

8th Workshop on Structural Analysis of Aperiodic Crystals

12 – 15 March 2015

Laboratory of Crystallography of the University of Bayreuth

Program

Lectures and registration are on the ground floor of building RW I, seminar rooms S57, S58 and S59, on the campus of the University of Bayreuth.

8th Workshop on Structural Analysis of Aperiodic Crystals

12 – 15 March 2015

at the Laboratory of Crystallography of the University of Bayreuth

Organized by the German Crystallographic Association (DGK)

Local organisation: Sander van Smaalen and Andreas Schönleber

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Venue

Building RW I – ground floor – rooms S57, S58, S59

on the campus of the University of Bayreuth, Universitätsstrasse 30, 95447 Bayreuth,
Germany.

Sponsored by the German Crystallographic Association (DGK) and the University of Bayreuth.

Thursday, 12 March 2015

Time		
15:00–18:00	<i>Registration</i>	
17:00–17:15	Opening	S. van Smaalen
17:15–18:00	From modulated compounds to quasicrystals—an introduction to aperiodic order	A. Schönleber
18:00–19:30	<i>Get together</i>	

Friday, 13 March 2015

Time		
9:00–10:30	The superspace method for incommensurately modulated structures	A. Schönleber
10:30–11:00	<i>Break</i>	
11:00–12:30	Superspace symmetry of modulated structures	S. van Smaalen
12:30–14:00	<i>Lunch in the Mensa</i>	
14:00–14:45	Introduction to JANA software	V. Petricek
14:45–18:00	Structural analysis of modulated crystals with JANA2006	*
15:30–16:00	<i>Break</i>	

*V. Petricek, M. Dusek, A. Schönleber, L. Palatinus and S. van Smaalen.

Saturday, 14 March 2015

Time		
9:00–10:30	Diffraction by aperiodic crystals, twinning and overlapping reflections	M. Dusek
10:30–11:00	<i>Break</i>	
11:00–12:30	Structure solution by Charge Flipping	L. Palatinus
12:30–13:15	<i>Lunch in the Mensa</i>	
13:15–14:00	<i>Poster session</i>	
14:00–15:00	Discussion of the problems in the script	A. Schönleber
14:00–18:00	Structural analysis of modulated crystals with JANA2006	*
15:30–16:00	<i>Break</i>	
19:00	<i>Conference Dinner</i>	

Sunday, 15 March 2015

Time		
9:00–9:45	Magnetic symmetry and magnetic structures	V. Petricek
9:45–10:30	Nuclear and magnetic modulated structures of FeOCl-type compounds	S. van Smaalen
10:30–11:00	<i>Break</i>	
11:00–11:30	Pressure-induced incommensurate phases of FeOCl-type compounds	M. Bykov
11:30–11:45	Closing remarks	S. van Smaalen
11:45–12:30	Discussion of the problems in the script	A. Schönleber
11:45–14:00	Structural analysis of modulated crystals with JANA2006	*
14:00	End of the Workshop	

*V. Petricek, M. Dusek, A. Schönleber, L. Palatinus and S. van Smaalen.

Poster presentations

Posters are on display during the entire workshop. The poster session is on Saturday, 13:15–14:00 hours.

1. S. Dey, A. Schönleber, S. van Smaalen and F. K. Larsen
Modulation, twinning and crystal structures of Co(sepulchrate) trinitrate at low temperatures
2. Ihab Eddine Yahiaouia, Yahia Bourourou and Mohamed Amine Benali
The first-principles study of Co₂VSi compounds with small concentration of the Er impurities
3. Sk Imran Ali, Swastik Mondal and Sander van Smaalen
Vacancy-Ordering in intercalated 2H-Cu_xTa_{1+y}Se₂ ($x, y = 0.52, 0$ and $0.16, 0.08$)

