QUANTUM ESPRESSO: from density-functional theory to dual wave-particle transport and device simulation

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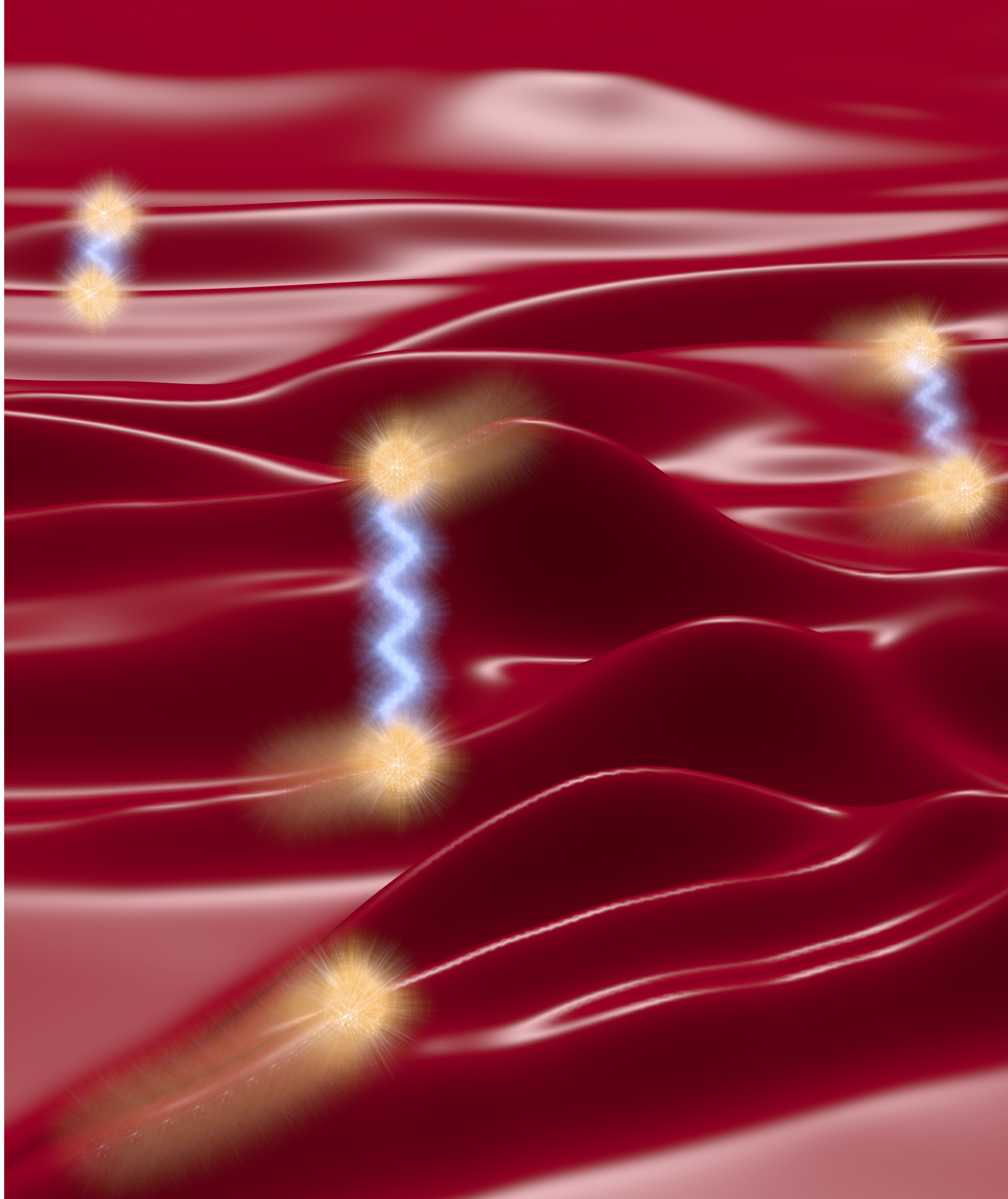
TCM



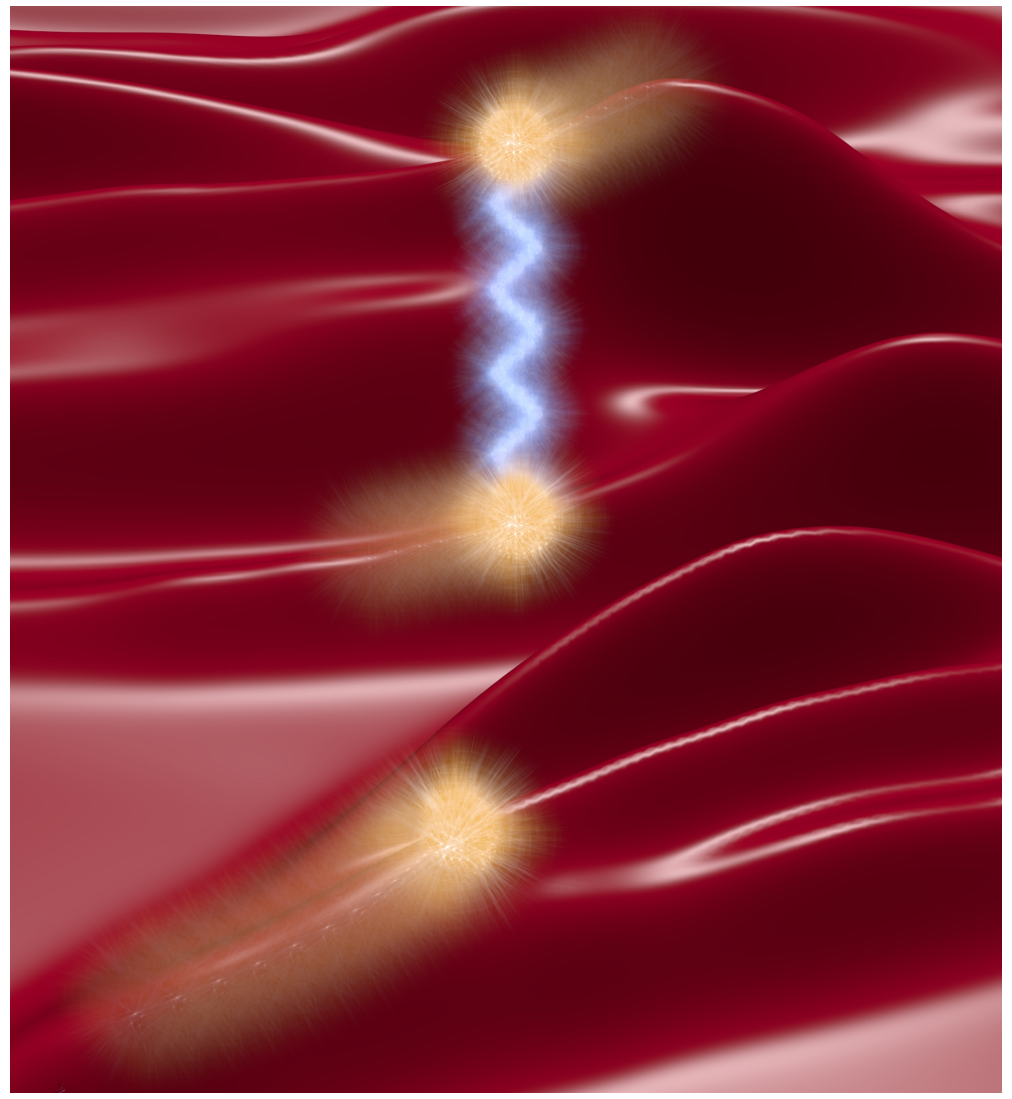
OUTLINE

Å — nm — μm — mm — Size

Density functional theory and dual wave-particle transport

Wigner formulation for electron and phonon transport

__Simoncelli__, Marzari, Mauri, Nat. Phys. 15 (2019)
__Simoncelli__, Marzari, Mauri, Phys. Rev. X 12 (2022)
Cepellotti and Kozinsky, Materials Today Physics 19 (2021)



Raman spectra: structural & quasiparticles' properties

Beyond band transport

Charge transport in solid state ionic conductors

Kahle, Marcolongo, & Marzari, Energy Environ. Sci. 13 (2020)

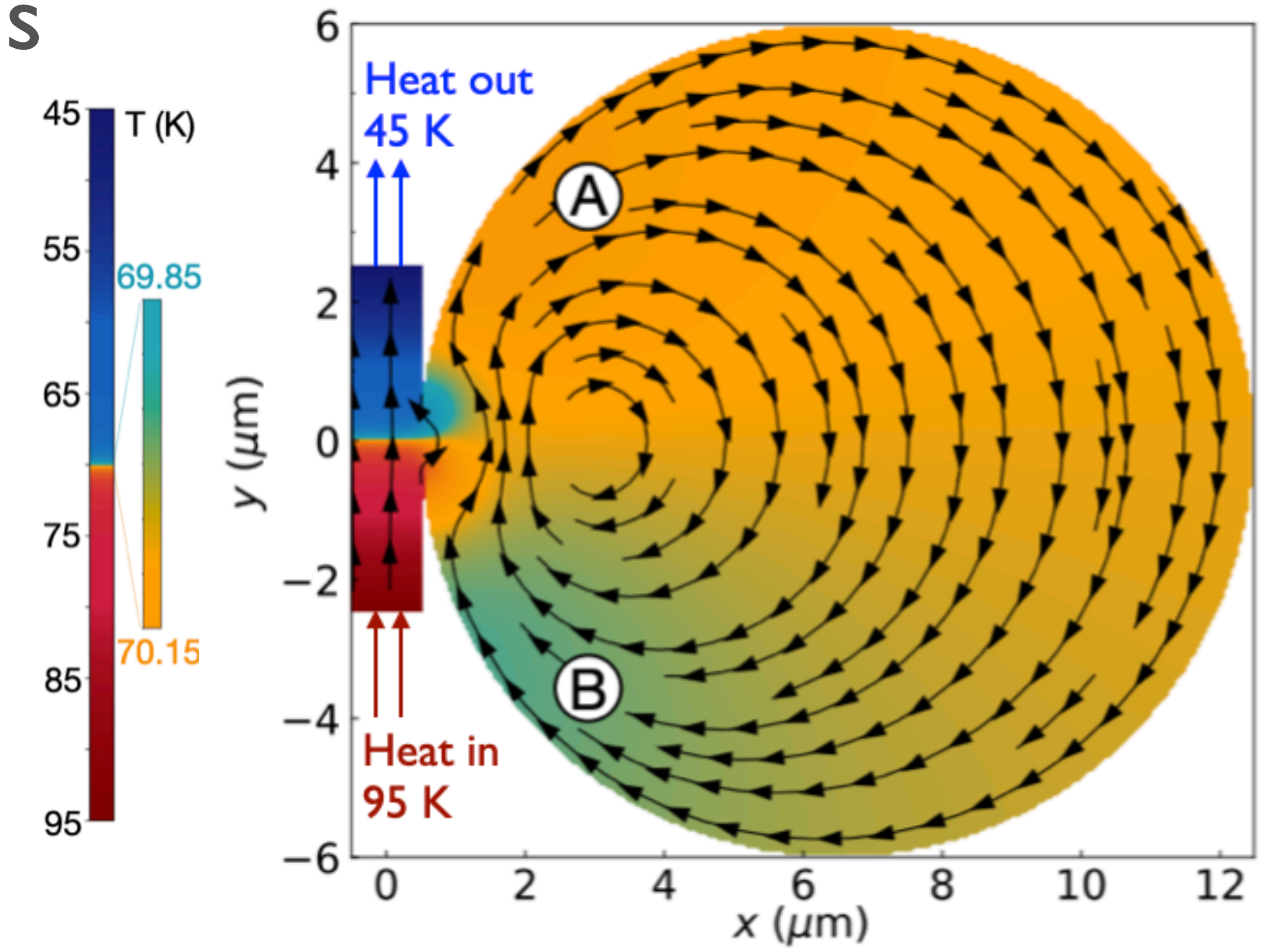
Thermal transport in glasses from first principles

__Simoncelli__, Mauri, Marzari, npj Comput. Mater. 9 (2023);
Harper, Iwanowski, Payne, __Simoncelli__ arXiv 2303.08637 (2023)

First-principles parametrisation of mesoscopic models

Viscous heat equations & diffusive-hydrodynamic crossover

__Simoncelli__, Marzari, Cepellotti, Phys. Rev. X 10 (2020)
Dragašević and __Simoncelli__, arXiv:2303.12777 (23.03.2023)



Predicting reflectivity and colour of metals

Prandini, Rignanese, & Marzari, npl Comput. Mater. 129 (2019)

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Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization

J. Phys.: Condens. Matter 21, 395502 (2009) and J. Phys.: Condens. Matter 29, 465901 (2017)

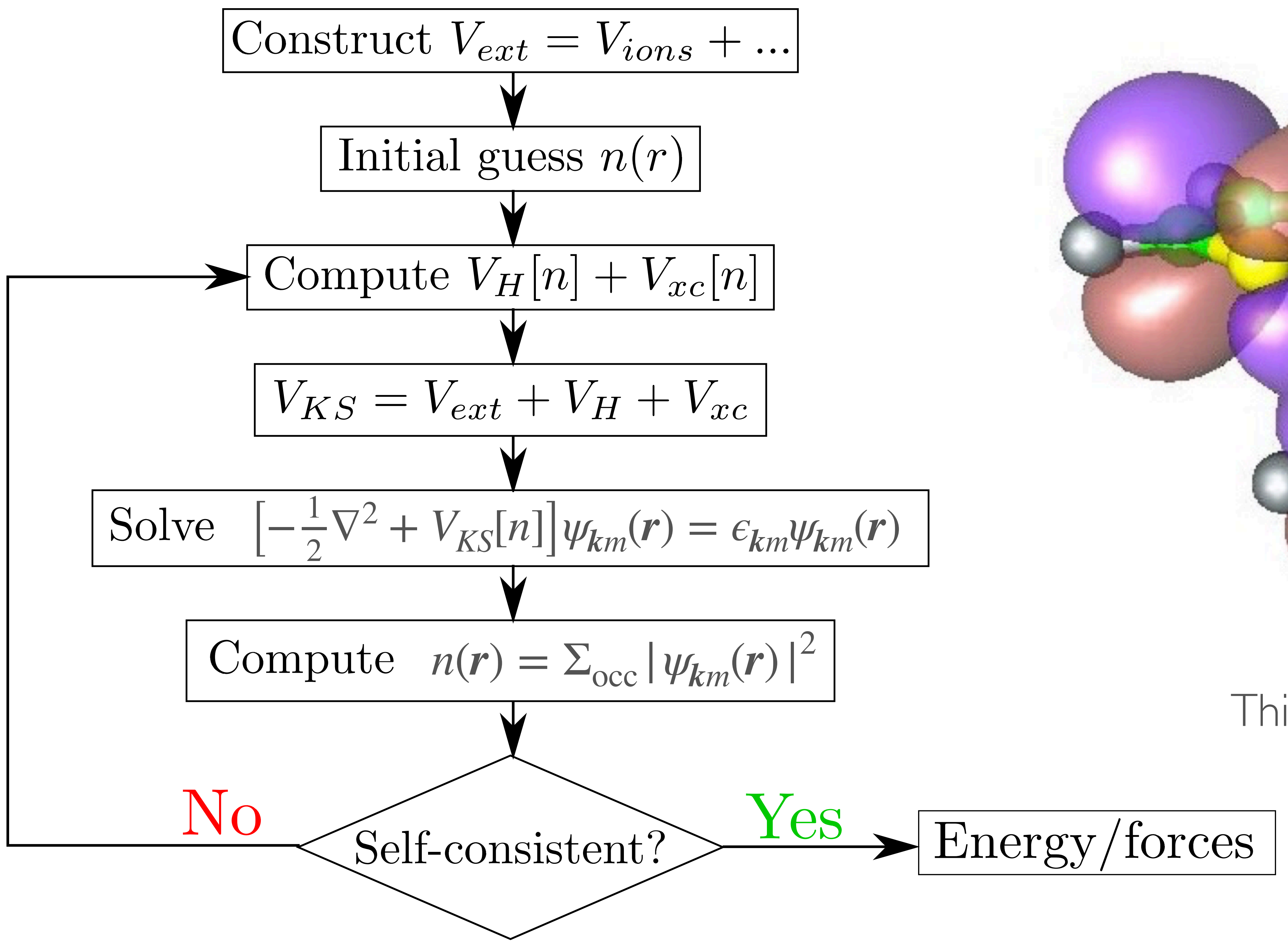
Composed of several packages:

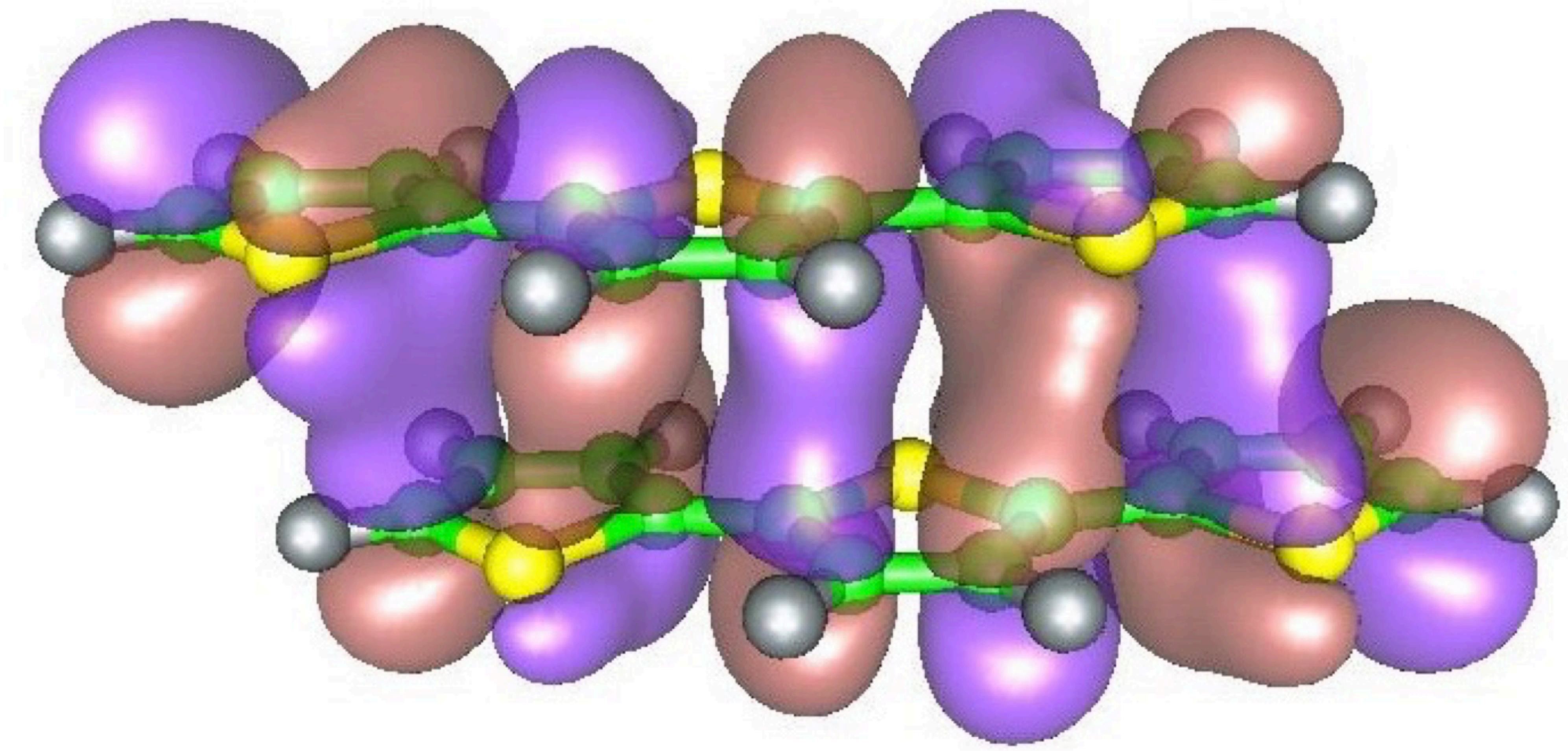
- **CP**: Car-Parrinello molecular dynamics
- **PWneb**: Nudged Elastic Band (NEB) for reaction pathways and barriers
- **atomic**: pseudopotential generation code
- **PWcond**: ballistic conductance
- **XSpectra**: Calculation of X-ray near-edge adsorption spectra (XANES)
- **GWL**: GW band structure with ultralocalized Wannier functions
- **TD-DFPT**: Time-Dependent Density-Functional Perturbation Theory
- **HP**: Hubbard parametes from linear response
- **turboMagnon**: spin-wave spectra using TD-DFPT
- **PWscf**: self-consistent electronic structure, structural optimization, molecular dynamics
- **PHonon**: linear-response calculations (phonons, dielectric properties)
- **D3Q**: Phonon-phonon interaction and thermal conductivity
- **EPW**: Electron-phonon coefficients and related properties

