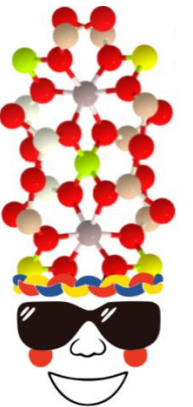


Electron-Phonon Physics using EPW

Sabyasachi Tiwari

Oden Institute for computational Engineering and Science
UT Austin



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

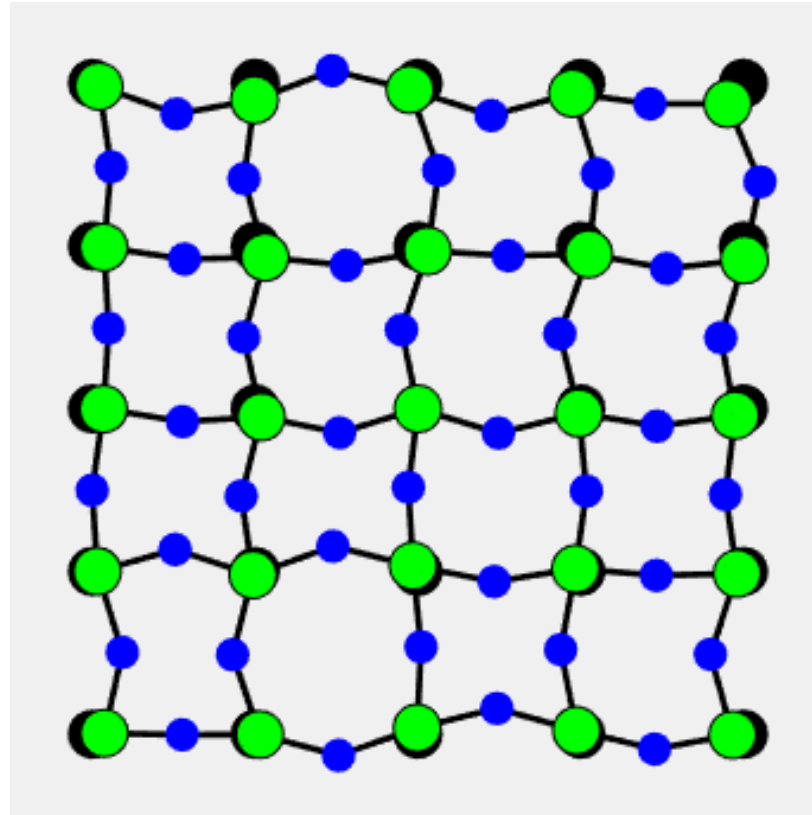
- Basic electron-phonon-physics
- EPW
- Practical calculations using EPW/EPWpy
- Conclusion



Developers

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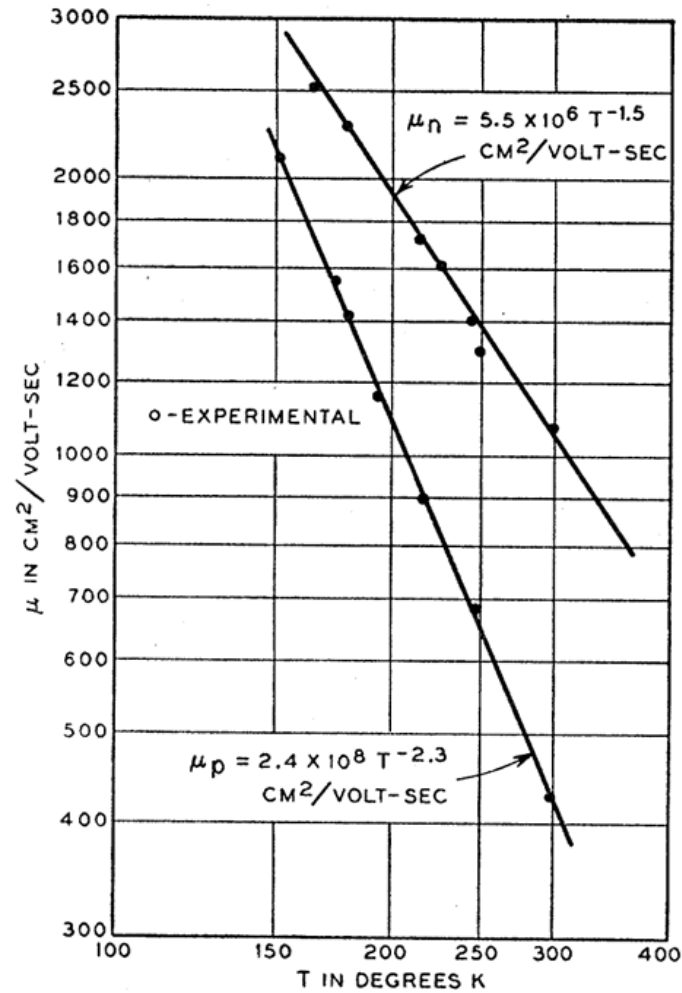
Why Electron-Phonon Physics?



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

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

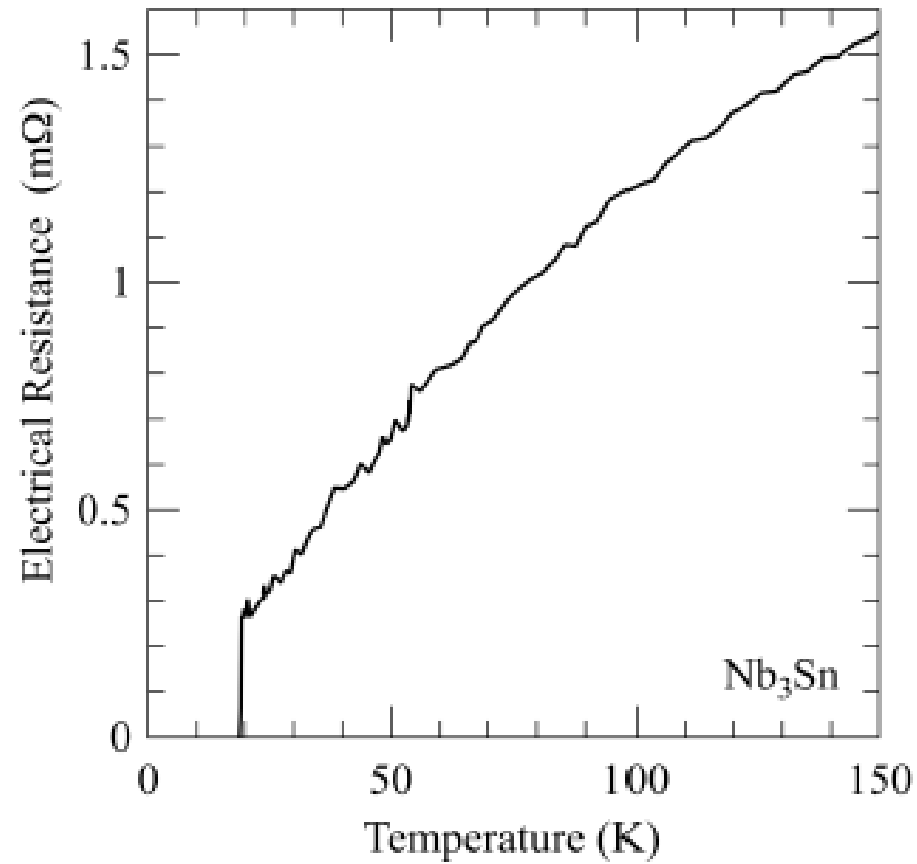
Why Electron-Phonon Physics?



