2024 School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

Interpolation of electron-phonon matrix elements

Hands-on session (Tue.6)

Hands-on based on QE-v7.3 and EPW-v5.8

In this session we will learn to use the core capabilities of EPW. In particular, we will focus on how to check the quality of Wannier interpolation of physical quantities for a future production run.

You are advised to run the calculations in your scratch directory and follow the instructions carefully. Unless you are an experienced user of EPW and Quantum ESPRESSO, do not change the directory structure and the parameters in jobscript. You can start by creating the working directory in your scratch folder and copying the tar file which contains all necessary files for this tutorial and extracting it. Then, go to the directory of the first exercise:

```
$ cd $SCRATCH
$ cp /work2/05193/sabyadk/stampede3/EPWSchool2024/tutorials/Tue.6.Lafuente.tar .
$ tar -xvf Tue.6.Lafuente.tar ; cd Tue.6.Lafuente/exercise1
```

Exercise 1

In this exercise we will calculate physical properties of metallic Pb using Quantum ESPRESSO and repeat the same calculations through Wannier interpolation using EPW. We will then compare them to check the interpolation quality. After assessing interpolation quality, we will calculate the phonon linewidth for Pb.

► 1st step: Run a self-consistent calculation on a homogeneous $8 \times 8 \times 8$ **k**-point grid and a phonon calculation on a homogeneous $3 \times 3 \times 3$ **q**-point grid using the following inputs and jobscript:

Note: The energy cutoff ecutwfc needed for convergence should be 90 Ry.

```
$ cd phonon
$ sbatch job.ph
```

job.ph

```
#!/bin/bash
#SBATCH -J myjob                 # Job name
#SBATCH -N 1                     # Total # of nodes
#SBATCH --ntasks-per-node 24
#SBATCH -t 01:00:00              # Run time (hh:mm:ss)
#SBATCH -A DMR23030
#SBATCH -p skx
#SBATCH --reservation=NSF_Summer_School_Tue

module list

# Launch MPI code...
export PATHQE=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e

ibrun $PATHQE/bin/pw.x -nk 4 -in scf.in > scf.out
ibrun $PATHQE/bin/ph.x -nk 4 -in ph.in > ph.out
```

```
--                                                                     scf.in
 &control
    calculation='scf'
    restart_mode='from_scratch',
    prefix='pb',
    pseudo_dir = '../',
    outdir='./'
 /
 &system
    ibrav=  2,
    celldm(1) = 9.2225583816,
    nat= 1,
    ntyp= 1,
    ecutwfc = 30.0
    occupations='smearing',
    smearing='marzari-vanderbilt',
    degauss=0.05
 /
 &electrons
    conv_thr =  1.0d-10
    mixing_beta = 0.7
 /
ATOMIC_SPECIES
 Pb 207.2 pb_s.UPF
ATOMIC_POSITIONS
 Pb 0.00 0.00 0.00
K_POINTS {automatic}
 8 8 8 0 0 0
```

```
--                                                                     ph.in
&inputph
prefix = 'pb',
fildyn = 'pb.dyn.xml',
fildvscf = 'dvscf',
ldisp = .true.,
nq1 = 3,
nq2 = 3,
nq3 = 3,
tr2_ph = 1.0d-16
/
```

The keyword fildvscf in `ph.in` tells the code to write on file the change of the self-consistent potential due to phonon perturbations, $\partial_{\mathbf{q}\nu} V^{\text{scf}}$, that is needed to compute the electron-phonon matrix elements.
In the output file of `ph.out`, locate the list of 4 irreducible $\mathbf{q}$ points in the Brillouin Zone (IBZ):

```
Dynamical matrices for ( 3, 3, 3)  uniform grid of q-points
(   4 q-points):
  N         xq(1)         xq(2)         xq(3)
  1   0.000000000   0.000000000   0.000000000
  2  -0.333333333   0.333333333  -0.333333333
  3   0.000000000   0.666666667   0.000000000
  4   0.666666667  -0.000000000   0.666666667
```

The list of irreducible $\mathbf{q}$ points is also written in the `pb.dyn0` file. If you type `ls`, you can see `pb.dynX.xml` file containing the dynamical matrix has been produced for each irreducible $\mathbf{q}$ point. The dvscf files are all named `pb.dvscf1` and are located inside the `_ph0/pb.q_X/` folders, except for the one corresponding to the first $\mathbf{q}$ point (Γ) that is located in _ph0/.

Note: The dynamical matrices files have been written in .xml format, which is advisable, because we specified it in the ph.in input with fildyn = 'pb.dyn.xml'.

▶ 2nd step: Calculate the phonon dispersion by using Fourier interpolation. This can be done in the following two steps:
(1) Bring the interatomic force constant to real space using a Fourier transformation with the program of q2r.x:

```
$ /work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/q2r.x -in q2r.in > q2r.out
```

```
--                                                                          q2r.in
&input
zasr='simple', fildyn='pb.dyn.xml', flfrc='pb333.fc'
/
```

Note in the output if the Fast Fourier transform (FFT) was successful:

```
fft-check success (sum of imaginary terms < 10^-12)
```

The matrix of interatomic force constants in real space should have been created (file pb333.fc.xml).

(2) Calculate the phonon dispersion along the high-symmetry lines using the program of matdyn.x:

```
$ /work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/matdyn.x -in matdyn.in > matdyn.out
```

```
--                                                                       matdyn.in
&input
  asr               = 'simple',
  flfrc             = 'pb333.fc.xml'
  flfrq             = 'pb.freq'
  q_in_band_form    = .true.
  q_in_cryst_coord = .true.
/
  6
  0.000 0.000 0.000   30 ! \Gamma
  0.500 0.000 0.500   30 ! X
  0.500 0.250 0.750   30 ! W
  0.500 0.500 0.500   30 ! L
  0.000 0.000 0.000   30 ! \Gamma
  0.375 0.375 0.750   30 ! K
```

This produces the file named pb.freq.gp with the phonon frequencies along the path, expressed in cm^{-1} unit. This will be checked against the phonon frequencies along the same path from EPW.

▶ 3rd step: Gather the .dyn and .dvscf files into a new save/ directory which EPW will read. The files in _ph0/pb.phsave/ containing the displacement patterns are also needed. This can be done using the pp.py python script which is included in the EPW/bin distribution:

```
$ python3 /work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/EPW/bin/pp.py
```

The script will ask you to enter the prefix of your calculation (pb):

```
Enter the prefix used for PH calculations (e.g. diam)
pb
```

Note: if this doesn't work when you do it after the school, you need to install numpy on your desktop. Just type "pip install numpy" and run the script again.
Note: if you want to make this more automatic, as part as a submission script for example, you can use:

```
python3 $PATHQE/EPW/bin/pp.py << EOF
pb
EOF
```

▶ 4th step: Run a non self-consistent calculation for electronic band structures using the charge density and other outputs from the previous self-consistent run:

```
$ cd ../band
$ sbatch job.band
```

```
--                                                                    job.band
#!/bin/bash
#SBATCH -J myjob             # Job name
#SBATCH -N 1                 # Total # of nodes
#SBATCH --ntasks-per-node 8
#SBATCH -t 01:00:00          # Run time (hh:mm:ss)
#SBATCH -A DMR23030
#SBATCH -p skx
#SBATCH --reservation=NSF_Summer_School_Tue

module list

# Launch MPI code...
export PATHQE=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e

mkdir pb.save
cp ../phonon/pb.save/charge-density.dat pb.save/
cp ../phonon/pb.save/data-file-schema.xml pb.save/

ibrun $PATHQE/bin/pw.x -nk 4 -in nscf.in > nscf.out
```

```
--                                                                     nscf.in
 &control
    calculation='bands'
    restart_mode='from_scratch',
    prefix='pb',
    pseudo_dir = '../',
    outdir='./'
 /
 &system
    ibrav=  2,
    celldm(1) = 9.2225583816,
    nat= 1,
    ntyp= 1,
    ecutwfc = 30.0
    occupations='smearing',
    smearing='marzari-vanderbilt',
    degauss=0.05
    nbnd=10
 /
 &electrons
    conv_thr =  1.0d-10
    mixing_beta = 0.7
 /
ATOMIC_SPECIES
 Pb 207.2 pb_s.UPF
ATOMIC_POSITIONS
```

```
 Pb 0.00 0.00 0.00
K_POINTS crystal_b
  6
  0.000 0.000 0.000  30 ! \Gamma
  0.500 0.000 0.500  30 ! X
  0.500 0.250 0.750  30 ! W
  0.500 0.500 0.500  30 ! L
  0.000 0.000 0.000  30 ! \Gamma
  0.375 0.375 0.750  30 ! K
```

Note: The difference between a `calculation='bands'` and `calculation='nscf'` is that the former uses exclusively the **k**-point provided while the latter might add points to respect crystal symmetry.