CHARGE DENSITY AND BAND STRUCTURE

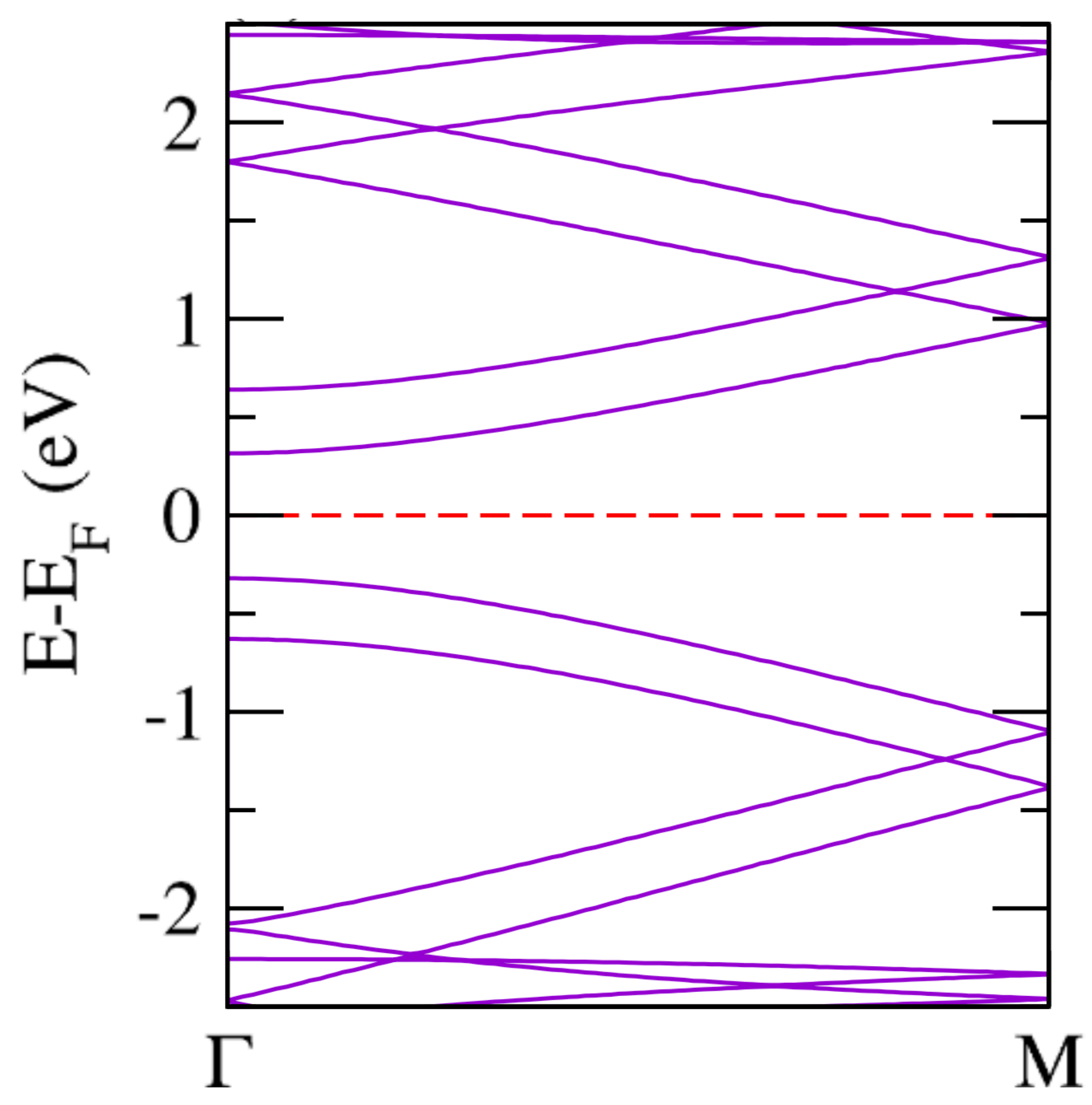
Ground state electronic energy and density, $n(\boldsymbol{r}) = \sum_{\boldsymbol{k}m \in \text{Occ}} |\psi_{\boldsymbol{k}m}(\boldsymbol{r})|^2$

Self-consistent solution of Kohn Sham equation: $\left[-\frac{1}{2}\nabla^2 + V_{\text{ext}} + V_H[n] + V_{xc}[n]\right]\psi_{\boldsymbol{k}m}(\boldsymbol{r}) = \epsilon_{\boldsymbol{k}m}\psi_{\boldsymbol{k}m}(\boldsymbol{r})$





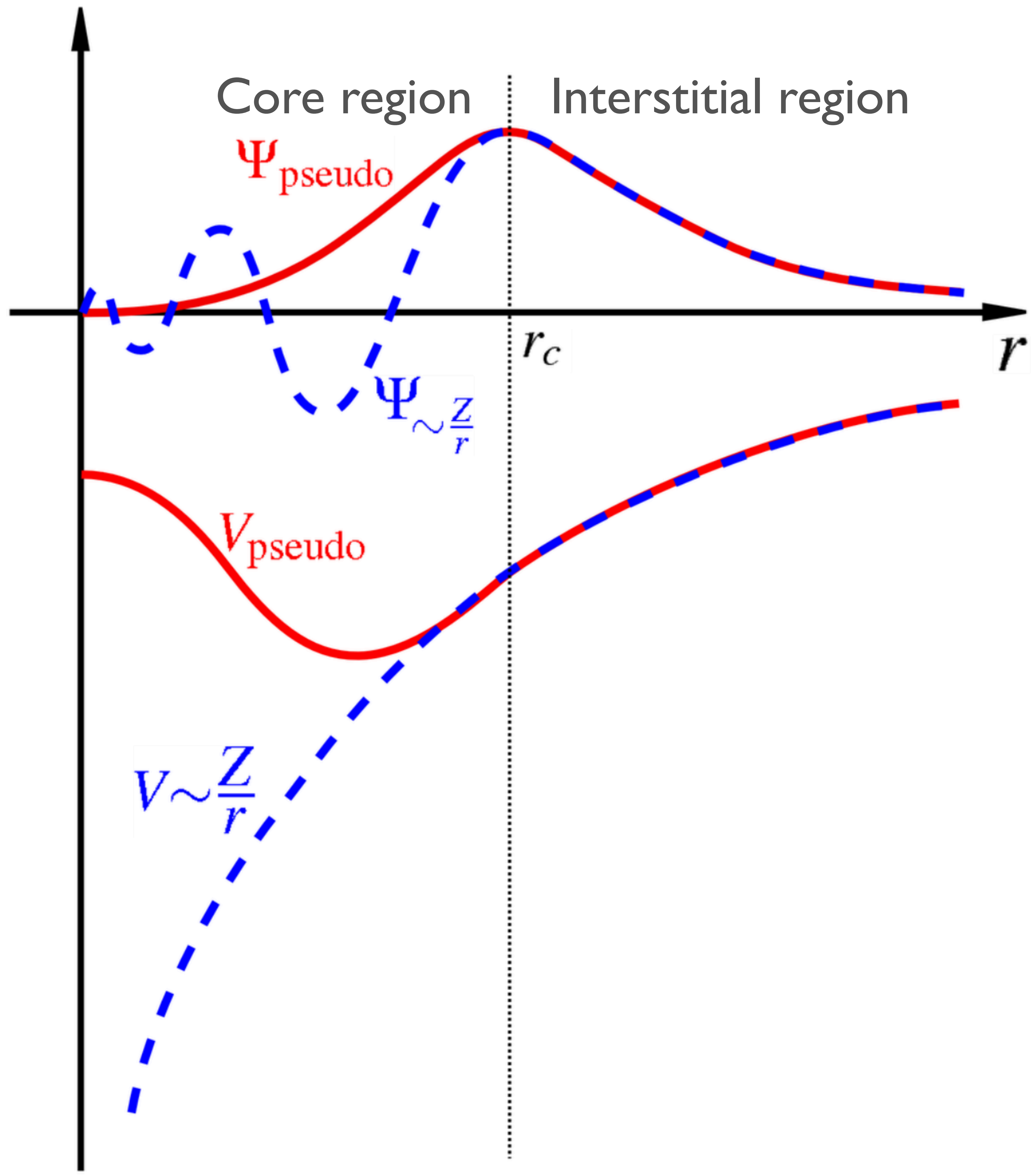
Thiophene (C_4H_4S), Scherlis and Marzari, JPCB (2004)

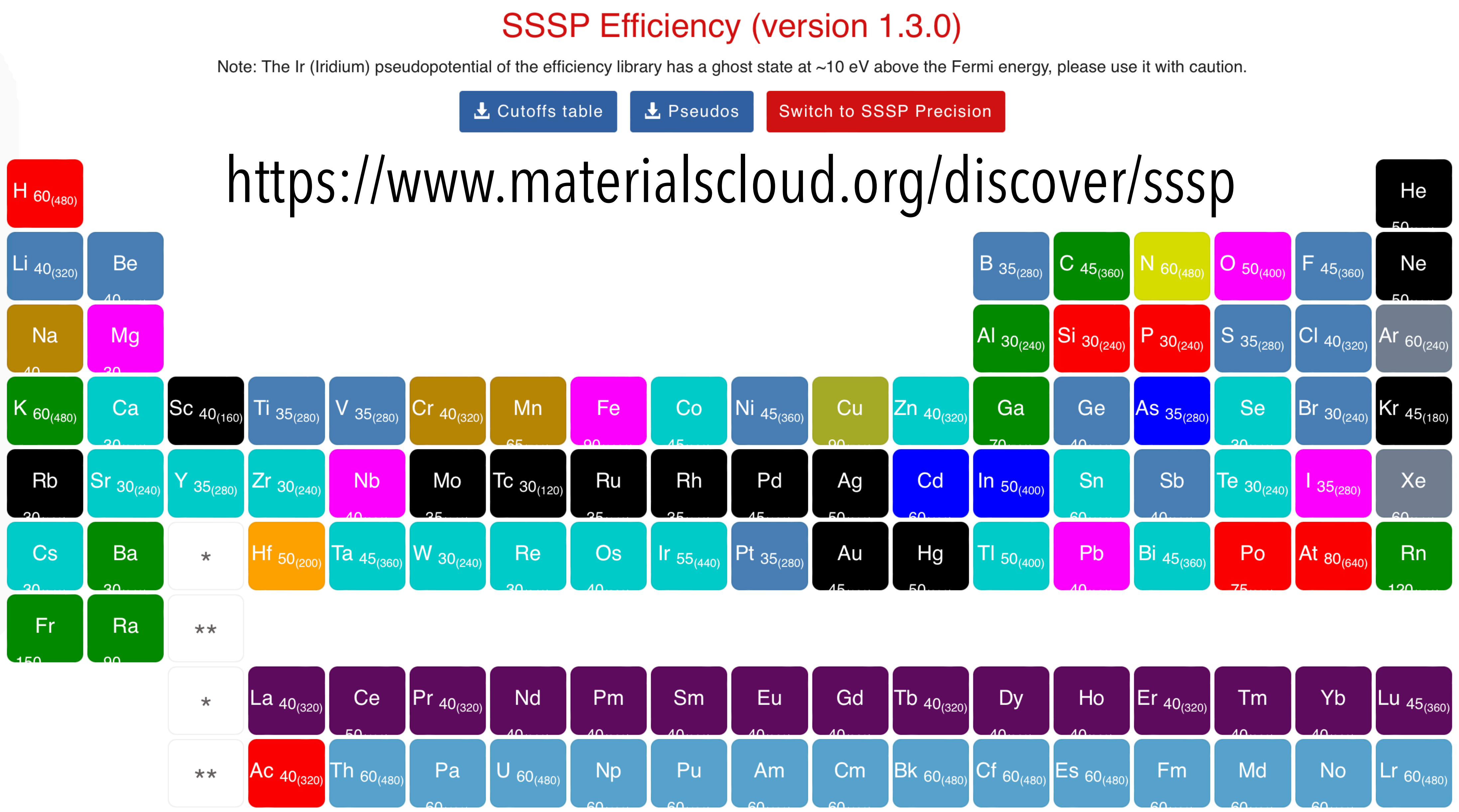


Kaloni et al, Sci. Rep. 6, 36554 (2016)

PSEUDOPOTENTIALS — SSSP LIBRARY

- Valence wavefunctions are ‘soft and smooth’ in the interstitial region, they strongly oscillate in the core region;
- Bonds are mainly determined by $\Psi_{km}(\boldsymbol{r})$ in the interstitial region;
- Core electrons are very localized;
- Approximation to reduce computational cost: freeze the core electrons & replace the real ionic potential with a ‘pseudopotential’.

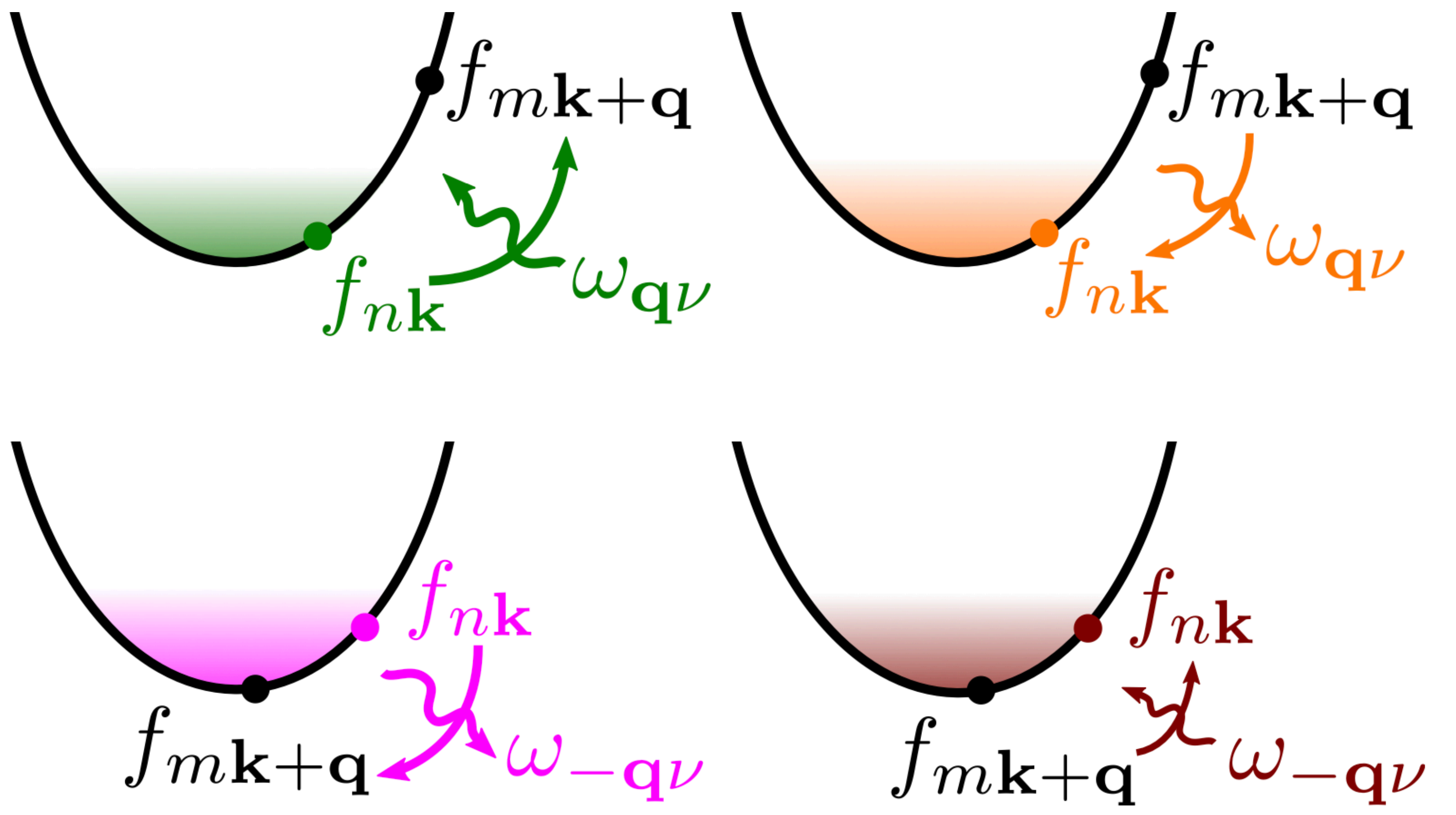




INTERACTIONS: BROADENING OF BANDS

Electron-phonon interaction

EPW



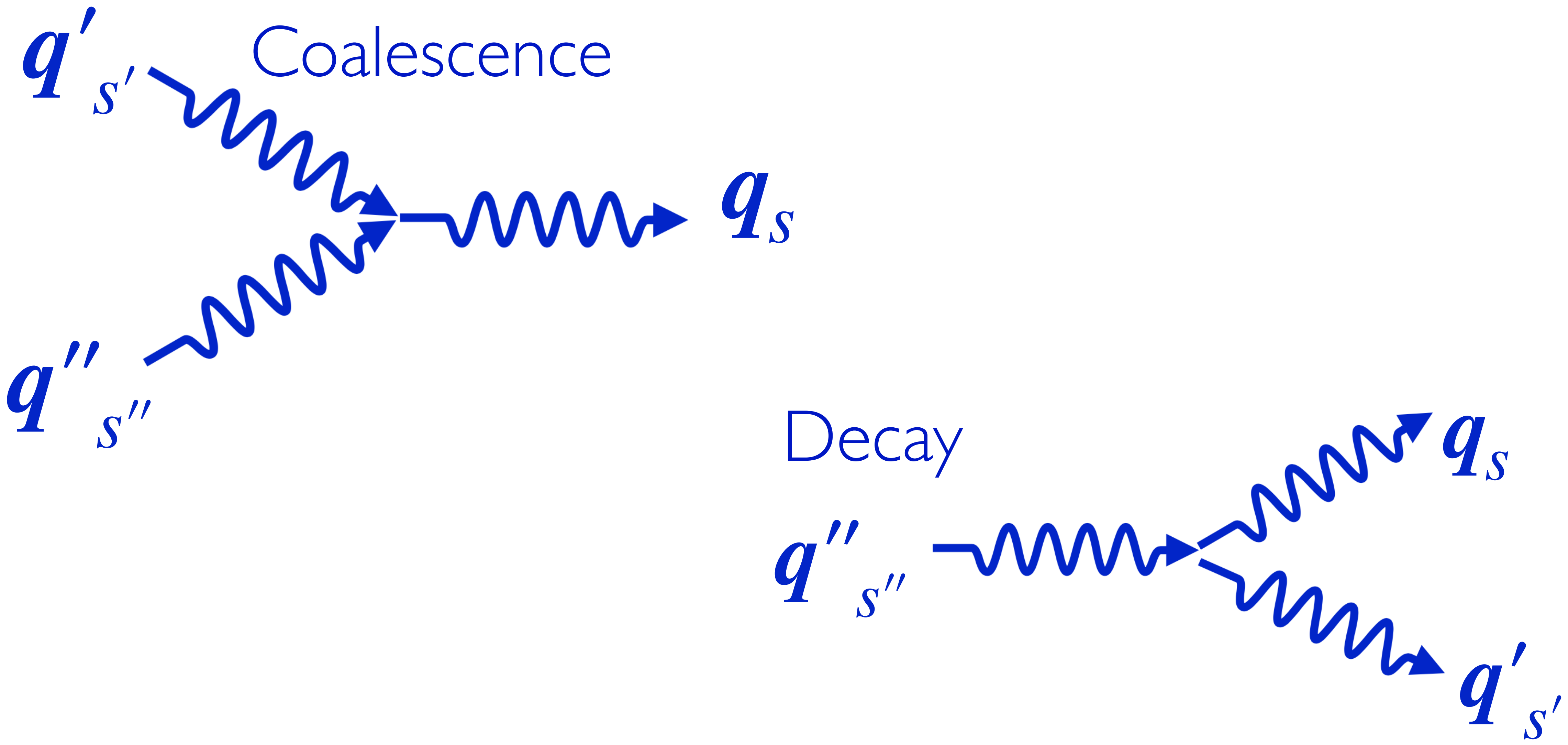
Electron-phonon matrix element $g_{m,m',s}(\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}) = \sqrt{\frac{\hbar}{2M_0\omega_{\boldsymbol{q}s}}}\left\langle \psi_{k'm'} | \partial_{\boldsymbol{q}s} V | \psi_{km} \right\rangle$

Self-consistent potential associated with phonon $\boldsymbol{q}s$

Poncé et al. Computer Phys. Commun, 209 (2016)
Poncé et al. Rep. Prog. Phys. 83 036501 (2020)

Phonon-phonon interaction

D3Q
d3q + thermal2



phonon-phonon matrix element $|V^{(3)}(\boldsymbol{q}s, -\boldsymbol{q}'s', -\boldsymbol{q}''s'')|^2$

