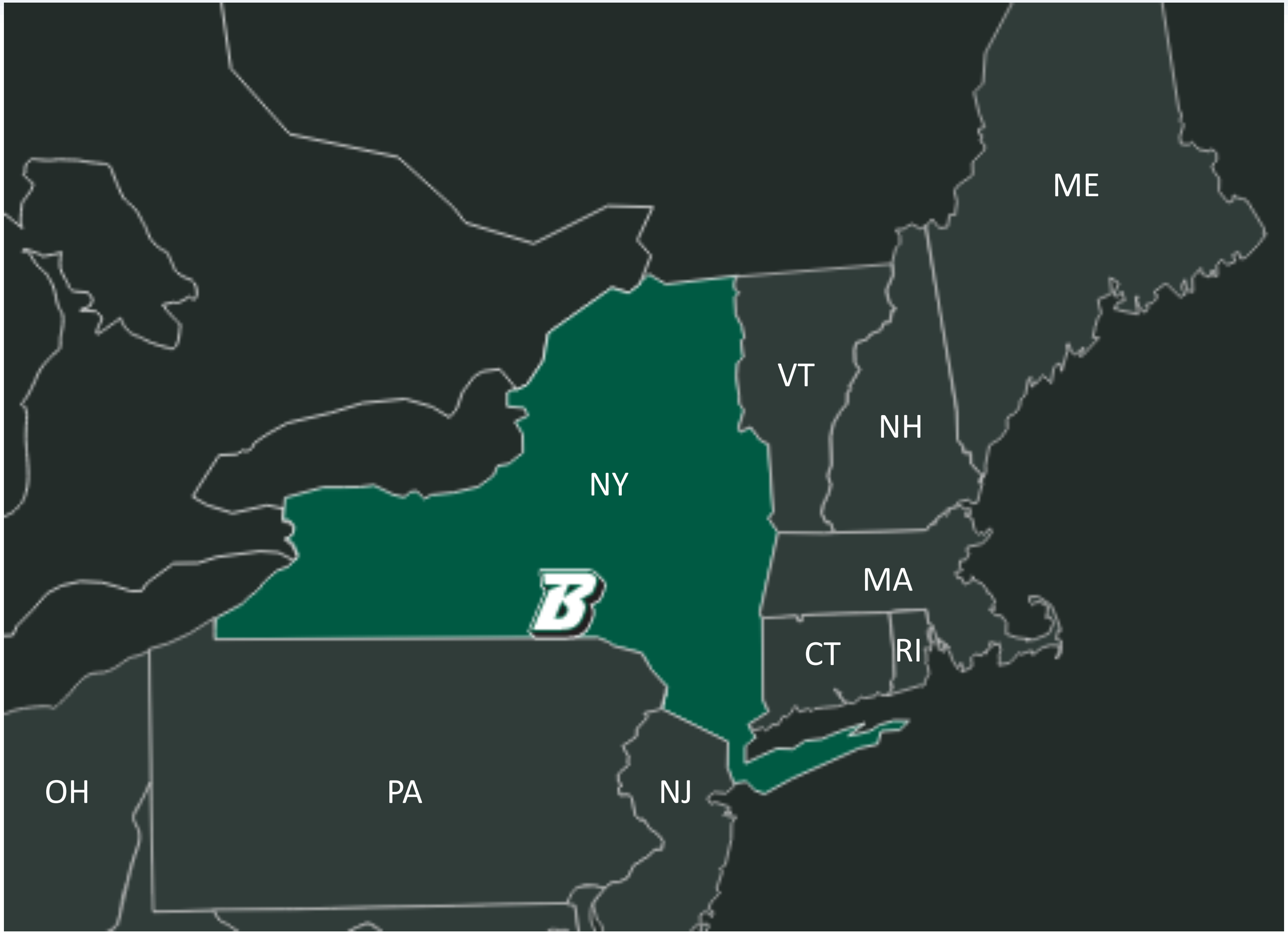
Superconductivity modeling with EPW

Roxana Margine

Department of Physics

Binghamton University - State University of New York

Binghamton University



BINGHAMTON UNIVERSITY
STATE UNIVERSITY OF NEW YORK

Binghamton University

https://www.nobelprize.org/prizes/chemistry/2019/whittingham/facts/

Nobel Prizes & Laureates | Nomination | Alfred Nobel | News & insights | Events | Educational

Chemistry | The Nobel Prize in Chemistry 2019 | M. Stanley Whittingham - Facts

The Nobel Prize in Chemistry 2019

John B. Goodenough
M. Stanley Whittingham
Akira Yoshino

Share this

M. Stanley Whittingham
Facts


© Nobel Media. Photo: A. Mahmoud

M. Stanley Whittingham
The Nobel Prize in Chemistry 2019

Born: 22 December 1941, United Kingdom

Affiliation at the time of the award: Binghamton University, State University of New York, New York, NY, USA

Prize motivation: "for the development of lithium-ion batteries"

Prize share: 1/3

BINGHAMTON UNIVERSITY
STATE UNIVERSITY OF NEW YORK

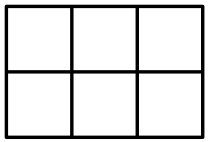
Superconductivity modeling with EPW: Outline

