Electron-Phonon Physics using EPW

Sabyasachi Tiwari

Oden Institute for computational Engineering and Science
UT Austin

60 ICTP
1964–2024

SLAFES
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Outline

- Basic electron-phonon-physics
- EPW
- Practical calculations using EPW/EPWpy
- Conclusion

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- EPW

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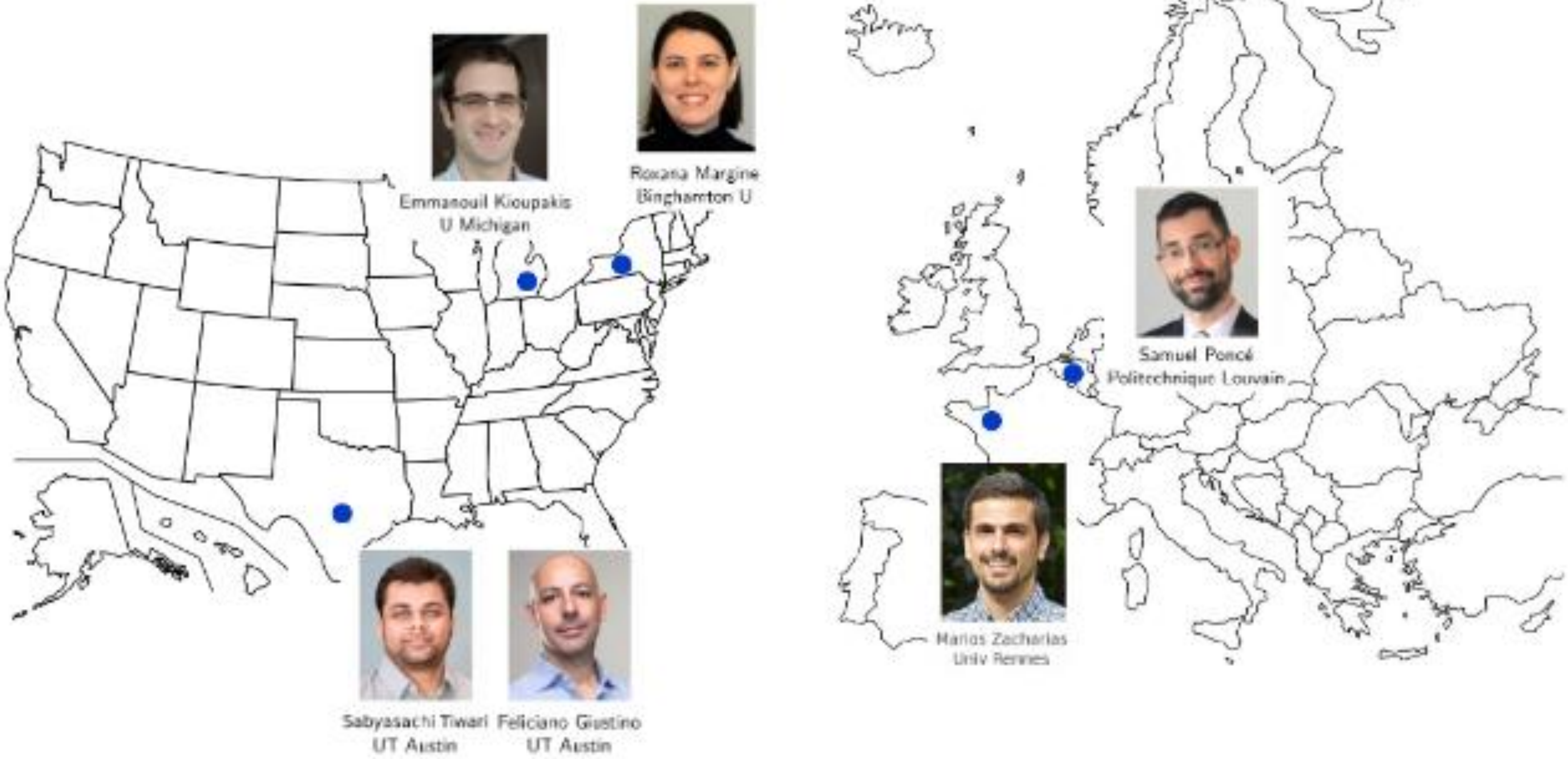
- Conclusion

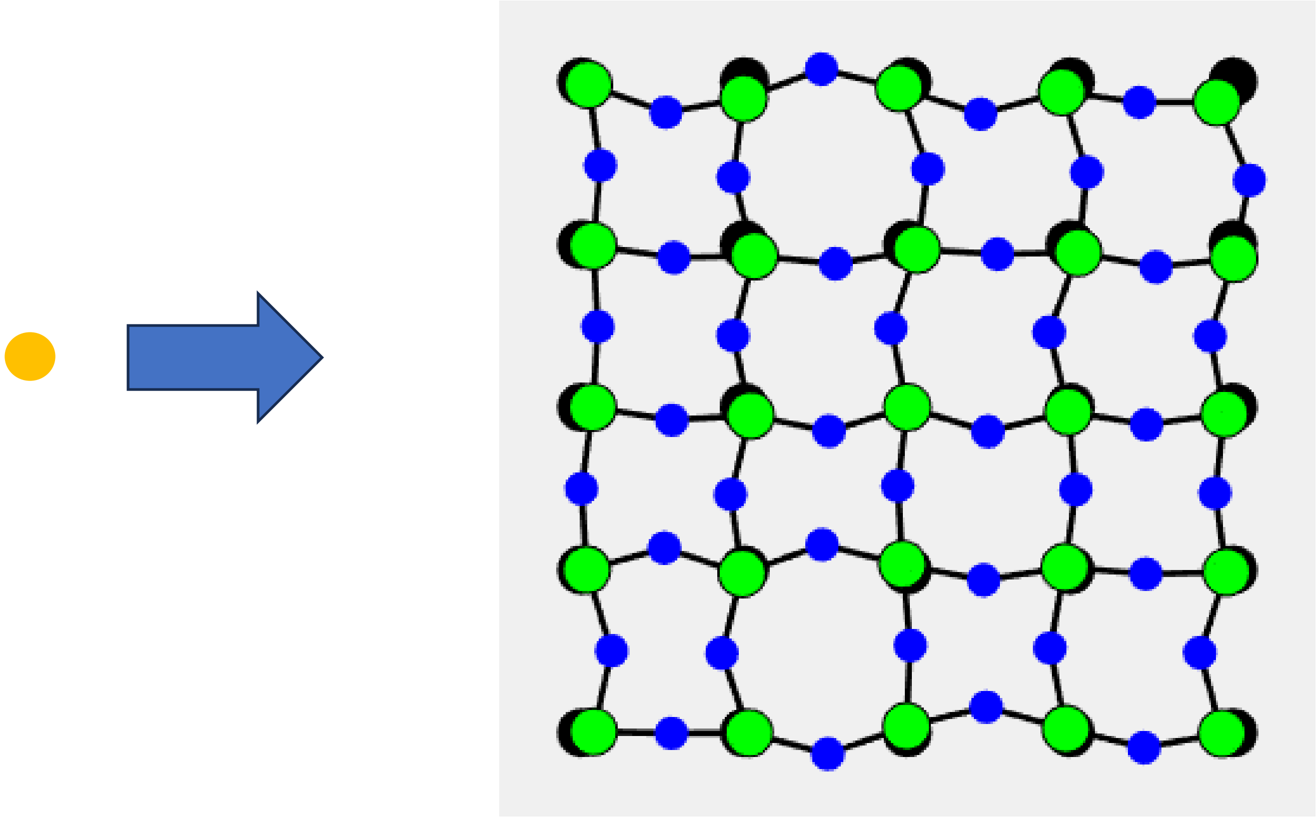
EPW collaboration



Developers

Kyle Bushick
Viet-Anh Ha
Samad Hajinazar
Jon Lafuente-Bartolomé
Hyungjun Lee
Johsua Leveillee
Chao Lian
Jae-Mo Lihm
Francesco Macheda
Hitoshi Mori
Hari Paudyal
Weng-Hong Sio
Aidan Thorn
Amanda Wang
Xiao Zhang

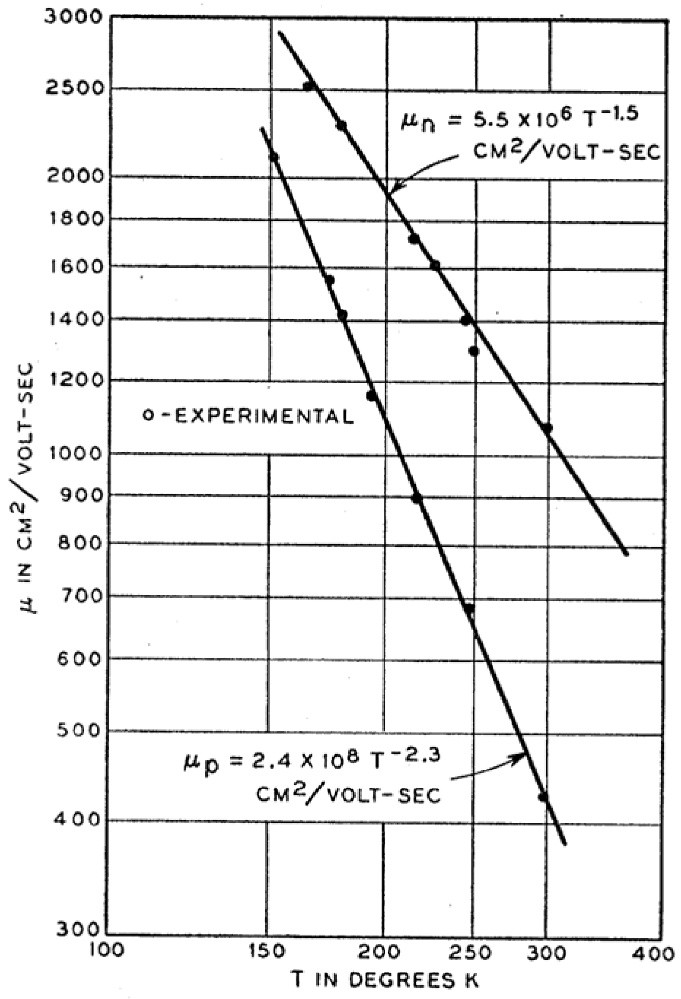
Why Electron-Phonon Physics?



