Vienna Ab Initio Package – Crash course

2nd Lecture – 08/09/21

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b-initio
VASP
ackage
ienna
imulation

ICIQ
Institut
Català
d'Investigació
Química

Structure of the course

Day / September	Hours / Madrid time	Location	Topic
Monday 6th	10:00-12:00	E4 / Zoom	Introduction + Handson 1 (molecules; frequencies; molecular dynamics)
Tuesday 7th	12:00-13:00	E4 / Zoom	Tutorial Handson 1
Wednesday 8th	10:00-12:00	E4 / Zoom	Correction exercises 1 + Handson 2 (bulk optimization and electronic properties) + Instructions for python / bash project
Thursday 9th	10:00-11:00	E3 / Zoom	Tutorial Handson 2
Friday 10th/ Wednesday 15th	Python / bash project		
Thursday 16th	10:00-12:00	E4 / Zoom	Correction exercises 2 and python / bash project + Handson 3 (surface optimization and electronic properties)
Friday 17th	10:00-11:00	E4 / Zoom	Tutorial Handson 3
Monday 20th	10:00-12:00	E4 / Zoom	Correction exercises 3 + Handson 4 (magnetic properties and Hubbard correction)
Tuesday 21th	10:00-11:00	E4 / Zoom	Tutorial Handson 4
Wednesday 22th	10:00-11:00	E4 / Zoom	Correction exercises 4

Materials

- Materials available on OneDrive;
- All lectures and tutorials will be registered and later available on OneDrive;
- Detailed explanation online. The current course gives only an introduction!
- Save the link to the VASP manual online: https://www.vasp.at/wiki/index.php/The_VASP_Manual

Today’s class

1. Correction of exercises of Handson 1;
2. Lecture 2 and instructions for Handson 2;
3. Instructions for python / bash project

Based on:
- 2_k-points

Further materials:
- 1_pseudopp2

Related handson session:
(2) Bulk optimization and electronic properties

Additional material
- personal notes taken during course given by Núria.

Handson 1

1_1_O_atom;
1_2_O_atomspin;
1_3_O_atomspinlowsym;
1_4_Odimer;
1_5_CO;
1_6_COvib;
1_7_H2O
1_8_H2Ovib;
1_9_COstates;
1_10_H2Omd.

```
SECOND DERIVATIVES (NOT SYMMETRIZED)
-----------------------------------
              1Z          2Z
 1Z  -114.847733  114.847733
 2Z   114.305971 -114.305971

Eigenvectors and eigenvalues of the dynamical matrix
---------------------------------------------------
  1 f  =   63.876494 THz   401.347846 2PiTHz 2130.690412 cm-1   264.172038 meV
            X         Y         Z           dx          dy          dz
     0.000000  0.000000  0.000000            0           0   -0.655709
     0.000000  0.000000  1.143000            0           0    0.755014
  2 f/i=    0.074763 THz     0.469753 2PiTHz    2.493841 cm-1     0.309197 meV
            X         Y         Z           dx          dy          dz
     0.000000  0.000000  0.000000            0           0   -0.755014
     0.000000  0.000000  1.143000            0           0   -0.655709
```

```
k-point   1 :       0.0000    0.0000    0.0000
 band No.  band energies     occupation
     1      -25.0761       1.00000
     2      -10.0715       1.00000
     3      -10.0715       1.00000
     4      -10.0715       1.00000
     5       -0.3997       0.00000
     6        1.6965       0.00000
     7        1.9499       0.00000
     8        1.9499       0.00000
```

PROCAR file:

```
band   3 # energy   -11.46549527 # occ.   2.00000000

ion       s     py     pz     px    dxy    dyz    d
  1   0.000  0.546  0.000  0.000  0.000  0.000  0.0
  2   0.000  0.157  0.000  0.000  0.000  0.000  0.0
tot   0.000  0.703  0.000  0.000  0.000  0.000  0.0
```

