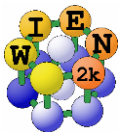
27th Wien2k Workshop, 8. - 20. April 2023, Trieste



PROGRAM

Day 1 (Monday, April 8th)

Time	*Activity*
Morning	• 8:30: Registration • 9:20: Welcome address • 9:30-10:30: **K. Schwarz**: Density functional theory (DFT) and the concepts of the augmented-plane-wave plus local orbitals (APW+lo) method • 11:00-12:30: **P. Blaha**: An overview of the WIEN2k package for beginners
Afternoon	• 14:00-15:00: **P. Blaha**: Input files of scf programs, Volume optimization • **L. Kalantari and all lecturers:** Exercises

Day 2 (Tuesday, April 9th)

Morning	• 9:00-10:00: **P. Blaha**: Forces, structure optimization, supercells, surfaces, phonons • 10:30-11:00: **K. Schwarz**: Magnetism (FM, FSM, AFM) • **L. Kalantari and all lecturers:** Exercises
Afternoon	• 14:00-15:00: **X. Roquefelte**: Relativistic effects • **L. Kalantari and all lecturers:** Exercises

Day 3 (Wednesday, April 10th)

Morning	• 9:00-10:00: **F. Tran**: Advanced DFT: mGGA, Hybrid-DFT, vdw-DFT, LDA+U, EECE, mBJ, KTBM-meta-GGAs • 10:30-11:30: **L. Marks**: Mixing + force minimization • **L. Kalantari and all lecturers:** Exercises
Afternoon	• 14:00-15:00: **P. Blaha**: Wien2k at the command line • **L. Kalantari and all lecturers:** Exercises

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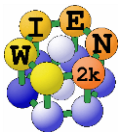


Day 4 (Thursday, April 11th)

Morning
- 9:00-10:00: **O. Rubel**: fold2Bloch. Wannier functions.
- 10:30-11:30: **A. Gomez**: Berry phases and topological materials.
- **L. Kalantari and all lecturers:** Exercises

Afternoon
- 14:00-15:00: **X. Roquefelte**: Optical properties
- **L. Kalantari and all lecturers:** Exercises

Day 5 (Friday, April 12th)

Morning
- 9:00-10:00: **S. Cottenier**: scientific talk: Precision of DFT calculations
- 10:30-11:30: **P. Blaha:** XPS, XES, XAS, EELS, BSE
- **L. Kalantari and all lecturers:** Exercises

Afternoon
- 14:00-15:00: **P. Blaha**: Wien2k goodies
- **L. Kalantari and all lecturers:** Exercises

Day 6 (Monday, April 15th)

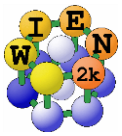
Morning
- 9:00-10:00: **S. Cottenier**: Hyperfine interactions
- 10:30-11:30: **P. Blaha:** NMR
- **L. Kalantari and all lecturers:** Exercises

Afternoon
- 14:00-15:00: **X. Roquefelte**: scientific talk: A Tale of Cuprates: The Good, the Bad and the Ugly!
- 15:30-17:30: **Poster session**

Day 7 (Tuesday, April 16th)

Morning
- 9:00-10:00: **N. Seriani**: scientific talk: Ab-initio simulations of materials for energy applications
- 10:30-11:30: **P. Blaha:** scientific talk: Surfaces and Catalysis
- **L. Kalantari and all lecturers:** Exercises

Afternoon
- 14:00-15:00 **N. Seriani/O. Rubel**: Small groups project on developing skills for presenting DFT results in publications



- **L. Kalantari and all lecturers:** Exercises

Day 8 (Wednesday, April 17th)

Morning
- 9:00-10:00: **G. Madsen:** Transport: Boltztrap
- 10:30-11:30: **L. Marks:** scientific talk: Fact, Fiction and Fantasy for Oxide Surfaces
- **L. Kalantari and all lecturers:** Exercises

Afternoon
- 14:00-15:00: **P. Blaha:** Installation of WIEN2k
- **L. Kalantari and all lecturers:** Exercises

Day 9 (Thursday, April 18th)

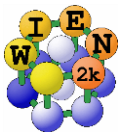
Morning
- 9:00-10:00: **G. Madsen**: Defect Thermochemistry (Spinney)
- **L. Kalantari and all lecturers:** Exercises

Afternoon
- 14:00-15:00: **G. Madsen**: Machine learned Force Fields
- **L. Kalantari and all lecturers:** Exercises

Day 10 (Friday, April 19th)

Morning
- 9:00-10:00: **O. Rubel:** scientific talk: Benchmarking exchange-correlation potentials with the mstar60 dataset
- **L. Kalantari and all lecturers:** Exercises

Afternoon
- 14:00-15:00: Discussion of Exercises, Round table, Poster award & closing
- **L. Kalantari and all lecturers:** Exercises



Topics of exercises

Basic tasks with w2web: setup, scf, DOS, bandstructure, electron density
Volume optimization, Optimization of free atomic positions, optimization of lattice parameters
Cohesive energies
Supercells, surfaces, adsorption energies
Commandline interface
Parallelization
Magnetism
meta-GGAs, mBJ and hybrid-DFT
DFT+U and EECE
Optical properties
Valence photoelectron spectra
Xspec (XANES), EELS and XPS
Phonons
Atoms-in-molecules
Hyperfine interactions (EFG, NMR chemical shifts)
Wannier functions, Polarization, Born effective charges
Topology, Cern number, Weyl points
Effective masses
Thermoelectric properties
Impurities, fold2Bloch