User guide for pvasp

Author: XY Ding

E-mail: `dxy_vasp@163.com`

Abstract. Please email me if there exist some bugs.

1. Installation instruction

The package of pvasp can be obtained from the github website:
$https://github.com/XVDing/pvasp$
First: uncompressing the pvasp-main.zip file, then go into the uncompressed file.
Second: find the pvasp file. Eiditing this file and modfying the file_path variable to the current path. (eg. file_path="/home/dxy/software/pvasp") .
Third: Entitle the pvasp executable authority: chmod +x pvasp
Fourth: Add the path for pvasp to the ~/.bashrc file.
(eg. export PATH=/home/dxy/software/pvasp:$PATH).
Note That: the path /home/dxy/software/pvasp above should change to your own file path of the location for pvasp executable file.

2. Introduction

pvasp is a pre- and post-processing software for vasp calculation. Fig.1 shows the main functions of pvasp.

The pre-processing of pvasp include the templates of INCAR file for vasp calculation: relax, scf, band, dos, phonon, elastic, HSE06 and molecular dynamics. (shows in Fig. 2)

The post-processing of pvasp include the visualization for vasp results: band ploting, dos ploting, hse06 band ploting, project band ploting and optical properties ploting. (shows in Fig. 3)

```
***********************************************************************
*This is a code used to simplify the vasp calculation, written by **
*****************              XY Ding               *****************
***********************************************************************
*************         (^o^)GOOD LUCK!(^o^)           **************


*********   Pre and post-preparation for vasp calculation  **********
*********   eg:(1) pre-processing: incar template    **************
*********   eg:(2) post-processing: band plot     ******************
***********************************************************************
(1) Incar template for vasp calculation
(2) Data processing for vasp calculation:eg. band and dos
(3) User defined plot scripts, data from first line
Input a number: █
```

Figure 1. Main functions of pvasp. (1) Generating the INCAR file for vasp calculation. (2) Post-processing for vasp results. (3) Waiting for update.

```
********   Incar template for vasp calculation !   *******
(1) optimization        (2) self-consistent
(3) band calculation    (4) dos calculation
(5) HSE06 calculation    (6) phonon
(7) Elastic calculation (8) md
Input a Number: █
```

Figure 2. INCAR templates for vasp calculation

```
********  Data processing for vasp calculation: band and dos ********
(1) band plot           (2) HSE06 band plot
(3) Projected band      (4) Density of state
(5) Optics properties
Input a Number: █
```

Figure 3. Vasp results visualization: band, dos and optical properties.

```
TET (tetragonal)
50
Line-mode
reciprocal
   0.0000    0.0000    0.0000    ! \Gamma
   0.0000    0.5000    0.0000    ! X

   0.0000    0.5000    0.0000    ! X
   0.5000    0.5000    0.0000    ! M

   0.5000    0.5000    0.0000    ! M
   0.0000    0.0000    0.0000    ! \Gamma

   0.0000    0.0000    0.0000    ! \Gamma
   0.0000    0.0000    0.5000    ! Z

   0.0000    0.0000    0.5000    ! Z
   0.0000    0.5000    0.5000    ! R

   0.0000    0.5000    0.5000    ! R
   0.5000    0.5000    0.5000    ! A

   0.5000    0.5000    0.5000    ! A
   0.0000    0.0000    0.5000    ! Z
```

Figure 4. KPOINTS file of PBE band formatting and KPATH.in file of HSE06 band formatting.

3. Noting

1. PBE BAND: Needing the INCAR, POSCAR, OUTCAR, KPOINTS and EIGEN-VAL, KPOINTS file store the high symmetry points information, and it must be for-mated as Fig. 4. Meanwhile, there must be have no blank in the tail of KPOINTS file.

2. HSE06 BAND: Needing the INCAR, POSCAR, OUTCAR, KPOINTS, EIGEN-VAL, and KPATH.in file, KPATH.in file store the high symmetry points information, and it must be formated as Fig. 4. (the same as KPOINTS for PBE band calculation). Meanwhile, there must be have no blank in the tail of KPATH.in file.

3. DOS: Needing the INCAR, POSCAR, DOSCAR file, and

This **scripts don't support to extract data of DOS including f orbitals**.