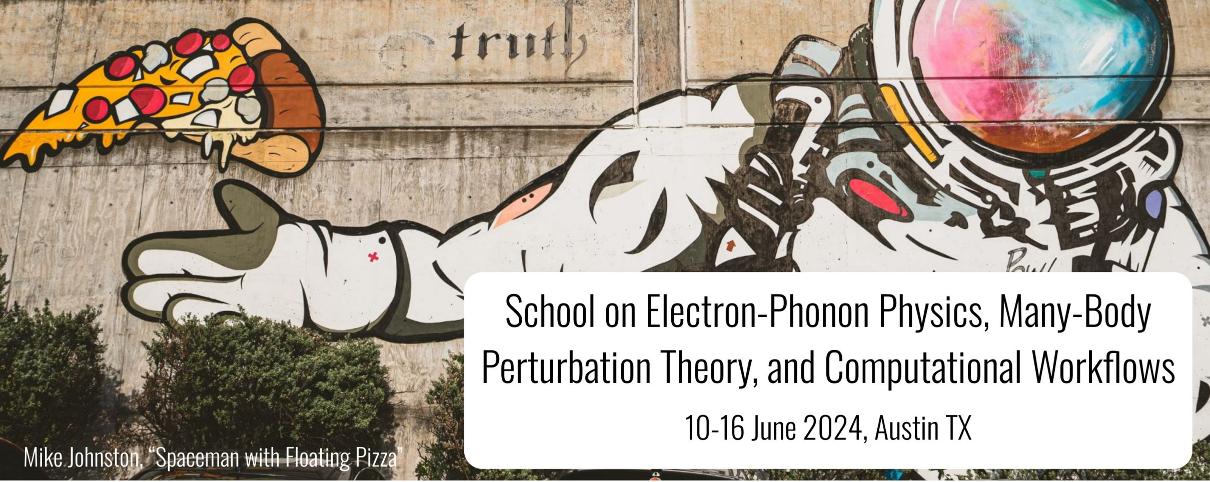
School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

10-16 June 2024, Austin TX



Mike Johnston, “Spaceman with Floating Pizza”

U.S. DEPARTMENT OF ENERGY

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Institute of Condensed Matter
and Nanosciences

Lecture Wed.1

Carrier transport in bulk and 2D materials

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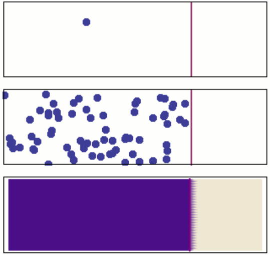
Lecture Summary

- The transport of charge carriers
- Quantum theory of mobility
- Mobility in simple semiconductors
- Hall mobility
- Carrier-impurity transport
- Resistivity in metals
- Outlook

Charges particles (electrons or holes) will move as a result of:

- a density gradient $\rightarrow$ **diffusion**

Fick's law (1855)
current density: $J = qD\nabla n$

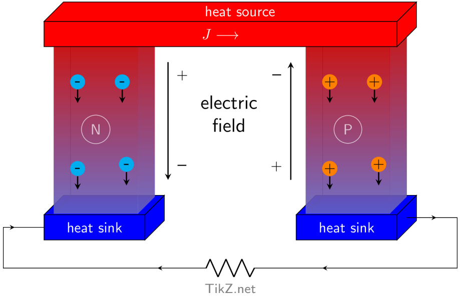


Wikipedia

Charges particles (electrons or holes) will move as a result of:

- a density gradient → **diffusion**
- a temperature gradient → **thermoelectricity**
  - Phonon-drag contribution - Gurevich (1945)

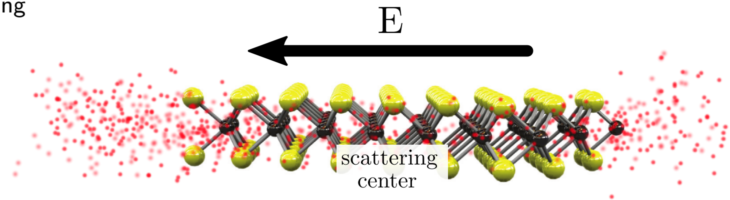
Seebeck effect (1821)
current density: $J \propto -\sigma S \nabla T$
S ∈ [-100$\mu V/K$, 1000$\mu V/K$]



Charges particles (electrons or holes) will move as a result of:

- a density gradient → **diffusion**
- a temperature gradient → **thermoelectricity**
  - Phonon-drag contribution - Gurevich (1945)
- an external electric field E → **drift**
  - lattice/phonon scattering
  - ionized impurity scattering
  - alloy scattering
  - defects scattering

Drude model (1900)
current density: $J = nq\mu E$



Mobility $\mu \propto \frac{\partial}{\partial E} \int d\mathbf{k} f_{\mathbf{k}} v_{\mathbf{k}}$

Quantum theory of mobility

Current density

$$\mathbf{J}(\mathbf{r}_1, t_1) = \frac{-e\hbar^2}{2m} \lim_{\mathbf{r}_2 \to \mathbf{r}_1} (\nabla_2 - \nabla_1) G^{<}(\mathbf{r}_1, \mathbf{r}_2; t_1, t_1)$$

$$G^{<}(\mathbf{r}_1, \mathbf{r}_2; t_1, t_2) \equiv \frac{i}{\hbar} \left\langle \hat{\psi}^{\dagger}_{\mathrm{H}}(\mathbf{r}_2, t_2) \hat{\psi}_{\mathrm{H}}(\mathbf{r}_1, t_1) \right\rangle$$

Quantum theory of mobility

Current density

$$\mathbf{J}(\mathbf{r}_1,t_1) = \frac{-e\hbar^2}{2m}\lim_{\mathbf{r}_2\to\mathbf{r}_1}(\nabla_2-\nabla_1)G^{<}(\mathbf{r}_1,\mathbf{r}_2;t_1,t_1)$$

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$$\hat{\psi}_{\mathrm{H}}(\mathbf{r},t) \equiv \overline{\mathcal{T}}\left[\mathrm{e}^{\frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\hat{H}(t')}\right]\hat{\psi}(\mathbf{r})\mathcal{T}\left[\mathrm{e}^{\frac{-i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\hat{H}(t')}\right]$$

$$\left\langle\hat{O}\right\rangle \equiv \frac{1}{Z}\mathrm{tr}\left[\mathrm{e}^{-\beta\hat{H}(t_0)}\hat{O}\right] \qquad \leftarrow \text{thermodynamical average}$$

$$Z \equiv \mathrm{tr}\left[\mathrm{e}^{-\beta\hat{H}(t_0)}\right] \qquad \leftarrow \text{partition function}$$

Current density

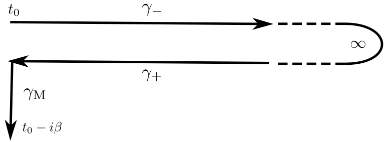
$$\mathbf{J}(\mathbf{r}_1,t_1) = \frac{-e\hbar^2}{2m}\lim_{\mathbf{r}_2\to\mathbf{r}_1}(\nabla_2-\nabla_1)G^{<}(\mathbf{r}_1,\mathbf{r}_2;t_1,t_1)$$

$$G^{<}(\mathbf{r}_1,\mathbf{r}_2;t_1,t_2) \equiv \frac{i}{\hbar}\left\langle \hat{\psi}^{\dagger}_{\mathrm{H}}(\mathbf{r}_2,t_2)\hat{\psi}_{\mathrm{H}}(\mathbf{r}_1,t_1)\right\rangle$$

Keldysh-Schwinger contour formalism

$$G(\mathbf{r}_1,\mathbf{r}_2;z_1,z_2) = \frac{-i}{\hbar}\frac{1}{Z}\mathrm{tr}\left\{\mathcal{T}_{\mathrm{C}}\left[\mathrm{e}^{\frac{-i}{\hbar}\int_{\gamma}\mathrm{d}z\,\hat{H}(z)}[\hat{\psi}(\mathbf{r}_1)]_{z_1}[\hat{\psi}^{\dagger}(\mathbf{r}_2)]_{z_2}\right]\right\}$$

$$\hat{H}(z) = \hat{H}_0+\hat{H}_{\mathrm{int}}+\hat{H}_{\mathrm{ext}}(z),$$



We can perform a perturbative expansion of the GF in powers of $\hat{H}_{\text{int}}$ and $\hat{H}_{\text{ext}}(z)$

$$G(\mathbf{r}_1,\mathbf{r}_2;z_1,z_2) = G_0(\mathbf{r}_1,\mathbf{r}_2;z_1,z_2) + \sum_{n,m=1}^{\infty}\frac{(-i/\hbar)^{n+m}}{n!m!}\int_\gamma \mathrm{d}z'_1 \dots \int_\gamma \mathrm{d}z'_n \int_\gamma \mathrm{d}z''_1 \dots \int_\gamma \mathrm{d}z''_m$$

$$\times \frac{1}{Z}\mathrm{tr}\Big[\mathcal{T}_{\mathrm{C}} e^{\frac{-i}{\hbar}\int_\gamma \mathrm{d}z\,[\hat{H}_0]_z}\big[\hat{H}_{\text{int}}\big]_{z'_1}\dots\big[\hat{H}_{\text{int}}\big]_{z'_n}\hat{H}_{\text{ext}}(z''_1)\dots\hat{H}_{\text{ext}}(z''_m)\big[\hat{\psi}(\mathbf{r}_1)\big]_{z_1}\big[\hat{\psi}^\dagger(\mathbf{r}_2)\big]_{z_2}\Big]$$

$$G_0(\mathbf{r}_1,\mathbf{r}_2;z_1,z_2) = \frac{-i}{\hbar}\frac{1}{Z_0}\mathrm{tr}\Big[\mathcal{T}_{\mathrm{C}} e^{\frac{-i}{\hbar}\int_\gamma \mathrm{d}z\,[\hat{H}_0]_z}\big[\hat{\psi}(\mathbf{r}_1)\big]_{z_1}\big[\hat{\psi}^\dagger(\mathbf{r}_2)\big]_{z_2}\Big]$$

Expressing the $\hat{H}$ in terms of $\hat{\psi}$ we can use Wick's theorem to write the perturbation series of G in terms of products of G_0 and then solve the expansion with Feynman diagram to obtain Dyson's equation

$$G(1,2) = G_0(1,2) + \int_\gamma \mathrm{d}3 \int_\gamma \mathrm{d}4\, G_0(1,3)\Sigma[G](3,4)G(4,2)$$

$$1 \equiv (\mathbf{r}_1, z_1)$$

Using Langreth rules, G_0^{-1}, explicit $\hat{H}_0$ and evaluating Dyson at equal time, we obtain the Kadanoff-Baym equation for $G^<$ in the limit $t_0 \to -\infty$:

$$i\hbar\frac{\partial}{\partial t}G^<(\mathbf{r}_1,\mathbf{r}_2;t,t) = \left[h_0(\mathbf{r}_1,-i\hbar\nabla_1) - h_0(\mathbf{r}_2,+i\hbar\nabla_2)\right]G^<(\mathbf{r}_1,\mathbf{r}_2;t,t)$$

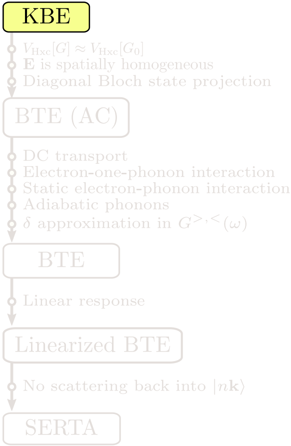
$$+\int \mathrm{d}^3 r_3 \left[\Sigma^\delta(\mathbf{r}_1,\mathbf{r}_3;t)G^<(\mathbf{r}_3,\mathbf{r}_2;t,t) - G^<(\mathbf{r}_1,\mathbf{r}_3;t,t)\Sigma^\delta(\mathbf{r}_3,\mathbf{r}_2;t)\right]$$

$$+\int_{-\infty}^{t}\mathrm{d}t'\int \mathrm{d}^3 r_3\Big[\Sigma^>(\mathbf{r}_1,\mathbf{r}_3;t,t')G^<(\mathbf{r}_3,\mathbf{r}_2;t',t)$$

$$+G^<(\mathbf{r}_1,\mathbf{r}_3;t,t')\Sigma^>(\mathbf{r}_3,\mathbf{r}_2;t',t)$$

$$-\Sigma^<(\mathbf{r}_1,\mathbf{r}_3;t,t')G^>(\mathbf{r}_3,\mathbf{r}_2;t',t) - G^>(\mathbf{r}_1,\mathbf{r}_3;t,t')\Sigma^<(\mathbf{r}_3,\mathbf{r}_2;t',t)\Big]$$

