


Basel 2016

ECM-30



**30th Meeting of the European
Crystallographic Association**
28 August – 1 September 2016
Congress Center Basel, Switzerland

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Final Programme

Sponsors

The organisers of the ECM-30 express their thanks and appreciation to all those who are generously contributing to the success of this meeting.

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Sponsors



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Focus Area Responsibilities

Focus Area 1: Michael Hennig, leadXpro AG, Villigen, for SIG 1
Focus Area 2: Jürg Schefer, Paul Scherrer Institute Villigen,
for SIG 5, 11, 12
Focus Area 3: Piero Macchi, Berne, for SIG 2, SIG 3, SIG 4
Focus Area 4: Katharina M. Fromm, Fribourg, for SIG 7 and SIG 13
Focus Area 5: Radovan Cerny, Geneva, for SIG 6, SIG 8 and SIG 9

Dear Colleagues and Friends, dear Participants of ECM-30,

On behalf of the European Crystallography Association as well as the Swiss Society for Crystallography, it is our pleasure to welcome you to Basel on the occasion of the 30th European Crystallography Meeting, ECM-30, held from 28 August until 1 September 2016.

The Swiss Society of Crystallography was born in 1968 and connects scientists from all disciplines for which crystallography is important. Together with the European Programme Committee from the SIGs and GIGs of the ECA, we have set up an exciting programme with excellent and fascinating science. With a total of 50 half-day microsymbiosia and 16 keynote speakers, as well as two plenary lectures by Nobel Laureates Professor Ada Yonath and Professor Jean-Marie Lehn, a large number of hot topics from biology, chemistry, physics and mineralogy will be covered.

ECM-30 will be a four-day vibrant and intensive scientific meeting with many learning opportunities in every current aspect of crystallography. In addition, there will be a Young Crystallographers meeting, workshops and user meetings, lunch meetings, and a social programme, which will allow you all to meet, connect and exchange. ***Do not miss out on the very first ever ECM-Science Slam***, which is organized on Tuesday evening together with the Bertaut prize ceremony. Check out also our satellite meetings as well as the conference excursion to the free electron laser SwissFEL at Paul Scherrer Institute.

Basel is a welcoming, active and enterprising city of open minded citizens who excel in business as well as in the arts, right at the Swiss-German-French border in the heart of Western Europe. The famous Basel mathematicians Bernoulli and Euler await you on the historical evening tour. In addition to the architecturally interesting campuses of some "big" pharmaceutical and chemical enterprises, world-renowned museums, like the Beyeler or the Vitra design museum, are ready to welcome you. Or join us Wednesday evening at the Conference Dinner at the Basel Zoo? Enquire ASAP at the registration desk if there are places left!

We thank also all the sponsors, exhibitors and science foundations for their support, our conference organizer Congrex Switzerland, all our volunteers and helpers as well as the organizers of previous ECMs, especially Zoran Štefanić for using and supporting his abstract submission system. And, last but not least, YOU for your participation, making this conference a success.

So, while you're here, please make sure to enjoy – at least for a short while – beautiful Basel and Switzerland.

Hoping to meet you all in person,

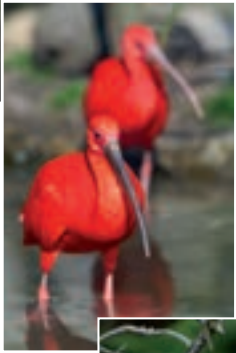
Jürg Schefer
Paul Scherrer Institut

Katharina M. Fromm
University of Fribourg

Welcome to Basel



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	Sydney	
08:00		Committees
08:15		
08:30		
08:45		
09:00		
09:15		
09:30		Welcome
09:45		
10:00		
10:15		
10:30		
10:45		
11:00		Programme Overview
11:15		
11:30		
11:45		
12:00		
12:15		
12:30		
12:45		
13:00		Venue Overview
13:15		
13:30		
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14:00		
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14:45		
15:00		Exhibition Floor Plan
15:15		
15:30		
15:45		
16:00		
16:15		
16:30		
16:45		
17:00		Scientific Programme
17:15	17:00–19:00	
17:30	Opening Session	
17:45		
18:00		
18:15		
18:30		
18:45		Poster Overview
19:00		
19:15		
19:30		
19:45		
20:00		
20:15		
20:30		
20:45		Social Events