- Computational flow of electron-phonon matrix elements in EPW
- BCS theory of superconductivity
- Eliashberg theory
- Application to layered materials and hydrides

BINGHAMTON UNIVERSITY
STATE UNIVERSITY OF NEW YORK

Computational flow of electron-phonon matrix elements in EPW

$g(\mathbf{k}_c, \mathbf{q}_c)$



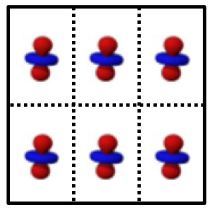
Coarse $\mathbf{k}_c/\mathbf{q}_c$ grid

Giannozzi et al., Comput. Phys. Commun. 29, 465901 (2017)

W90

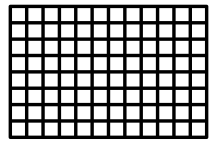
Pizzi et al., J. Phys. Cond. Matt. 32, 165902 (2020)

$g(\mathbf{R}_e, \mathbf{R}_p)$



Real-space supercell

$g(\mathbf{k}_f, \mathbf{q}_f)$



Fine $\mathbf{k}_f/\mathbf{q}_f$ grid

Poncé et al., Comput. Phys. Commun. 209, 116 (2016)

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

- $g_{mn\nu}(\mathbf{k}_c, \mathbf{q}_c)$: e-ph matrix coarse BZ grid
- $\Delta_{\mathbf{q}_c\nu} v^{\mathrm{KS}}$: lattice-periodic variation of Kohn-Sham potential
- $u_{m\mathbf{k}_c+\mathbf{q}_c}$, $u_{n\mathbf{k}_c}$: lattice-periodic part of wavefunction

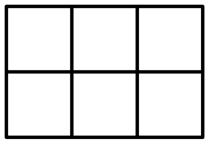
$$\Delta_{\mathbf{q}_c\nu} v^{\mathrm{KS}} = \sum_{\kappa\alpha} \sqrt{\frac{\hbar}{2M_\kappa \omega_{\mathbf{q}_c\nu}}} e_{\kappa\alpha,\nu}(\mathbf{q}_c) \, e^{-i\mathbf{q}_c\cdot\mathbf{r}} \sum_p e^{i\mathbf{q}_c\cdot\mathbf{R}_p} \frac{\partial V^{\mathrm{KS}}(\mathbf{r})}{\partial \tau_{\kappa\alpha p}}$$

- $\omega_{\mathbf{q}_c\nu}$: phonon frequency
- $e_{\kappa\alpha,\nu}(\mathbf{q}_c)$: phonon polarization
- $e^{-i\mathbf{q}_c\cdot\mathbf{r}}$, $e^{i\mathbf{q}_c\cdot\mathbf{R}_p}$: incommensurate modulation
- $\frac{\partial V^{\mathrm{KS}}(\mathbf{r})}{\partial \tau_{\kappa\alpha p}}$: potential change from ionic displacement

Giustino, Cohen, and Louie, Phys. Rev. B 76, 165108 (2007); Giustino, Rev. Mod. Phys. 89, 1 (2017)

Computational flow of electron-phonon matrix elements in EPW

$g(\mathbf{k}_\mathrm{c}, \mathbf{q}_\mathrm{c})$



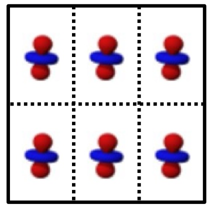
Coarse $\mathbf{k}_\mathrm{c}/\mathbf{q}_\mathrm{c}$ grid

Giannozzi et al., Comput. Phys. Commun. 29, 465901 (2017)

W90

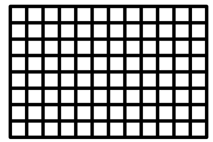
Pizzi et al., J. Phys. Cond. Matt. 32, 165902 (2020)

$g(\mathbf{R}_e, \mathbf{R}_p)$



Real-space supercell

$g(\mathbf{k}_\mathrm{f}, \mathbf{q}_\mathrm{f})$



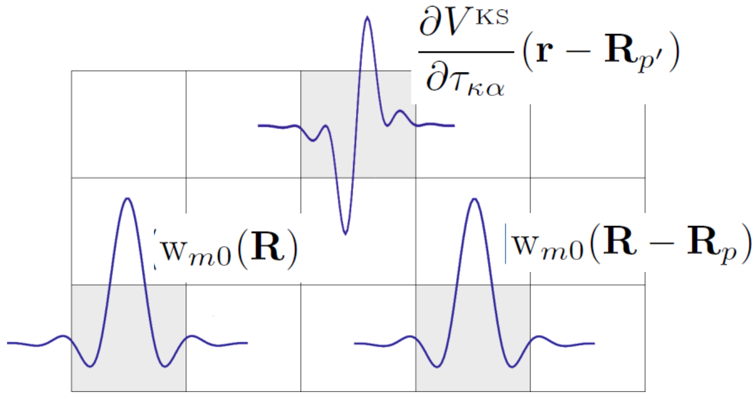
Fine $\mathbf{k}_\mathrm{f}/\mathbf{q}_\mathrm{f}$ grid

