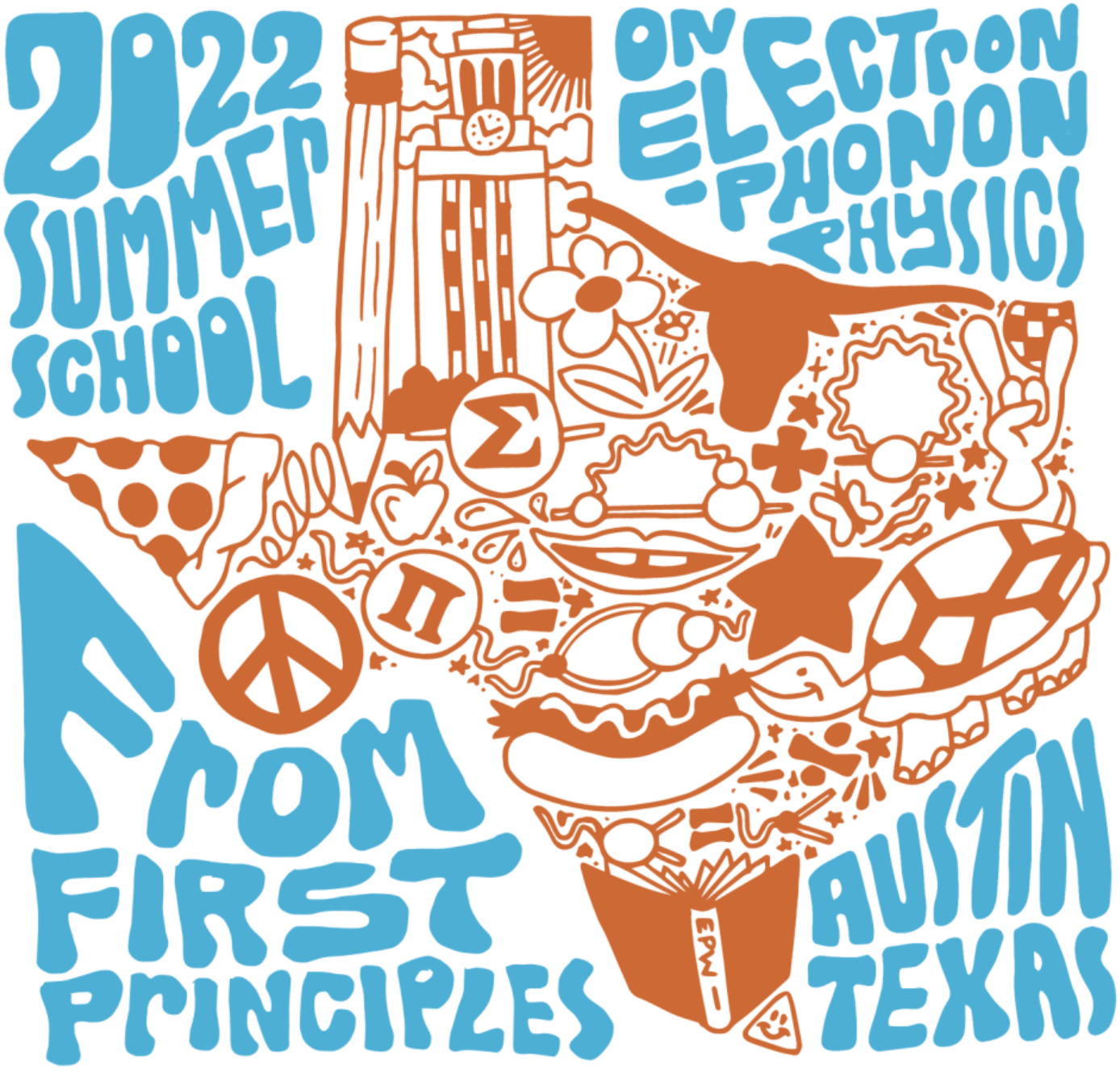

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U.S. DEPARTMENT OF ENERGY

TACC
TEXAS ADVANCED COMPUTING CENTER

ODEN

Intro to Hands-on Tutorial – Polarons

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Polaron without Supercell

Landau-Pekar Equation:

$$\underbrace{-\frac{\hbar^2}{2m^*}\nabla^2\psi(\mathbf{r})}_{\text{electron}} \underbrace{-\frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon_\infty}\right)\int\frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}\psi(\mathbf{r}')d\mathbf{r}'}_{\text{electron-lattice interaction}} = \varepsilon\psi(\mathbf{r})$$

W. H. Sio, C. Verdi, S. Poncé, and F. Giustino, Phys. Rev. Lett. 122, 246403 (2019); Phys. Rev. B 99, 235139 (2019)

Polaron without Supercell

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Full Ab initio description:

$$\underbrace{H_{\mathrm{KS}}\psi(\mathbf{r})}_{\text{electron}} \underbrace{-\left[\sum_{\kappa\alpha p}\sum_{\kappa'\alpha'p'} C^{-1}_{\kappa\alpha p\kappa'\alpha'p'}\frac{\partial V_{\mathrm{KS}}(\mathbf{r})}{\partial\tau_{\kappa\alpha p}}\int\frac{\partial V_{\mathrm{KS}}(\mathbf{r}')}{\partial\tau_{\kappa'\alpha'p'}}|\psi(\mathbf{r}')|^2 d\mathbf{r}'\right]\psi(\mathbf{r})}_{\text{electron-lattice interaction}} = \varepsilon\psi(\mathbf{r})$$

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Polaron without Supercell

Landau-Pekar Equation:

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Full Ab initio description:

$$\underbrace{H_{\mathrm{KS}}\psi(\mathbf{r})}_{\text{electron}} \underbrace{-\left[\sum_{\kappa\alpha p}\sum_{\kappa'\alpha'p'} C^{-1}_{\kappa\alpha p\kappa'\alpha'p'}\frac{\partial V_{\mathrm{KS}}(\mathbf{r})}{\partial\tau_{\kappa\alpha p}}\int\frac{\partial V_{\mathrm{KS}}(\mathbf{r}')}{\partial\tau_{\kappa'\alpha'p'}}|\psi(\mathbf{r}')|^2 d\mathbf{r}'\right]}_{\text{electron-lattice interaction}}\psi(\mathbf{r}) = \varepsilon\psi(\mathbf{r})$$

Reciprocal space:

$$N_p = N_1 \times N_2 \times N_3$$

$$\downarrow$$

$$N_k = N_1 \times N_2 \times N_3$$

$$H_{n\mathbf{k},n'\mathbf{k}'} = \delta_{n\mathbf{k},n'\mathbf{k}'}\epsilon_{n\mathbf{k}} - \frac{2}{N_p}\sum_\nu B^*_{\mathbf{k}-\mathbf{k}',\nu} g_{nn'\nu}(\mathbf{k}', \mathbf{k}-\mathbf{k}')$$

$$\sum_{n'\mathbf{k}'} H_{n\mathbf{k},n'\mathbf{k}'}A_{n'\mathbf{k}'} = \varepsilon A_{n\mathbf{k}} \longrightarrow B_{\mathbf{q}\nu} = \frac{1}{N_p}\sum_{mn\mathbf{k}} A_{m\mathbf{k}+\mathbf{q}}\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\omega_{\mathbf{q}\nu}}A_{n\mathbf{k}}$$