- Transport

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

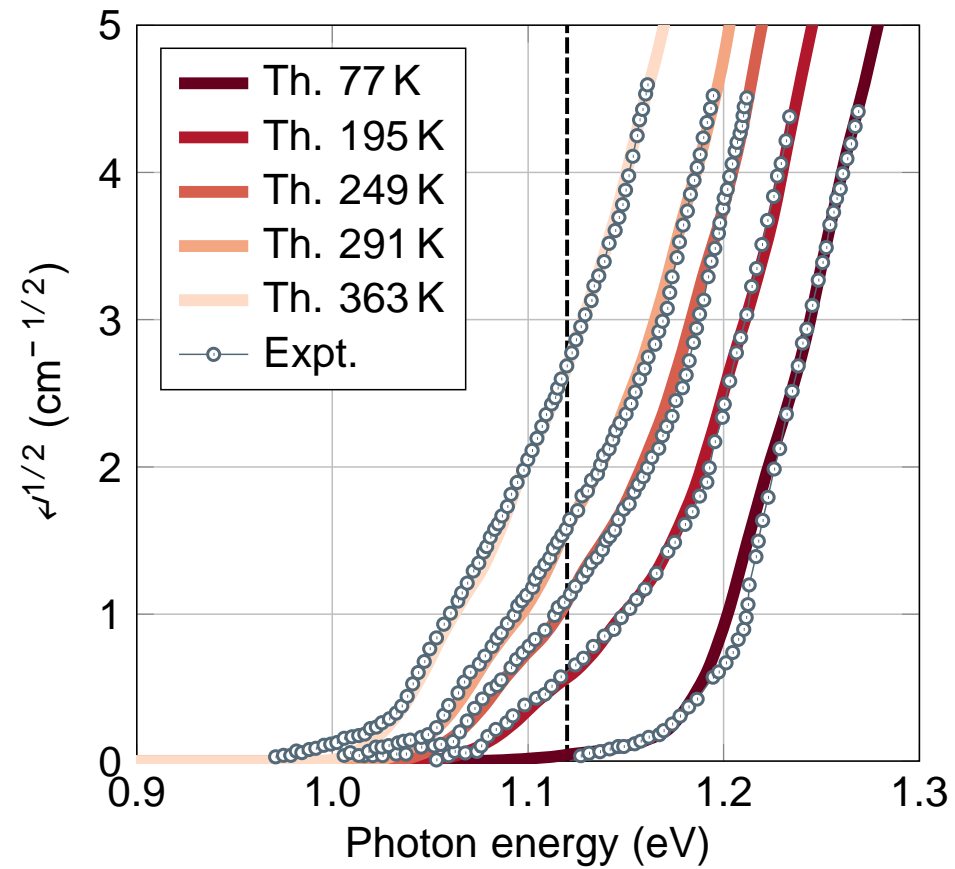
Why Electron-Phonon Physics ($T \approx 0$ K)?



- Superconductivity

Gabovich et.al., Supercond. (2014)

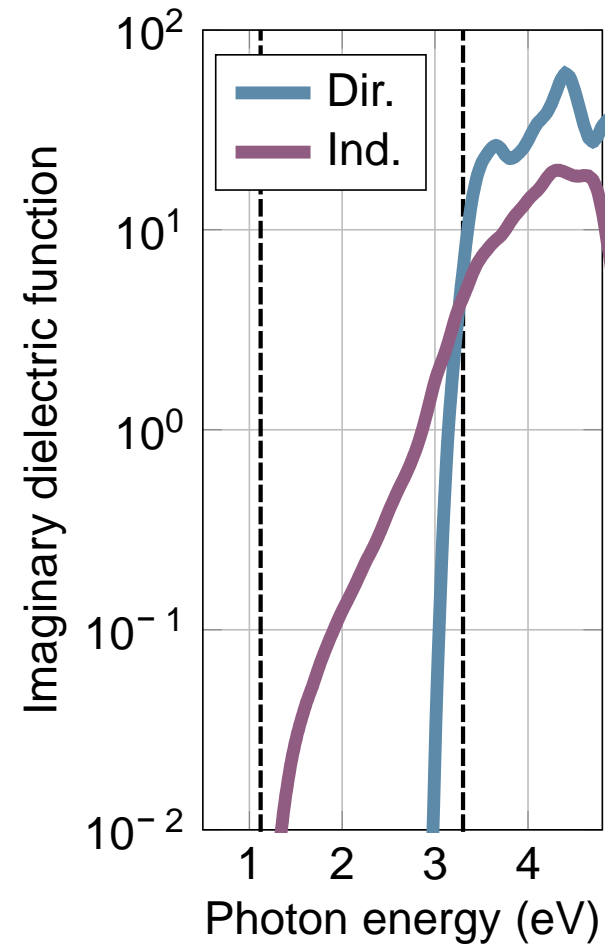
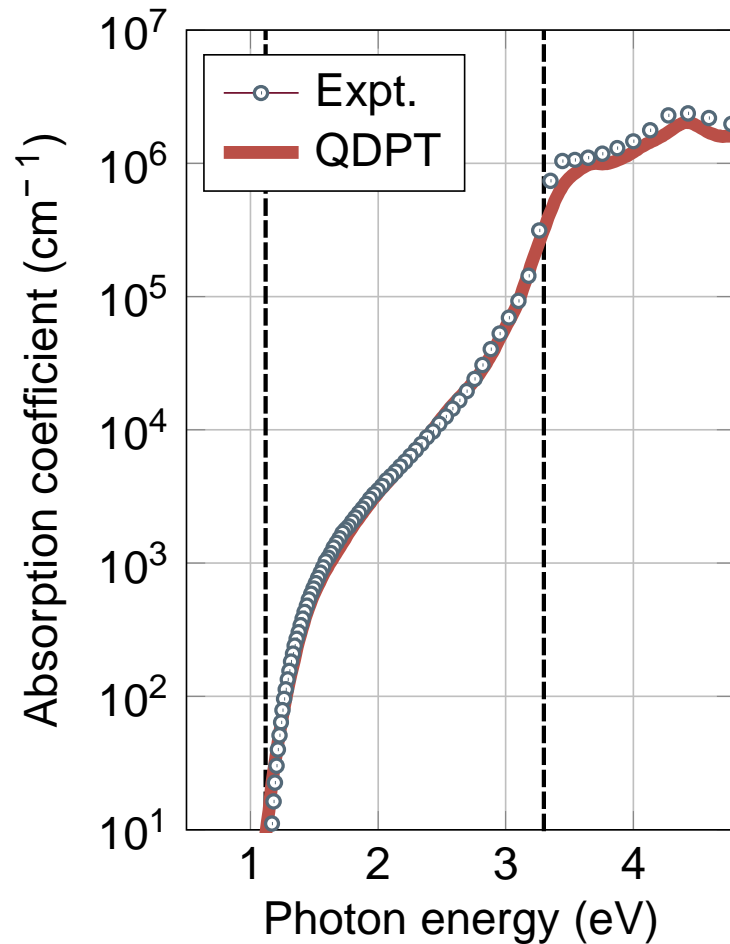
Why Electron-Phonon Physics (Light-Matter interaction)?



- Band-gap renormalization

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

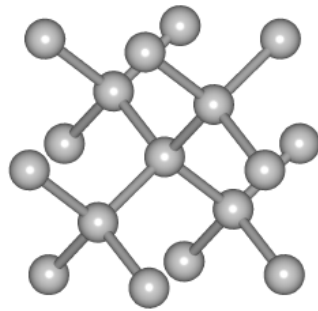
Why Electron-Phonon Physics (Light-Matter interaction)?



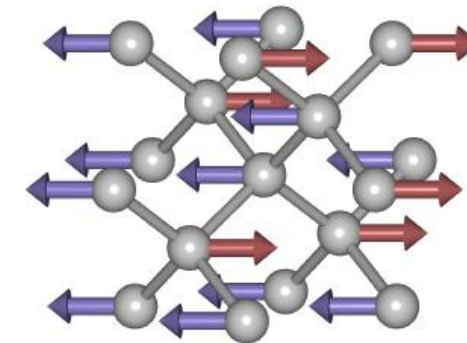
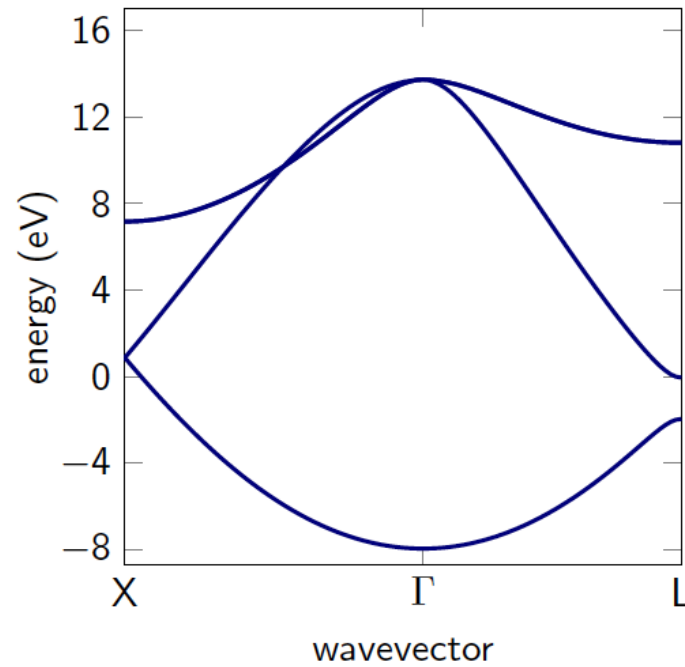
- Visible range: phonons

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

Where do phonons come from?