Then, run the program of `bands.x` to obtain the band structure data:

```
$ /work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/bands.x -in bands.in > bands.out
```

```
--                                                                     bands.in
&BANDS
  prefix = 'pb'
  lsym   = .false.
/
```

This will produce the file named `bands.out.gnu` which will be compared with the interpolated electronic band structure from EPW.

▶ 5th step: Run a non self-consistent calculation on a homogeneous $6 \times 6 \times 6$ $\mathbf{k}$-point grid for generating the input of wave functions for EPW and an EPW calculation for the Wannier interpolation of electronic band structure and phonon dispersion along the high-symmetry lines:

```
$ cd ../epw1
$ sbatch job.epw1
```

```
--                                                                     job.epw1
#!/bin/bash
#SBATCH -J myjob              # Job name
#SBATCH -N 1                  # Total # of nodes
#SBATCH --ntasks-per-node 8
#SBATCH -t 01:00:00           # Run time (hh:mm:ss)
#SBATCH -A DMR23030
#SBATCH -p skx
##SBATCH --reservation=NSF_Summer_School_Tue

module list

# Launch MPI code...
export PATHQE=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e

mkdir pb.save
cp ../phonon/pb.save/charge-density.dat pb.save/
cp ../phonon/pb.save/data-file-schema.xml pb.save/

ibrun $PATHQE/bin/pw.x -nk 4 -in nscf.in > nscf.out
ibrun $PATHQE/bin/epw.x -nk 8 -in epw1.in > epw1.out
```

```
--                                                                     nscf.in
 &control
    calculation='nscf'
```

```
    restart_mode='from_scratch',
    prefix='pb',
    pseudo_dir = '../',
    outdir='./'
 /
 &system
    ibrav=  2,
    celldm(1) = 9.2225583816,
    nat= 1,
    ntyp= 1,
    ecutwfc = 30.0
    occupations='smearing',
    smearing='marzari-vanderbilt',
    degauss=0.05
    nbnd=10
 /
 &electrons
    conv_thr =  1.0d-10
    mixing_beta = 0.7
 /
ATOMIC_SPECIES
 Pb 207.2 pb_s.UPF
ATOMIC_POSITIONS
 Pb 0.00 0.00 0.00
K_POINTS crystal
216
  0.00000000  0.00000000  0.00000000  4.629630e-03
  0.00000000  0.00000000  0.16666667  4.629630e-03
...
```

```
--                                                                                  epw1.in
&inputepw
  prefix      = 'pb',
  amass(1)    = 207.2
  outdir      = './'
  dvscf_dir   = '../phonon/save'

  etf_mem     = 0

  elph        = .true.
  epbwrite    = .true.
  epbread     = .false
  epwwrite    = .true.
  epwread     = .false.

  wannierize  = .true.
  nbndsub     =  4
  bands_skipped = 'exclude_bands = 1-5'
  num_iter    = 300
  dis_win_max = 21
  dis_froz_max= 13.5
  proj(1)     = 'Pb:sp3'
  wannier_plot= .true.
  wdata(1)    = 'bands_plot = .true.'
  wdata(2)    = 'begin kpoint_path'
  wdata(3)    = 'G 0.00 0.00 0.00 X 0.00 0.50 0.50'
  wdata(4)    = 'X 0.00 0.50 0.50 W 0.25 0.50 0.75'
  wdata(5)    = 'W 0.25 0.50 0.75 L 0.50 0.50 0.50'
  wdata(6)    = 'L 0.50 0.50 0.50 G 0.00 0.00 0.00'
  wdata(7)    = 'G 0.00 0.00 0.00 K 0.375 0.375 0.75'
  wdata(8)    = 'end kpoint_path'
```

```
  wdata(9)    = 'bands_num_points = 10'
  wdata(10)   = 'dis_num_iter      = 200'
  wdata(11)   = 'num_print_cycles  = 10'
  wdata(12)   = 'conv_tol = 1E-12'
  wdata(13)   = 'conv_window = 4'

  nkf1         = 1
  nkf2         = 1
  nkf3         = 1
  nqf1         = 1
  nqf2         = 1
  nqf3         = 1

  nk1         = 6
  nk2         = 6
  nk3         = 6
  nq1         = 3
  nq2         = 3
  nq3         = 3
 /
```

Note 1: In some cases, pw.x calculates additional **k**-points which are not provided in the **k**-point list of the input. If this happens, you need to use the keyword of calculation='bands' instead of calculation='nscf'. Also note that the **k** and **q** grids need to be **commensurate**, with the **k** grid at least of the size of the **q** grid. Since we chose a $6 \times 6 \times 6$ **k**-point grid, the $3 \times 3 \times 3$ **k**-point grid used in the phonon calculation is appropriate, however a $6 \times 6 \times 6$ **q**-point grid would be needed in order to interpolate more accurately the dynamical matrix and the electron-phonon matrix elements. For computational efficiency (see Phys. Rev. Research **3**, 043022 (2021)), we recommend using the same **k**-point and **q** grids.

Note 2: In dvscf_dir = '../phonon/save' we specify the directory where the .dyn, .dvscf and patterns files are stored.

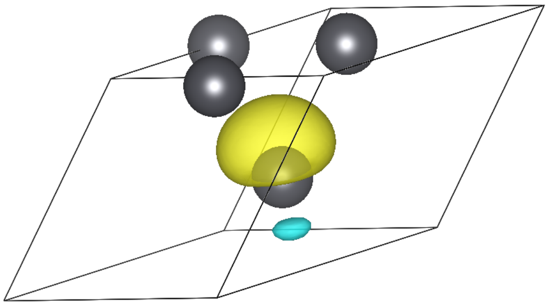
With this input, EPW will perform a Wannierzation, unfolding of the matrix elements from the IBZ on full BZ coarse grids, and Fourier transformation of the quantities into real space.

- Wannierization using Wannier90 as a library. In the output of epw1.out you can find the Wannier function centers and spreads obtained:

```
Wannier Function centers (cartesian, alat) and spreads (ang):

(    0.07779    0.07779    0.07779) :    2.22274
(    0.07779   -0.07779   -0.07779) :    2.22274
(   -0.07779    0.07779   -0.07779) :    2.22274
(   -0.07779   -0.07779    0.07779) :    2.22274
```

  while the full output from the Wannier90 run is in the file of pb.wout. The input keywords for the Wannierization are in the block following wannierize = .true.. nbndsub corresponds to the number of Wannier functions (4, starting from Pb sp^3 orbitals as the initial guess), while bands_skipped = ... specifies the list of bands not wannierized (generally a set of bands lying at lower energies, such as semicore states in this example). For the other input keywords you can refer to the page at https://docs.epw-code.org/doc/Inputs.html. It is also possible to add extra keywords that are read by Wannier90 by using the input keyword of wdata(index) with increasing index number. Here we are asking Wannier90 to plot the electronic band structure and we specify high symmetry points for this. As a result, the code will produce the following files pb_band.dat, pb_band.gnu, and pb_band.kpt.

