2021 Virtual School on Electron-Phonon Physics and the EPW code

Description of input variables for executables:
ZG.x, pp_spctrlfn.x, disca.x, pp_disca.x and bands_unfold.x.

Hands-on Session (Friday, 18th June)

▶ ZG.x (for optimum performance parallelize over all cpus X, i.e. mpirun -n X ZG.x -nk X)

```
ZG_conf       : Logical flag that enables the creation of the ZG-displacement.
                (default .true.)
T             : Real number specifying the temperature at which the calcula-
                tions will be performed. "T" essentially defines the amplitude
                of the normal coordinates through the Bose-Einstein factor.
                (default 0.00)
dim1, dim2,   : Integers specifying the dimensionality of the supercell i.e.:
dim3            size of supercell is [dim1 * a(1), dim2 * a(2), dim3 * a(3)],
                where a(1), a(2), a(3) are the lattice vectors of the unit-cell
                used to compute the phonons.
                (default 0, 0, 0)
atm_zg(i)     : String array describing the element of each atomic species
                (default "Element")
synch         : Logical flag that enables the synchronization of the modes.
                (default .false.)
compute_error: Logical flag: if set to .true. allows the code to find the opti-
                mal ZG configuration by minimizing the error based on the
                "error_thresh" flag (see below). Set it to .false. if speed up is
                required. This is useful when (i) large supercell sizes are consi-
                dered for which the error is minimized by the first set of signs,
                (ii) only single phonon displacements are of interest (see below)
                (default .true.)
niters        : Integer for the number of attempts the algorithm needs to go
                through for finding the optimum configuration. The algorithm
                generates a set of "+,-,+,- ..." signs and its possible permu-
                tations, trying to minimize the error coming from the coupling
                of modes with the same q-wavevector but at different branch.
                For a finite supercell size the order of using the "+,-,+,- ..."
                set and its permutations is important, giving different results.
                Therefore, the algorithm checks the combination that brings the
                error lower than a threshold (see "error_thresh" flag).
                (default 15000) - Meaningful if compute_error = .true.
error_thresh  : Real specifying the error at which the algorithm stops while
                it's looking for possible combinations of signs. Once this limit
                is reached, the ZG-displacement is constructed. The threshold is
                usually chosen to be less than 5%, which is a safe boundary for
                accurate non-perturbative calculations.
                (default 0.05) - Meaningful if compute_error = .true.
incl_qA       : Logical flag for including the phonons in set A, or not.
                (default .true.)
```

```
single_ph_displ : Logical flag that allows to displace the nuclei along single
                  phonon modes. Use output configurations to compute electron-
                  phonon matrix elements with a direct supercell calculation.
                  Set the displacement to the zero point by "T = 0". This fi-
                  nite displacement should carry precisely the effect of dia-
                  gonal elements of [g(q)+g(-q)]. New output files are:
                  "single_phonon-displacements.dat".
                  (default .false.)
q_external      : Logical flag that allows the use of a q-point list specified
                  by the user in the input file. If .false. the q-point list
                  is specified automatically by the supercell dimensions "dim1",
                  "dim2", and "dim3". If .true. the q-point list must be provi-
                  ded by the user (see "qlist_AB.txt"). It is advisable to keep
                  this flag to .false. except you know what you are doing.
qlist_AB.txt    : This file contains the external q-list in crystal coordinates,
                  see the example for "ZG_444.in", after the input flags. It co-
                  rresponds to the q-points commensurate to the supercell size.
                  Only one of the q-point time-reversal partners is kept for the
                  construction of the ZG-displacement, as done in the code. The
                  calculations, for the moment, assume systems with time-reversal
                  symmetry. For the generation of the "qlist_AB.txt" set the
                  q-grid in file  "example/silicon/input/qlist.in" and run
                  "../../../src/local/create_qlist.x < qlist.in > qlist.out".
                  One can modify the "create_qlist.f90" to generate a different
                  path for consecutive q-points. Paste the output of
                  "qlist_AB.txt" to "ZG.in" after namelist &input. Set the flag
                  "q_external = .true." for the code to read the list.
--------------------------------------------------------------------------------
The following input flags are as for matdyn.x:

flfrc           : String for the input file produced by q2r containing the
                  force constants.
                  (No default value: must be specified.)
asr             : Character indicating the type of Acoustic Sum Rule:
                  'no', 'simple', 'crystal', 'one-dim', and 'zero-dim'.
                  (default 'no')
amass(i)        : masses of atoms in the supercell in a.m.u., one per atom type
                  (default: masses from file flfrc)
loto_2d         : Logical flag. Set to .true. to activate two-dimensional
                  treatment of LO-TO splitting.
                  (default .false.)
--------------------------------------------------------------------------------
The following input flags are for the ZG structure factor calculation:

ZG_strf         : Logical flag for the calculation of the ZG structure factor.
                  (default .false.)
qpts_strf       : Integer specifying how many rows to read from the file
                  "qpts_strf.dat" containing the scattering vectors in crystal
                  coordinates. "qpts_strf.dat" can be automatically generated
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```
                from disca.x (see below).
                (default 0)
atmsf_zg_a(i,j): Parameters "a" and "b" that define the atomic scattering factor
atmsf_zg_b(i,j)  as a sum of Gaussians. 5 entries (j), per atom type (i).
                Parameters can be taken from Ref. [Micron 30, 625-648, (1999)].
                (default 0.d0)
```

