

DGK Ph.D. student/young scientist course

Rietveld and Pair distribution function (PDF) analysis workshop



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March 31st – April 4th, 2025

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in cooperation with
the universities of Tübingen and Stuttgart
and the committee Teaching of Crystallography of the German Society for Crystallography

<http://www.fkf.mpg.de/xray>

Course description:

In crystallography, the Rietveld method revolutionized the way in which we study the structure of materials to understand their properties. 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. Now more than ever, it is important to consider structure characterization methods for nanostructured and amorphous materials that diffract poorly. This workshop will serve as an introduction to the pair distribution function (PDF) method, a technique for determining the local structure in disordered materials. We will cover the basic theory of the method, data processing, and an in-depth tutorial on structure refinement implemented in TOPAS v.7.

In particular, the following topics will be covered:

- Basics of powder diffraction and Rietveld Refinement
- The profile of a Bragg reflection
- Determination of the Instrument Resolution Function (IRF) for powder diffractometers
- Whole Powder Pattern-Fitting techniques (WPPF)
- The intensity of a Bragg reflection
- Correction factors for diffraction angles and intensity
- 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)
- Different methods for quantifying the amorphous content
- Alternative ways of describing crystal structures
- Sequential and parametric Rietveld refinements
- Stacking faulted superstructures
- The making of Rietveld-Plots for publication
- Basics of total scattering and pair distribution function analysis
- Obtaining the pair distribution function from total scattering data
- Determining and accounting for effects of instrumental resolution
- Small-box crystal structure refinement
- Modelling nanoparticle structures and particle size distributions
- Simulated annealing and large-box approach

Place and Time:

Meeting point on Monday March 31st, 2025 at 8:30 am in front of the lecture hall 2D5 of the MPI-FKF (Heisenbergstraße 1). Please be there in time.

Duration of the course approx. 9.00 am – 4:00 m (Friday 9.00 am – 12:00 am)

More detailed schedule to follow.

Main tutors:

Sebastian Bette, Robert E. Dinnebier, Martin Etter, John Evans, Paolo Scardi, Maxwell W. Terban

Language:

Lectures and exercises in English.

Computer:

No computers can be supplied by the organizer. For the exercises, a contemporary laptop with a current Windows version with administrator rights is necessary. The licenses of Topas will be supplied using WiFi. A sufficient number of power outlets will be supplied. Bring an adapter if needed.

All programs and course material need to be downloaded and installed before the course. Installation instructions will be sent in due time.

Due to the large number of participants, there is no time for individual installation support.

Information:

More information will become available at: <http://www.fkf.mpg.de/xray>

Registration & Fee:

The course fee is 120 € for academic, 450 € for industrial users. Students can apply for a tuition waiver

To apply send an informal E-mail to r.dinnebier@fkf.mpg.de including name, address & position

Once accepted, send the registration fee to either:

Bank: Deutsche Bank AG

Account holder: Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V./MPI FKF

IBAN: DE98 7007 0010 0195 1300 38

BIC: DEUTDEMMXXX

or

paypal.me/FKFMPI

Purpose of use: Rietveld2025 + your name

Registration is valid only after receipt of payment.

Food:

The MPI canteen serves breakfast and lunch.

Lunch vouchers for the canteen might be distributed free of charge (depends on the funding situation).

ECTS:

2 ECTS (European Credit Transfer System) points can be awarded after passing a written test after the course.

Housing:

There is no support from the organizers but a limited number of rooms in the MPI guesthouse is available on a "first-come-first-served" base (Tel: +49-(0)711-689-1241).

Inexpensive accomodation is limited, therefore book you accommodation sufficiently early.

Here are some suggestions for nearby hotels:

RELEXA Waldhotel Schatten (15 min walking distance)

<http://www.relexa-hotel-stuttgart.de/en/hotel>

Vienna House Easy by Wyndham Stuttgart (15 min bus ride)

<https://www.wyndhamhotels.com>

Hotel Römerhof (convenient by car, 5 min)

<http://www.roemerhof-kulinarium.de/>

Pullmann Stuttgart Fontana Hotel (20 min bus ride, high budget)

<http://www.pullmanhotels.com>

Hotels in Stuttgart:

<https://book.stuttgart-tourist.de>

The internet is also a good resource: e.g.

<http://www.booking.com/Unterkunft-Stuttgart?>

<http://www.hrs.de>

<http://www.homeapartments.de/>

<http://www.nd-bed-breakfast.de/?>

<http://bbhappy.de/home>

Transportation:

How to find us: <http://www.fkf.mpg.de/92750/40> [How to find us](#)

Public transportation is quite good with a frequent bus stop close to the institute (stop: *Max-Planck-Institute*):
<http://www.vvs.de>

Number of participants:

Maximum of 65 participants - *first come, first served*.

This and that:

- If you want to bring your own data, please contact the organizer in time before the course starts, but no guarantee.
- **Should you not be able to attend the course, please notify the organizer in time. The course is non-profit.**
- **Out of respect for the other participants and the waiting list, participation for the full 5 days is mandatory.**

Contact details:

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