- Unperturbed time-evolution of $G^<$ in static $V(\mathbf{r})$
- Local time self-energy
- Internal dynamical correlations (collisions, scattering)



Nonequilibrium Many-Body Theory of Quantum Systems, Cambridge Uni. Press (2013)

SP *et al.*, Rep. Prog. Phys. **83**, 036501 (2020)

Approximation:

- $V_{\mathrm{Hxc}}[G] \approx V_{\mathrm{Hxc}}[G_0]$

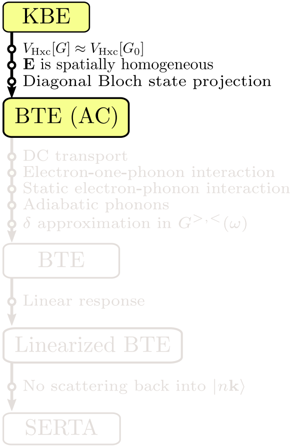
$$\Sigma^{\delta}(\mathbf{r}_1, \mathbf{r}_2; t) \approx -e\phi_{\mathrm{ext}}(\mathbf{r}_1, t)\delta^{(3)}(\mathbf{r}_1 - \mathbf{r}_2)$$

- **E** is spatially homogeneous

$$\phi_{\mathrm{ext}}(\mathbf{r}_1, t) - \phi_{\mathrm{ext}}(\mathbf{r}_2, t) = -\mathbf{E}(t) \cdot (\mathbf{r}_1 - \mathbf{r}_2)$$

$$\int \mathrm{d}^3 r_3 \left[\Sigma^{\delta}(\mathbf{r}_1, \mathbf{r}_3; t) G^{<}(\mathbf{r}_3, \mathbf{r}_2; t, t) - G^{<}(\mathbf{r}_1, \mathbf{r}_3; t, t)\Sigma^{\delta}(\mathbf{r}_3, \mathbf{r}_2; t)\right]$$

$$\approx e\mathbf{E}(t) \cdot (\mathbf{r}_1 - \mathbf{r}_2) G^{<}(\mathbf{r}_1, \mathbf{r}_2; t, t)$$



SP *et al.*, Rep. Prog. Phys. **83**, 036501 (2020)

We consider electrons in a solid and project the KBE in the $\{\varphi_{n\mathbf{k}}(\mathbf{r})\}$ basis.

Approximation:

- diagonal matrix elements of G and Σ (ok if no strong band mixing)

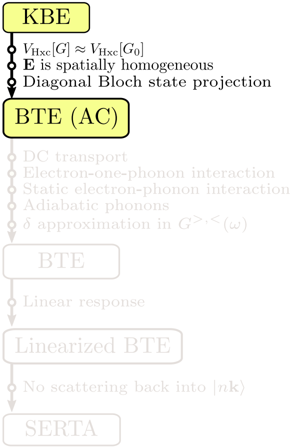
By expanding the Bloch WF in plane waves and taking the diagonal elements we have:

$$\int d^3r_1 \int d^3r_2\, \varphi^*_{n\mathbf{k}}(\mathbf{r}_1) e\mathbf{E}(t)\cdot(\mathbf{r}_1-\mathbf{r}_2) G^<(\mathbf{r}_1,\mathbf{r}_2;t,t)\varphi_{n\mathbf{k}}(\mathbf{r}_2)$$

$$= -e\mathbf{E}(t)\cdot\frac{1}{\hbar}\frac{\partial f^<_{n\mathbf{k}}}{\partial \mathbf{k}}(t,t)$$

where

$$\mp\frac{i}{\hbar} f^{>,<}_{n\mathbf{k}}(t,t') \equiv \int d^3r_1 \int d^3r_2\, \varphi^*_{n\mathbf{k}}(\mathbf{r}_1) G^{>,<}(\mathbf{r}_1,\mathbf{r}_2;t,t')\varphi_{n\mathbf{k}}(\mathbf{r}_2)$$



SP *et al.*, Rep. Prog. Phys. **83**, 036501 (2020)

Boltzmann transport equation

The quantum BTE is:

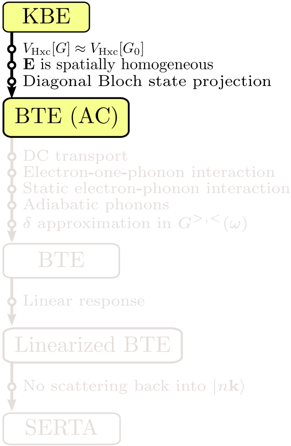
$$\frac{\partial f^{<}_{n\mathbf{k}}}{\partial t}(t,t) - e\mathbf{E}(t)\cdot\frac{1}{\hbar}\frac{\partial f^{<}_{n\mathbf{k}}}{\partial \mathbf{k}}(t,t) = -\Gamma^{(\mathrm{co})}_{n\mathbf{k}}(t)$$

where the *collision rate* is defined as:

$$\Gamma^{(\mathrm{co})}_{n\mathbf{k}}(t) \equiv \int_{-\infty}^{t} \mathrm{d}t' \left[\Gamma^{>}_{n\mathbf{k}}(t,t')\, f^{<}_{n\mathbf{k}}(t',t) + f^{<}_{n\mathbf{k}}(t,t')\, \Gamma^{>}_{n\mathbf{k}}(t',t) - \Gamma^{<}_{n\mathbf{k}}(t,t')\, f^{>}_{n\mathbf{k}}(t',t) - f^{>}_{n\mathbf{k}}(t,t')\, \Gamma^{<}_{n\mathbf{k}}(t',t) \right]$$

and

$$\mp i\hbar\, \Gamma^{>,<}_{n\mathbf{k}}(t,t') \equiv \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2\, \varphi^{*}_{n\mathbf{k}}(\mathbf{r}_1)\Sigma^{>,<}(\mathbf{r}_1,\mathbf{r}_2;t,t')\varphi_{n\mathbf{k}}(\mathbf{r}_2)$$



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Boltzmann transport equation

For time-independent $\mathbf{E}$ (DC) we can do a FT:

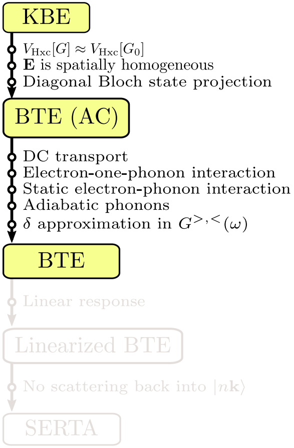
$$-e\mathbf{E}\cdot\frac{1}{\hbar}\frac{\partial f_{n\mathbf{k}}}{\partial\mathbf{k}} = -\int\frac{d\omega}{2\pi}\left[f^{<}_{n\mathbf{k}}(\omega)\Gamma^{>}_{n\mathbf{k}}(\omega) - f^{>}_{n\mathbf{k}}(\omega)\Gamma^{<}_{n\mathbf{k}}(\omega)\right]$$

where the $\mathbf{E}$-field dependent occupation number is

$$f_{n\mathbf{k}} \equiv \int\frac{d\omega}{2\pi}f^{<}_{n\mathbf{k}}(\omega).$$

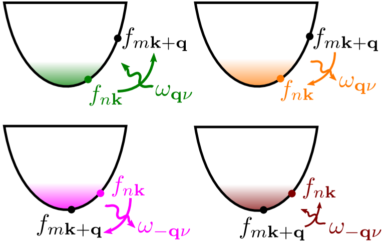
Approximations:

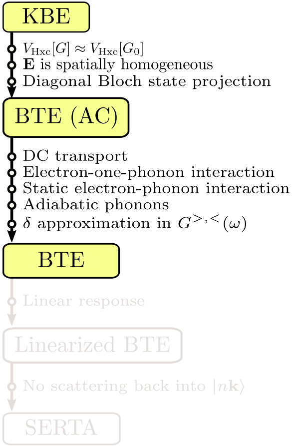
- Only scattering by lattice vibrations
- Neglect phonon-phonon interactions
- Frequency-independent el-ph matrix elements
- Phonon Green's function in the adiabatic approximation
- $f^{>,<}(\omega)$ is approximated at the level of $\hat{H}_0$ $[f^{<}_{n\mathbf{k}}(\omega) \approx 2\pi f_{n\mathbf{k}}\delta(\omega - \varepsilon_{n\mathbf{k}}/\hbar)]$



SP *et al.*, Rep. Prog. Phys. **83**, 036501 (2020)

$$
-e\mathbf{E}\cdot\frac{1}{\hbar}\frac{\partial f_{n\mathbf{k}}}{\partial\mathbf{k}} = \frac{2\pi}{\hbar}\sum_{m,\nu}\int\frac{\mathrm{d}^3q}{\Omega_{\mathrm{BZ}}}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2
\times\big[f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu}
+ f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}\nu})(n_{\mathbf{q}\nu}+1)
- (1-f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{n\mathbf{k}}+\hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu}
- (1-f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{n\mathbf{k}}-\hbar\omega_{\mathbf{q}\nu})(n_{\mathbf{q}\nu}+1)\big]
$$





SP *et al.*, Rep. Prog. Phys. **83**, 036501 (2020)

Linearized Boltzmann transport equation

Macroscopic average of the current density is

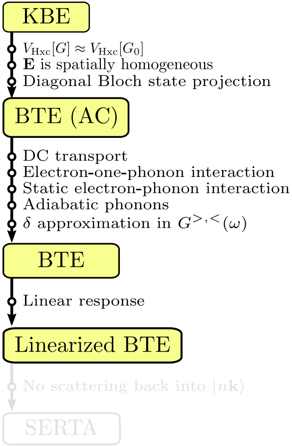
$$\mathbf{J}_{\mathrm{M}}(\mathbf{E}) = \frac{-e\hbar^2}{2m}\frac{1}{V}\int \mathrm{d}^3 r \lim_{\mathbf{r}_2\to\mathbf{r}_1} (\nabla_2 - \nabla_1) G^{<}(\mathbf{r}_1, \mathbf{r}_2; t, t; \mathbf{E})$$
$$= \frac{-e}{V_{\mathrm{uc}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} \mathbf{v}_{n\mathbf{k}} f_{n\mathbf{k}}(\mathbf{E})$$

For weak $\mathbf{E}$, we can use the *linear response* of the current density to define the *conductivity*:

$$\sigma_{\alpha\beta} \equiv \left.\frac{\partial J_{\mathrm{M},\alpha}}{\partial E_\beta}\right|_{\mathbf{E}=\mathbf{0}} = \frac{-e}{V_{\mathrm{uc}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

where $\partial_{E_\beta} f_{n\mathbf{k}} = (\partial f_{n\mathbf{k}}/\partial E_\beta)|_{\mathbf{E}=\mathbf{0}}$.
The *carrier drift mobility* is

$$\mu^{\mathrm{d}}_{\alpha\beta} \equiv \frac{\sigma_{\alpha\beta}}{e n_{\mathrm{c}}}$$



SP *et al.*, Rep. Prog. Phys. **83**, 036501 (2020)

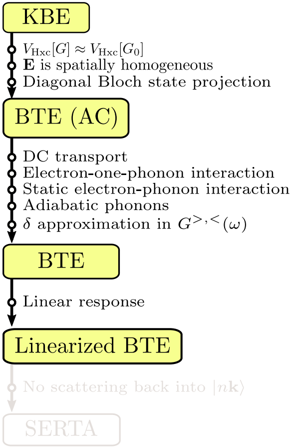
Linearized Boltzmann transport equation

$$\mu^{\mathrm{d}}_{\alpha\beta} = \frac{-1}{V_{\mathrm{uc}} n_{\mathrm{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

$$\partial_{E_\beta} f_{n\mathbf{k}} = e v^{\beta}_{n\mathbf{k}} \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \tau_{n\mathbf{k}} + \frac{2\pi \tau_{n\mathbf{k}}}{\hbar} \sum_{m\nu} \int \frac{\mathrm{d}^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \times \Big[(n_{\mathbf{q}\nu} + 1 - f^0_{n\mathbf{k}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{n\mathbf{k}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu})\Big] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}$$

where

$$\tau^{-1}_{n\mathbf{k}} \equiv \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \big[(n_{\mathbf{q}\nu} + 1 - f^0_{m\mathbf{k}+\mathbf{q}}) \times \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu})\big]$$