Poncé et al., Comput. Phys. Commun. 209, 116 (2016)

$$g_{mn\kappa\alpha}(\mathbf{R}_p, \mathbf{R}_{p'}) = \langle \mathrm{w}_{m0}(\mathbf{R}) | \frac{\partial V^{\mathrm{KS}}}{\partial \tau_{\kappa\alpha}}(\mathbf{r} - \mathbf{R}_{p'}) | \mathrm{w}_{m0}(\mathbf{R} - \mathbf{R}_p) \rangle_{\mathrm{sc}}$$

e-ph matrix real-space

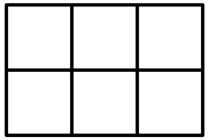
Wannier functions



Giustino, Cohen, and Louie, Phys. Rev. B 76, 165108 (2007); Giustino, Rev. Mod. Phys. 89, 1 (2017)

Computational flow of electron-phonon matrix elements in EPW

$g(\mathbf{k}_c, \mathbf{q}_c)$



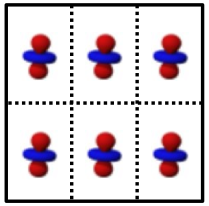
Coarse $\mathbf{k}_c/\mathbf{q}_c$ grid

Giannozzi et al., Comput. Phys. Commun. 29, 465901 (2017)

W90

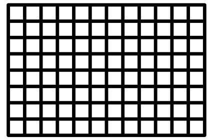
Pizzi et al., J. Phys. Cond. Matt. 32, 165902 (2020)

$g(\mathbf{R}_e, \mathbf{R}_p)$



Real-space supercell

$g(\mathbf{k}_f, \mathbf{q}_f)$



Fine $\mathbf{k}_f/\mathbf{q}_f$ grid

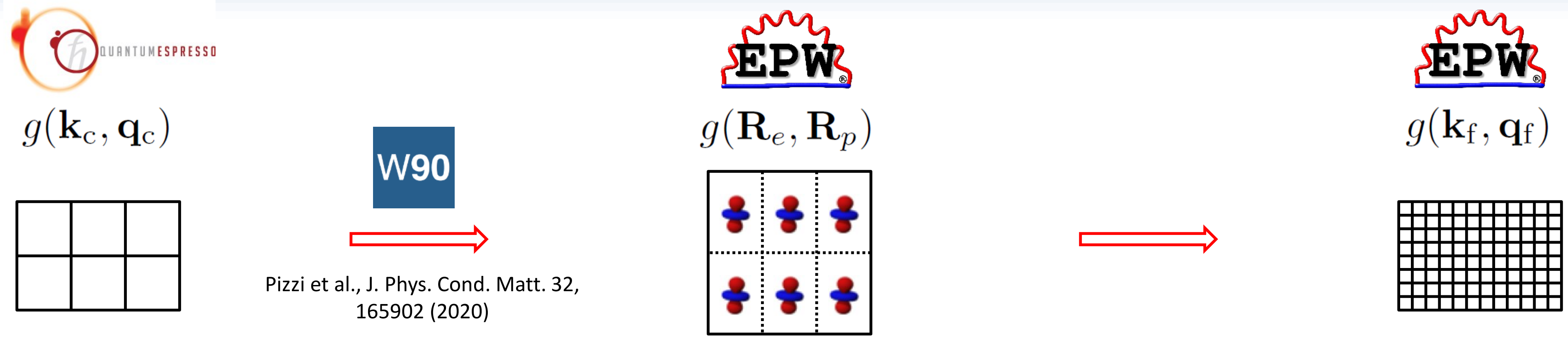
Poncé et al., Comput. Phys. Commun. 209, 116 (2016)

$$g_{mn\nu}(\mathbf{k}_f, \mathbf{q}_f) = \sqrt{\frac{\hbar}{2M_\kappa \omega_{\mathbf{q}_f \nu}}} \sum_{pp'} e^{i(\mathbf{k}_f \cdot \mathbf{R}_p + \mathbf{q}_f \cdot \mathbf{R}_{p'})} \left[U_{\mathbf{k}_f+\mathbf{q}_f}\, g(\mathbf{R}_p, \mathbf{R}_{p'}) \cdot e_{\kappa\alpha,\nu}(\mathbf{q}_f)\, U^\dagger_{\mathbf{k}_f}\right]_{mn}$$

- $g_{mn\nu}(\mathbf{k}_f, \mathbf{q}_f)$: e-ph matrix fine BZ grid
- U: rotation matrix
- $g(\mathbf{R}_p, \mathbf{R}_{p'})$: e-ph matrix real-space
- $e_{\kappa\alpha,\nu}$: phonon eigenmode

Giustino, Cohen, and Louie, Phys. Rev. B 76, 165108 (2007); Giustino, Rev. Mod. Phys. 89, 1 (2017)

Computational flow of electron-phonon matrix elements in EPW



Pizzi et al., J. Phys. Cond. Matt. 32, 165902 (2020)

Coarse $\mathbf{k}_c/\mathbf{q}_c$ grid

Giannozzi et al., Comput. Phys. Commun. 29, 465901 (2017)

Real-space supercell

Fine $\mathbf{k}_f/\mathbf{q}_f$ grid

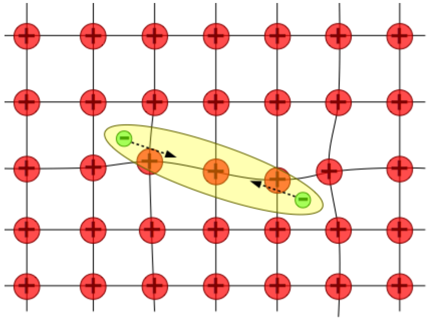
Poncé et al., Comput. Phys. Commun. 209, 116 (2016)