Wendt et.al., Sci. Adv. 10, 1126 (2019)

- Lattice vibrations : Phonons
- Electrons/excited particles
  - Interact with lattice
  - E-P coupling

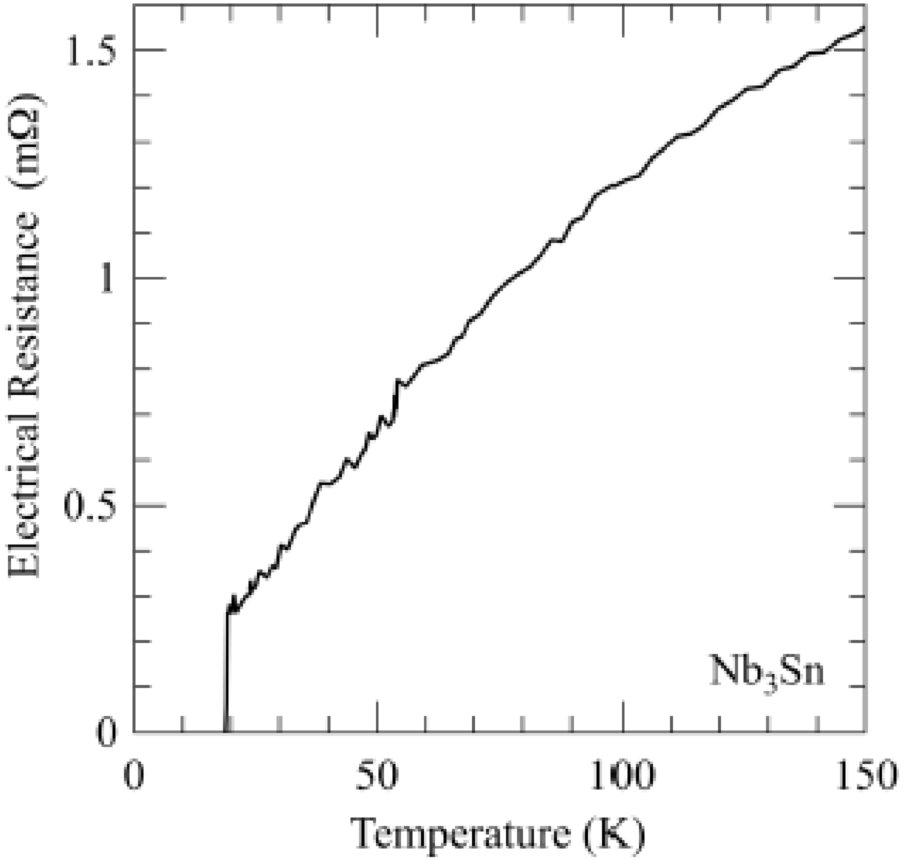
Why Electron-Phonon Physics?



Prince et.al., Phys. Rev. B. 93.1204 (1954)

- Transport

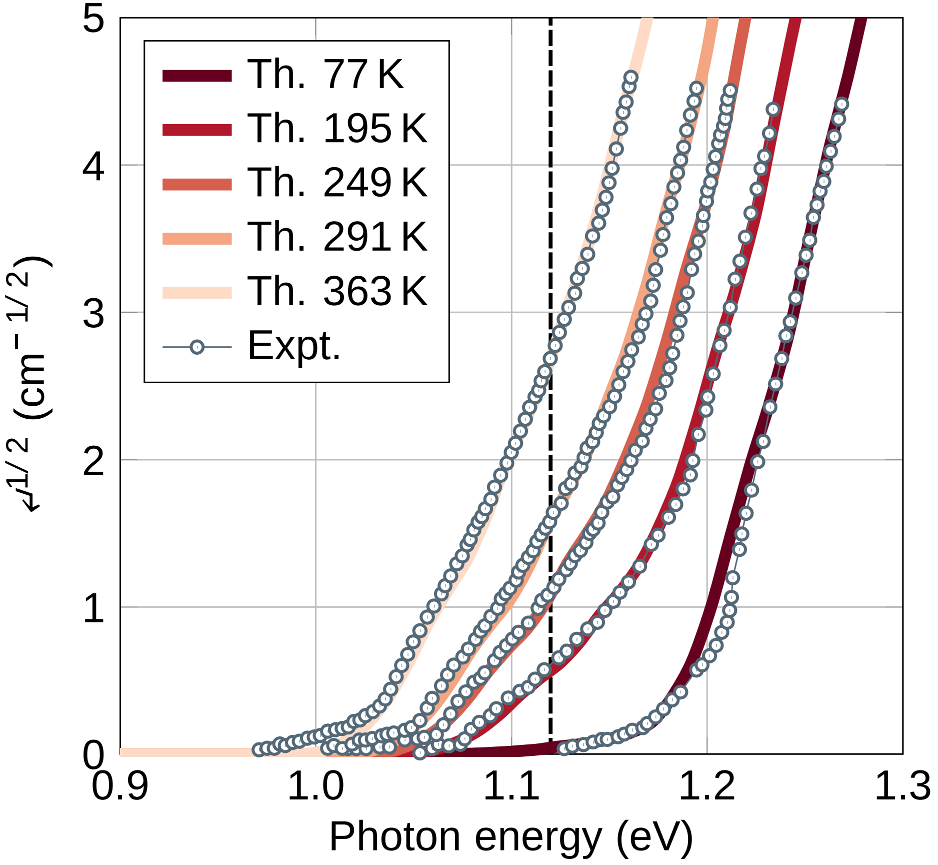
Why Electron-Phonon Physics (T ≈ 0 K)?



Gabovich et.al., Supercond. (2014)

- Superconductivity

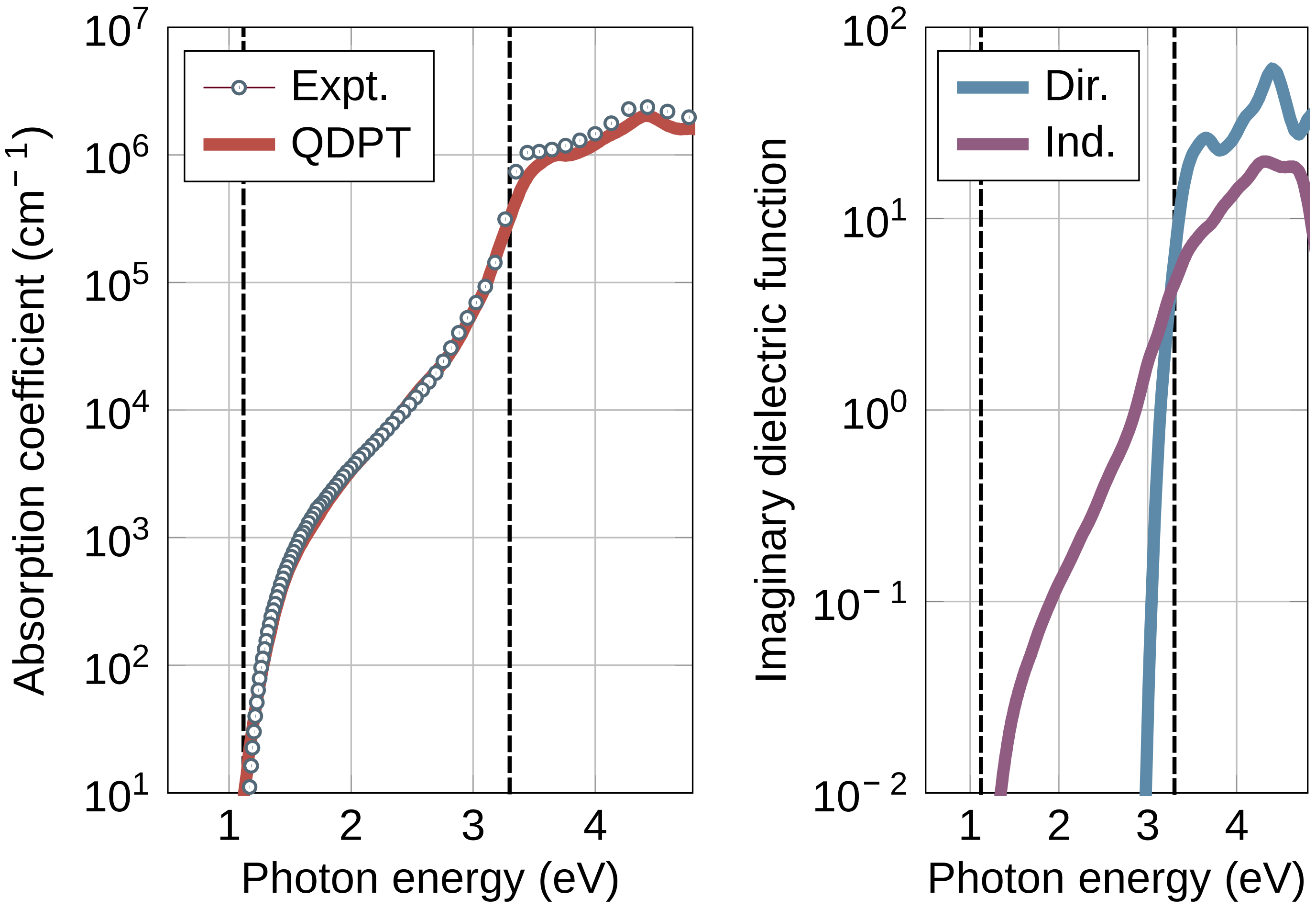
Why Electron-Phonon Physics (Light-Matter interaction)?



- Band-gap renormalization

Tiwari et.al., Phys. Rev. B. 109. 195137 (1954)

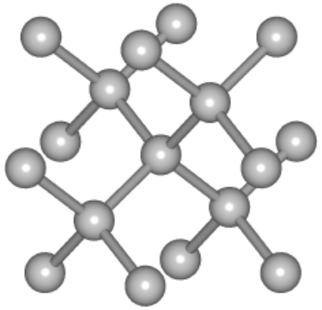
Why Electron-Phonon Physics (Light-Matter interaction)?



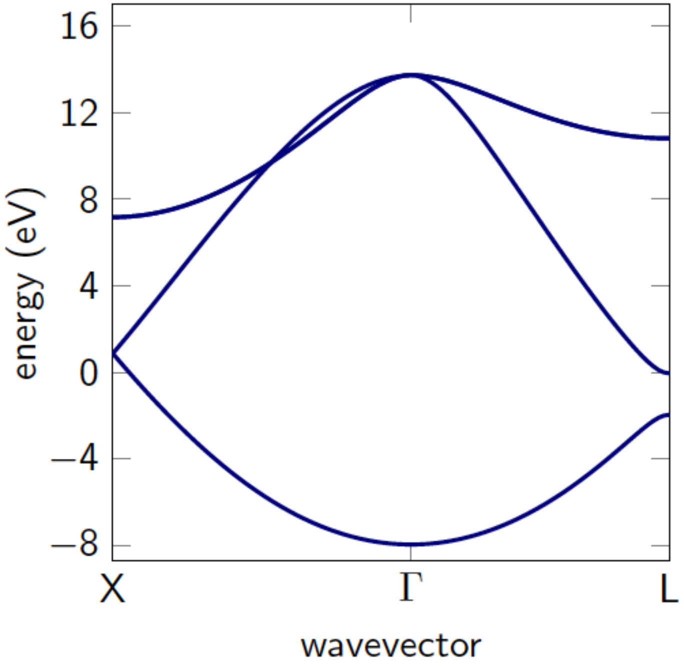
- Visible range: phonons

Tiwari et.al., Phys. Rev. B. 109. 195137 (1954)

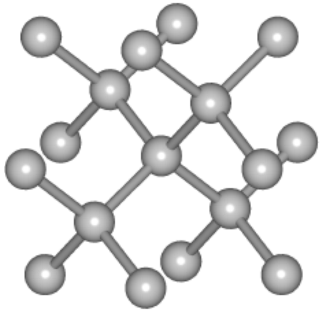
Where do phonons come from?



