

WIEN2k Hands-On Workshop for New and Existing Users

This 10-day workshop consists of lectures blended with hands-on sessions designed to introduce users to or advance skills in materials modelling with WIEN2k (a solid-state density-functional theory package). The event targets graduate students, early-career scientists, experienced users.

The WIEN2k code is one of the most accurate density functional theory (DFT) codes for solids and can be applied to all elements of the periodic table; it is currently the most popular all-electron DFT code for solids. Many materials characteristics can be calculated, ranging from the basic ones, such as the electronic band structure or the optimized atomic structure, to more specialized ones such as the nuclear magnetic resonance shielding tensor, the electric polarization, band topology. This event includes lectures that provide basic foundation, scientific talks that highlight illustrative examples on application of DFT to solving specific materials problems, and hands-on tutorials designed at the basic and advanced levels.

TOPICS:

- Foundations of augmented-plane-wave plus local orbitals (APW+lo) method
- Band structure (atom- and orbital-projected), density of states, effective masses
- Forces and stresses, structure optimization, phonons
- Magnetism
- Supercells, defects, effective band structure
- Surfaces and catalysis
- Exchange-correlation functionals beyond PBE
- Optical properties
- X-ray and electron energy loss spectroscopy
- Excitons (BSE)
- Hyperfine interactions
- Topological characteristics (Z₂, Chern number, chirality of Weyl points)
- Machine learning
- WIEN2k installation
- Pitching DFT results to scientific community

ABSTRACTS:

Applicants who want to present a poster are required to submit a research abstract for a poster session.



8 - 19 April 2024



Trieste, Italy



Application and Deadlines:

Requesting financial and/or visa support:

18 November 2023

For all other applicants:

5 February 2024

DIRECTORS:

Peter Blaha (TU Vienna, Austria)

Oleg Rubel (McMaster University, Canada)

LOCAL ORGANISER:

Nicola Seriani (ICTP)

GRANTS:

A limited number of grants are available to support the attendance of selected participants, with priority given to participants from developing countries. There is no registration fee.

FURTHER INFORMATION:



E-mail: smr3929@ictp.it

Web: <https://indico.ictp.it/event/10467/>

Female scientists are encouraged to apply.