<u>epw.f90</u>

```
CALL epw_readin()
..
IF (wannierize) CALL wann_run()
CALL elphon_shuffle_wrap()
    >> CALL elphon_shuffle()
         > CALL readdvscf
         > CALL elphel2_shuffle
    >> CALL ephwann_shuffle
..
```

- Read input keywords, read wfns and misc. data from pw.x
- Generate inputs to W90 and perform wannierization
- Read dvscf files from ph.x
- Calculate e-ph vertex on coarse grids
- Transform e-ph vertex from Bloch to Wannier and Wannier to Bloch

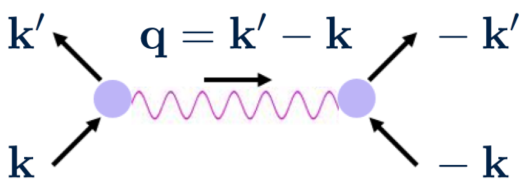
BCS theory

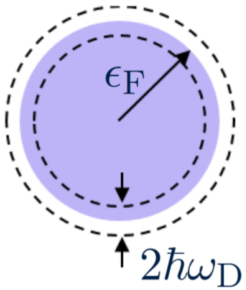


Bose-Einstein condensate
of (electron) Cooper pairs in a lattice

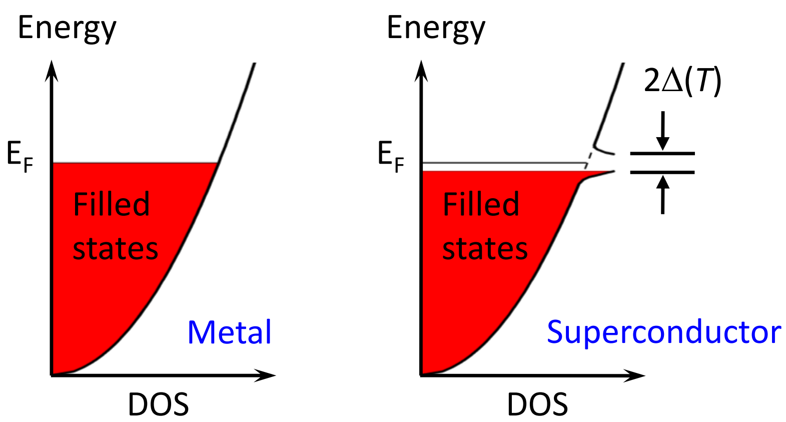
Bardeen, Cooper, and Schrieffer, Phys. Rev. 108, 1175 (1957)

BCS theory





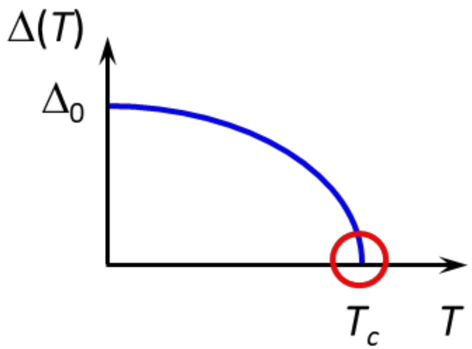
exchange of virtual phonons produces an attraction for electrons close to Fermi level



superconducting gap ↓ paring potential ↓

$$\Delta_{n\mathbf{k}} = \sum_m \int \frac{d\mathbf{q}}{\Omega_{BZ}} \tanh\left(\frac{E_{m\mathbf{k}+\mathbf{q}}}{2k_B T}\right) \frac{V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} \Delta_{m\mathbf{k}+\mathbf{q}}}{2E_{m\mathbf{k}+\mathbf{q}}}$$

quasiparticle excitation energy → $E_{n\mathbf{k}} = \sqrt{(\epsilon_{n\mathbf{k}} - \epsilon_F)^2 + |\Delta_{n\mathbf{k}}|^2}$



- describes in detail the phenomenology of superconductivity
- is a descriptive theory, material-independent → $2\Delta_0 = 3.53 k_B T_c$

Bardeen, Cooper, and Schrieffer, Phys. Rev. 108, 1175 (1957)

Eliashberg theory of superconductivity

A generalized 2 x 2 matrix Green's functions $\hat{G}_{n\mathbf{k}}(\tau)$ is used to describe the propagation of electron quasiparticles and of superconducting Cooper pairs on an equal footing.

