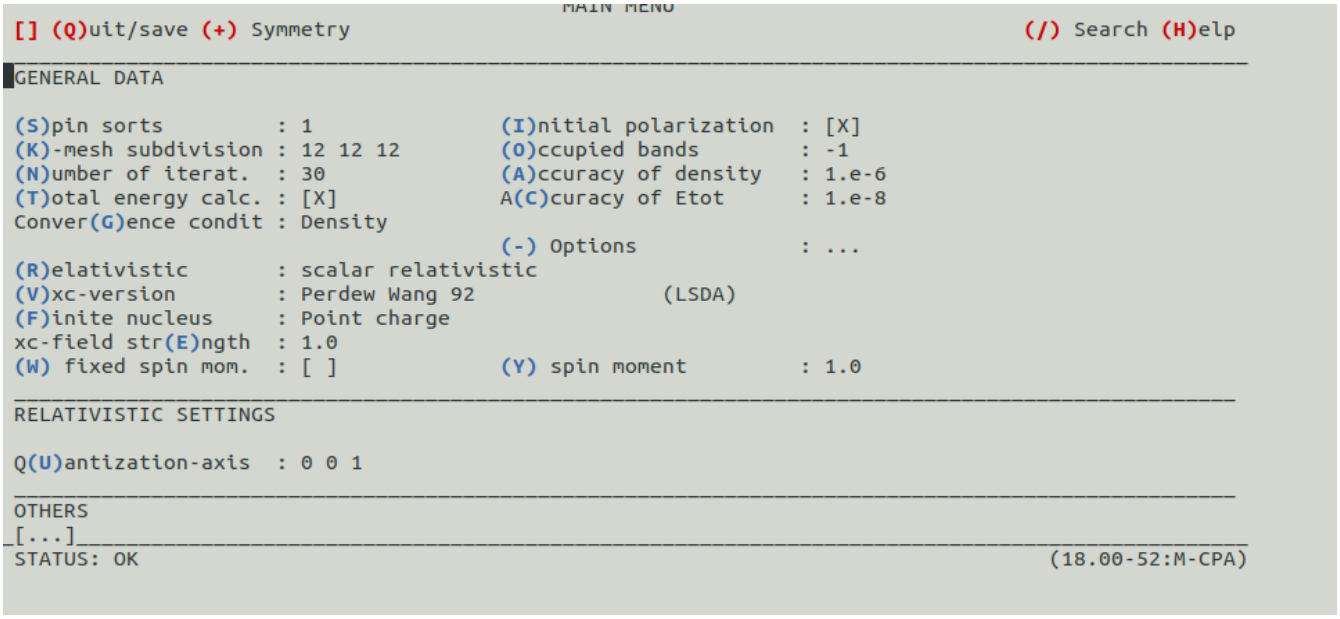
Optic Calculations in FPLO

Note: line with ! are suggestions and with $ are commands to be run on terminal.

! log in to your ssh
! navigate your home directory
! now make new directory
$ mkdir Al
$ cd Al
$ fedit18.00-52-x86_64
$ x
! set the input file as shown
! quit and save



! copy fplo.slurm file her in the directory Al ie.
scp -r path to your fplo.slurm your ssh id:path to your Al directory in ssh
$ scp -r /home/pawan/Downloads/fplo.slurm mpjoshi@202.70.90.210:/home/mpjoshi/storage0/fplo/Al

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############ Github: https://github.com/pawan054 ###### ############

! edit the fplo.slurm file and give proper output file name i.e. edit here sbatch name

```
#!/bin/bash
#SBATCH -J Mn              # Job name
#SBATCH -p fplo       # Partition name
#SBATCH -o job.%j.out    # Name of stdout output file (%j expands to jobId)
#SBATCH -N 1               # Total number of nodes requested
#SBATCH -n 1               # Total number of mpi tasks requested
#SBATCH -t Infinite       # Run time (hh:mm:ss)

# Launch MPI-based executable
#module load qe/6.8-gpu
module load gnu/5.4.0
module load fplo/18.52
#fedit18.00-52-x86_64
fplo18.00-52-x86_64
#python -u wpsearch.py > outwps
#python -u cherninsphere.py -i 0
#fdhva18.00-52-x86_64
#python -u fs.py > outfs
~
~
~
~
"fplo.slurm" 18L, 591C
```


```
~
~
"fplo.slurm" 18L, 591C
```