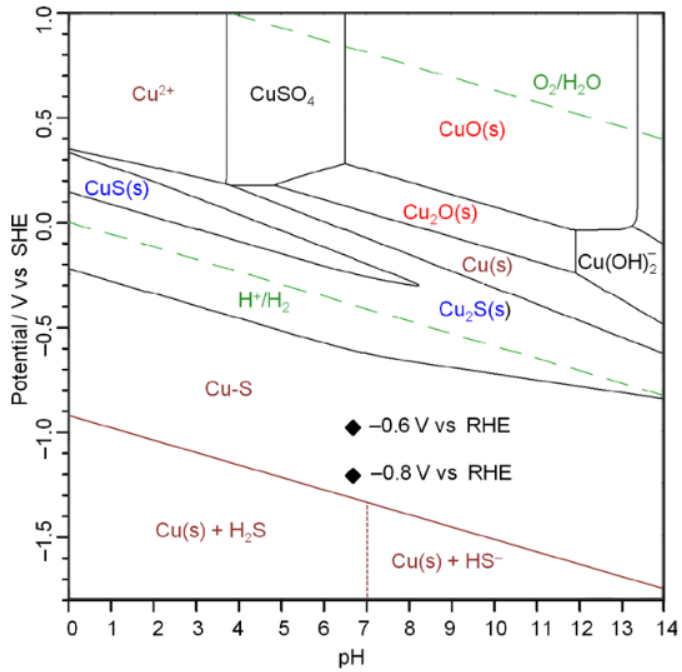
Handson 2

Exercises

- 2_1_fccSi
- 2_1_fccSi_opt
- 2_2_fccSi_dos
- 2_3_fccSi_band
- 2_4_diamondSi
- 2_4_diamondSi_vol_rex
- 2_5_beta-tinSi
- 2_6_diamond_relax_Si
- 2_7_fccNi
- 2_8_fccNi_dos

Investigations

- Most stable crystal structure;
- Comparison with experimental enthalpy of formation;
- Pourbaix diagram;
- Bandgap;
- Density of states.



Handson 2

Manual optimization of bulk (pg.35-48 of DFT book)

- 2_1_fccSi
- 2_4_diamondSi
- 2_7_fccNi

Internal energy is calculated for different lattice vector; energies saved in SUMMARY.fcc

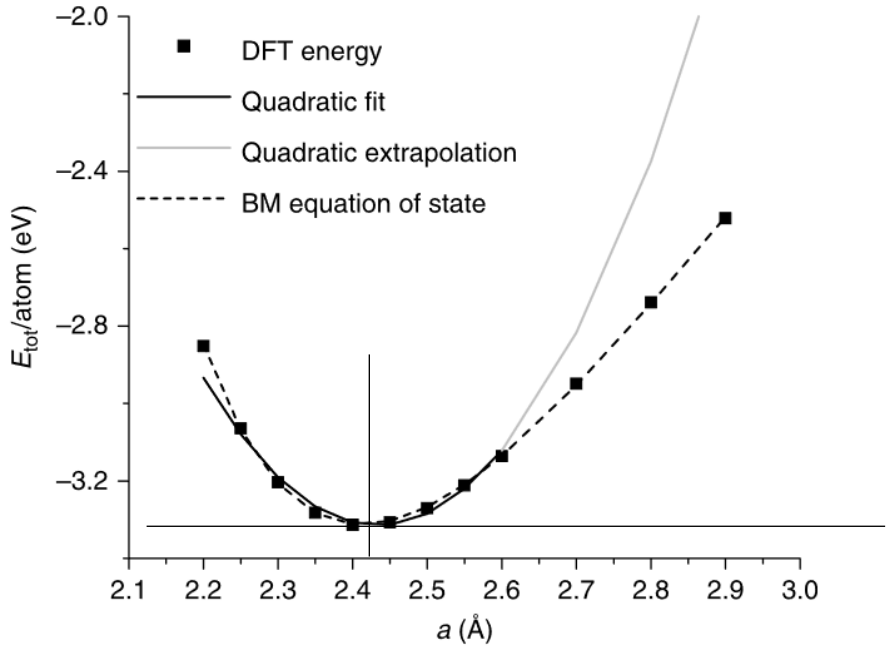


Figure 2.1 Total energy, E_{tot}, of Cu in the simple cubic crystal structure as a function of the lattice parameter, a. The filled symbols show the results of DFT calculations, while the three curves show the fits of the DFT data described in the text.

Quadratic fit

$$E(a) = p_1 + p_2 a + p_3 a^2;\ a_0 : \text{minimum}$$

Birch–Murnaghan equation of state

$$E(a) = E_0 + \frac{9V_0B_0}{16}\left\{\left[\left(\frac{a_0}{a}\right)^2 - 1\right]^3 B_0' + \left[\left(\frac{a_0}{a}\right)^2 - 1\right]^2 \left[6 - 4\left(\frac{a_0}{a}\right)^2\right]\right\}$$

Handson 2

Internal energy is calculated for different lattice vector; energies saved in SUMMARY.fcc

```
#!/bin/bash
### SGE Parameters ##########################
#$ -S /bin/bash
#$ -N test-2_2_fccSi_dos
#$ -cwd
#$ -masterq c4m8.q
#$ -pe c4m8_mpi 4
#$ -m ae
#$ -M fdattila@iciq.es
#$ -o o_$JOB_NAME.$JOB_ID
#$ -e e_$JOB_NAME.$JOB_ID
### Load Environment Variables ############
. /etc/profile.d/modules.sh
module load vasp/5.3.5
### Run Job ###############################
export OMP_NUM_THREADS=1
echo $PWD >> o_$JOB_NAME.$JOB_ID
echo $TMP >> o_$JOB_NAME.$JOB_ID
~/bin/savecalc ; mpirun -np $NSLOTS vasp ; # rm -f CHG
```