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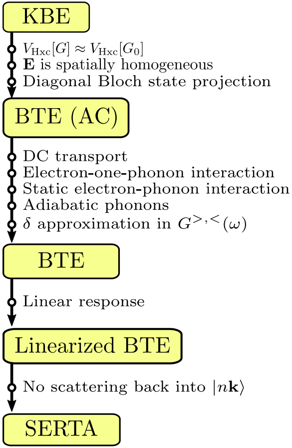
Self-energy relaxation time approximation

$$\mu^{\mathrm{d,SERTA}}_{\alpha\beta} = \frac{-1}{V_{\mathrm{uc}} n_{\mathrm{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

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

where

$$\tau^{-1}_{n\mathbf{k}} \equiv \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \big[(n_{\mathbf{q}\nu} + 1 - f^0_{m\mathbf{k}+\mathbf{q}}) \times \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu})\big]$$



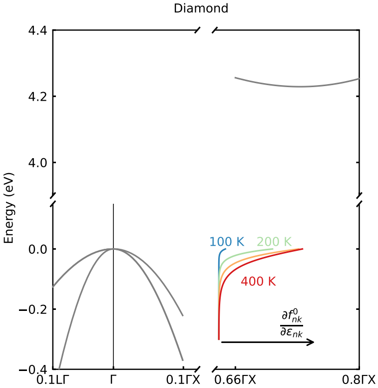
SP *et al.*, Rep. Prog. Phys. **83**, 036501 (2020)

$$\mu^{\mathrm{d}}_{\alpha\beta} = \frac{-1}{S_{\mathrm{uc}} n_{\mathrm{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{S_{\mathrm{BZ}}} v_{n\mathbf{k}\alpha} \, \partial_{E_\beta} f_{n\mathbf{k}}$$

$$\partial_{E_\beta} f_{n\mathbf{k}} = e v_{n\mathbf{k}\beta} \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \tau_{n\mathbf{k}} + \frac{2\pi \tau_{n\mathbf{k}}}{\hbar} \sum_{m\nu} \int \frac{\mathrm{d}^3 q}{S_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \Big[(n_{\mathbf{q}\nu} + 1 - f^0_{n\mathbf{k}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{n\mathbf{k}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) \Big] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}},$$

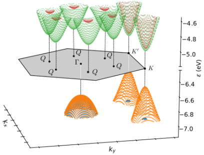
where the scattering rate is

$$\tau^{-1}_{n\mathbf{k}} \equiv \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{\mathrm{d}^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \big[(n_{\mathbf{q}\nu} + 1 - f^0_{m\mathbf{k}+\mathbf{q}}) \times \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{m\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) \big]$$



Ultra-dense sampling required !

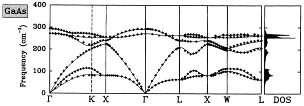
F. Macheda and N. Bonini, Phys. Rev. B **98**, 201201R (2018), SP *et al.*, Rep. Prog. Phys. **83**, 036501 (2020)
SP *et al.*, Phys. Rev. Research **3**, 043022 (2021)

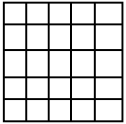


$$\Phi(\mathbf{q}) - \Phi^{\mathcal{L}}(\mathbf{q})$$
$$g(\mathbf{k},\mathbf{q}) - g^{\mathcal{L}}(\mathbf{k},\mathbf{q})$$

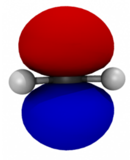
Real space

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

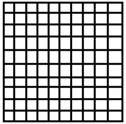




MLWF



MLWF



Coarse $\mathbf{k}/\mathbf{q}$ mesh

Dense $\mathbf{k}/\mathbf{q}$ mesh

P. Giannozzi *et al.*, Phys. Rev. B **43**, 7231 (1991), X. Gonze and C. Lee, Phys. Rev. B **55**, 10355 (1997), S. Baroni *et al.*, Rev. Mod. Phys. **73**, 515 (2001), F. Giustino *et al.*, Phys. Rev. B **76**, 165108 (2007), N. Marzari *et al.*, Rev. Mod. Phys. **84**, 1419 (2012), G. Pizzi *et al.*, Comput. Mater. Sci. **111**, 218 (2016), C. Verdi and F. Giustino, Phys. Rev. Lett. **115**, 176401 (2015), J. Sjakste *et al.*, Phys. Rev. B **92**, 054307 (2015), SP *et al.*, Comput. Phys. Commun. **209**, 116 (2016), T. Sohier *et al.*, Phys. Rev. X **9**, 031019 (2019), V. A. Jhalani *et al.*, Phys. Rev. Lett. **125**, 136602 (2020), G. Brunin *et al.*, Phys. Rev. Lett. **125**, 136601 (2020), M. Royo *et al.*, Phys. Rev. Lett. **125**, 217602 (2020), M. Royo and M. Stengel, Phys. Rev. X **11**, 041027 (2021), SP *et al.*, Phys. Rev. Lett. **130**, 166301 (2023)

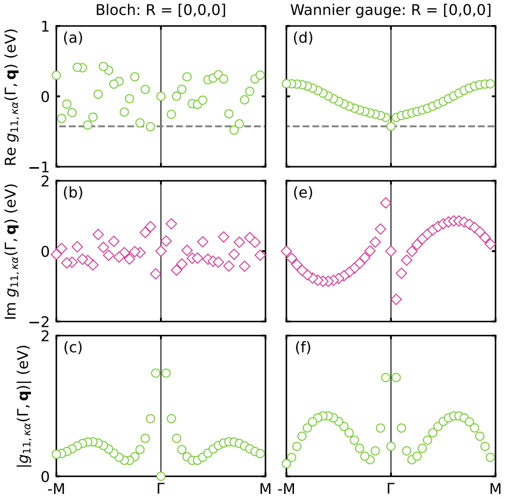
Long-range expressions

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) \equiv \langle \Psi_{m\mathbf{k}+\mathbf{q}} | \Delta_{\mathbf{q}\nu} V | \Psi_{n\mathbf{k}} \rangle$$

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = \left[\frac{\hbar}{2\omega_\nu(\mathbf{q})}\right]^{\frac{1}{2}} \sum_{\kappa\alpha} \frac{e_{\kappa\alpha\nu}(\mathbf{q})}{\sqrt{M_\kappa}} \, g_{mn,\kappa\alpha}(\mathbf{k},\mathbf{q})$$

$$g_{mn,\kappa\alpha}(\mathbf{k},\mathbf{q}) = g^{\mathcal{S}}_{mn,\kappa\alpha}(\mathbf{k},\mathbf{q}) + \sum_{\mathbf{G}\neq-\mathbf{q}} \sum_{sp} U_{ms\mathbf{k}+\mathbf{q}+\mathbf{G}} \langle u^{\mathrm{W}}_{s\mathbf{k}+\mathbf{q}+\mathbf{G}} | V^{\mathcal{L}}_{\mathbf{q}+\mathbf{G}\kappa\alpha} | u^{\mathrm{W}}_{p\mathbf{k}} \rangle U^{\dagger}_{pn\mathbf{k}}$$

$$|u_{n\mathbf{k}}\rangle = e^{-i\mathbf{k}\cdot\mathbf{r}} |\Psi_{n\mathbf{k}}\rangle = \sum_p U^*_{np\mathbf{k}} |u^{\mathrm{W}}_{p\mathbf{k}}\rangle$$



SP, M. Royo, M. Gibertini, N. Marzari and M. Stengel, Phys. Rev. Lett. **130**, 166301 (2023)

3D long-range scattering potential

$$V^{\mathcal{L}}_{\mathbf{q}\kappa\alpha}(\mathbf{r}) = \frac{4\pi e \, f(|\mathbf{q}|)}{\Omega |\mathbf{q}|^2 \, \tilde{\epsilon}(\mathbf{q})} e^{-i\mathbf{q}\cdot\boldsymbol{\tau}_\kappa} \Big(i\mathbf{q}\cdot\mathbf{Z}_{\kappa\alpha} + \frac{1}{2}\mathbf{q}\cdot\mathbf{Q}_{\kappa\alpha}\cdot\mathbf{q}\Big)\Big(1 + i\mathbf{q}\cdot V^{\mathrm{Hxc},\boldsymbol{\mathcal{E}}}(\mathbf{r})\Big)$$

$$\tilde{\epsilon}(\mathbf{q}) = \frac{\mathbf{q}\cdot\ \boldsymbol{\varepsilon}\cdot\mathbf{q}}{|\mathbf{q}|^2} f(|\mathbf{q}|) + 1 - f(|\mathbf{q}|)$$

$$f(|\mathbf{q}|) = e^{-\frac{|\mathbf{q}+\mathbf{G}|^2 L^2}{4}}$$

$$d(L) = \frac{1}{N} \sum^{*}_{\kappa\kappa' l} \sum_{\alpha\beta} |\Phi^{\mathcal{S}}_{\kappa\alpha,\kappa'\beta}(0,l)|$$

G. Brunin *et al.*, Phys. Rev. Lett. **125**, 136601 (2020), SP *et al.*, Phys. Rev. B **107**, 155424 (2023)

$$V^{\mathcal{L}}_{\mathbf{q}\kappa\alpha}(\mathbf{r}) = \frac{\pi e}{S}\frac{f(|\mathbf{q}|)}{|\mathbf{q}|}e^{-i\mathbf{q}\cdot\boldsymbol{\tau}_\kappa}\Bigg[\frac{1}{\tilde{\epsilon}^{\|}(\mathbf{q})}\Big\{2i\mathbf{q}\cdot\mathbf{Z}_{\kappa\alpha} + \mathbf{q}\cdot\mathbf{Q}_{\kappa\alpha}\cdot\mathbf{q} - |\mathbf{q}|^2 Q_{\kappa\alpha zz} - 2\mathbf{q}\cdot\mathbf{Z}_{\kappa\alpha}\mathbf{q}\cdot V^{\mathrm{Hxc},\boldsymbol{\mathcal{E}}}(\mathbf{r})/e\Big\}$$

$$+ \frac{1}{\tilde{\epsilon}^{\perp}(\mathbf{q})}\Big\{2|\mathbf{q}|^2 Z_{\kappa\alpha z}\big[z + V^{\mathrm{Hxc},\mathcal{E}_z}(\mathbf{r})/e\big]\Big\}\Bigg]$$

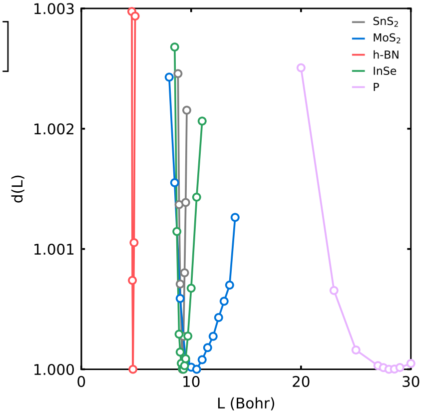
$$\tilde{\epsilon}^{\|}(\mathbf{q}) = 1 + \frac{2\pi f(|\mathbf{q}|)}{|\mathbf{q}|}\mathbf{q}\cdot\boldsymbol{\alpha}^{\|}\cdot\mathbf{q}$$

$$\tilde{\epsilon}^{\perp}(\mathbf{q}) = 1 - 2\pi|\mathbf{q}| f(|\mathbf{q}|)\,\alpha^{\perp}$$

$$\boldsymbol{\alpha}^{\|} = (\breve{\varepsilon}_{\alpha\beta} - \delta_{\alpha\beta})\frac{c}{4\pi}$$

$$\alpha^{\perp} = (1 - \breve{\varepsilon}^{-1}_{zz})\frac{c}{4\pi}$$

$$f(|\mathbf{q}|) = 1 - \tanh(|\mathbf{q}|\, L/2)$$



SP, M. Royo, M. Stengel, N. Marzari and M. Gibertini, Phys. Rev. B **107**, 155424 (2023)