- In addition, with the input keyword of `wannier plot= .true.` we can generate directly and efficiently in EPW the cube files containing real-space Wannier functions which can be plotted by using the plotting softwares such as VMD and VESTA; the plot of pb_00001.cube Wannier function should look like this:



- Calculate the electron-phonon matrix elements on the (**k**, **k** + **q**) points for each irreducible **q**-point in the Brillouin zone and unfold to the full Brillouin zone using symmetries. This is the most expensive part of the run. In the output you can see:

```
===================================================================
irreducible q point #    1
===================================================================

Symmetries of small group of q: 48
     in addition sym. q -> -q+G:

Number of q in the star =    1
List of q in the star:
     1   0.000000000   0.000000000   0.000000000
Imposing acoustic sum rule on the dynamical matrix

   q(    1 ) = (   0.0000000   0.0000000   0.0000000 )
...
```

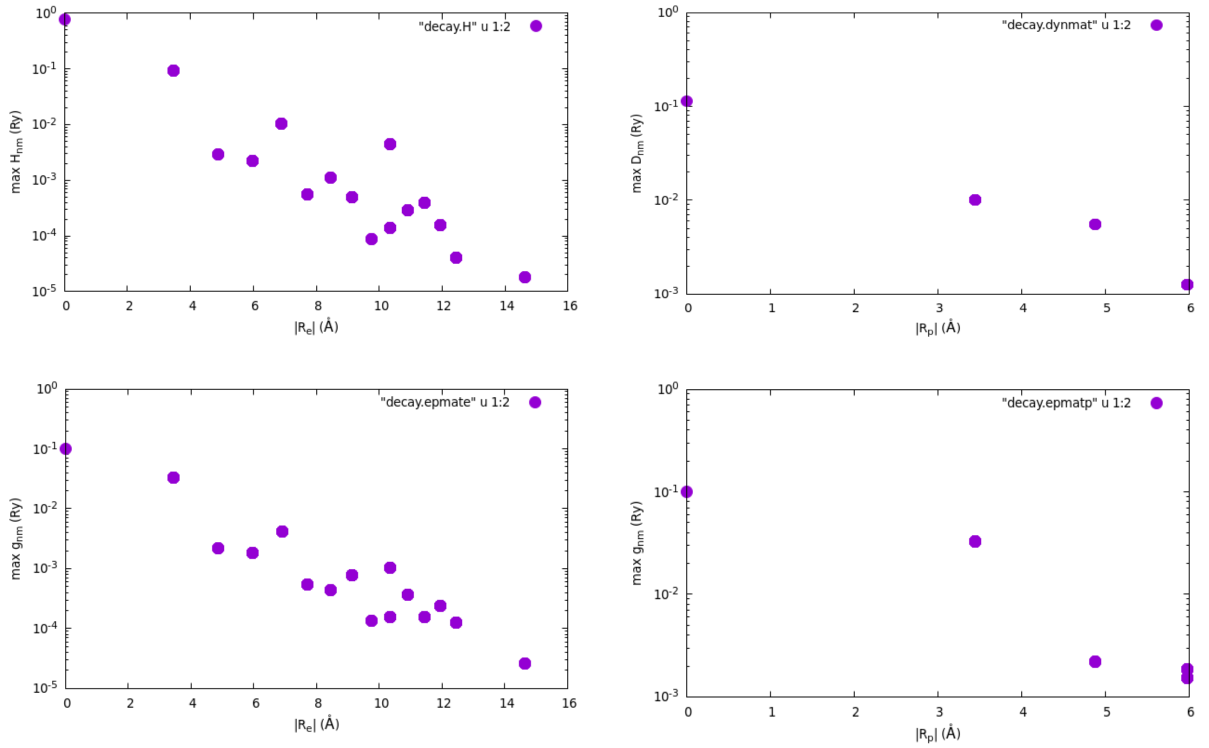
- Transform all quantities from reciprocal (Bloch) space to real (Wannier) space and store on file the resulting matrices and additional information needed for restarting a calculation (pb.epmatwp, crystal.fmt, vmedata.fmt, wigner.fmt, and epwdata.fmt files):

```
Writing Hamiltonian, Dynamical matrix and EP vertex in Wann rep to file
```

Finally, the Wannier-Fourier interpolation technique is based on the decay properties of the Wannier functions and of the phonon perturbation in real space. To check how each quantity is decaying within the supercell corresponding to our initial **k** and **q** grids, we can plot the files of decay.H (Hamiltonian), decay.dynmat (dynamical matrix) and decay.epmate (decay.epmatp) (electron-phonon matrix elements). You can obtain the following plots (note the log scale on the y axis) using gnuplot and assuming that you are connected with X11 support on Frontera and you are in the epw folder:

```
$ gnuplot
gnuplot> set encoding iso_8859_1
gnuplot> set logscale y
```

```
gnuplot> set format y "10^{%L}"
gnuplot> set pointsize 2
gnuplot> set xlabel "|R_e| (\305)"
gnuplot> set ylabel "max H_{nm} (Ry)"
gnuplot> plot "decay.H" u 1:2 w p pt 7
gnuplot> set xlabel "|R_p| (\305)"
gnuplot> set ylabel "max D_{nm} (Ry)"
gnuplot> plot "decay.dynmat" u 1:2 w p pt 7
gnuplot> set xlabel "|R_e| (\305)"
gnuplot> set ylabel "max g_{nm} (Ry)"
gnuplot> plot "decay.epmate" u 1:2 w p pt 7
gnuplot> set xlabel "|R_p| (\305)"
gnuplot> set ylabel "max g_{nm} (Ry)"
gnuplot> plot "decay.epmatp" u 1:2 w p pt 7
gnuplot> exit
```



From these plots we see clearly that we need a larger supercell (denser $\mathbf{q}$ grid) in order to interpolate more accurately the phonon properties, whereas the electronic part decays well (remember that we are using a $6 \times 6 \times 6$ $\mathbf{k}$ grid, and only a $3 \times 3 \times 3$ $\mathbf{q}$ grid).

▶ 6th step: Restart from the quantities in real space from the previous calculations and verify that the interpolated electronic and phonon bandstructure are the same as previously computed.

Note : In practice, you should also check the quality of your electron-phonon matrix element interpolation by comparing with direct DFPT calculations. We will perform such check in **Exercise 2**.

▶ Edit the `pb_band.kpt` file produced by `Wannier90` to specify that the points are in crystal units:

```
        43   crystal                                                    pb_band.kpt
    0.000000     0.000000     0.000000    1.0
    0.000000     0.050000     0.050000    1.0
    0.000000     0.100000     0.100000    1.0
    0.000000     0.150000     0.150000    1.0
```

```
    0.000000    0.200000    0.200000   1.0
    0.000000    0.250000    0.250000   1.0
    0.000000    0.300000    0.300000   1.0
    0.000000    0.350000    0.350000   1.0
...
```

Then move to the second folder for the restart calculation:

```
$ cd ../epw2
$ ln -s ../epw1/pb.epmatwp .
$ ln -s ../epw1/pb.ukk .
$ ln -s ../epw1/*.fmt .
$ ln -s ../epw1/pb_band.kpt .
$ sbatch job.epw2
```

job.epw2

```
#!/bin/bash
#!/bin/bash
#SBATCH -J myjob              # Job name
#SBATCH -N 1                  # Total # of nodes
#SBATCH --ntasks-per-node 8
#SBATCH -t 01:00:00           # Run time (hh:mm:ss)
#SBATCH -A DMR23030
#SBATCH -p skx
##SBATCH --reservation=NSF_Summer_School_Tue

module list

# Launch MPI code...
export PATHQE=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e

ibrun $PATHQE/bin/epw.x -nk 8 -in epw2.in > epw2.out
ibrun $PATHQE/bin/epw.x -nk 8 -in epw3.in > epw3.out
```

epw2.in

```
--
&inputepw
  prefix      = 'pb',
  amass(1)    = 207.2
  outdir      = './'
  dvscf_dir   = '../phonon/save'

  etf_mem     = 0

  elph        = .true.
  epbwrite    = .false.
  epbread     = .false
  epwwrite    = .false.
  epwread     = .true.

  wannierize  = .false.
  nbndsub     =  4
  bands_skipped = 'exclude_bands = 1-5'
  num_iter    = 300
  dis_win_max = 21
  dis_froz_max= 13.5
  proj(1)     = 'Pb:sp3'

  band_plot   = .true.
  fsthick     = 100    ! eV - should be large here for bandstructure plot

  filkf       = 'pb_band.kpt'
```

```
  filqf       = 'pb_band.kpt'

  nk1         = 6
  nk2         = 6
  nk3         = 6
  nq1         = 3
  nq2         = 3
  nq3         = 3
 /
```

