

DMG/DGK Ph.D. student course

Pair distribution function (PDF) analysis workshop



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October 11-12, 2018

Max Planck Institute for Solid State Research
Heisenbergstraße 1
D-70569 Stuttgart Germany

in cooperation with
the universities of Tübingen and Stuttgart
and the working committee Powder Diffraction of the DGK

<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. Now more than ever, it is important to consider structure characterization methods for nanostructured and amorphous materials that diffract poorly. This two-day 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.6. In particular, the following topics will be covered:

- Basics of total scattering and pair distribution function analysis
- Experimental setup and sample considerations
- Obtaining the pair distribution function from total scattering data: integration of 2D diffraction images, normalization, and transformation (considerations and pitfalls)
- Determining and accounting for effects of instrumental resolution
- Strategies for obtaining starting models and structure determination
- Small-box crystal structure refinement with x-ray or neutron data, and co-refinement of multiple datasets
- Modelling nanoparticle structures and particle size distributions
- Multi-phase refinement, dealing with mixed crystalline and amorphous systems, and phase quantification
- Local optimization of stacking faulted superstructures
- Strategies for investigating local symmetry broken states (box-car fitting and assessment of structure candidates)
- Sequential refinements for in situ data (temperature dependence etc.)
- Modelling strategies for small molecule and polymer structures: rigid bodies (RB), intra/intermolecular correlation
- Difference analysis
- Simulated annealing and large-box approach

Place and Time:

Meeting point on Thursday October 11th, 2018 at 8:30 am in front of the seminar room 2R4 of the MPI-IS (Heisenbergstraße 3). Please be there in time.

Duration of the course approx. 9.00 am – 4:00 pm

More detailed schedule to follow.

Tutors:

Maxwell Terban, Sebastian Bette, Luzia Germann, Gianpiero Gallo, Robert Dinnebier

Language:

Lectures and exercises in English.

Computer:

No computers can be supplied by the organizer. For the exercises, a contemporary laptop (Windows 7, 8, or 10) with administrator rights is necessary. The licenses of Topas will be supplied using WiFi. If you have your own license dongle for Topas, please take it with you. 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 is free of charge. Industrial users are asked to donate 250 Euros.

To apply send an informal E-mail to M. W. Terban (M.Terban@fkf.mpg.de) including name, address & position.

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>

Commundo Tagungshotel (5min bus ride, however heavily booked)

<https://www.campus-guest.de/>

ARCONA MO.HOTEL (15 min bus ride)

<http://stuttgart.arcona.de>

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/gb/hotel-5425-pullman-stuttgart-fontana/index.shtml>

Hotels in Stuttgart:

<https://book.stuttgart-tourist.de/stuttgart-en/ukv/result?tt=qoq3hco1ut85b4jqmldbgusri2>

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 40 participants (strictly limited) - 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 pro-bono.**
- **Out of respect for the other participants and the waiting list, participation for the full 2 days is mandatory.**

Contact details:

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