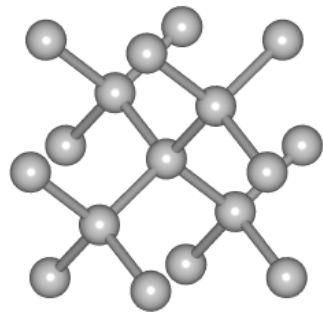


diamond

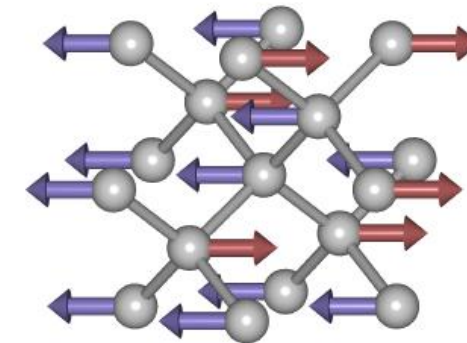
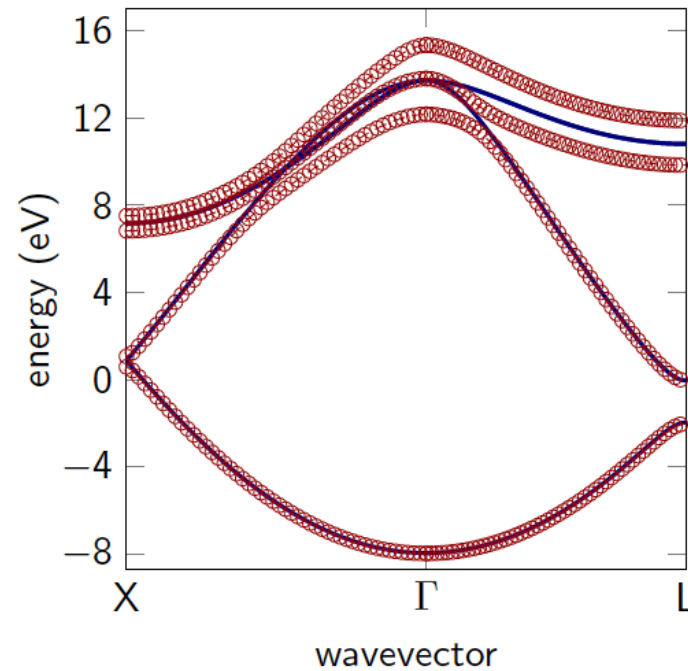


Move atoms along a mode

Where do phonons come from?



diamond



Move atoms along a mode

- Change in band structure

Where do phonons come from?

The diagram illustrates the self-consistent field (SCF) process. It starts with the Schrödinger equation for an electron in a potential V_{SCF} . This equation is used to calculate the electron density $n(r)$ by summing the squared magnitudes of the occupied orbitals. The electron density is then used to calculate the SCF potential $V_{\text{SCF}}(r)$, which includes the nuclear attraction and the Hartree potential, plus an exchange-correlation term $V_{\text{XC}}[n(r)]$. A feedback loop is shown by a blue arrow from the SCF potential back to the Schrödinger equation.

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_n + V_{\text{SCF}} \psi_n = \epsilon_n \psi_n$$
$$n(r) = \sum_{n \in \text{OCC}} |\psi_n|^2$$
$$V_{\text{SCF}}(r) = -\frac{e^2}{4\pi\epsilon_0} \left[\sum_{\kappa} \frac{Z_{\kappa}}{r - \tau_{\kappa}} + \int \frac{n(r') dr'}{r - r'} \right] + V_{\text{XC}}[n(r)]$$

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

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

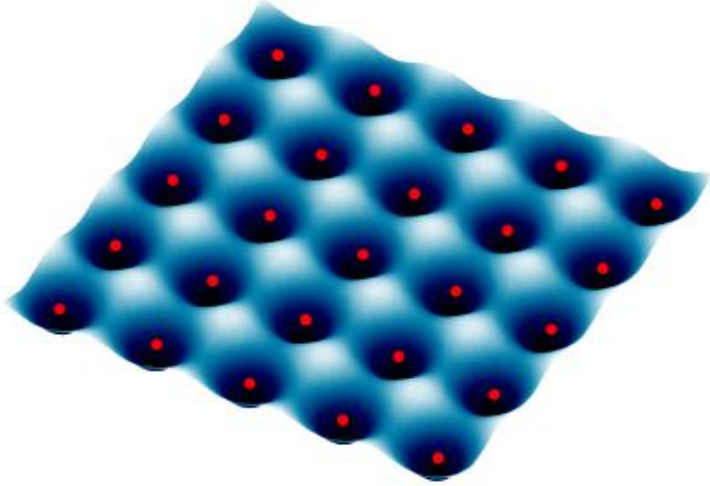
Displace atoms from equilibrium position: $\tau = \tau_0 + \Delta\tau$

$$V_{\text{SCF}}(\tau_0 + \Delta\tau) = V_{\text{SCF}}(\tau_0) + \frac{\partial V_{\text{SCF}}}{\partial \tau} \Delta\tau + \frac{1}{2} \frac{\partial^2 V_{\text{SCF}}}{\partial \tau^2} \Delta\tau^2 + \dots$$

- Perturbation to atomic positions
 - Temperature

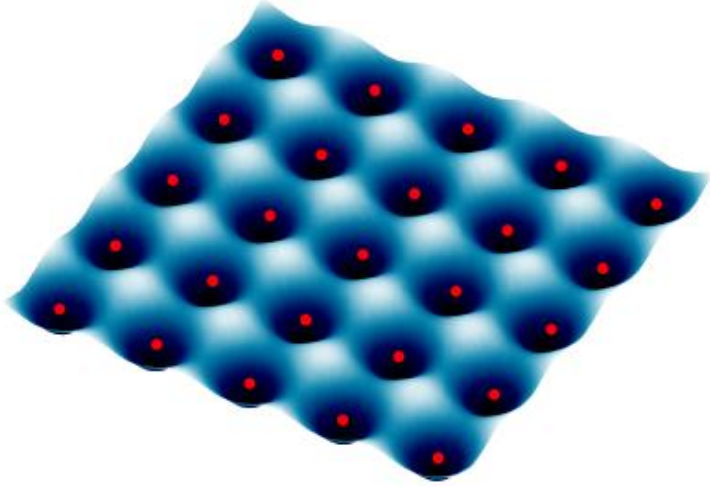
Where do phonons come from?

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

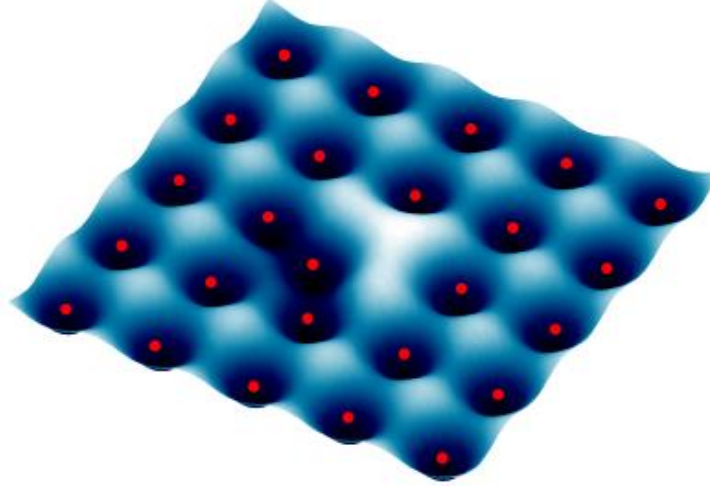


Where do phonons come from?