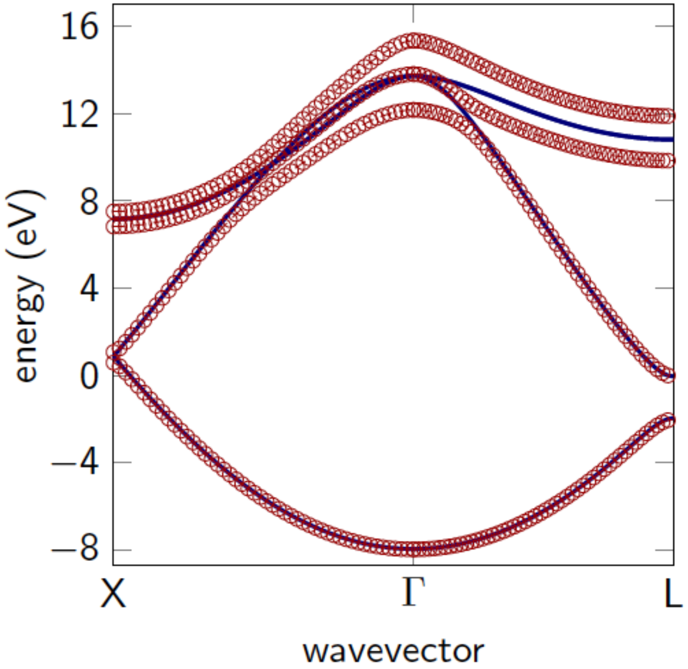
diamond

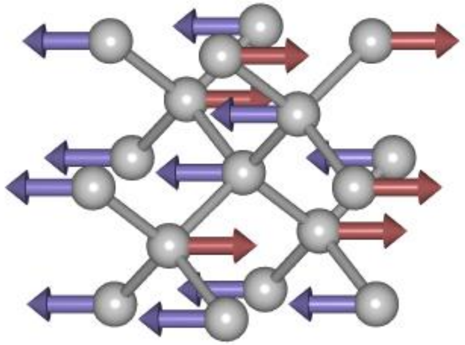


Where do phonons come from?



diamond





Move atoms along a mode

- Change in band structure

Where do phonons come from?

$$-\frac{\hbar^2}{2m}\nabla^2\psi_n + V_{\mathrm{SCF}}\psi_n = \epsilon_n\psi_n$$

$$n(r) = \sum_{n\in\mathrm{occ}} |\psi_n|^2$$

$$V_{\mathrm{SCF}}(r) = -\frac{e^2}{4\pi\epsilon_0}\left[\sum_{\kappa}\frac{Z_k}{r-\tau_\kappa} + \int\frac{n(r')dr'}{r-r'}\right] + V_{\mathrm{XC}}[n(r)]$$

- V_{SCF}: Depends on atomic positions (τ_κ)

Where do phonons come from?

$$V_{\mathrm{SCF}} = V_{\mathrm{SCF}}(r; \tau_{\kappa_1}, \tau_{\kappa_2}, \tau_{\kappa_3} .. \tau_{\kappa_N})$$

Displace atoms from equilibrium position: $\tau = \tau_0 + \Delta\tau$

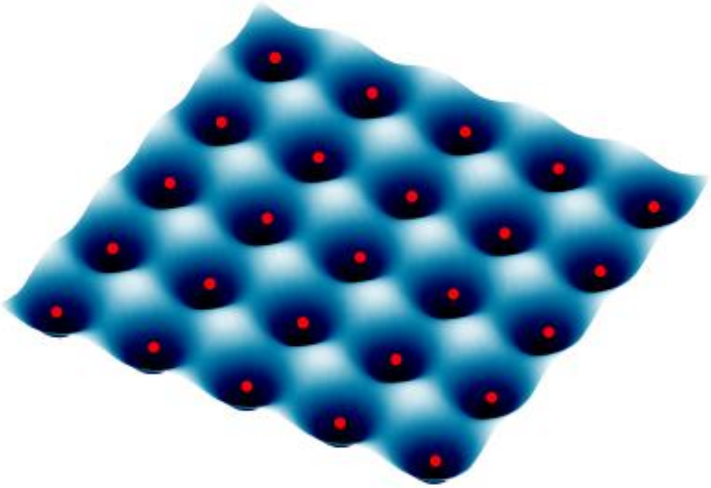
$$V_{\mathrm{SCF}}(\tau_0 + \Delta\tau) = V_{\mathrm{SCF}}(\tau_0) + \frac{\partial V_{\mathrm{SCF}}}{\partial \tau}\Delta\tau + \frac{1}{2}\frac{\partial^2 V_{\mathrm{SCF}}}{\partial \tau^2}\Delta\tau^2 + \ldots\ldots..$$

- Perturbation to atomic positions
  - Temperature

Baroni et.al., Rev. Mod. Phys. 73, 515 (2001)

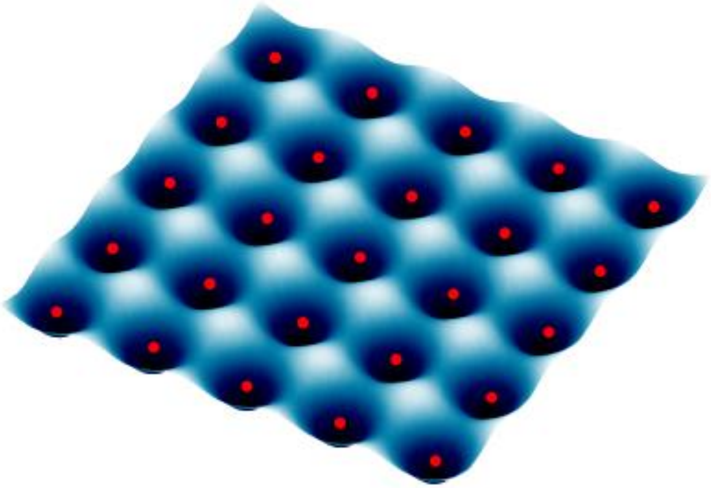
Where do phonons come from?

$V_{\mathrm{SCF}}(r;\tau)$

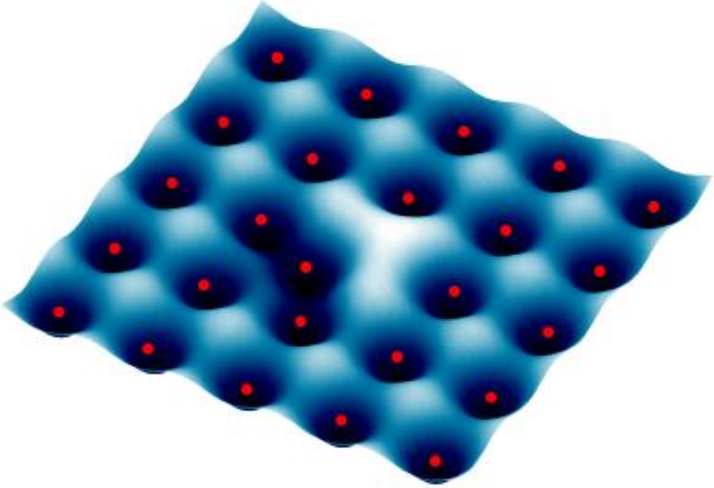


Where do phonons come from?

$V_{\mathrm{SCF}}(r;\tau)$

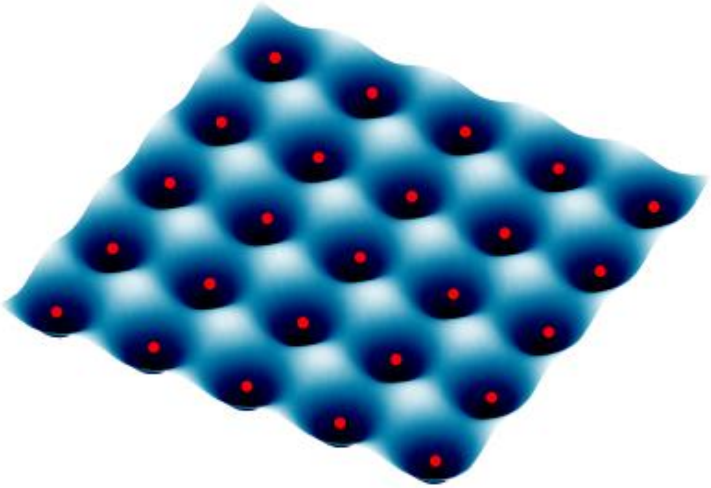


$V_{\mathrm{SCF}}(r;\tau+\Delta\tau)$

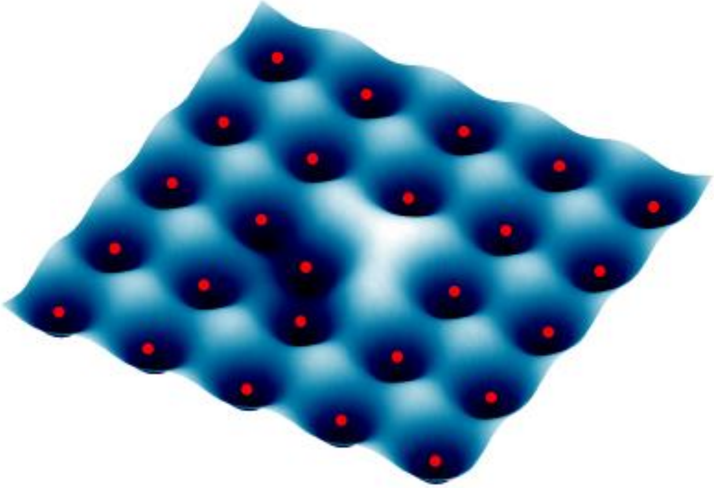


Where do phonons come from?

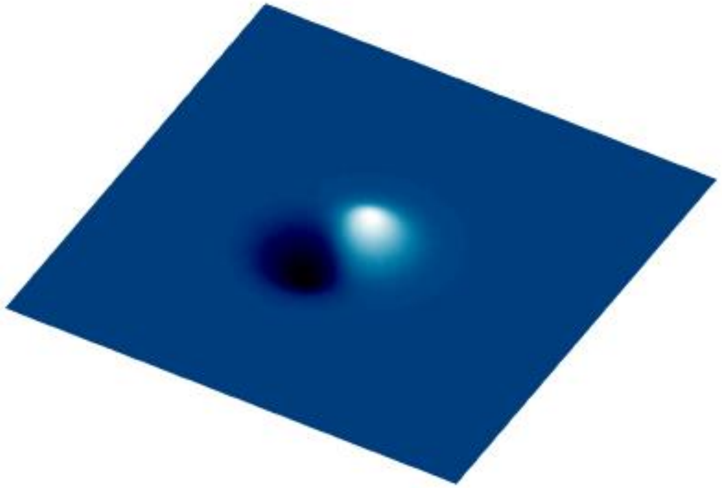
$V_{\mathrm{SCF}}(r;\tau)$



$V_{\mathrm{SCF}}(r;\tau+\Delta\tau)$



$V_{\mathrm{SCF}}(r;\tau)-V_{\mathrm{SCF}}(r;\tau+\Delta\tau)$



Perturbing potential

Use of potential

Energy $$\Delta E = \left\langle \psi_n \left| \frac{\partial V_{\mathrm{SCF}}}{\partial \tau} \Delta\tau \right| \psi_n \right\rangle$$ Band renormalization

Wavefunction $$\Delta\psi = \sum_{m\neq n} \frac{\left\langle \psi_m \left| \frac{\partial V_{\mathrm{SCF}}}{\partial \tau} \Delta\tau \right| \psi_n \right\rangle}{E_m - E_n} \psi_m$$ Optical transitions

Transition Rate $$\Gamma_{n\to m} = \frac{2\pi}{\hbar} \left| \left\langle \psi_m \left| \frac{\partial V_{\mathrm{SCF}}}{\partial \tau} \Delta\tau \right| \psi_n \right\rangle \right|^2 \delta(E_m - E_n)$$ Transport

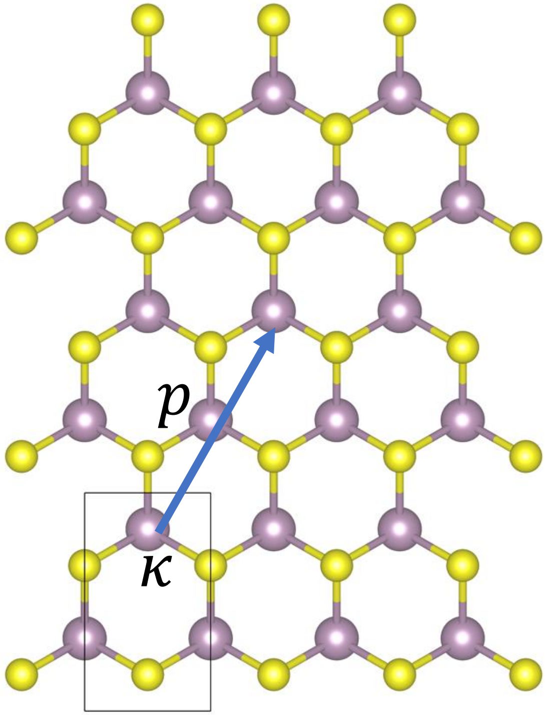
- Calculation of perturbation potential is key to calculating many properties