- Focus Area 1 (SIG 1)
- Focus Area 2 (SIG 5, 11, 12)
- Focus Area 3 (SIG 2, 3, 4)
- Focus Area 4 (SIG 7, 13)
- Focus Area 5 (SIG 6, 8, 9)
- General Microsymposia
- Keynote Lecture
- Plenary Lecture
- Commercial User Workshop / Presentation

Programme Overview – Monday, 29 August 2016

	Sydney	Singapore	Darwin	Boston 3
08:00				
08:15				
08:30	08:30–09:30			
08:45	Plenary Lecture			
09:00	Ada Yonath			
09:15	p. 23			
09:30				
09:45				
10:00	10:00–12:00	10:00–12:00	10:00–12:00	10:00–12:00
10:15	MS 7	MS 36	MS 23	MS 31
10:30	Protein & glycobiology structure determination	Crystallography in solid state reactions and catalysis	Charge and spin density of materials at extreme conditions	Crystal energy landscapes: computation and uses
10:45				
11:00				
11:15				
11:30				
11:45	p. 23	p. 24	p. 24	p. 25
12:00		12:00–13:00		12:00–13:00
12:15		SIG 1 Meeting		SIG 7 Meeting
12:30	12:30–13:30		12:30–13:30	
12:45	Commercial User Workshop hosted by Dectris	p. 62	Software Fayre	p. 62
13:00	p. 27	13:00–14:00		
13:15		SIG 5 Meeting	p. 60	
13:30				
13:45		p. 62		
14:00	14:00–16:00	14:00–16:00	14:00–16:00	14:00–16:00
14:15	MS 10	MS 34	MS 26	MS 42
14:30	H-bonding & weak interactions in crystals: neutrons and X-rays	Molecular recognition, supramolecular chemistry and crystal engineering	Incommensurate modulated and composite phases	Advances in neutron scattering under non-ambient conditions
14:45				
15:00				
15:15				
15:30				
15:45	p. 27	p. 28	p. 28	p. 29
16:00				
16:15				
16:30	16:30–17:30	16:30–17:30		
16:45	Keynote Lecture	Keynote Lecture		
17:00	Peter Schurtenberger	Francesca Fabbiani		
17:15	p. 31	p. 31		
17:30				
17:45				
18:00				
18:15				
18:30				
18:45				
19:00	19:00–20:00			
19:15	Commercial User Workshop hosted by Bruker			
19:30	p. 32			
19:45				
20:00				
20:15				
20:30				

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 ■ Focus Area 4 (SIG 7, 13)
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	Sydney	Singapore	Darwin
08:00			
08:15			
08:30	08:30–09:30	08:30–09:30	
08:45	Keynote Lecture	Keynote Lecture	
09:00	François Diederich	Birger Dittrich	
09:15	p. 33	p. 33	
09:30			
09:45			
10:00	10:00–12:00	10:00–12:00	10:00–12:00
10:15	MS 13	MS 3	MS 27
10:30	Hot structures	Data collection and	Dynamical refinement
10:45	in biology	processing software	of electron diffraction
11:00		(XFELS & synchrotrons)	data
11:15			
11:30			
11:45	p. 33	p. 34	p. 34
12:00			
12:15			
12:30	12:30–13:30		12:30–14:00
12:45	Commercial User		Software Fayre
13:00	Workshop hosted by		
13:15	Rigaku Oxford		
13:30	Diffraction p. 36		
13:45			p. 60
14:00	14:00–16:00	14:00–16:00	14:00–16:00
14:15	MS 32	MS 4	MS 43
14:30	Polymorphs, cocrystals,	New developments in	Combining x-ray
14:45	solvates, salts: a jungle	phasing and refinement	diffraction and other
15:00	for scientists and		techniques for in situ
15:15	industries		and operando studies
15:30			
15:45	p. 37	p. 37	p. 38
16:00			
16:15			
16:30	16:30–17:30	16:30–17:30	
16:45	Keynote Lecture	Keynote Lecture	
17:00	Sandra W. Jacob	Marcus Neumann	
17:15	p. 40	p. 41	
17:30			
17:45			
18:00			
18:15			
18:30			
18:45			
19:00	19:00–20:30		
19:15	The Bertaut Prize		
19:30	Ceremony and		
19:45	Science Slam		
20:00			
20:15	p. 41		
20:30			