W. H. Sio, C. Verdi, S. Poncé, and F. Giustino, Phys. Rev. Lett. 122, 246403 (2019); Phys. Rev. B 99, 235139 (2019)

Self-Consistent Solution of Polaron Equations

$$H_{n\mathbf{k},n'\mathbf{k}'} = \delta_{n\mathbf{k},n'\mathbf{k}'}\epsilon_{n\mathbf{k}} - \frac{2}{N_p}\sum_{\nu} B^{*}_{\mathbf{k}-\mathbf{k}',\nu} g_{nn'\nu}(\mathbf{k}', \mathbf{k}-\mathbf{k}')$$

$$\sum_{n'\mathbf{k}'} H_{n\mathbf{k},n'\mathbf{k}'} A_{n'\mathbf{k}'} = \varepsilon A_{n\mathbf{k}} \quad \longrightarrow \quad B_{\mathbf{q}\nu} = \frac{1}{N_p}\sum_{mn\mathbf{k}} A_{m\mathbf{k}+\mathbf{q}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\omega_{\mathbf{q}\nu}} A_{n\mathbf{k}}$$

Self-Consistent Solution of Polaron Equations: Preparation

Interpolated (ephwann_shuffle)

$$H_{n\mathbf{k},n'\mathbf{k}'} = \delta_{n\mathbf{k},n'\mathbf{k}'}\epsilon_{n\mathbf{k}} - \frac{2}{N_p}\sum_{\nu} B^{*}_{\mathbf{k}-\mathbf{k}',\nu} g_{nn'\nu}(\mathbf{k}', \mathbf{k}-\mathbf{k}')$$

$$\sum_{n'\mathbf{k}'} H_{n\mathbf{k},n'\mathbf{k}'} A_{n'\mathbf{k}'} = \varepsilon A_{n\mathbf{k}} \longrightarrow B_{\mathbf{q}\nu} = \frac{1}{N_p}\sum_{mn\mathbf{k}} A_{m\mathbf{k}+\mathbf{q}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\omega_{\mathbf{q}\nu}} A_{n\mathbf{k}}$$

Same k and q grid nkf1/2/3 = nqf1/2/3

nkf1 = 4, nkf2 = 4, nkf3 = 4
nqf1 = 4, nqf2 = 4, nqf3 = 4

nkf1 = 5, nkf2 = 4, nkf3 = 3
nqf1 = 5, nqf2 = 4, nqf3 = 3

Self-Consistent Solution of Polaron Equations: Initialization

$$H_{n\mathbf{k},n'\mathbf{k}'} = \delta_{n\mathbf{k},n'\mathbf{k}'}\epsilon_{n\mathbf{k}} - \frac{2}{N_p}\sum_{\nu} B^{*}_{\mathbf{k}-\mathbf{k}',\nu} g_{nn'\nu}(\mathbf{k}', \mathbf{k}-\mathbf{k}')$$

$$\sum_{n'\mathbf{k}'} H_{n\mathbf{k},n'\mathbf{k}'} A_{n'\mathbf{k}'} = \varepsilon A_{n\mathbf{k}} \longrightarrow B_{\mathbf{q}\nu} = \frac{1}{N_p}\sum_{mn\mathbf{k}} A_{m\mathbf{k}+\mathbf{q}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\omega_{\mathbf{q}\nu}} A_{n\mathbf{k}}$$

Initialization $A_{n\mathbf{k}} = \exp(-\sigma_p|\mathbf{k}-\mathbf{k}_M|)$

init_sigma_plrn (Bohr)

Self-Consistent Solution of Polaron Equations: When to End

1. When reaches the maximum iterations niter_plrn

$$H_{n\mathbf{k},n'\mathbf{k}'} = \delta_{n\mathbf{k},n'\mathbf{k}'}\epsilon_{n\mathbf{k}} - \frac{2}{N_p}\sum_{\nu} B^{*}_{\mathbf{k}-\mathbf{k}',\nu} g_{nn'\nu}(\mathbf{k}', \mathbf{k}-\mathbf{k}')$$

$$\sum_{n'\mathbf{k}'} H_{n\mathbf{k},n'\mathbf{k}'} A_{n'\mathbf{k}'} = \varepsilon A_{n\mathbf{k}} \longrightarrow B_{\mathbf{q}\nu} = \frac{1}{N_p}\sum_{mn\mathbf{k}} A_{m\mathbf{k}+\mathbf{q}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\omega_{\mathbf{q}\nu}} A_{n\mathbf{k}}$$

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1. When reaches the maximum iterations niter_plrn

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2. When lattice displacement changes below convergence threshold

$$\Delta\tau_{\kappa\alpha p} = -\sum_{\mathbf{q}\nu} C^{-1}_{\mathbf{q}\kappa\nu} B^*_{\mathbf{q}\nu} D_{\kappa\alpha\nu,p}(\mathbf{q}) \qquad \max|\Delta\tau^{\text{save}}_{\kappa\alpha p} - \Delta\tau_{\kappa\alpha p}| < \varepsilon_{\text{scf}}$$

conv_thr_plrn (Bohr)

$$C_{\mathbf{q}\kappa\nu} = N_p \left(\frac{M_\kappa \omega_{\mathbf{q}\nu}}{2\hbar}\right)^{\frac{1}{2}} \qquad D_{\kappa\alpha\nu,p}(\mathbf{q}) = e_{\kappa\alpha,\nu}(\mathbf{q}) \exp(i\mathbf{q}\cdot\mathbf{R}_p)$$

Self-Consistent Solution of Polaron Equations: After Convergence

1. Coefficient in Wannier $$A_{mp} = \frac{1}{N_p} \sum_{n\mathbf{k}} A_{n\mathbf{k}} \exp\left(i\mathbf{k}\cdot\mathbf{R}_p\right) U^{\dagger}_{mn\mathbf{k}}$$

2. Formation Energy $$E_{\mathrm{Form}} = \frac{1}{N_p} \sum_{n\mathbf{k}} |A_{n\mathbf{k}}|^2 \varepsilon_{n\mathbf{k}} - \frac{1}{N_p} \sum_{n\mathbf{k}} |B_{\mathbf{q}\nu}|^2 \omega_{\mathbf{q}\nu}$$

$$H_{n\mathbf{k},n'\mathbf{k}'} = \delta_{n\mathbf{k},n'\mathbf{k}'} \epsilon_{n\mathbf{k}} - \frac{2}{N_p} \sum_{\nu} B^{*}_{\mathbf{k}-\mathbf{k}',\nu} g_{nn'\nu}(\mathbf{k}', \mathbf{k}-\mathbf{k}')$$

$$\sum_{n'\mathbf{k}'} H_{n\mathbf{k},n'\mathbf{k}'} A_{n'\mathbf{k}'} = \varepsilon A_{n\mathbf{k}} \longrightarrow B_{\mathbf{q}\nu} = \frac{1}{N_p} \sum_{mn\mathbf{k}} A_{m\mathbf{k}+\mathbf{q}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\omega_{\mathbf{q}\nu}} A_{n\mathbf{k}}$$

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$$H_{n\mathbf{k},n'\mathbf{k}'} = \delta_{n\mathbf{k},n'\mathbf{k}'} \epsilon_{n\mathbf{k}} - \frac{2}{N_p} \sum_{\nu} B^{*}_{\mathbf{k}-\mathbf{k}',\nu} g_{nn'\nu}(\mathbf{k}', \mathbf{k}-\mathbf{k}')$$

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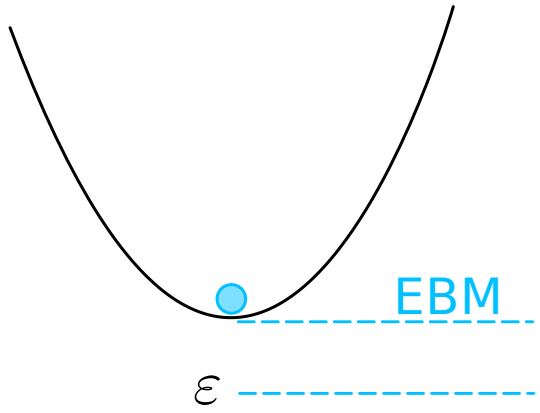
Write files: $B_{\mathbf{q}\nu}$ Bmat.plrn A_{mp} Amp.plrn $A_{n\mathbf{k}}$ Ank.plrn $\Delta\tau_{\kappa\alpha p}$ dtau.plrn/dtau.plrn.xsf