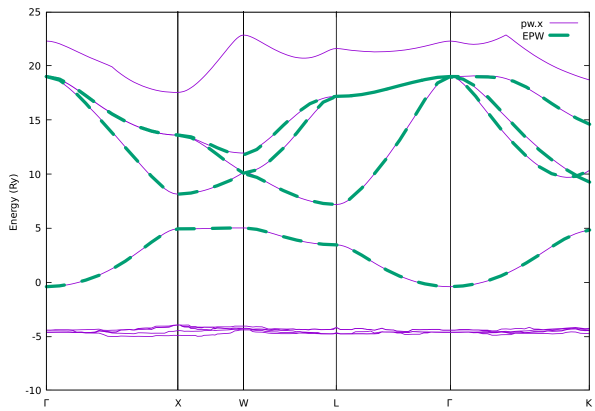
We should always check whether the Wannier-interpolated electron and phonon band structures match well to those calculated using pw.x and matdyn.x, respectively. With the input flag of band_plot = .true. in epw2.in we instructed EPW to save on files the interpolated electronic bands (band.eig) and phonon frequencies (phband.freq) and we chose to interpolate them onto the same Brillouin-zone path as previous pw.x and matdyn.x runs. This path is read from the file produced by wannier90 in the previous run and called pb_band.kpt, which is specified by the keywords of filkf and filqf. To extract easily the data to plot, you can run the plotband.x program from the Quantum ESPRESSO package and enter the input file (band.eig or phband.freq), the energy range (for example, -1 20), the output file with the data to plot (band.dat or freq.dat). The other inputs are not relevant and simply push the ENTER key when asked:

```
$ /work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/plotband.x
     Input file > band.eig
Reading    4 bands at     43 k-points
Range:   -0.4085   19.0142eV  Emin, Emax, [firstk, lastk] > -1 20
high-symmetry point:  0.0000 0.0000 0.0000   x coordinate   0.0000
high-symmetry point:  0.0000 1.0000 0.0000   x coordinate   1.0000
high-symmetry point: -0.5000 1.0000 0.0000   x coordinate   1.5000
high-symmetry point: -0.5000 0.5000 0.5000   x coordinate   2.2071
high-symmetry point:  0.0000 0.0000 0.0000   x coordinate   3.0731
high-symmetry point: -0.7500 0.7500 0.0000   x coordinate   4.1338
output file (gnuplot/xmgr) > band.dat
bands in gnuplot/xmgr format written to file band.dat
output file (ps) >
stopping ...

$ /work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/plotband.x
     Input file > phband.freq
Reading    3 bands at     43 k-points
Range:    0.0000   13.9958eV  Emin, Emax, [firstk, lastk] > 0 14
high-symmetry point:  0.0000 0.0000 0.0000   x coordinate   0.0000
high-symmetry point:  0.0000 1.0000 0.0000   x coordinate   1.0000
high-symmetry point: -0.5000 1.0000 0.0000   x coordinate   1.5000
high-symmetry point: -0.5000 0.5000 0.5000   x coordinate   2.2071
high-symmetry point:  0.0000 0.0000 0.0000   x coordinate   3.0731
high-symmetry point: -0.7500 0.7500 0.0000   x coordinate   4.1338
output file (gnuplot/xmgr) > freq.dat
bands in gnuplot/xmgr format written to file freq.dat
output file (ps) >
stopping ...
```

You can then compare your interpolated electronic band structure from EPW with the reference DFT calculation from pw.x:

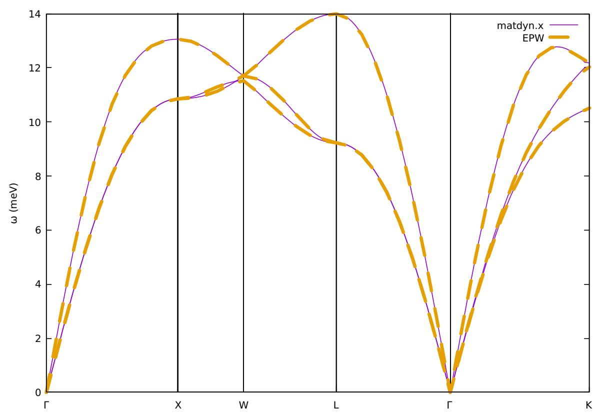
```
$ gnuplot
gnuplot> set terminal x11 enhanced
gnuplot> set encoding utf8
gnuplot> set ylabel "Energy (Ry)"
gnuplot> set xtics ("{/Symbol G}" 0, "X" 1, "W" 1.5, "L" 2.2071, "{/Symbol G}" 3.0731, "K" 4.1338)
gnuplot> set arrow from 1, graph 0 to 1, graph 1 nohead
gnuplot> set arrow from 1.5, graph 0 to 1.5, graph 1 nohead
gnuplot> set arrow from 2.2071, graph 0 to 2.2071, graph 1 nohead
gnuplot> set arrow from 3.0731, graph 0 to 3.0731, graph 1 nohead
```

```
gnuplot> plot "../band/bands.out.gnu" u 1:2 w l lw 3 title "pw.x","band.dat" u 1:2 w l lw 3 dt 2 title "EPW"
gnuplot> exit
```



We can also compare the phonon band structures:

```
$ gnuplot
gnuplot> set terminal x11 enhanced
gnuplot> set encoding utf8
gnuplot> set ylabel "{/Symbol w} (meV)"
gnuplot> set xtics ("{/Symbol G}" 0, "X" 1, "W" 1.5, "L" 2.2071, "{/Symbol G}" 3.0731, "K" 4.1338)
gnuplot> set arrow from 1, graph 0 to 1, graph 1 nohead
gnuplot> set arrow from 1.5, graph 0 to 1.5, graph 1 nohead
gnuplot> set arrow from 2.2071, graph 0 to 2.2071, graph 1 nohead
gnuplot> set arrow from 3.0731, graph 0 to 3.0731, graph 1 nohead
gnuplot> plot "../phonon/pb.freq.gp" u 1:($2/8.06554) w l lw 3 lt 1 title "matdyn.x", \
"" u 1:($3/8.06554) w l lw 3 lt 1 notitle, \
"" u 1:($4/8.06554) w l lw 3 lt 1 notitle, \
"freq.dat" u 1:2 w l lw 3 dt 2 title "EPW"
gnuplot> exit
```



▶ 7th step: We now calculate the phonon linewidths $\gamma_{\mathbf{q}\nu}$, the imaginary part of the phonon self-energy $\Pi''_{\mathbf{q}\nu}$, and the electron-phonon coupling strength $\lambda_{\mathbf{q}\nu}$ associated with a specific phonon mode ν and wavevector $\mathbf{q}$ within the double-delta approximation along high-symmetry lines by setting phonselfen=.true. delta_approx=.true.:

$$\gamma_{\mathbf{q}\nu} = \Pi''_{\mathbf{q}\nu} = 2\pi\omega_{\mathbf{q}\nu} \sum_{nm} \int_{\rm BZ} \frac{d\mathbf{k}}{\Omega_{\rm BZ}} |g_{nm\nu}(\mathbf{k},\mathbf{q})|^2 \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{\rm F})\delta(\varepsilon_{n\mathbf{k}+\mathbf{q}} - \varepsilon_{\rm F}), \quad (1)$$

where ε_{F} is the Fermi level and the coupling strength is defined as:

$$\lambda_{\mathbf{q}\nu} = \frac{1}{N(\varepsilon_{\mathrm{F}})\omega_{\mathbf{q}\nu}} \sum_{nm} \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{\Omega_{\mathrm{BZ}}} |g_{nm\nu}(\mathbf{k},\mathbf{q})|^2 \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{\mathrm{F}}) \delta(\varepsilon_{n\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathrm{F}}) = \frac{\gamma_{\mathbf{q}\nu}}{2\pi N(\varepsilon_{\mathrm{F}})\omega^2_{\mathbf{q}\nu}}, \quad (2)$$

where $N(\varepsilon_{\mathrm{F}})$ is the density of states per spin at the Fermi level.

```
--                                                                                     epw3.in
&inputepw
  prefix       = 'pb',
  amass(1)     = 207.2
  outdir       = './'
  dvscf_dir    = '../phonon/save'

  etf_mem      = 0

  elph         = .true.
  epbwrite     = .false.
  epbread      = .false
  epwwrite     = .false.
  epwread      = .true.

  wannierize   = .false.
  nbndsub      =  4
  bands_skipped = 'exclude_bands = 1-5'
  num_iter     = 300
  dis_win_max  = 21
  dis_froz_max= 13.5
  proj(1)      = 'Pb:sp3'

  phonselfen   = .true.
  delta_approx= .true.

  fsthick      = 1     ! eV
  temps        = 0.075 ! K
  degaussw     = 0.2   ! eV

  filqf        = 'pb_band.kpt'
  nkf1          = 20
  nkf2          = 20
  nkf3          = 20

  nk1          = 6
  nk2          = 6
  nk3          = 6
  nq1          = 3
  nq2          = 3
  nq3          = 3
 /
```

