User guide for CMPKIT: a tookit for condensed matter physics

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Abstract. **cmpkit** is a pre- and post-processing software for VASP and Quantum Espresso calculation. Fig.1 shows the main functions of cmpkit. It includes two components: P-VASP and P-Quantum Espresso.

Please email me if there exist some bugs.

1. Installation instruction

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

Introduction for P-VASP

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

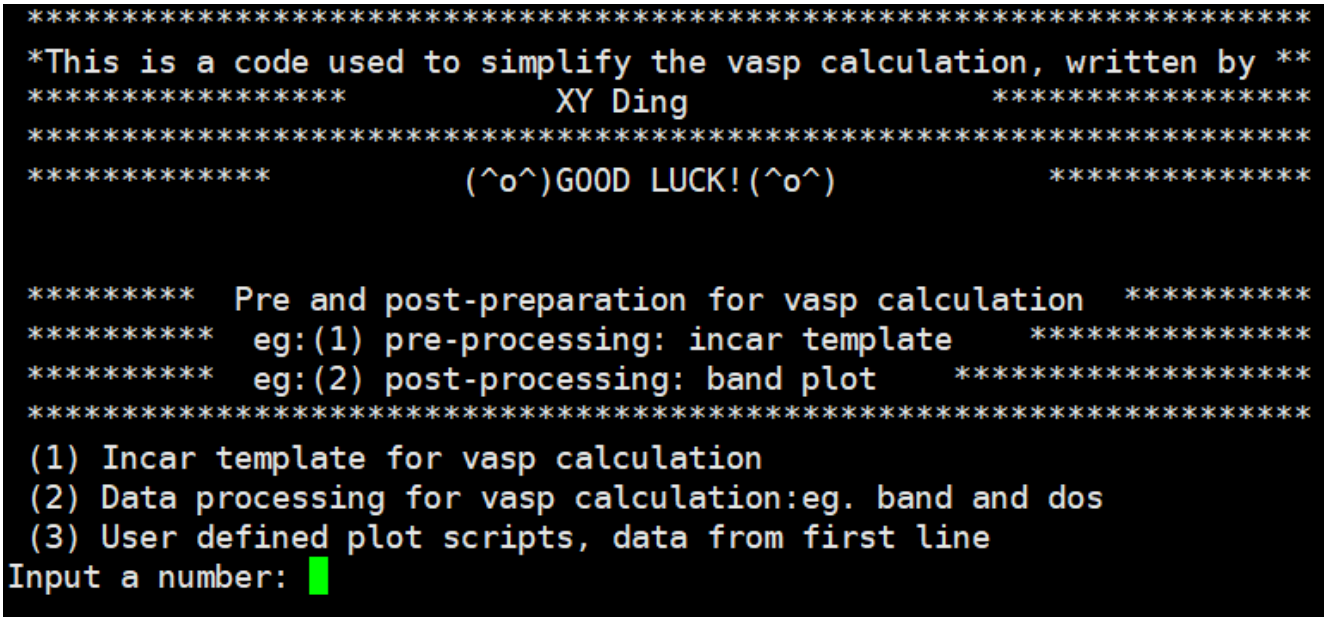


Figure 1. Main functions of VASP. (1) Generating the INCAR file for vasp calculation. (2) Post-processing for vasp results. (3) Waiting for update.

