README:

About:

MATLAB codes to read and process the Vienna Ab initio Simulation Package (VASP) outputs for electronic and optical properties analysis.

Requirements:

You need to have MATLAB software installed in your system.

Installation:

First copy the .m file to the folder where the VASP outputs are located. Then run the .m file with MATLAB.

Uses:

We have provided the step-by-step procedure in the comment lines of each code. The usage of each available code is summarized below.

(1) read_EIGVAL.m: Plot band structures along the calculated high symmetry k-path.

(2) read_DOSCAR_nosoc.m: Plot total and partial density of states where the calculations were performed without considering the spin-orbit coupling (soc).

(3) read_DOSCAR_soc.m: Plot total and partial density of states where the calculations were performed with the spin-orbit coupling (soc).

(4) read_PROCAR.m: This code reads the PROCAR file and gives the data of orbitals and site projected wave function characters in the 'procar_matlab.dat' output file. Additionally, 'kpoints.dat' and 'band_ene.dat' output files are generated which contain the information about k-points and band eigenvalues respectively.

(5) get_kpath_length.m: This file generates the k-length using the high symmetry k-points from the 'kpoints.dat' file. The output is generated in 'klenght.dat' file.

(6) get_2D_kmesh.m: This file generates the 2D k-mesh and output is stored in '2D_kmesh.dat' file.

(7) plot_spintexture.m: This file reads the output from 'read_PROCAR.m' and plots the spin texture in 2D k-plane.

(8) plot_3D_bands.m: This file reads the output from 'read_PROCAR.m' and plots the 3D bands in 2D k-plane.

N.B.

We are working on the codes for optical properties analysis. For further queries please contact mayank77338@gmail.com .