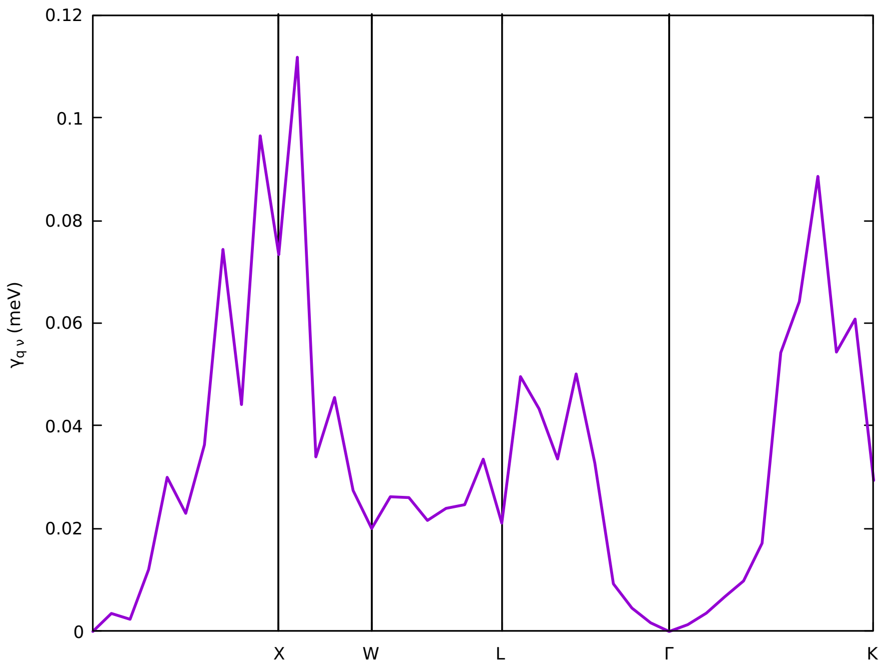
Note 1: The parameter fsthick determines the energy window around the Fermi level for which the electron-phonon matrix elements are interpolated. This can reduce significantly the cost of calculations: for example, only electronic states within a few phonon energies from the Fermi level will contribute to the phonon linewidth, therefore we can use fsthick $= 1$ (eV).

Note 2: Since calculating $\gamma_{\mathbf{q}\nu}$ and $\lambda_{\mathbf{q}\nu}$ requires an integration over **k**, we interpolate the electron-phonon matrix elements onto a denser $20 \times 20 \times 20$ **k**-point grid.

You can see that now the phonon linewidths and coupling strengths are printed in output for each phonon wavevector $\mathbf{q}$ and mode ν (`lambda___` and `gamma___`). The sum of $\lambda_{\mathbf{q}\nu}$ over all phonon modes, $\lambda_{\mathbf{q}}$, is also written (`lambda___( tot ))`. $\gamma_{\mathbf{q}\nu}$ and $\lambda_{\mathbf{q}\nu}$ are stored in the files `linewidth.phself.XXXK` and `lambda.phself.XXXK`, respectively. Inspect those files to familiarize yourself with the format and learn how to plot these quantities. For example, to plot the $\mathbf{q}$-dependent linewidth of the third phonon, you can type in `gnuplot`:

```
$ gnuplot
gnuplot> plot "linewidth.phself.0.075K" u 1:4 every 3::2 w l lw 2
```

and you should be able to produce a plot like this:



Exercise 2

In this exercise we will examine the electron-phonon interaction in semiconducting 3C-SiC which is a polar material where electrons interact with longitudinal optical modes, resulting in a Fröhlich divergence $1/|\mathbf{q}|$ divergence of the electron-phonon matrix elements for $|\mathbf{q}| \to 0$ (PRL **115**, 176401 (2015)) as well as a quadrupolar contribution in the long-wavelength limit (PRR **3**, 043022 (2021)). Here we start by checking the quality of Wannier interpolation as we did in **Exercise 1**; then we will see how to correctly interpolate the electron-phonon matrix elements in this case and calculate the electron linewidth.

▶ 1st step: Run a self-consistent calculation on a homogeneous $8 \times 8 \times 8$ **k**-point grid and a phonon calculation on a homogeneous $3 \times 3 \times 3$ $\mathbf{q}$-point grid using the following inputs and jobscript:

```
$ cd ../../exercise2
$ cd phonon
$ sbatch job.ph
```

job.ph

```
#!/bin/bash
#SBATCH -J myjob              # Job name
#SBATCH -N 1                  # Total # of nodes
#SBATCH --ntasks-per-node 8
#SBATCH -t 01:00:00           # Run time (hh:mm:ss)
#SBATCH -A DMR23030
#SBATCH -p skx
##SBATCH --reservation=NSF_Summer_School_Tue

module list

# Launch MPI code...
export PATHQE=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e

ibrun $PATHQE/bin/pw.x -nk 4 -in scf.in > scf.out
ibrun $PATHQE/bin/ph.x -nk 4 -in ph.in > ph.out
```

scf.in

```
--
 &control
    calculation     = 'scf'
    prefix          = 'sic'
    restart_mode    = 'from_scratch'
    pseudo_dir      = '../'
    outdir          = './'
 /
 &system
    ibrav           = 2
    celldm(1)       = 8.237
    nat             = 2
    ntyp            = 2
    ecutwfc         = 30.0
 /
 &electrons
    diagonalization = 'david'
    mixing_beta     = 0.7
    conv_thr        = 1.0d-10
 /
ATOMIC_SPECIES
  Si   28.0855     Si.pz-vbc.UPF
  C    12.01078    C.UPF
ATOMIC_POSITIONS alat
```

```
  Si  0.00  0.00  0.00
  C   0.25  0.25  0.25
K_POINTS automatic
8 8 8 0 0 0
```

```
--                                                                    ph.in
&inputph
  prefix   = 'sic'
  fildvscf = 'dvscf'
  ldisp    = .true
  fildyn   = 'sic.dyn.xml'
  nq1=3,
  nq2=3,
  nq3=3,
  tr2_ph   =  1.0d-16
 /
```

Note that the output of ph.out now contains also the Born effective charges Z^* and the electronic dielectric constant ϵ_∞:

```
     Electric Fields Calculation

     ....

     End of electric fields calculation

          Dielectric constant in cartesian axis

          (       7.214365306       0.000000000       0.000000000 )
     ....

          Effective charges (d Force / dE) in cartesian axis

           atom      1    Si
      Ex  (        2.67023         0.00000        -0.00000 )
      ....
```

These quantities are automatically calculated for an insulating system, using the response to a finite electric field, and determine the frequency splitting between LO and TO phonon modes.