■ Focus Area 1 (SIG 1)
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 ■ Focus Area 3 (SIG 2, 3, 4)

■ Focus Area 4 (SIG 7, 13)
 ■ Focus Area 5 (SIG 6, 8, 9)

Programme Overview – Tuesday, 30 August 2016

Rio	Osaka	Samarkand	Poster Area
			Poster Exhibition
			08:00
			08:15
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			20:00
			20:15
			20:30
10:00–12:00 MS 19 Solid state oxygen fuel cell, hydrogen storage & battery materials p. 35	10:00–12:00 MS 35 Simulation of dynamics in molecular compounds p. 35	10:00–12:00 MS 44 Total scattering: pdf analysis and diffuse scattering in X-Ray, neutron and electron diffraction p. 36	
12:00–13:00 SIG 12 Meeting p. 62	12:00–14:00 ECM-31 Programme Committee Meeting p. 62		
13:00–14:00 GIG 3 Meeting p. 62			
14:00–16:00 MS 20 Materials for energy conversion and harvesting p. 39	14:00–16:00 MS 28 New approaches in electron crystallography p. 39	14:00–16:00 MS 47 Teaching & Education p. 40	
			p. 63
			Poster Session 2 p. 41

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	Sydney	Singapore	Darwin
08:00			
08:15			
08:30	08:30–09:30 Keynote Lecture Jan Pieter Abrahams p. 42	08:30–09:30 Keynote Lecture Simon Parsons p. 42	
08:45			
09:00			
09:15			
09:30			
09:45			
10:00	10:00–12:00 MS 38 Nanomaterials & graphene p. 42	10:00–12:00 MS 11 Hybrid approaches and validation (X-ray and electron microscopy) p. 43	10:00–12:00 MS 21 Structural disorder and materials' properties at ambient and non-ambient conditions p. 43
10:15			
10:30			
10:45			
11:00			
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11:30			
11:45			
12:00	12:00–13:00 SIG 11 Meeting p. 62		
12:15			
12:30			
12:45			
13:00		13:00–14:00 SIG 13 Meeting p. 62	13:00–14:00 Software Fayre p. 61
13:15			
13:30			
13:45			
14:00	14:00–16:00 MS 6 Molecular machines and big complexes p. 46	14:00–16:00 MS 37 Molecular compounds and MOFs at ambient conditions and under high pressure p. 47	14:00–16:00 MS 30 Hydrogen bonding from theory to applications p. 47
14:15			
14:30			
14:45			
15:00			
15:15			
15:30			
15:45			
16:00			
16:15			
16:30	16:30–17:30 Keynote Lecture Makoto Fujita p. 50	16:30–17:30 Keynote Lecture Olivier Thomas p. 50	
16:45			
17:00			
17:15			
17:30	17:30–18:30 Keynote Lecture Robert von Dreele p. 50	17:30–18:30 Keynote Lecture Petra Fromme p. 50	
17:45			
18:00			
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20:30			

■ Focus Area 1 (SIG 1)
 ■ Focus Area 2 (SIG 5, 11, 12)
 ■ Focus Area 3 (SIG 2, 3, 4)
 ■ Focus Area 4 (SIG 7, 13)
 ■ Focus Area 5 (SIG 6, 8, 9)

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Rio	Osaka	Samarkand	Poster Area	
			Poster Exhibition	08:00
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10:00–12:00 MS 5 Structural information in drug design p. 44	10:00–12:00 MS 48 Crystallography in art and cultural heritage p. 45	10:00–12:00 MS 46 Computational tools for theoretical chemistry in crystallography p. 45		
12:00–14:00 General Assembly SGK/SSCr p. 62	12:00–13:00 GIG 1 Meeting p. 62 13:00–14:00 SIG 2 Meeting p. 62	12:00–14:00 ECA Council 2 Meeting p. 62		
14:00–16:20 MS 14 Biominerological crystallography and bioinspired inorganic materials p. 48	14:00–16:00 MS 22 Beyond multipolar refinement p. 49	14:00–16:00 MS 45 Measuring data quality p. 49		
				p. 63

