Calculate Band Structure Using VASP
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VASP Version : 4.6
A complete tutorial on VASP is available at
http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html

In this article, I will describe how to calculate the Band Structure using VASP, taking Si as an example. The Si crystal are just two sets of FCC lattice with a displacement of (a/4,a/4,a/4), where a is the length of the conventional cubic lattice. In the calculation, I chose a FCC primitive unit cell with 2 atoms in the unit cell.

Files need by vasp: INCAR, KPOINTS, POSCAR, POTCAR

INCAR : Contains all the control parameter
KPOINTS : Contains the K-point Sampling scheme
POSCAR : Contains information on unit cell and the basis atoms
POTCAR : Pseudo-Potential File used by VASP

To calculate the Band structure, we need to first run self-consistently to get the charge density, and then fix the charge density and do a non-self consistent run at desired K points to get the band structure.

Step 1.--Run self-consistently to get the charge density.
Here are the sample files:
The INCAR file

```
SYSTEM = Si
 Startparameter for this run:
   NWRITE =      2;   LPETIM=F    write-flag & timer
   PREC   = medium    medium, high low
   ISTART =      0    job   : 0-new  1-cont  2-samecut
   ICHARG =      2   charge: 1-file 2-atom 10-const
   ISPIN  =      1    spin polarized calculation?

 Electronic Relaxation 1
   NELM   =     90;   NELMIN=  8; NELMDL= 10     # of ELM steps
   EDIFF  = 0.1E-03   stopping-criterion for ELM
   LREAL  = .FALSE.     real-space projection

 Ionic relaxation
   EDIFFG = 0.1E-02   stopping-criterion for IOM
   NSW    =      0    number of steps for IOM
   IBRION =      2    ionic relax: 0-MD 1-quasi-New 2-CG
   ISIF   =      2    stress and relaxation
```

POTIM = 0.10 time-step for ionic-motion
TEIN = 0.0 initial temperature
TEBEG = 0.0; TEEND = 0.0 temperature during run

DOS related values:
ISMEAR = 0 ; SIGMA = 0.10 broadening in eV -4-tet -1-fermi 0-gaus

Electronic relaxation 2 (details)

Write flags
LWAVE = T write WAVECAR
LCHARG = T write CHGCAR

VASP sets defaults for almost every parameter, so you can use a much simpler INCAR file if you are not too familiar with the Control Parameters. Here is a simpler version of the INCAR file:

SYSTEM = Si
Startparameter for this run:
PREC = medium medium, high low
ISTART = 0 job : 0-new 1-cont 2-samecut
ICHARG = 2 charge: 1-file 2-atom 10-const
EDIFF = 0.1E-03 stopping-criterion for ELM
NSW = 0 number of steps for IOM
IBRION = 2 ionic relax: 0-MD 1-quasi-New 2-CG
ISIF = 2 stress and relaxation

The KPOINT file:
We use the Automatic Mesh generation. For semiconductors, a 4x4x4 mesh is usually good enough.

Monkhorst Pack
0
Monkhorst Pack
4 4 4
0 0 0

The POSCAR file:
We use the FCC primitive unit cell for Si, Thus there are 2 atoms in a unit cell.

Si
5.38936
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
2
Cartesian

0.0000000000000 0.00000000000 0.0000000000000
0.2500000000000 0.25000000000 0.2500000000000

The POTCAR file
You don't need to worry about this file since it is provided by VASP. All you need to do is to copy the correct file from the VASP pseudo-potential library. If you are dealing with a compound, then you need to concat multiple files together, using Unix command "cat".

Once we have all the files, we issue a command to run vasp, such as "./vasp>&output&" (This depends on your system, if a queue system is running, then you need to write a simple script to queue the job)

After this step is completed, we should now have the charge density, which is contained in CHGCAR file. In order to get band structure, we need to do non-self consistent run on each desired K point, by connecting these information, we can get the E~K dispersion relation, which is the Band structure.

Step 2.—Get energy for each K points based on the charge density we got from the first job.

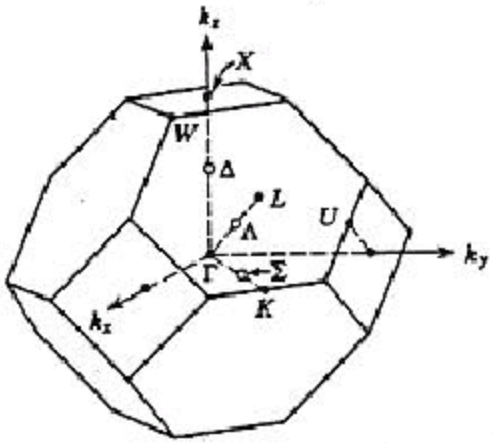
We need to modify one line in INCAR, which is
ICHARG = 11 charge: 1-file 2-atom 10-const
ICHARG=11 means reading charge density from CHGCAR and kept constant during the subsequent run.

