



Workshop on Structural Analysis of Aperiodic Crystals 23rd – 26th March 2017 University of Bayreuth, Germany

Organisation:

German Association for
Crystallography (DGK)



Local Organisation:

Sander van Smaalen
Andreas Schönleber
Laboratory of Crystallography
University of Bayreuth

Venue:

University of Bayreuth
Germany



Dates:

Start: Thursday, 23rd March 2017, 17.00 hours
Registration desk open: 15.00 hours
End: Sunday, 26th March 2017, 14.00 hours

Registration Fee:

Students: 55 EUR
PhD students: 55 EUR
Academics: 110 EUR
Full fee: 490 EUR

Contact:

Prof. dr. Sander van Smaalen
Laboratory of Crystallography
University of Bayreuth
95440 Bayreuth
Germany
Phone: +49-921-553886
Email: smash@uni-bayreuth.de

Description:

An overview will be provided of the methods of structural analysis of incommensurately modulated crystals and composite crystals. Lectures will cover the basic principles of the superspace approach. A presentation of recent developments includes special modulation functions.

Participants will have the opportunity to practice structural analysis in superspace with the computer programs Superflip and JANA2006 (by V. Petricek, M. Dusek and L. Palatinus, Prague). A step-by-step tutorial will guide you through structure determination, symmetry analysis, structure refinement and *t*-plots for crystal-chemical analysis of selected examples of modulated structures and composite crystals.

The maximum number of participants is 40.

Topics:

- Aperiodic order of matter
- Superspace theory of modulated crystals
- Symmetry and superspace groups
- Diffraction
- Structure solution and charge flipping
- Structural analysis and refinement in superspace
- Crystal chemistry and *t*-plots

Tutorials:

A practical course on structural analysis of modulated crystals with JANA2006 and Superflip.

Lecturers:

- M. Dusek, Prague, Czech Republic
- L. Palatinus, Prague, Czech Republic
- V. Petricek, Prague, Czech Republic
- O. Pérez, Caen, France
- S. van Smaalen, Bayreuth, Germany
- A. Schönleber, Bayreuth, Germany

Website:

http://aperiodic.uni-bayreuth.de/workshop_2017