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	Sydney	Singapore	Darwin
08:00			
08:15			
08:30	08:30–09:30	08:30–09:30	
08:45	Keynote Lecture	Keynote Lecture	
09:00	Werner Paulus	Bob Cernik	
09:15	p. 51	p. 51	
09:30			
09:45			
10:00	10:00–12:00	10:00–12:00	10:00–12:00
10:15	MS 9	MS 33	MS 1
10:30	Enzyme reactions and	Hot structures of small	SAXS in
10:45	dynamics in crystals	molecules	Structural Biology
11:00			
11:15			
11:30			
11:45	p. 51	p. 52	p. 52
12:00			12:00–14:00
12:15			Software Fayre
12:30			
12:45			
13:00		13:00–14:00	
13:15		ECA Council 3	
13:30		Meeting	
13:45		p. 62	p. 61
14:00	14:00–16:00	14:00–16:00	14:00–16:00
14:15	MS 8	MS 29	MS 24
14:30	Membranes and	Molecular interactions	Inorganic and metal-
14:45	membrane interacting	in crystal packing and	organic magnetic
15:00	proteins	molecular assemblies	structures
15:15			
15:30			
15:45	p. 55	p. 55	p. 56
16:00			
16:15			
16:30	16:30–17:30	16:30–17:30	
16:45	Keynote Lecture	Keynote Lecture	
17:00	Marek Grzelczak	Martin Schmidt	
17:15	p. 58	p. 58	
17:30	17:30–18:30		
17:45	Plenary Lecture		
18:00	Jean-Marie Lehn		
18:15	p. 58		
18:30	18:30–19:30		
18:45	ECM Closing		
19:00	Ceremony and Poster		
19:15	Prizes		
19:30	p. 59		
19:45			
20:00			
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20:30			

■ Focus Area 1 (SIG 1)
 ■ Focus Area 2 (SIG 5, 11, 12)
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■ Focus Area 4 (SIG 7, 13)
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Rio	Osaka	Samarkand	Poster Area	
			Poster Exhibition	08:00
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10:00–12:00
MS 41
The use of X-ray, electron and neutron scattering in nanoscience
p. 53

10:00–12:00
MS 17
Minerals, materials and polymorphs
p. 53

10:00–12:00
MS 25
Quasicrystal and approximant: structure and properties
p. 54

12:00–13:00
SIG 6 Meeting
p. 62

12:00–14:00
ECA Executive Committee meets SIGs
p. 62

13:00–14:00
GIG 2 Scientific Committee Meeting
p. 62

14:00–16:00
MS 16
Structure-property relationships in high pressure crystallography
p. 56

14:00–16:00
MS 40
New detectors for high energy x-ray applications
p. 57

14:00–16:00
MS 50
History of ECA, history of crystallography: contributions to and of crystallography
p. 58