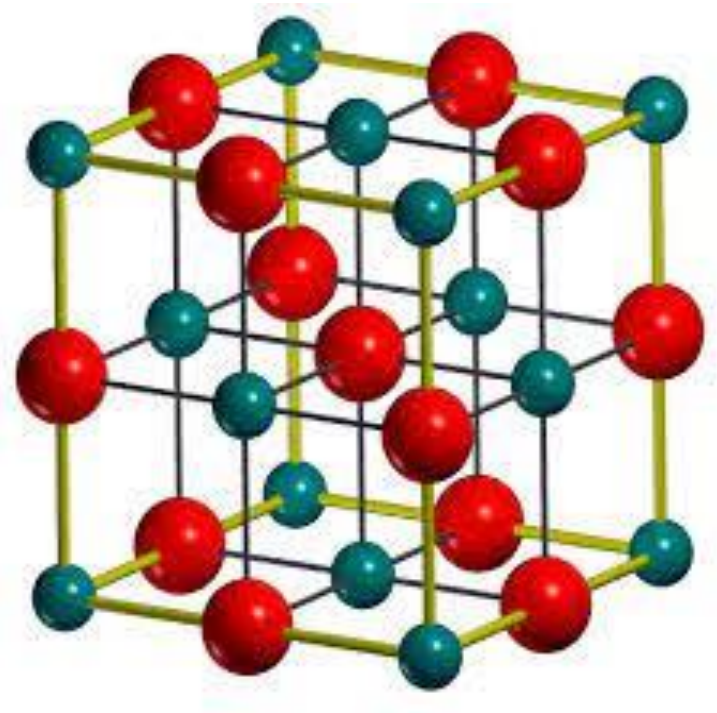
Job start here!

```
for i in  3.5 3.6 3.7 3.8 3.9 4.0 4.1 4.2 4.3 ; do
cat >POSCAR <<!
fcc:
   $i
 0.5 0.5 0.0
 0.0 0.5 0.5
 0.5 0.0 0.5
   1
cartesian
0 0 0
!
echo "a= $i" ;
export OMP_NUM_THREADS=1
echo $PWD >> o_$JOB_NAME.$JOB_ID
echo $TMP >> o_$JOB_NAME.$JOB_ID
mpirun -np $NSLOTS vasp # rm CHG
E=`tail -1 OSZICAR` ; echo $i $E  >>SUMMARY.fcc
done
cat SUMMARY.fcc
```

Handson 2

Automation optimization of bulk (ISIF = 2,3)

- 2_4_diamondSi_vol_rex (ISIF = 3);
- 2_5_beta-tinSi (ISIF = 3);
- 2_6_diamond_relax_Si (ISIF = 2).



ISIF	calculate		degrees-of-freedom		
	forces	Stress tensor	positions	cell shape	cell volume
0	yes	no	yes	no	no
1	yes	trace only	yes	no	no
2	yes	yes	yes	no	no
3	yes	yes	yes	yes	yes
4	yes	yes	yes	yes	no
5	yes	yes	no	yes	no
6	yes	yes	no	yes	yes
7	yes	yes	no	no	yes

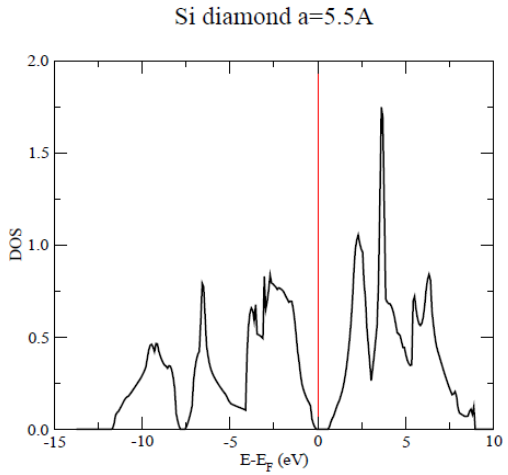
Question:
(1) What is the most stable crystal structure of Si?
Does your prediction agree with experiments?

