

A Hands-on Tutorial: Quantum Chemical Computations

Workshop: Computational Chemistry and Machine Learning for Chemical
Physics, CY Cergy Paris Université.
June 8-12, 2026

The ORCA 6.1 electronic structure program will be used during the practical sessions. All participants must download and install ORCA 6.1 on their personal computers before the tutorials begin. For detailed installation instructions, please visit:

https://www.faccts.de/docs/orca/6.1/tutorials/first_steps/install.html

Additionally, please install Avogadro (<https://two.avogadro.cc/install/index.html>), which will be used as the graphical interface for building and visualising molecular structures.

Participants should ensure that both software applications are installed and ready to run calculations.

Schedule

9.00 - 9.20: Introduction to computational chemistry

9.20 - 09.40: Introduction to ORCA6.1 program

9.40 - 10.00: preparation for tutorials

10.00 - 10.15: Coffee break

10.15 – 11.00: Geometry optimisation, Vibrational frequencies

11.00 – 12.00: Finding Transition States

12.00 – 13.00: Lunch

13.00 – 15.00: Thermodynamics

15.00- 15.15: Coffee break

15.15- 16.00: Kinetic Isotope Effects

16.00- 17.00: Multiscale models