

2021 Virtual School on Electron-Phonon Physics and the EPW code

June 14-18 2021



U.S. DEPARTMENT OF
ENERGY

Lecture Wed.1

Transport module of EPW

Samuel Poncé

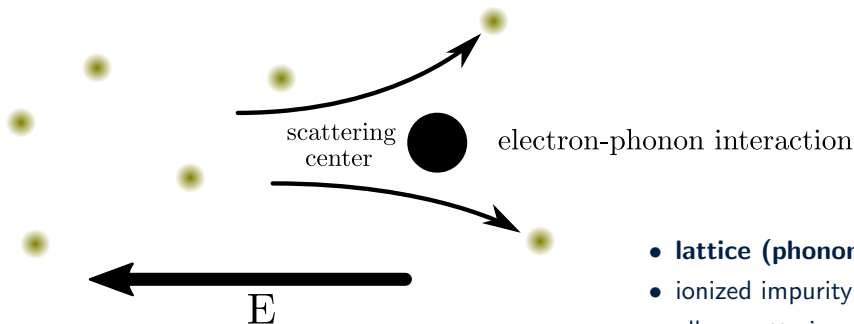
Theory and Simulation of Materials (THEOS)

École Polytechnique Fédérale de Lausanne

- Carrier transport
- Quantum theory of mobility
- Boltzmann transport equation
- Technical details
- Applications to semiconductors
- Ionized impurity scattering

Carrier transport: experimental evidences

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



- **lattice (phonon) scattering**
- ionized impurity scattering
- alloy scattering
- defects scattering

Carrier transport: experimental evidences

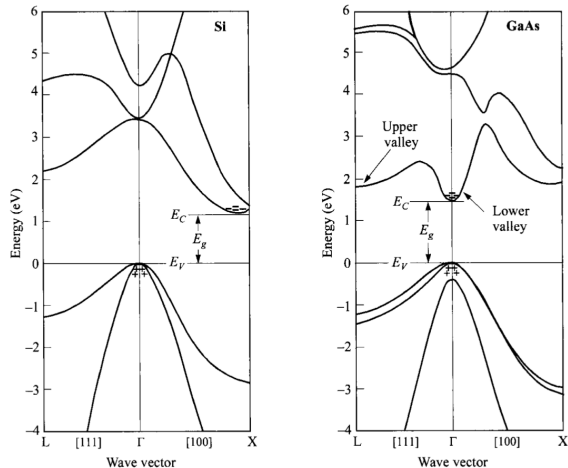
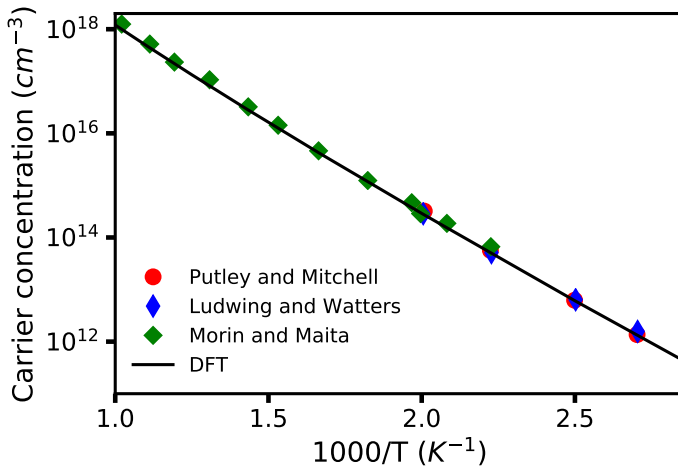


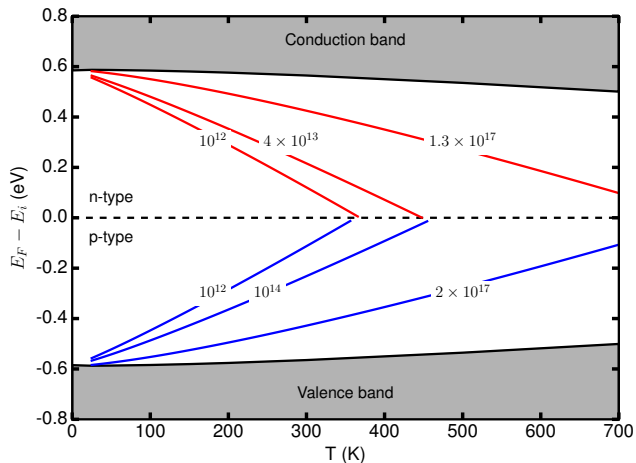
Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Carrier transport: experimental evidences



Carrier transport: experimental evidences

Calculated evolution of the Fermi level of Si as a function of temperature and impurity concentration.



Carrier transport: experimental evidences

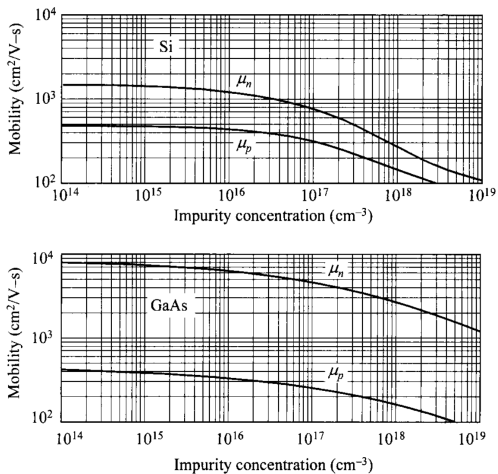


Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Carrier transport: experimental evidences

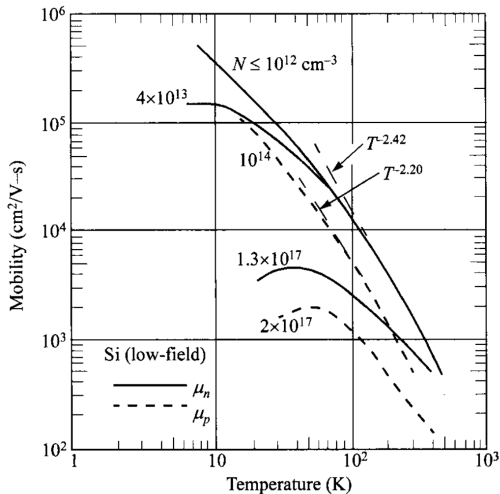


Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Current density

$$\mathbf{J}(\mathbf{r}_1, t_1) = \frac{-e\hbar^2}{2m} \lim_{\mathbf{r}_2 \rightarrow \mathbf{r}_1} (\nabla_2 - \nabla_1) G^<(\mathbf{r}_1, \mathbf{r}_2; t_1, t_1)$$
$$G^<(\mathbf{r}_1, \mathbf{r}_2; t_1, t_2) \equiv \frac{i}{\hbar} \left\langle \hat{\psi}_H^\dagger(\mathbf{r}_2, t_2) \hat{\psi}_H(\mathbf{r}_1, t_1) \right\rangle$$

Quantum theory of mobility

Current density

$$\mathbf{J}(\mathbf{r}_1, t_1) = \frac{-e\hbar^2}{2m} \lim_{\mathbf{r}_2 \rightarrow \mathbf{r}_1} (\nabla_2 - \nabla_1) G^<(\mathbf{r}_1, \mathbf{r}_2; t_1, t_1)$$
$$G^<(\mathbf{r}_1, \mathbf{r}_2; t_1, t_2) \equiv \frac{i}{\hbar} \left\langle \hat{\psi}_H^\dagger(\mathbf{r}_2, t_2) \hat{\psi}_H(\mathbf{r}_1, t_1) \right\rangle$$

$$\hat{\psi}_H(\mathbf{r}, t) \equiv \overline{\mathcal{T}} \left[e^{\frac{i}{\hbar} \int_{t_0}^t dt' \hat{H}(t')} \right] \hat{\psi}(\mathbf{r}) \mathcal{T} \left[e^{\frac{-i}{\hbar} \int_{t_0}^t dt' \hat{H}(t')} \right]$$
$$\langle \hat{O} \rangle \equiv \frac{1}{Z} \text{tr} \left[e^{-\beta \hat{H}(t_0)} \hat{O} \right] \quad \leftarrow \text{thermodynamical average}$$
$$Z \equiv \text{tr} \left[e^{-\beta \hat{H}(t_0)} \right] \quad \leftarrow \text{partition function}$$