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

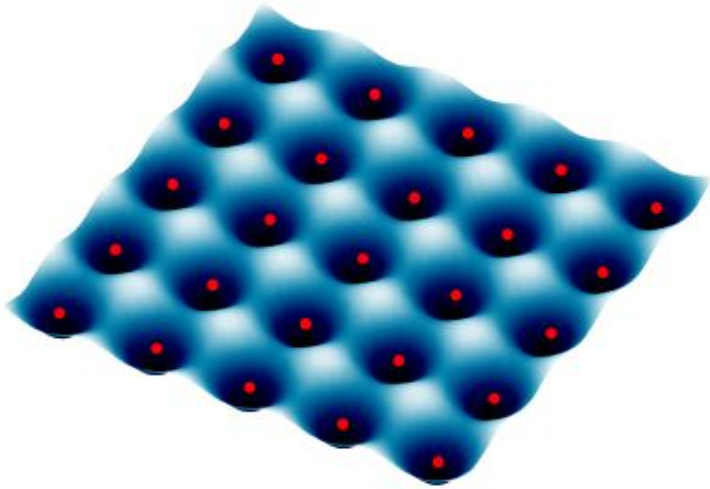


$$V_{\text{SCF}}(r; \tau + \Delta\tau)$$

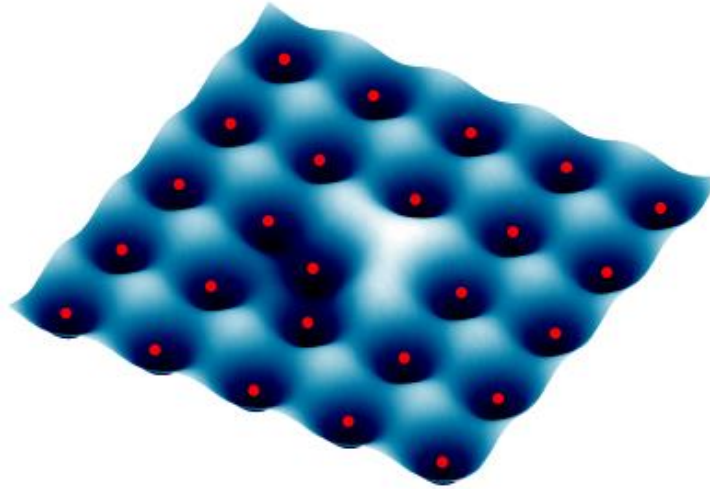


Where do phonons come from?

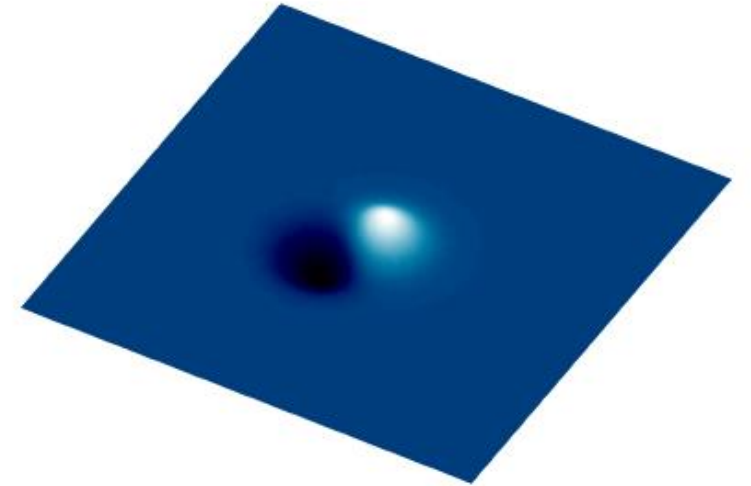
$$V_{\text{SCF}}(r; \tau)$$



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



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



Perturbing potential

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

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

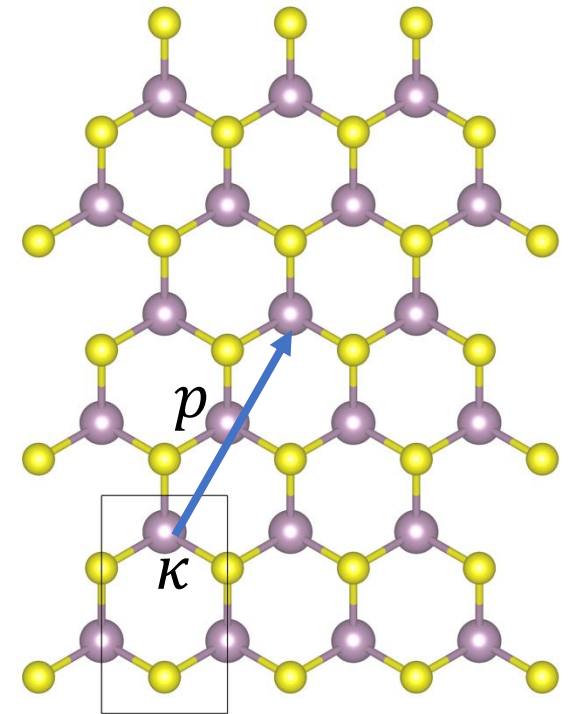
Transition Rate $\Gamma_{n \rightarrow m} = \frac{2\pi}{\hbar} \left| \left\langle \psi_m \left| \frac{\partial V_{\text{SCF}}}{\partial \tau} \Delta \tau \right| \psi_n \right\rangle \right|^2 \delta(E_m - E_n)$ Transport

- Calculation of perturbation potential is key to calculating many properties

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

Supercell

Unit-cell



- Go from supercell to unit-cell
 - Cheaper calculations

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

$$\sum_{\kappa\alpha p} \frac{\partial V_{\text{SCF}}}{\partial \tau_{\kappa\alpha p}} \Delta\tau_{\kappa\alpha p} \rightarrow \sum_{\mathbf{q}\nu} \Delta_{\mathbf{q}\nu} V_{\text{SCF}} (\hat{a}_{\mathbf{q}\nu} + \hat{a}_{-\mathbf{q}\nu}^{\dagger})$$

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

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

Phonon polarization



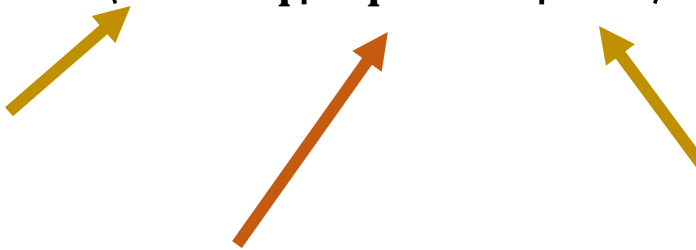
$$\hat{V}_{\text{ep}} = \frac{1}{N_p} \sum_{mnkq}^{\nu} g_{mn}^{\nu}(\mathbf{k}, \mathbf{q}) c_{m\mathbf{k}+\mathbf{q}}^{\dagger} c_{n\mathbf{k}} (\hat{a}_{\mathbf{q}\nu} + \hat{a}_{-\mathbf{q}\nu}^{\dagger})$$

- Electron-phonon Hamiltonian in second quantization

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

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

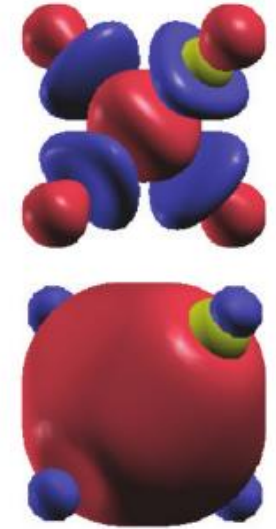
- Dense \mathbf{k}, \mathbf{q} grids needed for calculating observables
- Wavefunctions: NSCF calculations (DFT)
 - Cheap for unit-cells
- Displacements/derivatives V_{SCF} : Linear response/DFPT
 - Expensive
 - Dense grids not possible

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


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

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

$$w_m(r; R_p) = \frac{1}{N_p} \sum_{nk} \exp(i\mathbf{k} \cdot R_p) U_{nm}^{\mathbf{k}} |\psi_{n\mathbf{k}}\rangle$$
$$|\psi_{n\mathbf{k}}\rangle = \sum_{mR_p} \exp(-i\mathbf{k} \cdot R_p) U_{mn}^{\mathbf{k}*} w_m(r; R_p)$$



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

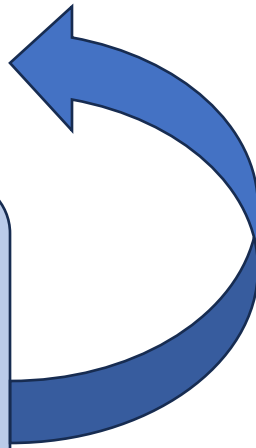
Marzari et.al., Rev. Mod. Phys. 84, 1419 (2012)

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

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

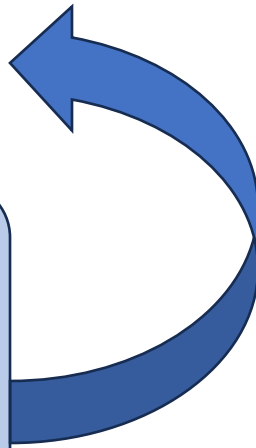
- Notice the summation is over Wigner-Seitz vectors in case of Wannier
 - Much smaller than plane waves since Wannier functions are localized

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

$$w_m(r; R_p) = \frac{1}{N_p} \sum_{nk} \exp(i\mathbf{k} \cdot R_p) U_{nm}^{\mathbf{k}} |\psi_{n\mathbf{k}}\rangle$$
$$|\psi_{n\mathbf{k}}\rangle = \sum_{mR_p} \exp(-i\mathbf{k} \cdot R_p) U_{mn}^{\mathbf{k}*} w_m(r; R_p)$$