Hole Polaron vs Electron Polaron



Electron Polaron

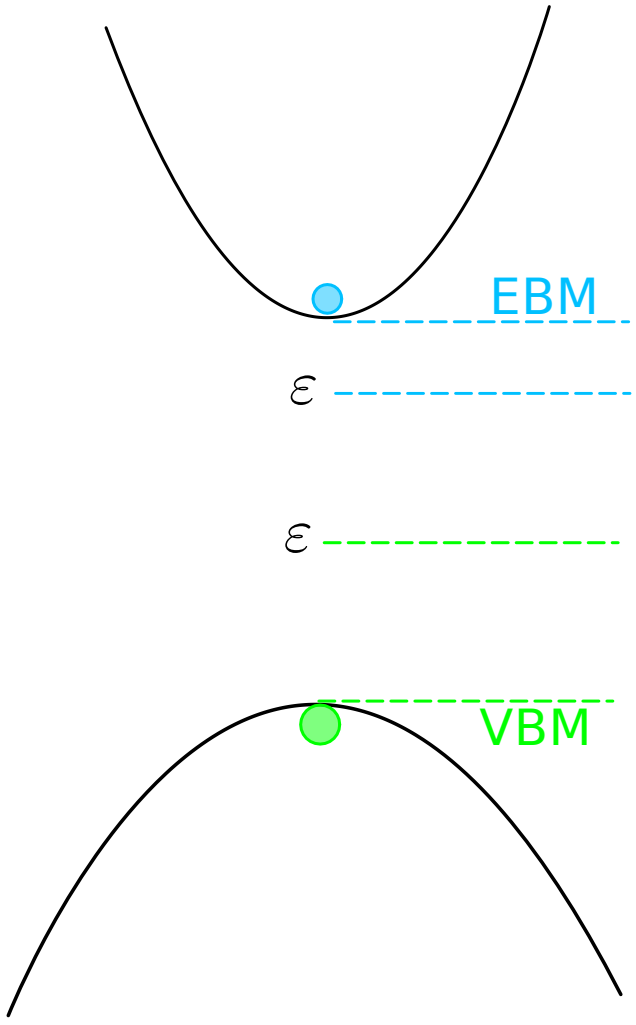
type_plrn = - 1

Reference energy EBM = 0

Electron energy $\varepsilon - \varepsilon_{\mathrm{EBM}}$

Lowest eigenvalue

Hole Polaron vs Electron Polaron



Electron Polaron

type_plrn = - 1

Reference energy EBM = 0

Electron energy $\varepsilon - \varepsilon_{\mathrm{EBM}}$

Lowest eigenvalue

Hole Polaron

type_plrn = 1

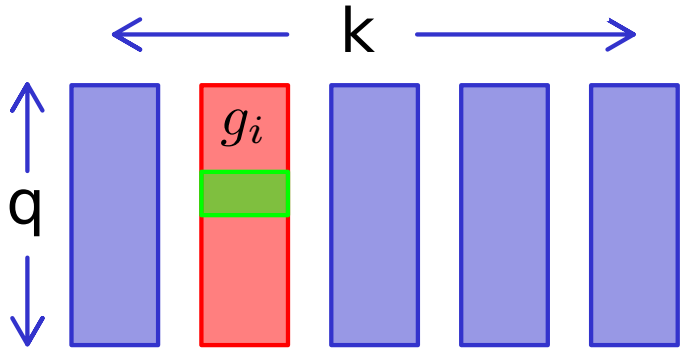
Reference energy VBM = 0

Electron energy $\varepsilon_{\mathrm{VBM}} - \varepsilon$

Highest eigenvalue

Parallelization and Diagonalization

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



mpirun -np N epw.x -nk N

Needed RAM: $(N_b \times N_k)^2 \times N_\nu \times 16/1024^4$ TB

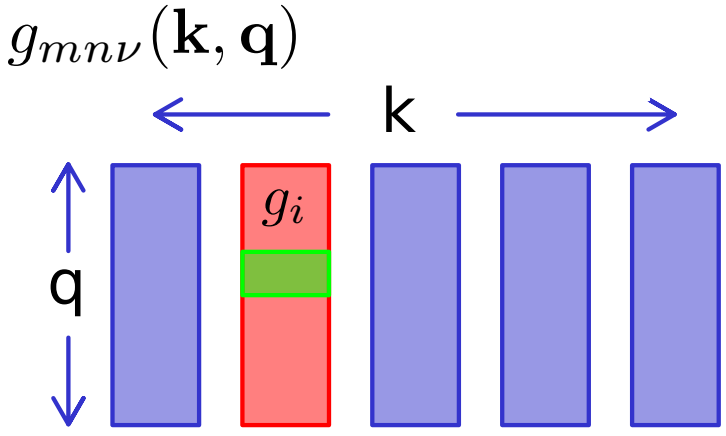
LiF electron (exercise)

$(1 \times 12 \times 12 \times 12)^2 \times 6 \times 16/1024^4 = 266$ MB

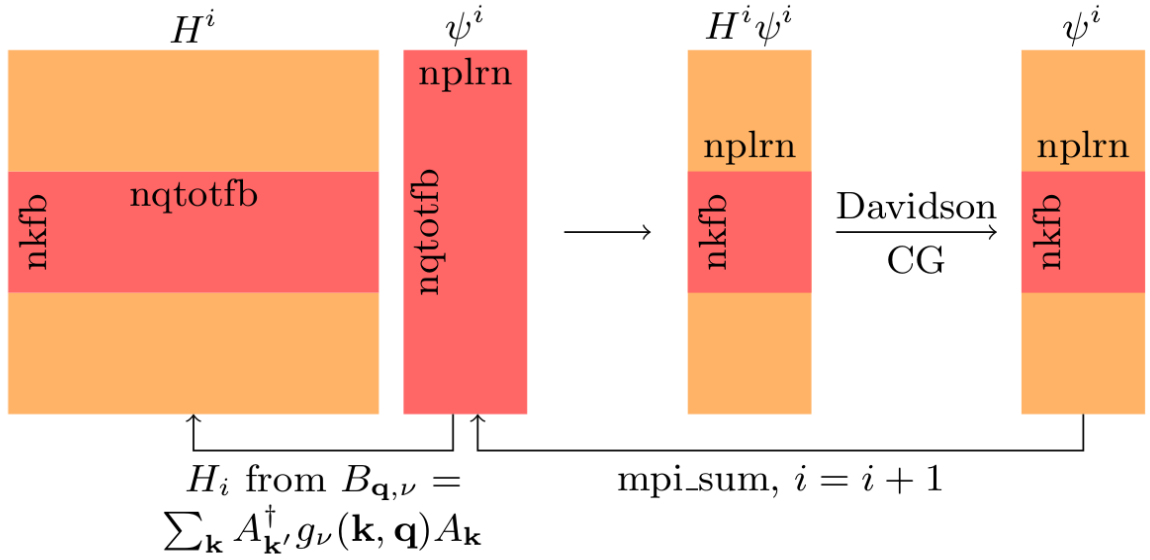
GaN hole (production)

$(6 \times 60 \times 60 \times 30)^2 \times 12 \times 16/1024^4 = 73.3$ TB

Parallelization and Diagonalization



mpirun -np N epw.x -nk N



Needed RAM: $(N_b \times N_k)^2 \times N_\nu \times 16/1024^4$ TB

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$(1 \times 12 \times 12 \times 12)^2 \times 6 \times 16/1024^4 = 266$ MB