Matrix overlap

$$g_{mn,\kappa\alpha}(\mathbf{k},\mathbf{q}) = g^{\mathcal{S}}_{mn,\kappa\alpha}(\mathbf{k},\mathbf{q}) + \sum_{\mathbf{G}\neq-\mathbf{q}} \sum_{sp} U_{ms\mathbf{k}+\mathbf{q}+\mathbf{G}} \langle u^{\mathrm{W}}_{s\mathbf{k}+\mathbf{q}+\mathbf{G}} | V^{\mathcal{L}}_{\mathbf{q}+\mathbf{G}\kappa\alpha} | u^{\mathrm{W}}_{p\mathbf{k}} \rangle U^{\dagger}_{pn\mathbf{k}}$$

Wannier gauge is smooth everywhere in BZ and for $\mathbf{q} \to 0$:

$$\langle u^{\mathrm{W}}_{s\mathbf{k}+\mathbf{q}}| = \langle u^{\mathrm{W}}_{s\mathbf{k}}| + \sum_{\alpha} q_{\alpha} \left\langle \frac{\partial u^{\mathrm{W}}_{s\mathbf{k}}}{\partial k_{\alpha}} \right| + \cdots$$

The **r**-dependent part:

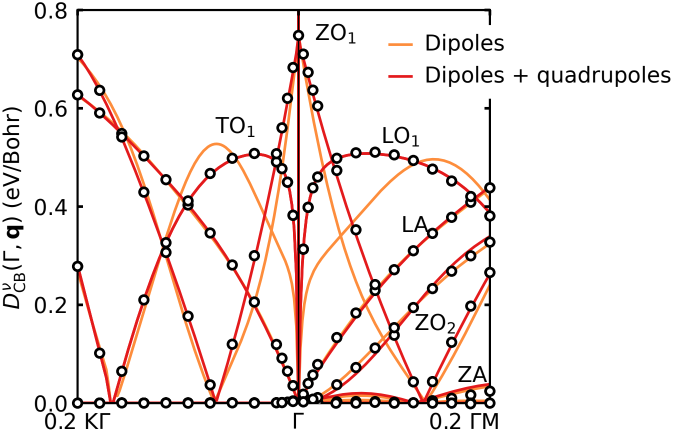
$$\langle \psi_{m\mathbf{k}+\mathbf{q}} | e^{i\mathbf{q}\cdot\mathbf{r}} [1 + i\mathbf{q}\cdot V^{\mathsf{Hxc},\boldsymbol{\mathcal{E}}}(\mathbf{r})] | \psi_{n\mathbf{k}} \rangle = \sum_{sp} U_{ms\mathbf{k}+\mathbf{q}} \Big[\delta_{sp} + i\mathbf{q}\cdot \Big(\mathbf{A}^{\mathrm{W}}_{sp\mathbf{k}} + \langle u^{\mathrm{W}}_{s\mathbf{k}} | V^{\mathsf{Hxc},\boldsymbol{\mathcal{E}}}(\mathbf{r}) | u^{\mathrm{W}}_{p\mathbf{k}} \rangle \Big) \Big] U^{\dagger}_{pn\mathbf{k}},$$

where $A^{\mathrm{W}}_{sp\mathbf{k},\alpha} = -i\langle \frac{\partial u^{\mathrm{W}}_{s\mathbf{k}}}{\partial k_{\alpha}} | u^{\mathrm{W}}_{p\mathbf{k}} \rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \mathbf{r}_{sp,\mathbf{R}}$ is the Berry connection

$V^{\mathrm{Hxc},\boldsymbol{\mathcal{E}}}(\mathbf{r})$ has been found to be small and is neglected.

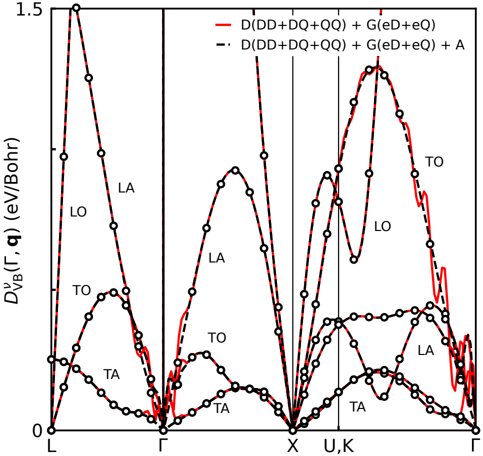
SP, M. Royo, M. Stengel, N. Marzari and M. Gibertini, Phys. Rev. B **107**, 155424 (2023)

$$D^{\nu}(\Gamma,\mathbf{q}) =$$
$$\frac{1}{\hbar N_{\rm w}}\left[2\rho S_{\rm uc}\hbar\omega_{\mathbf{q}\nu}\sum_{mn}|g_{mn\nu}(\Gamma,\mathbf{q})|^2\right]^{1/2}$$



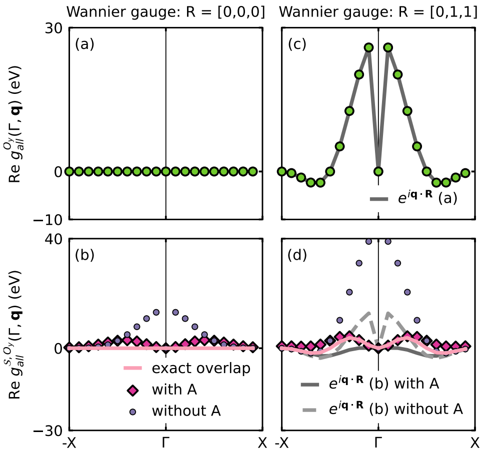
SP, M. Royo, M. Stengel, N. Marzari and M. Gibertini, Phys. Rev. B **107**, 155424 (2023)

1. Improves the interpolation quality - quadrupolar order term

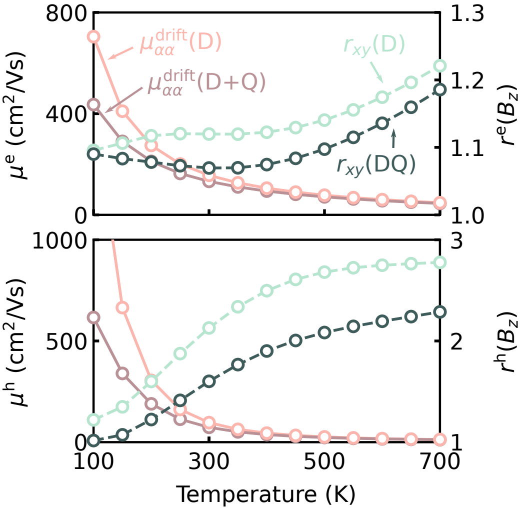


SP, M. Royo, M. Stengel, N. Marzari and M. Gibertini, Phys. Rev. B **107**, 155424 (2023)

2. Restores gauge covariance in the long-wavelength limit



SP, M. Royo, M. Stengel, N. Marzari and M. Gibertini, Phys. Rev. B **107**, 155424 (2023)



SP, M. Royo, M. Gibertini, N. Marzari and M. Stengel, Phys. Rev. Lett. **130**, 166301 (2023)

Electronic velocities

$$\mu^{\mathrm{d}}_{\alpha\beta} = \frac{-1}{V_{\mathrm{uc}} n_{\mathrm{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

Obtained from the commutator:

$$\hat{\mathbf{v}} = (i/\hbar)[\hat{H}, \hat{\mathbf{r}}]$$

$$\mathbf{v}_{nm\mathbf{k}} = \langle \psi_{m\mathbf{k}} | \hat{\mathbf{p}}/m_e + (i/\hbar)[\hat{V}_{\mathrm{NL}}, \hat{\mathbf{r}}] | \psi_{n\mathbf{k}} \rangle,$$

where $\hat{\mathbf{p}} = -i\hbar\partial/\partial\mathbf{r}$ is the momentum operator.
$P_{\mathrm{c}} r_\alpha |\psi_{n\mathbf{k}}\rangle$ are the solution of the linear system:

$$[H - \varepsilon_{n\mathbf{k}} S] P_{\mathrm{c}} r_\alpha |\psi_{n\mathbf{k}}\rangle = P_{\mathrm{c}}^{\dagger} [H - \varepsilon_{n\mathbf{k}} S, r_\alpha] |\psi_{n\mathbf{k}}\rangle,$$

where S is the overlap matrix and P_{c} the projector over the empty states.

In the local approximation (neglecting $\hat{V}_{\mathrm{NL}}$):

$$v_{mn\mathbf{k}\mathbf{k}'\alpha} \approx \langle \psi_{m\mathbf{k}'} | \hat{p}_\alpha | \psi_{n\mathbf{k}} \rangle = \delta(\mathbf{k} - \mathbf{k}') \left(k_\alpha \delta_{mn} - i \int d\mathbf{r} u^*_{m\mathbf{k}'}(\mathbf{r}) \nabla_\alpha u_{n\mathbf{k}}(\mathbf{r}) \right)$$

J. Tóbik and A. D. Corso, J. Chem. Phys. **120**, 9934 (2004)

Electronic velocities

$$\mu^{\mathrm{d}}_{\alpha\beta} = \frac{-1}{V_{\mathrm{uc}} n_{\mathrm{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

Wannier interpolated velocities:

$$v_{nm\mathbf{k}',\alpha} = \frac{1}{\hbar} H_{nm\mathbf{k}',\alpha} - \frac{i}{\hbar}(\varepsilon_{m\mathbf{k}'} - \varepsilon_{n\mathbf{k}'}) A_{mn\mathbf{k}',\alpha}$$

$$A_{mn\mathbf{k}',\alpha} = \sum_{m'n'} U^{\dagger}_{mm'\mathbf{k}'} A^{(\mathrm{W})}_{m'n'\mathbf{k}',\alpha} U_{n'n\mathbf{k}'}$$

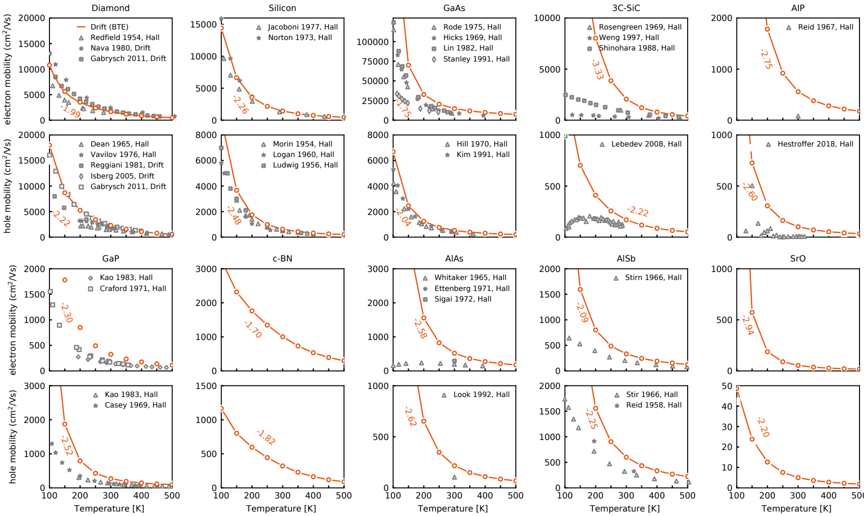
$$A^{(\mathrm{W})}_{nm\mathbf{k},\alpha} = i \sum_{\mathbf{b}} w_b b_\alpha \left(\langle u^{(\mathrm{W})}_{n\mathbf{k}} | u^{(\mathrm{W})}_{m\mathbf{k}+\mathbf{b}} \rangle - \delta_{nm} \right),$$

$\mathbf{b}$ are the vectors connecting $\mathbf{k}$ to its nearest neighbor and overlap matrices are:

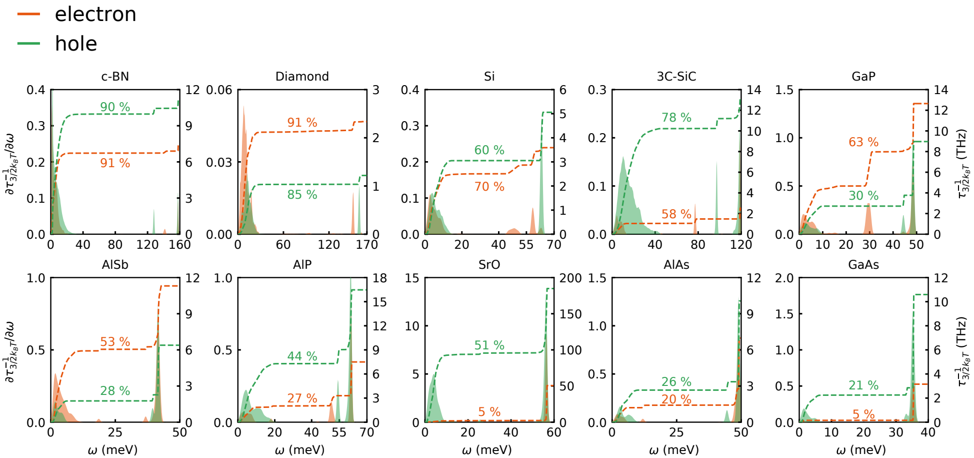
$$\langle u^{(\mathrm{W})}_{n\mathbf{k}} | u^{(\mathrm{W})}_{m\mathbf{k}+\mathbf{b}} \rangle = \sum_{n'm'} U^{\dagger}_{mm'\mathbf{k}} M_{mn\mathbf{k}} U_{nn'\mathbf{k}+\mathbf{b}},$$

$M_{mn\mathbf{k}} = \langle u_{n\mathbf{k}} | u_{m\mathbf{k}+\mathbf{b}} \rangle$ is the phase relation between neighboring Bloch orbitals.

X. Wang, J. R. Yates, I. Souza, and D. Vanderbilt, Phys. Rev. B **74**, 195118 (2006)

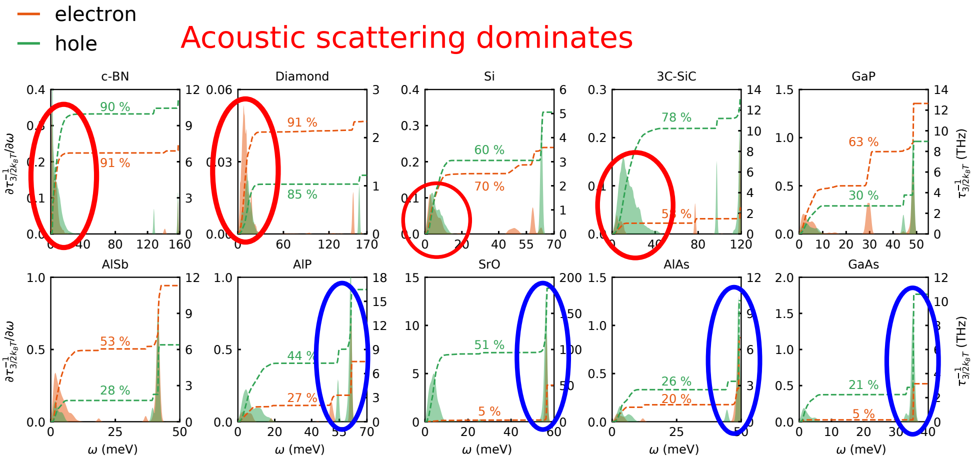


SP, F. Macheda, E. R. Margine, N. Marzari, N. Bonini, and F. Giustino, Phys. Rev. Research **3**, 043022 (2021)

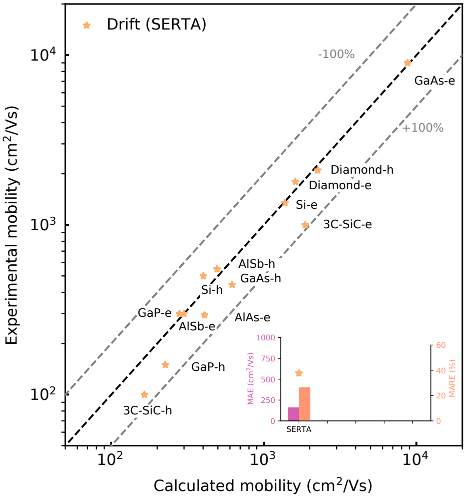


SP, F. Macheda, E. R. Margine, N. Marzari, N. Bonini, and F. Giustino, Phys. Rev. Research **3**, 043022 (2021)

Spectral decomposition: dominant scattering

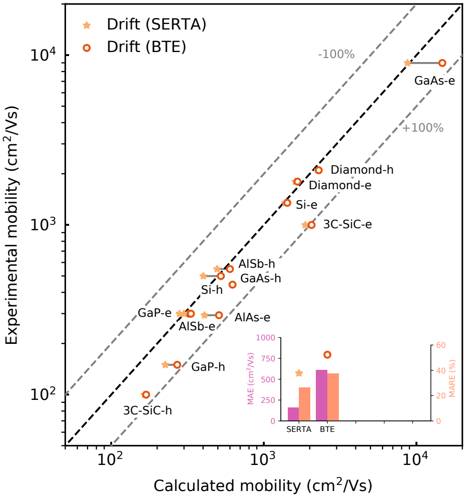


SP, F. Macheda, E. R. Margine, N. Marzari, N. Bonini, and F. Giustino, Phys. Rev. Research **3**, 043022 (2021)

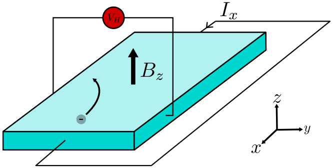


SP, F. Macheda, E. R. Margine, N. Marzari, N. Bonini, and F. Giustino, Phys. Rev. Research **3**, 043022 (2021)

Experimental comparison



SP, F. Macheda, E. R. Margine, N. Marzari, N. Bonini, and F. Giustino, Phys. Rev. Research **3**, 043022 (2021)



$$\mu^{\text{Hall}}_{\alpha\beta}(\hat{\mathbf{B}}) = \sum_{\gamma} \mu^{\text{drift}}_{\alpha\gamma} \, r_{\gamma\beta}(\hat{\mathbf{B}})$$

$$r_{\alpha\beta}(\hat{\mathbf{B}}) \equiv \lim_{\mathbf{B}\to 0} \sum_{\delta\epsilon} \frac{[\, \mu^{\text{drift}}_{\alpha\delta} \,]^{-1} \mu_{\delta\epsilon}(\mathbf{B}) \, [\, \mu^{\text{drift}}_{\epsilon\beta} \,]^{-1}}{|\mathbf{B}|}$$

$$\mu_{\alpha\beta}(B_\gamma) = \frac{-1}{S_{\text{uc}} n_{\text{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{S_{\text{BZ}}} v_{n\mathbf{k}\alpha} \big[\, \partial_{E_\beta} f_{n\mathbf{k}}(B_\gamma) - \partial_{E_\beta} f_{n\mathbf{k}} \,\big]$$

$$\mu^{\text{drift}}_{\alpha\beta} = \frac{-1}{S_{\text{uc}} n_{\text{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{S_{\text{BZ}}} v_{n\mathbf{k}\alpha} \, \partial_{E_\beta} f_{n\mathbf{k}}$$

F. Macheda and N. Bonini, Phys. Rev. B **98**, 201201R (2018)
SP, W. Li, S. Reichardt, and F. Giustino, Rep. Prog. Phys. **83**, 036501 (2020)
SP, F. Macheda, E. R. Margine, N. Marzari, N. Bonini, and F. Giustino, Phys. Rev. Research **3**, 043022 (2021)

Hall mobility

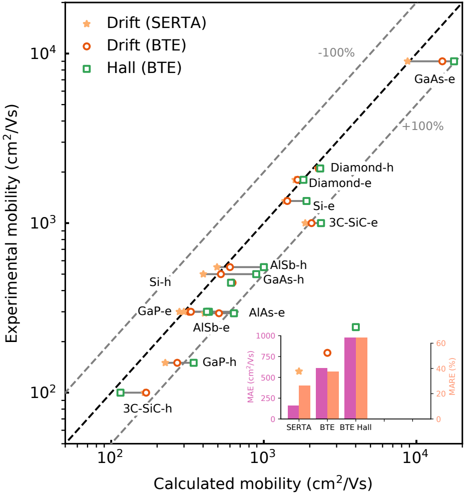
$$\left[1 - \frac{e}{\hbar}\tau_{n\mathbf{k}}(\mathbf{v}_{n\mathbf{k}} \times \mathbf{B}) \cdot \nabla_{\mathbf{k}}\right] \partial_{E_\beta} f_{n\mathbf{k}}(\mathbf{B}) = e v_{n\mathbf{k}\beta} \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \tau_{n\mathbf{k}}$$
$$+ \frac{2\pi \tau_{n\mathbf{k}}}{\hbar} \sum_{m\nu} \int \frac{\mathrm{d}^3 q}{S_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \Big[(n_{\mathbf{q}\nu} + 1 - f^0_{n\mathbf{k}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu})$$
$$+ (n_{\mathbf{q}\nu} + f^0_{n\mathbf{k}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu})\Big] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}(\mathbf{B}),$$

where the scattering rate is

$$\tau^{-1}_{n\mathbf{k}} \equiv \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \big[(n_{\mathbf{q}\nu} + 1 - f^0_{m\mathbf{k}+\mathbf{q}})$$
$$\times \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu})\big]$$

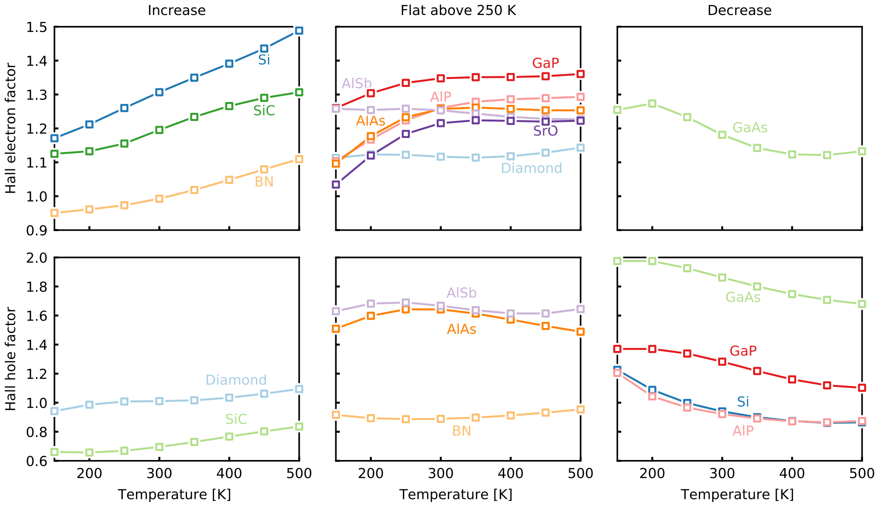
F. Macheda and N. Bonini, Phys. Rev. B **98**, 201201R (2018)
SP, W. Li, S. Reichardt, and F. Giustino, Rep. Prog. Phys. **83**, 036501 (2020)
SP, F. Macheda, E. R. Margine, N. Marzari, N. Bonini, and F. Giustino, Phys. Rev. Research **3**, 043022 (2021)