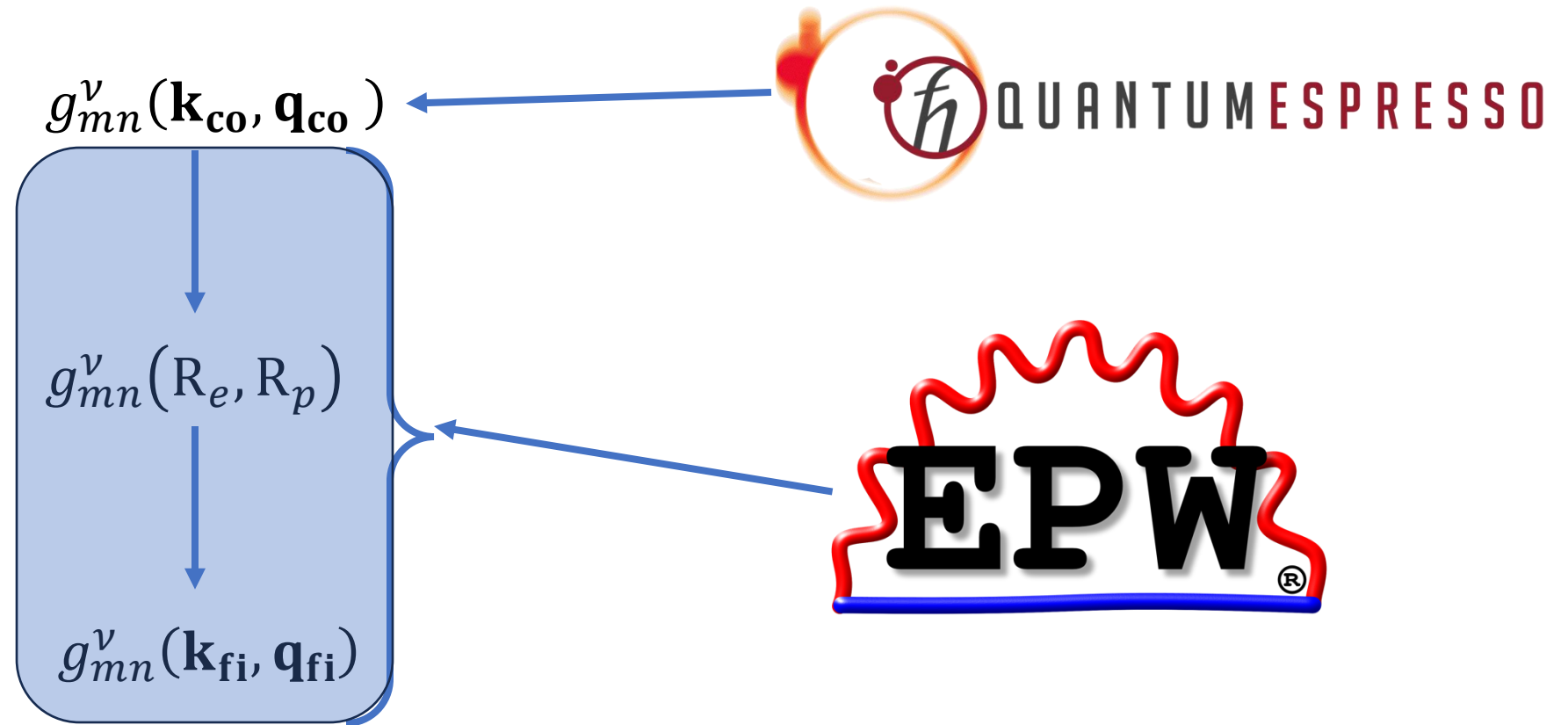
$$g_{mn}^{\nu}(\mathbf{k}, \mathbf{q}) = \langle u_{m\mathbf{k}+\mathbf{q}} | \Delta_{\mathbf{q}\nu} v_{\text{SCF}} | u_{n\mathbf{k}} \rangle$$

$$w_m(r; R_p) = \frac{1}{N_p} \sum_{nk} \exp(i\mathbf{k} \cdot R_p) U_{nm}^{\mathbf{k}} | \psi_{n\mathbf{k}} \rangle$$

$$| \psi_{n\mathbf{k}} \rangle = \sum_{mR_p} \exp(-i\mathbf{k} \cdot R_p) U_{mn}^{\mathbf{k}*} w_m(r; R_p)$$


$$g_{mn}^{\nu}(\mathbf{k}_{\text{co}}, \mathbf{q}_{\text{co}}) \rightarrow g_{mn}^{\nu}(R_e, R_p) \rightarrow g_{mn}^{\nu}(\mathbf{k}_{\text{fi}}, \mathbf{q}_{\text{fi}})$$

- A method for reliably interpolating g



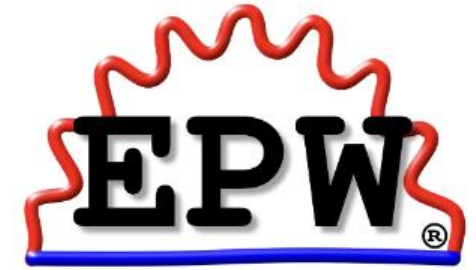
- QE: $\Delta_{q\nu} V_{SCF}; \Delta\tau$
- EPW: Wannierization and interpolation

Ponce et.al., Comput. Phys. Comm, 209, 116-133 (2016)

Lee, ... Tiwari et.al., npj comput. mater., 9, 156 (2023)

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

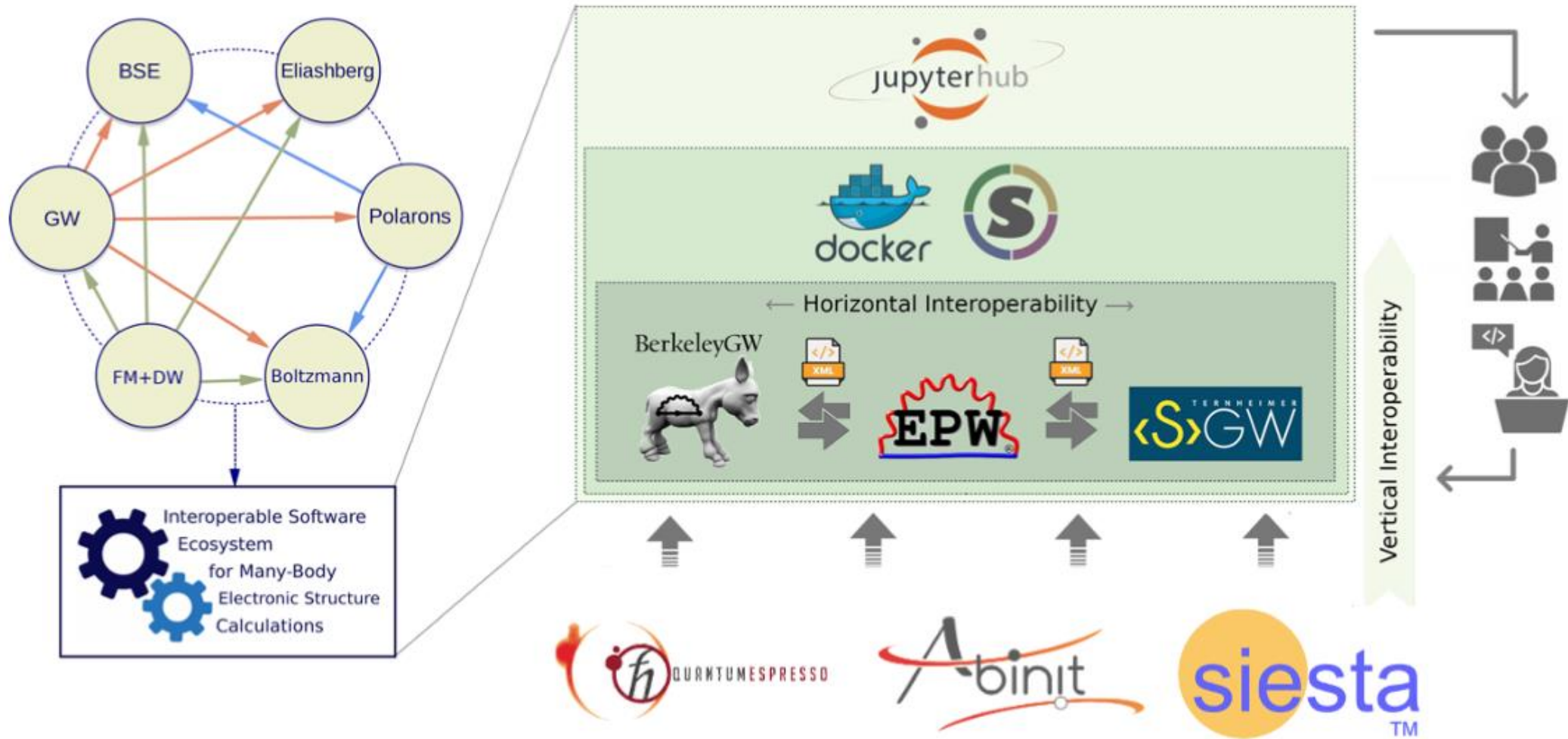
- Electron-Phonon Wannier code
 - A sub-package within the Quantum Espresso DFT package
 - Interpolates e-p matrix elements obtained from DFPT (QE)
 - Allows calculations on very fine \mathbf{k} and \mathbf{q} grids
 - Transport (IBTE)
 - Superconductivity
 - Polarons
 - Temperature dependent Bandgap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