- `pp_spctrlfn.x` (for optimum performance parallelize over all cpus `X`,
  i.e. `mpirun -n X pp_spctrlfn.x -nk X`)

```
flin   : String for specifying the name of the input file that contains the
         momentum (first column), energies (second column), and the
         spectral weights (third column).
         (No default value: must be specified.)
steps  : Integer specifying how many entries from file "flin" are included in
         the computation of the spectral function, starting from the first one.
         (default 5000)
ksteps : Integer that defines the smearing along the momentum-axis as:
         (kmax - kmin) / ksteps. For kmax, kmin see below.
         (default 200)
esteps : Integer that defines the smearing along the energy-axis as:
         (emax - emin) / esteps. For emax, emin see below.
         (default 200)
kmin   : Real indicating the minimum value of the momentum axis.
         (default 0.d0)
kmax   : Real indicating the maximum value of the momentum axis.
         (default 1.d0)
emin   : Real indicating the minimum value of the energy axis.
         (default -5.d0)
emax   : Real indicating the maximum value of the energy axis.
         (default -5.d0)
flspfn : String for specifying the output file that contains the
         momentum (first column), energies (second column), and the
         spectral function (third column).
         (No default value: must be specified.)
```

▶ `disca.x` (for optimum performance parallelize over all cpus `X`, i.e. `mpirun -n X disca.x -nk X`)

```
disca          : Logical flag for the calculation of the diffuse scattering.
                 (default .true.)
T              : Real number specifying the temperature at which the calcula-
                 tions will be performed. "T" essentially defines the amplitude
                 of the normal coordinates through the Bose-Einstein factor.
                 (default 0.00)
dim1, dim2,    : Integers specifying the dimensionality of the supercell i.e.:
dim3             size of supercell is [dim1 * a(1), dim2 * a(2), dim3 * a(3)],
                 where a(1), a(2), a(3) are the lattice vectors of the unit-cell
                 used to compute the phonons.
                 (default 0, 0, 0)
atm_zg(i)      : String array describing the element of each atomic species
                (default "Element")
atmsf_zg_a(i,j): Parameters "a" and "b" that define the atomic scattering factor
atmsf_zg_b(i,j)  as a sum of Gaussians. 5 entries (j), per atom type (i).
                 Parameters can be taken from Ref. [Micron 30, 625-648, (1999)].
                (default 0.d0)
zero_one_phonon: Logical flag for the calculation of the one-phonon contribution
                 to diffuse scattering (including Bragg scattering).
                 (default .true.)
full_phonon    : Logical flag for the calculation of the all-phonon contribution
                 to diffuse scattering (including Bragg scattering).
                 (default .false.)
atom_resolved  : Logical flag for the calculation of the atom resolved contribu-
                 bution to diffuse scattering.
                 (default .false.)
nks1, nks2,    : Integers specifying the initial coordinates of the reciprocal
nks3             lattice vector Gi = [nks1 * b1 + nks2 * b2 + nks3 * b3],
                 where b1, b2, b3 are the reciprocal lattice vectors of
                 the unit-cell.
                 (default 0, 0, 0)
nksf1, nksf2,  : Integers specifying the final coordinates of the reciprocal
nksf3            lattice vector Gf = [nksf1 * b1 + nksf2 * b2 + nksf3 * b3],
                 where b1, b2, b3 are the reciprocal lattice vectors of
                 the unit-cell. Reciprocal lattice vectors from Gi to Gf
                 define the centers of the Brillouin zones for which the
                 scattering vectors Q are computed.
                 (default 6, 6, 6)
plane_val      : Real number that defines the plane for which the structure