Third derivative of the Born-Oppenheimer potential

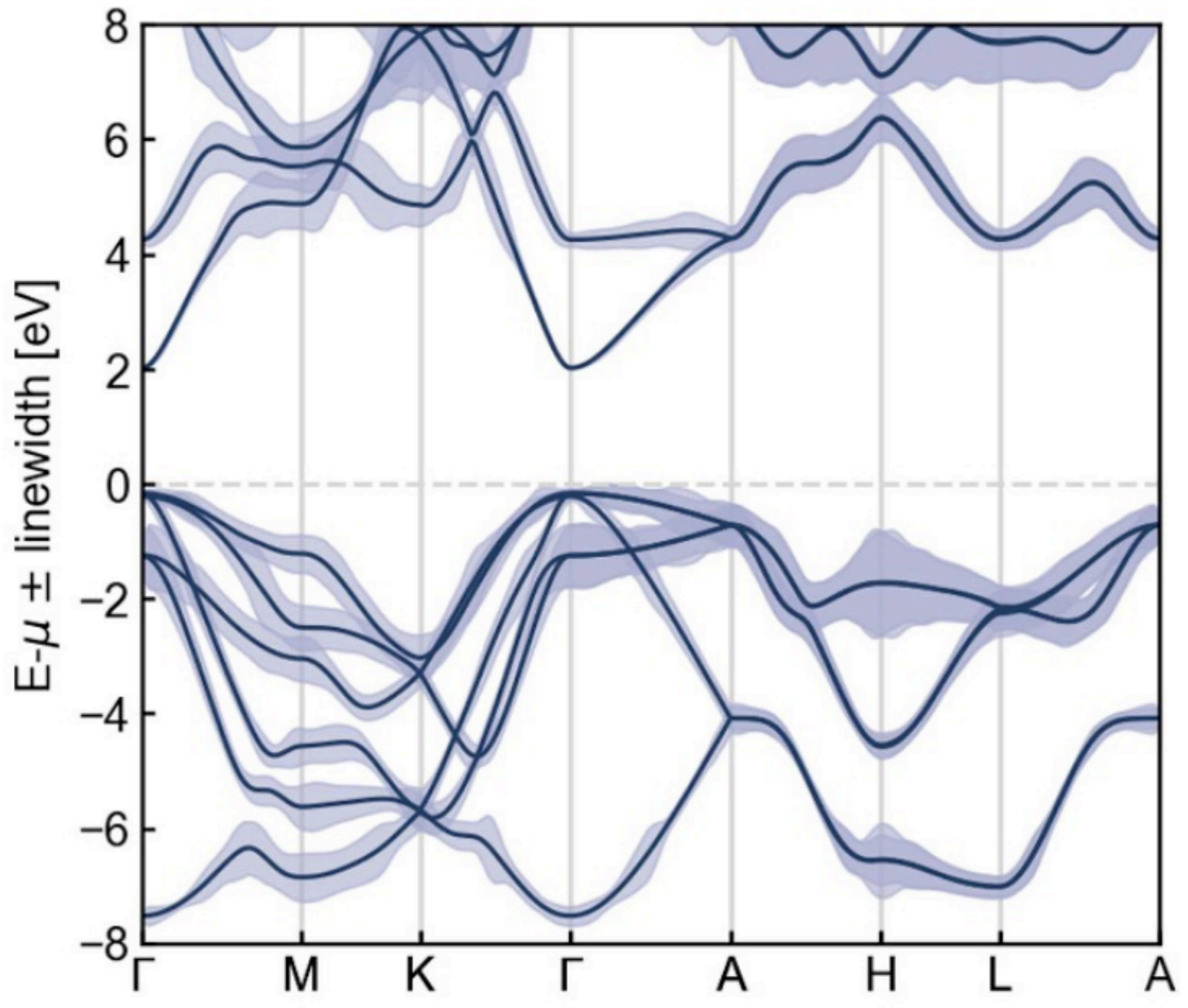
Paulatto et al. PRB 87 (2013)
Fugallo et al. PRB 88 (2013)

‘BROADENED’ BAND STRUCTURE FROM DFT

Electrons

— $\epsilon(\boldsymbol{k})_m$

$$\Gamma(\boldsymbol{k})_m = \frac{1}{\mathcal{N}_{\boldsymbol{k}}\mathcal{V}} \sum_{\boldsymbol{k}''m'',\boldsymbol{q}s} \frac{2\pi}{\hbar} |g_{m,m'',s}(\boldsymbol{k},\boldsymbol{k}'',\boldsymbol{q})|^2 \delta_{\boldsymbol{k}''-\boldsymbol{k}-\boldsymbol{q},\boldsymbol{G}} \Big[\big(\bar{N}(\boldsymbol{q})_s + \bar{F}(\boldsymbol{k}'')_{m''}\big) \times \delta\big[\epsilon(\boldsymbol{k}'')_{m''} - \epsilon(\boldsymbol{k})_m - \hbar\omega(\boldsymbol{q})_s\big] + \big(1 - \bar{F}(\boldsymbol{k}'')_{m''} + \bar{N}(\boldsymbol{q})_s\big)\delta\big[\epsilon(\boldsymbol{k}'')_{m''} - \epsilon(\boldsymbol{k})_m + \hbar\omega(\boldsymbol{q})_s\big]\Big]$$

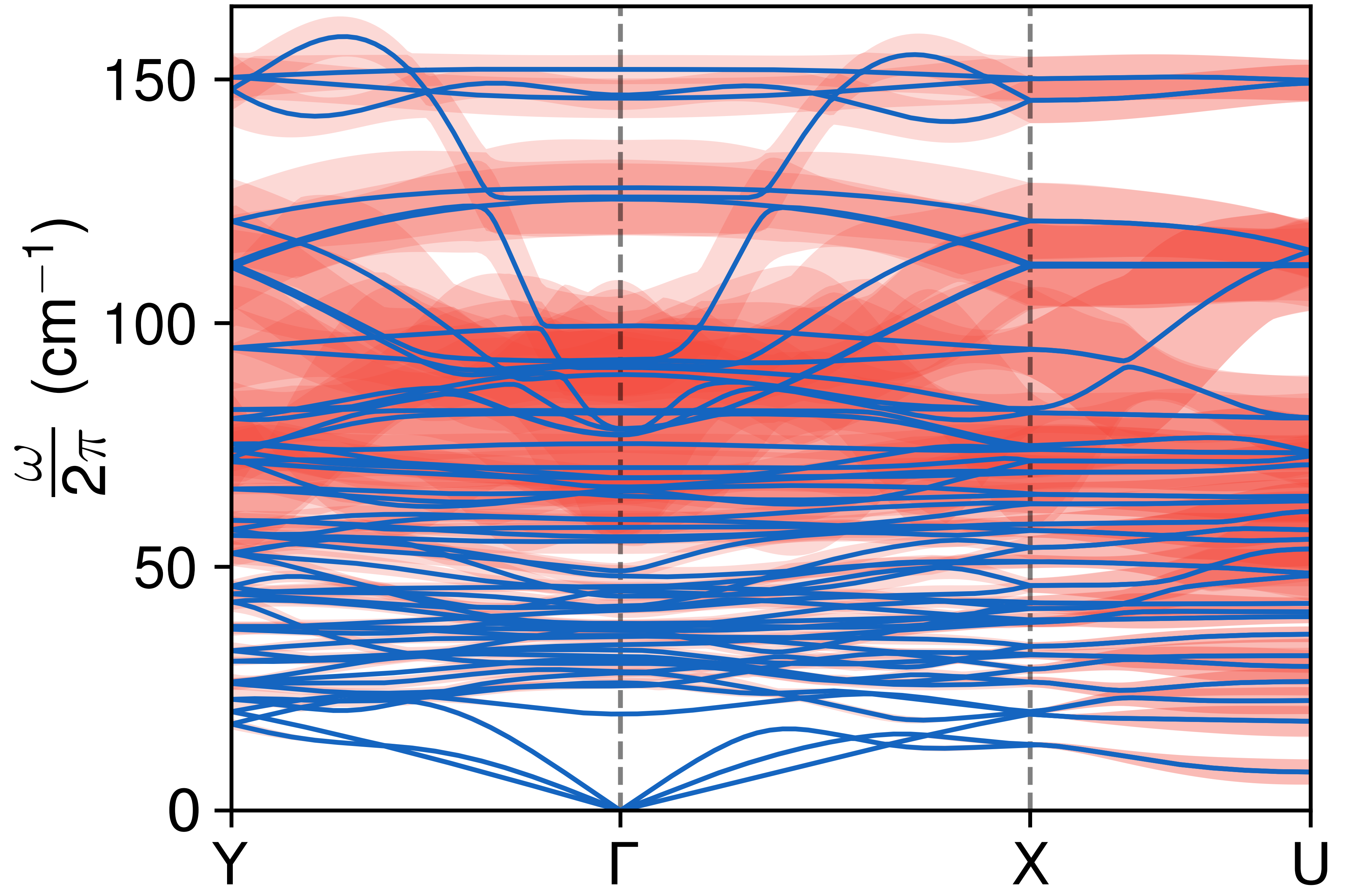


GaN, from Cepellotti et al, J. Phys. Mater. 5 (2022)

Phonons

— $\omega(\boldsymbol{q})_s$

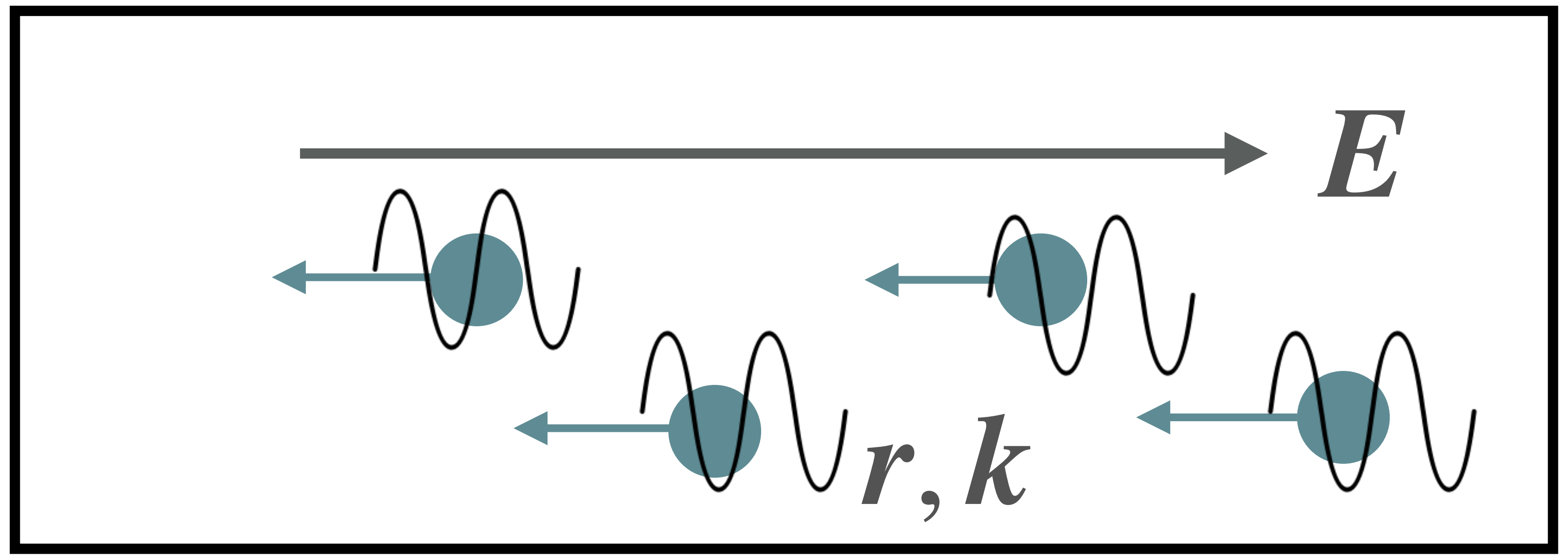
$$\Gamma(\boldsymbol{q})_s = \frac{36\pi}{\hbar N_q} \sum_{\boldsymbol{q},\boldsymbol{q}',s,s'} |V^{(3)}(\boldsymbol{q}s, -\boldsymbol{q}'s', -\boldsymbol{q}''s'')|^2 \delta_{\boldsymbol{q}-\boldsymbol{q}'-\boldsymbol{q}'',\boldsymbol{G}} \Big[\big(\bar{N}_{\boldsymbol{q}'s'} + \bar{N}_{\boldsymbol{q}''s''} + 1\big) \times \delta\big(\hbar\omega_{\boldsymbol{q}s} - \hbar\omega_{\boldsymbol{q}'s'} - \hbar\omega_{\boldsymbol{q}''s''}\big) + \big(\bar{N}_{\boldsymbol{q}'s'} - \bar{N}_{\boldsymbol{q}''s''}\big)\big[\delta\big(\hbar\omega_{\boldsymbol{q}s} + \hbar\omega_{\boldsymbol{q}'s'} - \hbar\omega_{\boldsymbol{q}''s''}\big) - \delta\big(\hbar\omega_{\boldsymbol{q}s} - \hbar\omega_{\boldsymbol{q}'s'} + \hbar\omega_{\boldsymbol{q}''s''}\big)\big]\Big]$$



*$CsPbBr_3$, from **Simoncelli**, Marzari, Mauri, Nat. Phys. 15 (2019)*

FROM BAND STRUCTURE TO TRANSPORT COEFFICIENTS

Wigner transport equation for electrons



electron Wigner distribution $F(\boldsymbol{r}, \boldsymbol{k}, t)_{m,m'}$

At equilibrium, diagonal elements = Fermi-Dirac

Electronic velocity operator (diagonal $\frac{\partial \epsilon(\boldsymbol{k})_m}{\partial \boldsymbol{k}}$) $\boldsymbol{V}(\boldsymbol{k})_{m,m'}$

$$\frac{\partial F(\boldsymbol{r},\boldsymbol{k},t)}{\partial t} + i[\mathcal{E}(\boldsymbol{k}) + \boldsymbol{d}(\boldsymbol{k}) \cdot \boldsymbol{E}, F(\boldsymbol{r},\boldsymbol{k},t)]$$

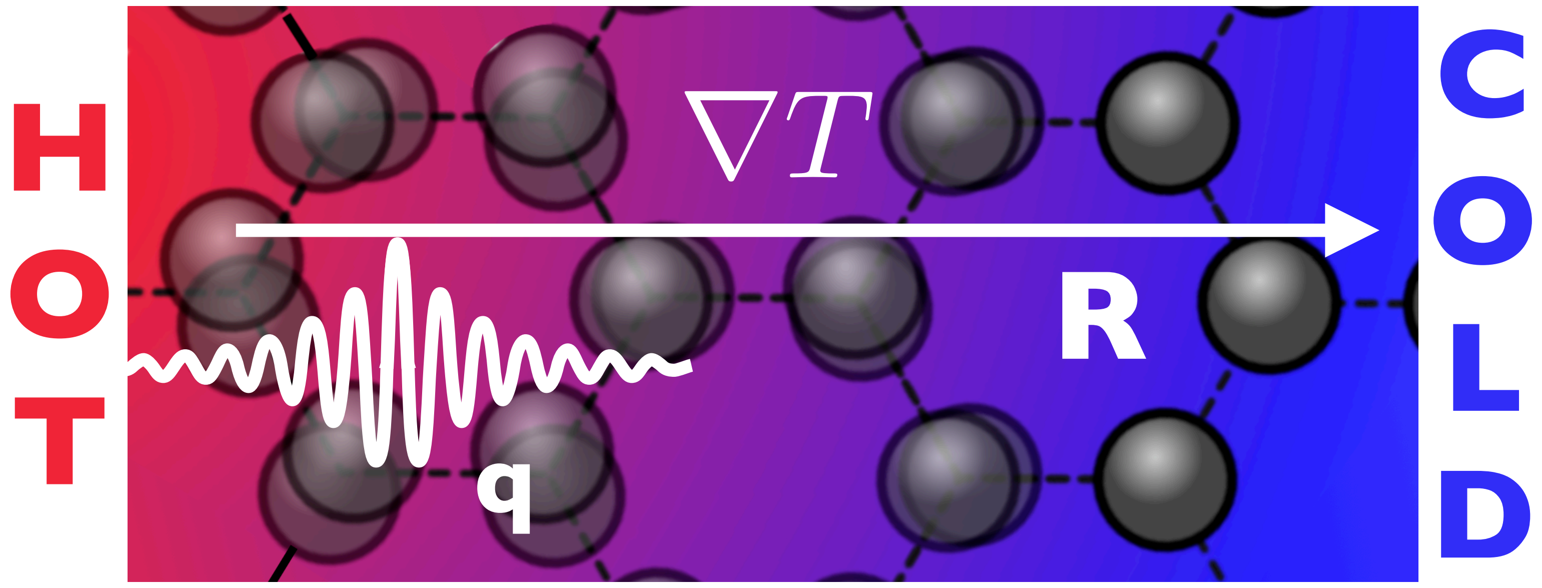
$$+ \frac{1}{2}\{\boldsymbol{V}(\boldsymbol{k}), \cdot \nabla_{\boldsymbol{r}} F(\boldsymbol{r},\boldsymbol{k},t)\} - e\boldsymbol{E} \cdot \nabla_{\boldsymbol{k}} F(\boldsymbol{r},\boldsymbol{k},t) = \left.\frac{\partial F(\boldsymbol{r},\boldsymbol{k},t)}{\partial t}\right|_{\text{coll}}$$

Iafrate, Sokolov, Krieger, Phys. Rev. B 96, 144303 (2017);
Cepellotti & Kozinsky, Materials Today Physics 19 (2021) 100412

coherences / populations

couplings / Group velocity

Wigner transport equation for phonons



$N(\boldsymbol{R}, \boldsymbol{q}, t)_{s,s'}$ **phonon Wigner distribution**

At equilibrium, diagonal elements = Bose-Einstein

$\boldsymbol{V}(\boldsymbol{q})_{s,s'}$ **Phonon velocity operator** (diagonal $\frac{\partial \omega(\boldsymbol{q})_s}{\partial \boldsymbol{q}}$)

$$\frac{\partial}{\partial t}\mathsf{N}(\boldsymbol{R},\boldsymbol{q},t) + i\Big[\boldsymbol{\Omega}(\boldsymbol{q}), \mathsf{N}(\boldsymbol{R},\boldsymbol{q},t)\Big] +$$

$$+ \frac{1}{2}\Big\{\vec{\mathsf{V}}(\boldsymbol{q}), \cdot \vec{\nabla}_{\boldsymbol{R}} \mathsf{N}(\boldsymbol{R},\boldsymbol{q},t)\Big\} = \left.\frac{\partial}{\partial t}\mathsf{N}(\boldsymbol{R},\boldsymbol{q},t)\right|_{\mathrm{H^{col}}}$$

Simoncelli, Marzari and Mauri, Nat. Phys. ***15*** *(2019)*
Simoncelli, Marzari and Mauri, Phys. Rev. X ***12*** *(2022)*

WIGNER CONDUCTIVITIES FOR ELECTRONS AND PHONONS

linear response in ∇T of phonon Wigner equation yields the heat flux $\mathbf{Q}$, thus thermal conductivity ($\mathbf{Q} = -\kappa \nabla T$)

$$\kappa^{\alpha\beta} = \kappa_P^{\alpha\beta} + \frac{1}{VN_q} \sum_{\boldsymbol{q},s\neq s'} \frac{\omega(\boldsymbol{q})_s + \omega(\boldsymbol{q})_{s'}}{4} \left[\frac{C(\boldsymbol{q})_s}{\omega(\boldsymbol{q})_s} + \frac{C(\boldsymbol{q})_{s'}}{\omega(\boldsymbol{q})_{s'}}\right] v^\alpha(\boldsymbol{q})_{s,s'} v^\beta(\boldsymbol{q})_{s',s} \frac{\frac{1}{2}\left[\Gamma(\boldsymbol{q})_s + \Gamma(\boldsymbol{q})_{s'}\right]}{[\omega(\boldsymbol{q})_{s'} - \omega(\boldsymbol{q})_s]^2 + \frac{1}{4}[\Gamma(\boldsymbol{q})_s + \Gamma(\boldsymbol{q})_{s'}]^2}$$