imaginary time

Wick's time-ordering operator

$$\hat{G}_{n\mathbf{k}}(\tau) = -\langle T_\tau \mathbf{\Psi}_{n\mathbf{k}}(\tau)\mathbf{\Psi}^\dagger_{n\mathbf{k}}(0)\rangle$$

two-component field operator

$$\mathbf{\Psi}_{n\mathbf{k}} = \begin{bmatrix} \hat{c}_{n\mathbf{k}\uparrow} \\ \hat{c}^\dagger_{n-\mathbf{k}\downarrow} \end{bmatrix}$$

$$\hat{G}_{n\mathbf{k}}(\tau) = -\begin{bmatrix} \langle T_\tau \hat{c}_{n\mathbf{k}\uparrow}(\tau)\hat{c}^\dagger_{n\mathbf{k}\uparrow}(0)\rangle & \langle T_\tau \hat{c}_{n\mathbf{k}\uparrow}(\tau)\hat{c}_{n-\mathbf{k}\downarrow}(0)\rangle \\ \langle T_\tau \hat{c}^\dagger_{n-\mathbf{k}\downarrow}(\tau)\hat{c}^\dagger_{n\mathbf{k}\uparrow}(0)\rangle & \langle T_\tau \hat{c}^\dagger_{n-\mathbf{k}\downarrow}(\tau)\hat{c}_{n-\mathbf{k}\downarrow}(0)\rangle \end{bmatrix}$$

Allen and MitrovÍc, Solid State Phys. 37, 1 (1982); Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Eliashberg theory of superconductivity

$$\hat{G}_{n\mathbf{k}}(\tau) = -\begin{bmatrix} \langle T_\tau \hat{c}_{n\mathbf{k}\uparrow}(\tau)\hat{c}^\dagger_{n\mathbf{k}\uparrow}(0)\rangle & \langle T_\tau \hat{c}_{n\mathbf{k}\uparrow}(\tau)\hat{c}_{n-\mathbf{k}\downarrow}(0)\rangle \\ \langle T_\tau \hat{c}^\dagger_{n-\mathbf{k}\downarrow}(\tau)\hat{c}^\dagger_{n\mathbf{k}\uparrow}(0)\rangle & \langle T_\tau \hat{c}^\dagger_{n-\mathbf{k}\downarrow}(\tau)\hat{c}_{n-\mathbf{k}\downarrow}(0)\rangle \end{bmatrix}$$

- Diagonal elements are the normal state Green's functions and describe single-particle electronic excitations.
- Off-diagonal elements are the anomalous Green's functions and describe Cooper pairs amplitudes.

$\hat{G}_{n\mathbf{k}}(\tau)$ is periodic in τ and can be expanded in a Fourier series:

$$\hat{G}_{n\mathbf{k}}(\tau) = T\sum_{i\omega_j} e^{-i\omega_j\tau}\hat{G}_{n\mathbf{k}}(i\omega_j) \longrightarrow \hat{G}_{n\mathbf{k}}(i\omega_j) = \begin{bmatrix} G_{n\mathbf{k}}(i\omega_j) & F_{n\mathbf{k}}(i\omega_j) \\ F^*_{n\mathbf{k}}(i\omega_j) & -G_{-n\mathbf{k}}(-i\omega_j) \end{bmatrix}$$

↑ Matsubara frequencies

Allen and MitrovÍc, Solid State Phys. 37, 1 (1982); Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Eliashberg theory of superconductivity

Fan-Migdal self energy

GW self energy

pairing self-energy

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\hat{\tau}_3\hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_3 \times [\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j-\omega_{j'}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j-i\omega_{j'})]$$

↑ interacting Green's function

↑ anisotropic e-ph coupling strength

↑ screened Coulomb interaction

$\hat{G}_{n\mathbf{k}}(i\omega_j)$ obeys the Dyson's equation in Matsubara space:

$$\hat{G}^{-1}_{n\mathbf{k}}(i\omega_j) = \hat{G}^{-1}_{0,n\mathbf{k}}(i\omega_j) - \hat{\Sigma}_{n\mathbf{k}}(i\omega_j)$$

non-interacting Green's function

$$\hat{G}^{-1}_{0,n\mathbf{k}}(i\omega_j) = i\omega_j\hat{\tau}_0 - (\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})\hat{\tau}_3$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = i\omega_j\,[1 - Z_{n\mathbf{k}}(i\omega_j)]\,\hat{\tau}_0 + \chi_{n\mathbf{k}}(i\omega_j)\hat{\tau}_3 + \Delta_{n\mathbf{k}}(i\omega_j)Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_1$$

↑ mass renormalization function

↑ energy shift

↑ superconducting gap function

Allen and MitrovÍc, Solid State Phys. 37, 1 (1982); Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Eliashberg theory of superconductivity

$$\hat{G}_{n\mathbf{k}}(i\omega_j) = -\frac{i\omega_j Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_0 + [(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)]\,\hat{\tau}_3 + \Delta_{n\mathbf{k}}(i\omega_j) Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_1}{\Theta_{n\mathbf{k}}(i\omega_j)}$$

$$\Theta_{n\mathbf{k}}(i\omega_j) = [\omega_j Z_{n\mathbf{k}}(i\omega_j)]^2 + [(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)]^2 + [Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j)]^2$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\hat{\tau}_3\hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_3 \times [\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'})]$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - N_{\mathrm{F}} V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}$$
$$\times \{i\omega_{j'} Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_0 + [(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\mathrm{F}}) + \chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})]\,\hat{\tau}_3 - \Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'}) Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_1\}$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = i\omega_j\,[1 - Z_{n\mathbf{k}}(i\omega_j)]\,\hat{\tau}_0 + \chi_{n\mathbf{k}}(i\omega_j)\hat{\tau}_3 + \Delta_{n\mathbf{k}}(i\omega_j) Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_1$$

Equating the scalar coefficients of the Pauli matrices leads to the anisotropic Eliashberg equations.

