Phonon-limited DC electrical conductivity for metals in Abinit

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Theoretical analysis

From the relaxation time approximation (RTA), the electrical conductivity tensor σ induced by phonon is

$$\sigma = e^2 \sum_n \int \frac{d\vec{k}}{4\pi^3} \tau_n(k) v_{\alpha n}(k) v_{\beta_n}(k) \left(\frac{-\partial f}{\partial \epsilon} \right)_{\epsilon=\epsilon_n(k)} \tag{1.1}$$

where

- $\tau_n(\epsilon)$ is the electron lifetime
- $v_{\alpha_n}(k)$ $v_{\beta n}(k)$ is the velocity tensor
- f is the fermi-dirac occupation

For metals, this is approximated as

$$\sigma = \frac{e^2}{\hbar} \sum_n \int_{S_F} \frac{dS}{4\pi^3} \tau_n[\epsilon_F(k)] v_\alpha(k) v_\beta(k) \tag{1.2}$$

The electron lifetime $\tau(e_F)$ can be calculated using 2 approximations

$$\tau^{-1} = 2 \cdot Im[\Sigma_{nk}^{FM}(\epsilon_{n_k})] \tag{1.3}$$

1. Self Energy Relaxation Time Approximation (SERTA)

$$\begin{aligned} Im[\Sigma_{nk}^{FM}(\epsilon_{n_k})] =& \pi \sum_{m,\nu} \int_{BZ} \frac{dq}{\Omega_{BZ}} |g_{mn\nu}(k,q)|^2 \\ & \times [(n_{q\nu} + f_{m,k+q})\delta(\epsilon_{n,k} - \epsilon_{m,k+q} + \omega_{q\nu})] \\ & \times [(n_{q\nu} + 1 - f_{m,k+q})\delta(\epsilon_{n,k} - \epsilon_{m,k+q} - \omega_{q\nu})] \end{aligned} \tag{1.4}$$

2. Momentum Relaxation Time Approximation (MRTA)

$$\begin{aligned} Im[\Sigma_{nk}^{FM}(\epsilon_{n_k})] =& \pi \sum_{m,\nu} \int_{BZ} \frac{dq}{\Omega_{BZ}} |g_{mn\nu}(k,q)|^2 \left(1 - \frac{v_{nk} \cdot v_{mk+q}}{|v_{nk}|^2}\right) \\ & \times [(n_{q\nu} + f_{m,k+q})\delta(\epsilon_{n,k} - \epsilon_{m,k+q} + \omega_{q\nu})] \\ & \times [(n_{q\nu} + 1 - f_{m,k+q})\delta(\epsilon_{n,k} - \epsilon_{m,k+q} - \omega_{q\nu})] \end{aligned} \tag{1.5}$$

Abinit Implementation

Without Kerange

WFK

DDB
DVDB

1. Conductivity

- **optdriver** : 7 for eph calculations
- **eph_task** : -4 to compute the imaginary part of the Fan-Migdal Self Energy
- **ddb_ngqpt** : The qpt grid in DDB and DVDB file
- **eph_ngqpt_fine** : The interpolated phonon grid
- **tmesh** : Temperature mesh
- **sigma_erange** : The range around the fermi level to calculate the conductivity

With Kerange

WFK

1. Interpolate k-point grid

- **optdriver** : 8 for post-processing of WFK file
- **wfk_task** : "wfk_kpts_erange" to interpolate electron energies onto sigma_ngkpt mesh
- **sigma_erange** : The range around the fermi level to calculate the conductivity
- **einterp** : Electron bands interpolation
- **sigma_ngkpt** : Fine grid to interpolate the WFK

KERANGE.nc

DEN

2. NSCF Band Structure

- **ddb_ngqpt** : The qpt grid in DDB and DVDB file
- **getkerange_filepath** : Path to Kerange.nc file

WFK

DDB
DVDB

3. Conductivity

- **optdriver** : 7 for eph calculations
- **eph_task** : -4 to compute the imaginary part of the Fan-Migdal Self Energy
- **ddb_ngqpt** : The qpt grid in DDB and DVDB file
- **eph_ngqpt_fine** : The interpolated phonon grid
- **tmesh** : Temperature mesh
- **sigma_erange** : The range around the fermi level to calculate the conductivity

Convergence Study

Convergence parameters :

1. ecut
2. ngkpt (coarse)
3. tsmear
4. ngqpt (coarse)
5. ngkpt (nscf)
6. ngqpt (fine)

If using kerange :