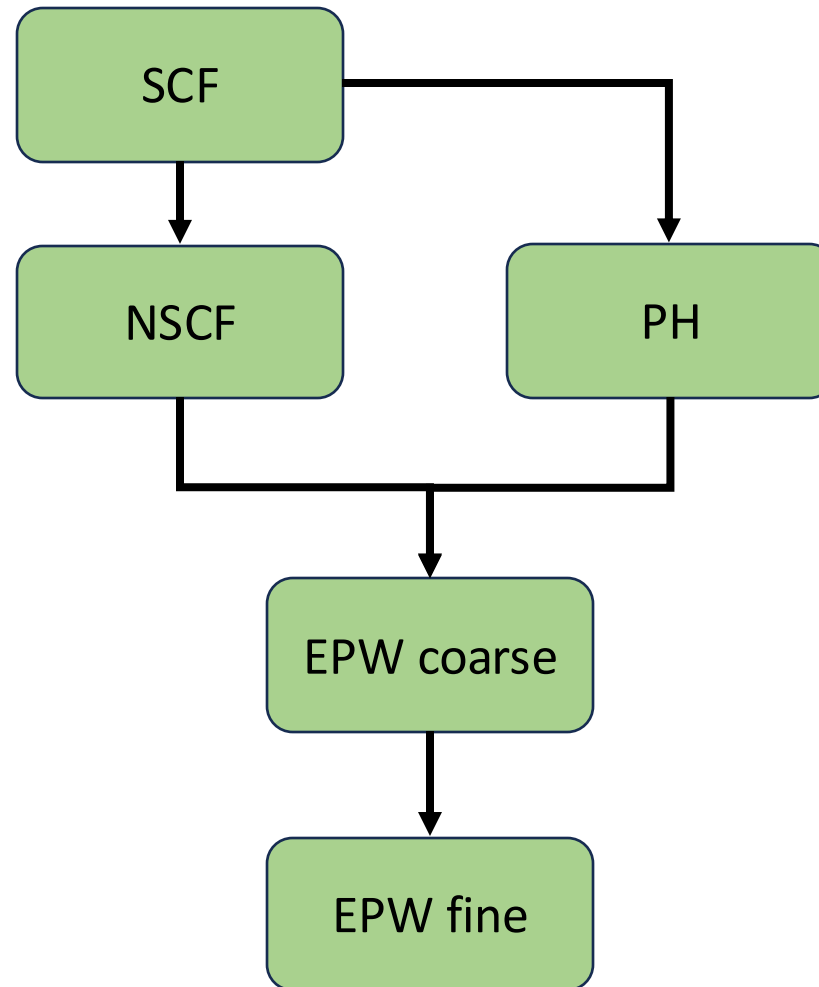
- Basic electron-phonon-physics
- EPW
- **Practical calculations using EPW/EPWpy**
- Conclusion

EPWpy

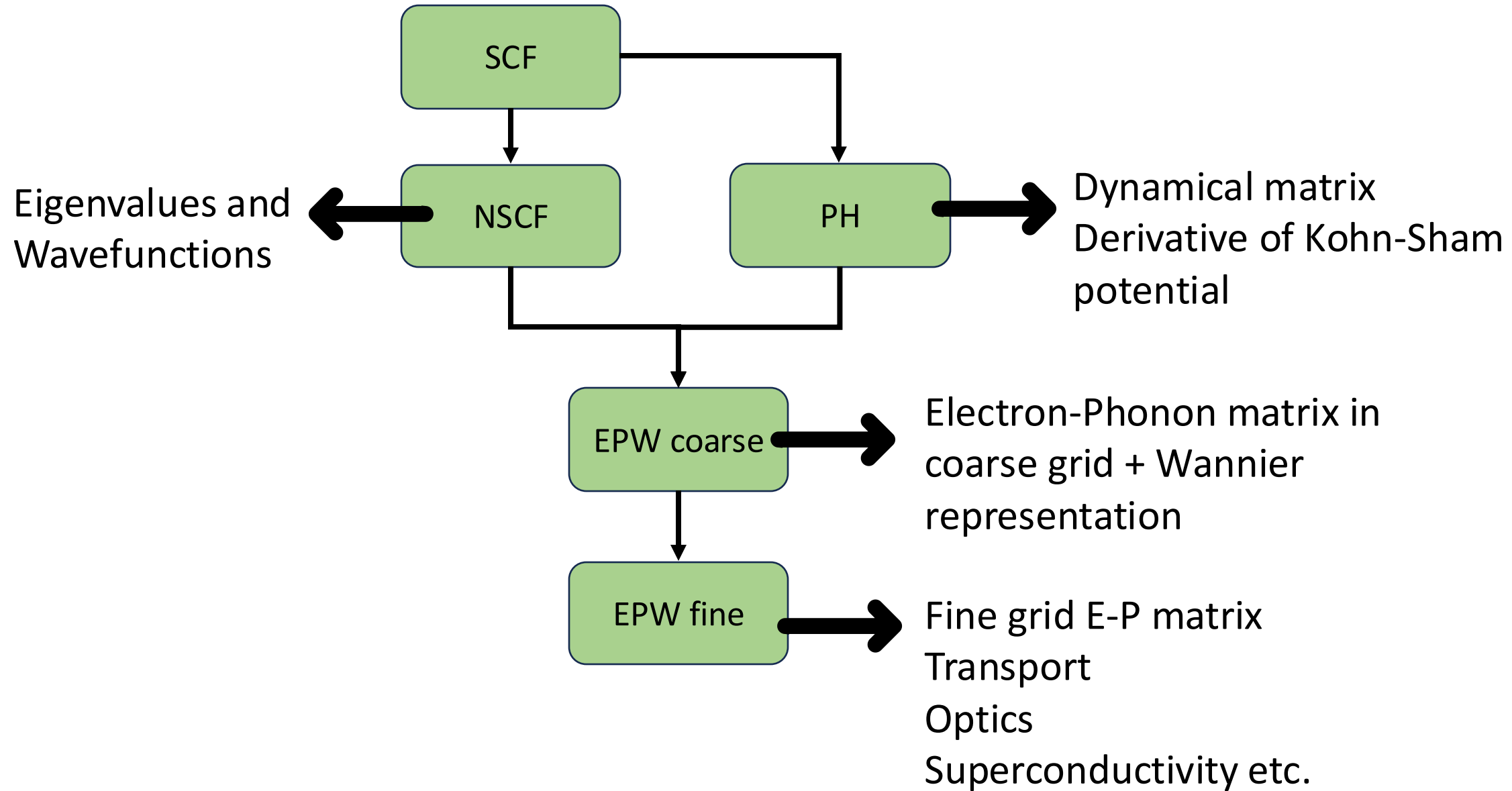
Enabling interoperable software environment