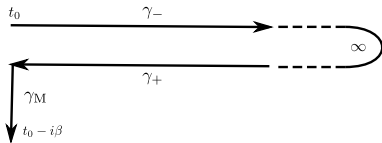
Quantum theory of mobility

Current density

$$\mathbf{J}(\mathbf{r}_1, t_1) = \frac{-e\hbar^2}{2m} \lim_{\mathbf{r}_2 \rightarrow \mathbf{r}_1} (\nabla_2 - \nabla_1) G^<(\mathbf{r}_1, \mathbf{r}_2; t_1, t_1)$$
$$G^<(\mathbf{r}_1, \mathbf{r}_2; t_1, t_2) \equiv \frac{i}{\hbar} \left\langle \hat{\psi}_H^\dagger(\mathbf{r}_2, t_2) \hat{\psi}_H(\mathbf{r}_1, t_1) \right\rangle$$

Keldysh-Schwinger contour formalism

$$G(\mathbf{r}_1, \mathbf{r}_2; z_1, z_2) = \frac{-i}{\hbar} \frac{1}{Z} \text{tr} \left\{ \mathcal{T}_C \left[e^{\frac{-i}{\hbar} \int_\gamma dz \hat{H}(z)} [\hat{\psi}(\mathbf{r}_1)]_{z_1} [\hat{\psi}^\dagger(\mathbf{r}_2)]_{z_2} \right] \right\}$$
$$\hat{H}(z) = \hat{H}_0 + \hat{H}_{\text{int}} + \hat{H}_{\text{ext}}(z)$$



Quantum theory of mobility

Perturbative expansion of the GF in powers of $\hat{H}_{\text{int}}$ and $\hat{H}_{\text{ext}}(z)$

$$G(\mathbf{r}_1, \mathbf{r}_2; z_1, z_2) = G_0(\mathbf{r}_1, \mathbf{r}_2; z_1, z_2) + \sum_{n,m=1}^{\infty} \frac{(-i/\hbar)^{n+m}}{n!m!} \int_{\gamma} dz'_1 \dots$$
$$\times \frac{1}{Z} \text{tr} \left[\mathcal{T}_C e^{\frac{-i}{\hbar} \int_{\gamma} dz [\hat{H}_0]_z} [\hat{H}_{\text{int}}]_{z'_1} \dots \hat{H}_{\text{ext}}(z''_m) [\hat{\psi}(\mathbf{r}_1)]_{z_1} [\hat{\psi}^{\dagger}(\mathbf{r}_2)]_{z_2} \right]$$
$$G_0(\mathbf{r}_1, \mathbf{r}_2; z_1, z_2) = \frac{-i}{\hbar} \frac{1}{Z_0} \text{tr} \left[\mathcal{T}_C e^{\frac{-i}{\hbar} \int_{\gamma} dz [\hat{H}_0]_z} [\hat{\psi}(\mathbf{r}_1)]_{z_1} [\hat{\psi}^{\dagger}(\mathbf{r}_2)]_{z_2} \right]$$

Express $\hat{H}$ in $\hat{\psi} \rightarrow$ Wick's theorem to write G as products of G_0 and then solve the expansion with Feynman diagram $\rightarrow$ Dyson's eq:

$$G(1, 2) = G_0(1, 2) + \int_{\gamma} d3 \int_{\gamma} d4 G_0(1, 3) \Sigma[G](3, 4) G(4, 2)$$
$$1 \equiv (\mathbf{r}_1, z_1)$$

Kadanoff-Baym equation of motion

Using Langreth rules, G_0^{-1} , explicit $\hat{H}_0$ and evaluating Dyson at equal time $\rightarrow G^<$ in the limit $t_0 \rightarrow -\infty$:

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

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

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

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

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

KBE

- $V_{\text{Hxc}}[G] \approx V_{\text{Hxc}}[G_0]$
- $\mathbf{E}$ is spatially homogeneous
- Diagonal Bloch state projection

BTE (AC)

- DC transport
- Electron-one-phonon interaction
- Static electron-phonon interaction
- Adiabatic phonons
- δ approximation in $G^>, <(\omega)$

BTE

- Linear response

Linearized BTE

- No scattering back into $|nk\rangle$

SERTA

Rep. Prog. Phys. **83**, 036501 (2020)

Boltzmann transport equation (AC)

We consider electrons in a solid and choose:

$$h_0(\mathbf{r}, -i\hbar\nabla) = \frac{-\hbar^2\nabla^2}{2m} + V_{\text{lat}+\text{Hxc}}(\mathbf{r})$$

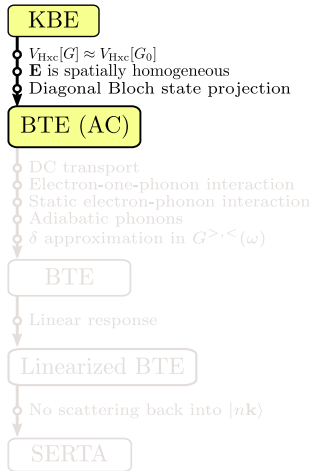
$$\rightarrow [h_0(\mathbf{r}_1, -i\hbar\nabla_1) - h_0(\mathbf{r}_2, +i\hbar\nabla_2)] G^<(\mathbf{r}_1, \mathbf{r}_2; t, t) = 0$$

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

$$\int d^3r_3 \left[\Sigma^\delta(\mathbf{r}_1, \mathbf{r}_3; t) G^<(\mathbf{r}_3, \mathbf{r}_2; t, t) - G^<(\mathbf{r}_1, \mathbf{r}_3; t, t) \Sigma^\delta(\mathbf{r}_3, \mathbf{r}_2; t) \right] \\ \approx -e\mathbf{E}(t) \cdot \frac{1}{\hbar} \frac{\partial f_{n\mathbf{k}}^<}{\partial \mathbf{k}}(t, t)$$

where

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



Rep. Prog. Phys. **83**, 036501 (2020)

Boltzmann transport equation (AC)

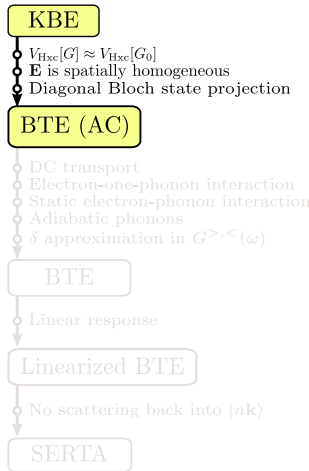
$$\frac{\partial f_{n\mathbf{k}}^{<}}{\partial t}(t, t) - e\mathbf{E}(t) \cdot \frac{1}{\hbar} \frac{\partial f_{n\mathbf{k}}^{<}}{\partial \mathbf{k}}(t, t) = -\Gamma_{n\mathbf{k}}^{(\text{co})}(t)$$

where the *collision rate* is defined as:

$$\Gamma_{n\mathbf{k}}^{(\text{co})}(t) \equiv \int_{-\infty}^t dt' [\Gamma_{n\mathbf{k}}^{>}(t, t') f_{n\mathbf{k}}^{<}(t', t) + f_{n\mathbf{k}}^{<}(t, t') \Gamma_{n\mathbf{k}}^{>}(t', t) \\ - \Gamma_{n\mathbf{k}}^{<}(t, t') f_{n\mathbf{k}}^{>}(t', t) - f_{n\mathbf{k}}^{>}(t, t') \Gamma_{n\mathbf{k}}^{<}(t', t)]$$

and

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



Rep. Prog. Phys. **83**, 036501 (2020)