7. sigma_ngkpt : Finer k-point grid in the erange interval
8. einterp[1] : Number of star function per kpts

Abipy Implementation

Abipy Step :

1. Create a scf input and a nscf input.
2. Create a |MultiDataset| object.
   a. abipy.abio.factories.conduc_from_inputs()
   b. abipy.abio.factories.conduc_kerange_from_inputs()
3. Create the |ConducWork|.
   a. If DDB and DVDB already exist :
      abipy.ConducWork.from_filepath()
   b. If DDB and DVDB need to be computed :
      abipy.ConducWork.from_phwork()

See : abipy/examples/flows/run_conducwork.py

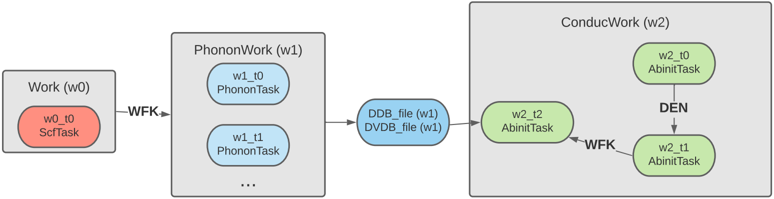
Conductivity Without Kerange

Abipy Function :

conduc_from_inputs(scf_input, nscf_input, tmesh, ddb_ngqpt,
eph_ngqpt_fine, sigma_erange,
boxcutmin=1.1, mixprec=1)

a. from_filepath(ddb_path, dvdb_path, multi, nbr_proc=None,
flow=None, with_kerange=False,
omp_nbr_thread=1, manager=None)

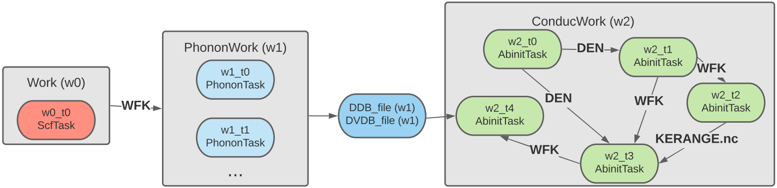
b. from_phwork(phwork, [...])



Conductivity with Kerange

conduc_kerange_from_inputs(scf_input, nscf_input, tmesh,
ddb_ngqpt, eph_ngqpt_fine, **sigma_ngkpt**,
sigma_erange, **einterp=(1, 5, 0, 0)**,
boxcutmin=1.1, mixprec=1)

einterp[0] = 1 for star functions
einterp[1] = Number of stars per kpts
einterp[2-3] = If artificial high frequency oscillations appears [1]



[1] Uehara, Kentaro & Tse, John. (2000). *Calculations of transport properties with the linearized augmented plane-wave method.* Phys. Rev. B.

Conductivity of bulk Cu

Conductivity in $(\mu\Omega cm)^{-1}$

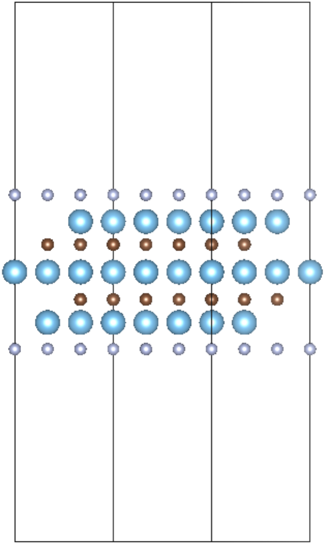
T(K)	Reference[2]	tests/v9/Input/t65.abi[3]	High Convergence
73-77	5.00	1.80	1.80
273	0.64	0.50	0.63
373	0.45	0.37	0.46

Variables	tests/v9/Input/t65.abi	High Convergence
ngqpt	2x2x2	8x8x8
eph_ngqpt_fine	16x16x16	64x64x64
ngkpt	4x4x4	16x16x16
ngkpt(Interpolated)	4x4x4	32x32x32
ngkpt_sigma	16x16x16	64x64x64
sigma_erange	[-0.2, -0.2, 'eV']	[-0.3, -0.3, 'eV']
einterp	[1, 5, 0, 0]	[1, 5, 0, 0]

[2] Ashcroft, N. W. & Mermin, N. D. (1976), Solid State Physics

[3] With tmesh changed to [73,100,4]

