How to Plot Fatband with PDOS

The following instruction is written with the help of bryanalchemist fatband instruction.

Pros : You can plot the fatband along with pdos.

Cons: More time consuming then bryanalchemist fatband instruction.

To plot Fatband with DOS we need to do following calculations.

1. scf calculations

```
pw.x -in scf.in > scf.out
```

2. bands calculations

```
pw.x -in bands.in > bands.out
```

3. bands.x calculations

```
bands.x -in band.in > band.out
```

4. projwfc.x calculation

```
projwfc.x -in pdos.in > pdos.out
```

5. nscf calculations (tetrahedra with dense k points)

```
pw.x -in nscf.in > nscf.out
```

6. dos calculations

```
dos.x -in dos.in > dos.out
```

Post-Processing step-1 : PDOS

7. Sumpdos orbitals (Together): it will sum all the orbital together e.g. P_orbital.

```
./sumpdos_tog.sh
```

8. Sumpdos orbitals (individual) : it will sum orbitals individually e.g. px py pz.

```
./sumpdos_indi.sh
```

Post-Processing step-2: Fatband with PDOS

9. Make a soft link of projwfc calc (required for plotband.x)

```
ln -s *up bands.dat.proj
```

10. To list all the valence electron of element edit the list.sh script for each element and run

```
./list.sh
```

11. From the above steps we can select specific orbitals e.g. s, p, d, f. We need to run the select.sh script for each orbital mentioned in the output of list.sh.

```
./select.sh
```

12. use the 1st column of select.sh output as a 2nd row input for plotband input and then run plotband script for each orbital e.g. for p orbital

```
./plotband_p_orb.sh
```

13. Above steps will create too many output files it is better to create individual directory and subdirectory for each element and respective orbitals e.g. s p and d_band. After this we need to copy some important files to each directory. then use the sumplot.sh script to some all the orbitals.

```
cp sumplot.sh atom-* sum-ud-* dos.dat nscf.in scf.out bands.in
band.out bands.dat.gnu /home/sai/fatband/silicon/s_band

cp sumplot.sh atom-* sum-ud-* dos.dat nscf.in scf.out bands.in band.out
bands.dat.gnu /home/sai/fatband/silicon/p_band

cp sumplot.sh atom-* sum-ud-* dos.dat nscf.in scf.out bands.in band.out
bands.dat.gnu /home/sai/fatband/silicon/p_band/px

cp sumplot.sh atom-* sum-ud-* dos.dat nscf.in scf.out bands.in band.out
bands.dat.gnu /home/sai/fatband/silicon/p_band/py

cp sumplot.sh atom-* sum-ud-* dos.dat nscf.in scf.out bands.in band.out
bands.dat.gnu /home/sai/fatband/silicon/p_band/pz

./sumplot.sh
```

14. Plot the all and individual bands with the help of gnuplot given.

```
gnuplot p-all-gnufatpdos.gp
gnuplot pxgnufatpdos.gp
gnuplot sgnufatpdos.gp
```