Boltzmann transport equation

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

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

$$f_{n\mathbf{k}} \equiv \int \frac{d\omega}{2\pi} f_{n\mathbf{k}}^<(\omega) \quad \leftarrow \text{occupation function}$$

Approximate the self-energy:

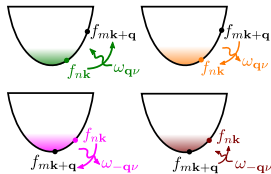
$$-e\mathbf{E} \cdot \frac{1}{\hbar} \frac{\partial f_{n\mathbf{k}}}{\partial \mathbf{k}} = \frac{2\pi}{\hbar} \sum_{m,\nu} \int \frac{d^3q}{\Omega_{\text{BZ}}} |g_{m\nu}(\mathbf{k}, \mathbf{q})|^2$$

$$\times [f_{n\mathbf{k}}(1 - f_{m\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) n_{\mathbf{q}\nu}$$

$$+ f_{n\mathbf{k}}(1 - f_{m\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) (n_{\mathbf{q}\nu} + 1)$$

$$- (1 - f_{n\mathbf{k}}) f_{m\mathbf{k}+\mathbf{q}} \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} + \hbar\omega_{\mathbf{q}\nu}) n_{\mathbf{q}\nu}$$

$$- (1 - f_{n\mathbf{k}}) f_{m\mathbf{k}+\mathbf{q}} \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu}) (n_{\mathbf{q}\nu} + 1)]$$



KBE

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BTE

Linear response

Linearized BTE

No scattering back into $|n\mathbf{k}\rangle$

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Rep. Prog. Phys. **83**, 036501 (2020)

The electron-phonon matrix element

(Lecture Tue.1)

Variation of the Kohn-Sham potential

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

Lattice-periodic part of wavefunction

Incommensurate modulation

$$\Delta_{\mathbf{q}\nu} v_{\text{SCF}} = \sum_{\kappa\alpha p} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_p)} \sqrt{\frac{\hbar}{2M_\kappa\omega_{\mathbf{q}\nu}}} e_{\kappa\alpha,\nu}(\mathbf{q}) \frac{\partial V_{\text{SCF}}(\mathbf{r})}{\partial \tau_{\kappa\alpha p}}$$

κ Atom in the unit cell

α Cartesian direction

p Unit cell in the equivalent supercell

Zero-point amplitude

Phonon polarization

Displacement of a single ion

KBE

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Rev. Mod. Phys. **89**, 015003 (2017)

Linearized Boltzmann transport equation

Macroscopic average of the current density is

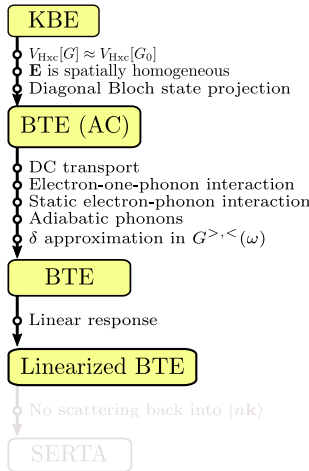
$$\begin{aligned}\mathbf{J}_M(\mathbf{E}) &= \frac{-e\hbar^2}{2m} \frac{1}{V} \int d^3r \lim_{\mathbf{r}_2 \rightarrow \mathbf{r}_1} (\nabla_2 - \nabla_1) G^<(\mathbf{r}_1, \mathbf{r}_2; t, t; \mathbf{E}) \\ &= \frac{-e}{V_{uc}} \sum_n \int \frac{d^3k}{\Omega_{BZ}} \mathbf{v}_{n\mathbf{k}} f_{n\mathbf{k}}(\mathbf{E})\end{aligned}$$

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

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

where $\partial_{E_\beta} f_{n\mathbf{k}} = (\partial f_{n\mathbf{k}} / \partial E_\beta)|_{\mathbf{E}=0}$.

The *carrier drift mobility* is $\mu_{\alpha\beta}^d \equiv \frac{\sigma_{\alpha\beta}}{en_c}$



Rep. Prog. Phys. **83**, 036501 (2020)

Drift mobility

$$\mu_{\alpha\beta}^d = \frac{-e}{V_{uc}n_c} \sum_n \int \frac{d^3k}{\Omega_{BZ}} v_{n\mathbf{k}}^\alpha \partial_{E_\beta} f_{n\mathbf{k}}$$

where

$$\partial_{E_\beta} f_{n\mathbf{k}} = ev_{n\mathbf{k}}^\beta \frac{\partial f_{n\mathbf{k}}^0}{\partial \varepsilon_{n\mathbf{k}}} \tau_{n\mathbf{k}} + \frac{2\tau_{n\mathbf{k}}}{\hbar} \sum_{m\nu} \int \frac{d^3q}{\Omega_{BZ}} |g_{m\nu}(\mathbf{k}, \mathbf{q})|^2 \times \left[(n_{\mathbf{q}\nu} + 1 - f_{n\mathbf{k}}^0) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f_{n\mathbf{k}}^0) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) \right] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}$$

where the scattering rate is:

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

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BTE

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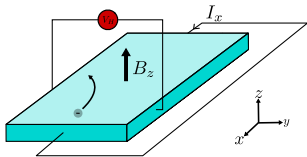
Linearized BTE

- No scattering back into $|n\mathbf{k}\rangle$

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Rep. Prog. Phys. **83**, 036501 (2020)

Hall mobility



$$\mu_{\alpha\beta\gamma}^H = \frac{-e}{V_{uc}n_c} \sum_n \int \frac{d^3k}{\Omega_{BZ}} v_{n\mathbf{k}}^\alpha \partial_{E_\beta} f_{n\mathbf{k}}(B_\gamma)$$

BTE:

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

Hall factor:

$$\mu_{\alpha\beta\gamma}^H = r_{\alpha\beta\gamma}^H \mu_{\alpha\beta}^d \\ r_{\alpha\beta\gamma}^H \equiv \sum_{\delta\epsilon} \frac{(\mu_{\alpha\delta}^d)^{-1} \mu_{\delta\epsilon\gamma}^H (\mu_{\epsilon\beta}^d)^{-1}}{B_\gamma},$$

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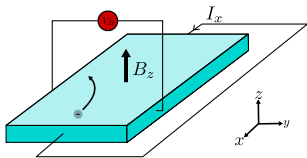
Linearized BTE

○ No scattering back into $|n\mathbf{k}\rangle$

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Rep. Prog. Phys. **83**, 036501 (2020)

Self energy relaxation time approximation



$$\mu_{\alpha\beta\gamma}^H = \frac{-e}{V_{uc}n_c} \sum_n \int \frac{d^3k}{\Omega_{BZ}} v_{n\mathbf{k}}^\alpha \partial_{E_\beta} f_{n\mathbf{k}}(B_\gamma)$$

BTE:

$$\left[1 - \frac{e}{\hbar} \tau_{n\mathbf{k}} (\mathbf{v}_{n\mathbf{k}} \times \mathbf{B}) \cdot \nabla_{\mathbf{k}} \right] \partial_{E_\beta} f_{n\mathbf{k}}(B_\gamma) = e v_{n\mathbf{k}}^\beta \frac{\partial f_{n\mathbf{k}}^0}{\partial \epsilon_{n\mathbf{k}}} \tau_{n\mathbf{k}}$$

