GW Band Structure

In this tutorial we are going to learn how to calculate GW band structure using YAMBO. Apply the following command inside the "MoS2.save" directory to generate the input file for the GW calculation using a Hartree-Fock method and the plasmon-pole approximation,

```
$ ./yambo -x -g n -p p
```

Options:

-x: Hartree-Fock method,

-g n: to calculate G_0W_0 quasiparticle (QP) energies using Newton algorithm (other option: -g s)

(The QP equation is a non-linear equation whose solution must be found using a suitable numerical algorithm. A widely used method is the Newton method based on the linearization of the self-energy operator. YAMBO can also perform a search of the QP energies using a non-linear iterative method based on the Secant iterative method. In any case it is worth testing these methods during the convergence procedure.)

-p p: for plasmon-pole approximation.

For available options and general details about the YAMBO input structure please refer to the YAMBO site, where all the options are listed.

The command above will generate the input file (yambo.in) for GW calculations and immediately open the following input file in vi editor. If you are not familiar with the vi editor, please refer to a tutorial with basic vi commands.

```
#  __  __   _________   ___ __ __    _______   ______
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# GPL Version 4.2.1 Revision 110. (Based on r.14778 h.7b4dc3
#                        MPI Build
#                http://www.yambo-code.org
HF_and_locXC               # [R XX] Hartree-Fock Self-energy and Vxc
gw0                        # [R GW] GoWo Quasiparticle energy levels
ppa                        # [R Xp] Plasmon Pole Approximation
em1d                       # [R Xd] Dynamical Inverse Dielectric Matrix
EXXRLvcs=  4985        RL      # [XX] Exchange RL components
Chimod= ""                 # [X] IP/Hartree/ALDA/LRC/BSfxc
% BndsRnXp
   1 |  50 |                 # [Xp] Polarization function bands
%
```

```
NGsBlkXp= 1             RL      # [Xp] Response block size
% LongDrXp
 1.000000 | 0.000000 | 0.000000 |        # [Xp] [cc] Electric Field
%
PPAPntXp= 27.21138      eV      # [Xp] PPA imaginary energy
% GbndRnge
   1 |  50 |                    # [GW] G[W] bands range
%
GDamping=  0.10000      eV      # [GW] G[W] damping
dScStep=  0.10000       eV    # [GW] Energy step to evaluate Z factors
DysSolver= "n"                # [GW] Dyson Equation solver ("n","s","g")
%QPkrange                     # [GW] QP generalized Kpoint/Band indices
  1| 43|  1| 50|
%
```

The default values generated in the input may not be sufficient for your calculations. Convergence tests are required for values of EXXRLvcs, NGsBlkXp, BndsRnXp, GbndRnge, and QPkrange. To keep the calculation simple for the purpose of this tutorial, we simply set them to the values indicated above. Click here if you would like to explore details about these variables.

The following is a sample job submission file to perform a GW calculation. This will submit your job to the parallel queue by the qsub/sbatch command (this is a long job compared to Quantum Espresso calculations and it will take a while to finish). For details of how to submit jobs in MARCC, please refer to the running jobs page.

```
#!/bin/bash -l
#SBATCH --job-name=job-gw
#SBATCH --time=06:00:00
#SBATCH --partition=parallel
#SBATCH --nodes=4
#SBATCH --ntasks-per-node=24
mpirun -np 96 ./yambo -F yambo.in > yambo.out
```

After you finish the GW calculation with the above job script, the system will generate an output file “o.qp” with quasiparticle corrections to the band gap.