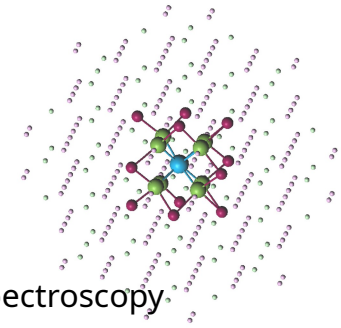
Wavefunction methods for solid state matter (WFS-2026)

What is the workshop about?
This five-days workshop provides an overview of modern methods for accurate theoretical description of the electronic structure of impurities in solids. The focus will be on multiconfigurational methods and embedding cluster techniques. In particular, calculations of local excited states associated with lanthanide dopant of the crystal matrix. In addition to lectures, participants will take part in intensive hands-on sessions.

Who should attend?
The workshop is aimed at Master's students, PhD students and postdocs in chemistry, physics, materials science, and related fields - both experimental and theoretical. No prior experience with electronic structure calculations is required. However, participants are expected to have a basic understanding of computational methods such as Hartree-Fock and Density Functional Theory.

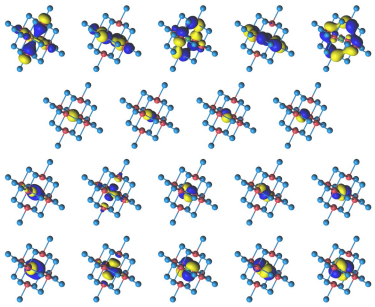
Please, bring your laptop: all hands-on sessions will use computational codes, accessed via a web based interface. Any laptop, with any operating system, will be sufficient.



The main topics to be covered include:
- Basic crystallography
- Periodic and cluster models of solids
- Basis sets and embedding techniques
- Multiconfigurational theory
- Properties, based on electronic structure.
- Relativistic effect and Lanthanide electronic spectroscopy

Dates and Venue:
The workshop will be given from 23/03- 27/03 2026
at Arche Dwor Uphagena, Gdansk, Poland

Visit our web page to register:
https://klar.ug.edu.pl/workshop-wfs-2026/



Entrance fee: 0 PLN
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