Linked with the imaginary part of the electron-phonon self-energy:

$$\tau_{n\mathbf{k}} = \frac{1}{2\Im\Sigma_{n\mathbf{k}}}$$

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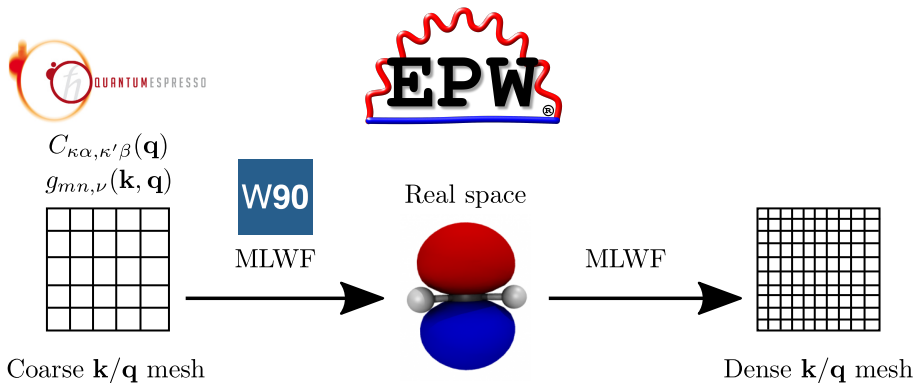
- No scattering back into $|n\mathbf{k}\rangle$

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Rep. Prog. Phys. **83**, 036501 (2020)

Electron-phonon interpolation

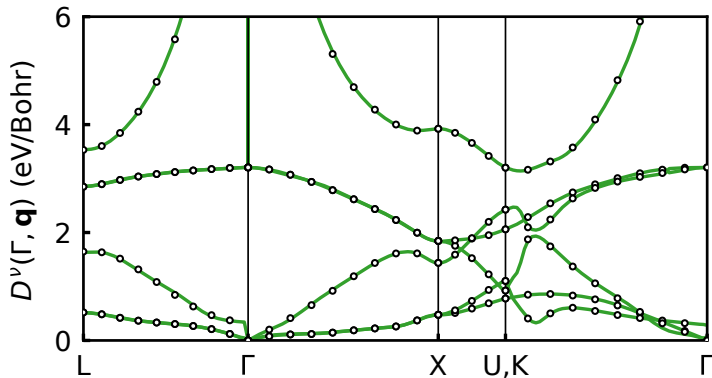
EPW relies on Maximally Localized Wannier Function to interpolate electron-phonon matrix elements.



Comp. Phys. Commun. **209**, 116 (2016)

Deformation potential of c-BN

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



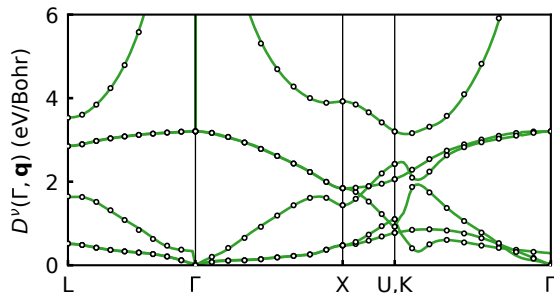
arXiv:2105.04192 (2021)

Long-range interaction: Fröhlich dipole

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

$$g_{mn\nu}^{\mathcal{L}}(\mathbf{k}, \mathbf{q}) \hat{=} g_{mn\nu}^{\mathcal{L},D}(\mathbf{k}, \mathbf{q}) + \dots$$

$$g_{mn\nu}^{\mathcal{L},D}(\mathbf{k}, \mathbf{q}) = i \frac{4\pi}{V_{uc}} \frac{e^2}{4\pi\epsilon^0} \sum_{\kappa} \left[\frac{\hbar}{2N_{p'} M_{\kappa} \omega_{\mathbf{q}\nu}} \right]^{\frac{1}{2}} \sum_{\mathbf{G} \neq -\mathbf{q}} \\ \times \frac{(\mathbf{G} + \mathbf{q}) \cdot \mathbf{Z}_{\kappa}^* \cdot \mathbf{e}_{\kappa\mathbf{q}\nu}}{(\mathbf{G} + \mathbf{q}) \cdot \boldsymbol{\epsilon}^{\infty} \cdot (\mathbf{G} + \mathbf{q})} e^{-i(\mathbf{G} + \mathbf{q}) \cdot \boldsymbol{\tau}_{\kappa}} \\ \times \langle \Psi_{m\mathbf{k}+\mathbf{q}} | e^{i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} | \Psi_{n\mathbf{k}} \rangle,$$



Phys. Rev. Lett. **115**, 176401 (2015)

Phys. Rev. B **92**, 054307 (2015)

arXiv:2105.04192 (2021)

Long-range interaction: Fröhlich dipole

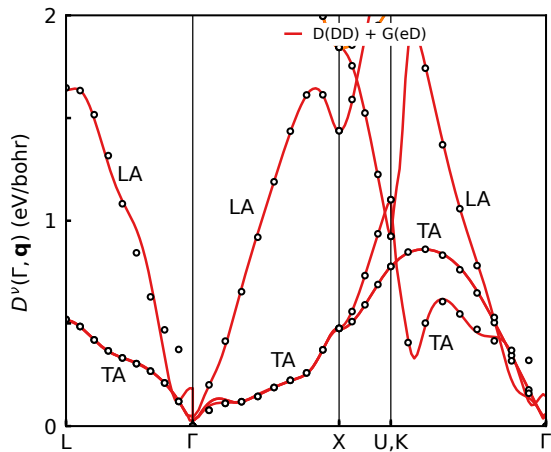
$$g_{mn\nu}(\mathbf{k}, \mathbf{q}) = g_{mn\nu}^S(\mathbf{k}, \mathbf{q}) + g_{mn\nu}^{\mathcal{L}}(\mathbf{k}, \mathbf{q})$$

$$g_{mn\nu}^{\mathcal{L}}(\mathbf{k}, \mathbf{q}) \hat{=} g_{mn\nu}^{\mathcal{L},D}(\mathbf{k}, \mathbf{q}) + \dots$$

$$g_{mn\nu}^{\mathcal{L},D}(\mathbf{k}, \mathbf{q}) = i \frac{4\pi}{V_{uc}} \frac{e^2}{4\pi\epsilon^0} \sum_{\kappa} \left[\frac{\hbar}{2N_{p'} M_{\kappa} \omega_{\mathbf{q}\nu}} \right]^{\frac{1}{2}} \sum_{\mathbf{G} \neq -\mathbf{q}} \times \frac{(\mathbf{G} + \mathbf{q}) \cdot \mathbf{Z}_{\kappa}^* \cdot \mathbf{e}_{\kappa\mathbf{q}\nu}}{(\mathbf{G} + \mathbf{q}) \cdot \boldsymbol{\epsilon}^{\infty} \cdot (\mathbf{G} + \mathbf{q})} e^{-i(\mathbf{G} + \mathbf{q}) \cdot \boldsymbol{\tau}_{\kappa}} \times \langle \Psi_{m\mathbf{k}+\mathbf{q}} | e^{i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} | \Psi_{n\mathbf{k}} \rangle,$$

Phys. Rev. Lett. **115**, 176401 (2015)

Phys. Rev. B **92**, 054307 (2015)



arXiv:2105.04192 (2021)