Experimental comparison



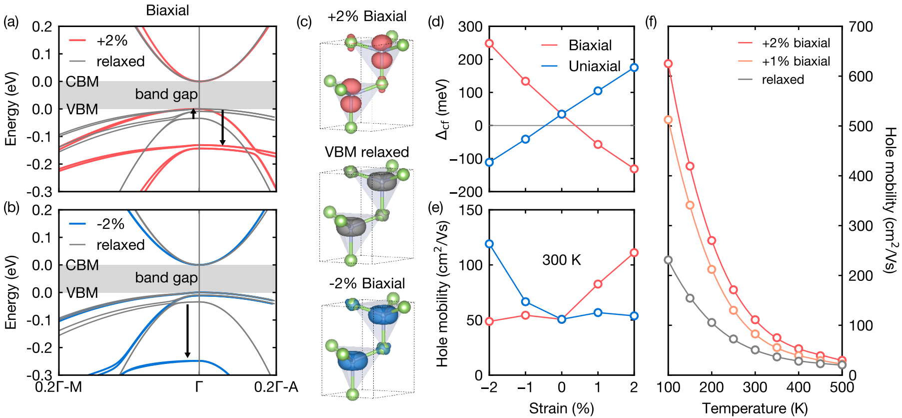
SP, F. Macheda, E. R. Margine, N. Marzari, N. Bonini, and F. Giustino, Phys. Rev. Research **3**, 043022 (2021)

Hall factor is not unity



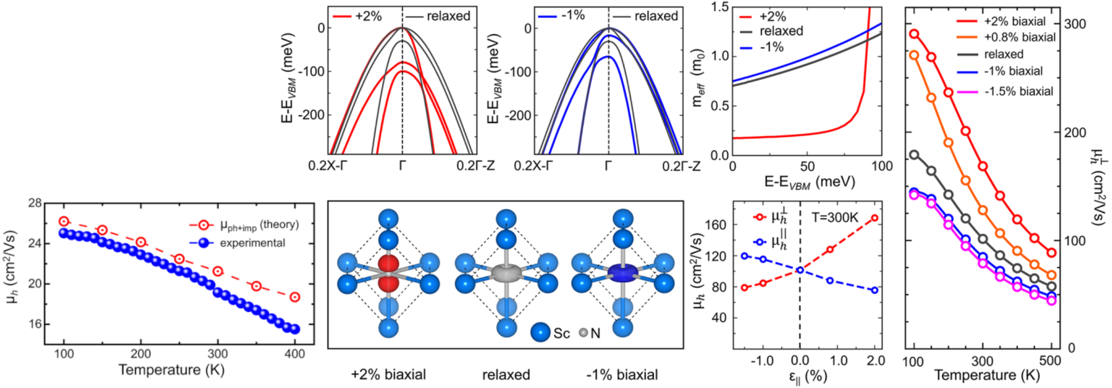
SP, F. Macheda, E. R. Margine, N. Marzari, N. Bonini, and F. Giustino, Phys. Rev. Research **3**, 043022 (2021)

Wurtzite GaN: Reversing the sign of the crystal-field splitting with strain
Can be lattice matched to $ZnGeN_2$ (+50%) and $MgSiN_2$ (+260%)



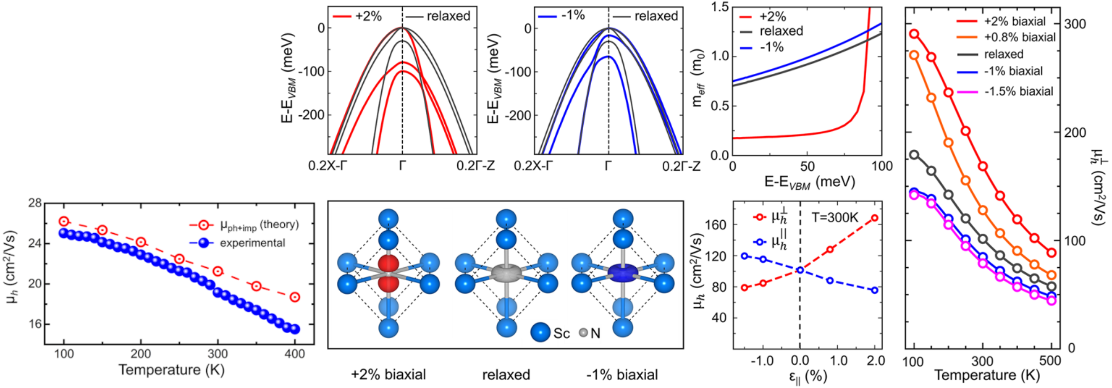
SP, D. Jena, and F. Giustino, Phys. Rev. Lett. **123**, 096602 (2019)
J. Leveillee, SP, N. L. Adamski, C. G. Van de Walle, and F. Giustino, App. Phys. Lett. **120**, 202106 (2022)

High hole mobility in strained p-type ScN



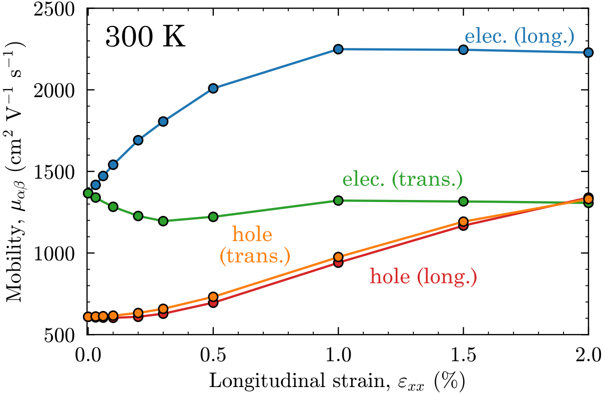
S. Rudra, D. Rao, SP, and B. Saha, Nano Lett. **23**, 8211 (2023)

High hole mobility in strained p-type ScN



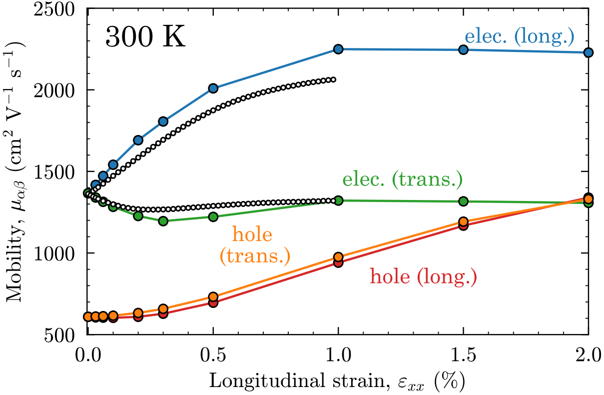
S. Rudra, D. Rao, SP, and B. Saha, Nano Lett. **23**, 8211 (2023)

Impact on mobility of highly-strained silicon

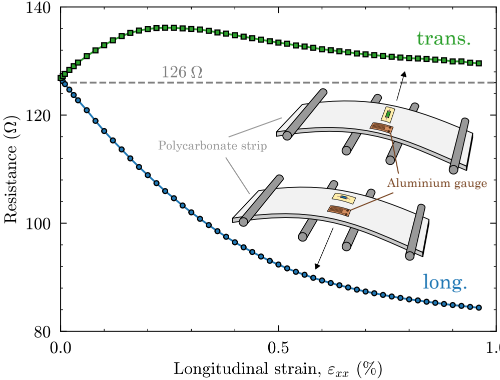


N. Roisin, G. Brunin, G.-M. Rignanese, D. Flandre, J.-P. Raskin, and SP, submitted (2024)

Impact on mobility of highly-strained silicon



Lab-on-a-chip: 4-point bending measurements



N. Roisin, G. Brunin, G.-M. Rignanese, D. Flandre, J.-P. Raskin, and SP, submitted (2024)

Approximations:

- point charge impurity embedded in the dielectric continuum of the host material
- $\tau^{\mathrm{imp},-1}$ within the first Born approximation (single-impurity scattering)
- dilute limit (additive $\tau^{\mathrm{imp},-1}$) + randomly distributed impurities

Charged impurity scattering:

$$\frac{1}{\tau^{\mathrm{imp}}_{n\mathbf{k}}} = N^{\mathrm{imp}} \frac{2\pi}{\hbar} \sum_{m\mathbf{q}} |g^{\mathrm{imp}}_{mn}(\mathbf{k},\mathbf{q})|^2 \, \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}})$$

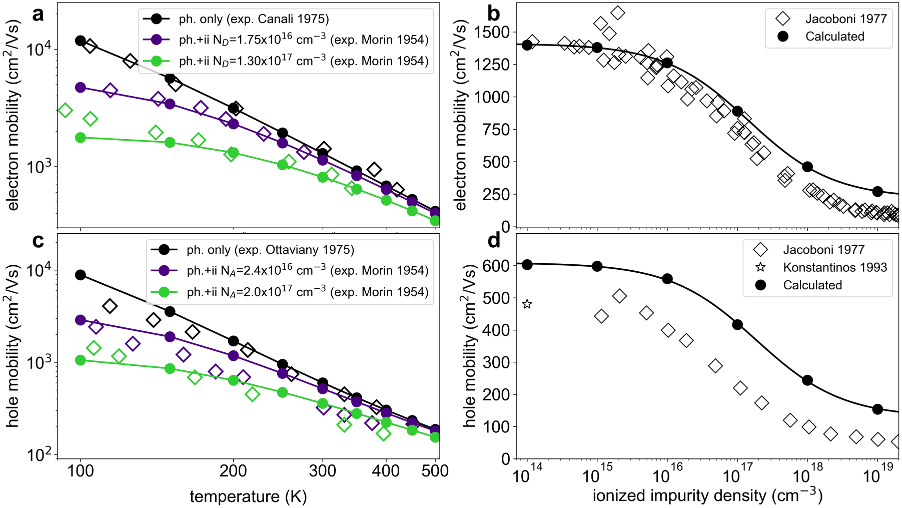
$$|g^{\mathrm{imp}}_{mn}(\mathbf{k},\mathbf{q})|^2 = \left[\frac{e^2}{4\pi\epsilon^0}\frac{4\pi Z}{\Omega}\right]^2 \sum_{\mathbf{G}\neq-\mathbf{q}} \frac{|\langle\psi_{m\mathbf{k}+\mathbf{q}}|e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|\psi_{n\mathbf{k}}\rangle|^2}{|(\mathbf{q}+\mathbf{G})\cdot\boldsymbol{\epsilon}^0\cdot(\mathbf{q}+\mathbf{G})|^2},$$

with a non-integrable divergence $|\mathbf{q}|^{-4}$ $\rightarrow$ free carrier screening in the $\mathbf{q}\rightarrow\mathbf{0}$ limit:

$$\boldsymbol{\epsilon}^0 \rightarrow \boldsymbol{\epsilon}^0 + \frac{(q^{\mathrm{TF}})^2}{q^2}\boldsymbol{\mathcal{I}}$$

$$(q^{\mathrm{TF}})^2 = \frac{e^2}{4\pi\epsilon^0}\frac{4\pi}{\Omega} 2\sum_n \int \frac{d\mathbf{k}}{\Omega_{\mathrm{BZ}}}\left|\frac{\partial f^0_{n\mathbf{k}}}{\partial\varepsilon_{n\mathbf{k}}}\right|$$

J. Leveillee, X. Zhang, E. Kioupakis, and F. Giustino, Phys. Rev. B **107**, 125207 (2023)



J. Leveillee, X. Zhang, E. Kioupakis, and F. Giustino, Phys. Rev. B **107**, 125207 (2023)

Matthiessen's rule:

$$\frac{1}{\mu} = \frac{1}{\mu^{\text{ph}}} + \frac{1}{\mu^{\text{imp}}}$$

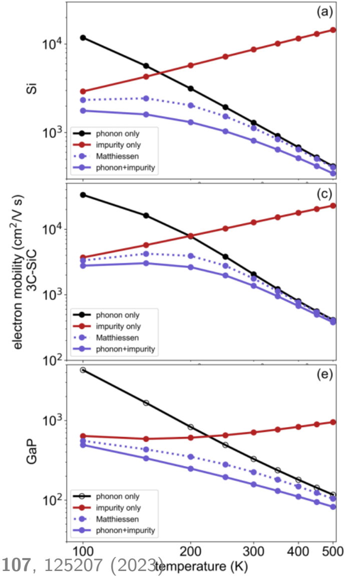
versus aiBTE:

$$\partial_{E_\beta} f_{n\mathbf{k}}(\mathbf{B}) = e v_{n\mathbf{k}\beta} \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \left[\tau_{n\mathbf{k}} + \tau^{\text{imp}}_{n\mathbf{k}}\right] + \frac{2\pi}{\hbar}\left[\tau_{n\mathbf{k}} + \tau^{\text{imp}}_{n\mathbf{k}}\right] \sum_m$$

$$\times \int \frac{\mathrm{d}^3 q}{S_{\text{BZ}}} \Bigg[\sum_\nu |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \Big\{ (n_{\mathbf{q}\nu} + 1 - f^0_{n\mathbf{k}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu})$$

$$+ (n_{\mathbf{q}\nu} + f^0_{n\mathbf{k}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) \Big\}$$

$$+ |g^{\text{imp}}_{mn}(\mathbf{k},\mathbf{q})|^2 \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}}) \Bigg] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}(\mathbf{B})$$