Supercell to unit-cell

$$\left\langle \psi_m \left| \frac{\partial V_{\mathrm{SCF}}}{\partial \tau_{\kappa \alpha p}} \right| \psi_n \right\rangle \to \langle u_{m\mathbf{k}+\mathbf{q}} | \Delta_{\mathbf{q}\nu} v_{\mathrm{SCF}} | u_{n\mathbf{k}} \rangle_{\mathrm{uc}} = g_{mn}^{\nu}(\mathbf{k}, \mathbf{q})$$

Supercell

Unit-cell



- Go from supercell to unit-cell
  - Cheaper calculations

Giustino et.al., Rev. Mod. Phys. 89, 015013 (2017)

Interaction Hamiltonian

$$\left\langle \psi_m \left| \frac{\partial V_{\mathrm{SCF}}}{\partial \tau_{\kappa\alpha p}} \right| \psi_n \right\rangle \rightarrow \langle u_{m\mathbf{k}+\mathbf{q}} | \Delta_{\mathbf{q}\nu} v_{\mathrm{SCF}} | u_{n\mathbf{k}} \rangle = g_{mn}^{\nu}(\mathbf{k},\mathbf{q})$$

$$\sum\nolimits_{\kappa\alpha p} \frac{\partial V_{\mathrm{SCF}}}{\partial \tau_{\kappa\alpha p}} \Delta\tau_{\kappa\alpha p} \rightarrow \sum\nolimits_{\mathbf{q}\nu} \Delta_{\mathbf{q}\nu} V_{\mathrm{SCF}} \left(\hat{a}_{\mathbf{q}\nu} + \hat{a}^{+}_{-\mathbf{q}\nu}\right)$$

$$\Delta_{\mathbf{q}\nu} V_{\mathrm{SCF}} = \exp(i\mathbf{q}.r)\Delta_{\mathbf{q}\nu} v_{\mathrm{SCF}}$$

Phonon polarization

$$\Delta_{\mathbf{q}\nu} v_{\mathrm{SCF}} = \sum\nolimits_{\kappa\alpha p} \exp\left(-i\mathbf{q}.\left(r - R_p\right)\right) \sqrt{\frac{\hbar}{2M_\kappa \omega_{\mathbf{q}\nu}}}\, e_{\kappa\alpha,\nu}(\mathbf{q}) \frac{\partial V_{\mathrm{SCF}}(r)}{\partial \tau_{\kappa\alpha p}}$$

$$\hat{V}_{\mathrm{ep}} = \frac{1}{N_p} \sum\nolimits_{mnkq}^{\nu} g_{mn}^{\nu}(\mathbf{k},\mathbf{q}) c^{+}_{m\mathbf{k}+\mathbf{q}} c_{n\mathbf{k}} (\hat{a}_{\mathbf{q}\nu} + \hat{a}^{+}_{-\mathbf{q}\nu})$$

- Electron-phonon Hamiltonian in second quantization
  - Giustino et.al., Rev. Mod. Phys. 89, 015013 (2017)

Electron-Phonon matrix element

$$g_{mn}^{\nu}(\mathbf{k},\mathbf{q}) = \langle u_{m\mathbf{k}+\mathbf{q}} | \Delta_{\mathbf{q}\nu} v_{\mathrm{SCF}} | u_{n\mathbf{k}} \rangle$$

- Dense **k, q** grids needed for calculating observables
- Wavefunctions: NSCF calculations (DFT)
  - Cheap for unit-cells
- Displacements/derivatives V_{SCF}: Linear response/DFPT
  - Expensive
  - Dense grids not possible

Electron-Phonon matrix element

$$g_{mn}^{\nu}(\mathbf{k},\mathbf{q}) = \langle u_{m\mathbf{k}+\mathbf{q}} | \Delta_{\mathbf{q}\nu} v_{\mathrm{SCF}} | u_{n\mathbf{k}} \rangle$$

- Can we do some kind of interpolation?
- Interpolate the potential:
  - Heavy on memory since we need dense grid wavefunctions
- Interpolate the wavefunctions

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- Basic electron-phonon-physics
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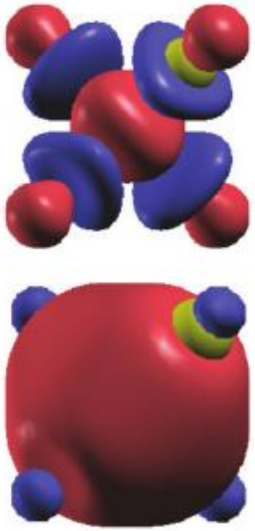
Wannier functions

$$w_m(r;\mathrm{R}_p) = \frac{1}{N_p}\sum_{nk} \exp(i\mathbf{k}.\mathrm{R}_p)U_{nm}^{\mathbf{k}}\,|\psi_{n\mathbf{k}}\rangle$$

$$|\psi_{n\mathbf{k}}\rangle = \sum_{m\mathrm{R}_p} \exp(-i\mathbf{k}.\mathrm{R}_p)U_{mn}^{\mathbf{k}*}\,w_m(r;\mathrm{R}_p)$$



- Wavefunctions can be localized using Wannier representation
- Interpolated to arbitrary wavevectors using Fourier transform
  - $U_{mn}^{\mathbf{k}}$: Obtained by diagonalizing Wannier Hamiltonian

Marzari et.al., Rev. Mod. Phys. 84, 1419 (2012)

Wannier functions

$$O_{mn} = \sum_{G,G'} \langle \psi_m(G) \big| \hat{O} \big| \psi_n(G') \rangle$$

$$O_{mn} = \sum_{R_p,R_{p'}} \langle w_m\left(r; R_p\right) \big| \hat{O} \big| w_n\left(r; R_{p'}\right) \rangle$$

- Notice the summation is over Wigner-Seitz vectors in case of Wannier
    - Much smaller than plane waves since Wannier functions are localized

Marzari et.al., Rev. Mod. Phys. 84, 1419 (2012)

Wannier interpolation

$$g_{mn}^{\nu}(\mathbf{k},\mathbf{q}) = \left\langle u_{m\mathbf{k}+\mathbf{q}} \middle| \Delta_{\mathbf{q}\nu} v_{\mathrm{SCF}} \middle| u_{n\mathbf{k}} \right\rangle$$

$$w_m(r;\mathrm{R}_p) = \frac{1}{N_p}\sum_{nk} \exp(i\mathbf{k}.\,\mathrm{R}_p)U_{nm}^{\mathbf{k}}\,|\psi_{n\mathbf{k}}\rangle$$

$$|\psi_{n\mathbf{k}}\rangle = \textstyle\sum_{m\mathrm{R}_p} \exp(-i\mathbf{k}.\,\mathrm{R}_p)U_{mn}^{\mathbf{k}*}\,w_m(r;\mathrm{R}_p)$$

Giustino et.al., Phys. Rev. B. 76, 165108 (2007)

Wannier interpolation

$$g^{\nu}_{mn}(\mathbf{k},\mathbf{q}) = \langle u_{m\mathbf{k}+\mathbf{q}} | \Delta_{\mathbf{q}\nu} v_{\mathrm{SCF}} | u_{n\mathbf{k}} \rangle$$

$$w_m(r;\mathrm{R}_p) = \frac{1}{N_p}\sum_{nk} \exp(i\mathbf{k}.\,\mathrm{R}_p) U^{\mathbf{k}}_{nm} \, |\psi_{n\mathbf{k}}\rangle$$

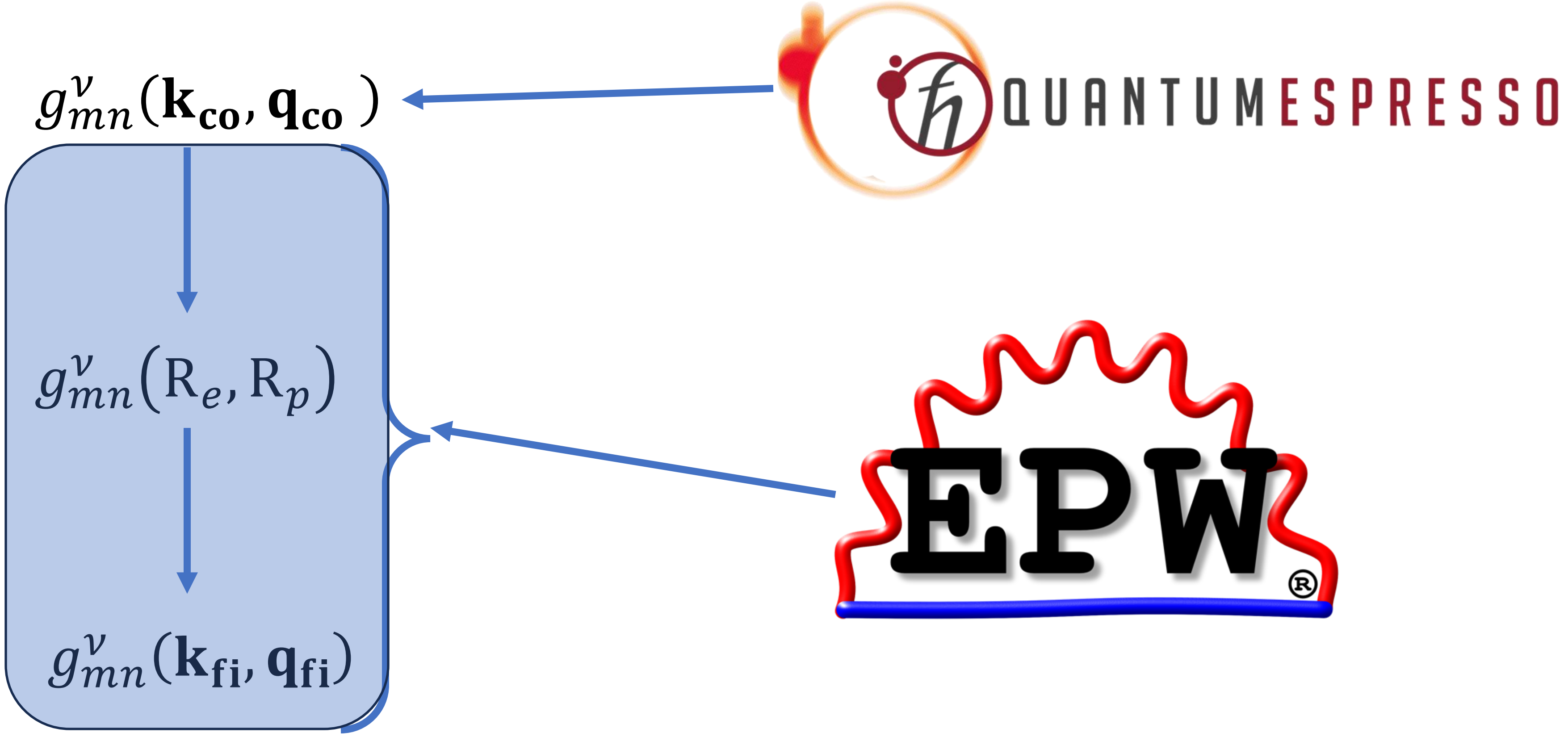
$$|\psi_{n\mathbf{k}}\rangle = \sum\nolimits_{m\mathrm{R}_p} \exp(-i\mathbf{k}.\,\mathrm{R}_p) U^{\mathbf{k}*}_{mn} \, w_m(r;\mathrm{R}_p)$$

$$g^{\nu}_{mn}(\mathbf{k}_{\mathbf{co}},\mathbf{q}_{\mathbf{co}}) \rightarrow g^{\nu}_{mn}(\mathrm{R}_e,\mathrm{R}_p) \rightarrow g^{\nu}_{mn}(\mathbf{k}_{\mathbf{fi}},\mathbf{q}_{\mathbf{fi}})$$