Long-range interaction: dynamic quadrupole

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

$$g_{mn\nu}^{\mathcal{L}}(\mathbf{k}, \mathbf{q}) \approx g_{mn\nu}^{\mathcal{L},D}(\mathbf{k}, \mathbf{q}) + g_{mn\nu}^{\mathcal{L},Q}(\mathbf{k}, \mathbf{q}) + \dots$$

$$g_{mn\nu}^{\mathcal{L},D}(\mathbf{k}, \mathbf{q}) = i \frac{4\pi}{V_{uc}} \frac{e^2}{4\pi\epsilon^0} \sum_{\kappa} \left[\frac{\hbar}{2N_{p'} M_{\kappa} \omega_{\mathbf{q}\nu}} \right]^{\frac{1}{2}} \sum_{\mathbf{G} \neq -\mathbf{q}}$$

$$\times \frac{(\mathbf{G} + \mathbf{q}) \cdot \mathbf{Z}_{\kappa}^* \cdot \mathbf{e}_{\kappa\mathbf{q}\nu}}{(\mathbf{G} + \mathbf{q}) \cdot \boldsymbol{\epsilon}^{\infty} \cdot (\mathbf{G} + \mathbf{q})} e^{-i(\mathbf{G} + \mathbf{q}) \cdot \boldsymbol{\tau}_{\kappa}}$$

$$\times \langle \Psi_{m\mathbf{k}+\mathbf{q}} | e^{i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} | \Psi_{n\mathbf{k}} \rangle,$$

$$g_{mn\nu}^{\mathcal{L},Q}(\mathbf{k}, \mathbf{q}) = \frac{4\pi}{V_{uc}} \frac{e^2}{4\pi\epsilon^0} \sum_{\kappa} \left[\frac{\hbar}{2N_{p'} M_{\kappa} \omega_{\mathbf{q}\nu}} \right]^{\frac{1}{2}} \sum_{\mathbf{G} \neq -\mathbf{q}}$$

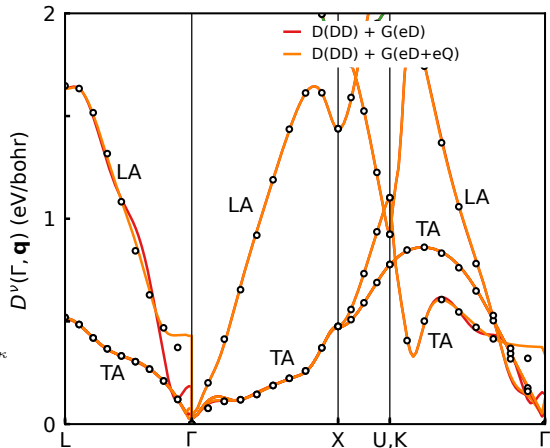
$$\times \frac{(\mathbf{G} + \mathbf{q}) \cdot (\mathbf{G} + \mathbf{q}) \cdot \mathbf{e}_{\kappa\mathbf{q}\nu} \cdot \tilde{\mathbf{Q}}_{mn\kappa}(\mathbf{k}, \mathbf{q})}{(\mathbf{G} + \mathbf{q}) \cdot \boldsymbol{\epsilon}^{\infty} \cdot (\mathbf{G} + \mathbf{q})} e^{-i(\mathbf{G} + \mathbf{q}) \cdot \boldsymbol{\tau}_{\kappa}}$$

Phys. Rev. Lett. **115**, 176401 (2015)

Phys. Rev. B **92**, 054307 (2015)

Phys. Rev. Lett. **125**, 136601 (2020)

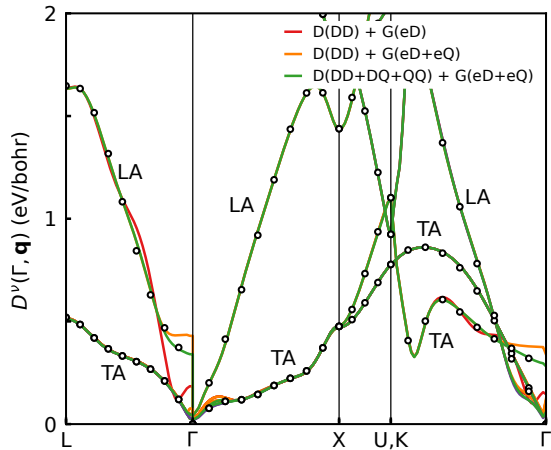
Phys. Rev. Lett. **125**, 136602 (2020)



arXiv:2105.04192 (2021)

Long-range interaction: dynamical matrix

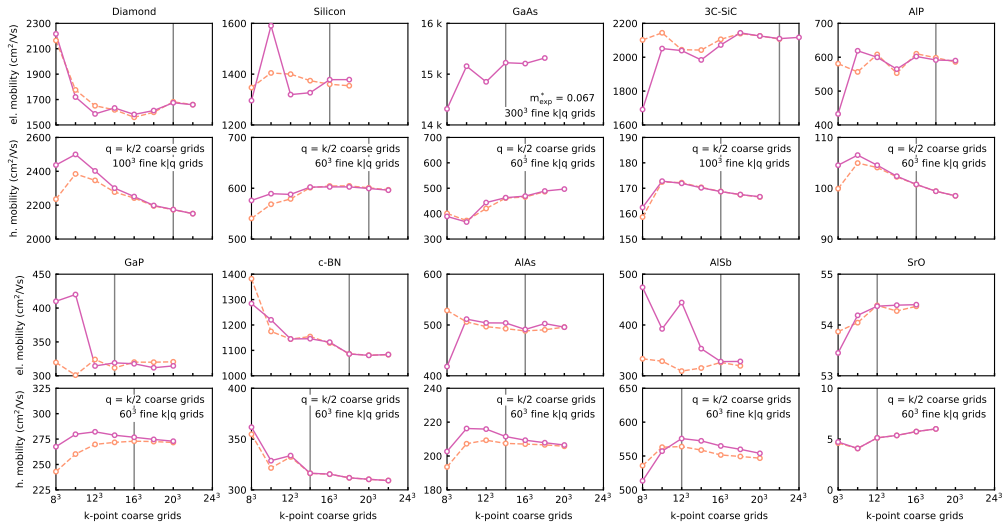
$$D_{\kappa\alpha,\kappa'\beta}^{\mathcal{L},D+Q}(\mathbf{q}) = \frac{e^{i\mathbf{q}\cdot(\boldsymbol{\tau}_{\kappa}-\boldsymbol{\tau}_{\kappa'})} e^{\frac{-\mathbf{q}\cdot\boldsymbol{\epsilon}^{\infty}\cdot\mathbf{q}}{4\Lambda^2}}}{\mathbf{q}\cdot\boldsymbol{\epsilon}^{\infty}\cdot\mathbf{q}} \left[\mathbf{q}\cdot\mathbf{Z}_{\kappa\alpha}^*\cdot\mathbf{q}\cdot\mathbf{Z}_{\kappa'\beta}^* \right. \\ \left. + \frac{1}{4}\mathbf{q}\cdot\mathbf{q}\cdot\mathbf{Q}_{\kappa\alpha}\cdot\mathbf{q}\cdot\mathbf{q}\cdot\mathbf{Q}_{\kappa'\beta} + \frac{i}{2}\mathbf{q}\cdot\mathbf{Z}_{\kappa\alpha}^*\cdot\mathbf{q}\cdot\mathbf{q}\cdot\mathbf{Q}_{\kappa'\beta} \right. \\ \left. - \frac{i}{2}\mathbf{q}\cdot\mathbf{q}\cdot\mathbf{Q}_{\kappa\alpha}\cdot\mathbf{q}\cdot\mathbf{Z}_{\kappa'\beta}^* \right]$$



Phys. Rev. Lett. **125**, 217602 (2020))

arXiv:2105.04192 (2021)

