Hands-on Tue.4

Hands-On Intro: Running EPW

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EPW

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Structure of the input data

title_line

&inputepw

...

/

nqs {cartesian}

xq(1) xq(2) xq(3) wq

Note: the k/q-points of the fine grids have to be provided in crystal coordinate only.

&inputepw

A a2f, amass, asr_typ, assume_metal

B band_plot, bands_skipped, bnd_cum, broyden_beta, broyden_ndim

C carrier, conv_thr_iaxis, conv_thr_racon, conv_thr_raxis, cumulant

D degaussq, degaussw, delta_approx, delta_qsmear, delta_smear, dvscf_dir

E efermi_read, eig_read, elecselfen, eliashberg, elph, ep_coupling, epbwrite, epbread, epexst, ephwrite, eps_acustic, epsiHEG, epwread, epwwrite, etf_mem

F fermi_diff, fermi_energy, fila2f, fildvscf, filkf, filqf, filukk, filukq, fsthick

G gap_edge

I imag_read, int_mob, iterative_bte, iverbosity

K kerread, kerwrite, kmaps

L lacon, laniso, lifc, limag, lindabs, liso, longrange, lpade, lphase, lpolar, lreal, lscreen, lunif

M max_memlt, meff, mob_maxiter, mp_mesh_k, mp_mesh_q, muc

N nbndsub, ncarrier, nc, nel, nest_fn, ngaussw, nk1, nk2, nk3, nkf1, nkf2, nqf3, nq1, nq2, nq3, nqf1, nqf2, nqf3, nqsmear, nqstep, n_r, nsiter, nsmear, nstemp, nswi, nswc, nswfc, nw, nw_specfun

O omegamax, omegamin, omegastep

P phonselfen, plselfen, prefix, prtgkk, pwc

R rand_nq, rand_nk, rand_q, rand_k, restart, restart_step

S scr_typ, scattering, scattering_serta, scissor, smear_rpa, specfun_el, specfun_ph, specfun_pl, system_2d, shortrange

T temps

V vme

W wannierize, wepexst, wmax, wmax_specfun, wmin, wmin_specfun, wscut, wsfc

/

nqs, xq(1) xq(2) xq(3)

https://docs.epw-code.org/doc/Inputs.html (to be updated)

Basic input templates

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

  elph        = .true.
  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.

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

Input&Output

Control

Wannierization

k, **q** coarse grids

Basic input templates

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

  elph        = .true.
  epwwrite    = .true.
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  num_iter    = 300
  dis_win_max = 21
  dis_froz_max= 13.5
  proj(1)     = 'Pb:sp3'
  wannier_plot= .true.

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

1. outdir/prefix.save dir. points to the directory where nscf results are stored.
2. prefix is a prefix of EPW outputs.
3. Most (not all) EPW outputs are stored in outdir.

Basic input templates

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

  elph        = .true.
  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.

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

1. Not important. Overwritten by the nscf data.

Basic input templates

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

  elph        = .true.
  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.

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

1. dvscf_dir points to the directory where outputs from ph.x are stored; they can be simply collected by the script pp.py.

Basic input templates

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

  elph        = .true.
  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.

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

1. *e*-ph vertex calculation is done only when elph=.true. (in default, .false.)