Allen and MitrovÍc, Solid State Phys. 37, 1 (1982); Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Anisotropic Eliashberg equations on imaginary axis

mass renormalization function

$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{T}{\omega_j} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{\omega_{j'} Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})} \frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'})}{N_{\mathrm{F}}}$$

energy shift

$$\chi_{n\mathbf{k}}(i\omega_j) = -T \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\mathrm{F}}) + \chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})} \frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'})}{N_{\mathrm{F}}}$$

$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = T \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})} \left[\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'})}{N_{\mathrm{F}}} - V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'})\right]$$

superconducting gap function

electron number

$$n_e = 1 - 2T \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\mathrm{F}}) + \chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}$$

eliashberg = .true.
laniso = .true.
limag = .true.
fbw=.true.
muchem=.true.

Margine and Giustino, PRB 87, 024505 (2013)

Eliashberg equations on imaginary axis

$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{\pi T}{\omega_j N_\mathrm{F}} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_\mathrm{BZ}} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta^2_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}} \times \lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_\mathrm{F})$$

mass renormalization function

$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{N_\mathrm{F}} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_\mathrm{BZ}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta^2_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}} \times \left[\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - \mu_\mathrm{c}^*\right] \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_\mathrm{F})$$

superconducting gap function

Margine and Giustino, PRB 87, 024505 (2013)

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

anisotropic e-ph coupling strength

→ EPW

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

$$\mu_\mathrm{c}^* = \frac{\mu_\mathrm{c}}{1 + \mu_\mathrm{c} \log(\omega_\mathrm{el}/\omega_\mathrm{ph})}$$

Coulomb repulsion

Morel and Anderson, Phys. Rev. 125, 1263 (1962)

$$\mu_\mathrm{c} = N_\mathrm{F} \langle\langle V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} \rangle\rangle_\mathrm{FS}$$

screened Coulomb interaction → SGW

Schlipf, Lambert, Zibouche and Giustino, Comput. Phys. Commun. 247, 106856 (2020)

Eliashberg equations on imaginary axis

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

$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{N_{\mathrm{F}}} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \times \left[\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - \mu_{\mathrm{c}}^*\right] \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\mathrm{F}})$$

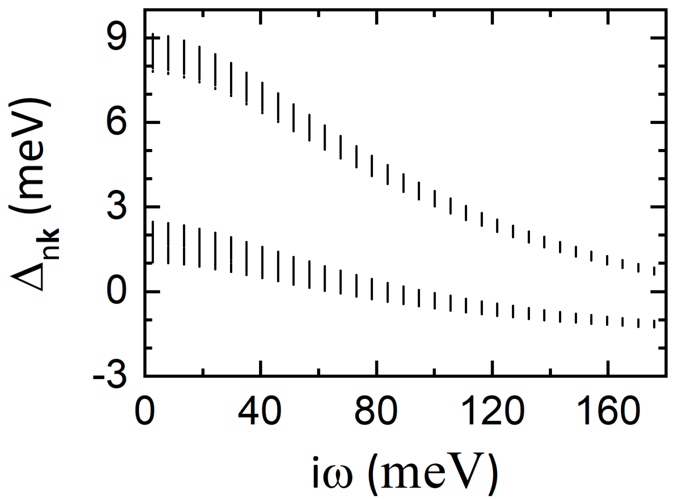
- The coupled nonlinear equations need to be solved self-consistently at each temperature T
- The equations must be evaluated on dense electron **k**- and phonon **q**-meshes to properly describe anisotropic effects
- The sum over Matsubara frequencies must be truncated (a typical cutoff of the order of 1 eV)
- The solutions are only meaningful for ***n*k** states at or near the Fermi surface

```
eliashberg = .true.
laniso = .true.
limag = .true.
```

```
muc = 0.1
temps = 10 20
degaussw = 0.1
```

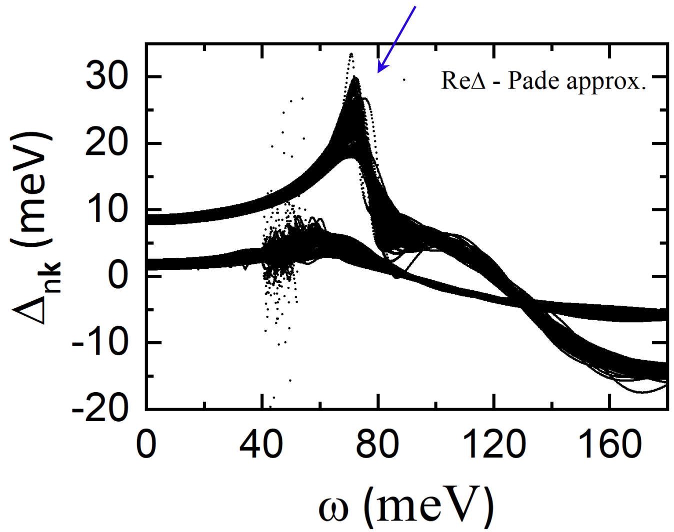
Eliashberg equations on real axis

- Eliashberg equations on the imaginary frequency axis are computationally efficient and they are adequate for calculating the critical temperature and the superconducting gap.
- To extract information about the spectral properties, the Eliashberg equations need to be solved on the real energy axis.
- Solutions on the real energy axis can be obtained by an analytic continuation using Padé approximants (lpade = .true., very light computationally) or an iterative procedure (lacon = .true., very heavy computationally).