GaN hole (production)

$(6 \times 60 \times 60 \times 30)^2 \times 12 \times 16/1024^4 = 73.3$ TB

Same iterative diagonalizer as PWscf (Davidson)

Convergence threshold for iterative diagonalization ethrdg_plrn

Post-Self-consistent Mode

calculate the real-space wavefunction of polaron

cal_psir_plrn = .true.

$$\psi(\mathbf{r}) = \sum_{mp} A_{mp} w_m(\mathbf{r} - \mathbf{R}_p)$$

Read Amp.plrn and prefix000x.cube
Write psir_plrn.xsf

Post-Self-consistent Mode

calculate the real-space wavefunction of polaron

cal_psir_plrn = .true.

$$\psi(\mathbf{r}) = \sum_{mp} A_{mp} w_m(\mathbf{r} - \mathbf{R}_p)$$

Read Amp.plrn and prefix000x.cube
Write psir_plrn.xsf

interpolate Ank on a line-mode k points

interp_Ank_plrn = .true.

$$A_{n\mathbf{k}} = \sum_{mp} A_{mp} \exp(-i\mathbf{k} \cdot \mathbf{R}_p) U_{mn\mathbf{k}},$$

Read Amp.plrn
Write Ank.band.plrn

Post-Self-consistent Mode

calculate the real-space wavefunction of polaron

cal_psir_plrn = .true.

$$\psi(\mathbf{r}) = \sum_{mp} A_{mp} w_m(\mathbf{r} - \mathbf{R}_p)$$

Read Amp.plrn and prefix000x.cube
Write psir_plrn.xsf

interpolate Ank on a line-mode k points

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$$A_{n\mathbf{k}} = \sum_{mp} A_{mp} \exp(-i\mathbf{k} \cdot \mathbf{R}_p) U_{mn\mathbf{k}},$$

Read Amp.plrn
Write Ank.band.plrn

interpolate Bqu on a line-mode q points

interp_Bqu_plrn = .true.

$$B_{\mathbf{q}\nu} = -\frac{1}{N_p} \sum_{\kappa\alpha p} C_{\mathbf{q}\kappa\nu} \Delta\tau_{\kappa\alpha p} D_{\kappa\alpha\nu,p}(\mathbf{q})$$

Read dtau.plrn
Write Bmat.band.plrn

Post-Self-consistent Mode

calculate the real-space wavefunction of polaron

cal_psir_plrn = .true.

$$\psi(\mathbf{r}) = \sum_{mp} A_{mp} w_m(\mathbf{r} - \mathbf{R}_p)$$

Read Amp.plrn and prefix000x.cube
Write psir_plrn.xsf

interpolate Ank on a line-mode k points

interp_Ank_plrn = .true.

$$A_{n\mathbf{k}} = \sum_{mp} A_{mp} \exp(-i\mathbf{k} \cdot \mathbf{R}_p) U_{mn\mathbf{k}},$$

Read Amp.plrn
Write Ank.band.plrn

interpolate Bqu on a line-mode q points

interp_Bqu_plrn = .true.

$$B_{\mathbf{q}\nu} = -\frac{1}{N_p} \sum_{\kappa\alpha p} C_{\mathbf{q}\kappa\nu} \Delta\tau_{\kappa\alpha p} D_{\kappa\alpha\nu,p}(\mathbf{q})$$

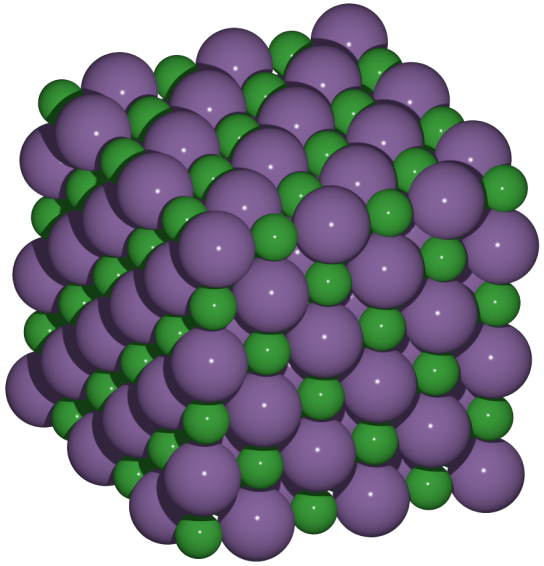
Read dtau.plrn
Write Bmat.band.plrn

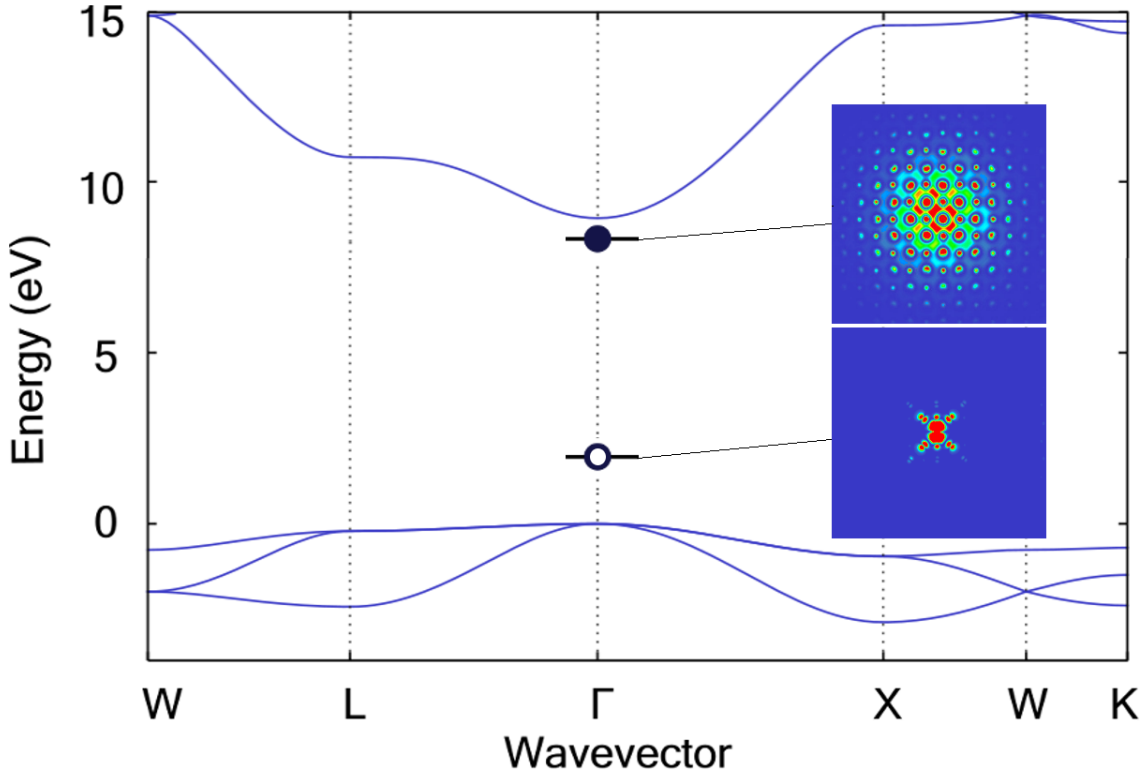
mamually generated line-mode k/q path

filkf = './path.kpt'
filqf = './path.kpt'