J. Leveillee, X. Zhang, E. Kioupakis, and F. Giustino, Phys. Rev. B **107**, 125207 (2023)

Resistivity in metals

Can be obtained from the solution of the BTE:

$$\rho_{\alpha\beta} = \sigma^{-1}_{\alpha\beta}$$

$$\sigma_{\alpha\beta} = \frac{-e}{V_{\rm uc}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\rm BZ}}\, v^{\alpha}_{n\mathbf{k}}\, \partial_{E_\beta} f_{n\mathbf{k}}$$

Further approximation:

- constant $g_{mn\nu}(\mathbf{k},\mathbf{q})$ close to the Fermi level
- $-\frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \approx \delta(\varepsilon^{\rm F} - \varepsilon_{n\mathbf{k}})$

Lowest-order variational approximation (LOVA) / Ziman formula:

$$\rho(T) = \frac{4\pi m_e}{ne^2 k_B T} \int_0^\infty d\omega\, \hbar\omega\, \alpha^2_{\rm tr} F(\omega)\, n(\omega,T)\big[1 + n(\omega,T)\big],$$

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

Lowest-order variational approximation (LOVA) / Ziman formula:

$$\rho(T) = \frac{4\pi m_e}{ne^2 k_B T}\int_0^\infty d\omega\,\hbar\omega\,\alpha^2_{\text{tr}}F(\omega)\,n(\omega,T)\big[1+n(\omega,T)\big],$$

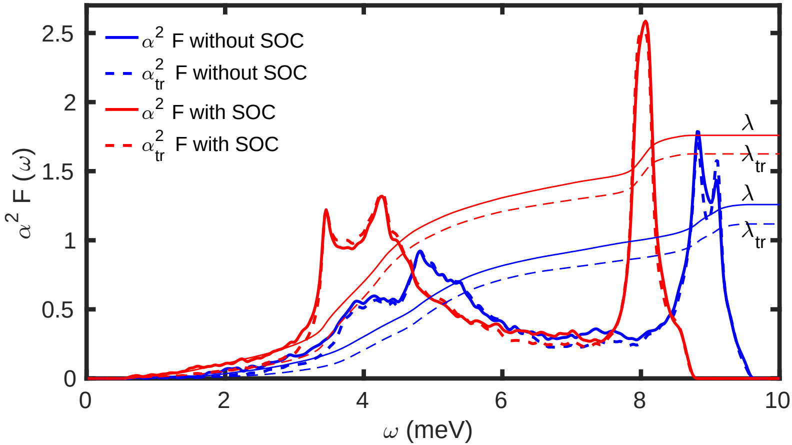
Isotropic Eliashberg transport spectral function:

$$\alpha^2_{\text{tr}}F(\omega) = \frac{1}{2}\sum_{\nu}\int_{\text{BZ}}\frac{d\mathbf{q}}{\Omega_{\text{BZ}}}\omega_{\mathbf{q}\nu}\,\lambda_{\text{tr},\mathbf{q}\nu}\,\delta(\omega-\omega_{\mathbf{q}\nu}),$$

Mode-resolved transport coupling strength is defined by:

$$\lambda_{\text{tr},\mathbf{q}\nu} = \frac{1}{N(\varepsilon_F)\omega_{\mathbf{q}\nu}}\sum_{nm}\int_{\text{BZ}}\frac{d\mathbf{k}}{\Omega_{\text{BZ}}}|g_{mn,\nu}(\mathbf{k},\mathbf{q})|^2\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{\text{F}})\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{\text{F}})\left(1-\frac{v_{n\mathbf{k}}\cdot v_{m\mathbf{k}+\mathbf{q}}}{|v_{n\mathbf{k}}|^2}\right).$$

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



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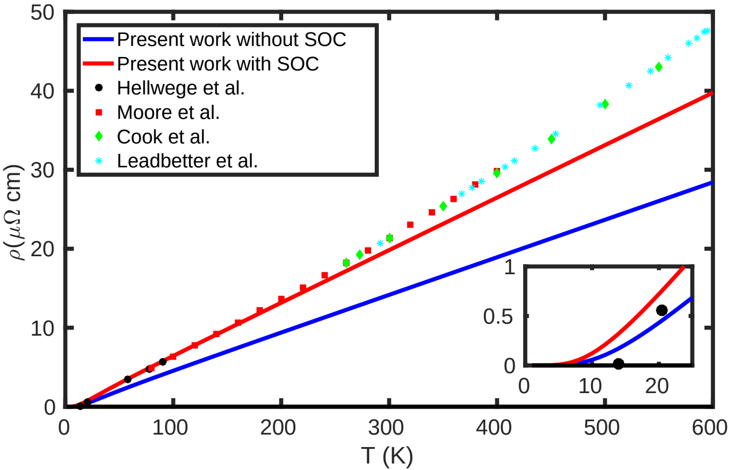
Ziman's formula



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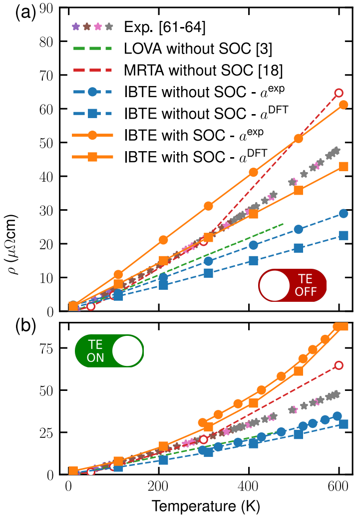
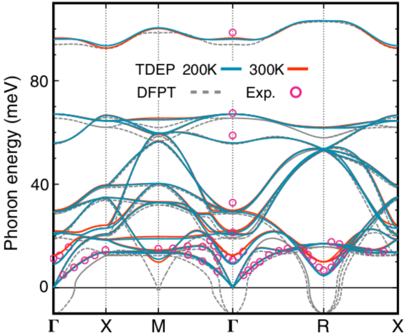


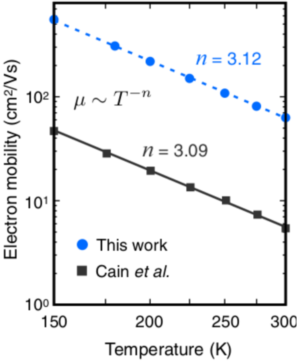
F. Goudreault, SP, F. Giustino, and M. Côté, unpublished (2024)

Anharmoncity can be treated with:

- TDEP, SSCHA
- d3q, phono3py, ShengBTE
- Alamode,
- ZG.x

Perturbo





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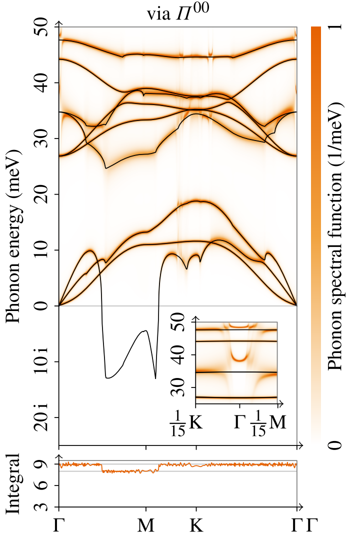
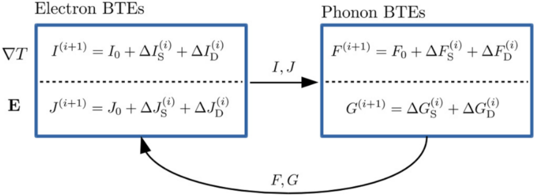
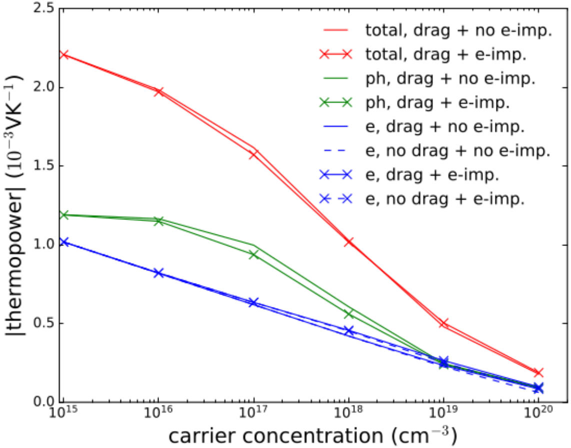


- Phonon spectral function $\Pi_{\mathbf{q}}(T, \omega)$ at 12 K - monolayer TaS_2
- Many Kohn anomalies are revealed

J. Berges, N. Girotto, T. Wehling, N. Marzari, and SP, Phys. Rev. X **13**, 041009 (2023) elphbolt





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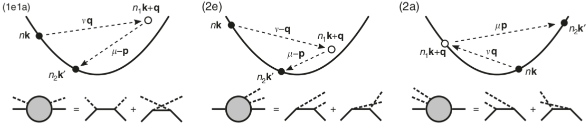
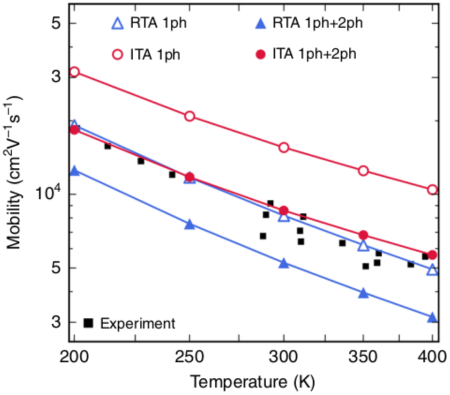
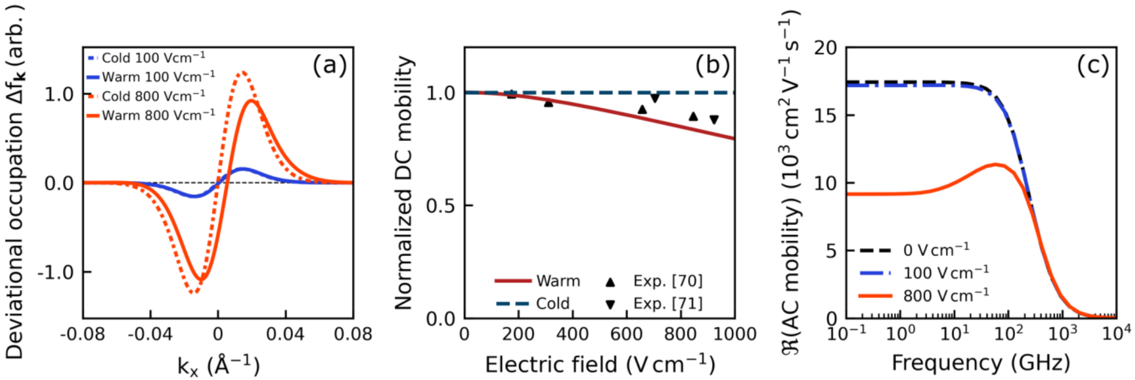




GaAs

N.-E. Lee, J.J. Zhou, H.-Y. Chen, and M. Bernardi, Nature Commun. **11**, 1607 (2020)



GaAs

A. Y. Choi, P. S. Cheng, B. Hatanpää, and A. J. Minnich, Phys. Rev. Materials **5**, 044603 (2021)

Recent developments: Electron-neutral defect scattering

Perturbo

DFT: $\Delta V_{\mathrm{e-d}}$

DFT: $|n\boldsymbol{k}_{\mathrm{c}}\rangle$

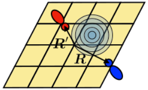
WF: $|j\boldsymbol{R}\rangle \longleftrightarrow U_{\boldsymbol{k}_{\mathrm{c}}}$