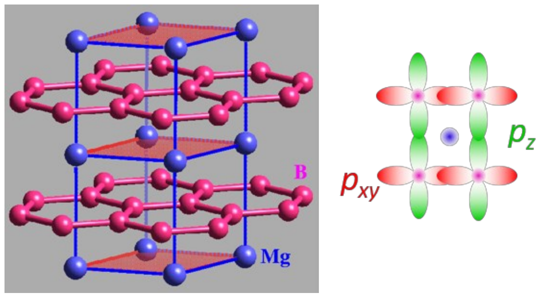


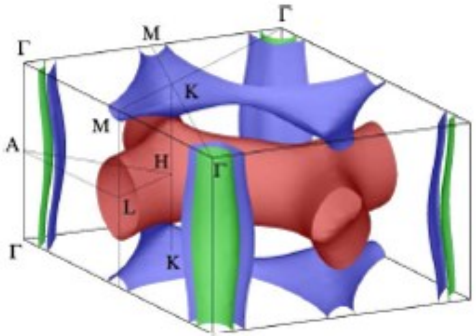
analytic continuation from imaginary-to-real axis

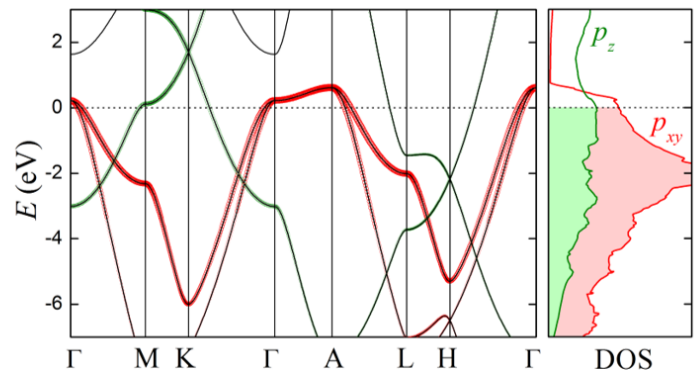
structure in the real axis solutions on the scale of the phonon energy



Example 1: Superconductivity in MgB_2

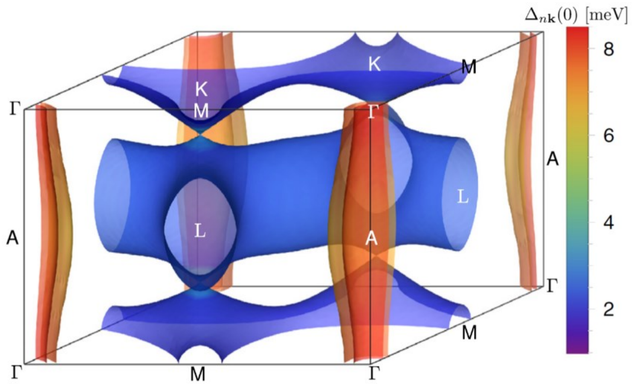






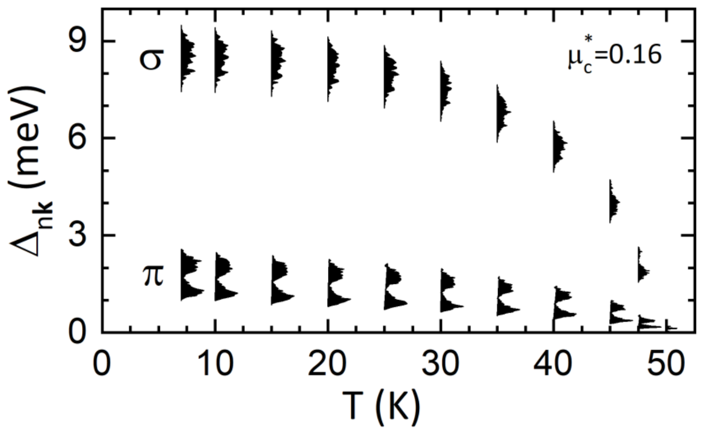
Kortus, Mazin, Belashchenko, Antropov, and L. L. Boyer, Phys. Rev. Lett. 86, 4656 (2001)

superconducting gap on FS



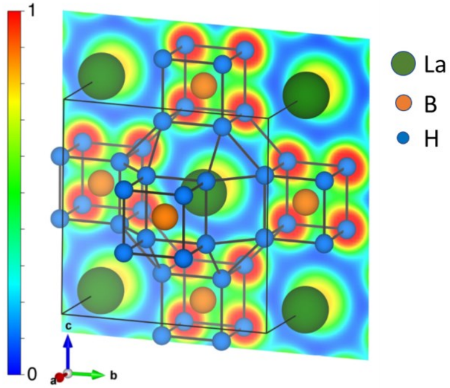
Poncé, Margine, Verdi, and Giustino, Comput. Phys. Commun. 209, 116 (2016)

