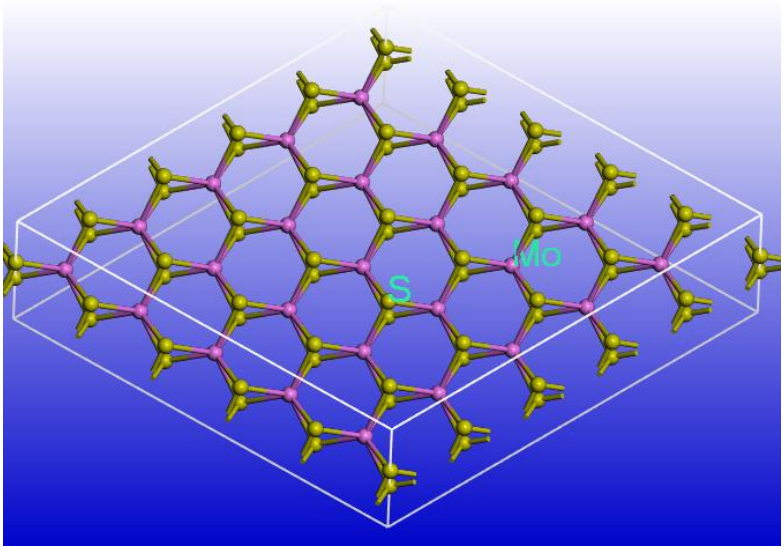
Ground State Calculation as Starting Point for YAMBO

YAMBO is a code for many-body calculations in solid state and molecular physics. YAMBO relies on the Kohn-Sham wavefunctions generated by DFT codes such as Quantum Espresso (QE).

In this tutorial we are going to calculate the ground state wavefunction with Quantum Espresso. Please go to the Quantum Espresso Tutorial for instructions on how to configure QE. We will be using MoS_2 as an example system for our QE ground state calculation. Details about the material are listed below.

System of Interest for this Tutorial



2D MoS_2

- Hexagonal lattice
- Three atoms per cell, 1 Mo and 2 S (26 electrons). Each Mo atom is covalently bonded with six adjacent S atoms to form a hexagonal network.
- Lattice constant 3.17 Å

Once QE is configured and the executable “pw.x” is ready, both self-consistency (SCF) and non-self-consistency (NSCF) runs need to be completed to obtain the ground state wavefunction which we will then use for YAMBO calculations. Note, we assume that you are already familiar with QE. If not, please refer to our QE tutorials.

Please find below the QE input files (SCF and NSCF) for MoS_2,

SCF input file

```
&control
 calculation   = 'scf',
 restart_mode  = 'from_scratch',
 pseudo_dir    = './',
 prefix        = 'MoS2',
 outdir        = './',
 nstep         = 100,
 wf_collect    = .true.,
 verbosity     = 'high',
/
&system
 ibrav = 4,
 a     = 3.17520e+00,
 c     = 2.00000e+01,
 nat   = 3,
 ntyp  = 2,
 ecutwfc     = 10,
 occupations = 'fixed',
 smearing    = 'gauss',
 vdw_corr    = 'DFT-D',
 force_symmorphic = .true.,
/
&electrons
 conv_thr = 1.0d-6,
/
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
12 12 1 0 0 0
```

YAMBO can work only with symmorphic symmetries. QE has an input variable *force_symmorphic* to force the symmetry group to be symmorphic by disabling symmetry operations having an associated fractional translation. This flag has to be set to ‘.true.’ for all calculations with YAMBO.

You can download pseudopotential files for Mo and S directly by executing the following commands,

```
$ wget http://www.quantum-simulation.org/potentials/sg15_oncv/upf/Mo_ONCV_PBE-1.0.upf

$ wget http://quantum-simulation.org/potentials/sg15_oncv/upf/S_ONCV_PBE-1.0.upf
```

NSCF input file

```
&control
 calculation   = 'nscf',
 restart_mode  = 'from_scratch',
 pseudo_dir    = './',
 prefix        = 'MoS2',
 outdir        = './',
 nstep         = 100,
 wf_collect    = .true.,
 verbosity     = 'high',
/
&system
 ibrav = 4,
 a     = 3.17520e+00,
 c     = 2.00000e+01,
 nat   = 3,
 ntyp  = 2,
 nbnd  = 50,
 ecutwfc     = 10,
 occupations = 'fixed',
 smearing    = 'gauss',
 vdw_corr    = 'DFT-D',
 force_symmorphic = .true.,
/
&electrons
 conv_thr = 1.0d-6,
/
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
12 12 1 0 0 0
```

At the end of the SCF and NSCF calculations it will create a “MoS2.save” directory inside the current working directory.

Energy cutoff (*ecutwfc*), the Brillouin zone sampling k-points, and the self-consistency energy convergence threshold (*conv_thr*) used in this example is only to reduce the computational time. An accurate calculation requires specific parameters for the material of interest and their convergence. To obtain accurate results, one should optimize these parameters. Please go to the Quantum Espresso Tutorial for a hands-on exercise to better understand the convergence of these parameters in general and other related calculations.

Please note that the values for ***nbnd***, *ecutwfc, conv_thr*, k-points are reduced for the purpose of the tutorial. If you are interested in further details of publication quality convergence parameters for MoS_2, please refer to Molina-Sánchez *et.* al., Phys. Rev. **B 88**, 045412 (2013), **https://arxiv.org/abs/1306.4257**.