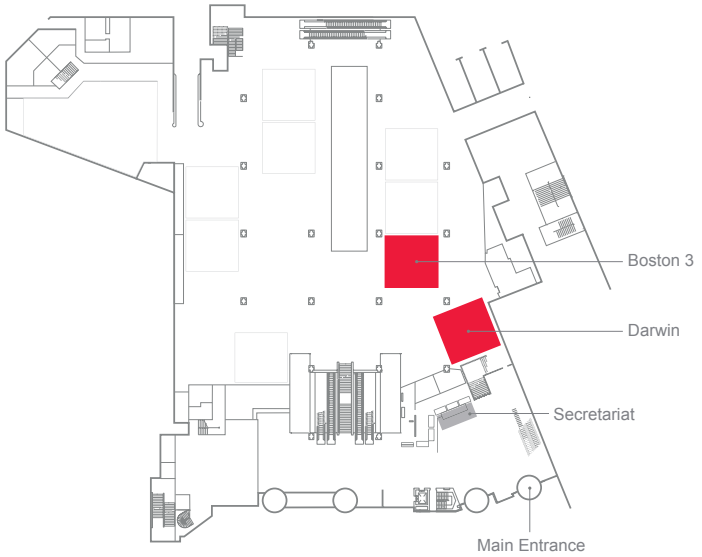
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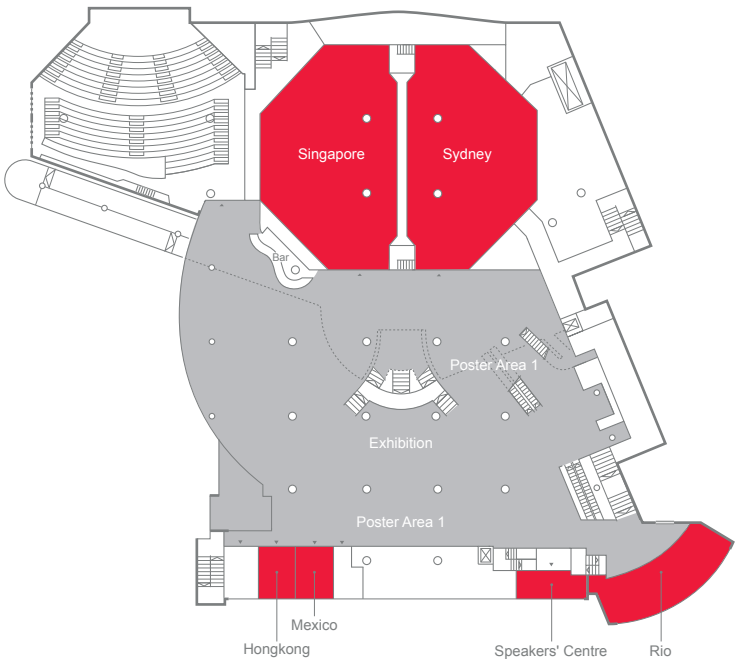
Venue Overview

Ground Floor



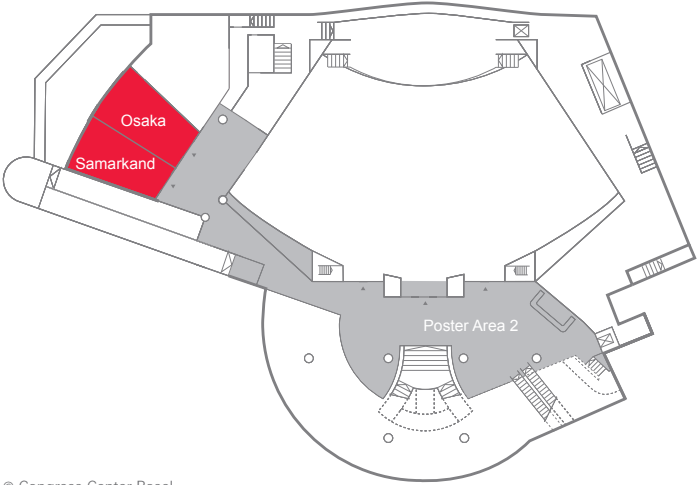
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2nd Floor