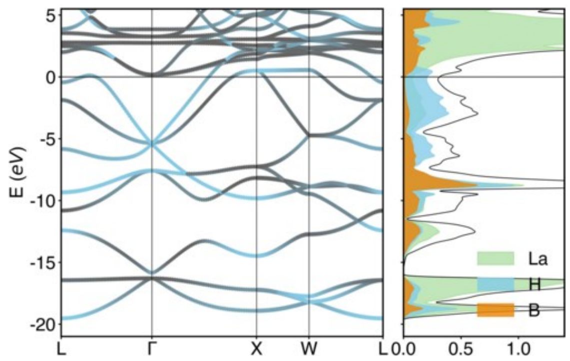
anisotropic superconducting gap

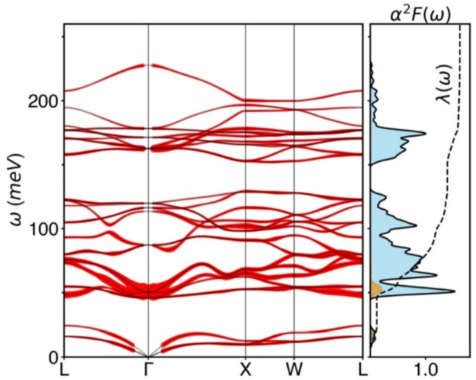


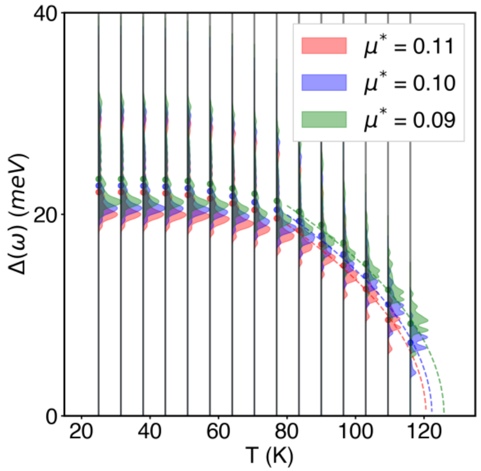
Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

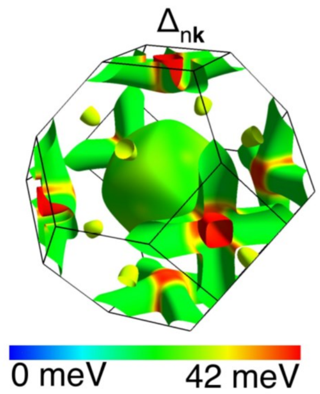
Example 2: Superconductivity in $LaBH_8$











$LaBH_8$ predicted to be a conventional HTSC with a T_c of 126 K at 50 GPa

Di Cataldo, Heil, von der Linden, and Boeri, Phys. Rev. B 104, L020511 (2021).

Superconductivity modeling with EPW: Summary

Key points

Anisotropic superconducting properties can now be obtained with the implemented Eliashberg theory.

Accurate solution requires fine sampling of the electron-phonon matrix elements across the Brillouin zone.

References

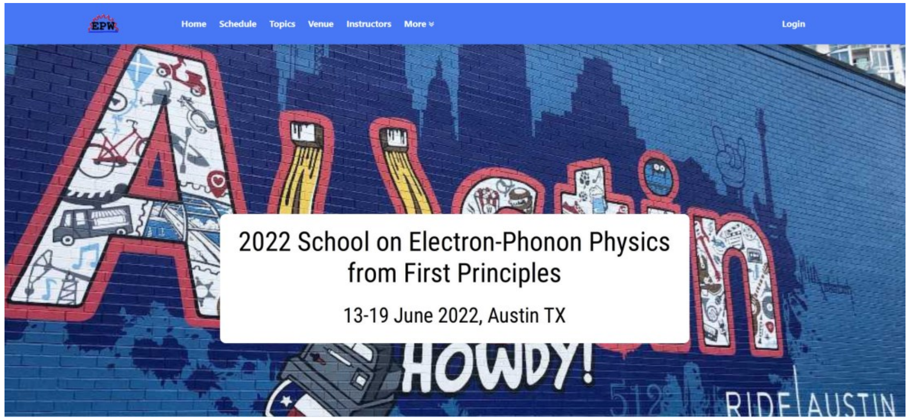
1. F. Giustino, M. Cohen and S. G. Louie, Phys. Rev. B 76, 165108 (2007)
2. E. R. Margine and F. Giustino, Phys. Rev. B 87, 024505 (2013)
3. S. Poncé, C. Verdi, E. R. Margine and F. Giustino, Comput. Phys. Commun. 209, 116 (2016)
4. F. Giustino, Rev. Mod. Phys. 89, 1 (2017)

NSF OAC-2103991
NSF DMR-2035518

Key points

Anisotropic superconducting properties can now be obtained with the implemented Eliashberg theory.

Accurate solution requires fine sampling of the electron-phonon matrix elements across the Brillouin zone.



Postdoctoral position

This position is part of a collaborative effort supported by the NSF Cyberinfrastructure for Sustained Scientific Innovation (CSSI) program. The project aims to develop an interoperable software ecosystem for many-body electronic structure calculations at finite temperature, with a focus on the EPW, BerkeleyGW, and SternheimerGW codes. The four-year project is a collaboration with Prof. Giustino at the University of Texas at Austin, Prof. Louie at the University of California at Berkeley, and Dr. Stanzione at the Texas Advanced Computing Center (TACC).

NSF OAC-2103991
NSF DMR-2035518