Simoncelli, Marzari and Mauri, Nat. Phys. ***15*** *(2019)*

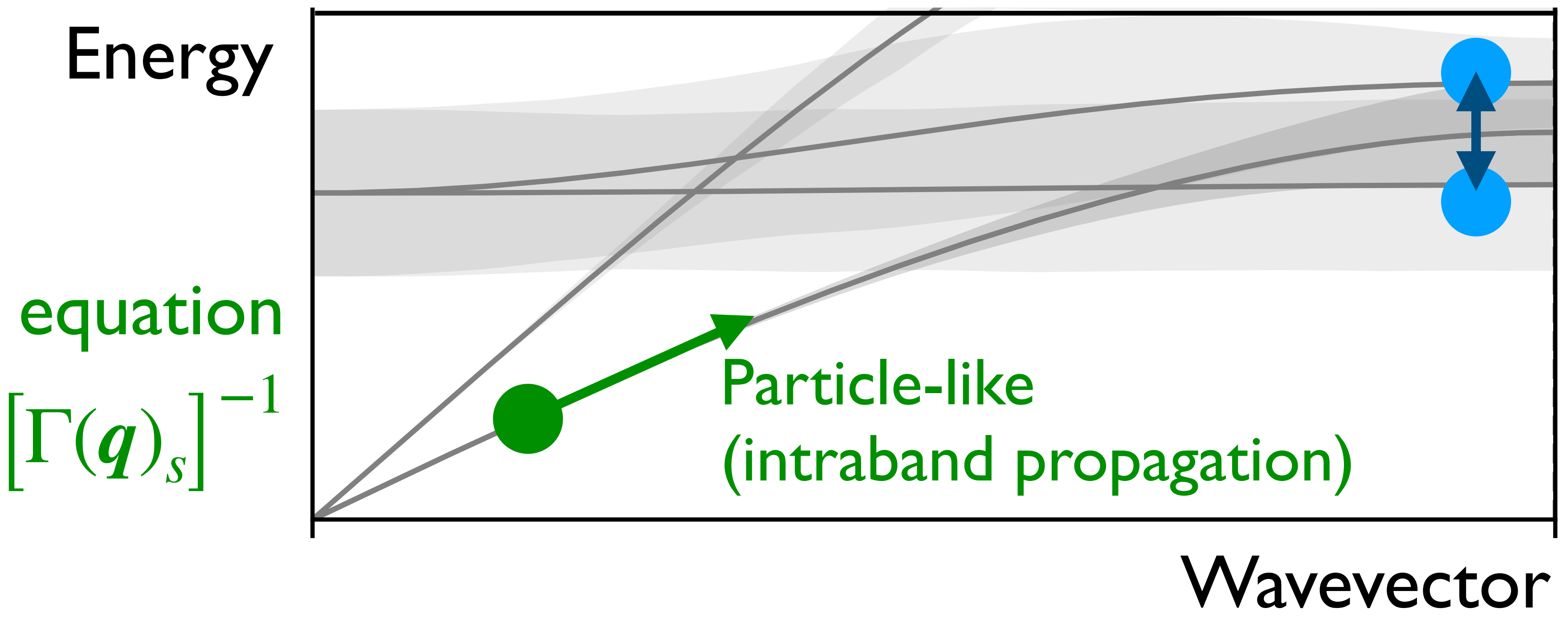
linear response in $\boldsymbol{E}$ of electron Wigner equation yields the charge current $\mathbf{J}$, thus electrical conductivity $\mathbf{J} = -\sigma\mathbf{E}$

$$\sigma^{\alpha\beta} = \sigma_P^{\alpha\beta} + \frac{g_s}{VN_k} \sum_{\boldsymbol{k},m\neq m'} \frac{f(\boldsymbol{k}')_{m'} - f(\boldsymbol{k})_m}{\epsilon(\boldsymbol{k}')_{m'} - \epsilon(\boldsymbol{k})_m} v^\alpha(\boldsymbol{k})_{m,m'} v^\beta(\boldsymbol{k})_{m',m} \frac{\frac{1}{2}\left[\Gamma(\boldsymbol{k})_m + \Gamma(\boldsymbol{k})_{m'}\right]}{[\epsilon(\boldsymbol{k})_{m'} - \epsilon(\boldsymbol{k})_m]^2 + \frac{1}{4}[\Gamma(\boldsymbol{k})_m + \Gamma(\boldsymbol{k})_{m'}]^2}$$

Cepellotti and Kozinsky, Materials Today Physics 19 (2021)

Equivalent to Boltzmann transport equation

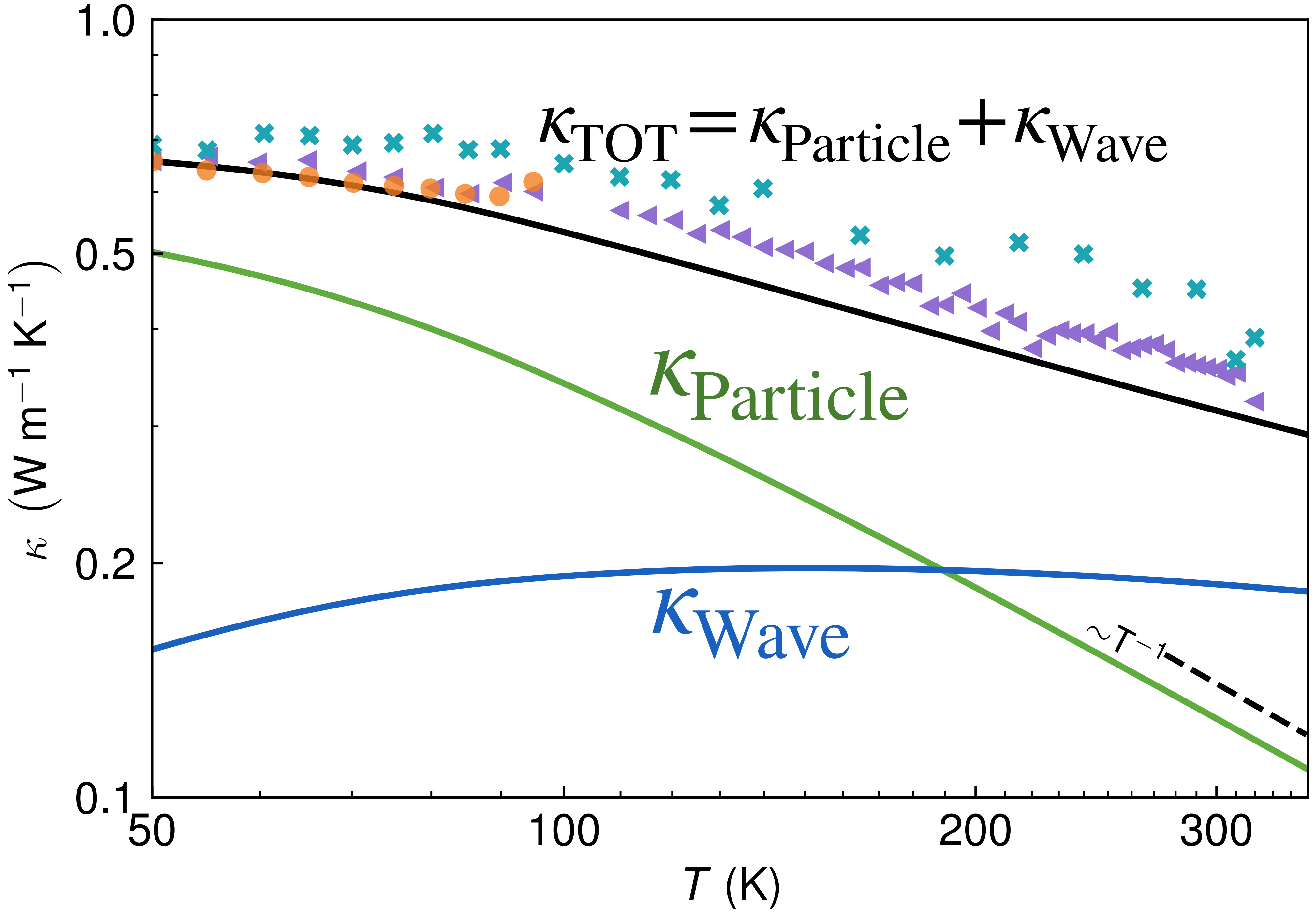
$$\kappa_P \sim \frac{1}{3VN_q} \sum_{\boldsymbol{q}s} C(\boldsymbol{q})_s \boldsymbol{v}^2(\boldsymbol{q})_s \left[\Gamma(\boldsymbol{q})_s\right]^{-1}$$



Wave-like
(interband tunnelling)

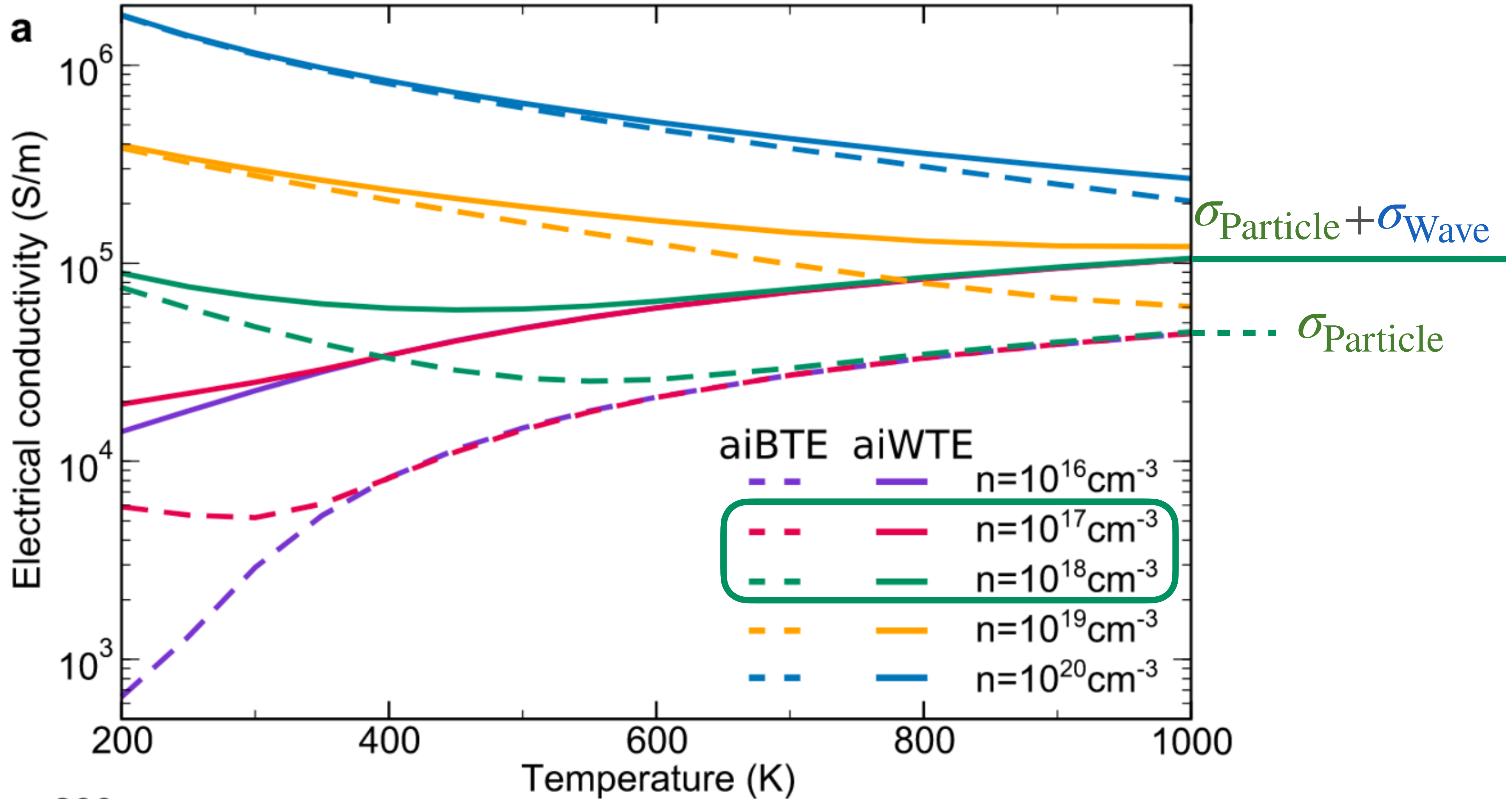
DUAL WAVE-PARTICLE TRANSPORT

Phonon transport in $CsPbBr_3$



Simoncelli, Marzari, Mauri, Nat. Phys. 15 (2019)

Electron transport in Bi_2Se_3



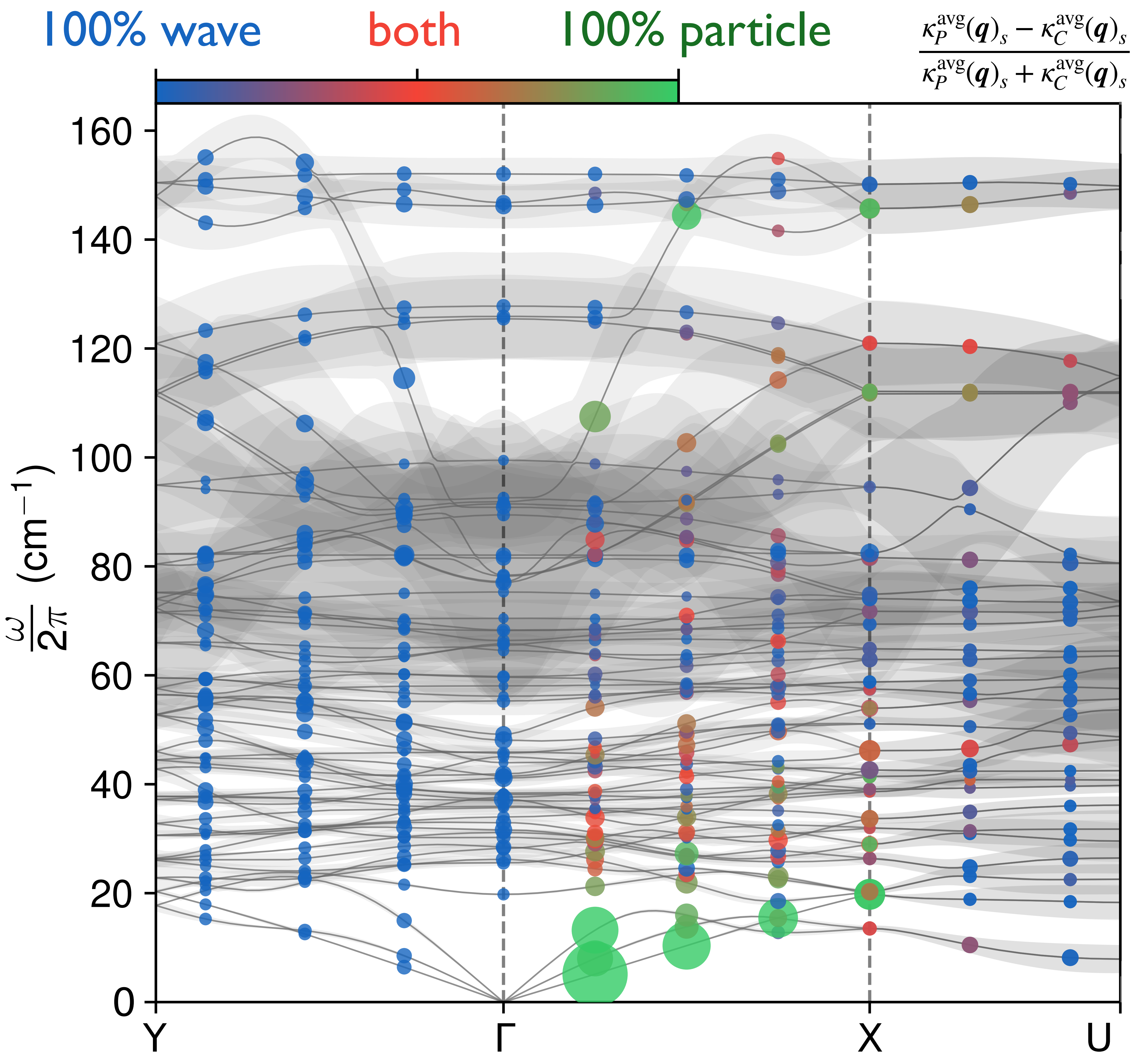
Cepellotti and Kozinsky, Materials Today Physics 19 (2021)

QUANTUM ESPRESSO + D3Q (d3q + thermal2) or phono3py or ALAMODE or Phoebe

QUANTUM ESPRESSO + Phoebe or EPW

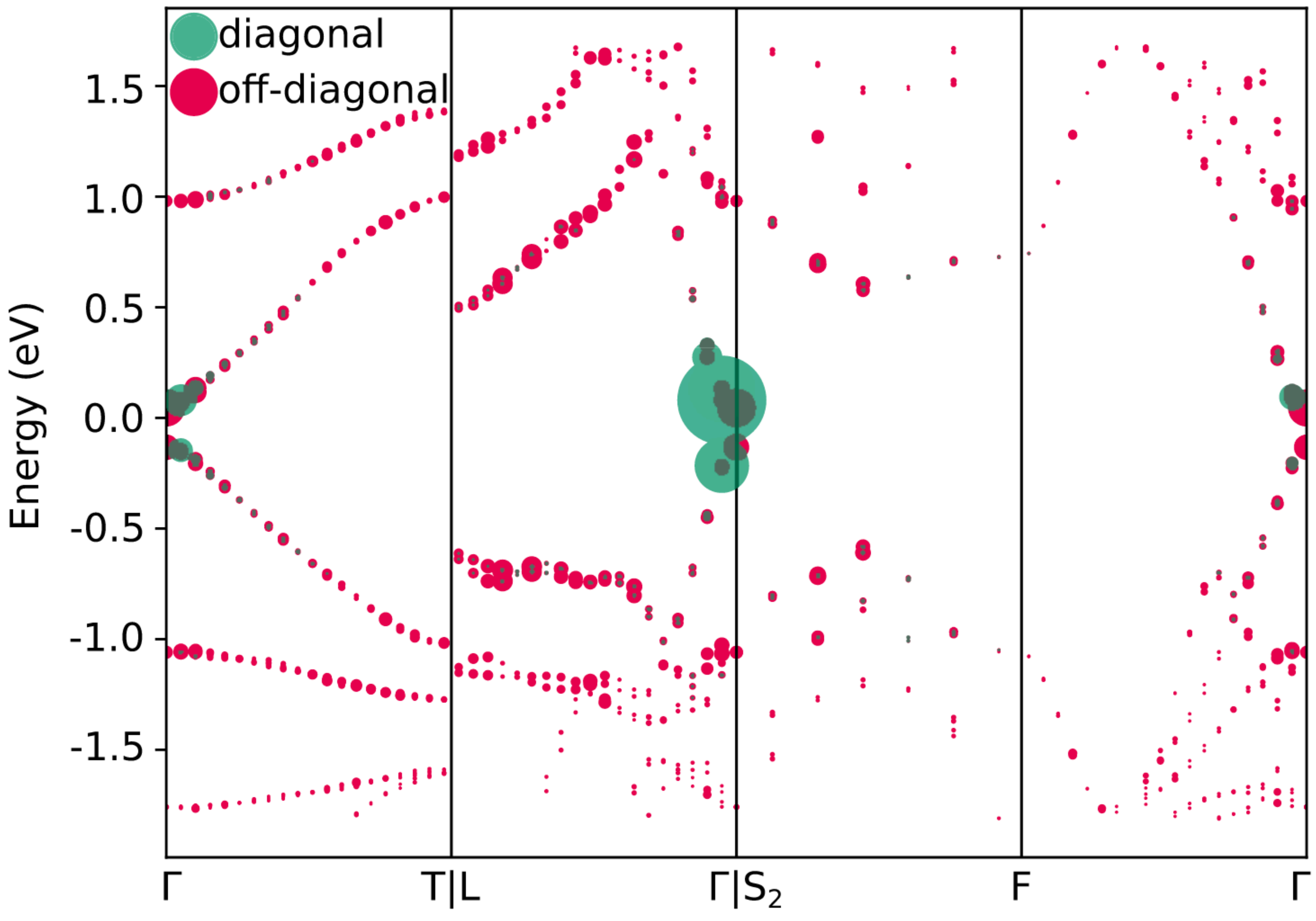
DUAL WAVE-PARTICLE TRANSPORT

Phonon transport in $CsPbBr_3$



Simoncelli, Marzari, Mauri, Nat. Phys. 15 (2019)