(i)

$$M_{mn}(\boldsymbol{k}'_{\mathrm{c}},\boldsymbol{k}_{\mathrm{c}}) = \langle m\boldsymbol{k}'_{\mathrm{c}}\,|\,\Delta V_{\mathrm{e-d}}\,|\,n\boldsymbol{k}_{\mathrm{c}}\rangle$$

(ii)

$$M_{ij}(\boldsymbol{R}',\boldsymbol{R}) = \langle i\boldsymbol{R}'\,|\,\Delta V_{\mathrm{e-d}}\,|\,j\boldsymbol{R}\rangle = \left(\frac{1}{N_{\boldsymbol{k}_{\mathrm{c}}}}\right)^2 \sum_{\boldsymbol{k}'_{\mathrm{c}}\boldsymbol{k}_{\mathrm{c}}} e^{i(\boldsymbol{k}'_{\mathrm{c}}\cdot\boldsymbol{R}'-\boldsymbol{k}_{\mathrm{c}}\cdot\boldsymbol{R})}\left[U^{\dagger}_{\boldsymbol{k}'_{\mathrm{c}}} M(\boldsymbol{k}'_{\mathrm{c}},\boldsymbol{k}_{\mathrm{c}}) U_{\boldsymbol{k}_{\mathrm{c}}}\right]_{ij}$$

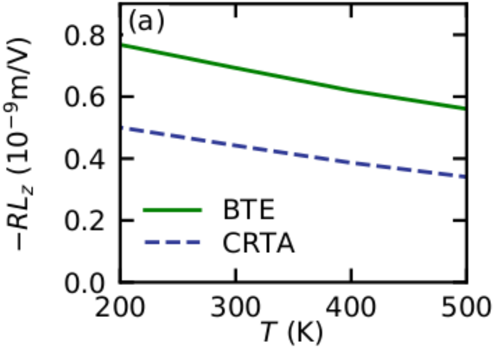


(iii) $H(\boldsymbol{R}) \longrightarrow H(\boldsymbol{k}_{\mathrm{f}}) \longrightarrow U_{\boldsymbol{k}_{\mathrm{f}}}$

(iv)

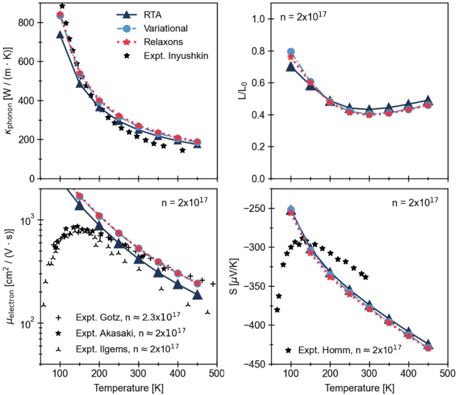
$$M_{mn}(\boldsymbol{k}'_{\mathrm{f}},\boldsymbol{k}_{\mathrm{f}}) = \sum_{\boldsymbol{R}'\boldsymbol{R}} e^{-i(\boldsymbol{k}'_{\mathrm{f}}\cdot\boldsymbol{R}'-\boldsymbol{k}_{\mathrm{f}}\cdot\boldsymbol{R})}\left[U_{\boldsymbol{k}'_{\mathrm{f}}} M(\boldsymbol{R}',\boldsymbol{R}) U^{\dagger}_{\boldsymbol{k}_{\mathrm{f}}}\right]_{mn}$$

I.-T. Lu, J. Park, J.-J. Zhou, and M. Bernardi, npj Comput. Mater. **6**, 17 (2020)



Current responsivity in GeTe

$$R = \frac{1}{L_z}\frac{\sigma^{z;xx}_{\mathrm{NLH}}}{\sigma^{xx}_{\mathrm{L}}}$$

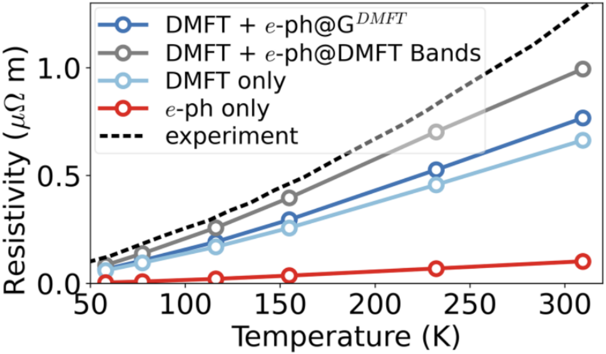


Thermal and carrier transport of doped GaN

J.-M. Lihm and C.-H. Park, Phys. Rev. Lett. **132**, 106402 (2024)
A. Cepellotti, J. Coulter, A. Johansson, N. S. Fedorova, and B. Kozinsky, J. Phys: Mater. 5, 035003 (2022)

Perturbo

TRIQS



Transport in Sr_2RuO_4

D. J. Abramovitch, J.-J. Zhou, J. Mravlje, A. Georges, and M. Bernardi, Phys. Rev. Mater. **7**, 093801 (2023)
+ cumulant → J.-J. Zhou and M. Bernardi, Phys. Rev. Research **1**, 033138 (2019)

Recent developments: rise of the machine ...

PHYSICAL REVIEW APPLIED **19,** 064049 (2023)

Physics-Informed Deep Learning for Solving Coupled Electron and Phonon Boltzmann Transport Equations

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Electron-phonon (*e*-ph) coupling and transport are ubiquitous in modern electronic devices. The coupled electron and phonon Boltzmann transport equations (BTEs) hold great potential for the simulation of thermal transport in metal and semiconductor systems. However, solving the BTEs is often computationally challenging owing to their high dimensional complexity and a wide span of heat carrier properties, which

Machine learning electron-phonon interactions in 2D materials

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(Dated: August 10, 2023)

Accelerating the calculation of electron-phonon coupling by machine learning methods

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PHYSICAL REVIEW LETTERS **132,** 096401 (2024)

Editors' Suggestion

Deep-Learning Density Functional Perturbation Theory

He Li,[1,2,*] Zechen Tang,[1,*] Jingheng Fu,[1] Wen-Han Dong,[1] Nianlong Zou,[1] Xiaoxun Gong,[1,3] Wenhui Duan,[1,2,4,†] and Yong Xu[1,4,5,‡]
[1]*State Key Laboratory of Low Dimensional Quantum Physics and Department of Physics, Tsinghua University, Beijing 100084, China*
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Calculating perturbation response properties of materials from first principles provides a vital link between theory and experiment, but is bottlenecked by the high computational cost. Here, a general framework is proposed to perform density functional perturbation theory (DFPT) calculations by neural networks, greatly improving the computational efficiency. Automatic differentiation is applied on neural networks, facilitating accurate computation of derivatives. High efficiency and good accuracy of the approach are demonstrated by studying electron-phonon coupling and related physical quantities. This work brings deep-learning density functional theory and DFPT into a unified framework, creating opportunities for developing *ab initio* artificial intelligence.

DOI: 10.1103/PhysRevLett.132.096401

PHYSICAL REVIEW X **14,** 021023 (2024)

Data-Driven Compression of Electron-Phonon Interactions

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First-principles calculations of electron interactions in materials have seen rapid progress in recent years, with electron-phonon (*e*-ph) interactions being a prime example. However, these techniques use large matrices encoding the interactions on dense momentum grids, which reduces computational efficiency and obscures interpretability. For *e*-ph interactions, existing interpolation techniques leverage locality in real space, but the high dimensionality of the data remains a bottleneck to balance cost and accuracy. Here we show an efficient way to compress *e*-ph interactions based on singular value decomposition (SVD), a widely used matrix and image compression technique. Leveraging (un)constrained SVD methods, we accurately predict material properties related to *e*-ph interactions—including charge mobility, spin relaxation times, band renormalization, and superconducting critical temperature—while using only a small fraction (1%–2%) of the interaction data. These findings unveil the hidden low-dimensional nature of

R. Li, E. Lee, and T. Luo, Phys. Rev. Appl. **19**, 064049 (2023)
H. Li, Z. Tang, J. Fu, W.-H. Dong, N. Zou, X. Gong, W. Duan, and Y. Xu, Phys. Rev. Lett. **132**, 0.96401 (2024)
Y. Luo, D. Desai, B. K. Chang, J. Park, and M. Bernardi, Phys. Rev. X **14**, 021023 (2024)

Recent developments: rise of the machine ...

PHYSICAL REVIEW APPLIED **19,** 064049 (2023)

Physics-Informed Deep Learning for Solving Coupled Ele
Boltzmann Transport Equations

Ruiyang Li,[1] Eungkyu Lee,[2,*] and Tengfei Lu
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Accelerating the calculation of electron-phonon coupling
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PHYSICAL REVIEW LETTERS **132,** 096401 (2024)

Editors' Suggestion

Deep-Learning Density Functional Perturbation Theory

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PHYSICAL REVIEW X **14,** 021023 (2024)

riven Compression of Electron-Phonon Interactions

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Y. Luo, D. Desai, B. K. Chang, J. Park, and M. Bernardi, Phys. Rev. X **14**, 021023 (2024)

Conclusion

- The Boltzmann transport equation can be obtained from a rigorous many-body framework
- Long-range electrostatics is important for accurate interpolation
- The Hall factor is temperature dependent and can deviate from unity
- BTE mobilities overestimates experiment
- Carrier-impurity scattering is crucial for high-carrier concentrations

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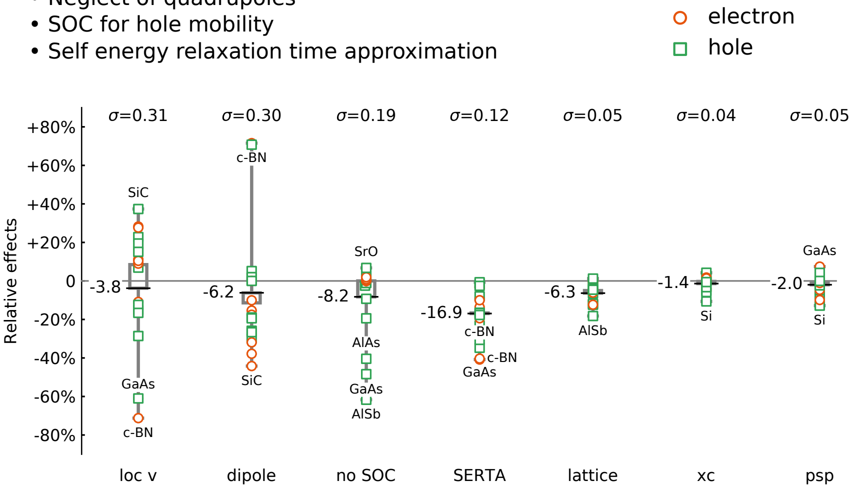
Supplemental Slides

Strongest approximations

- Local velocity approximation
- Neglect of quadrupoles
- SOC for hole mobility
- Self energy relaxation time approximation



Linearized Boltzmann transport equation

Side note

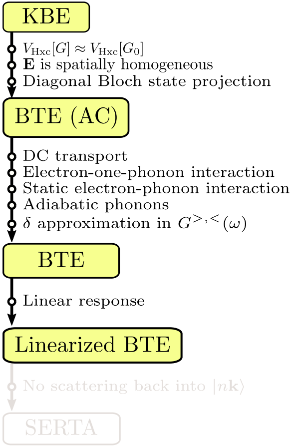
Berryology [TM Ivo Souza]:

$$j_\alpha = -e \int_{\mathbf{k}} \dot{r}_a f(\varepsilon)$$
$$= -e \int_{\mathbf{k}} [\underbrace{v_a}_{\text{band}} + \underbrace{(e/\hbar)\Omega_{ab} E_b}_{\text{anomalous}} + \dots][f_0 + \tau e v_c E_c f_0' + \dots]$$
$$= C + \sigma_{ab} E_b + \sigma_{abc} E_b E_c + \dots$$

$$\sigma_{ab} = -e^2\tau \int_{\mathbf{k}} v_a v_b f_0' - \frac{e^2}{\hbar} \int_{\mathbf{k}} \Omega_{ab} f_0$$

Linear Ohmic + Hall

In system with TR symmetry: $\int_{\mathbf{k}} \Omega_{ab} f_0 = 0$



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