Mobility convergece with coarse BZ grids

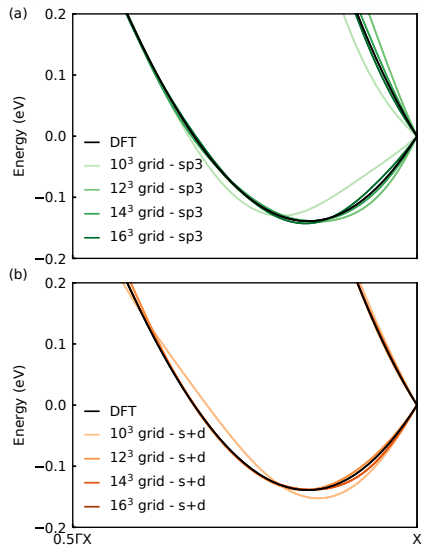


arXiv:2105.04192 (2021)

Convergence of Wannier functions

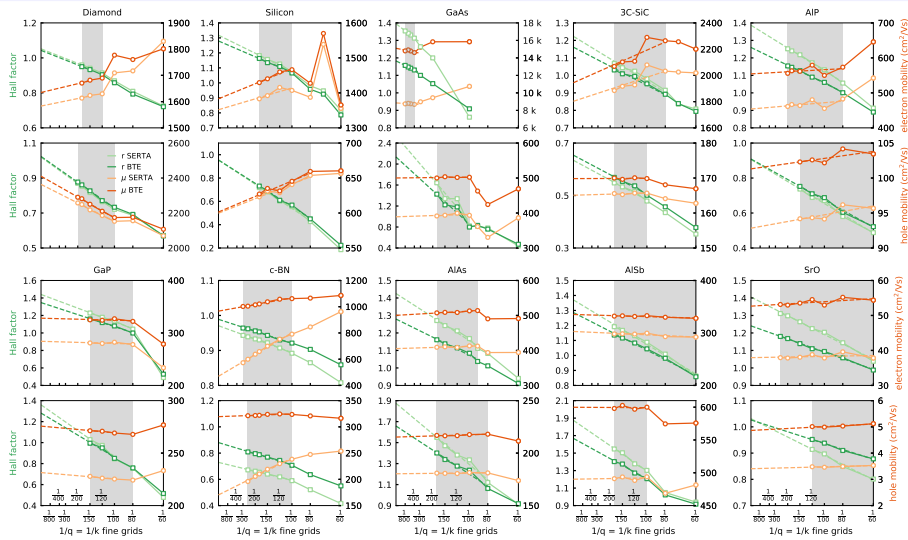
Slower convergence of Wannier function when:

- CBM/VBM not at a high symmetry point
- SOC is used
- conduction manifold only is Wannierized
- Ex: CB of silicon with SOC



arXiv:2105.04192 (2021)

Mobility convergece with fine BZ grids



arXiv:2105.04192 (2021)

Gaussian or adaptative smearings - [c-BN]

$$\tau_{n\mathbf{k}}^{-1} = \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d^3q}{\Omega_{\text{BZ}}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \times \left[(n_{\mathbf{q}\nu} + 1 - f_{m\mathbf{k}+\mathbf{q}}^0) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f_{m\mathbf{k}+\mathbf{q}}^0) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) \right].$$

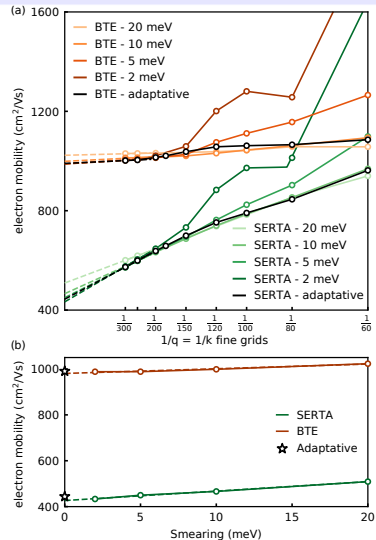
Adaptative broadening:

$$\eta_{n\mathbf{k}}(\mathbf{q}\nu) = \frac{\hbar}{\sqrt{12}} \sqrt{\sum_{\alpha} \left[\left(\mathbf{v}_{\mathbf{q}\nu\nu} - \mathbf{v}_{n\mathbf{k}+\mathbf{q}} \right) \cdot \frac{\mathbf{G}_{\alpha}}{N_{\alpha}} \right]^2},$$

where the phonon velocity is:

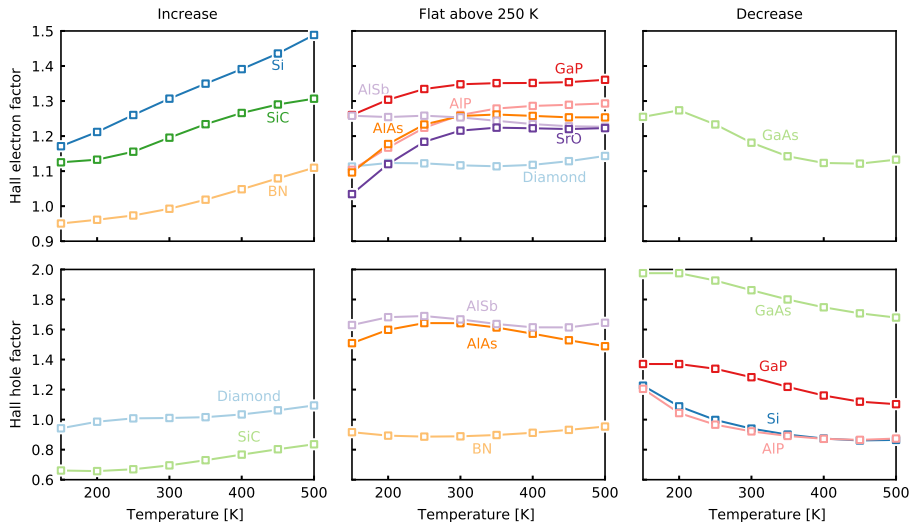
$$v_{\mathbf{q}\mu\nu\beta} = \frac{1}{2\omega_{\mathbf{q}\nu}} \frac{\partial D_{\mu\nu}(\mathbf{q})}{\partial q_{\beta}} = \frac{1}{2\omega_{\mathbf{q}\nu}} \sum_{\mathbf{R}} iR_{\beta} e^{i\mathbf{q} \cdot \mathbf{R}} D_{\mu\nu}(\mathbf{R}).$$

Comput. Phys. Commun. **185**, 1747 (2014)



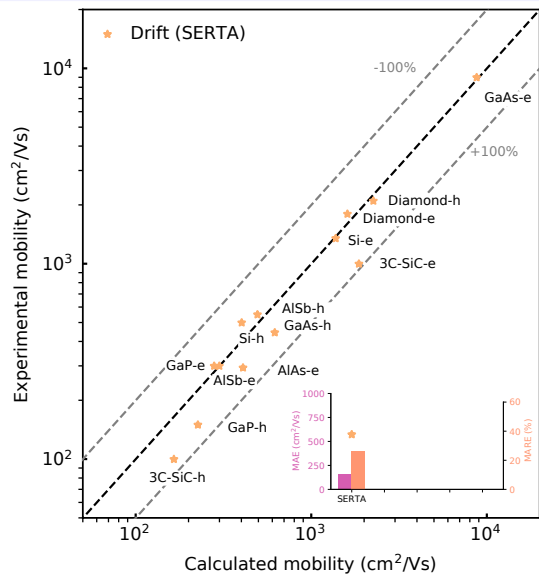
arXiv:2105.04192 (2021)