- A method for reliably interpolating g

Giustino et.al., Phys. Rev. B. 76, 165108 (2007)

Electron-Phonon-Wannier method (EPW)



$g_{mn}^{\nu}(\mathbf{k}_{\mathbf{co}}, \mathbf{q}_{\mathbf{co}})$

$g_{mn}^{\nu}(\mathrm{R}_e, \mathrm{R}_p)$

$g_{mn}^{\nu}(\mathbf{k}_{\mathbf{fi}}, \mathbf{q}_{\mathbf{fi}})$

- QE: $\Delta_{\mathbf{q}\nu} V_{\mathrm{SCF}}; \Delta\tau$
- EPW: Wannierization and interpolation

Ponce et.al., Comput. Phys. Comm, 209, 116-133 (2016)
Lee, … Tiwari et.al., npj comput. mater., 9, 156 (2023)

Notes about e-p matrix elements

- $g_{mn}^{\nu}(\mathbf{k},\mathbf{q}) = \langle u_{m\mathbf{k}+\mathbf{q}} | \Delta_{\mathbf{q}\nu} v_{\mathrm{SCF}} | u_{n\mathbf{k}} \rangle$
- Complex quantity and has a gauge dependence and requires a series of consistent calculations
- Since, the Wannier functions depend on the gauge of starting Wavefunctions: $|u_{n\mathbf{k}}\rangle$; the gauge consistency should be maintained all across the calculations
- g can only be used for calculations with the same initial SCF calculation

EPW

- Electron-Phonon Wannier code
  - A sub-package within the Quantum Espresso DFT package
  - Interpolates e-p matrix elements obtained from DFPT (QE)
  - Allows calculations on very fine **k** and **q** grids
    - Transport (IBTE)
    - Superconductivity
    - Polarons
    - Temperature dependent Bandgap
    - Optical absorption

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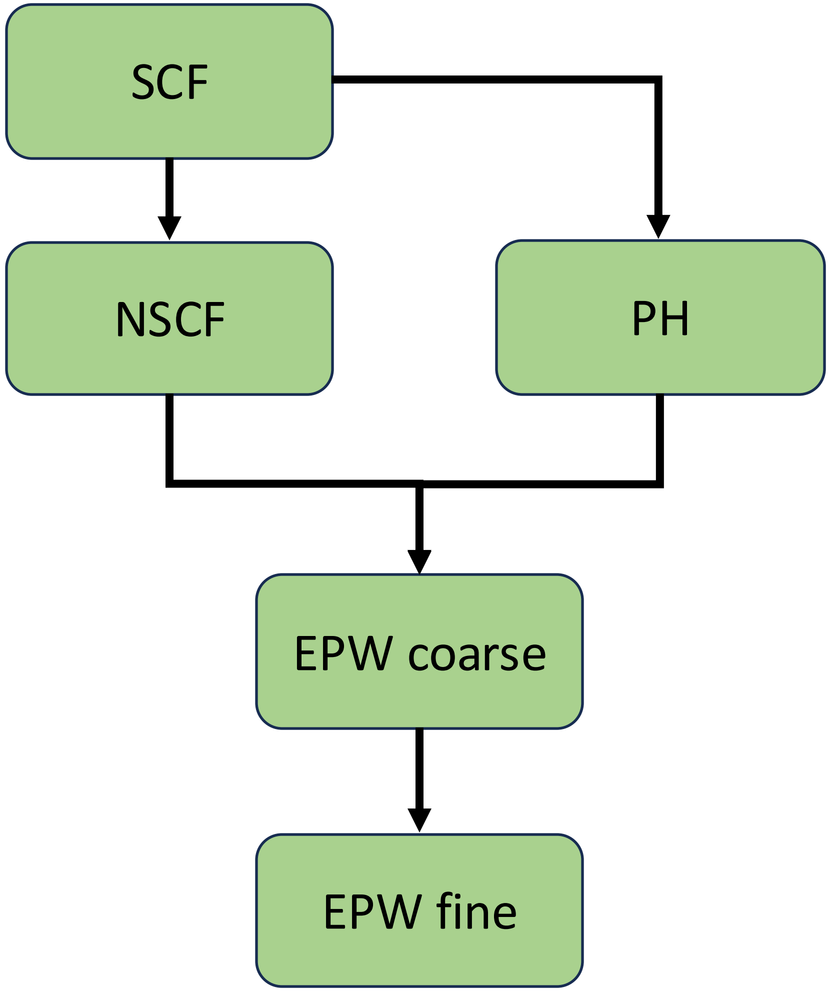
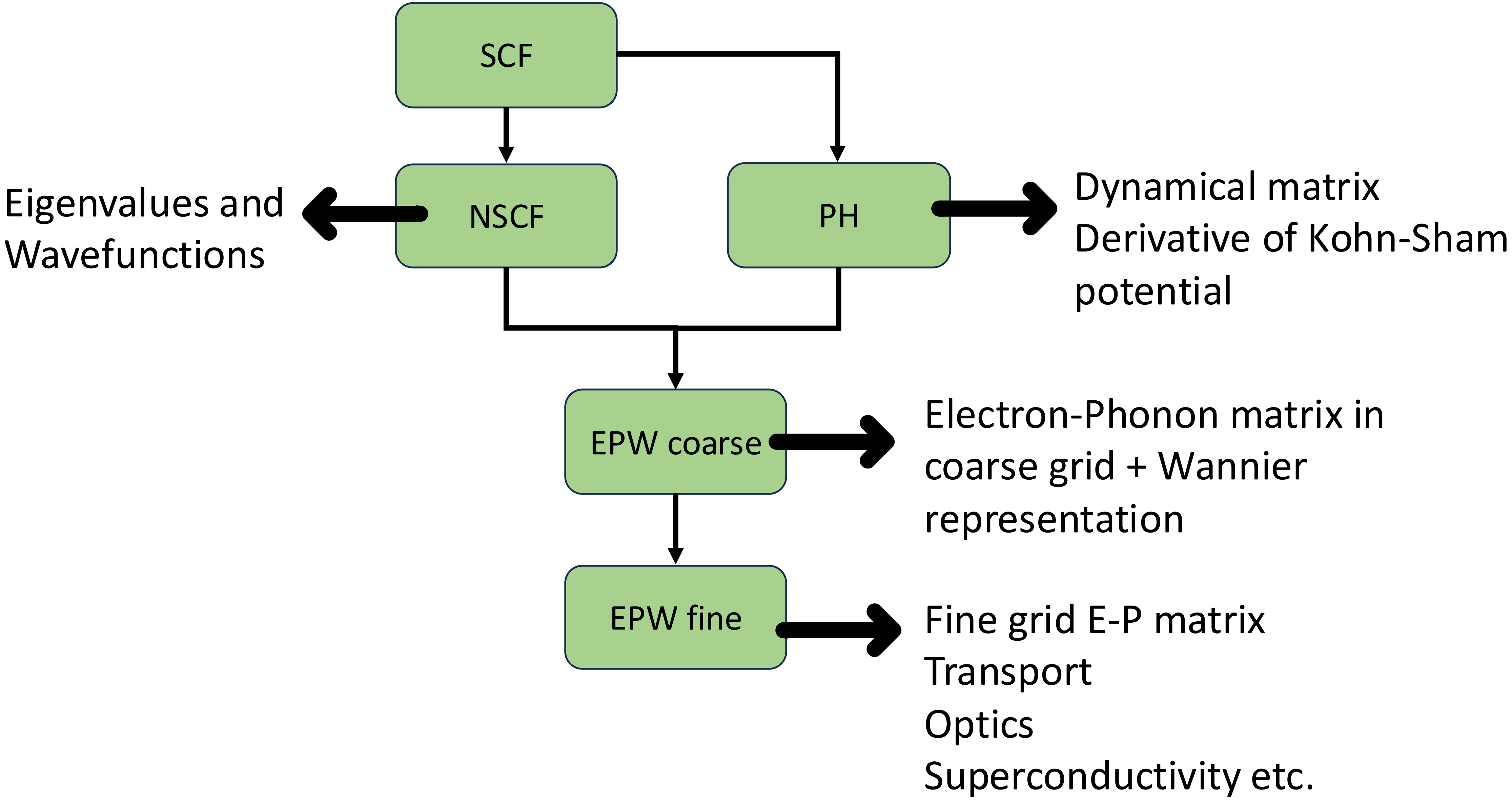
A typical workflow for EPW



A typical workflow for EPW



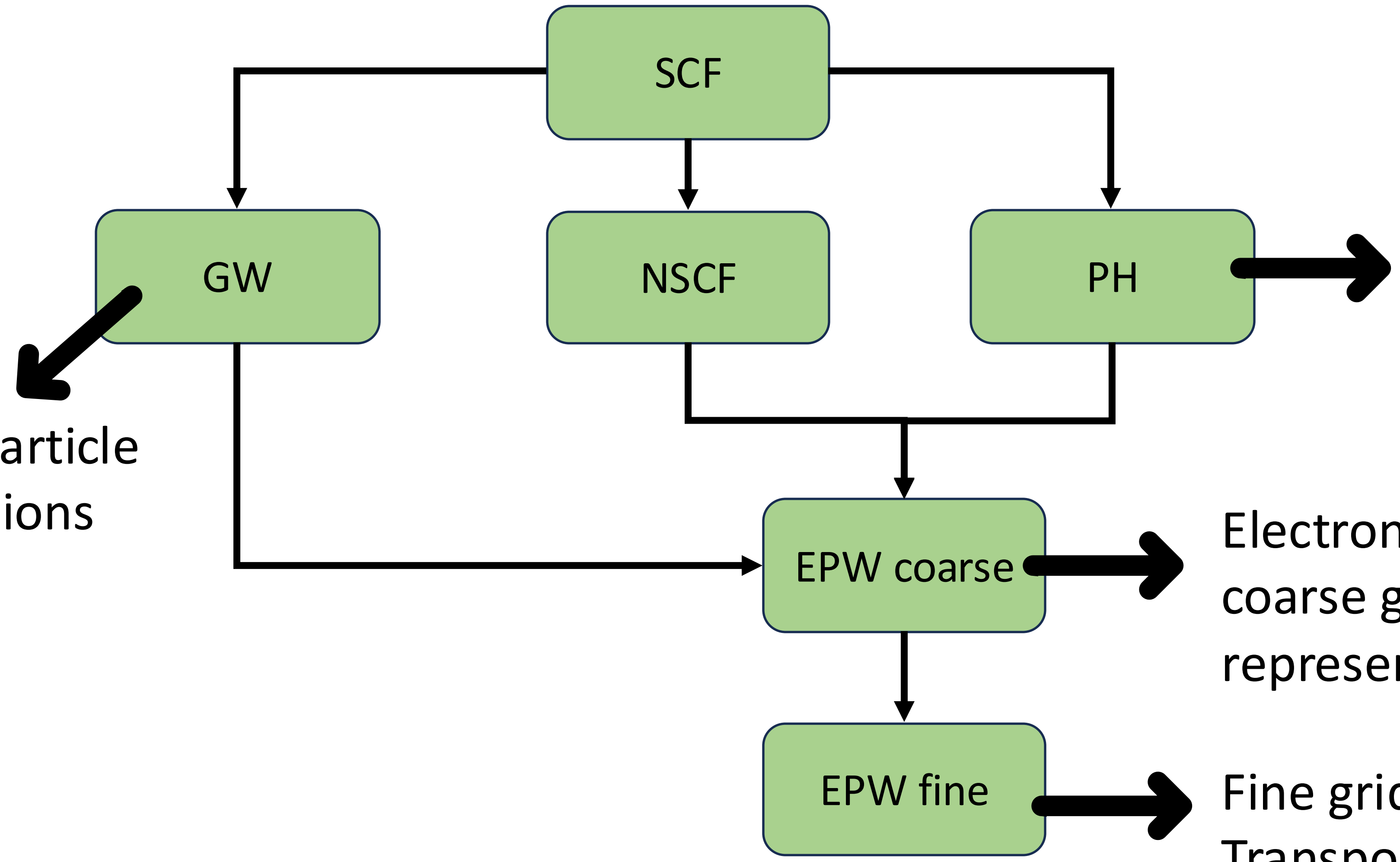
Eigenvalues and Wavefunctions

Dynamical matrix
Derivative of Kohn-Sham potential

Electron-Phonon matrix in coarse grid + Wannier representation

Fine grid E-P matrix
Transport
Optics
Superconductivity etc.