Example: Polaron in LiF

Determine the suitable manifold for polaron calculations





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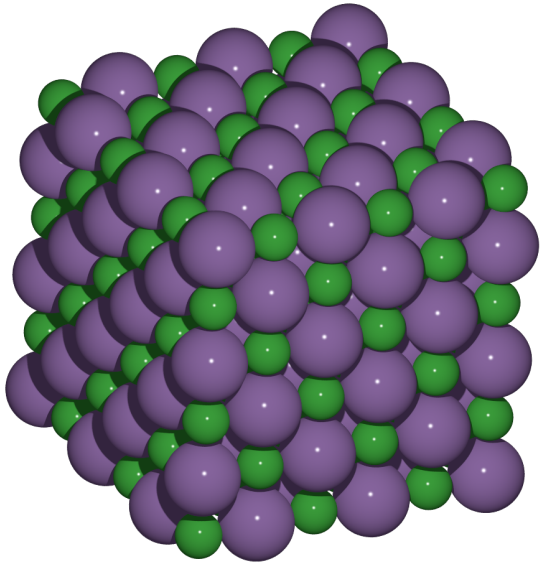

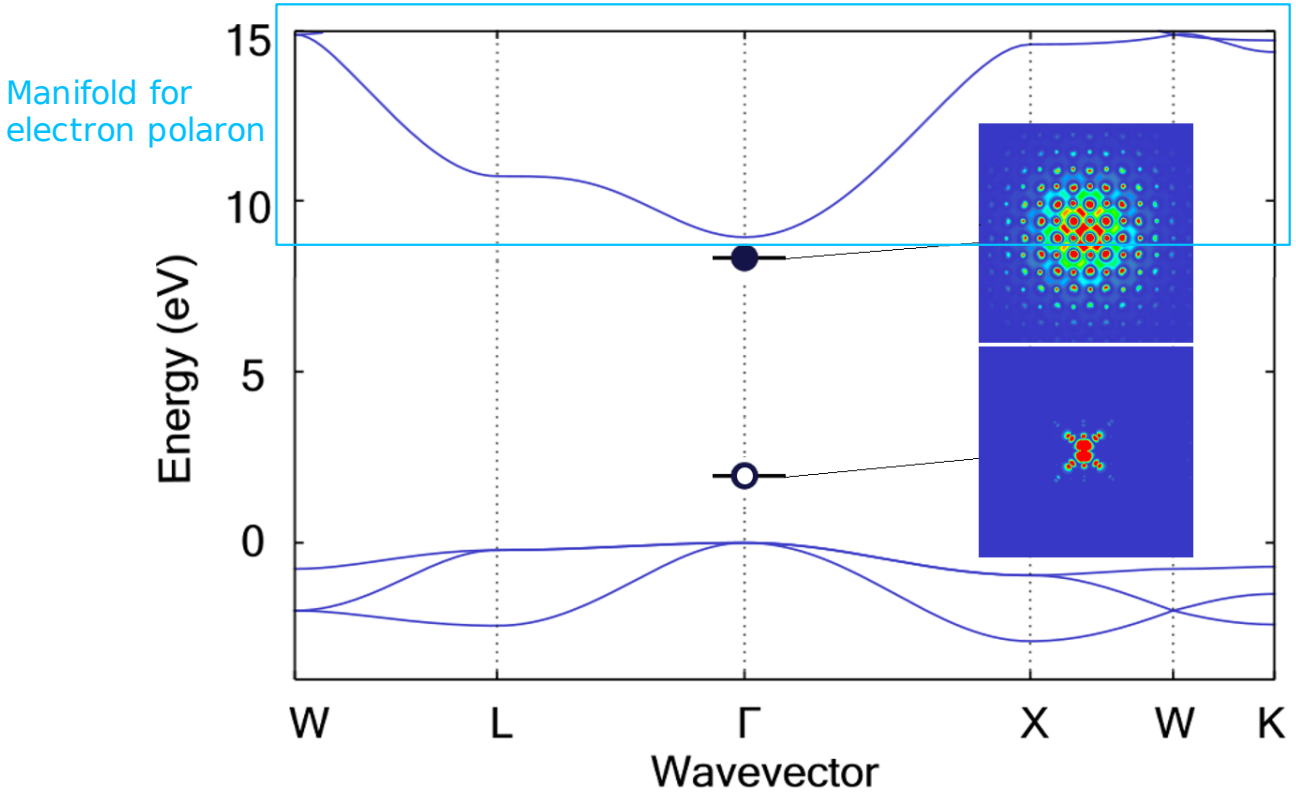

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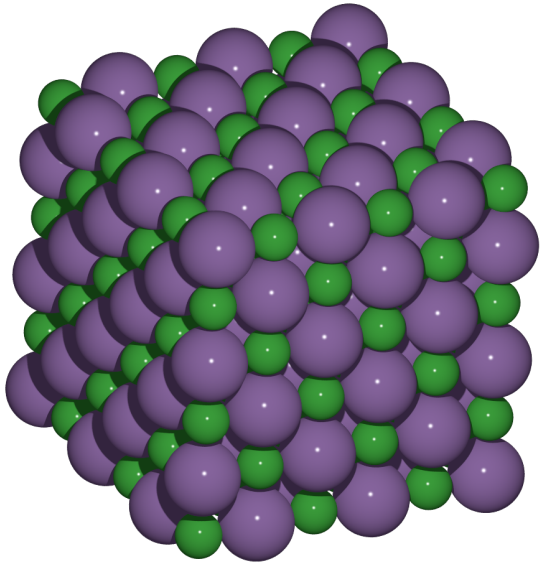