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3rd Floor



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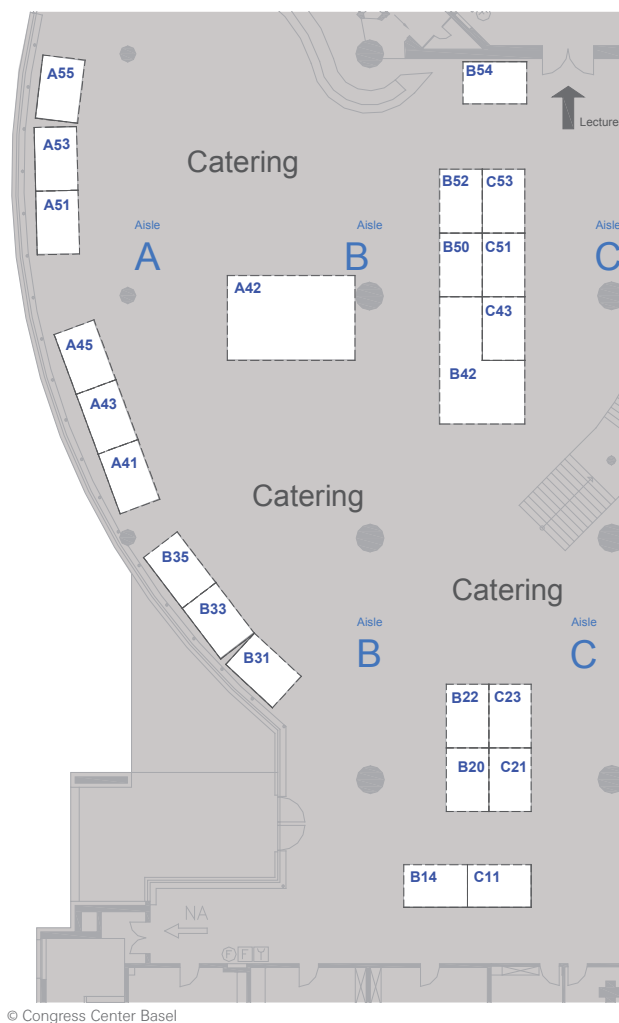
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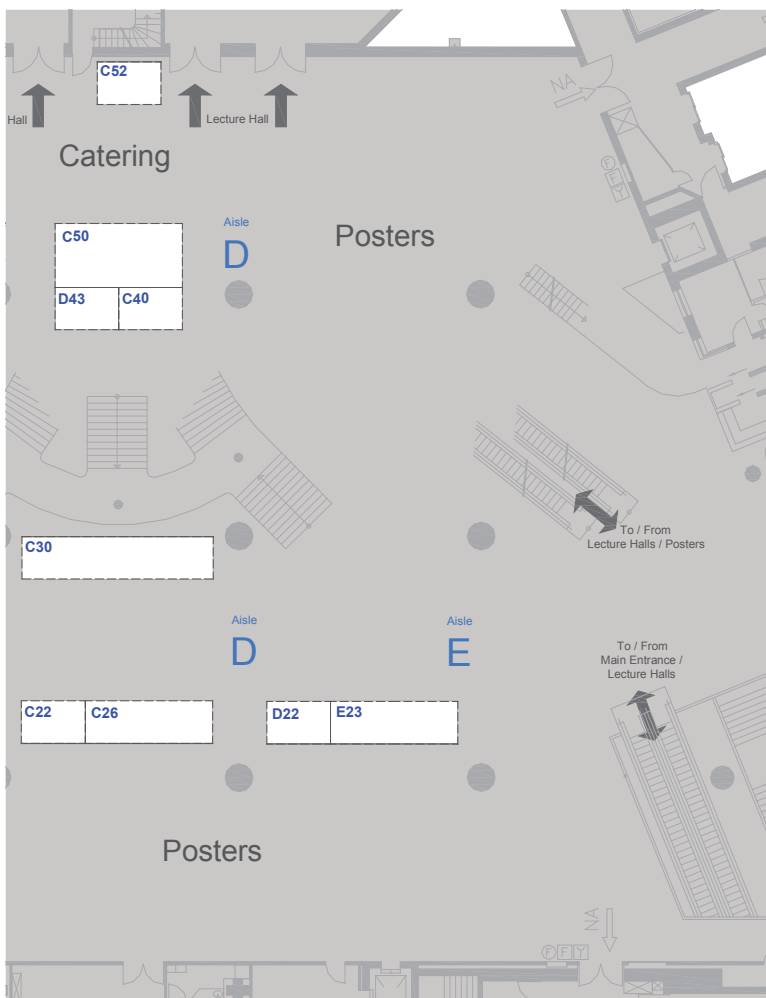
General
Information