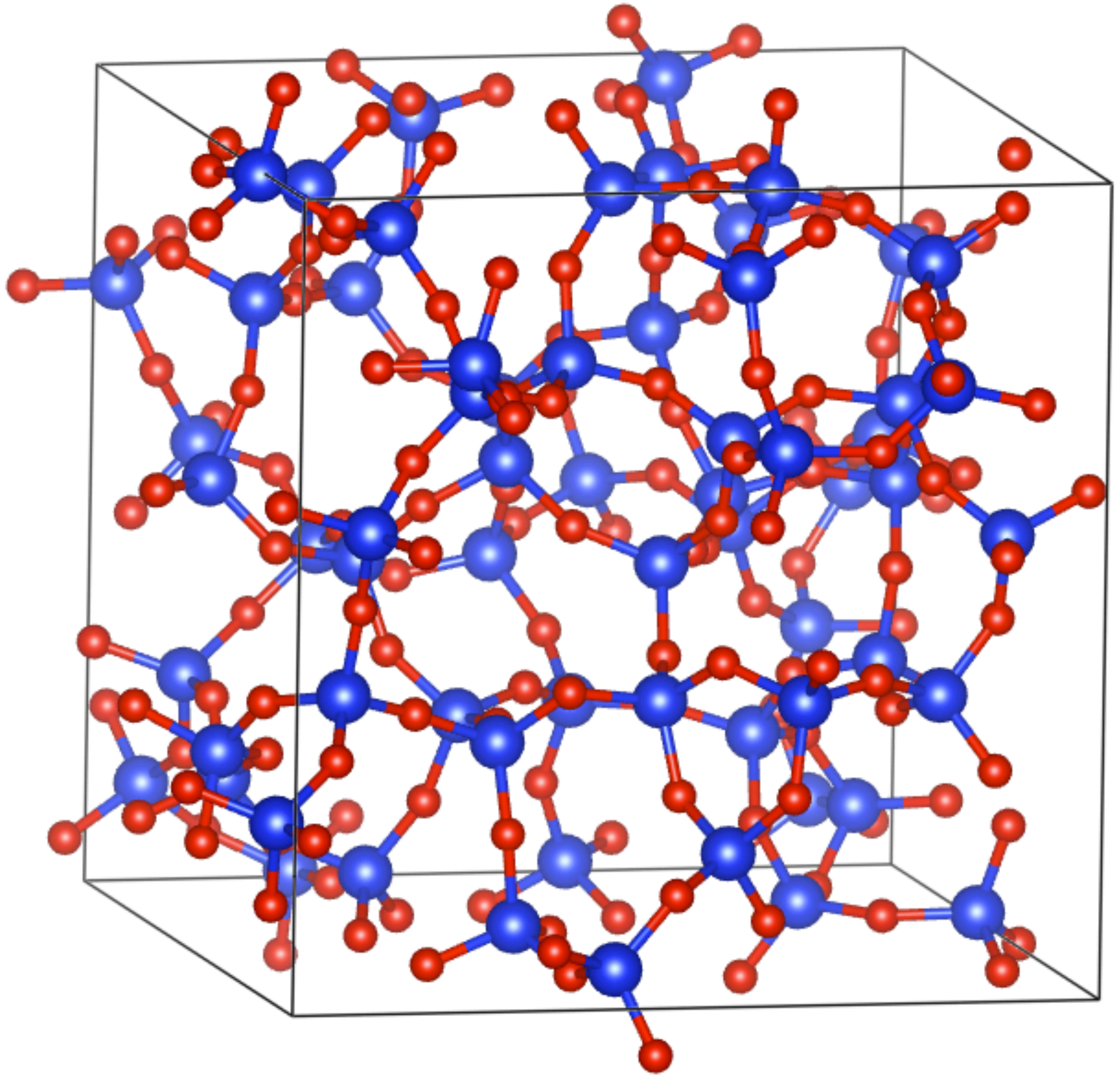
Electron transport in Bi_2Se_3



Cepellotti and Kozinsky, Materials Today Physics 19 (2021)

BEYOND BAND TRANSPORT

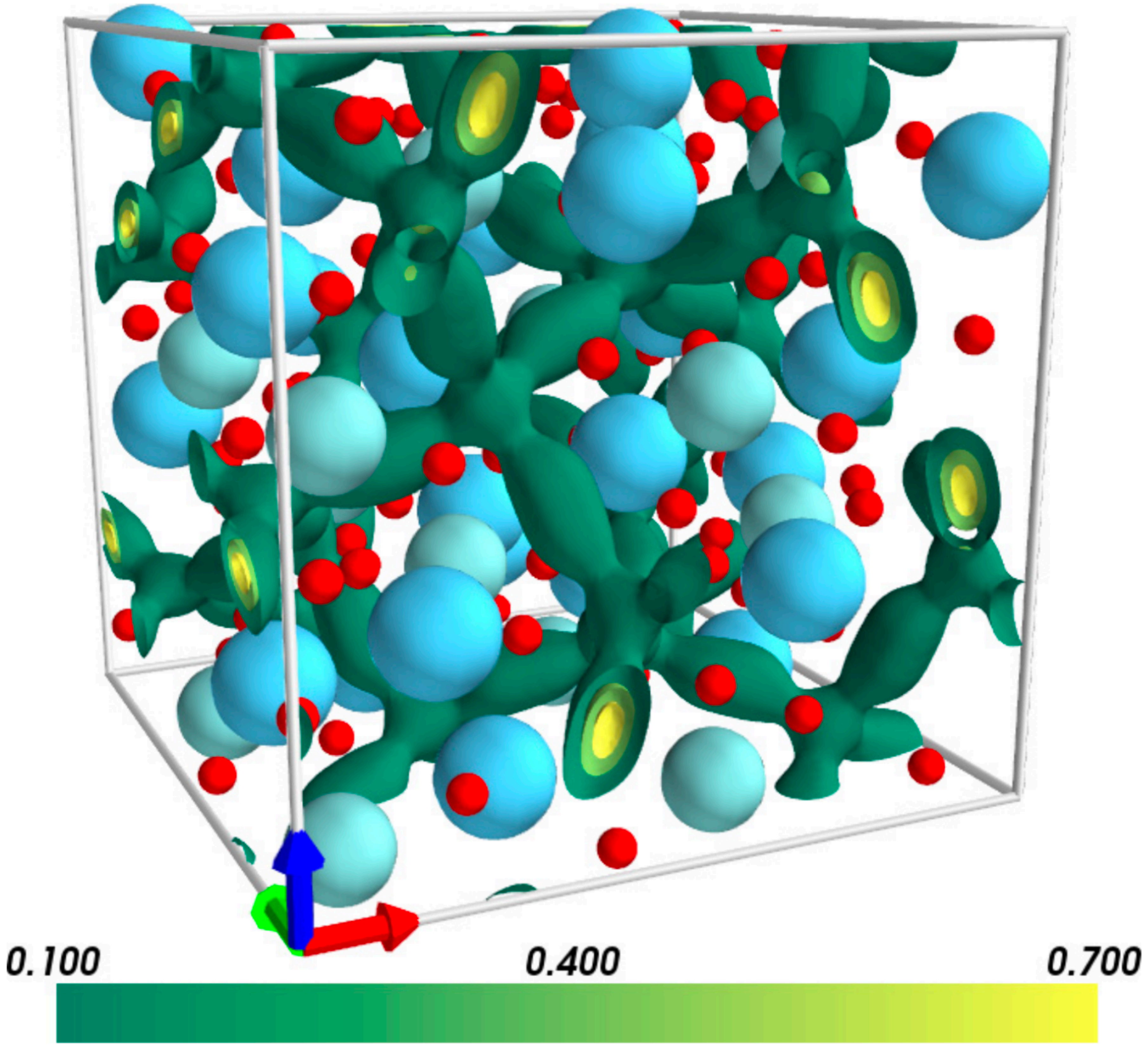
Heat transfer in amorphous solids



Atomistic model of SiO_2 generated from first principles

***Simoncelli**, Mauri, Marzari, npj Comput. Mater. 9 (2023);*

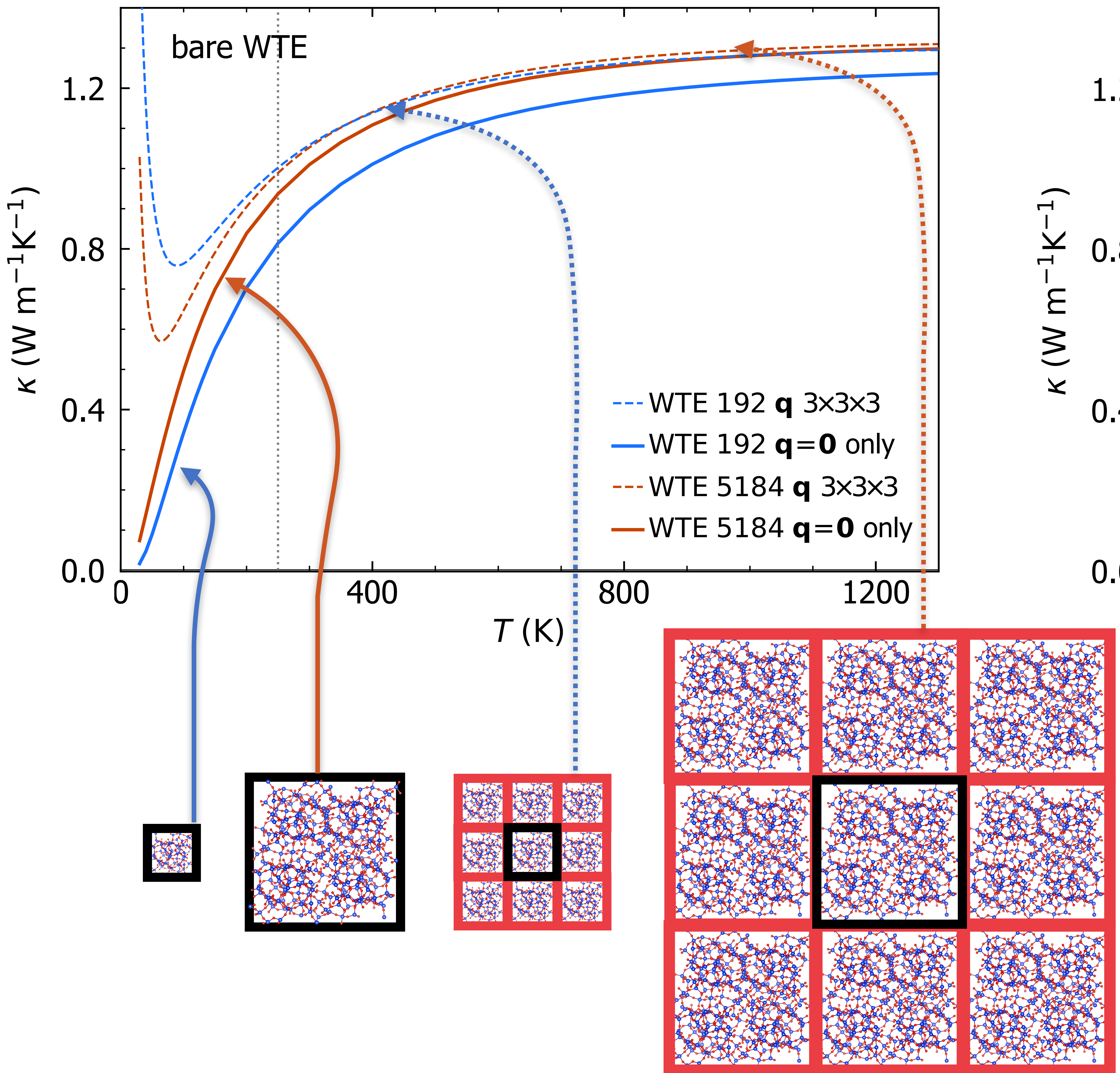
Charge transfer in solid-state ionic conductors

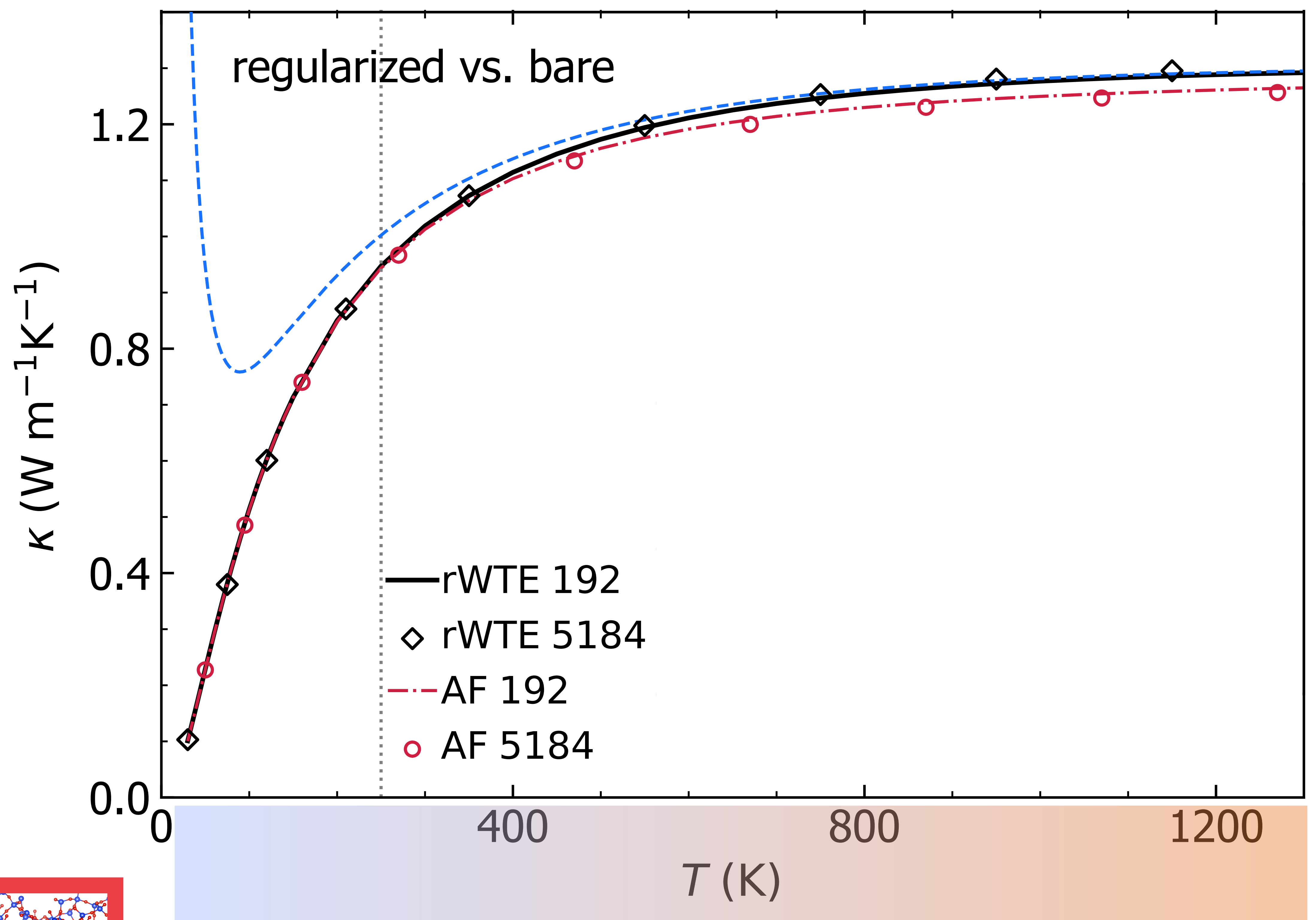


Li-Ion percolation pathways in $Li_7La_3Zr_2O_{12}$

Kahle et al., Phys. Rev. Materials 3, 055404 (2019)

PROTOCOL FOR HEAT TRANSPORT IN GLASSES





$$\frac{1}{\sqrt{2\pi}\eta}e^{-\frac{(\omega(\boldsymbol{q})_s-\omega(\boldsymbol{q})_{s'})^2}{2\eta^2}}$$

$$\frac{1}{\pi}\frac{\frac{1}{2}(\Gamma(\boldsymbol{q})_s+\Gamma(\boldsymbol{q})_{s'})}{(\omega(\boldsymbol{q})_s-\omega(\boldsymbol{q})_{s'})^2+\frac{1}{4}(\Gamma(\boldsymbol{q})_s+\Gamma(\boldsymbol{q})_{s'})^2}$$

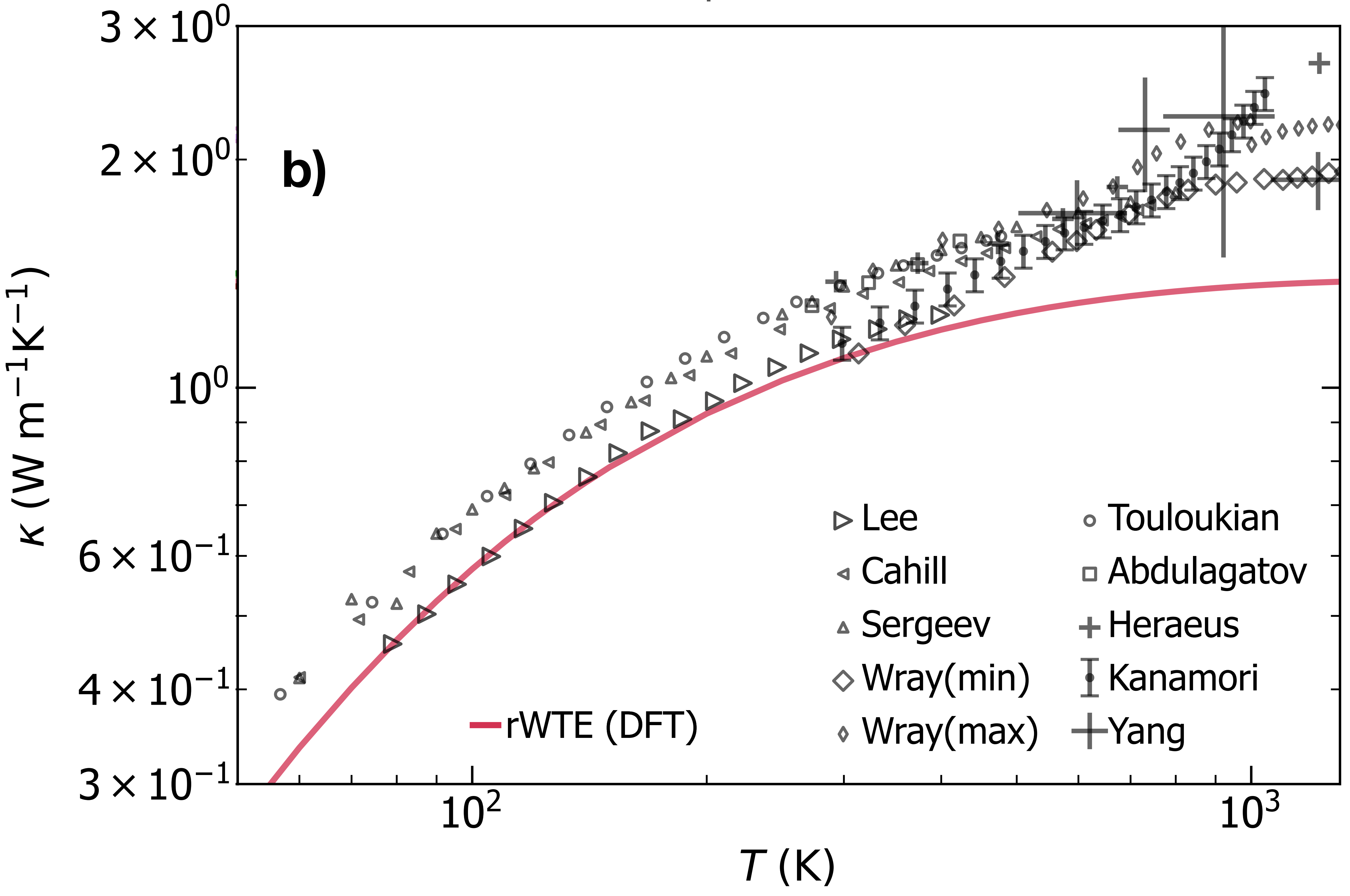
$\Gamma(\boldsymbol{q})_s \ll \eta$ $\Gamma(\boldsymbol{q})_s \gg \eta$

Voigt profile $\mathcal{F}_{[\eta;\Gamma(\boldsymbol{q})_s+\Gamma(\boldsymbol{q})_{s'}]}(\omega(\boldsymbol{q})_s-\omega(\boldsymbol{q})_{s'})$

Erhard et al.. Npj Comput. Mater. 8 (2022)
***Simoncelli**, Mauri, Marzari, npj Comput. Mater. 9 (2023)*