                 factor (one-phonon or all-phonon) is calculated for.
                 (default 0.d0 in units of 2pi/alat)
plane_dir      : Integer number that defines the Cartesian direction
                 perpendicular to the plane (1 --> x, 2 --> y, and 3 --> z)
                 for which the structure factor (one-phonon or all-phonon)
                 is calculated for.
                 (default 3)
qstart, qfinal : Integers that define how many scattering vectors Q will be
```

```
                included in the present run. These flags enable, essentially,
                the splitting of the full calculation into different runs.
                (default 1, 2)
-------------------------------------------------------------------------------
The following input flags are as for matdyn.x:

flfrc          : String for the input file produced by q2r containing the
                 force constants.
                 (No default value: must be specified.)
asr            : Character indicating the type of Acoustic Sum Rule:
                 'no', 'simple', 'crystal', 'one-dim', and 'zero-dim'.
                 (default 'no')
amass          : masses of atoms in the supercell in a.m.u., one per atom type
                 (default: masses from file flfrc)
```

▶ pp_disca.x (for optimum performance parallelize over all cpus X,
i.e. mpirun -n X pp_disca.x -nk X)

```
flstrfin : String for specifying the name of the input file that contains the
           scattering vectors' coordinates (columns 1:3), and the
           scattering intensity (column 4).
           (No default value: must be specified.)
  steps  : Integer specifying how many entries from file "flstrfin" are included
           in the computation of the scattering intensity, starting from the
           first row.
           (default 10000)
 ksteps1 : Integer that defines the smearing along the first momentum-axis as:
           (kmax - kmin) / ksteps1. For kmax, kmin see below.
           (default 250)
 ksteps2 : Integer that defines the smearing along the second momentum-axis as:
           (kmax - kmin) / ksteps2. For kmax, kmin see below.
           (default 250)
  kmin   : Real indicating the minimum value of the momentum axis.
           (default -5.d0)
  kmax   : Real indicating the maximum value of the momentum axis.
           (default 5.d0)
  dim1   : Integer from 1 to 3 for specifying the first Cartesian direction of
           the scattering vectors in the 2D map. Code reads the column "dim1"
           from "flstrfin" (1 --> x, 2 --> y, and 3 --> z).
           (default 1)
  dim2   : Integer from 1 to 3 for specifying the second Cartesian direction of
           the scattering vectors in the 2D map. Code reads the column "dim2"
           from "flstrfin" (1 --> x, 2 --> y, and 3 --> z).
           (default 2)
   Np    : Integer that defines the number of reduced wavevectors (q-points)
           used to sample each Brillouin zone of reciprocal space. This number
           is equal to (dim1 * dim2 * dim3) as specified in disca.in (see above).
           The code divides the scattering intensity for every Q by Np**2 for
           normalization reasons. One can specify a different value.
           (default 400000)
flstrfout: String for specifying the output file that contains the
           momentum (first column), energies (second column), and the
           spectral function (third column).
           (No default value: must be specified.)
```

▶ Input variables' description for bands_unfold.x are as for bands.x of Quantum Espresso.
(see → https://www.quantum-espresso.org/Doc/INPUT_BANDS.html)
The only difference is that, here, we introduce the flags dim1, dim2, dim3 which specify the dimensions of the supercell used. This routine is general and can be used for band structure unfolding of ZG supercell structures, supercells with defects, or any other distorted configuration. It is implemented to deal with norm-conserving, paw, and us pseudopotentials.