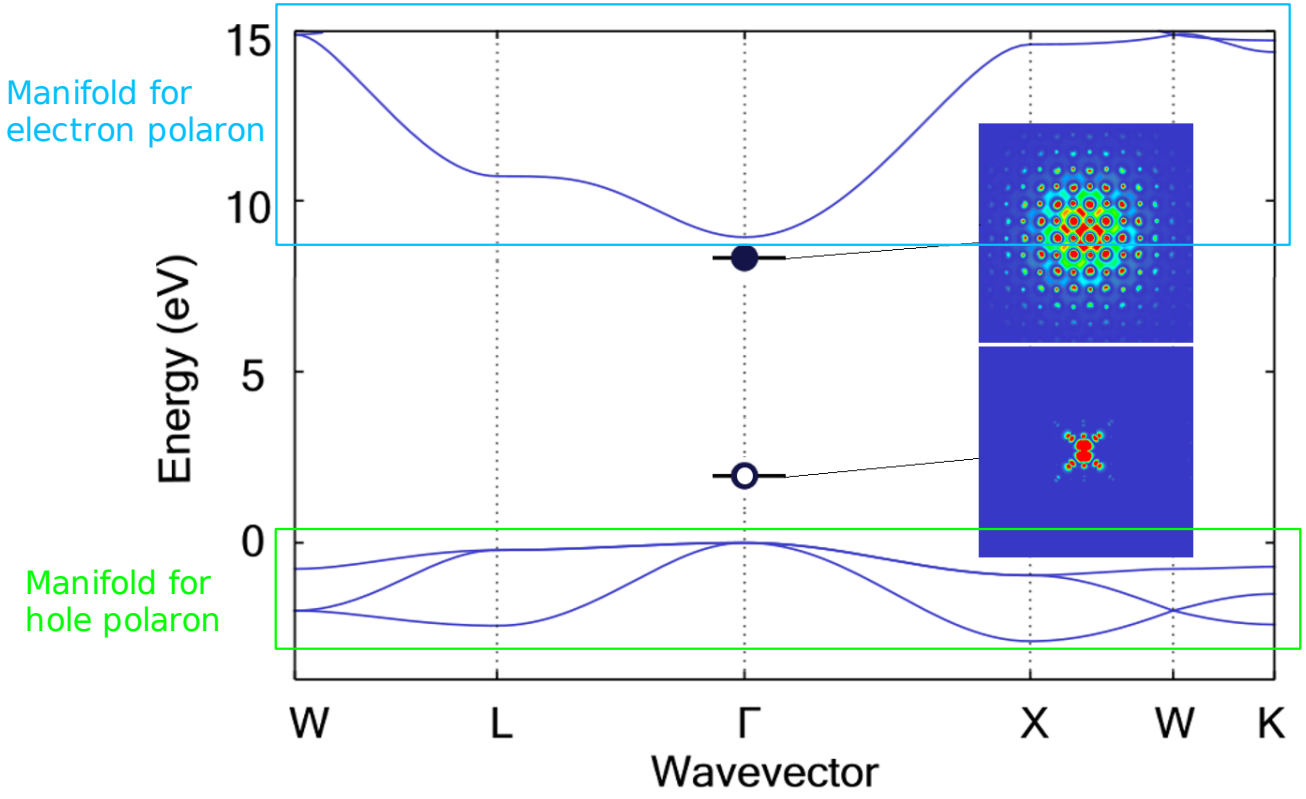

Example: Polaron in LiF

DFT and DFPT calculations

lif.scf.in → lif.save/charge-density.dat

lif.ph.in → save

lif.nscf.in → lif.save/wfc.dat

Example: Polaron in LiF

DFT and DFPT calculations

lif.scf.in

lif.ph.in

lif.nscf.in

lif.save/charge-density.dat

save

lif.save/wfc.dat

Wannierization and Coarse grid

```
elph          = .true.

epwwrite      = .true.

lpolar        = .true.

nbndsub       =  3

dvscf_dir     = './save/'

bands_skipped = 'exclude_bands = 1:2, 6:15'
wannierize    = .true.
num_iter      = 500

proj(1)       = 'F:p'

wannier_plot  = .true.
wannier_plot_supercell = 6 6 6

nk1  = 6, nk2  = 6, nk3   = 6
nq1  = 6, nq2  = 6, nq3  = 6

band_plot     = .true.
```

prefix0000x.cube
prefix.epmatwp

Example: Polaron in LiF

DFT and DFPT calculations

lif.scf.in

lif.ph.in

lif.nscf.in

lif.save/charge-density.dat

save

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wannier_plot_supercell = 6 6 6

nk1  = 6, nk2  = 6, nk3  = 6
nq1  = 6, nq2  = 6, nq3  = 6

band_plot     = .true.
```

prefix0000x.cube
prefix.epmatwp

Polaron

```
elph          = .true.

epwread       = .true.

lpolar        = .true.

plrn          = .true.

type_plrn     = 1

init_sigma_plrn  = 10.0

niter_plrn    = 500

conv_thr_plrn    = 1E-4

ethrdg_plrn      = 1E-5

nkf1  = 4, nkf2 = 4,  nkf3  = 4
nqf1  = 4, nqf2 = 4,  nqf3 = 4
```

Bmat.plrn
Amp.plrn
Ank.plrn
dtau.plrn
dtau.plrn.xsf

Example: Polaron in LiF

In standard output (lif.epw2.out)

Information of SC processes

```
Starting the self-consistent process
------------------------------------------------------------------------
 iter    Phonon/eV  Electron/eV  Formation/eV   Error/Bohr   Eigval/eV
    1  -0.2546E-02  -0.6857E-02   0.4311E-02  0.9932E-02  0.7131E-02
    2  -0.2163E-01  -0.5192E-01   0.3029E-01  0.2343E-01  0.6673E-01
    3  -0.1844E+00  -0.2167E+00   0.3226E-01  0.8901E-01  0.4747E+00
    ...
```

Example: Polaron in LiF

In standard output (lif.epw2.out)

Information of SC processes

```
Starting the self-consistent process
-------------------------------------------------------------------
 iter    Phonon/eV  Electron/eV  Formation/eV   Error/Bohr   Eigval/eV
    1  -0.2546E-02  -0.6857E-02   0.4311E-02  0.9932E-02  0.7131E-02
    2  -0.2163E-01  -0.5192E-01   0.3029E-01  0.2343E-01  0.6673E-01
    3  -0.1844E+00  -0.2167E+00   0.3226E-01  0.8901E-01  0.4747E+00
    ...
```

Energies

1
2
3
4