We also need to modify the KPOINT file, to specify along which direction(Usually some high symmetry direction) we need VASP to calculate the energy. In VASP4.6 and higher, there is an easy way of doing this.

```
k-points along high symmetry lines
 10  ! 10 intersections
Line-mode
rec
  0   0   0   ! gamma
  0.5 0.5 0   ! X

  0.0 0.0 0   ! gamma
  0.5 0.5 0.5  ! L
```

By specifying the Line-mode, VASP automatically interpolate between the points you want to calculate. The above file instructs VASP to calculate the energy at each K point between Gamma point and X point, Gamma point and L point. Along each line, 10 K points are calculated.



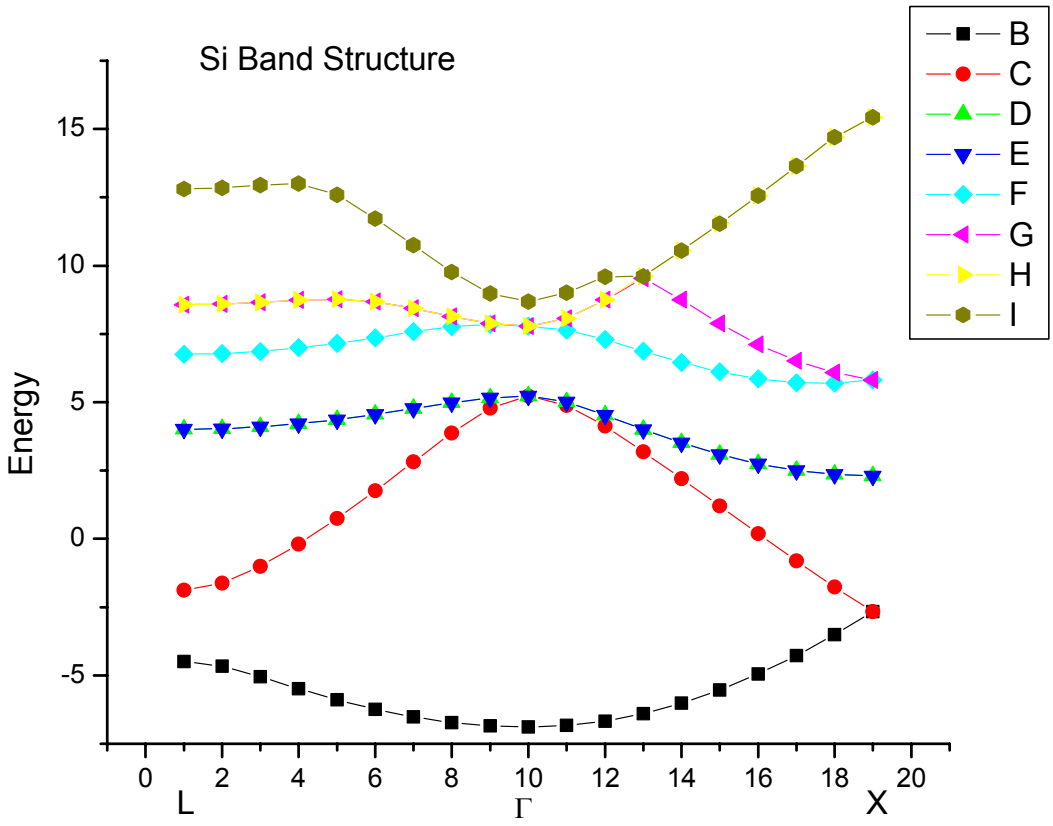
First Brillouin Zone for FCC lattic.

Having modified these two files, we rerun the vasp again and we will get all the information we need to plot the band structure.(contained in EIGENVAL file)

In EIGENVAL file, there would be lines like this

0.5555556E-01 0.5555556E-01 0.0000000E+00 0.5000000E-01
1 -6.8356
2 4.8911
3 5.0077
4 5.0079
5 7.6438
6 8.0693
7 8.0694
8 9.0057

the first line is just the K point, the following 8 lines tell us the energy of 8 bands at that particular energy point. You can visualize these information using any plotting tool like EXCEL or ORIGIN(nicer!). Since you have the Enegy of the bands at each K point, this is exactly what you want – the Band Structure. The following is the result generated by the above files. We can see that Si is not a direct gap material. (Of course you can get much more than this from the information of Band Structure)


Si Band Structure
Energy
15
10
5
0
-5
0
2
4
6
8
10
12
14
16
18
20
L
Γ
X
B
C
D
E
F
G
H
I