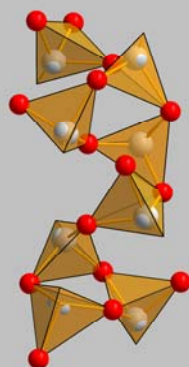


Programme

of the

Workshop

*Computer methods
in
crystal structure systematics*



Organized by:

M. Jansen

R. E. Dinnebier

September 19 – 22, 2011

Max Planck Institute for Solid State Research
Heisenbergstrasse 1
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<http://www.fkf.mpg.de/xray>

under the auspices of the GDCh and the MPG

September 19, 2011

Time (24 hrs format)		Topic	Speaker
9.00 - 9:05	5	Welcome remarks	Dinnebier
9.05 – 10:00	55	Introductory talk	Jansen
10.00 -10:15	15	Coffee break (in front of lecture hall)	
10:15 – 11:45	90	Theory Part 1	Blatov, Proserpio
11:45 – 12:45	60	Lunch in cafeteria (self paid)	
12.45 -14:15	90	Theory Part 2	Blatov, Proserpio
14.15 - 15:45	90	Theory Part 3	Blatov, Proserpio
15:45 – 16:00	15	Coffee break (in front of lecture hall)	
16:00 – 17:30	90	Theory Part 3	Blatov, Proserpio
17:30 – 18:30	60	Group–subgroup relations Part 1	Ulrich Müller

September 20, 2011

Time (24 hrs format)		Topic	Speaker
9.00 – 10:30	90	Standard topological analysis and classification of nets in inorganic crystals Part 1	Blatov, Proserpio
10.30 -10:45	15	Coffee break (in front of lecture hall)	
10:45 – 12:15	90	Standard topological analysis and classification of nets in inorganic crystals Part 2	Blatov, Proserpio
12:15 – 13:15	60	Lunch in cafeteria (self paid)	
13.15 -14:45	90	Standard topological analysis and classification of nets in inorganic crystals Part 3	Blatov, Proserpio
14:45 – 15:00	15	Coffee break (in front of lecture hall)	
15:10 – 16:30	90	Standard topological analysis and classification of nets in inorganic crystals Part 4	Blatov, Proserpio
16:30 – 17:30	60	Group–subgroup relations Part 2	Ulrich Müller
17:30 – 18:30	60	Application of Group-subgroup relations to symmetry modes	Melanie Müller, Dinnebier

September 21, 2011

Time (24 hrs format)		Topic	Speaker
9.00 – 10:30	90	Special topological methods of searching for building units in crystal structures	Blatov, Proserpio
10.30 -10:45	15	Coffee break (in front of lecture hall)	
10:45 – 12:15	90	Analysis of microporous materials and fast-ion conductors with natural tilings Part 1	Blatov, Proserpio
12:15 – 13:15	60	Lunch in cafeteria (self paid)	
13.15 -14:45	90	Analysis of microporous materials and fast-ion conductors with natural tilings Part 2	Blatov, Proserpio
14:45 – 15:00	15	Coffee break (in front of lecture hall)	
15:10 – 16:30	90	Crystal design and topological relations between crystal structures Part 1	Blatov, Proserpio
16:30 – 18:00	90	Crystal design and topological relations between crystal structures Part 2	Blatov, Proserpio
19:00 –		Conference dinner in the cafeteria with great wine and beer	

September 22, 2011

Time (24 hrs format)		Topic	Speaker
9.00 – 10:30	90	Analysis and systematics of large samples of crystal data	Blatov, Proserpio
10.30 -10:45	15	Coffee break (in front of lecture hall)	
10:45 – 12:15	90	Analysis of periodic structures using KPLOT Part 1	Schön, Hundt
12:15 – 13:15	60	Lunch in cafeteria (self paid)	
13:15 – 14:45	90	Analysis of periodic structures using KPLOT Part 2	Schön, Hundt
14:45 – 16:15	90	Open discussion and closing remarks	Dinnebier, Jansen