

# Vienna Ab Initio Package – Crash course

1<sup>st</sup> Lecture – 06/09/21

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# Structure of the course

Day / September	Hours / Madrid time	Location	Topic
Monday 6 <sup>th</sup>	10:00-12:00	E4 / Zoom	Introduction + Handson 1 (molecules; frequencies; molecular dynamics)
Tuesday 7 <sup>th</sup>	12:00-13:00	E4 / Zoom	Tutorial Handson 1
Wednesday 8 <sup>th</sup>	10:00-12:00	E4 / Zoom	Correction exercises 1 + Handson 2 (bulk optimization and electronic properties)
Thursday 9 <sup>th</sup>	10:00-11:00	E4 / Zoom	Tutorial Handson 2
Monday 13 <sup>th</sup>	10:00-12:00	E4 / Zoom	Correction exercises 2 + Handson 3 (surface optimization and electronic properties)
Tuesday 14 <sup>th</sup>	10:00-11:00	E4 / Zoom	Tutorial Handson 3
Wednesday 15 <sup>th</sup>	10:00-12:00	E4 / Zoom	Correction exercises 3 + Handson 4 (magnetic properties and Hubbard correction)
Thursday 16 <sup>th</sup>	10:00-11:00	E4 / Zoom	Tutorial Handson 4
Monday 20 <sup>th</sup>	10:00-11:00	E4 / Zoom	Correction exercises 4

# Lectures vs Tutorials

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|--|--|
| <ul style="list-style-type: none"><li>• Overview about theory and exercises (1h)</li><li>• Correction of previous exercises (1h)</li><li>• Notebook;</li><li>• Please stop me for questions.</li></ul> | <ul style="list-style-type: none"><li>• Discussion of main problems</li><li>• 15 minutes each</li><li>• Bring laptop with virtual machine o Anydesk)</li><li>• Focus on main issues!</li></ul> |
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# 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](https://www.vasp.at/wiki/index.php/The_VASP_Manual)

# Elevator pitch – 2 minutes to present yourself

- Federico;
- Enric;
- Maryam;
- Santiago;
- Sichen.

# Today's class

Based on:

- [DFT section of my thesis](#);

Further materials:

- [1\\_comput\\_mat](#);
- [2\\_dft\\_introd](#);
- [3\\_pseudopp](#).

Related handson session:

[\(1\)](#) molecules; frequencies; molecular dynamics

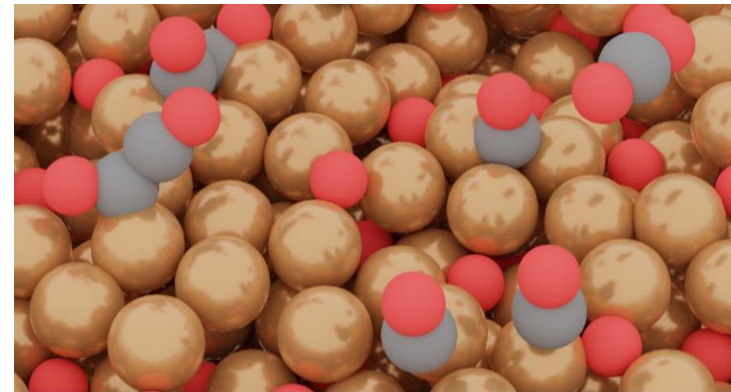
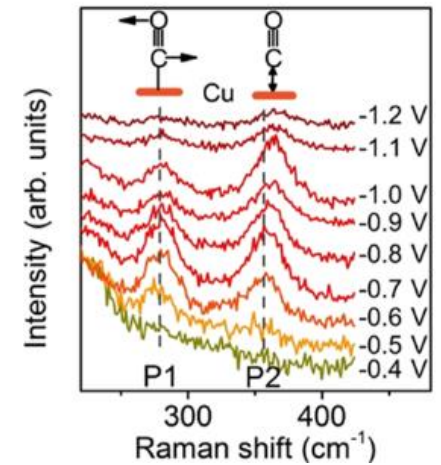
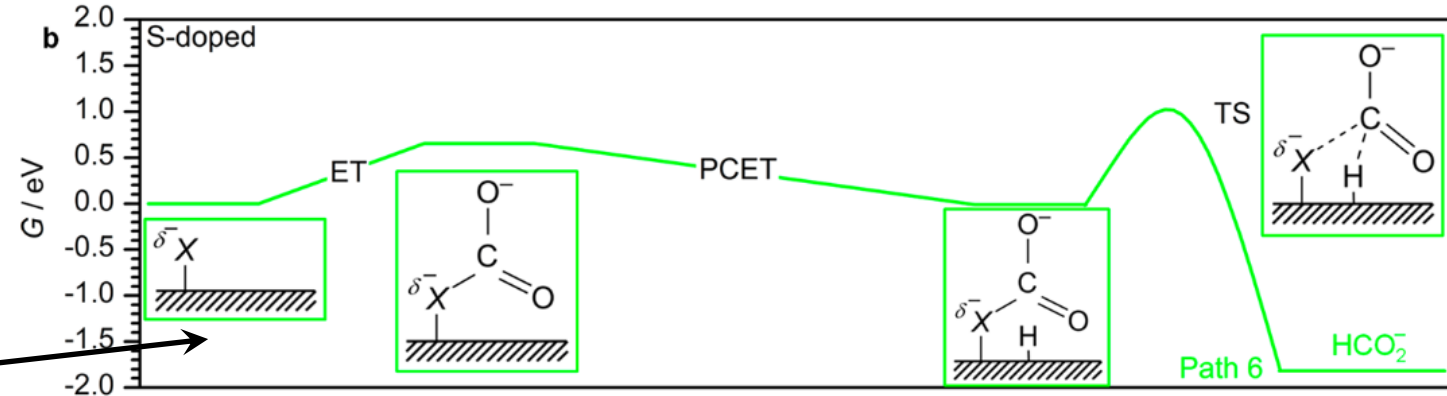
# Handson 1

- 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.

Reference energies

Spectroscopy

Dynamic processes



# Handson 1 – copy the exercises (supercomputer)

- Enter the virtual machine (password: guest1\$) or AnyDesk;
- Open a terminal: *Ctrl + Alt + t*
- Enter tekla home (from ICIQ workstation): *ssh tekla2.iciq.es*
- From outside ICIQ: enable Betelgeuse tunnel and then enter tekla home  
*ssh -p2004 -X [yourusername@betelgeuse.iciq.es](mailto:yourusername@betelgeuse.iciq.es)*  
*ssh tekla2.iciq.es*
- Make a directory *handson* and a subdirectory *1*  
*mkdir handson ; mkdir handson/1*
- Copy the exercises from my tekla home to yours  
*cp -r /home/fdattila/00-vasp-course/handson1/\* ~/handson/1*
- Enter the folder and check to have successfully copied the files  
*cd handson/1 ; ls -lt ; cd ../..*



# Handson 1 – check the exercises

## Check the VASP input (supercomputer / locally)

- Enter each simulation (e.g. 1\_1\_O\_atom) and check INCAR / KPOINTS / POSCAR  
*cd handson/1 ; cd 1\_1\_O\_atom ; vi INCAR ; cd .. ; cd ../..*
  - Use the [VASP manual](#) to understand properly all the tag of the INCAR. Check as well the [Handson](#).
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## Check the structures (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 tekla home folder  
*cd ~/tekla/home*
- Enter a simulation and check the structure through the p4v utility  
*cd handson/1 ; cd 1\_1\_O\_atom ; p4v POSCAR ; cd .. ; cd ../..*

# Handson 1 – submit simulation (supercomputer)

- 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/1 folder and create a run.sh file in each simulation to be run (e.g. 1\_1\_O\_atom)  
`cd handson/1/1_1_O_atom; 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/1/1_1_O_atom; 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/1 ; for i in 1_* ; do cd $i ; action-to-be-performed ; cd .. ; done ; cd ../../..`

# Handson 1 – 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 tekla home folder  
*cd ~/tekla/home*
- Enter a simulation and check the structure through the p4v utility  
*cd handson/1 ; cd 1\_1\_O\_atom ; p4v vasprun.xml ; cd .. ; cd ../..*