A typical workflow for EPW



Quasiparticle corrections

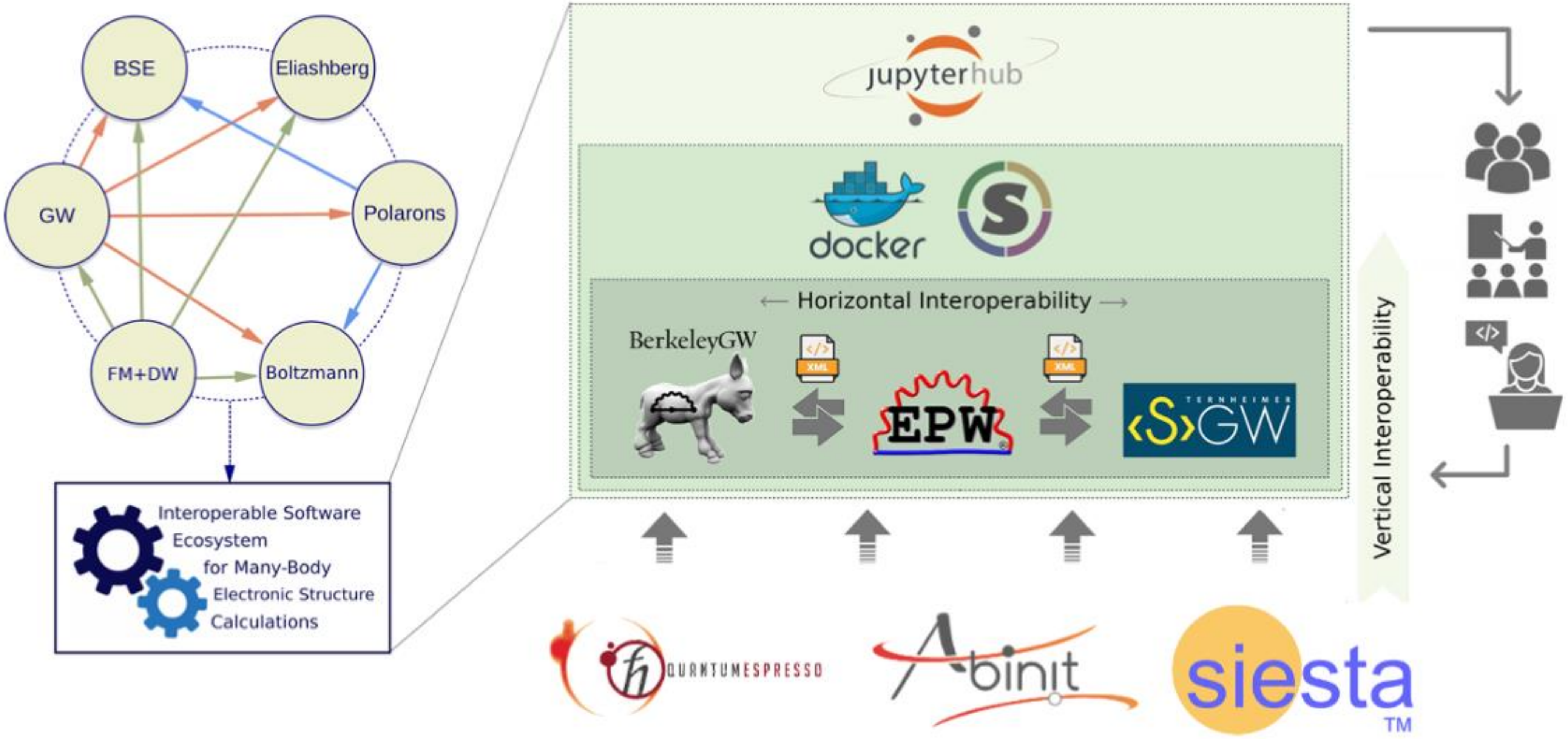
Dynamical matrix
Derivative of Kohn-Sham potential

Electron-Phonon matrix in coarse grid + Wannier representation

Fine grid Ep matrix
Transport
Optics
Superconductivity etc.

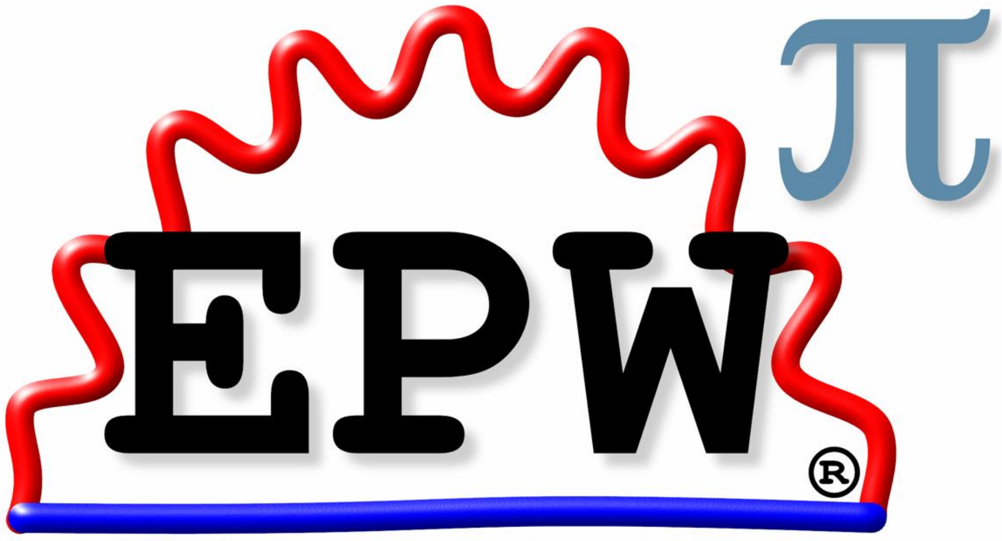
EPWpy

Enabling interoperable software environment

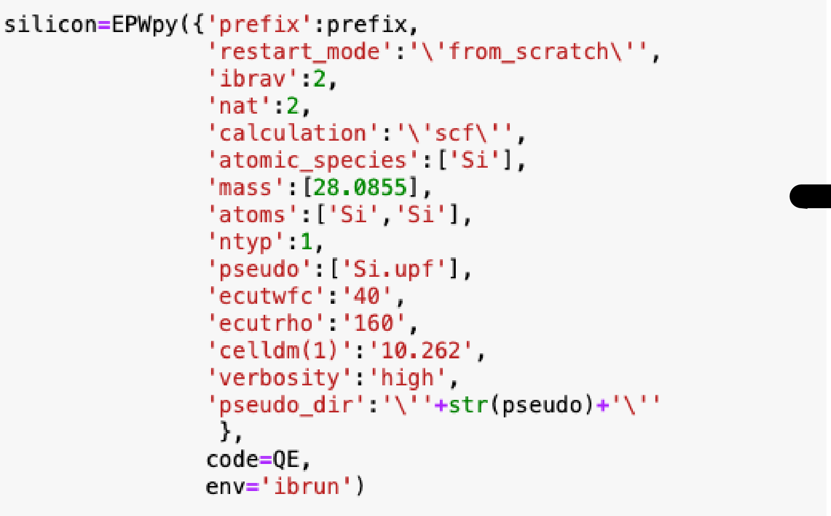

BSE
Eliashberg
GW
Polarons
FM+DW
Boltzmann
Interoperable Software Ecosystem for Many-Body Electronic Structure Calculations
jupyterhub
docker
← Horizontal Interoperability →
BerkeleyGW
XML
EPW
XML
TERNHEIMER
‹S›GW
Vertical Interoperability
QUANTUMESPRESSO
Abinit
siesta
TM

EPWpy

- Python package
  - Wrap various codes to work with EPW
  - Easy to use and develop
  - Streamline calculations
    - Parallelly run multiple calculations
  - High level access to data (for analysis)
  - Makes it possible to use EPW using a Jupyter notebook

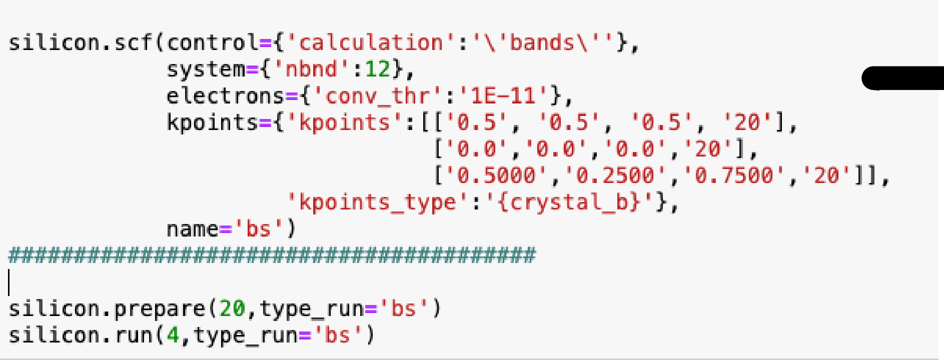


A typical EPWpy workflow



```
silicon=EPWpy({'prefix':prefix,
               'restart_mode':'\'from_scratch\'',
               'ibrav':2,
               'nat':2,
               'calculation':'\'scf\'',
               'atomic_species':['Si'],
               'mass':[28.0855],
               'atoms':['Si','Si'],
               'ntyp':1,
               'pseudo':['Si.upf'],
               'ecutwfc':'40',
               'ecutrho':'160',
               'celldm(1)':'10.262',
               'verbosity':'high',
               'pseudo_dir':'\''+str(pseudo)+'\''
                },
               code=QE,
               env='ibrun')
```

