

Location

Werner-Köster
Lecture Hall 2R4

MPI for Intelligent Systems
Heisenbergstraße 3
70569 Stuttgart

More Information

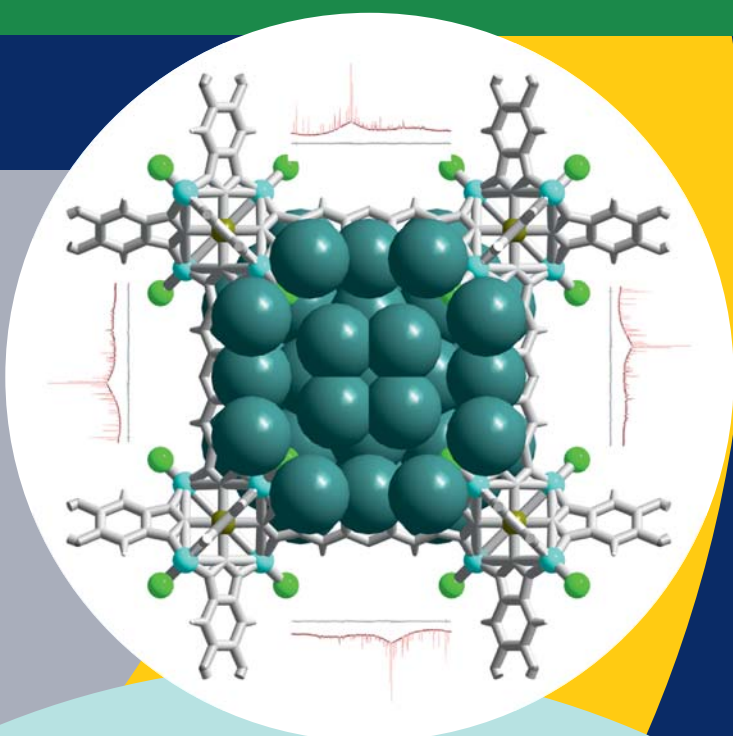
Please consult our web pages:

www.fkf.mpg.de/xray

DMG/DGK Ph.D. student course

Basics and Applications of the Rietveld Method

March 6 – 9, 2017



Max Planck Institute for Solid State Research
in cooperation with the
universities of Tübingen and Stuttgart
and the working committee
Powder Diffraction of the DGK

Course description

It is the aim of this intensive course to impart the Rietveld method in theory and practice. Using selected examples the entire process from profile fitting using fundamental parameters towards crystal structure determination and refinement will be explained.

In particular the following topics will be covered:

- Basics of powder diffraction and Rietveld Refinement
- Whole Powder Pattern-Fitting (WPPF), fundamental parameters (FP), complex reflection profiles
- Determination of the Instrument Resolution Function (IRF) for powder diffractometers
- Angular and intensity corrections (LP-Faktor, absorption, microabsorption, extinction, preferred orientation, sample height, zero error, ...)
- Methods to develop a starting model for crystal structure determination
- Penalty-functions, constraints, restraints
- Rigid Bodies (RB) (flexible polyhedra, molecules, z-matrices)
- Strategies for structure determination, global optimization in direct space, Charge-Flipping (CF)
- Difference-Fourier-analysis in combination with Rietveld refinement
- Isotropic and anisotropic microstructural parameters
- Quantitative Phase Analysis (QPA) with the Rietveld method
- Different methods for quantifying the amorphous content
- Symmetry and rotation modes as alternatives ways of describing crystal structures
- Parametric Rietveld refinements (includes basic macro-programming)
- Local and global optimization of stacking faulted superstructures
- Local and global optimization of the Pair-Distribution-Function (PDF)
- The making of Rietveld-Plots for publications

Contact

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