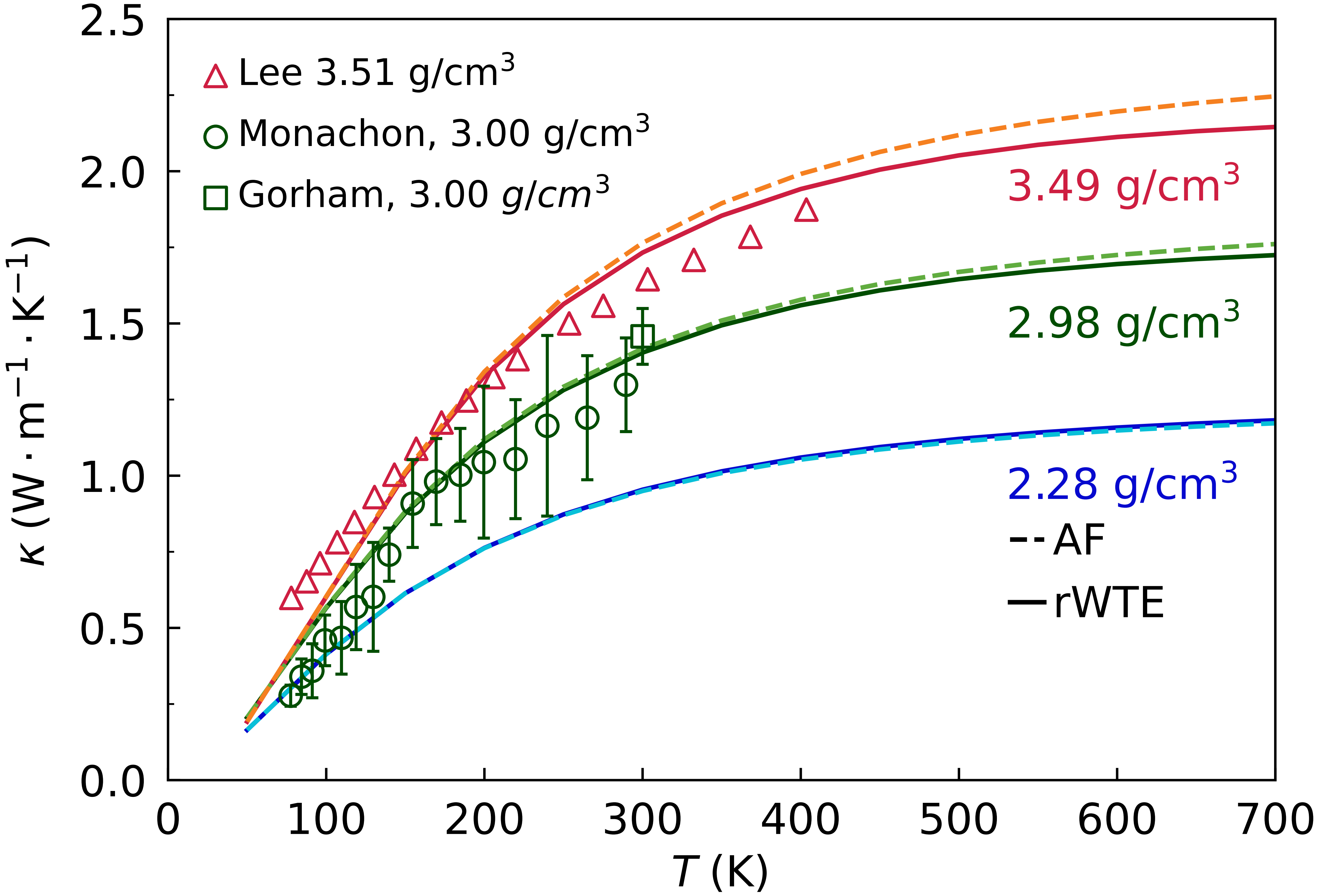
CONDUCTIVITY OF GLASSES FROM FIRST PRINCIPLES

Amorphous SiO_2



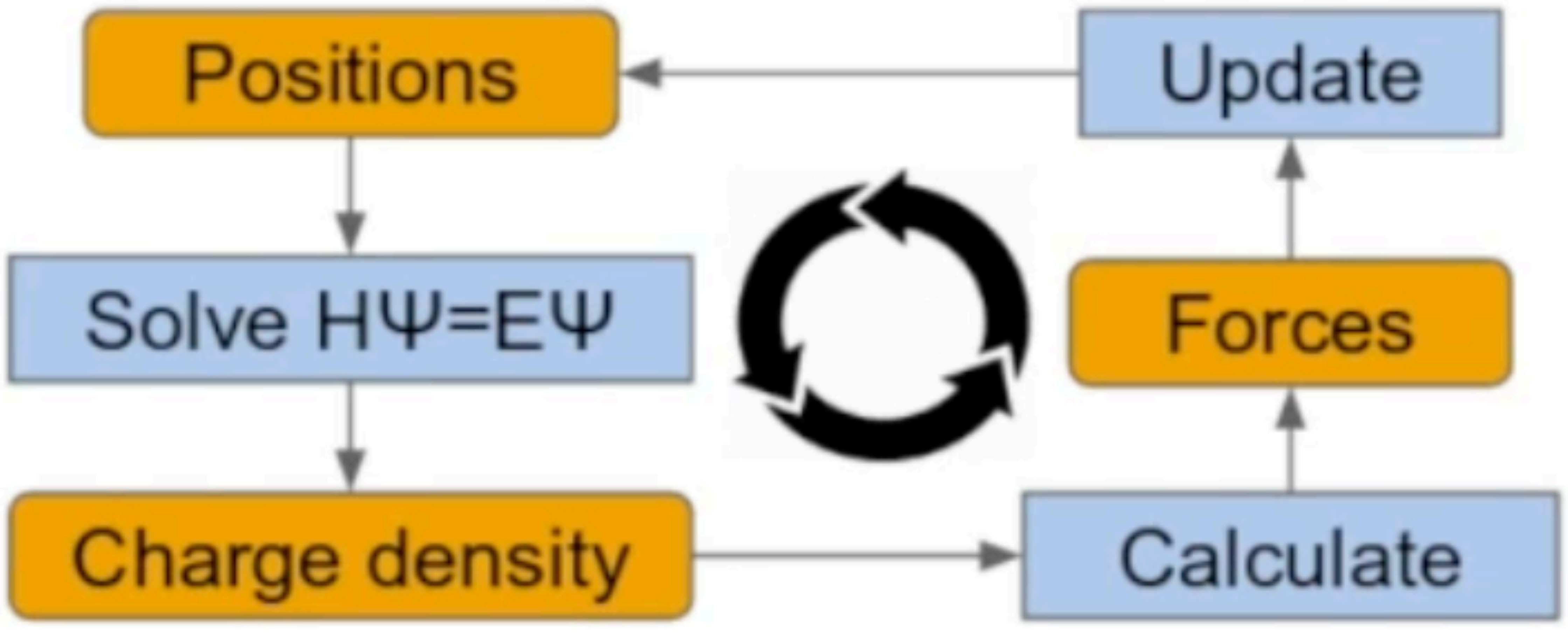
Simoncelli, Mauri, Marzari, npj Comput. Mater. 9 (2023)

Amorphous Al_2O_3

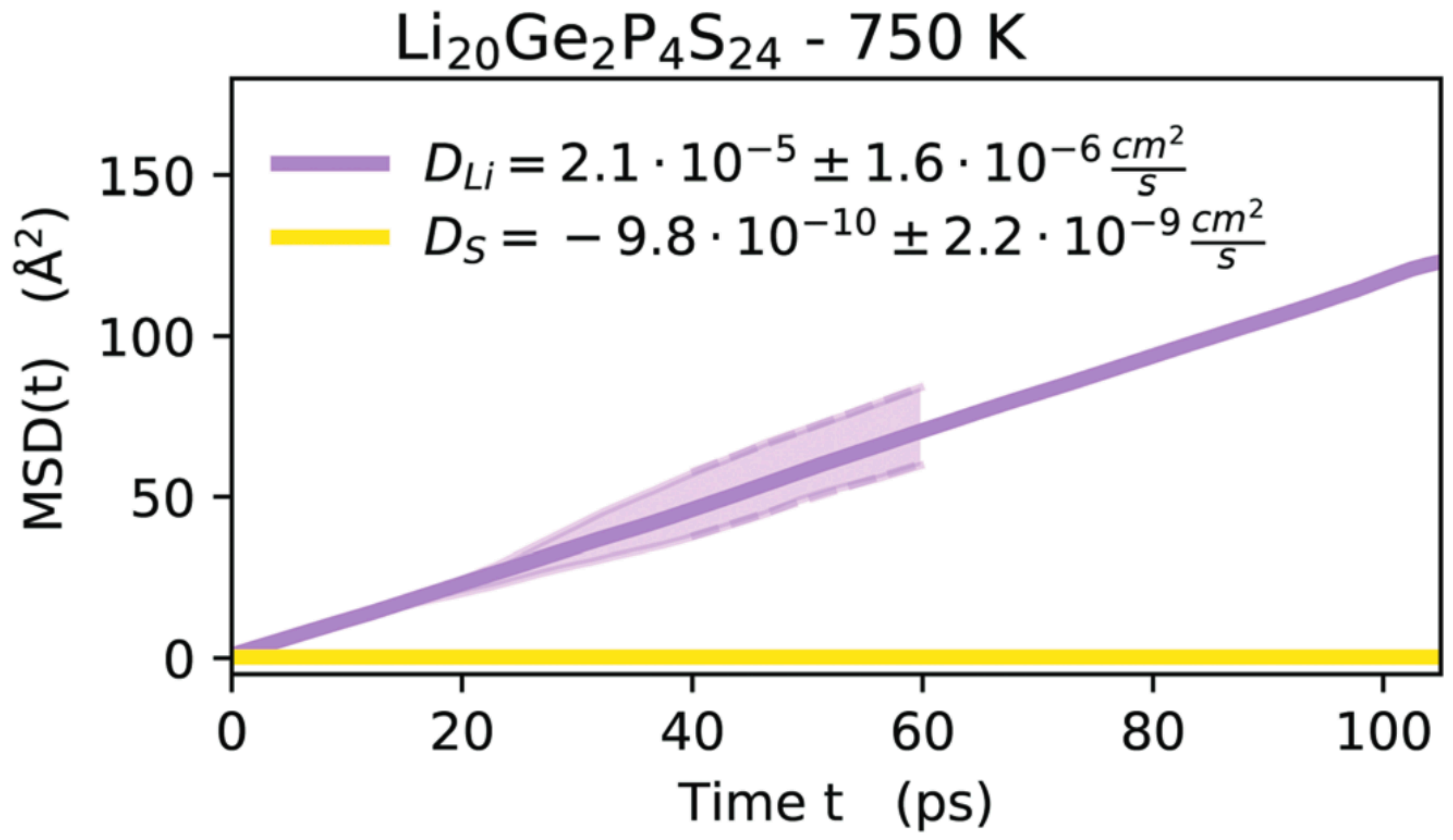


Harper, Iwanowski, Payne, *Simoncelli* arXiv 2303.08637 (2023)

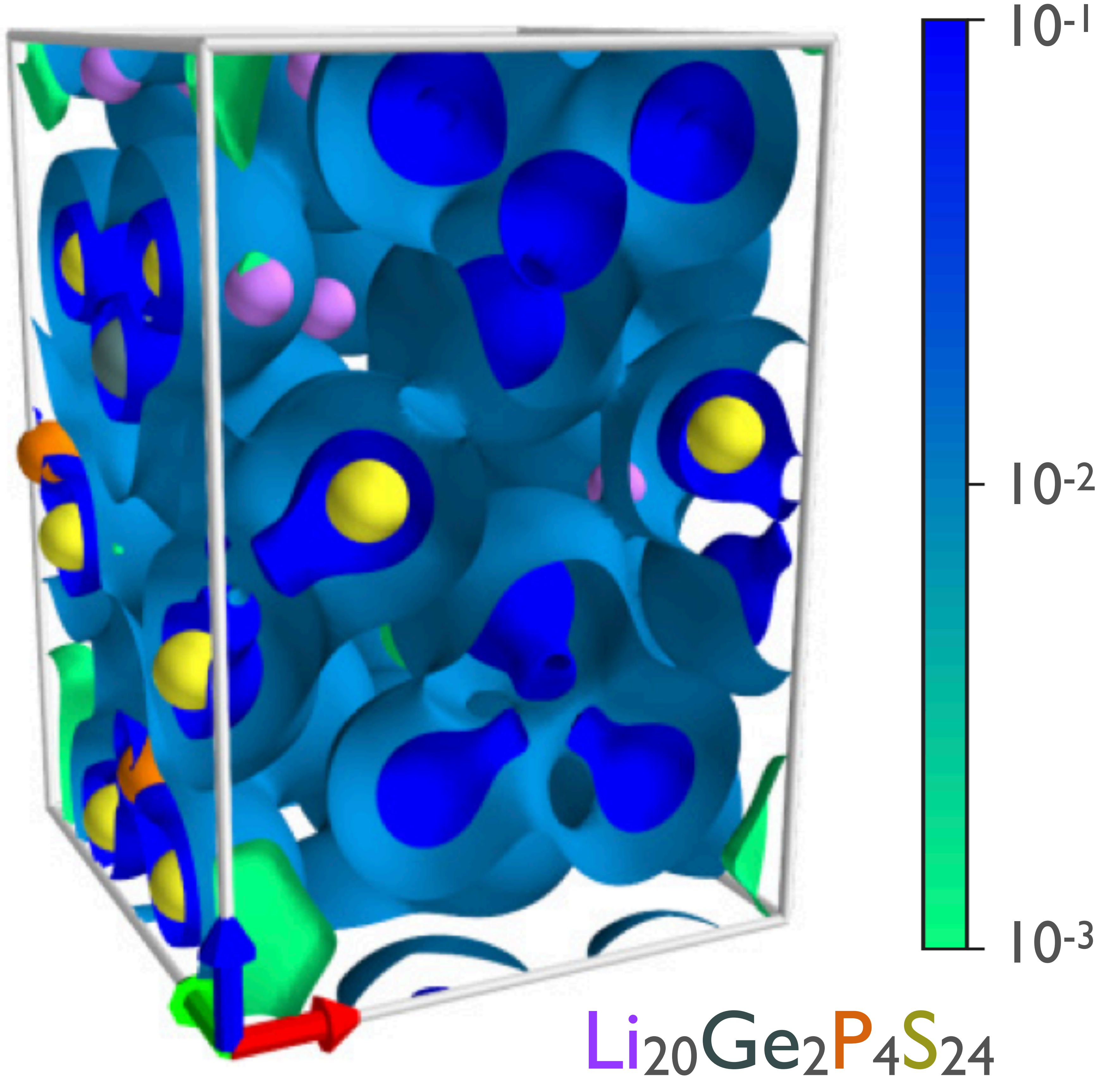
IONIC DIFFUSIVITY FROM AB INITIO MOLECULAR DYNAMICS



Ionic conductors: $D_{\mathrm{tr}}^{\mathrm{Li}} = \lim_{t \to \infty} \frac{1}{6t} \frac{1}{N_{\mathrm{Li}}} \sum_{l}^{\mathrm{Li}} \langle |\mathbf{R}_l(t+\tau) - \mathbf{R}_l(\tau)|^2 \rangle_\tau$



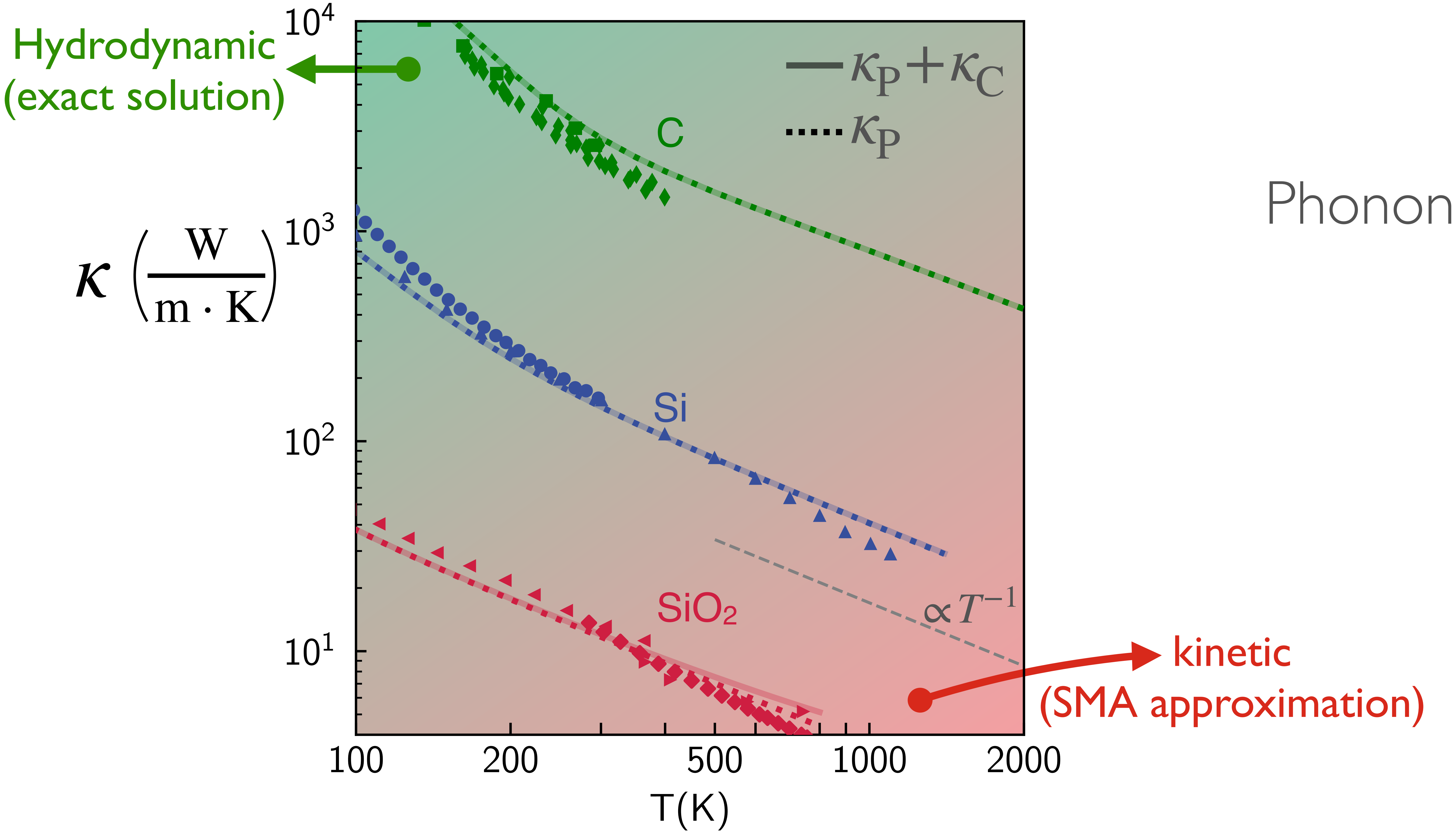
Isosurfaces of valence electronic charge density

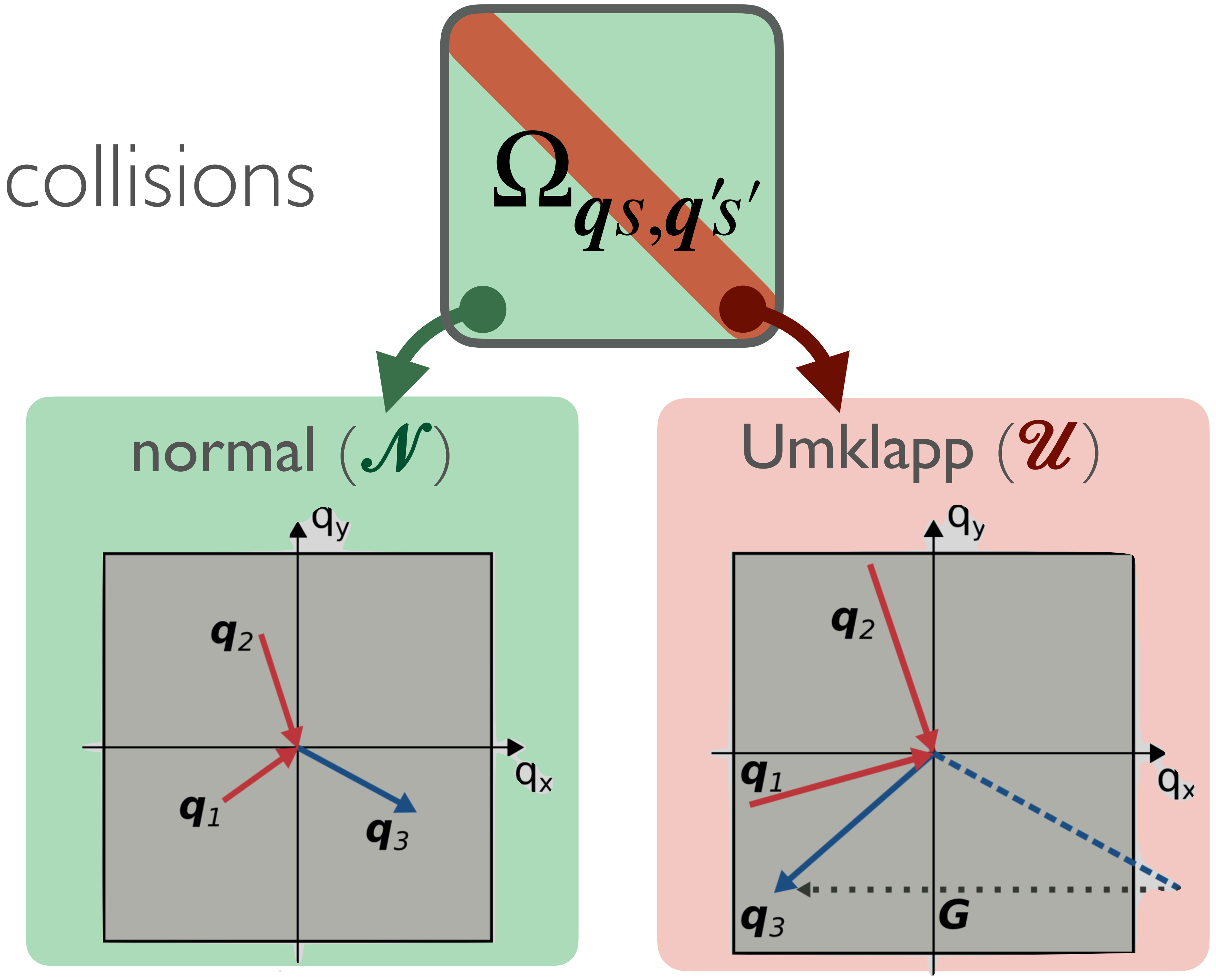


Kahle, Marcolongo, & Marzari, Phys. Rev. Materials 2 (2018)
Kahle, Marcolongo, & Marzari, Energy Environ. Sci. 13 (2020)