Structure of 2D $Ti_3C_2F_2$



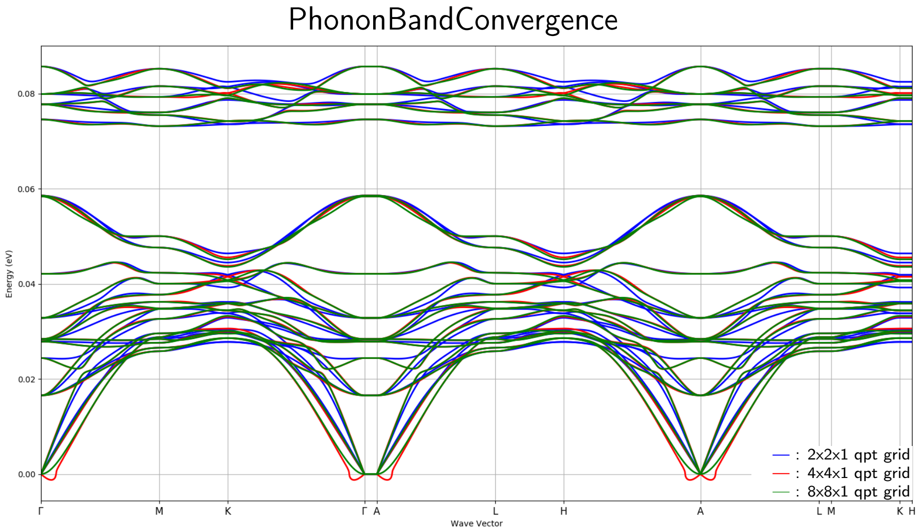
Atoms

- Titanium
- Carbone
- Fluorine

Converged parameters

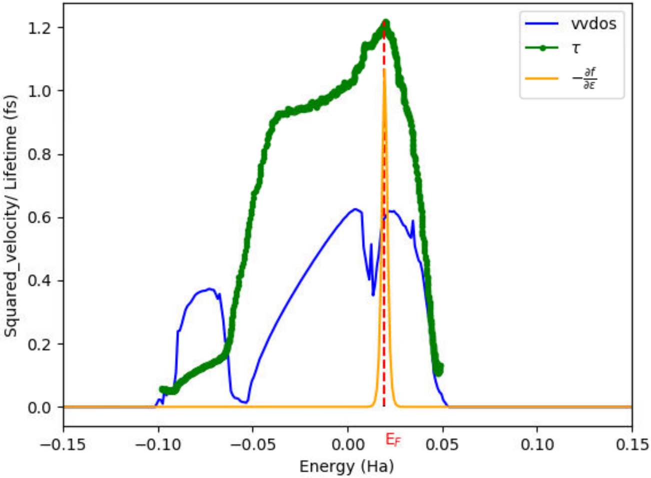
Ecut : 35 Ha
tsmear : 0.005 Ha
ngkpt(coarse) : 16x16x1
ngkpt(interpolated) : 16x16x1
ngqpt(coarse) : 8x8x1
sigma_erange : [-0.09, -0.09, eV]

Convergence study 2D $Ti_3C_2F_2$



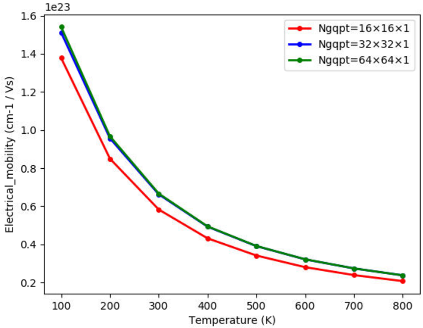
Components of the conductivity

ngqpt(fine) : 32x32x1 ngkpt(nscf) : 64x64x1 Temp : 300K



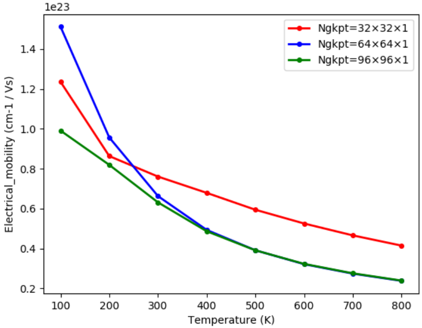
Ngqpt Grid convergence

ngkpt(nscf) = 64x64x1



Ngkpt Grid convergence

ngqpt_fine = 32x32x1



Conclusion

Summary :

- At room temperature, we can get good agreements with experimental result considering only phonon-limited conductivity
- To do so, we need to use a really fine kpt and qpt grid
- The kpt grid can be interpolated only around the fermi level
- These calculations can be automatized using |ConducWork| from Abipy

Possible improvements :

- Solve the BTE equation iteratively

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