▶ 2nd step: You should now know well how to plot the phonon dispersions using q2r.x and matdyn.x with the inputs:

```
--                                                                    q2r.in
&input
  zasr='simple', fildyn='sic.dyn.xml', flfrc='sic333.fc'
/
```

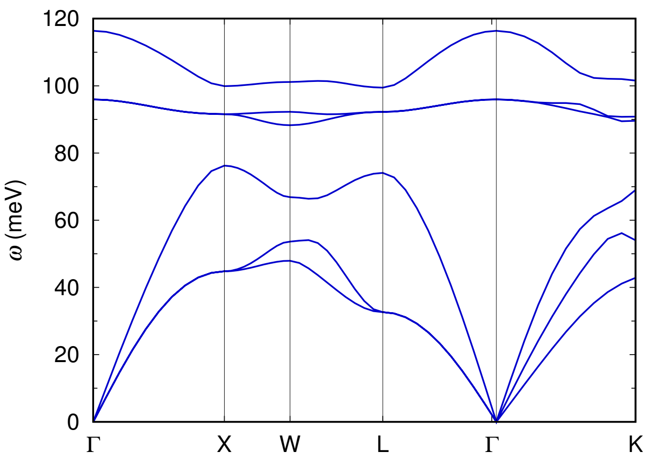
```
--                                                                 matdyn.in
&input
  asr              = 'simple',
  flfrc            = 'sic333.fc.xml'
  flfrq            = 'sic.freq'
  q_in_band_form   = .true.
  q_in_cryst_coord = .true.
/
```

```
6
0.000 0.000 0.000  30
0.500 0.000 0.500  30
0.500 0.250 0.750  30
0.500 0.500 0.500  30
0.000 0.000 0.000  30
0.375 0.375 0.750  30
```

You can plot the phonon dispersion using `sic.freq.gp`.

```
$ gnuplot
gnuplot> plot for [col=2:7] "sic.freq.gp" using 1:col w l lt 1 notitle
```

The plot should look like this:



Note that now there are 3 acoustic and 3 optical branches, separated by an energy gap, and that the so-called LO-TO splitting is present around Γ.

▶ 3rd step: Gather the `.dyn`, `.dvscf` and `patterns` files into a `save/` directory as in Exercise 1 using the `pp.py` script:

```
$ python3 /work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/EPW/bin/pp.py
```

Enter the `prefix` of your calculation (sic):

```
Enter the prefix used for PH calculations (e.g. diam)
sic
```

▶ 4th step: Run a calculation for the direct evaluation of electron-phonon matrix elements along the selected high-symmetry lines using density-functional perturbation theory.

```
$ cd ../ephline
$ sbatch job.ph
```

```
--                                                                  job.ph
#!/bin/bash
#!/bin/bash
#SBATCH -J myjob               # Job name
#SBATCH -N 1                   # Total # of nodes
#SBATCH --ntasks-per-node 18
#SBATCH -t 01:00:00            # Run time (hh:mm:ss)
#SBATCH -A DMR23030
```

```
#SBATCH -p skx
##SBATCH --reservation=NSF_Summer_School_Tue

module list

# Launch MPI code...
export PATHQE=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e

ibrun $PATHQE/bin/pw.x -nk 18 -in scf.in > scf.out
ibrun $PATHQE/bin/ph.x -nk 18 -in ephline.in > ephline.out
```

```
--                                                              ephline.in
&inputph
  prefix   = 'sic'
  fildvscf = 'dvscf'
  ldisp    = .true.
  fildyn   = 'sic.dyn.xml'
  tr2_ph   =  1.0d-16
  qplot    = .true.
  q_in_band_form = .true.
  electron_phonon = 'prt'
  kx = 0.0
  ky = 0.0
  kz = 0.0
/
3
  1.0000 0.0000 0.0000 20 # X
  0.0000 0.0000 0.0000 20 # Gamma
 -0.5000 0.5000 0.5000 1  # L
```

The electron-phonon matrix elements for $\mathbf{k} = \Gamma$ (default) and each $\mathbf{q}$ along the BZ path are written in the output of `ephline.out`, with columns corresponding to each band and phonon mode. Since electron-phonon matrix elements are gauge-dependent, an (gauge-invariant) average of their norm over degenerate subspaces of bands and modes has been performed. If you want to change the wavevector $\mathbf{k}$ of the initial state, you can do it by specifying the input flags of `kx`, `ky`, `kz` (in Cartesian $2\pi/a$ units).

To extract and plot the electron-phonon matrix elements for the valence-band top (n = m = 4) and a given frequency phonon branch (ν = 1 for example), you can type with the eight spaces between digits:

```
$ grep "4        4        1" ephline.out > data1
$ grep "4        4        3" ephline.out > data3
$ grep "4        4        4" ephline.out > data4
$ grep "4        4        6" ephline.out > data6
```

where mode index 2 and 5 are degenerate with 1 and 4, respectively. This data will be processed together with the corresponding data from EPW for comparison.

▶ 5th step: Run a non self-consistent calculation on a homogeneous $6 \times 6 \times 6$ $\mathbf{k}$-point grid for generating the input of wave functions for EPW and for the Wannier interpolation of electron-phonon matrix elements along the high-symmetry lines.

```
$ cd ../epw
$ sbatch job.epw1
```

```
--                                                                    job.epw1
#!/bin/bash
#SBATCH -J myjob              # Job name
#SBATCH -N 1                  # Total # of nodes
#SBATCH --ntasks-per-node 8
#SBATCH -t 01:00:00           # Run time (hh:mm:ss)
#SBATCH -A DMR23030
#SBATCH -p skx
##SBATCH --reservation=NSF_Summer_School_Tue

module list

# Launch MPI code...
export PATHQE=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e

mkdir sic.save
cp ../phonon/sic.save/charge-density.dat sic.save/
cp ../phonon/sic.save/data-file-schema.xml sic.save/

ibrun $PATHQE/bin/pw.x -nk 4 -in nscf.in > nscf.out
ibrun $PATHQE/bin/epw.x -nk 8 -in epw1.in > epw1.out
```

```
--                                                                    nscf.in
 &control
    calculation     = 'nscf'
    prefix          = 'sic'
    pseudo_dir      = '../'
    outdir          = './'
 /
 &system
    ibrav           = 2
    celldm(1)       = 8.237
    nat             = 2
    ntyp            = 2
    ecutwfc         = 30.0
    nbnd            = 4
 /
 &electrons
    diagonalization = 'david'
    mixing_beta     = 0.7
    conv_thr        = 1.0d-10
 /
ATOMIC_SPECIES
  Si  28.0855     Si.pz-vbc.UPF
  C   12.01078    C.UPF
ATOMIC_POSITIONS alat
  Si  0.00  0.00  0.00
  C   0.25  0.25  0.25
K_POINTS crystal
216
  0.00000000  0.00000000  0.00000000  4.629630e-03
  0.00000000  0.00000000  0.16666667  4.629630e-03
  0.00000000  0.00000000  0.33333333  4.629630e-03
...
```

```
--                                                                    epw1.in
&inputepw
  prefix      = 'sic'
  amass(1)    = 28.0855
  amass(2)    = 12.0107
```

```
  outdir      = './'
  dvscf_dir   = '../phonon/save'

  elph        = .true.
  epwwrite    = .true.
  epwread     = .false.
  lpolar      = .true.
  vme         = 'dipole'

  wannierize  = .true.
  nbndsub     =  4
  num_iter    = 300
  proj(1)     = 'Si:sp3'

  prtgkk      = .true.

  filqf       = 'path1.dat'
  nkf1        = 1
  nkf2        = 1
  nkf3        = 1

  nk1         = 6
  nk2         = 6
  nk3         = 6
  nq1         = 3
  nq2         = 3
  nq3         = 3
 /
```

Note that in order to speed up the calculation, we chose to print the electron-phonon matrix elements for the initial electronic states only at $\mathbf{k} = \Gamma$ (nkf1=nkf2=nkf3=1).

In this calculation, we consider the BZ path of X-Γ-L by providing the file path1.dat along the same direction as in the ../ephline folder but with more points:

```
101 cartesian                                                              path1.dat
    1.0000000000  0.000000000  0.000000000  1.0
    0.9800000000  0.000000000  0.000000000  1.0
    0.9600000000  0.000000000  0.000000000  1.0
    0.9400000000  0.000000000  0.000000000  1.0
    0.9200000000  0.000000000  0.000000000  1.0
    0.9000000000  0.000000000  0.000000000  1.0
    0.8800000000  0.000000000  0.000000000  1.0
    0.8600000000  0.000000000  0.000000000  1.0
....
```

This file can be generated directly using Wannier90 called in library mode from EPW or with the following python scrip:

```
import numpy as np
for ii in np.linspace(1,0,51):
    print( '{:16.10f}  0.000000000  0.000000000  1.0'.format(ii))
for ii in np.linspace(0+0.5/50,0.5,50):
    print( '{:16.10f}  {:16.10f}  {:16.10f}  1.0'.format(-ii,ii,ii))
```

Note that the printing of interpolated electron-phonon matrix elements to the output file is activated in EPW with the input variable prtgkk = .true..