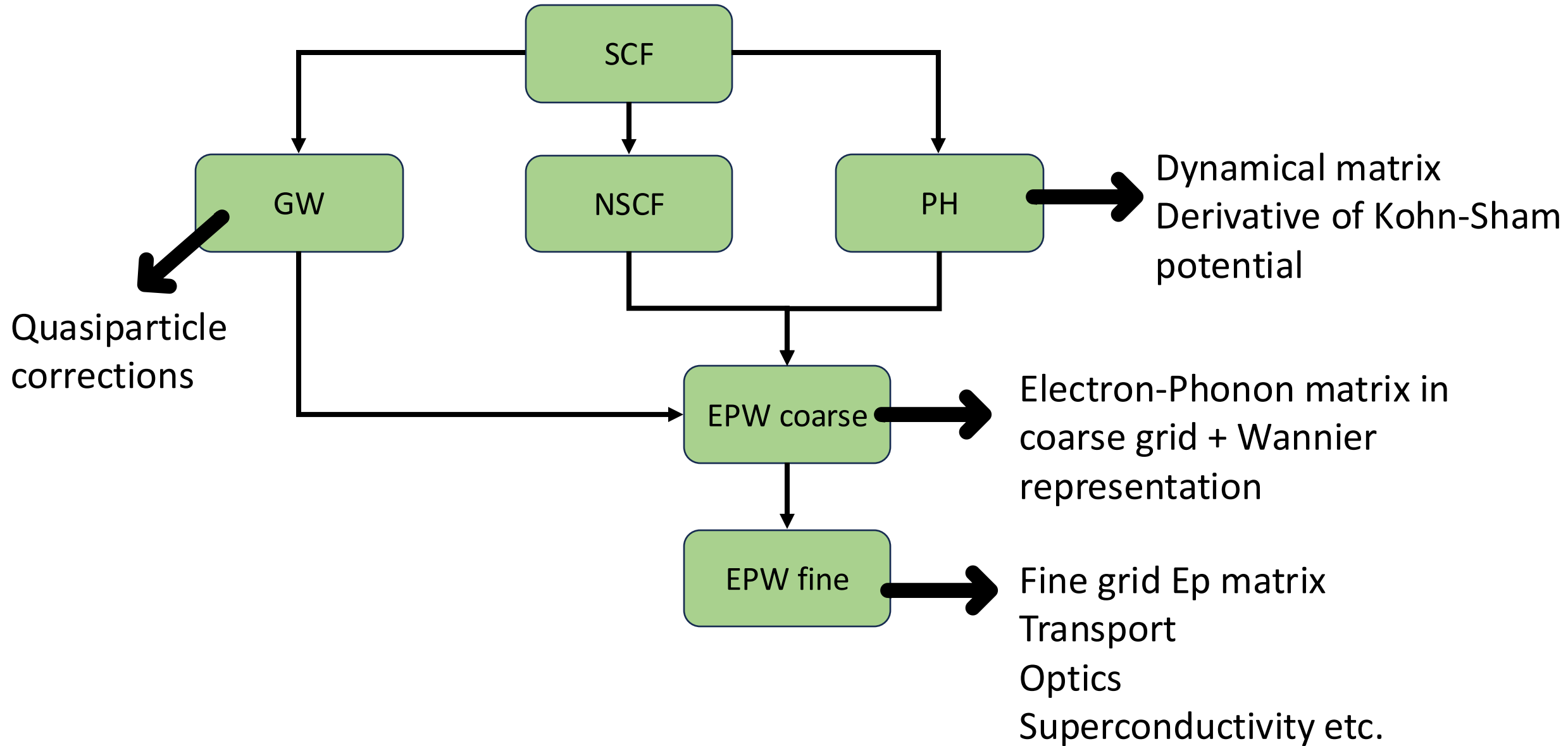
A typical workflow for EPW



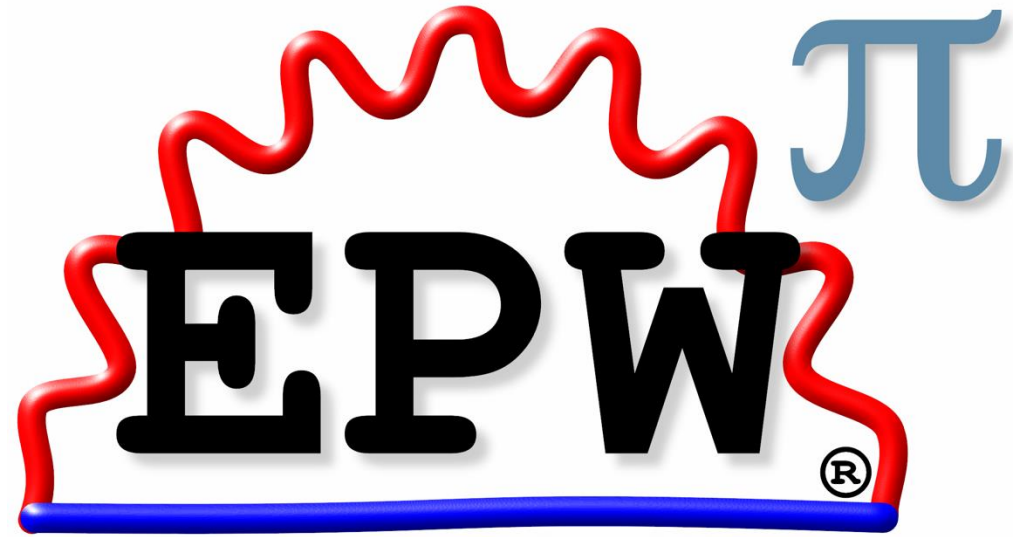
A typical workflow for EPW



A typical workflow for EPW



- Python package
 - Wrap various codes to work with EPW
 - Easy to use and develop
 - Streamline calculations
 - Parallely 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