FIRST PRINCIPLES PARAMETRISATION OF MESOSCOPIC MODELS FOR DEVICES

HEAT HYDRODYNAMICS IN SIMPLE CRYSTALS WITH $\kappa_P \gg \kappa_C$





Particle-like conduction dominates, Peierls-Boltzmann equation is accurate

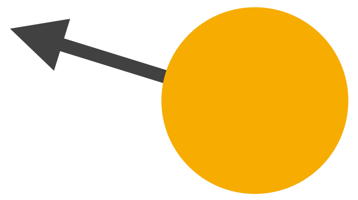
$$\frac{\partial N(\boldsymbol{x},\boldsymbol{q},t)_s}{\partial t} + \vec{V}(\boldsymbol{q})_s \cdot \nabla_{\boldsymbol{x}} N(\boldsymbol{x},\boldsymbol{q},t)_s = -\sum_{\boldsymbol{q}'s'} \Omega_{\boldsymbol{q}s,\boldsymbol{q}'s'}\left[N(\boldsymbol{x},\boldsymbol{q}',t)_{s'} - \bar{N}(\boldsymbol{q}')_{s'}\right]$$

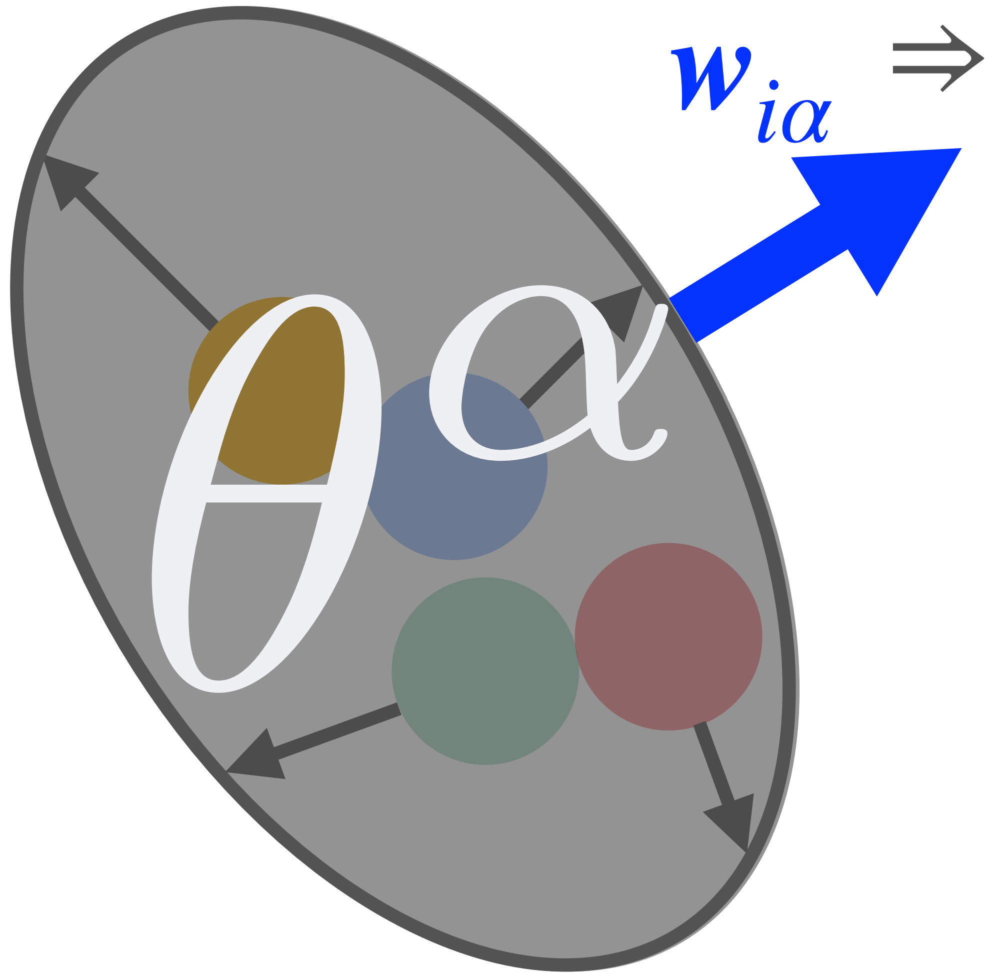
Berman, Phys. Rev. B ***45*** *(1992)*

RELAXONS: EXACT SOLUTION & MICROSCOPIC INSIGHTS

How to define heat carriers and relaxation time in the hydrodynamic regime?

$$\frac{\partial N(\boldsymbol{x},\boldsymbol{q},t)_s}{\partial t} + \vec{V}(\boldsymbol{q})_s \cdot \nabla_{\boldsymbol{x}} N(\boldsymbol{x},\boldsymbol{q},t)_s = -\sum_{\boldsymbol{q}'s'} \Omega_{\boldsymbol{q}s,\boldsymbol{q}'s'} \left[N(\boldsymbol{x},\boldsymbol{q}',t)_{s'} - \bar{N}(\boldsymbol{q}')_{s'} \right]$$



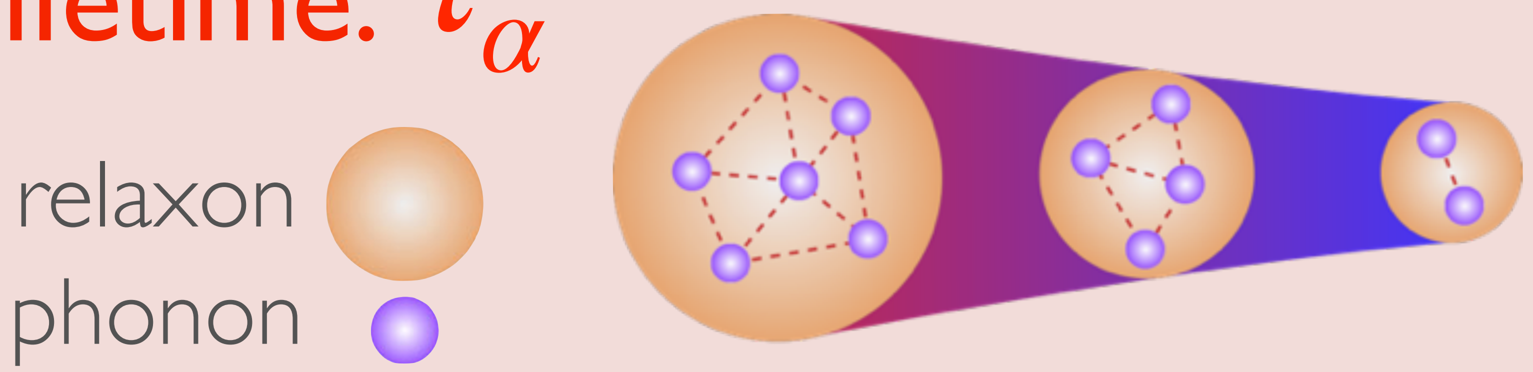


⇒ Symmetrise and diagonalise the scattering matrix

$$-\sum_{q's'} \tilde{\Omega}_{qs,q's'} \left| \theta(q')^{\alpha}_{s'} \right\rangle = -\frac{1}{\tau_{\alpha}} \left| \theta(q)^{\alpha}_{s} \right\rangle$$

Relaxon $\left| \theta(q)^{\alpha}_{s} \right\rangle$ = cloud of interacting phonons having:

1) Exact lifetime: τ_{α}



2) Velocity:

$$w_{i\alpha} = \frac{1}{V} \sum_{q,s} \left\langle \phi(q)^{i}_{s} \middle| V(q)_s \middle| \theta(q)^{\alpha}_{s} \right\rangle$$

Cepellotti and Marzari, Phys. Rev. X **6** *(2016)*

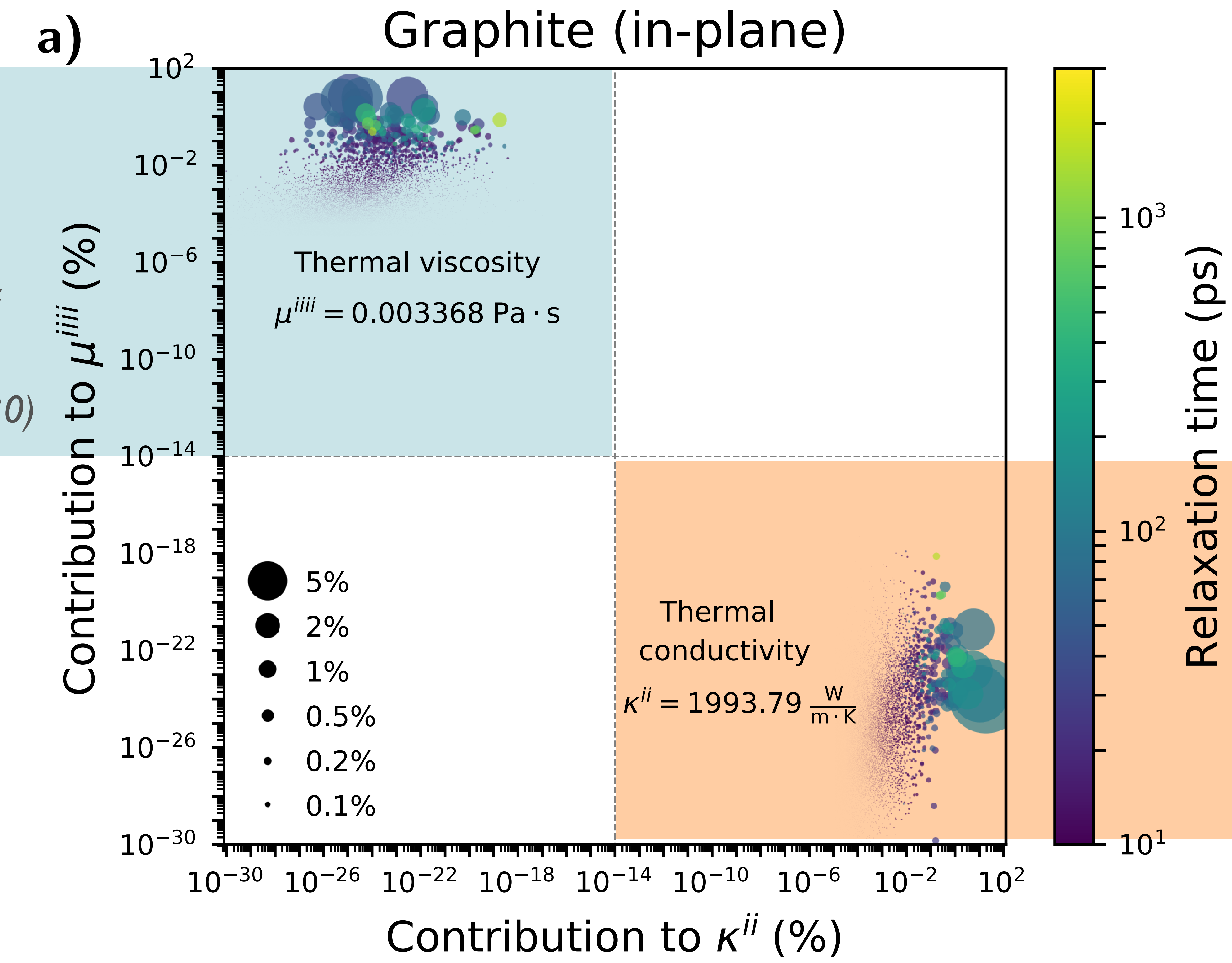
ODD & EVEN RELAXONS: CONDUCTIVITY & VISCOSITY

Relaxons have parity: even $\left|\theta(-\boldsymbol{q})^{\alpha}_{s}\right\rangle = +\left|\theta(\boldsymbol{q})^{\alpha}_{s}\right\rangle$ or odd $\left|\theta(-\boldsymbol{q})^{\beta}_{s}\right\rangle = -\left|\theta(\boldsymbol{q})^{\beta}_{s}\right\rangle$

Even relaxons → $\boldsymbol{\mu}$

$$\mu^{ijkl} = \sqrt{A^i A^k} \sum_{\alpha>0} \frac{w^j_{i\alpha} w^l_{k\alpha} + w^l_{i\alpha} w^j_{k\alpha}}{2} \tau_\alpha$$

*Simoncelli, Marzari, & Cepellotti, PRX **10** (2020)*



Odd relaxons → κ

$$\kappa^{ij} = C \sum_{\alpha} w^i_{0\alpha} w^j_{0\alpha} \tau_\alpha$$

*Cepellotti and Marzari, PRX **6** (2016)*

QUANTUMESPRESSO

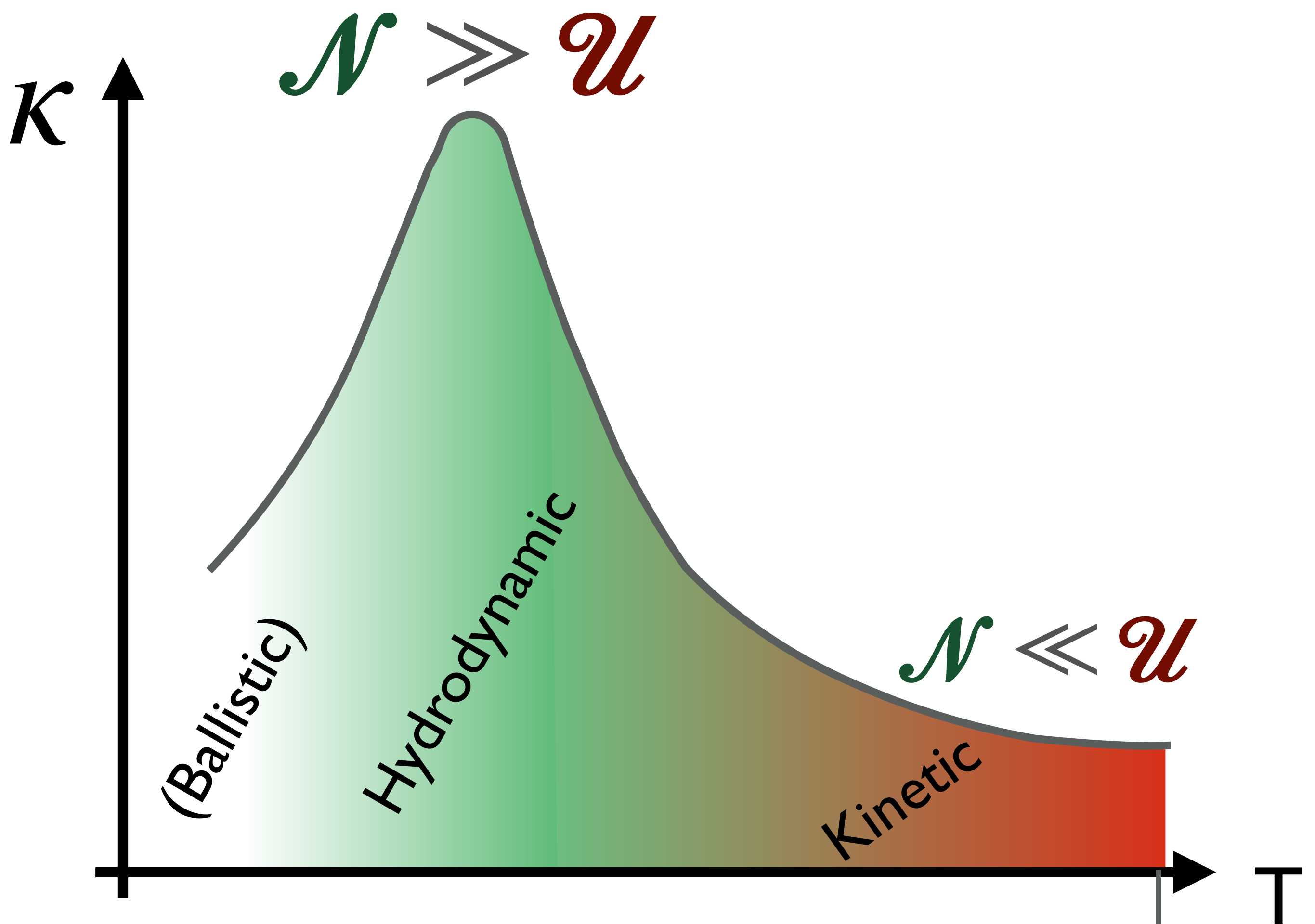
Phoebe

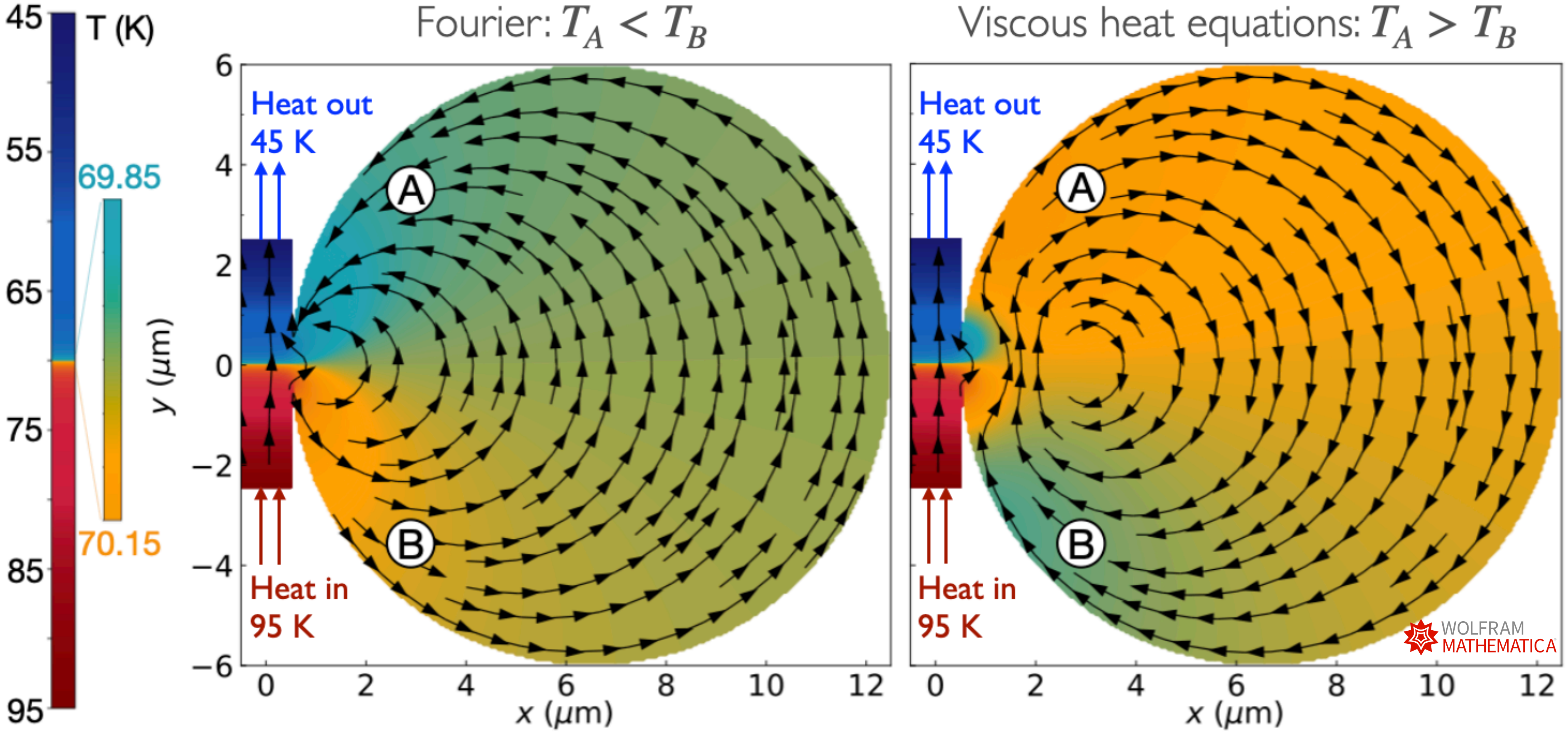
Simoncelli, Marzari and Cepellotti, PRX, 10 (2020);

