Practice: VASP

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VASP units

Energy	-	eV
Length	-	Å
Force	-	eV/Å
Stresses	-	kB, divide by 10 to get GPa

How to use VASP

go to Lab3_silicon/sampleinputs

4 input files are required

POSCAR - contains crystal structure

INCAR - control parameters

KPOINTS - k-mesh in reciprocal space

POTCAR - PAW potential file

POSCAR

```
Si                                  # just any name
1.000                               # multiplier for vec
 0.00   2.71   2.71                 # Lattice vec 1, A
 2.71   0.00   2.71                 # Lattice vec 2, A
 2.71   2.71   0.00                 # Lattice vec 3, A
Si C
2  2                               # N atom for each type
Direct                              # type of coordinates
 0.00   0.00   0.00                 # atom 1 Si
 0.25   0.25   0.25                 # atom 2 Si
 0.00   0.00   0.00                 # atom 1 C
 0.25   0.25   0.25                 # atom 2 Ce
```

Minimum INCAR

```
ENCUT = 300     # eV, energy cut-off
ISIF = 3        # full optimization
ISMEAR = 2      # Smearing method, Methfessel-Paxton

KSPACING = 0.1 # spacing of k points, can be used instead of
KPOINTS file
```

INCAR, reasonable

```
SYSTEM =  2 Li;# name
EDIFF = 0.0001 # eV,   stopping criteria of SCF
EDIFFG = -0.01 # eV/A, stopping criteria of relaxation
NSW = 20       # number of relaxation steps
ENCUT = 150    # eV, energy cut-off
IBRION = 1     # optimization algo;
ISIF = 3       # full optimization
ISMEAR = 2     # Smearing method, Methfessel-Paxton
SIGMA = 0.2    # eV,  smearing broadening
NBANDS = 4     # number of bands
```

INCAR for structural optimization of Si

```
ENCUT = 600    # eV, energy cut-off
EDIFFG = -0.01 # force stopping criteria, 0.01 eV/A or
ISIF = 3       # full optimization
IBRION = 2     # Quasi-Newton
NSW    = 100   # Maximum Number of steps for optimization
ISMEAR = 0     # Smearing method, Gaussian
SIGMA  = 0.1   # Smearing
LWAVE = .FALSE. # do not save WAVECAR - usually huge ~1-10 GB


# EDIFFG reads as eV/A^3 for stresses. See “Total” in OUTCAR and
divide by Nat
```

KPOINTS, normal calculation

```
Automatic Mesh
0
Monkhorst Pack
9 9 9
0 0 0
```

KPOINTS, band structure, CHGCAR required

```
kpoints for bandstructure L-G-X-U K-G
 40         ! 40 intersections
line        ! line mode
reciprocal  ! type of coordinates
  0.50000  0.50000  0.50000    !L
  0.00000  0.00000  0.00000    !G

  0.00000  0.00000  0.00000    !G
  0.00000  0.50000  0.50000    !X

  0.00000  0.50000  0.50000    !X
  0.25000  0.62500  0.62500    !U

  0.37500  0.7500   0.37500    !K
  0.00000  0.00000  0.00000    !G
```

POTCAR - Potential file, with VASP

```
 PAW_PBE Li 17Jan2003   # version
 1.00000000000000000   # N valence
 parameters from PSCTR are:
 VRHFIN =Li: s1p0 # electronic conf
 LEXCH  = PE       # exch. cor PBE
 EATOM  =  5.3001 eV # energy of
atom in vacuum, it is subtracted
from output total energy
```

Creating POTCAR for multiple elements

e. g. for SiC system you should run

```
cat Si/POTCAR C/POTCAR > POTCAR
```

The order should be the same as types of atoms follow in POSCAR

OUTPUT

CONTCAR - file with output structure, the same format as **POSCAR**

OUTCAR - main file with energies, etc.

CHGCAR - charge density file

WAVECAR - wave function file

EIGENVAL - Kohn-Sham energies at k - required for band structure ploting

and others, see VASP manual

OUTCAR, check that is finished

```
grep reached OUTCAR
```

OUTCAR, read final energies

```
grep TOTEN OUTCAR
```

Print total energy at each SCF step

```
grep 'energy  without entropy'  OUTCAR
```

print total energy after each relax step

use energy(sigma->0) extrapolated energy

OUTCAR, read stresses and forces

```
grep  'in kB'  OUTCAR
```

Print stress tensor after each relax step,

multiply by 100 to get MPa

residual stress of 100 MPa is OK for most solids

```
grep -A 3 TOTAL OUTCAR
```

Print positions and forces

why forces are zero?

OUTCAR, More

```
grep E-fermi OUTCAR
```

Print Fermi energy in eV

residual stress of 100 MPa is OK for most solids

Eigenvectors and eigenvalues of the dynamical matrix