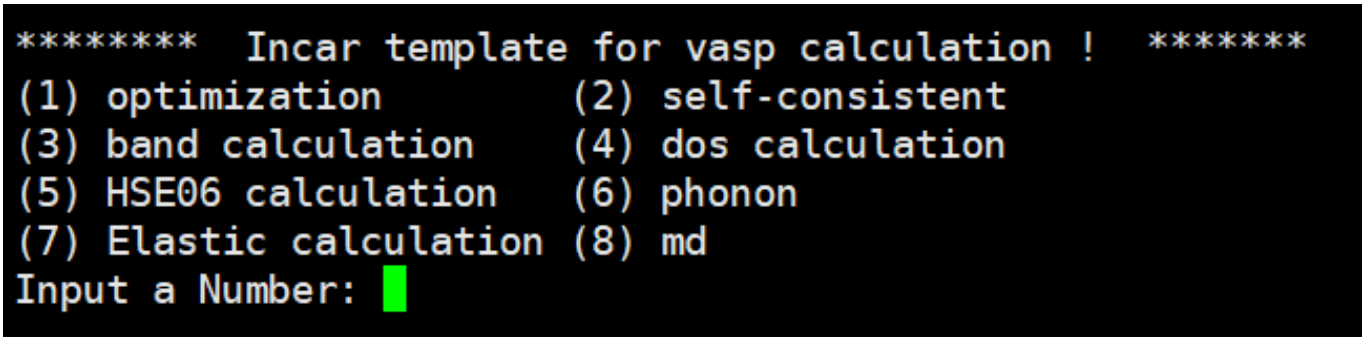


Figure 2. INCAR templates for vasp calculation

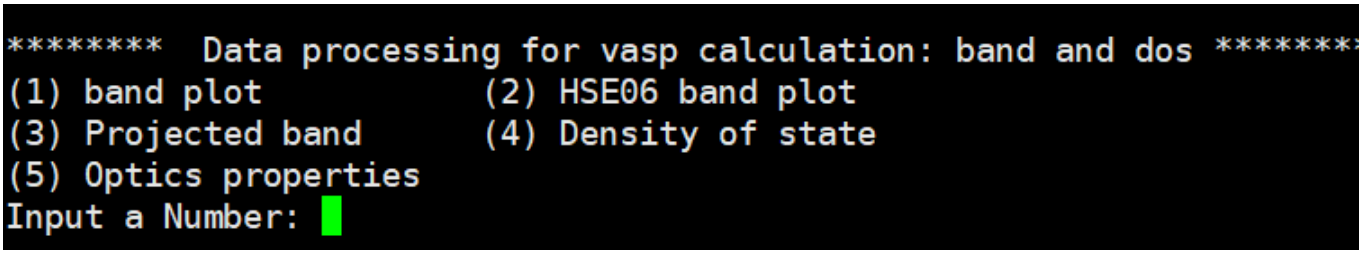
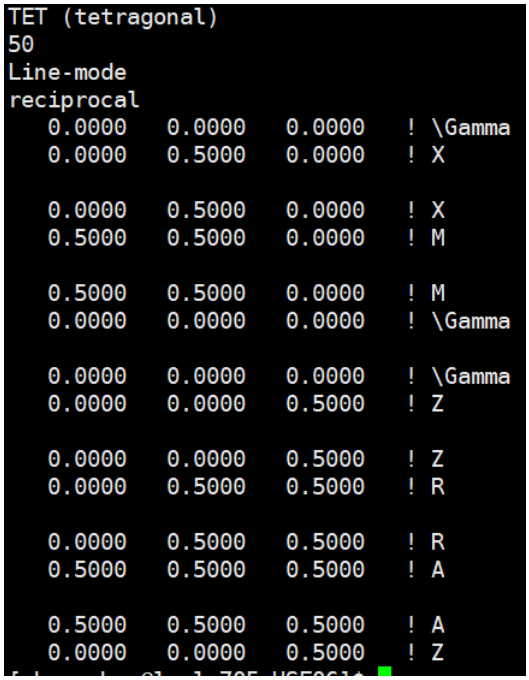


Figure 3. Vasp results visualization: band, dos and optical properties.



```
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.

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**.

Introduction for P-Quantum Espresso

Noting

1. PBE BAND: Needing the **relax**, **relax.out**, **band**, **band.dat** and **scf.out**

relax (input file for relaxation): Needing this file to exact data for cell parameters, if you implent the 'relax' calculation, not the 'vc-relax'.
Noting that the calculation parameter in the relax file must use ', not " to bracket relax or vc-relax. eg. calculation = 'relax', not calculation = "relax"

relax.out (output file for relaxation): Needing this file for exacting coordinates of your structure.
band (input file for band calculation): Needing this file for obtaining the high-symmetry points information. you must calculate with K_POINTS crystal_b.
band.dat (output file for band calculation, the eigenval data for band): the data extracted after using bands.x for band calculation.
scf.out (output file for scf calculation): Needing this file to obtain the Fermi level energy.

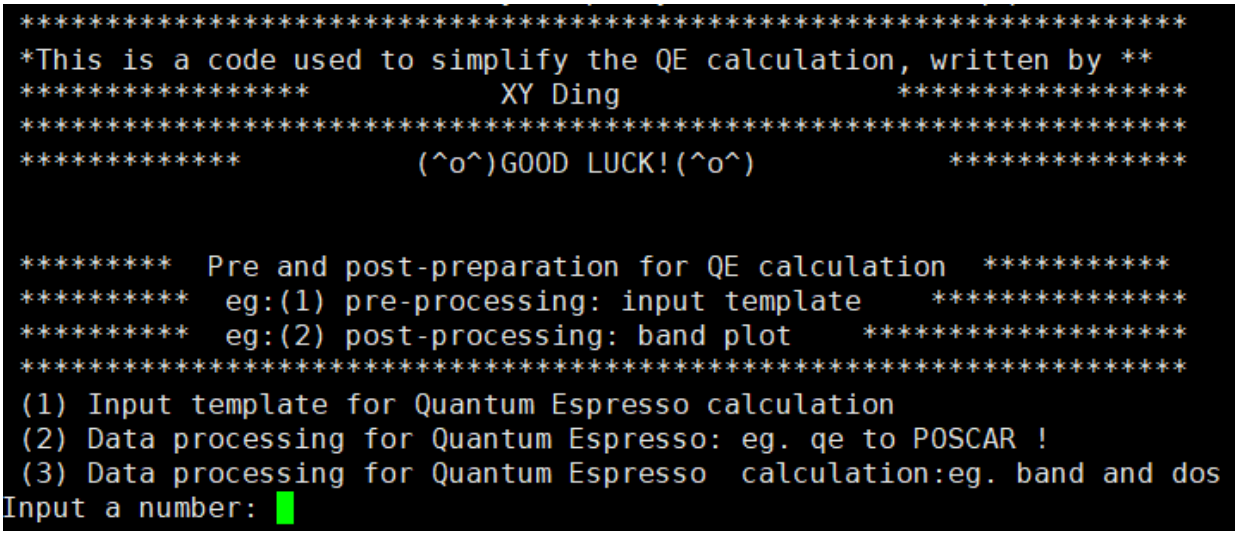


Figure 5. Main functions of pqe. (1) Generating the input file for QE calculation, Including transform the POSCAR formate to QE formate (**Needing the POSCAR file.**). (2) Transforming the output file of relaxation to CONTCAR file (vasp formate). (3) Post-processing for QE results.