```
End of self-consistent cycle
          Eigenvalue (eV):      3.6726401
        Phonon part (eV):      -2.2480230
       Electron part (eV):       0.8181848
 Formation Energy (eV):      -1.4298381
```

Energies: 4 = - (1 + 2) = 2 + 3

Example: Polaron in LiF

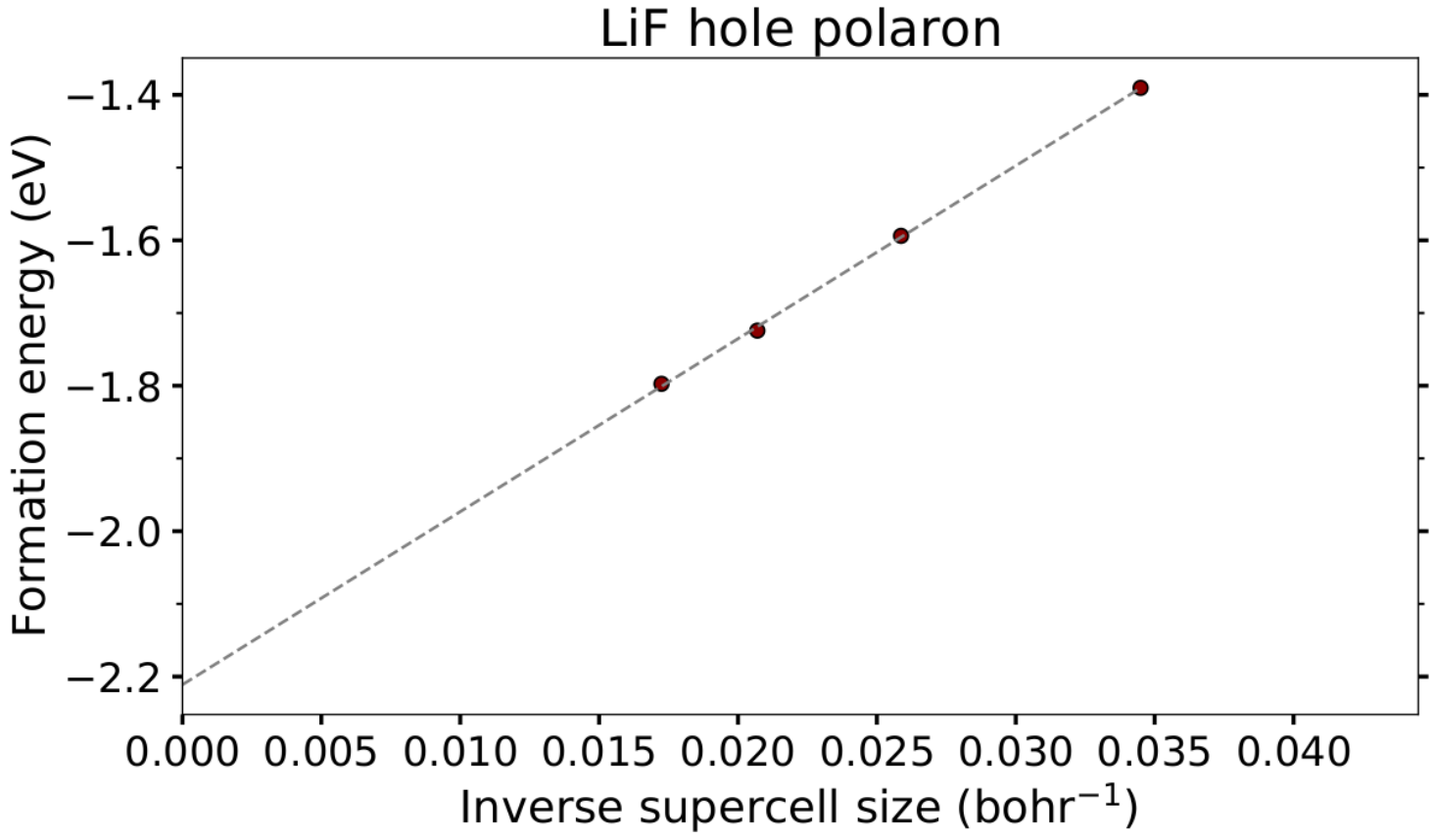
nkf1/2/3 -> supercell nkf1 x nkf2 x nkf3

Change the values of nkf1/2/3 and plot the formation energies as a function of supercell size

Example: Polaron in LiF

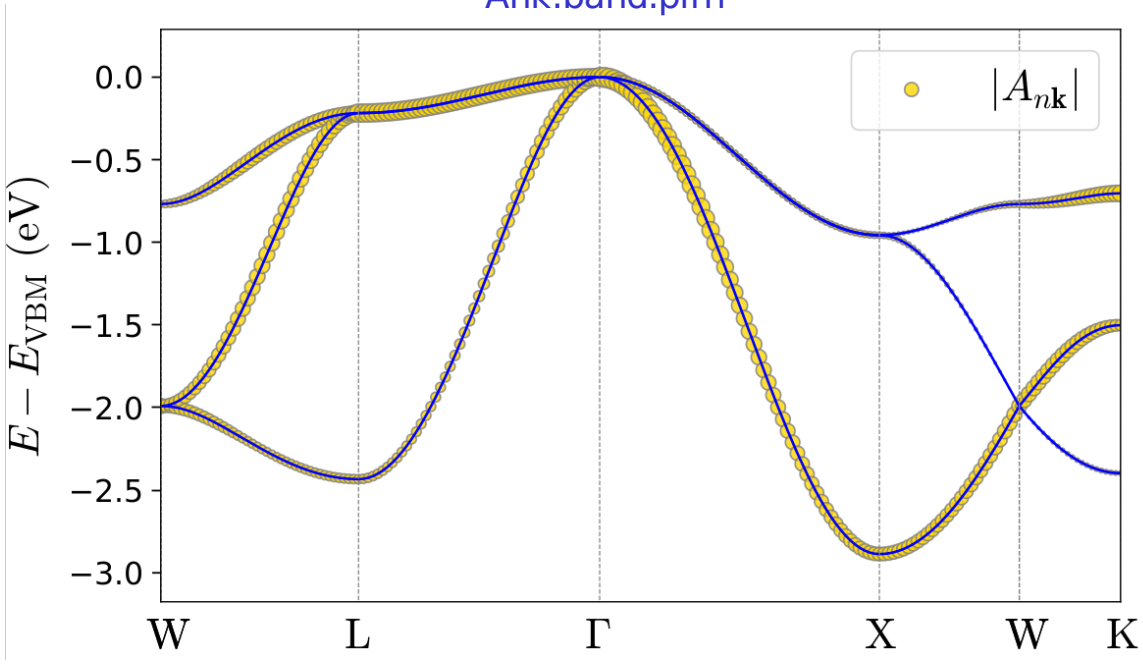
nkf1/2/3 -> supercell nkf1 x nkf2 x nkf3

Change the values of nkf1/2/3 and plot the formation energies as a function of supercell size



Example: Polaron in LiF

Ank.band.plrn



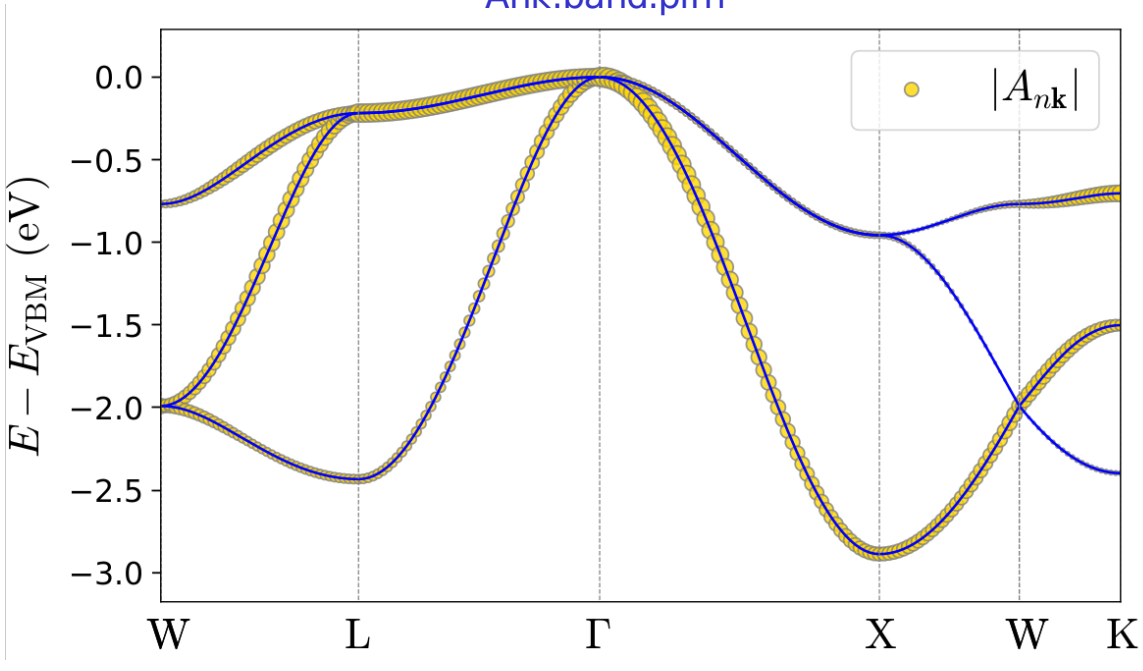
interp_Ank_plrn = .true.

$$A_{n\mathbf{k}} = \sum_{mp} A_{mp} \exp(-i\mathbf{k} \cdot \mathbf{R}_p) U_{mn\mathbf{k}},$$

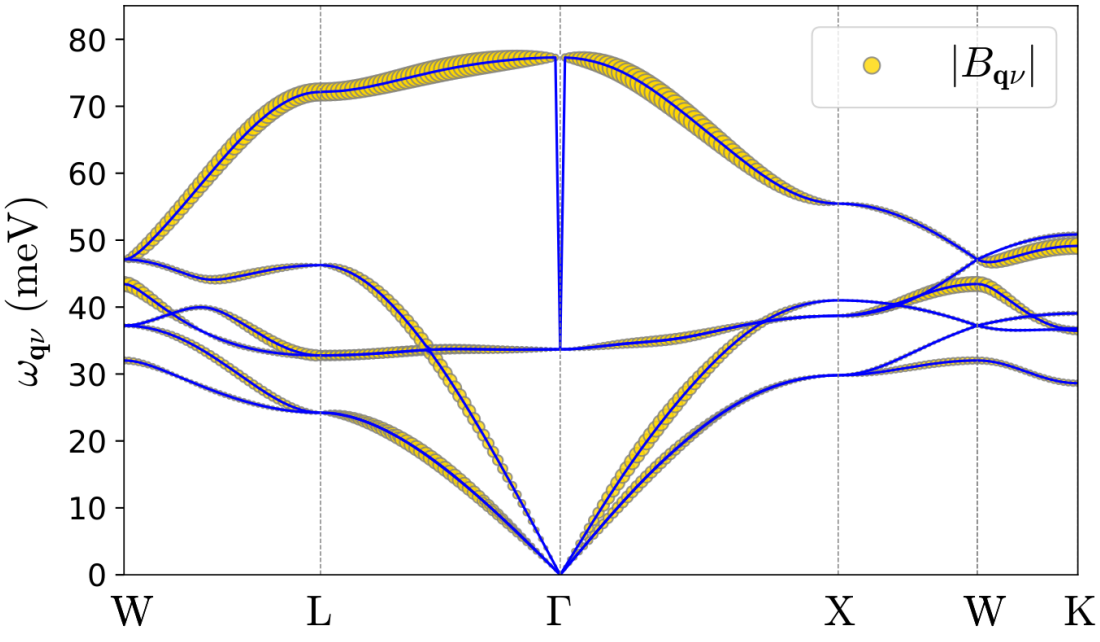
filkf = './path.kpt'