Since 3C-SiC is not a metal, we set lpolar = .true. in order to correctly treat the long-range interaction in bulk crystals. The strategy consists in subtracting the long-range component $g^{\mathcal{L}}$ from the full matrix element g before interpolation and adding it back after interpolation (see e.g. npj Comput Mater **9**, 156 (2023) for more details). An analogous strategy is implemented to correctly interpolate the dynamical matrix including the long-range interactions which result in the LO-TO splitting.

In EPW, two long-range contributions can be considered: dipoles and quadrupoles. By default, only the dipoles will be considered when `lpolar = .true.`. To include quadrupoles, you need to provide a `quadrupole.fmt` file. The file must have that name and be located in the folder in which you run the calculation. We have taken the quadrupole value from Table II of Ref. PRR **3**, 043022 (2021) and the quadrupole files (3 lines per atoms) is as follow:

```
atom  dir     Qxx        Qyy        Qzz        Qyz        Qxz        Qxy
  1    1   0.000000   0.000000   0.000000   6.870000   0.000000   0.000000
  1    2   0.000000   0.000000   0.000000   0.000000   6.870000   0.000000
  1    3   0.000000   0.000000   0.000000   0.000000   0.000000   6.870000
  2    1   0.000000   0.000000   0.000000  -2.440000   0.000000   0.000000
  2    2   0.000000   0.000000   0.000000   0.000000  -2.440000   0.000000
  2    3   0.000000   0.000000   0.000000   0.000000   0.000000  -2.440000
```

Note : You can compute the quadrupole tensor for your materials via fitting of the perturbed density or fitting of direct electron-phonon matrix elements (see here or here for example). Alternatively (easiest option), you can use perturbation theory and the Abinit code to compute quadrupole tensor, see https://docs.abinit.org/topics/longwave.

You can verify that quadrupoles are correctly included in the calculation by looking at the `epw1.out` where you should find:

```
------------------------------------
Quadrupole tensor is correctly read:
------------------------------------
atom   dir        Qxx       Qyy       Qzz       Qyz       Qxz       Qxy
  1      x      0.00000   0.00000   0.00000   6.87000   0.00000   0.00000
  1      y      0.00000   0.00000   0.00000   0.00000   6.87000   0.00000
  1      z      0.00000   0.00000   0.00000   0.00000   0.00000   6.87000
  2      x      0.00000   0.00000   0.00000  -2.44000   0.00000   0.00000
  2      y      0.00000   0.00000   0.00000   0.00000  -2.44000   0.00000
  2      z      0.00000   0.00000   0.00000   0.00000   0.00000  -2.44000
```

The electron-phonon matrix elements for $\mathbf{k} = \Gamma$ and each $\mathbf{q}$ along the BZ path are written in the output of `epw1.out`, with columns corresponding to each band and phonon mode. Since electron-phonon matrix elements are gauge-dependent, an (gauge-invariant) average of their norm over degenerate subspaces of bands and modes has been performed. To extract and plot the electron-phonon matrix elements for the valence-band top (n = m = 4) and the phonon branches, as done in the 4th step, you can type with eight spaces between digits:

```
$ grep "4        4        1" epw1.out > epwdata1
$ grep "4        4        3" epw1.out > epwdata3
$ grep "4        4        4" epw1.out > epwdata4
$ grep "4        4        6" epw1.out > epwdata6
```

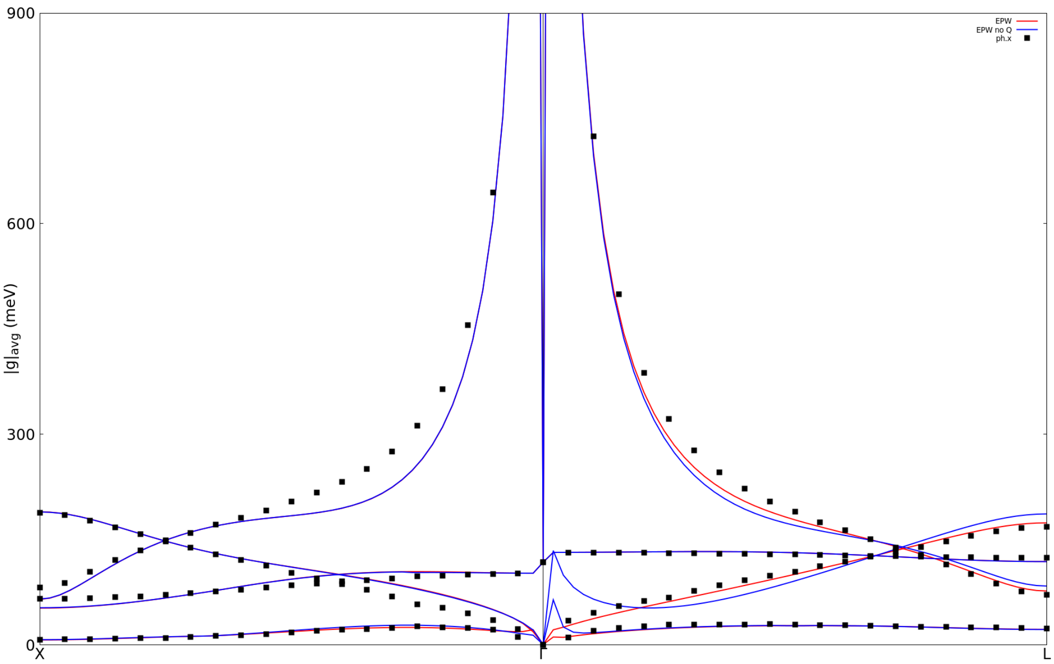
You can now compare the direct DFPT calculation made before with the interpolated results using gnuplot (assume you connected with X11 support on Frontera and you are in the epw folder):

```
$ gnuplot
gnuplot> set terminal x11 enhanced
gnuplot> set encoding utf8
gnuplot> set ylabel "|g|_{avg} (meV)" font ",20"
```

```
gnuplot> set xtics ("X" 0, "{/Symbol G}" 50, "L" 100) font ",20"
gnuplot> set ytics (0,300,600,900) font ",20"
gnuplot> set arrow from 50, graph 0 to 50, graph 1 nohead
gnuplot> set yrange[0:900]

gnuplot> plot "epwdata1" u 7 w l lw 2 lc rgb "red" title "EPW",\
     "epwdata3" u 7 w l lw 2 lc rgb "red" notitle,\
     "epwdata4" u 7 w l lw 2 lc rgb "red" notitle,\
     "epwdata6" u 7 w l lw 2 lc rgb "red" notitle

gnuplot> replot "../ephline/data1" u ($0*2.5):7 w p pt 5 ps 1.5 lc rgb "black" title "ph.x"
    "../ephline/data3" u ($0*2.5):7 w p pt 5 ps 1.5 lc rgb "black" notitle,\
    "../ephline/data4" u ($0*2.5):7 w p pt 5 ps 1.5 lc rgb "black" notitle,\
    "../ephline/data6" u ($0*2.5):7 w p pt 5 ps 1.5 lc rgb "black" notitle

gnuplot> exit
```

Note : We multiply the DFPT x-axis by 2.5 simply because this is the ratio of number of points computed with `EPW`.

You should obtain the following figure:



Note that we are also showing the results without quadrupole in that figure (blue line). You can try to obtain this by simply removing the quadrupole.fmt file and re-running `epw1.in`. In addition, note that the interpolated ones are not fully accurate, since a larger coarse $\mathbf{q}$-grid is needed in order to accurately interpolate the electron-phonon matrix elements.

Note: if you want to inspect the results of the interpolation when the long-range contribution to the matrix elements is not taken into account, you can run a new calculation using `lpolar=.false.`. Remember to run this test in a new directory, or to run again an `EPW` calculation from scratch using `lpolar=.true.`.