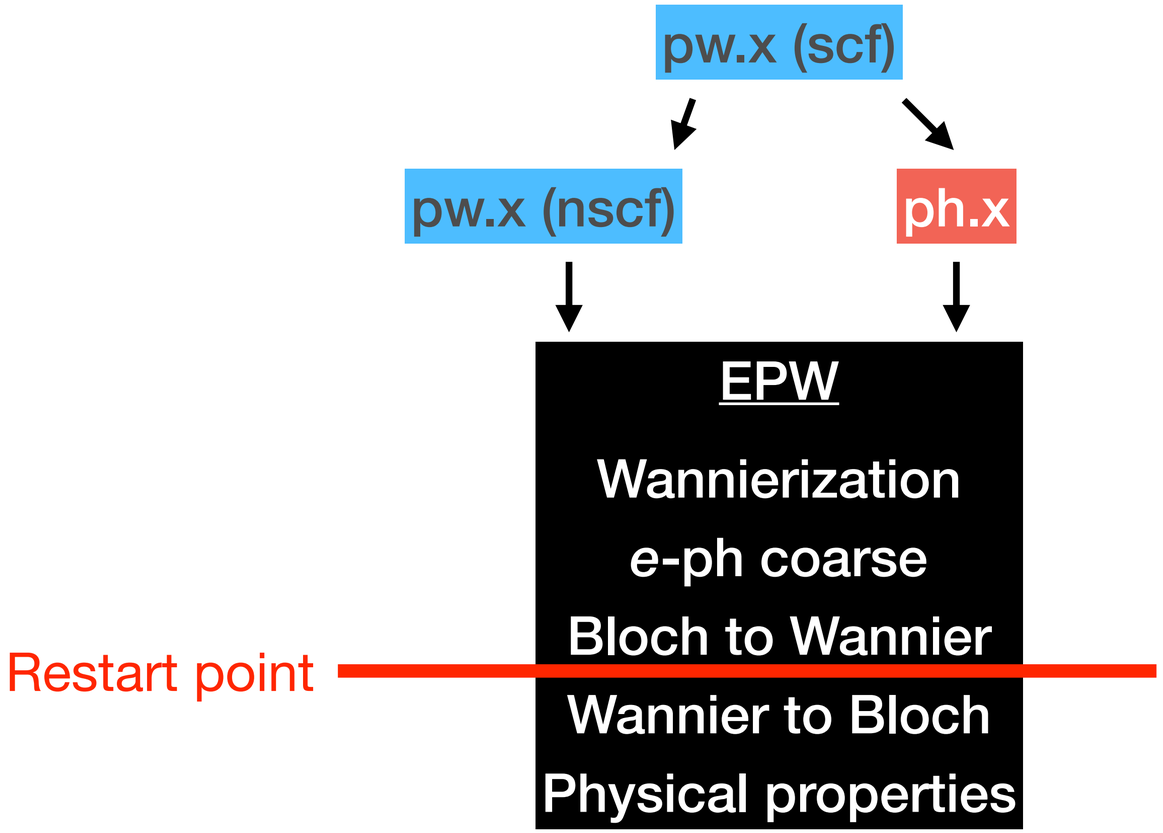
Basic input templates

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

  elph        = .true.
  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.

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



1. For future restart from the Wannier basis, it is desirable to set epwwrite=.true. and epwread=.false. .
2. When restarting from the Wannier basis, set epwread=.true. and epwwrite=.false.

Basic input templates

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

  elph        = .true.
  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.

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

1. To reduce computing load, exclude unnecessary bands from the band manifold; ex) low-lying semi-core states

Basic input templates

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

  elph        = .true.
  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.

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

1. If necessary, we can directly generate cube files in EPW.

Basic input templates

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

  elph        = .true.
  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.

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

1. If additional W90 inputs are needed, use the keywords wdata .

```
Ex)
  wdata(1) = 'bands_plot = .true.'
  wdata(2) = 'begin kpoint_path'
  wdata(3) = 'G 0.00 0.00 0.00 M 0.50 0.00 0.00'
  wdata(4) = 'G 0.00 0.00 0.00 K 0.33333333333 0.33333333333 0.00'
  wdata(5) = 'G 0.00 0.00 0.00 A 0.00 0.00 0.50'
  wdata(6) = 'end kpoint_path'
  wdata(7) = 'bands_plot_format = gnuplot'
```