Hall factor is not unity



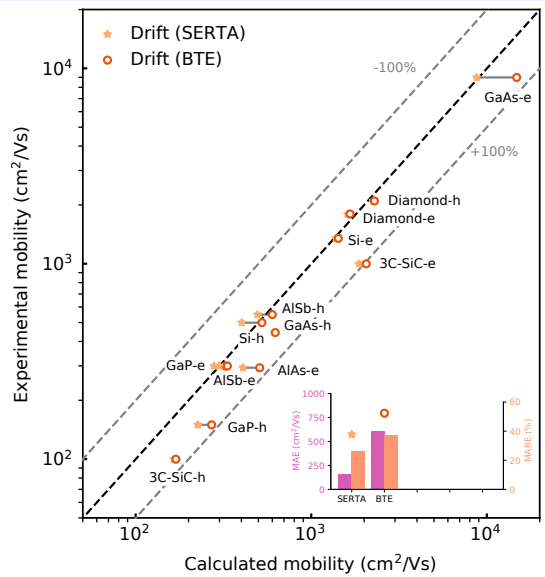
arXiv:2105.04192 (2021)

Experimental comparison



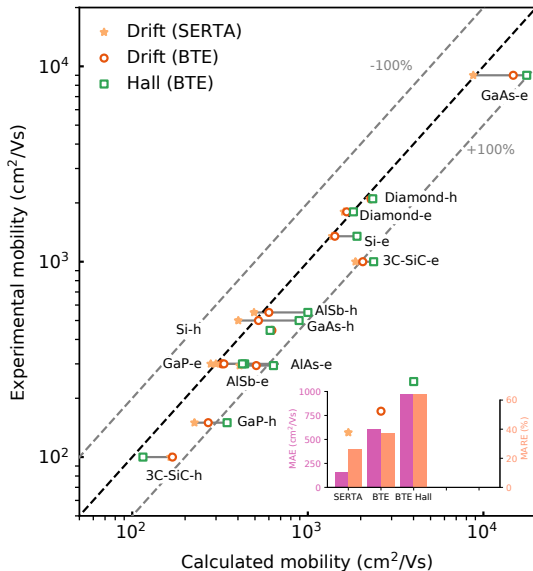
arXiv:2105.04192 (2021)

Experimental comparison



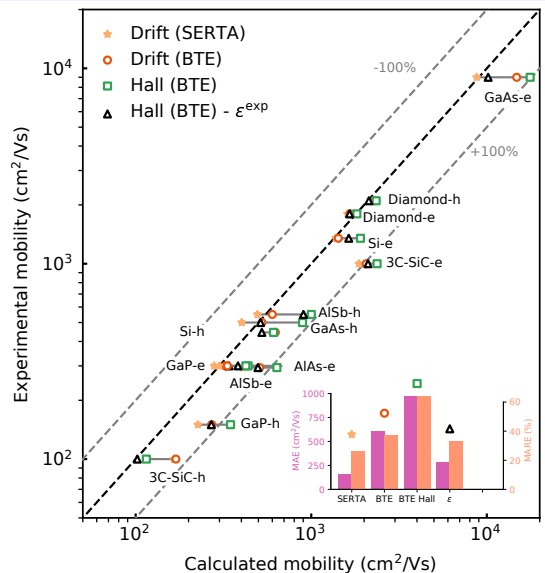
arXiv:2105.04192 (2021)

Experimental comparison



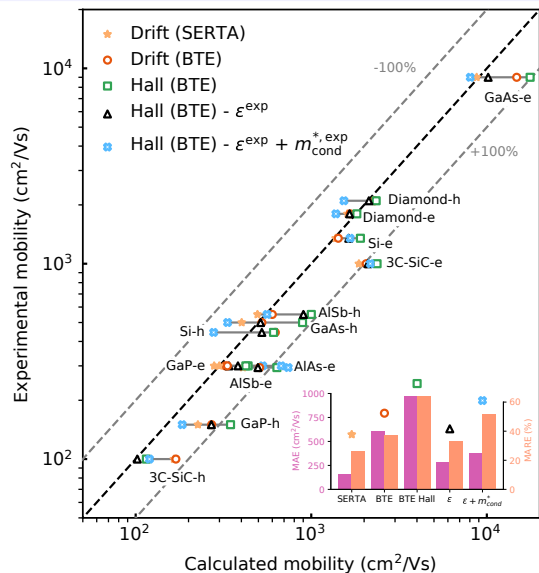
arXiv:2105.04192 (2021)

Experimental comparison



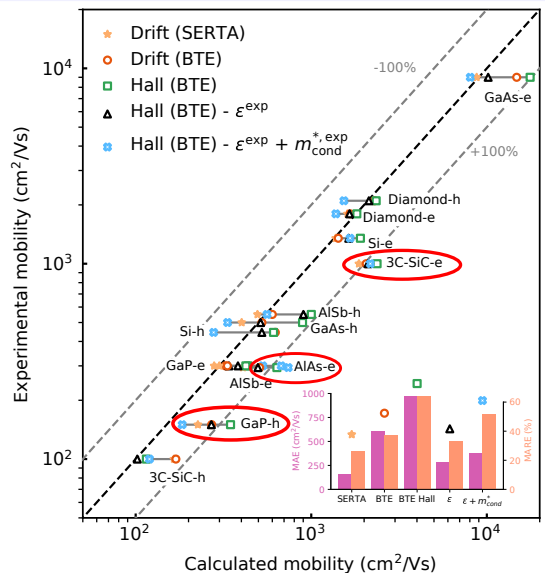
arXiv:2105.04192 (2021)

Experimental comparison



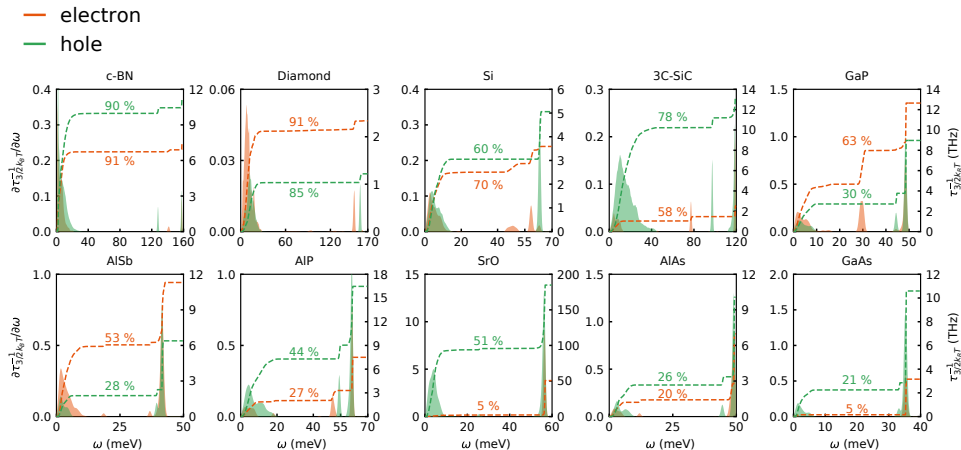
arXiv:2105.04192 (2021)

Experimental comparison



arXiv:2105.04192 (2021)

Spectral decomposition: dominant scattering

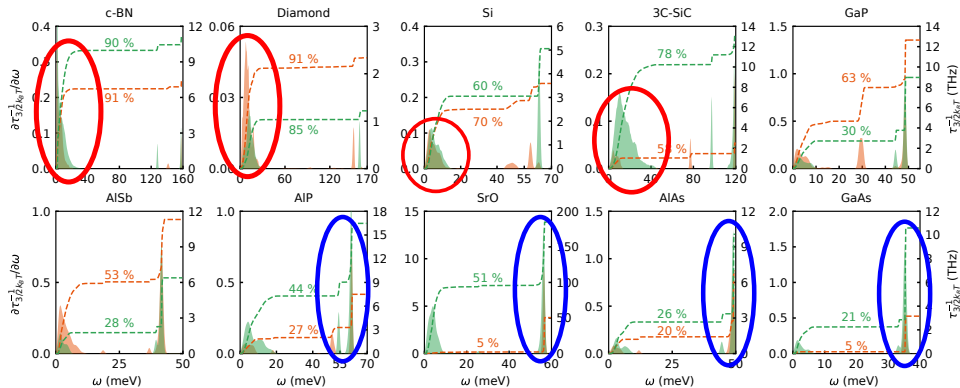


arXiv:2105.04192 (2021)

