**Advanced Computational Materials Research Laboratory**

**Chittagong University of Engineering and Technology**

**VASP MANUAL**

**Step 1:Determination of cut-off energy(ENCUT) and kpoints**

Cut-off Energy trial should begin from **ENMAX** in **POTCAR** with a fixed kpoints

* After getting enough data of Cut-off energy vs final total free energy**(E0)**, we have to find a saturated point from the curve and fix the final cut-off energy for our further calculation.

→ Final total free energy**(E0)** can be get from **OSZICAR /** type **vasp.out**

* After that we have to follow the same path to get the suitable kpoints where trial should be done with the final cut-off energy with respect to different kpoints.

**Step 2: Relaxation/Geometry Optimization of the Structure**

Input files: INCAR,POSCAR,POTCAR,KPOINTS

* Create **POSCAR** from .cif or get from available database(Materials Project)

→ Standardize it by vaspkit (602) and rename it as POSCAR

* Create **POTCAR** :

→ cat ~/vasp/potpaw\_PBE.64/H/POTCAR > POTCAR

→ cat ~/vasp/potpaw\_PBE.64/O/POTCAR >> POTCAR

→ check that all the potentials are set sequentially wrt POSCAR: CTRL+F ( End of Dataset)

* Create **KPOINTS** (102) and set the suitable kpoints got from the trial to get more accuracy.
* Create **INCAR** (available in the folder)

→ INCAR parameters should be same always for the structure to any calculation

* **Run**

→ for run: mpirun -np 36 vasp\_std

→ for non-collinear spin mode: mpirun -np 36 vasp\_ncl

**Step 3: SCF optimization**

Input files: INCAR,POTCAR,KPOINTS,CONTCAR from geometry optimization

* copy the required input files from geo\_opt folder

→ cp INCAR POTCAR KPOINTS CONTCAR ~/vasp/…../scf

(**CONTCAR** is the relaxed structure file)

* rename CONTCAR as POSCAR

→ mv CONTCAR POSCAR

* Run

**Step 4: Determination of the BAND structure and DOS**

Input files: INCAR,POTCAR,POSCAR,**CHGCAR,WAVECAR** from scf optimization

* copy the required input files from scf\_opt folder

→ cp INCAR POSCAR POTCAR CHGCAR WAVECAR ~/vasp/…../band

* create **KPATH.in**(303) and rename it as KPOINTS

→ mv KPATH.in KPOINTS

* RUN
* Get the band structure data (211)
* Get the dos data (111)

For hybrid calculation:

* Do hybrid scf\_opt

→ same as mentioned earlier just with hybrid INCAR(available in the folder)

* Create KPATH.in (303)
* Generate KPONTS(251)
* RUN
* Get the band structure data (252)
* Get the dos data (111)

**Step 5: Determination of the mechanical properties**

Input files: INCAR,POSCAR,POTCAR,KPOINTS(accuracy should be good enough: 0.01)

* Prepare VPKIT.in file and set the value of first line to 1

1 ! 1 for pre-processing; 2 for post-processing

3D ! 2D for two-dimentional, 3D for bulk

7 ! number of strain case

-0.015 -0.010 -0.005 0.000 0.005 0.010 0.015 ! Strain range

* After that to get

→ Elastic-Constants Using Stress-Strain Method (200) [faster and preferable]

→ Elastic-Constants Using Energy-Strain Method (201)

* Do batch Run all the elastic constants created in a folder
* Modify the value of the first line in VPKIT.in file to 2
* Get all the mechanical data (200/201)

**Step 6: Determination of the optical properties**

Input files: INCAR,POTCAR,POSCAR,KPOINTS,**CHGCAR,WAVECAR** from scf optimization

* copy the required input files from scf\_opt folder

→ cp INCAR POSCAR POTCAR CHGCAR WAVECAR KPOINTS ~/vasp/…../optical

* RUN
* Get the optical properties data (71)

**Thank You**

To Be Continued after further research ……………

The updated manual and INCAR files can be found from the following link:

https://github.com/Kashfi-uddin/vasp

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