! edit the fplo.slurm file and give proper output file name i.e. edit here sbatch name

! save and quit

$ sbatch fplo.slurm

! wait for scf convergence

! Now, do

$ fedit18.00-52-x86_64

! make initialization polarization False

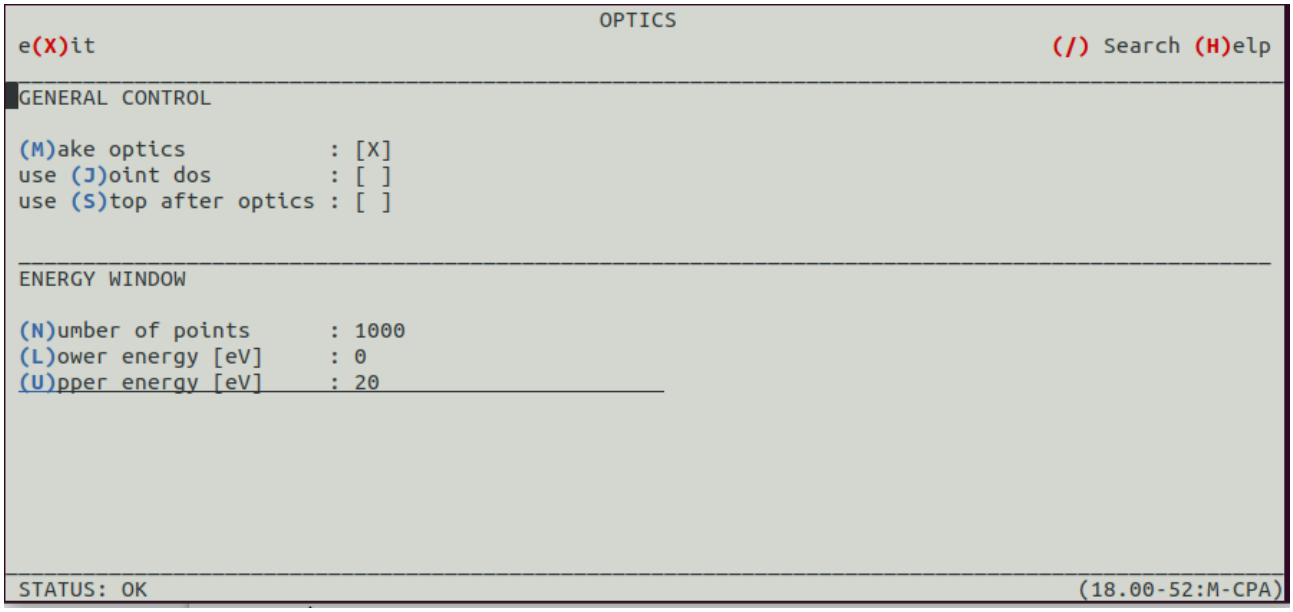
$ space key ! enter space key (two times)

$ c ! choose option c

$ m ! make optic True

! Shown below

$ u >> 20 ! set upper energy 20eV
! again open fplo.slurm and edit sbatch name as .outoptic and save



$ sbatch fplo.slurm
$ ls
! hope, you got the file : +imeps
! Now just run
$ foptics18.00-52-x86_64
! just hit enter to use default value
$ ls
$ xfbp im_eps
$ xfbp re_eps
$ xfbp re_sigma
$ xfbp loss
$ xfbp +imeps

Contgratulations. You did this.

Note: These calculations are just for default cases but please make sure that you use convergence values and proper input values according to your crystal system for your publication or thesis but methods are applicable to all system in general.

! For specific system with converging input parameters, I will upload on Github. Please, check the Github link.