▶ 6th step: We now calculate the linewidths of the valence states in SiC along high-symmetry lines, which correspond to twice the imaginary part of the electron self-energy $\Sigma''_{n\mathbf{k}}$:

$$\Sigma''_{n\mathbf{k}}(\omega,T) = \pi \sum_{m\nu} \int_{\rm BZ} \frac{d\mathbf{q}}{\Omega_{\rm BZ}} |g_{mn,\nu}(\mathbf{k},\mathbf{q})|^2 \Big\{ [n_{\mathbf{q}\nu}(T) + f_{m\mathbf{k+q}}(T)]\delta(\omega - (\varepsilon_{m\mathbf{k+q}-\varepsilon_{\rm F}}) + \omega_{\mathbf{q}\nu}) + [n_{\mathbf{q}\nu}(T) + 1 - f_{m\mathbf{k+q}}(T)]\delta(\omega - (\varepsilon_{m\mathbf{k+q}-\varepsilon_{\rm F}}) - \omega_{\mathbf{q}\nu}). \quad (3)$$

To do so, we need to use the input variable `elecselfen = .true.`, the $\mathbf{k}$-point path, and a homogeneous $\mathbf{q}$ grid for the integration.

```
$ sbatch job.epw2
```

```
--                                                                                   job.epw2
#!/bin/bash
#SBATCH -J myjob              # Job name
#SBATCH -N 1                  # Total # of nodes
#SBATCH --ntasks-per-node 8
#SBATCH -t 01:00:00           # Run time (hh:mm:ss)
#SBATCH -A DMR23030
#SBATCH -p skx
##SBATCH --reservation=NSF_Summer_School_Tue

module list

# Launch MPI code...
export PATHQE=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e

ibrun $PATHQE/bin/epw.x -nk 8 -in epw2.in > epw2.out
```

```
--                                                                                   epw2.in
&inputepw
  prefix      = 'sic'
  amass(1)    = 28.0855
  amass(2)    = 12.0107
  outdir      = './'
  dvscf_dir   = '../phonon/save'

  etf_mem     = 0

  elph        = .true.
  epwwrite    = .false.
  epwread     = .true.
  lpolar      = .true.
  vme         = 'dipole'

  wannierize  = .false.
  nbndsub     =  4
  num_iter    = 300
  proj(1)     = 'Si:sp3'

  elecselfen  = .true.
  efermi_read = .true.
  fermi_energy= 9.6

  fsthick     = 7.0
  temps       = 20
  degaussw    = 0.05

  filkf       = 'path2.dat'
  nqf1        = 20
```

```
  nqf2        = 20
  nqf3        = 20

  nk1         = 6
  nk2         = 6
  nk3         = 6
  nq1         = 3
  nq2         = 3
  nq3         = 3
 /
```

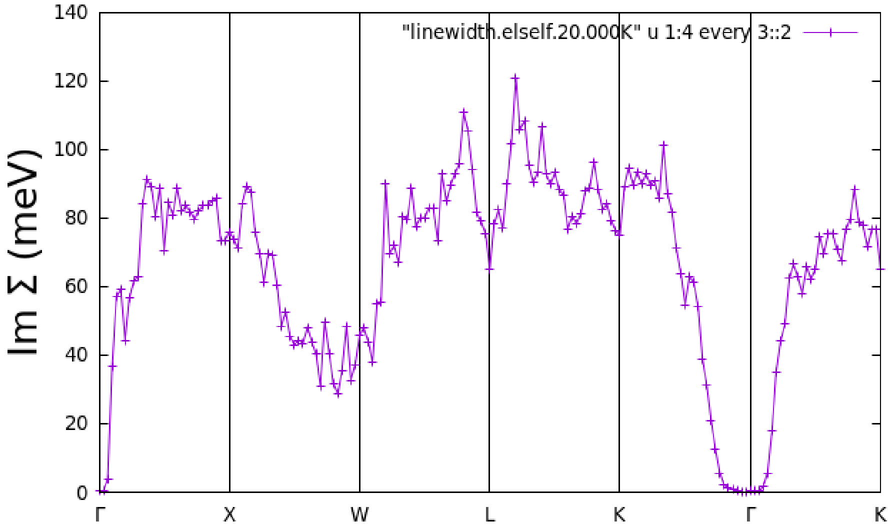
Note that since we use a $\mathbf{k}$ path, the Fermi energy calculated from the fine (interpolated) grid will not be accurate. To overcome this problem, we provide the Fermi energy in the input by using `efermi_read = .true.` and fermi_energy=9.6 (just above the valence-band top).

In the output you can monitor the progression of the $\mathbf{q}$ integration, before reading the electron self-energy for each $\mathbf{k}$ point:

```
     Progression iq (fine) =         50/       8000
     Progression iq (fine) =        100/       8000
     ...
     ...
     Average over degenerate eigenstates is performed
     Temperature:   20.000K
     WARNING: only the eigenstates within the Fermi window are meaningful

     ik =        1 coord.:     0.0000000    0.0000000    0.0000000
     -------------------------------------------------------------------
     E(    2 )=  -0.2406 eV   Re[Sigma]=      96.661664 meV Im[Sigma]=       0.240285 meV
     E(    3 )=  -0.2406 eV   Re[Sigma]=      96.661664 meV Im[Sigma]=       0.240285 meV
     E(    4 )=  -0.2406 eV   Re[Sigma]=      96.661664 meV Im[Sigma]=       0.240285 meV
     -------------------------------------------------------------------
...
```

Note that the electron energies are now reported with respect to E_{F}. Moreover, the self-energy for the first valence band is not computed since fsthick is 7 eV. To plot the linewidths you can use the file `linewidth.elself` that has been created. For example, ImΣ for the highest valence band should look like:

```
$ gnuplot
gnuplot> set terminal x11 enhanced
gnuplot> set encoding utf8
gnuplot> set ylabel "Im {/Symbol S} (meV)" font ",20"
gnuplot> set xtics ("{/Symbol G}" 1, "X" 31, "W" 61, "L" 91, "K" 121, "{/Symbol G}" 151, "K
gnuplot> set arrow from 31, graph 0 to 31, graph 1 nohead
gnuplot> set arrow from 61, graph 0 to 61, graph 1 nohead
gnuplot> set arrow from 91, graph 0 to 91, graph 1 nohead
gnuplot> set arrow from 121, graph 0 to 121, graph 1 nohead
gnuplot> set arrow from 151, graph 0 to 151, graph 1 nohead
gnuplot> set yrange[0:140]
gnuplot> plot "linewidth.elself.20.000K" u 1:4 every 3::2 w lp
gnuplot> exit
```



Note1: If you want to plot the electron lifetimes, these are given by $\tau_{n\mathbf{k}} = \hbar/(2\text{Im}\Sigma_{n\mathbf{k}})$.

Note2: Can you understand the behavior of the linewidths along the Brillouin-zone path? It is useful to look also at the electronic band structure.

Note3: You can also look at the contribution of each phonon mode by using `iverbosity = 3` in the input. The file `linewidth.elself` will then contain the mode-resolved linewidths. Can you tell which phonon has the largest contribution and why?

▶ Try increasing the $\mathbf{q}$ grid, and also using a random set of $\mathbf{q}$ points: you will see the linewidths are not well converged yet. For polar materials it is indeed more difficult to converge Brillouin-zone integrals, due to the $1/|\mathbf{q}|$ divergence of the Fröhlich matrix elements.

Extra exercise

Repeat the 4th and 6th steps of Exercise 2 with the wavevector $\mathbf{k}$ of the initial state set to (-0.5,-1.0,0.0) (in Cartesian $2\pi/a$ units).

Hint: You can proceed in the following way:

```
$ cd ephline
* Modify the following lines in ephline.in:
! kx = 1.2500000
! ky = 0.8750000
! kz = 1.2500000
$ sbatch job.ph
$ cd ../epw/
* Modify the following lines in epw1.in:
nkf1 = 1
nkf2 = 1
nkf3 = 1
* And create a necessary file.
$ sbatch job.epw1
```