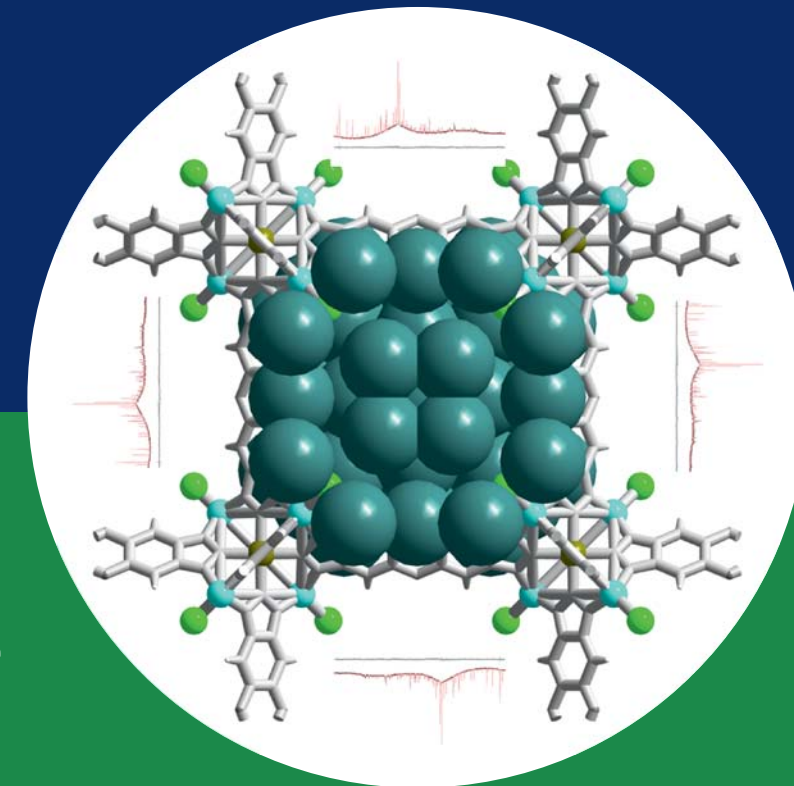**Location**

Werner-Köster Lecture Hall 2R4

MPI for Intelligent Systems
Heisenbergstraße 3
70569 Stuttgart

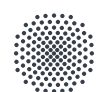## DMG/DGK Ph.D. student course

Basics and Applications of the Rietveld Method

Schedule (time estimates):

Monday, March 6, 2017

Time	Topic
8:00 – 9:00	Registration in front of 2P4 lecture hall
9:00 – 9:15	Welcome, organization
9:15 – 10:00	Introduction to the Rietveld method. Information content of a powder diffraction pattern
10:00 – 10:30	Break (coffee/tea/water/cookies)
10:30 – 11:15	Theory of the Bragg reflection: position, peak shape, intensity
11:15 – 12:00	Concept of convolution, fundamental parameters versus phenomenological peak shape functions, isotropic and anisotropic peak broadening, microstructural properties
12:00 – 13:00	Lunch (canteen)
13:00 – 13:45	Single peak fits, Whole Powder Pattern-Fitting (Pawley, LeBail, Rietveld), powder pattern calculation
13:45 – 14:30	Exercises
14:30 – 15:00	Break (coffee/tea/water/cookies)
15:00 – 16:30	Determination of the instrumental resolution function

Tuesday, March 7, 2017

Time	Topic
9:00 – 10:00	Indexing, space group determination (with exercises).
10:00 - 10:30	Break (coffee/tea/water/cookies)
10:30 – 11:15	Crystal structure determination in direct space (simulated annealing) and reciprocal space (charge-flipping)
11:15 – 12:00	Exercises
12:00 – 13:00	Lunch (canteen)
13:00 – 13:45	Correction functions (LP-factor, absorption, microabsorption, extinction, preferred orientation etc. (with exercises)
13:45 – 14:30	The pair distribution function (PDF) and its combination with Rietveld analysis
14:30 – 15:00	Break (coffee/tea/water/cookies)
15:00 – 16:30	Exercises
16:30 – 17:00	Success in structure solution as a result of specific data collection strategy (Dubravka Sisak Jung, Dectris GmbH)
17:30 – 21:00	Evening buffet with beverages
21:00 – 22:00	Scientific discussion I

Wednesday, March 8, 2017

Time	Topic
9:00 – 10:00	Penalty-functions in global and local minimization (constraints, restraints and rigid bodies (with exercises)
10:00 - 10:30	Break (coffee/tea/water/cookies)
10:30 – 11:15	How to set up rigid bodies (flexible polyhedra, molecules, z-matrices)
11:15 – 12:00	Exercises
12:00 – 13:00	Lunch (canteen)
13:00 – 13:45	Combining Rietveld refinement with difference Fourier analysis and global optimization
13:45 – 14:30	Exercises
14:30 – 15:00	Break (coffee/tea/water/cookies)
15:00 – 16:00	Quantitative Phase Analysis (QPA) with the Rietveld method. Quantifying the amorphous content (with exercises), PONCS

Thursday, March 9, 2017

Time	Topic
9:00 – 10:00	Refinement of crystal structures with stacking faults using Rietveld analysis (exercises)
10:00 - 10:30	Break (coffee/tea/water/cookies)
10:30 – 11:15	Symmetry/distortion mode analysis
11:15 – 12:00	Exercises
12:00 – 13:00	Lunch (canteen)
13:00 – 13:45	Sequential and parametric Rietveld refinement in dependence on external variables. Macro programming
13:45 – 14:30	Exercises
14:30 – 15:00	Break (coffee/tea/water/cookies)
15:00 – 16:00	Macro programming/ Making of Rietveld plots/ Critical analysis of results
16:00 –	Scientific discussion II – The future

Max Planck Institute for Solid State Research

University of Stuttgart Germany

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

DMG Deutsche Mineralogische Gesellschaft

DECTRIS®

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STOE since 1887

ICDD International Centre for Diffraction Data

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CRYSTAL IMPACT