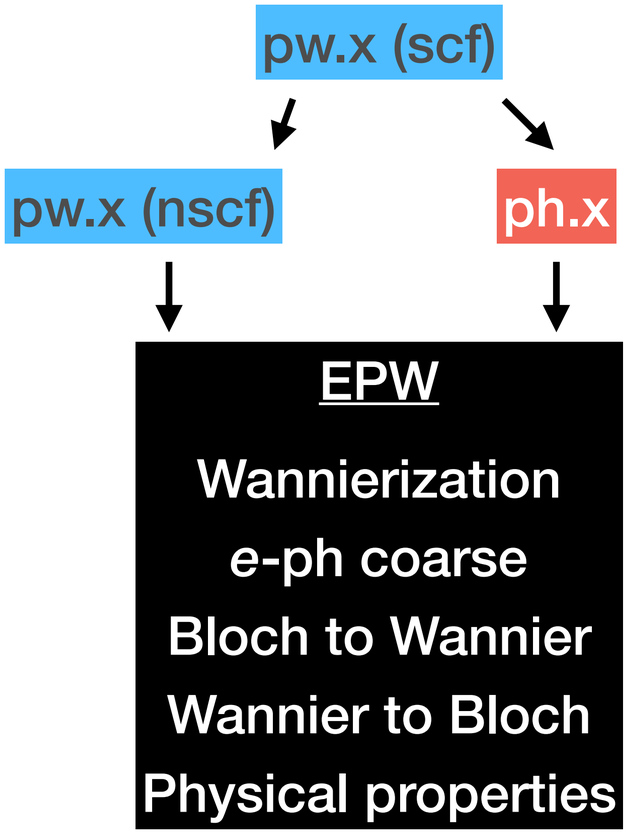
Basic input templates

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

  elph        = .true.
  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.

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



1. Set coarse **k** grids (same as those in nscf) and **q** grids (same as those in ph)
2. **k** and **q** grids should be commensurate and nkX>=nqX (X=1,2,3)

Additional inputs depending on calculations

Added to the basic template

```
band_plot    = .true.

filkf        = 'path2.dat'
filqf        = ‘path2.dat'
```

If you want to plot electronic bands and phonon dispersions, set **band_plot=.true.** .
Additionally, provide the **k** (**q**)-point lists .

Additional inputs depending on calculations

Added to the basic template

```
prtgkk       = .true.

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

If you want to plot *e*-ph vertex along **k** (or **q**)-point path, set **prtgkk=.true.** .
Additionally, provide the **k** (or **q**)-point lists .

Additional inputs depending on calculations

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

Added to the basic template

```
phonselfen  = .true.
delta_approx= .true.

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

filqf       = 'path2.dat'
nkf1         = 20
nkf2         = 20
nkf3         = 20
```

If you want to calculate phonon self-energy within the delta approximation,

1. set **phonselfen=.true.** and **delta_approx= .true.**
2. **degaussw** for the Gaussian width of the Gaussian function for the approx. of the Delta function
3. Fine **k**- and **q**-point lists
4. Fermi window, **fsthick** : consider only states within Fermi energy +- fsthick
5. temps (temperature) is not used within Delta approximation

Additional inputs depending on calculations

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

Added to the basic template

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

fsthick     = 7.0
temps       = 20
degaussw    = 0.05
```

If you want to calculate electron self-energy,

1. set **elecselfen=.true. .**
2. **degaussw** for the Gaussian width of the Gaussian function for the approx. of the Delta function
3. Fine **k**- and **q**-point lists
4. Fermi window, **fsthick** : consider only states within Fermi energy +- fsthick
5. **temps** (temperature)
6. **efermi_read** and **fermi_energy** for Fermi energy (in default, Fermi energy is calculated)

Supp.1) Restart input flags

- **epbread** and **epbwrite**: enable restart from the *e*-ph vertex in the Bloch basis on coarse grids
- **epwread** and **epwwrite**: enable restart from the e-ph vertex in the Wannier basis
- + several restart flags [will be covered during other Hands-on sessions]

Supp.2) specification of k (q) points

- (Γ-centered) Regular grids: (coarse) **nkX** , **nqX**, (fine) **nkfX** , **nqfX** (X=1,2,3)
- **k** (**q**)-point lists: **filkf** (**filqf**)
- Random grids.

Example of file for **k** (**q**)-points lists

# of points cartesian or crystal

```
41 cartesian
   1.000000000   0.000000000   0.000000000   1.0
   0.950000000   0.000000000   0.000000000   1.0
..
```

weights
(usually, not meaningful)

Supp.3) lpolar for polar materials

- Enable the correct Wannier interpolation in case of polar materials

Summary of Exercises and Problem

- Practice for how to check the quality of Wannier interpolation of physical quantities for a future production run
- Exercise 1: Pb
  - Electron and phonon band structures & phonon linewidth
- Exercise 2: SiC (polar material, **lpolar=.true.**)
  - *e*-ph vertex, electron and phonon band structures & electron linewidth
- Problem: SiC (polar material, **lpolar=.true.**)
  - *e*-ph vertex, but different wave vector for initial states.
  - Check different convergence behavior

More Info

- https://docs.epw-code.org/doc/Inputs.html (to be updated)
- https://forum.epw-code.org