Material definition

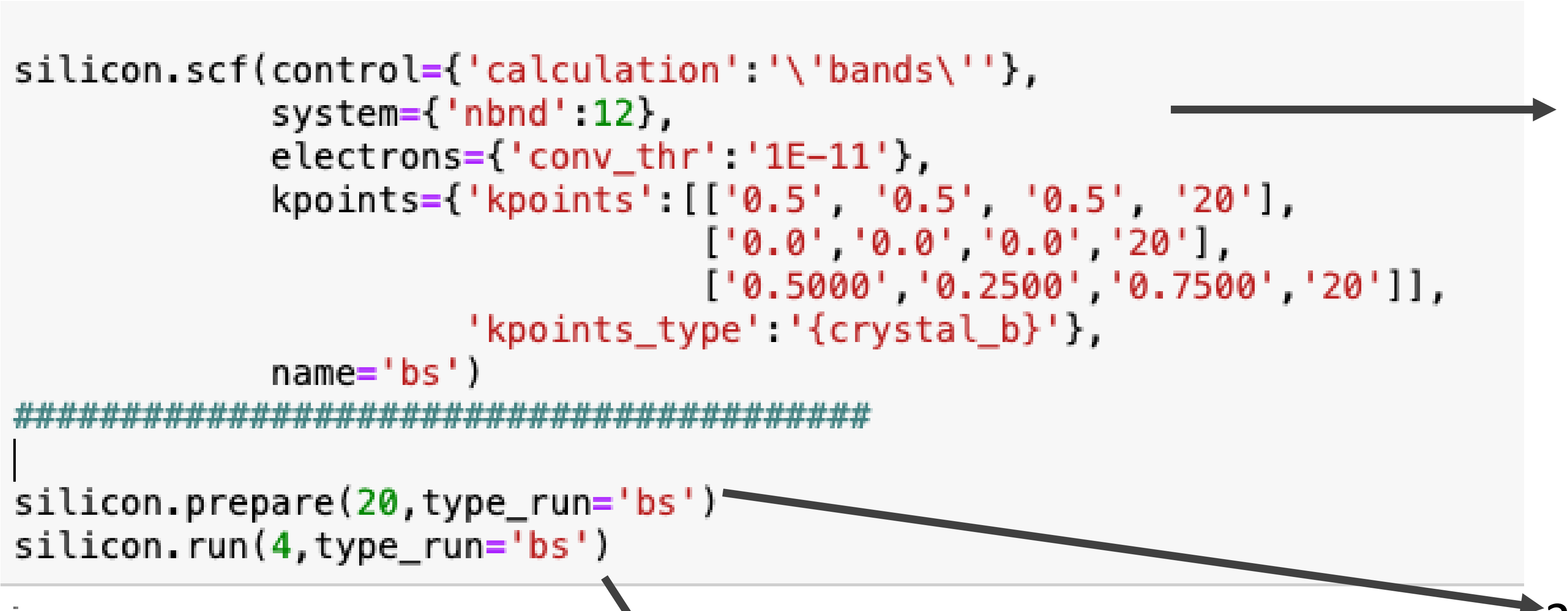


```
silicon.scf(control={'calculation':'\'bands\''},
            system={'nbnd':12},
            electrons={'conv_thr':'1E-11'},
            kpoints={'kpoints':[['0.5', '0.5', '0.5', '20'],
                                ['0.0','0.0','0.0','20'],
                                ['0.5000','0.2500','0.7500','20']],
                     'kpoints_type':'{crystal_b}'},
            name='bs')
########################################
|
silicon.prepare(20,type_run='bs')
silicon.run(4,type_run='bs')
```

Preparation and calculation

- Definition not needed, most of the things are automated

Three-step process



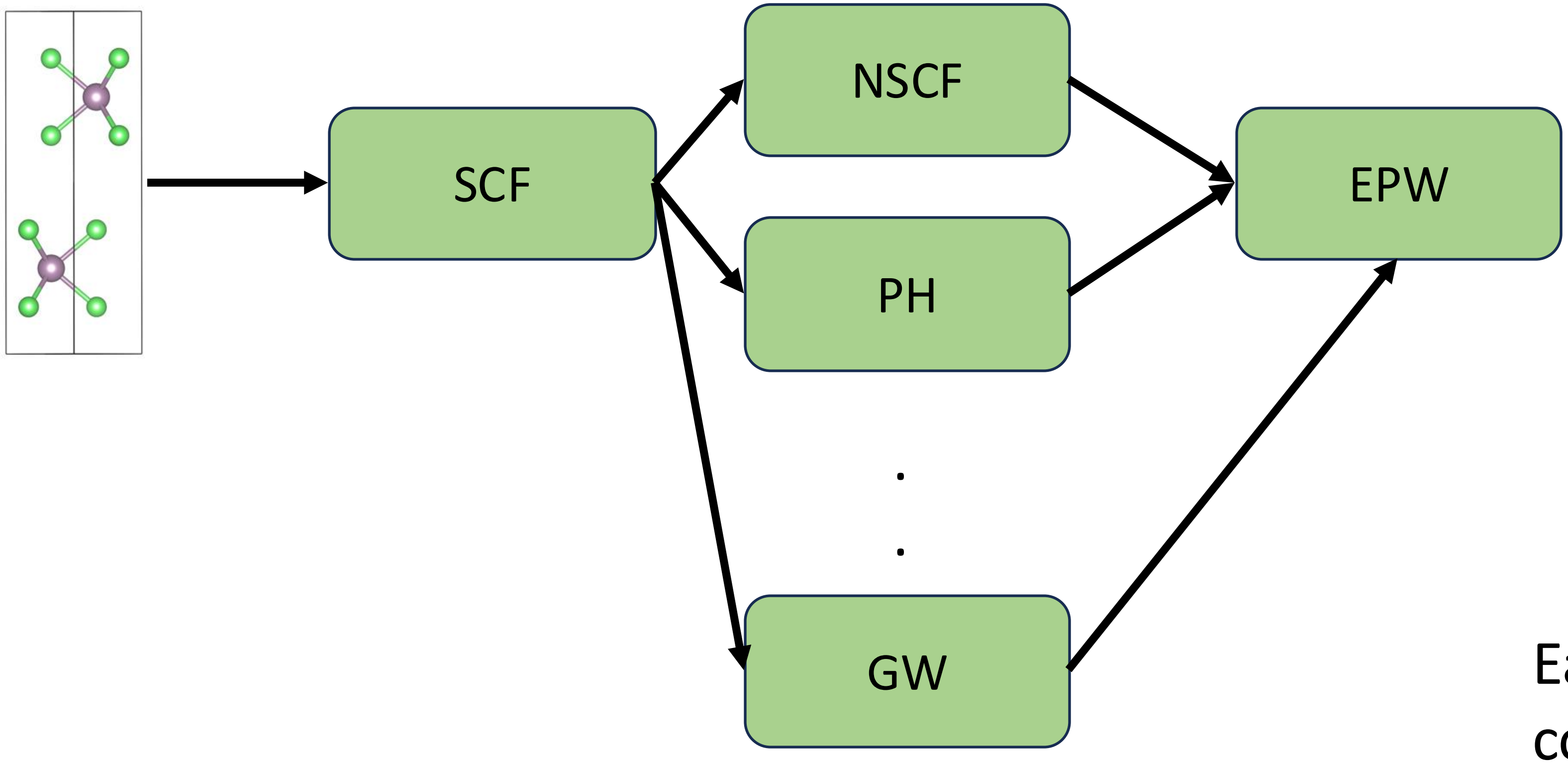
```
silicon.scf(control={'calculation':'\'bands\''},
            system={'nbnd':12},
            electrons={'conv_thr':'1E-11'},
            kpoints={'kpoints':[['0.5', '0.5', '0.5', '20'],
                                ['0.0','0.0','0.0','20'],
                                ['0.5000','0.2500','0.7500','20']],
                     'kpoints_type':'{crystal_b}'},
            name='bs')
########################################

silicon.prepare(20,type_run='bs')
silicon.run(4,type_run='bs')
```

1. Calling the method prepares and writes inputs

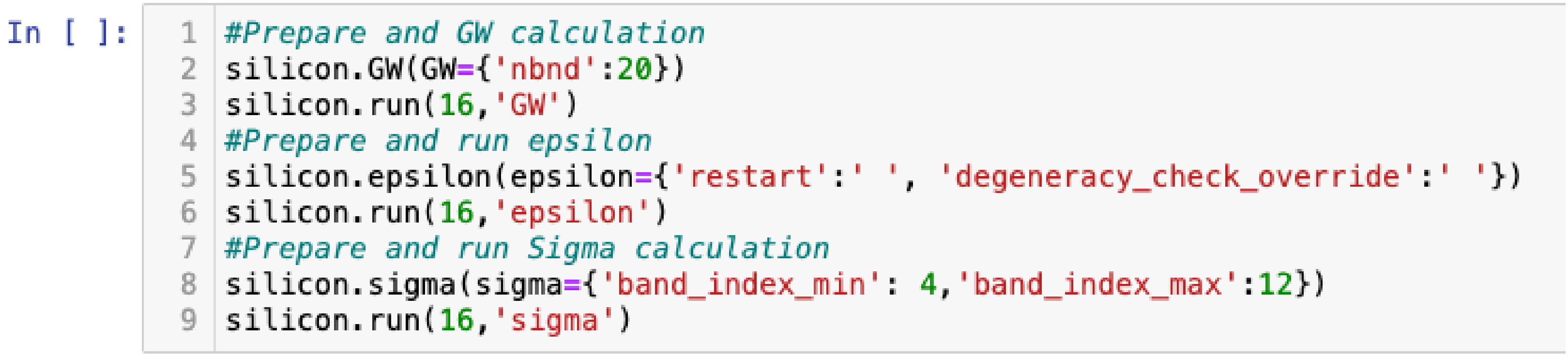
2. Prepares files needed for calculation

3. Runs the calculation

Adding blocks of calculation



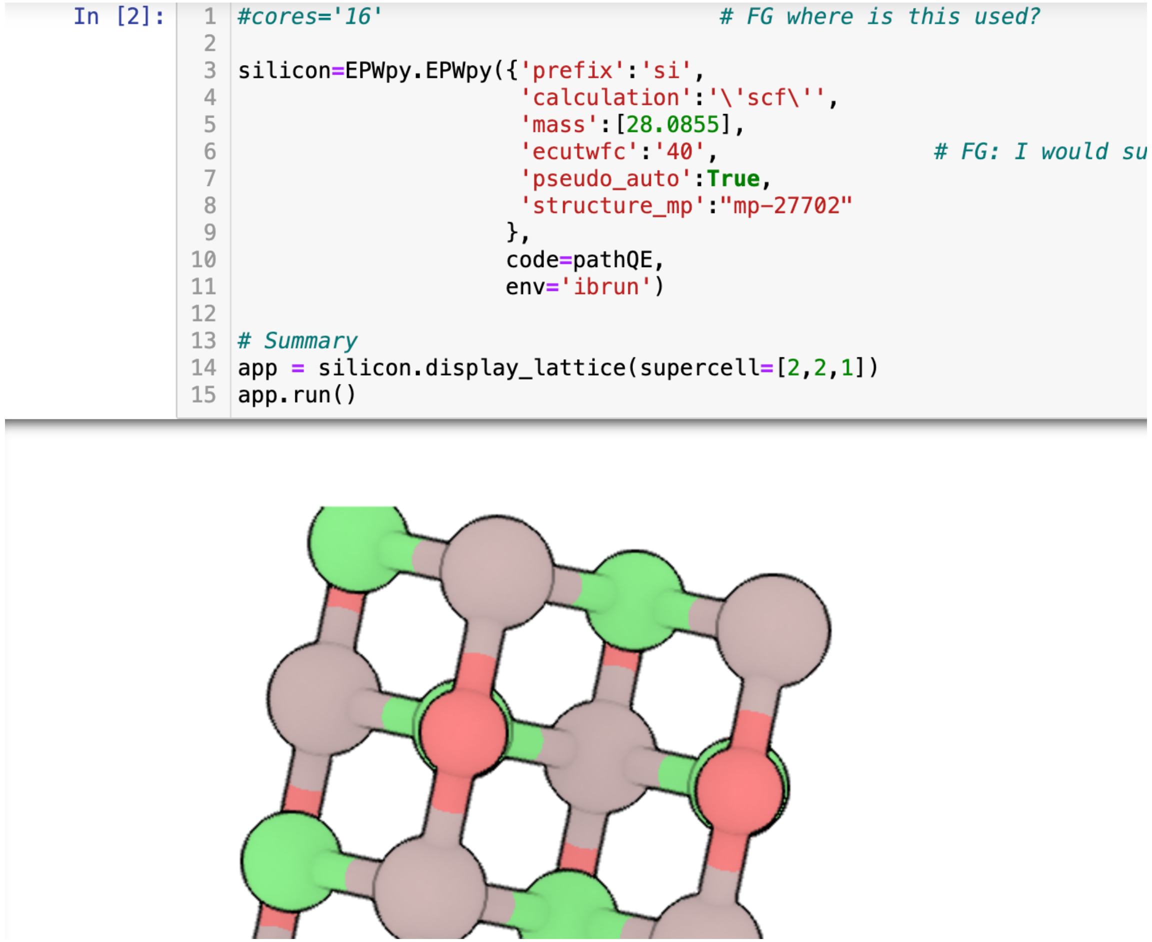
Easily added as a block or combination of blocks



```
#Prepare and GW calculation
silicon.GW(GW={'nbnd':20})
silicon.run(16,'GW')
#Prepare and run epsilon
silicon.epsilon(epsilon={'restart':' ', 'degeneracy_check_override':' '})
silicon.run(16,'epsilon')
#Prepare and run Sigma calculation
silicon.sigma(sigma={'band_index_min': 4,'band_index_max':12})
silicon.run(16,'sigma')
```

