Phase transition from T-carbon to bct-C_{16}

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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 changed 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 moleculat 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)

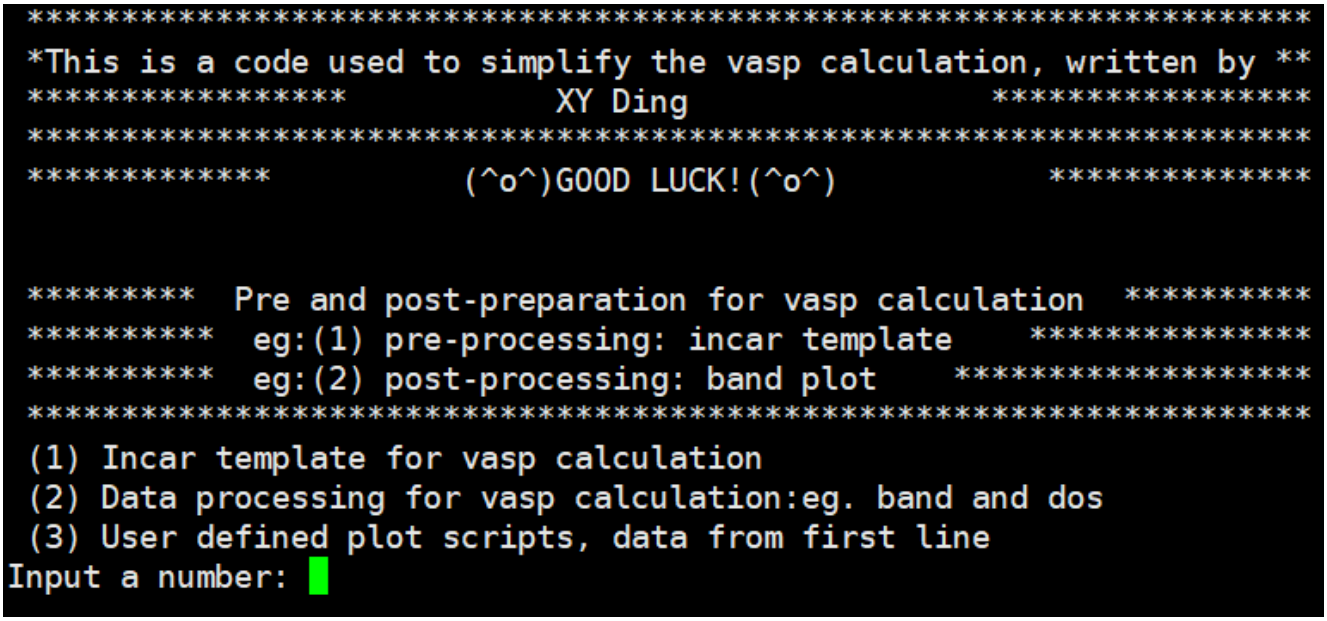

Figure 1. Main functions of pvasp. (1) Generating the INCAR file for vasp calculation. (2) Post-processing for vasp results. (3) Waiting for update.

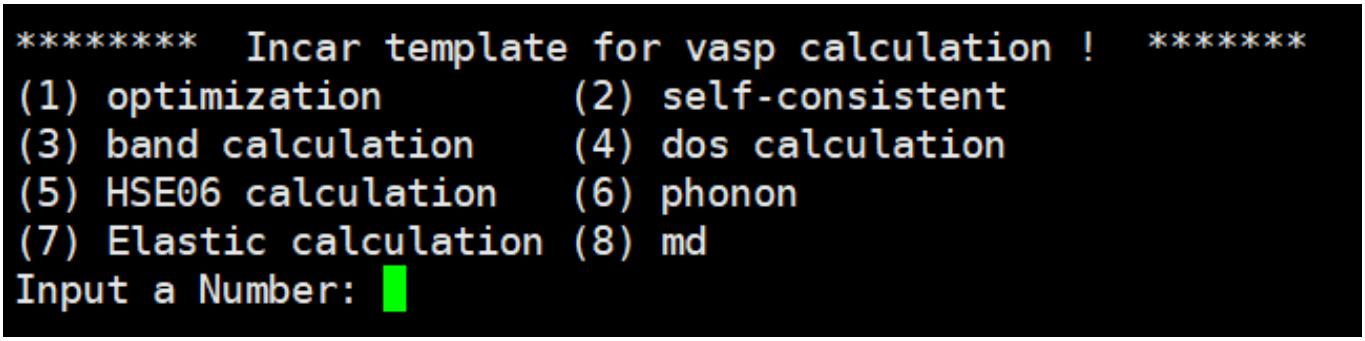

Figure 2. INCAR templates for vasp calculation

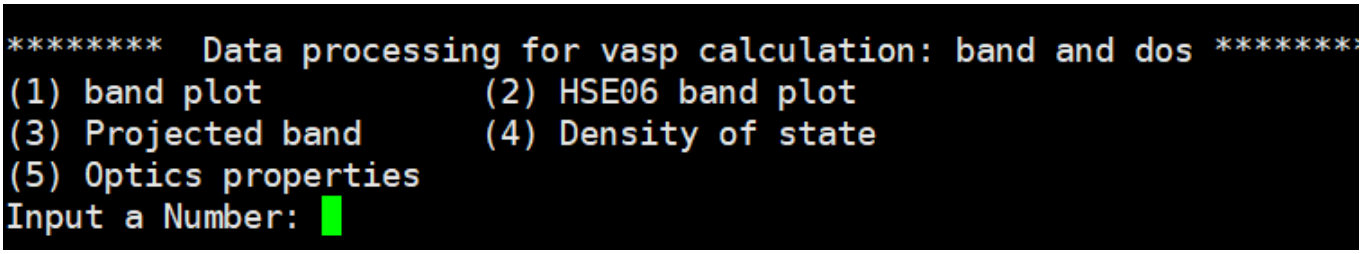

Figure 3. Vasp results visualization: band, dos and optical properties.

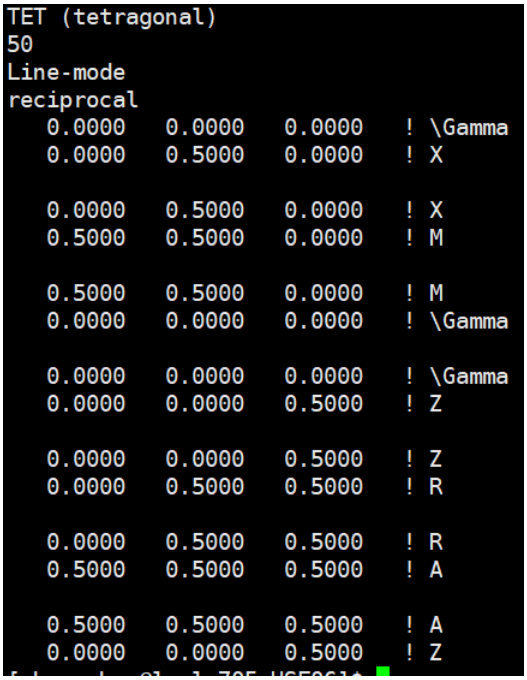

Figure 4. KPOINTS file of PBE band formatting and KPATH.in file of HSE06 band formatting.

3. Noting

1. PBE BAND: Needing the INCAR, POSCAR, OUTCAR, KPOINTS and EIGENVAL, KPOINTS file store the high symmetry points information, and it must be formated 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, EIGENVAL, 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**.