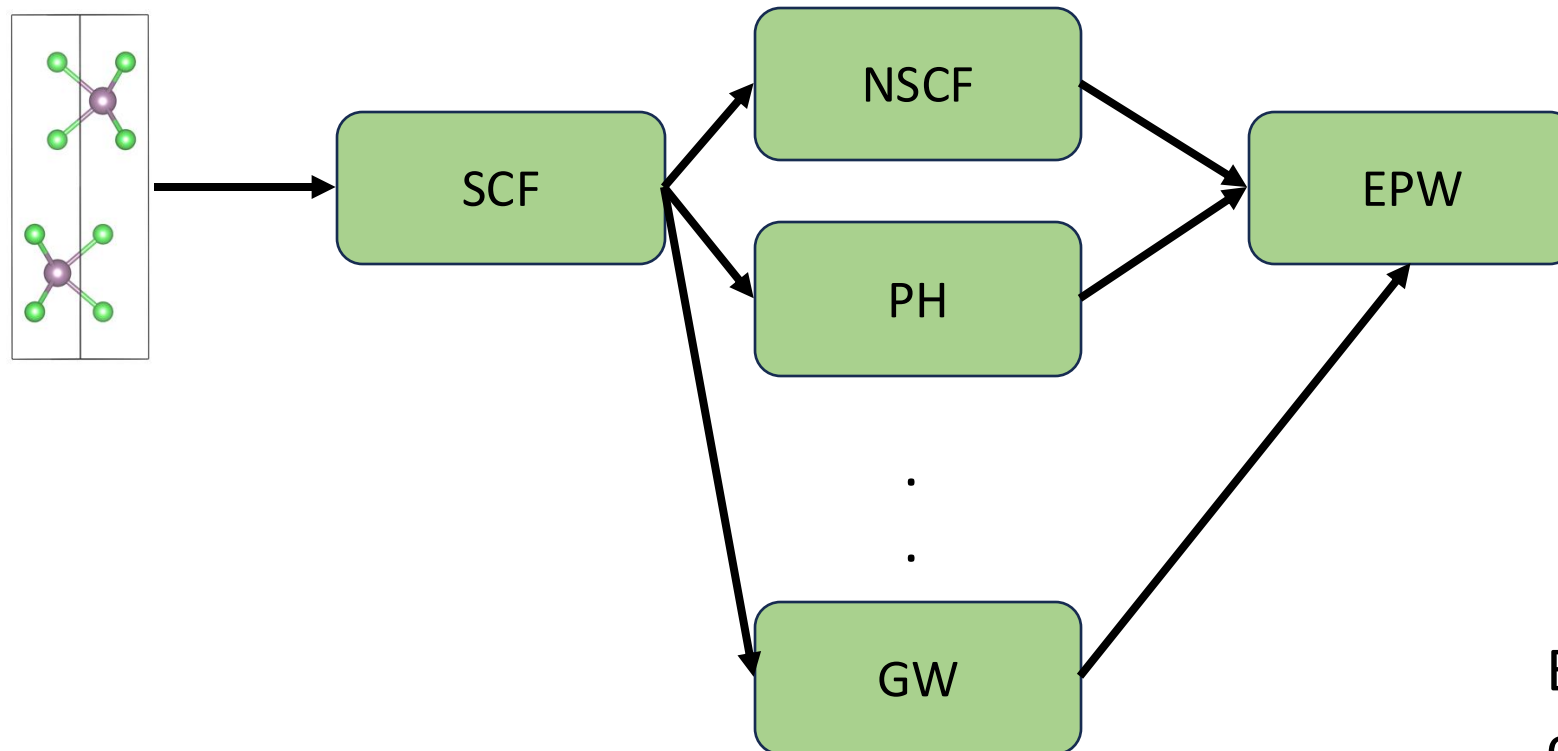
```
silicon.scf(control={'calculation':'\bands\'},
            system={'nbnd':12},
            electrons={'conv_thr':'1E-11'},
            kpoints={'kpoints':[['0.5', '0.5', '0.5', '20'],
                                ['0.0', '0.0', '0.0', '20'],
                                ['0.5000', '0.2500',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

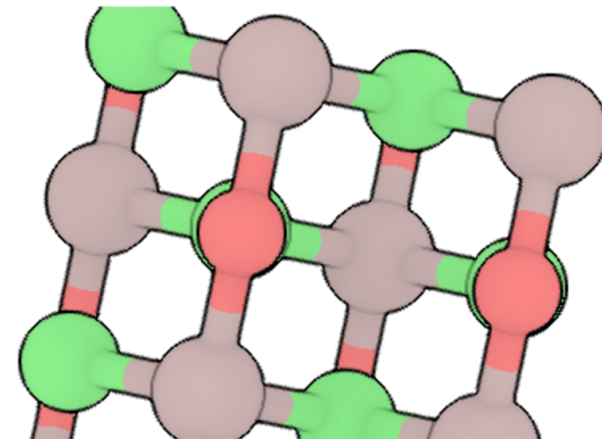


Easily added as a block or combination of blocks

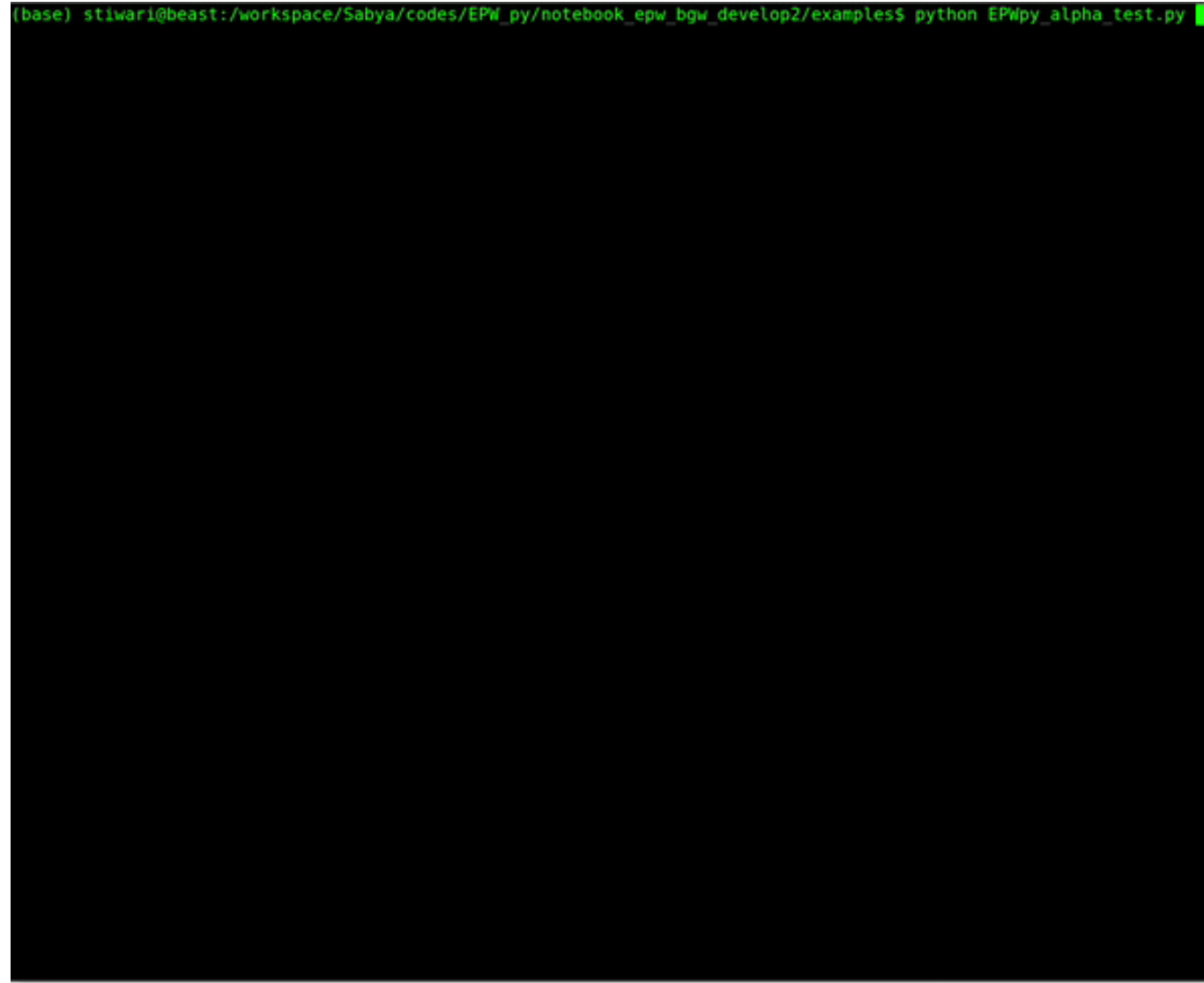
```
In [ ]: 1 #Prepare and GW calculation
2 silicon.GW(GW={'nbnd':20})
3 silicon.run(16,'GW')
4 #Prepare and run epsilon
5 silicon.epsilon(epsilon={'restart':' ', 'degeneracy_check_override':' '})
6 silicon.run(16,'epsilon')
7 #Prepare and run Sigma calculation
8 silicon.sigma(sigma={'band_index_min': 4,'band_index_max':12})
9 silicon.run(16,'sigma')
```

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

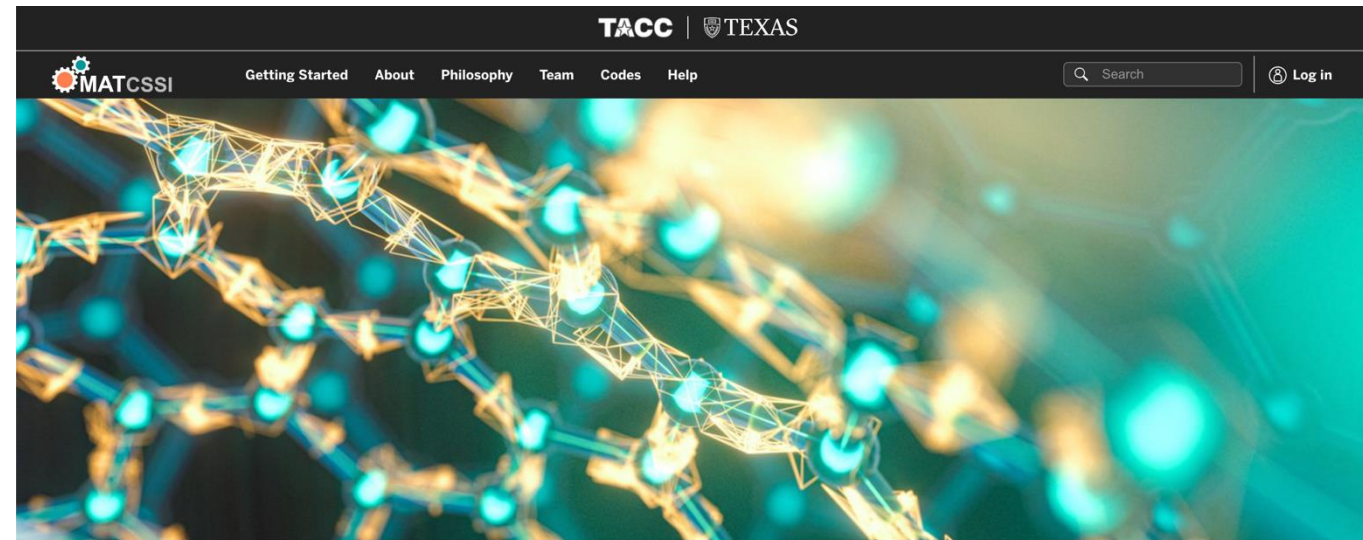
```
In [2]: 1 #cores='16' # FG where is this used?
2
3 silicon=EPWpy.EPWpy({'prefix':'si',
4                      'calculation':'\scf\'',
5                      'mass':[28.0855],
6                      'ecutwfc':'40', # FG: I would su
7                      'pseudo_auto':True,
8                      'structure_mp':"mp-27702"
9                      },
10                      code=pathQE,
11                      env='ibrun')
12
13 # Summary
14 app = silicon.display_lattice(supercell=[2,2,1])
15 app.run()
```




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



- 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.

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