Example: Polaron in LiF

Ank.band.plrn



Bqu.band.plrn



interp_Ank_plrn = .true.

$$A_{n\mathbf{k}} = \sum_{mp} A_{mp} \exp(-i\mathbf{k}\cdot\mathbf{R}_p) U_{mn\mathbf{k}},$$

filkf = './path.kpt'

interp_Bqu_plrn = .true.

$$B_{\mathbf{q}\nu} = -\frac{1}{N_p} \sum_{\kappa\alpha p} C_{\mathbf{q}\kappa\nu} \Delta\tau_{\kappa\alpha p} D_{\kappa\alpha\nu,p}(\mathbf{q})$$

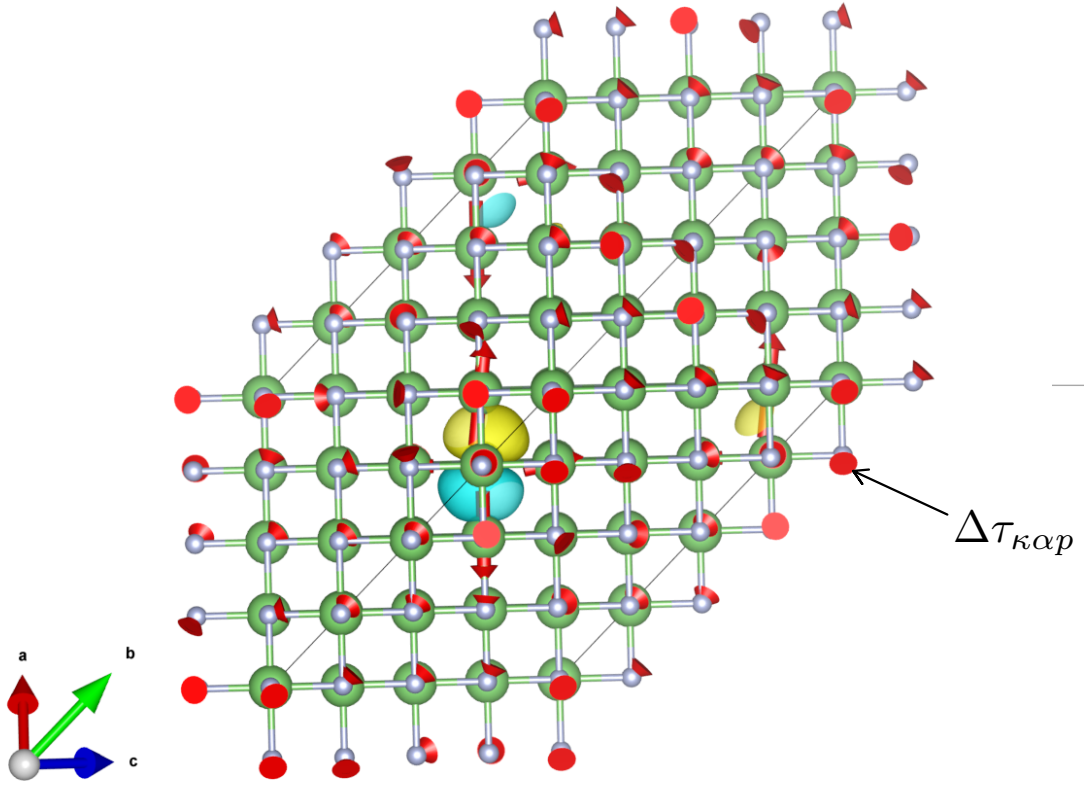
filqf = './path.kpt'

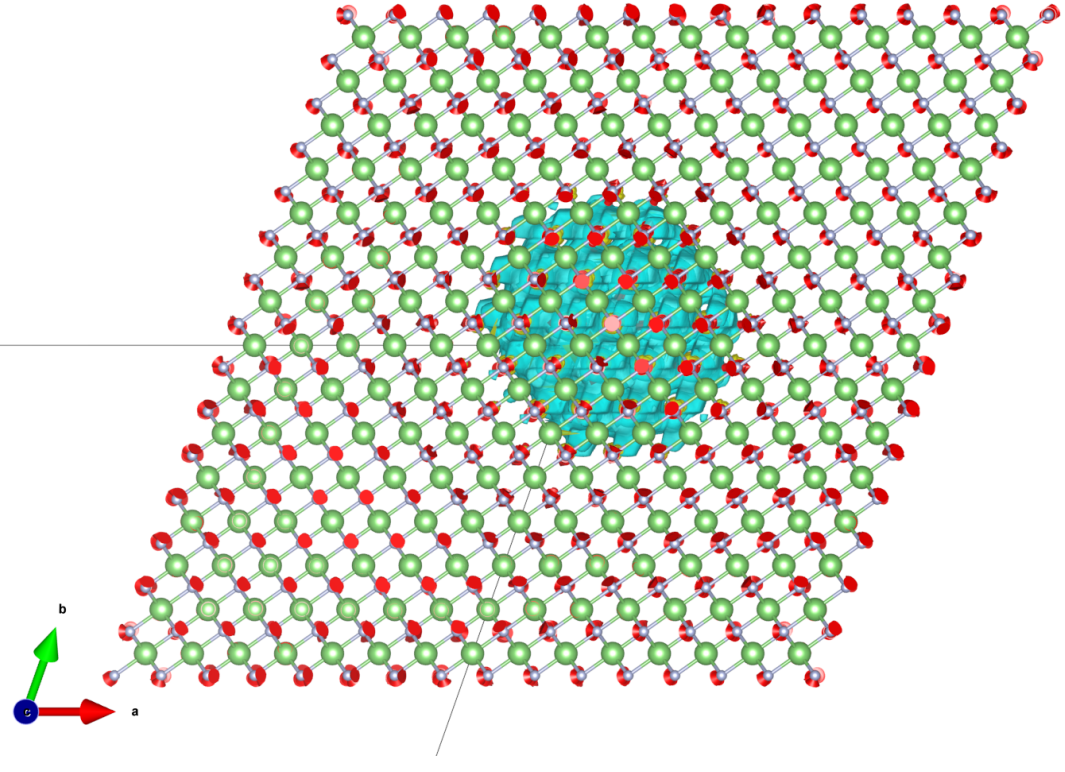
Example: Polaron in LiF

cal_psir_plrn = .true.

$$\psi(\mathbf{r}) = \sum_{mp} A_{mp} w_m(\mathbf{r} - \mathbf{R}_p)$$

psir_plrn.xsf





Summary of Parameters

plrn = .true.

SCF Mode

PP Mode

type_plrn = 1 or -1

init_sigma_plrn = 10.0 (Bohr)

niter_plrn = 500

conv_thr_plrn = 1E-4 (Bohr)

ethrdg_plrn = 1E-5

nkf1/2/3 = nqf1/2/3

interp_Ank_plrn = .true.

interp_Bqu_plrn = .true.

cal_psir_plrn = .true.

filkf = './path.kpt'