# Vienna Ab Initio Package – Crash course

## 4th Lecture – 20/09/21

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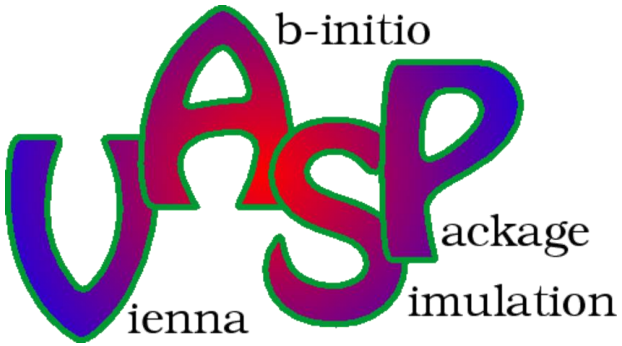


# Structure of the course

| 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 21st | 10:00-11:00 | E4 / Zoom | Tutorial Handson 4 |
| Wednesday 22nd | 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 3;
2. Lecture 4 and instructions for Handson 4.

Based on:

- 0_vasp_summary (summary of all the important information)

Further materials:

- 1_accuracy
- 2_pseudoppdatabase
- 3_dft_depth
- 4_magnetism

Related handson session:
(4) Magnetic properties and Hubbard correction

# Handson 3

Question:

Define the surface energies for Ni(100) and Ni(111). Which is the most stable crystalline facet between Ni(100) and Ni(111)? Compare with experimental values. Which facet is the most abundant on a Ni nanoparticle?

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

$A$ = Area = $a_x \times b_y$
$E_{\text{unrel}}$ = energy of the first ionic step
(*grep "energy  w" OUTCAR | head –n 1*)
$E_{\text{rel}}$ = energy of the last ionic step
(*grep "energy  w" OUTCAR | tail –n 1* )
$\Delta E_{\text{rel}} = E_{\text{rel}} - E_{\text{unrel}}$
$E_{\text{bulk}}$ = energy of the bulk crystal structure (2_7_fccNi_opt)
$n$ = number of unit cell in the surface

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| | *n* unit cell | $a_x$ / Å | $b_y$ / Å | $A$ / Å$^2$ | $E_{unrel}$ / eV | $E_{rel}$ / eV | $\Delta E_{rel}$ / eV | $\gamma$ / eV Å$^{-2}$ | $\gamma$ / J m$^{-2}$ |
|---|---|---|---|---|---|---|---|---|---|
| Ni(100) | 5 | 1.8 | 1.8 | 3.1 | -25.6 | -25.6 | -0.014 | 0.4 | 5.6 |
| **Ni(111)** | **5** | **2.5** | **2.2** | **5.4** | **-25.7** | **-25.7** | **-0.001** | **0.2** | **3.0** |
| bulk | 1 | | | | | -5.6 | | | |

$\gamma$ (J m$^{-2}$)

(111) 2.011

(100) 2.426 2.380 [c],2.450 [a]

(110) 2.368

*Surf. Sci.* **1998**, *411*, 186–202.

# Handson 3

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| **Ads / eV** | **–0.3** |

TABLE I. Calorimetric heat of adsorption at initial low coverage ($q_i$), at final steady state coverage, $1.0\times10^{15}$ /cm$^2$ ($q_f$), the differential entropy of the adsorbate layer at steady state ($\bar{S}$), and the desorption preexponential at steady state ($\upsilon$).

| System | $q_i$ (kJ/mol) | $q_f$ (kJ/mol) | $\bar{S}$ (J/K/mol) | $\upsilon$ (s$^{-1}$) |
|---|---|---|---|---|
| CO/Ni(111) | 130 | 95 | 71 | $3\times10^{14}$ |
| CO/Ni(100) | 123 | 99 | 58 | $1\times10^{15}$ |
| CO/Ni(110) | 133 | 101 | 50 | $3\times10^{15}$ |

*J. Chem. Phys.* **1993**, *99*, 2202.

| ΔG / eV | low coverage | steady state |
|---|---|---|
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Why does DFT underestimate the experimental value?

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# Handson 3

Question:

List Ni-CO vibrational frequencies and compare with experimental values.

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```
fdattila@tekla2:~/00-vasp-course/handson3-sol/3_8_COonNi111_freq> grep cm-1 OUTCAR
   1 f  =    64.129566 THz    402.937946 2PiTHz 2139.131995 cm-1    265.218661 meV
   2 f  =    12.470844 THz     78.356621 2PiTHz  415.982553 cm-1     51.575282 meV
```

49.7 meV (401 $cm^{-1}$) for Ni–CO stretch, Exp 59.5 meV

264.0 meV (2129 $cm^{-1}$) for CO stretch,

40.5 meV (327 $cm^{-1}$) for NiCO bend.

*Surf. Sci.* **1982**, *115*, 553–568.

# Handson 4 – 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 *4*
  *mkdir handson ; mkdir handson/4*
- Copy the exercises from my teklahome to yours
  *cp –r /home/fdattila/00-vasp-course/handson4/* ~/handson/4*
- Enter the folder and check to have successfully copied the files
  *cd handson/4 ; ls –lt ; cd ../..*

# Handson 4 – check the exercises

**Check the VASP input (supercomputer / locally)**

- Enter each simulation and check INCAR / KPOINTS
  *cd handson/4 ; cd simulation-folder ; vi INCAR ; cd .. ; cd ../..*

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

# Handson 4 – submit simulation (supercomputer)

Only for Maryam!

- Create a bin directory and copy the rungen file
  *mkdir /home/yourusername/bin ; cp –r /home/fdattila/bin/rungen ~/bin/.*
- Check the file with the vi editor. Change all the fdattila to yourusername through the editor
  *vi ~/bin/rungen ;*
- Alternatively, replace all the fdattila in rungen with yourusername automatically
  *sed –i "s/fdattila/yourusername/g" ~/bin/rungen*

- Enter the handson/4 folder and create a run.sh file in each simulation to be run (e.g. 4_1_Ni)
  *cd handson/4/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/4/simulation-folder; qsub run.sh; cd ../../..*

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**Tip**: consider iterating the creation of run.sh file and the submission of each simulation with the for command. E.g. *cd handson/4 ; for i in 4_* ; do cd $i ; action-to-be-performed ; cd .. ; done ; cd ../..*

# Handson 4 – 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/4 ; cd simulation-folder; p4v vasprun.xml ; cd .. ; cd ../..*