Step-by-Step Guide to Plot Spin-Texture Using QE Data

1. Parse bands data (.dat) will be written in the format of kx ky kz nbnd_1 nbnd_2[in the nbnd column there will be energy].

band data parser.ipynb

2. Parse spin data(.dat.1,.dat.2,.dat.3) will be written in the format of kx ky kz nbnd_1 nbnd_2[in the nbnd column there will be expectation value of spin operator].

band data parser.ipynb

- 3. To plot the individual band's spin texture make an Excel file of kx, ky,sx,sy and sz for a particular band from the previously generated .csv file.
- 4. To plot the spin texture of individual bands with sz as background and sx,sy as vector arrow in the kx-ky plane.

background_sz_arrow_sx_sy.ipynb

5. To plot the spin texture of individual bands with sz as the colour of the (sx,sy) vector arrow in the kx-ky plane.

spin texture with sz color arrow sx sy.ipynb

6. To make the bands parse data [E-E_f]

fermi_energy_subtracted_band_data.ipynb

7. To make the bands parse data [E-E_f] and up to three-digit precision

band data fermi subtracted with three digit prec.ipynb

8. To find the considerable bands that are cutting an iso-energy surface with the whole kx,ky range and plot them.

isosurface band plot for fix kx ky.ipynb

9. To find the considerable bands which are cutting an iso-energy surface with varying kx,ky range.

isosurface band plot changing kx ky range.ipynb

10. To get the data of bands that are cutting the iso-energy surface and the plot

crssing_band_filtered.ipynb

11. To get the kx, ky value where particular bands are crossing the iso-energy surface and with a data file [kx_nbnd_ky_nbnd_nbnd_energy]

kx ky data of each particular interested band.ipynb

12. Extract the sx,sy and sz values of a particular band three .csv file for three spin projection.

to extract partcular band.ipynb

13. Find the sx,sy,sz value of the particular band at those kx,ky point where bands are crossing the isosurface.

collecting intersecting band kx ky and s.ipynb

- 14. Make an excel with the kx,ky,s file from the previous .csv data file
- 15. To plot them separately

spin-texture plot for two band.ipynb

16. To plot the spin-texture combined

spin-texture plot.ipynb