Structure of the QE Input File

Quantum Espresso's input file consists of 3 major sections (&control, &system, &electrons) and 2 optional sections (&ions, &cell) depending on the type of calculation to be performed. Sections must appear in the order given below,

&CONTROL
&SYSTEM
&ELECTRONS
&IONS
&CELL

A "/" indicates the end of a section.

After listing all required sections, additional information about your molecule or the crystal system has to be specified such as

ATOMIC_SPECIES
ATOMIC_POSITIONS
K_POINTS
CELL_PARAMETERS

For a full list of sections and other options refer to the QE website.

Find below an example input file for a self-consistant calculation of single layer MoS_2.

Example QE Input File for Monolayer MoS_2

```
&control
 calculation   = 'scf',
 restart_mode  = 'from_scratch',
 pseudo_dir    = './',
 prefix        = 'MoS2',
 outdir        = './',
 nstep         = 100,
/

&system
 ibrav = 4,
 a     =  3.16000e+00,
 c     =  2.00000e+01,
 nat   = 3,
 ntyp  = 2,
 ecutwfc     = 60,
 occupations = 'fixed',
 smearing    = 'gauss',
 vdw_corr    = 'DFT-D',
/

&electrons
 conv_thr = 1.0d-9,
/


ATOMIC_SPECIES
 Mo     95.94000  Mo_ONCV_PBE-1.0.upf
 S      32.06600  S_ONCV_PBE-1.0.upf

ATOMIC_POSITIONS (angstrom)
S         0.002804304   0.001613133   8.429890591
S         0.002804304   0.001613133  11.570109409
Mo        1.582007393   0.913365735  10.000000000

K_POINTS automatic
51 51 1 0 0 0
```

For further details please click on the highlighted input parameter.

In line 2 of the input file, we list the type of calculation we ask to perform. Available types of calculations include,

- *SCF* - Single point energy calculation without changing atomic coordinates or the cell parameters, i.e., no structure relaxation.

- *NSCF*- Non-self-consistency calculation to extract the desired properties such as the DOS in case you need a denser electronic momentum mesh (k-mesh), based on the previous *SCF* calculation.

- *BANDS* - Calculation of electronic bands along a path of high-symmetry k-points based on the previous *SCF* calculation.

- *RELAX* - Optimization of the atomic coordinates to minimize the forces while keeping the cell fixed. This calculation requires section &ions. All options for a single *SCF* calculation apply, plus a few others.

- *VC-RELAX* - Optimization of both atomic coordinates and the cell parameters. Structure relaxation is important to minimize forces acting on the atoms as well as to reduce the stress in the cell. This calculation requires section &cell.

Important Convergence Parameters

Accurate DFT calculations require specific parameters for the material of interest and their convergence. These parameters for any type of DFT calculation include the planewave kinetic energy cutoff (*ecutwfc*), the Brillouin zone sampling k-points, and the self-consistency energy convergence threshold (*conv_thr*). To obtain accurate results, one should optimize these parameters with energy minimization.

Please see the following links below for a hands-on exercise to better understand these parameters and other related calculations.