Spectral decomposition: dominant scattering

— electron
— hole

Acoustic scattering dominates

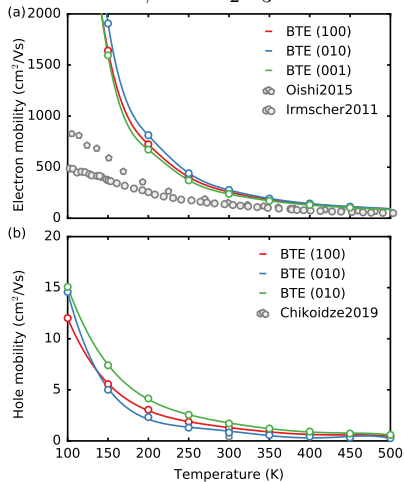


Optical scattering dominates

arXiv:2105.04192 (2021)

Examples of mobility with T done with EPW

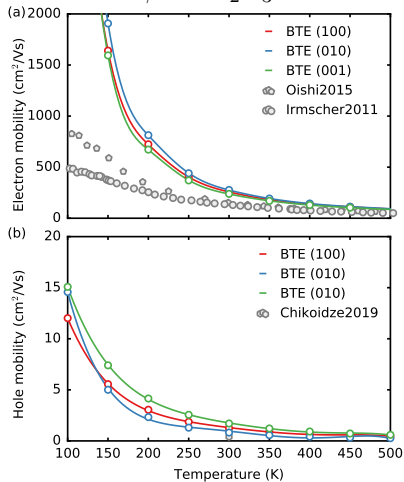
$\beta - \text{Ga}_2\text{O}_3$



Phys. Rev. Res. 2, 033102 (2020)

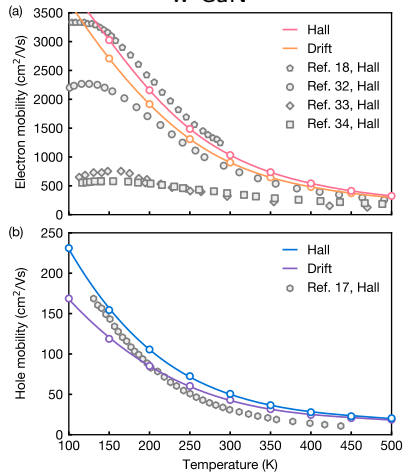
Examples of mobility with T done with EPW

$\beta - \text{Ga}_2\text{O}_3$



Phys. Rev. Res. **2**, 033102 (2020)

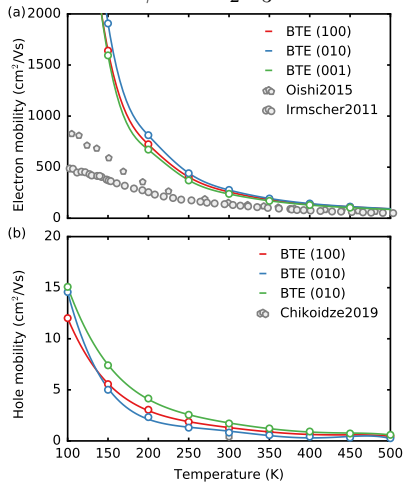
w-GaN



Phys. Rev. Lett. **123**, 096602 (2019)

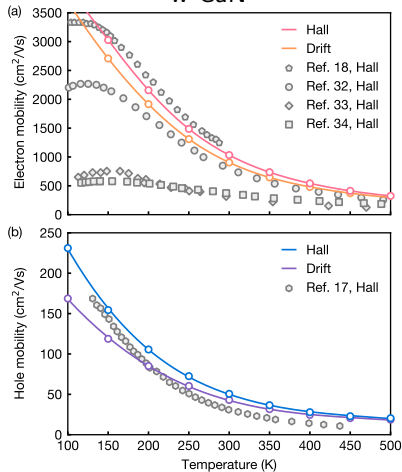
Examples of mobility with T done with EPW

$\beta - \text{Ga}_2\text{O}_3$



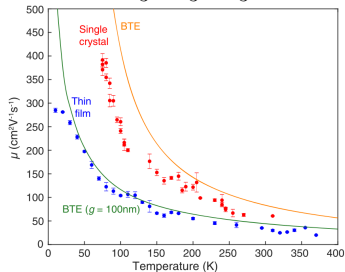
Phys. Rev. Res. **2**, 033102 (2020)

w-GaN



Phys. Rev. Lett. **123**, 096602 (2019) J. Phys. Chem. Lett. **12**, 3607 (2021)

$\text{CH}_3\text{NH}_3\text{PbI}_3$



Brooks-Herring model for impurity scattering

Semi-empirical Brooks-Herring model for the hole of silicon:

$$\mu_i = \frac{2^{7/2} \epsilon_s^2 (k_B T)^{3/2}}{\pi^{3/2} e^3 \sqrt{m_d^*} n_i G(b)} \left[\frac{\text{cm}^2}{\text{Vs}} \right],$$

where $G(b) = \ln(b+1) - b/(b+1)$, $b = 24\pi m_d^* \epsilon_s (k_B T)^2 / e^2 h^2 n'$, and $n' = n_h(2 - n_h/n_i)$. Here $m_d^* = 0.55m_0$ is the silicon hole density-of-state effective mass.

H. Brooks, Phys. Rev. **83**, 879 (1951)

S. S. Li and W. R. Thurber, Solid-State Electronics **20**, 609 (1977)

Brooks-Herring model for impurity scattering

Because the electron mass is anisotropic in silicon, we used the Long-Norton model:

$$\mu_i^{\text{LN}} = \frac{7.3 \cdot 10^{17} T^{3/2}}{n_i G(b)} \left[\frac{\text{cm}^2}{\text{Vs}} \right],$$

The mobility total phonon (μ_l) and impurity (μ_i) mobility is:

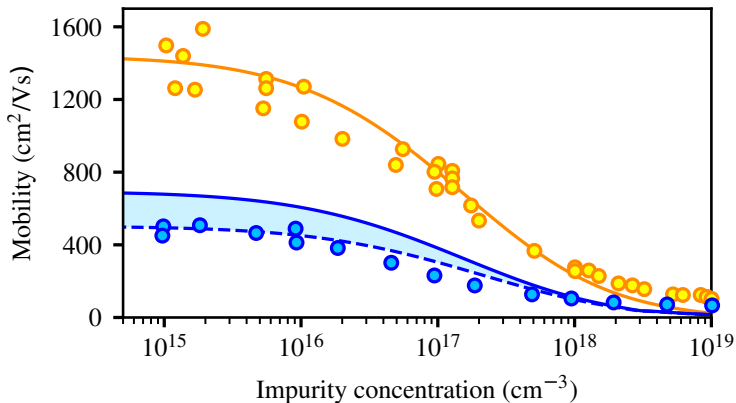
$$\mu = \mu_l \left[1 + X^2 \{ \text{ci}(X) \cos(X) + \sin(X) (\text{si}(X) - \frac{\pi}{2}) \} \right]$$

$X^2 = 6\mu_l/\mu_i$ and $\text{ci}(X)$ and $\text{si}(X)$ are the cosine and sine integrals.

P. Norton, T. Braggins, and H. Levinstein, Phys. Rev. B **8**, 5632 (1973)

Brooks-Herring model for impurity scattering

Electron and hole mobility in silicon (EPW)



Phys. Rev. B **97**, 121201 (2018)

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Supplemental Slides

A supplemental slide

Some extra information.