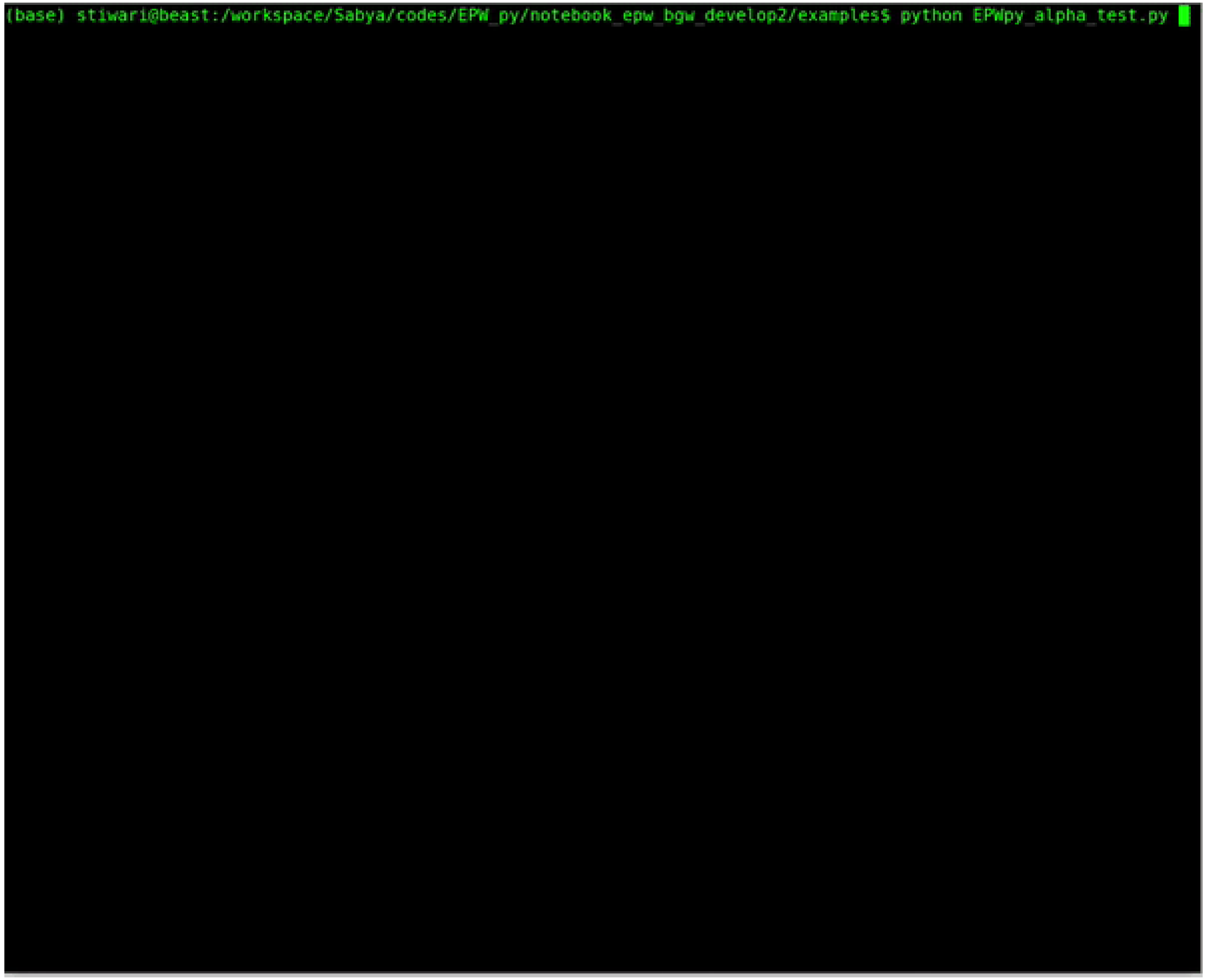
Utilities

- Structure view
- Analysis class
  - Further calculations
- High-throughput calculations



```
In [2]:
#cores='16'                         # FG where is this used?

silicon=EPWpy.EPWpy({'prefix':'si',
                     'calculation':'\'scf\'',
                     'mass':[28.0855],
                     'ecutwfc':'40',                # FG: I would su
                     'pseudo_auto':True,
                     'structure_mp':"mp-27702"
                    },
                    code=pathQE,
                    env='ibrun')

# Summary
app = silicon.display_lattice(supercell=[2,2,1])
app.run()
```

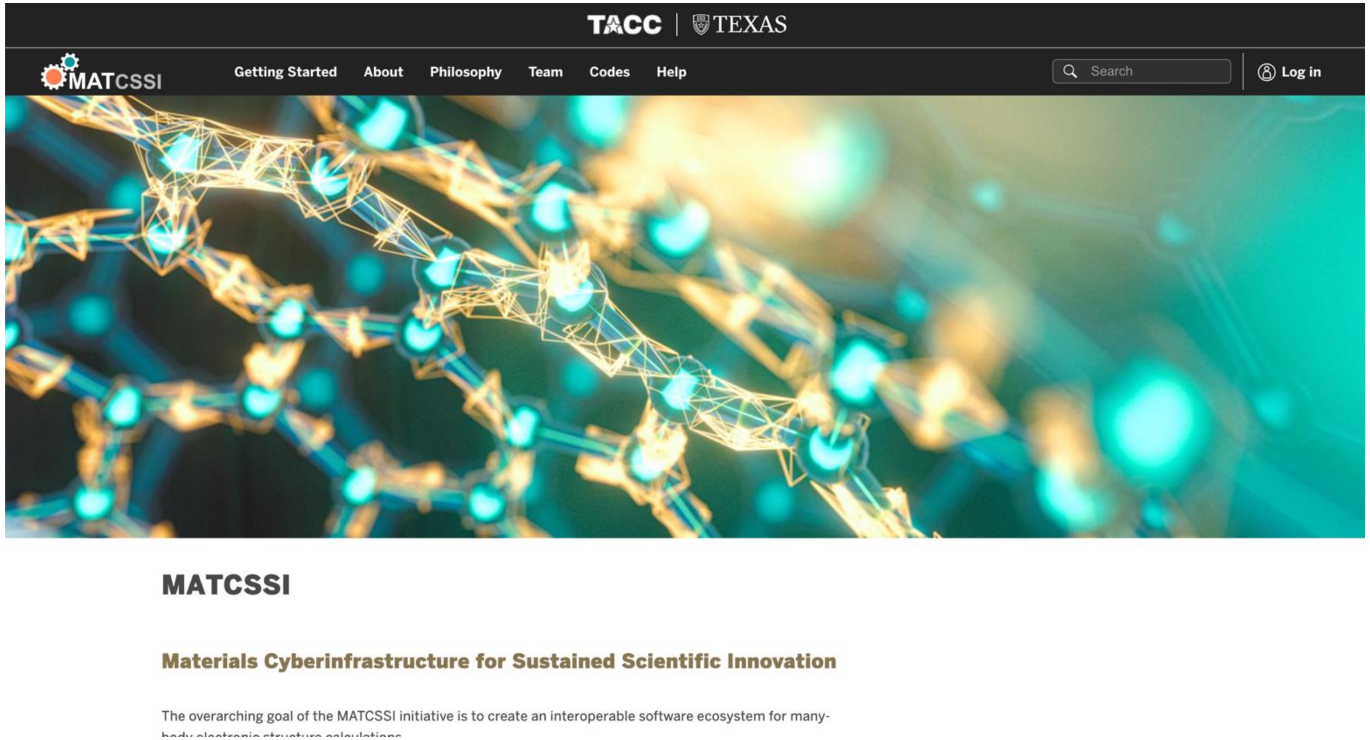
EPWpy in action



```
(base) stiwari@beast:/workspace/Sabya/codes/EPW_py/notebook_epw_bgw_develop2/examples$ python EPWpy_alpha_test.py
```

MATCSSI

- Cyberinfrastructure development for ab-initio calculations
- Interactive Jupyter notebooks which run on Frontera TACC
- Can be accessed from anywhere



MATCSSI

Materials Cyberinfrastructure for Sustained Scientific Innovation

The overarching goal of the MATCSSI initiative is to create an interoperable software ecosystem for many-body electronic structure calculations

Outline

- Basic electron-phonon-physics
- EPW
- Practical calculations using EPW/EPWpy
- Conclusion

Conclusion

- Electron-Phonon physics is important for many physical properties
- EPW and EPWpy provide a convenient tool for exploring electron-phonon physics
- EPW GitLab: https://gitlab.com/epw/q-e
- EPWpy GitLab: https://gitlab.com/matcssi/notebook_epw_bgw

Trying out EPWpy today

1. Add these lines in your .bashrc

```
# >>> conda initialize >>>
# !! Contents within this block are managed by 'conda init' !!
__conda_setup="$('/leonardo_scratch/large/userexternal/stiwari0/Conda_install/build/bin/conda' 'shell.bash' 'hook' 2> /dev/null)"
if [ $? -eq 0 ]; then
    eval "$__conda_setup"
else
    if [ -f "/leonardo_scratch/large/userexternal/stiwari0/Conda_install/build/etc/profile.d/conda.sh" ]; then
        . "/leonardo_scratch/large/userexternal/stiwari0/Conda_install/build/etc/profile.d/conda.sh"
    else
        export PATH="/leonardo_scratch/large/userexternal/stiwari0/Conda_install/build/bin:$PATH"
    fi
fi
unset __conda_setup
# <<< conda initialize <<<
```

2. Copy two files from stiwari0 repo

```
cp leonardo_scratch/large/userexternal/stiwari0/Jupyter_test/launcher.sh <your location>
cp –r leonardo_scratch/large/userexternal/stiwari0/tutorials/ <your location>
cd <your location> ; sbatch launcher.sh
```

3. Launcher will launch a job on a compute node; ssh into that compute node and run the tutorials

```
cd <your location>/tutorials/transport
python transport.py
```

4. Eventually, this calculation will return you the mobility of Si at 300 K