Handson 2

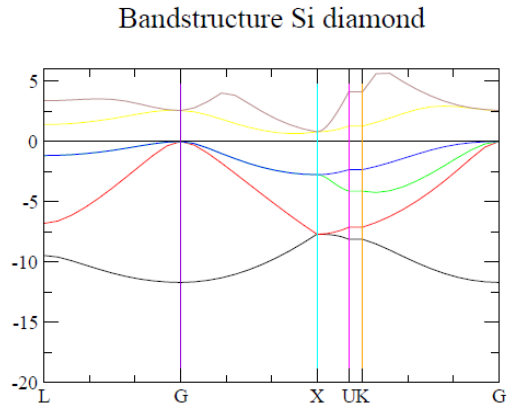
Electronic properties

- 2_1_fccSi_opt (lattice vector *a* from 2_1_fccSi)
- 2_2_fccSi_dos (copy CHGCAR from 2_1_fccSi_opt; use CONTCAR from 2_1_fccSi_opt as POSCAR).
- 2_3_fccSi_band (copy CHGCAR from 2_1_fccSi_opt; use CONTCAR from 2_1_fccSi_opt as POSCAR)
- 2_8_fccNi_dos (lattice vector *a* from 2_7_fccNi)

Density of States



Bandstructure



Question:
(2) From the density of states, do you consider Si and Ni metals or semiconductors? Motivate the answer.

Handson 2

Questions:

(1) What is the most stable crystal structure of Si? Does your prediction agree with experiments?

(2) From the density of states, do you consider Si and Ni metals or semiconductors? Motivate the answer.

Handson 2 – copy the exercises (supercomputer)

- Enter the virtual machine (password: guest1$) or AnyDesk;
- Open a terminal: *Ctrl + Alt + t*
- Enter teklahome (from ICIQ workstation): *ssh tekla2.iciq.es*
- From outside ICIQ: enable Betelgeuse tunnel and then enter teklahome
  ssh -p2004 -X yourusername@betelgeuse.iciq.es
  ssh tekla2.iciq.es
- Make a directory *handson* and a subdirectory *2*
  mkdir handson ; mkdir handson/2
- Copy the exercises from my teklahome to yours
  cp –r /home/fdattila/00-vasp-course/handson2/ ~/handson/2*
- Enter the folder and check to have successfully copied the files
  cd handson/2 ; ls –lt ; cd ../..

Handson 2 – check the exercises

Check the VASP input (supercomputer / locally)

- Enter each simulation and check INCAR / KPOINTS
  cd handson/2 ; cd simulation-folder ; vi INCAR ; cd .. ; cd ../..

- Use the VASP manual to understand properly all the tag of the INCAR.

Handson 2 – submit simulation (supercomputer)

- Enter the handson/1 folder and create a run.sh file in each simulation to be run (e.g. 1_1_O_atom)
  cd handson/2/simulation-folder; ~/bin/rungen name-of-sim 4 4 5.3.5 ; sed –i "s/vasp_std/vasp/g" run.sh ; cd ../../..

- Enter the handson folder, check that you have INCAR, KPOINTS, POTCAR, POSCAR and run.sh, submit the simulation.
  cd handson/2/simulation-folder; qsub run.sh; cd ../../..

Tip: consider iterating the creation of run.sh file and the submission of each simulation with the for command. E.g. *cd handson/2 ; for i in 2_* ; do cd $i ; action-to-be-performed ; cd .. ; done ; cd ../..*

Handson 2 – check the VASP output (locally)

- Only if you access through virtual machine. Run the commands tunnel1 and tunnel2 in 2 terminals
  tunnel1 yourusername (terminal 1)
  tunnel2 yourusername (terminal 2)

- Open a new terminal and enter the teklahome folder
  cd ~/teklahome

- Enter a simulation and check the structure through the p4v utility
  cd handson/2 ; cd simulation-folder; p4v vasprun.xml ; cd .. ; cd ../..

Python / Bash projects

Maryam / Santiago – Python

- Cut surface facets from bulk (input: POSCAR: output: POSCAR_xyz)

In case you finish the first (or it is too complex):

- Calculate the surface energy *γ* for a facet in J m^{-2} or eV $Å^{-2}$ (input: POSCAR surface/bulk, OUTCAR surface/bulk; output: the value of *γ*)

Enric / Sichen – bash

- Order a surface and fix bulk layer (input: POSCAR; output: POSCAR);
- Generate *k*-points mesh (input: POSCAR; output: KPOINTS);

In case you finish the first two:

- Add a molecule on top of an ordered POSCAR (input: CONTCAR; output: POSCAR)

```
fdattila@tekla2:~/00-vasp-course/scripting> for i in bash python ; do echo $i ; cd $i ; ls ; cd .. ; done
bash
add-mol  k-gen  ordtor
python
get-surface-energy  slab-gen
```

Python / Bash projects

Maryam / Santiago – Python

- Work on jupyter notebook;
- Add # comments to explain each step;
- Check the pymatgen library: https://pymatgen.org/pymatgen.core.surface.html;
- Use numpy to solve equations (*import numpy as np*);

$$\gamma = \frac{1}{A}\left\{\frac{1}{2}\left[E_{\text{unrel}} - n \cdot (E_{\text{bulk}})\right] + \Delta E_{\text{rel}}\right\}$$

A = Area = $a_x \times b_y$

Enric / Sichen – bash

- Work on bash;
- Add # comments to explain each step;
- Check suggestions and tips on the script.