VISCOUS HEAT EQUATIONS GENERALISE FOURIER'S LAW

$$\partial_t T + \overleftrightarrow{A} \otimes \nabla_{\boldsymbol{x}} \boldsymbol{u} - \overleftrightarrow{\kappa} \otimes \nabla^2_{\boldsymbol{x}} T = 0$$

$$\partial_t \boldsymbol{u} + \overleftrightarrow{B} \otimes \nabla_{\boldsymbol{x}} T - \overleftrightarrow{\mu} \otimes \nabla^2_{\boldsymbol{x}} \boldsymbol{u} = -\overleftrightarrow{D} \otimes \boldsymbol{u}$$





1822: Fourier's law
diffusion

1948: Cattaneo's equation
large-scale temperature waves

1989: dual-phase-lag equation
small-time and small-scale inviscid waves

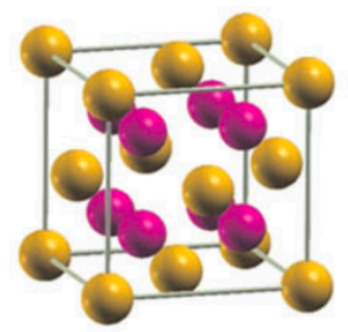
2020: Viscous heat equations
steady-state hydrodynamic signatures
viscous waves

__Simoncelli__, Marzari and Cepellotti, PRX, 10 (2020); Dragašević and __Simoncelli__, arXiv:2303.12777

PREDICTING REFLECTIVITY AND COLOUR OF METALS

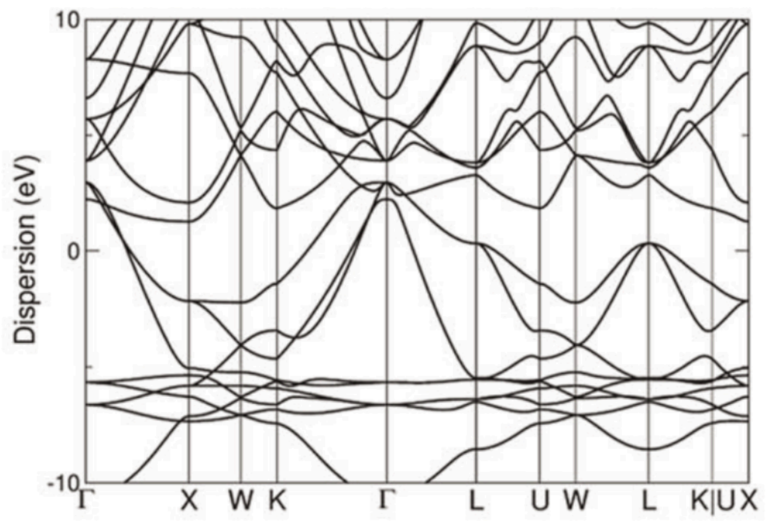
ColourWorkflow

Crystal structure



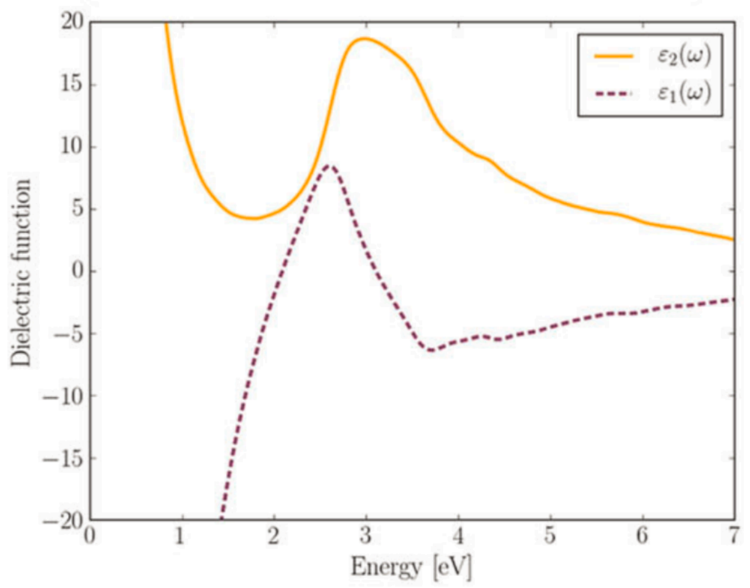
→

(i) Band structure



→

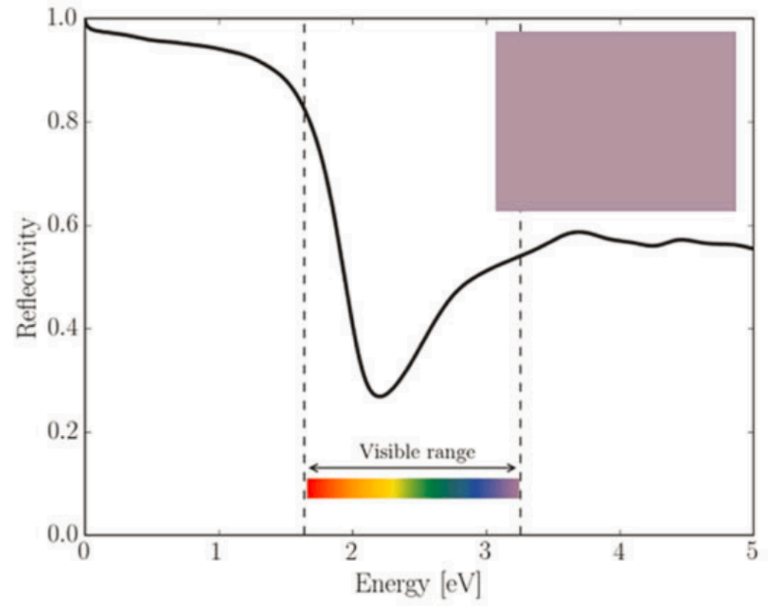
(ii) Dielectric function (interband + intraband)



$$\varepsilon(\hat{\mathbf{q}},\omega) = 1 - \frac{4\pi}{V}\sum_{\mathbf{k}}\sum_{\substack{n,n' \\ n\neq n'}} \frac{|\langle\psi_{n'\mathbf{k}}|\hat{\mathbf{q}}\cdot\mathbf{v}|\psi_{n\mathbf{k}}\rangle|^2}{(E_{n'\mathbf{k}} - E_{n\mathbf{k}})^2} \frac{f_{n\mathbf{k}} - f_{n'\mathbf{k}}}{\omega - (E_{n'\mathbf{k}} - E_{n\mathbf{k}}) + i\eta} - \frac{\omega_D^2(\hat{\mathbf{q}})}{\omega(\omega + i\gamma)}$$

→

(iii) Reflectivity and colour

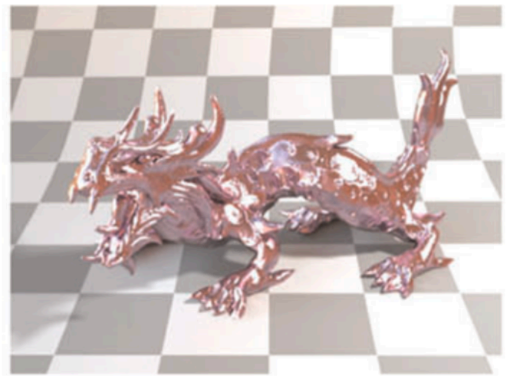


$$\varepsilon(\omega) = [n(\omega) + ik(\omega)]^2$$

$$R(\omega) = \frac{[n(\omega) - 1]^2 + k(\omega)^2}{[n(\omega) + 1]^2 + k(\omega)^2}$$

→

(iv) Photorealistic rendering



Mitsuba
Physically Based Renderer

Prandini, Rignanese, & Marzari, npj Comput. Mater. 129 (2019)

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Evidence of near-ambient superconductivity in a N-doped lutetium hydride

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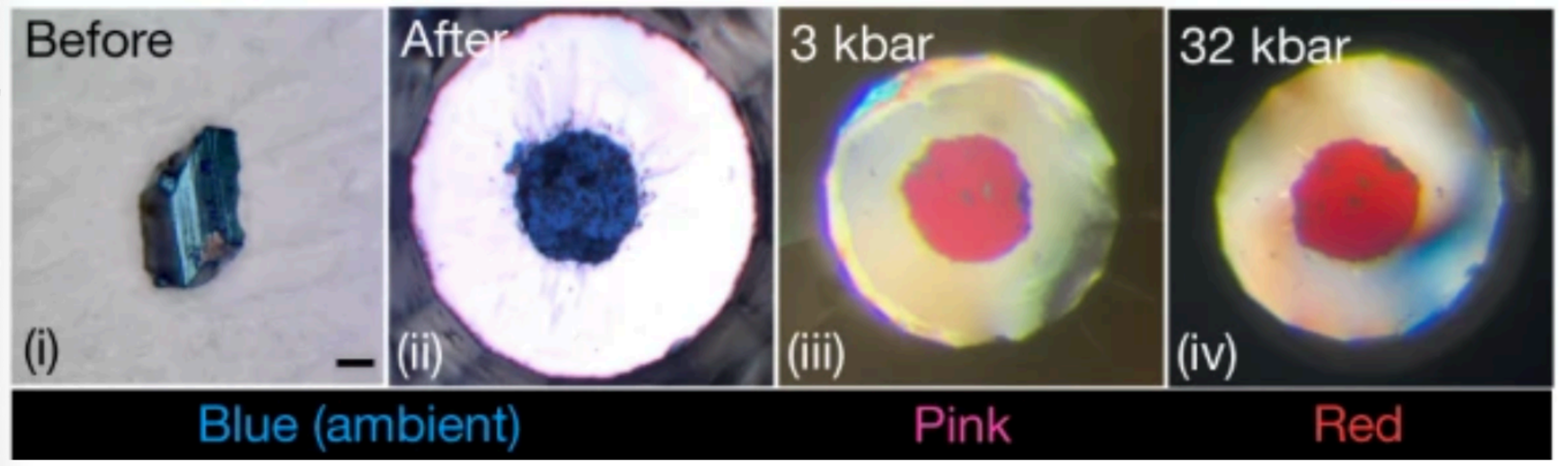

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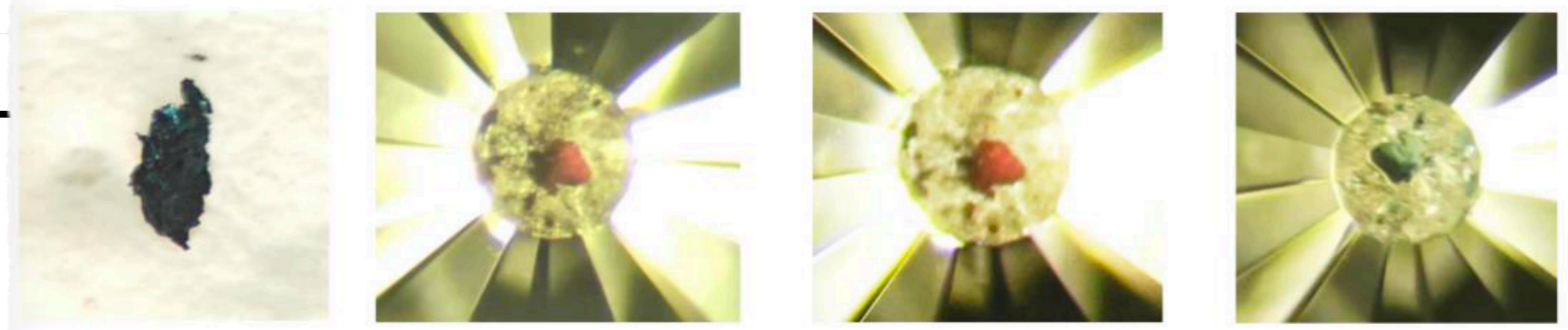
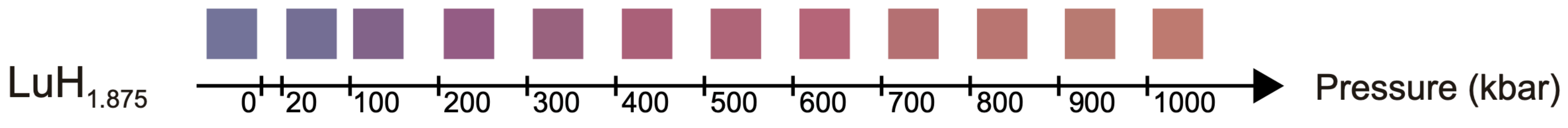
Article | Published: 11 May 2023

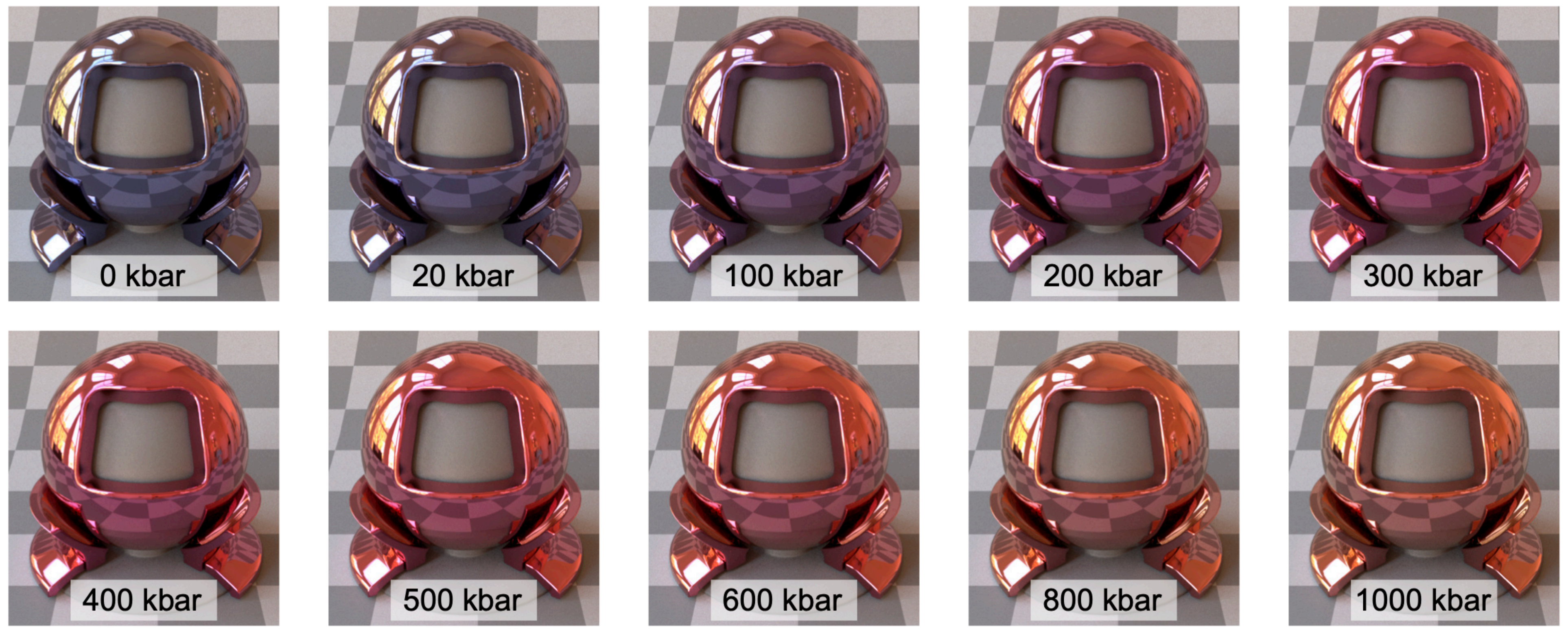
Absence of near-ambient superconductivity in $LuH_{2\pm x}N_y$

Xue Ming, Ying-Jie Zhang, Xiyu Zhu, Qing Li, Chengping He, Yuecong Liu, Tianheng Huang, Gan Liu, Bo Zheng, Huan Yang, Jian Sun, Xiaoxiang Xi & Hai-Hu Wen



As grown Ambient pressure | 2.5 GPa | 5.0 GPa | Released to ambient pressure



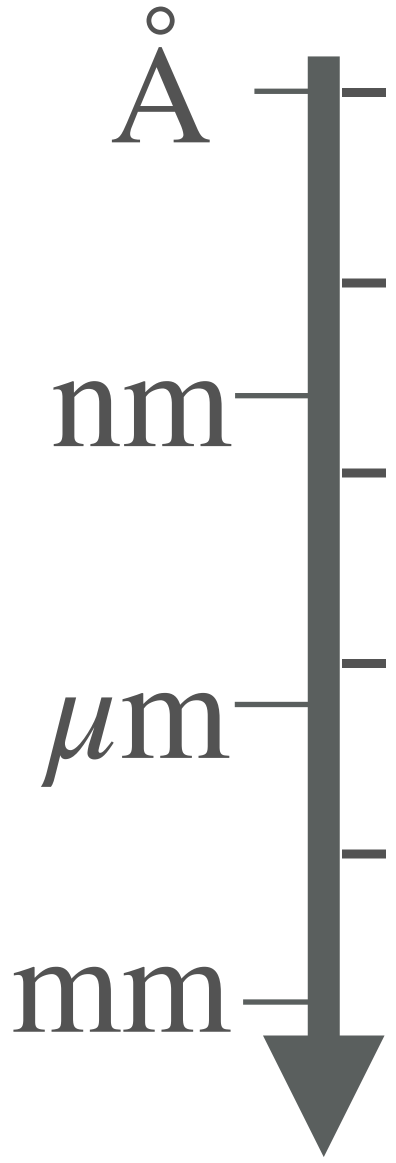


Ab-initio theory predicts color change but no superconductivity

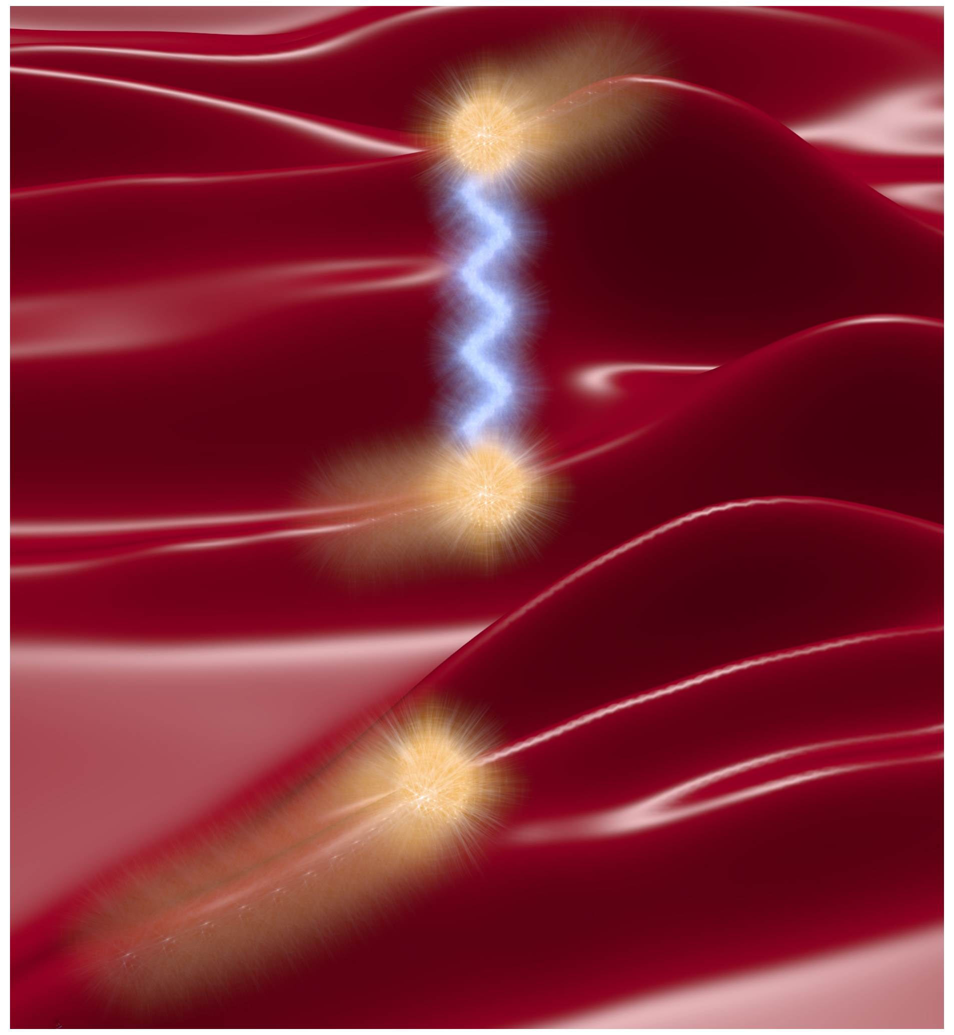
Kim, Conway, Pickard, Pascut, & Monserrat, arXiv:2304.07326

CONCLUSIONS

QUANTUMESPRESSO allows to predict from first principles:



- **Bands** for electrons and phonons, and **broadening** due to interactions;
- **electrical and thermal conductivity** beyond semiclassical theory;
- Ionic diffusion or heat transport in **disordered materials**;
- **Raman spectra**, useful to characterise structural properties;
- parameters for **mesoscopic models** for **devices.**



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