

WIEN2k & TURBOMOLE WORKSHOP



November 16th to 20th

Alba Synchrotron Light Source

Carrer de la Llum, 2-26

Cerdanyola del Vallès, 08290

PROGRAM

Monday, November 16th

09:00 - 10:00	Registration
10:00 - 11:00	Introduction into Linux and computer cluster usage
11:00 - 11:15	Coffee break
11:15 - 13:00	Lecture I: "Introduction to Density Functional Theory and the LAPW method"
13:00 - 14:00	Lunch
14:00 - 16:00	Lecture II: "Introduction to WIEN2k package"
16:00 - 16:30	Coffee break
16:30 - 18:00	Exercise I: Getting started: struct file, init, scf, charge density, DOS, bands

Tuesday, November 17th

09:30 - 11:00	Exercise II: Volume and structure optimization
11:00 - 11:30	Coffee break
11:30 - 13:00	Exercise III: Testing accuracy: RKmax and k-points
13:00 - 14:00	Lunch
14:00 - 16:00	Exercise IV: Testing exchange potentials
16:00 - 16:30	Coffee break
16:30 - 18:00	Exercise V: Magnetism

Wednesday, November 18th

09:30 - 11:00	Exercise VI: Hybrid-DFT
11:00 - 11:30	Coffee break
11:30 - 13:00	Exercise VI: Hybrid-DFT
13:00 - 14:00	Lunch
14:00 - 16:00	Exercise VII: Core level spectroscopy (XSPEC)
16:00 - 16:30	Coffee break
16:30 - 18:00	Exercise VII: Core level spectroscopy (XSPEC) and core-hole effects

PROGRAM

Thursday, November 19th

09:00 - 10:00	Registration
10:00 - 11:00	Introduction into Linux and computer cluster usage
11:00 - 11:15	Coffee break
11:15 - 13:00	Lecture I: "Exploring Potential Energy Surface" Lecture II: "Hartree-Fock method and beyond"
13:00 - 14:00	Lunch
14:00 - 16:00	Lecture III: "Chemically biased introduction to Density Functional Theory" Lecture IV: "Introduction to Turbomole package"
16:00 - 16:30	Coffee break
16:30 - 18:00	Exercise I: The first steps with Turbomole: preparing input files, geometry optimization

Friday, November 20th

09:30 - 11:00	Exercise II: Further steps in Turbomole: vibrational analysis, electronic properties
11:00 - 11:30	Coffee break
11:30 - 13:00	Exercise III: Transition metal compounds
13:00 - 14:00	Lunch
14:00 - 16:00	Exercise IV: Intermolecular interactions
16:00 - 16:30	Coffee break
16:30 - 18:00	Exercise V: Selected spectroscopies (NMR, UV-Vis) in Turbomole



Lectures; Marie Curie Meeting Room



Exercises; Tesla Training Room

EVENT COMMITTEE

Scientific program: Dr. Eric Pellegrin
Secretary: Mrs. Inma Hernandez

CONTRIBUTORS

IRAIDA DEMCHENKO
PAVLO KONSTANTYNOV
YEVGEN MELIKHOV
PAWEL REJMAK
YEVGEN SYRYANY