Floor Plan and List of Exhibitors



Exhibitor Name	Booth #		
Anton Paar GmbH	A43	ECM-31 / ECM-32	B14
Bruker	A42	Excillum	D22
CCDC - Cambridge	C53	Formulatrix	B50
Crystallographic Data Centre		Huber Diffraktions-technik	B52
CSEM SA	D43	imXPAD	C51
Dectris	C50	Incaotec	A42
Douglas Instruments	B22	IUCr	A41
ECA	C11	marXperts	B35

Floor Plan and List of Exhibitors



Exhibitor Name	Booth #		
Molecular Dimensions	E23	STOE	C26
NanoTemper	C40	Taylor & Francis	C22
NatX-ray	C43	TTP Labtech	B33
Oxford Cryosystems	C23	Walter De Gruyter GmbH	C52
Oxford University Press	A55	Xtal	B31
PANalytical	B42		
PDBe	A51		
Rigaku	C30		
SCANZ	A53		

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Scientific Programme – Introduction

The scientific programme of the ECM-30 is organised into the following microsymbiosia which are promoted by the Programme Committee, the Special Interest Groups (SIGs 1-13) and the General Interest Groups (GIG 1-2). Throughout the programme book the microsymbiosia are colour-coded according to their respective focus areas.

Focus Area 1 (SIG 1)

- SAXS in structural biology
- Development of new types of sample preparation (both XFEL & synchrotrons)
- Data collection and processing software (XFELS & synchrotrons)
- New developments in phasing and refinement
- Structural information in drug design
- Molecular machines and big complexes
- Protein & glycobiology structure determination
- Membranes and membrane interacting proteins
- Enzyme reactions and dynamics in crystals
- H-bonding & weak interactions in crystals: neutrons and X-rays
- Hybrid approaches and validation (X-ray and electron microscopy)
- Biophysical characterization and crystallization
- Hot structures in biology

Focus Area 2 (SIG 5, 11, 12)

- Biomineralogical crystallography and bioinspired inorganic materials
- Minerals and materials
- Structure-property relationships in high pressure crystallography
- Crystal chemistry of C-bearing materials and minerals at extreme conditions
- Structural studies of meteoritic, extra-terrestrial, and planetary materials
- Solid state oxygen fuel cell, hydrogen storage & battery materials
- Materials for energy conversion and harvesting
- Structural disorder and materials' properties at ambient and non-ambient conditions

Focus Area 3 (SIG 2, 3, 4)

- Beyond multipolar refinement
- Charge and spin density of materials at extreme conditions
- Inorganic and metal-organic magnetic structures
- Quasicrystal and approximant: structure and properties
- Incommensurate modulated and composite phases
- Dynamical refinement of electron diffraction data
- New approaches in electron crystallography

Focus Area 4 (SIG 7, 13)

- Molecular interactions in crystal packing and molecular assemblies
- Hydrogen bonding from theory to applications
- Crystal energy landscapes: computation and uses
- Polymorphs, cocrystals, solvates, salts: a jungle for scientists and industries
- Hot structures of small molecules
- Molecular recognition, supramolecular chemistry and crystal engineering
- Simulation of dynamics in molecular compounds
- Crystallography in solid state reactions and catalysis
- Molecular compounds and MOFs at ambient conditions and under high pressure
- Nanomaterials & graphene

Focus Area 5 (SIG 6, 8, 9)

- X-Ray diffraction on the μs to ps time scale
- New detectors for high energy X-ray applications
- The use of X-ray, electron and neutron scattering in nanoscience
- Advances in neutron scattering under non-ambient conditions
- Combining X-ray diffraction and other techniques for in situ and operando studies
- Total scattering: pdf analysis and diffuse scattering in X-Ray, neutron and electron diffraction
- Measuring data quality
- Computational tools for theoretical chemistry in crystallography

General Microsymposia

- Teaching & Education
- Crystallography in art and cultural heritage
- How to...: crystallization for small and large molecules
- History of ECA, history of crystallography: contributions to and of crystallography

The programme of the ECM-30 contains 2 plenary lectures, 16 keynote lectures and 50 microsymposia. The keynote talks are held typically at 08:30 and 16:30/17:30, the oral contributions of the microsymposia are running in 6 (7) parallel sessions, in the mornings from 10:00–12:00 and in the afternoons from 14:00–16:00. In each microsymposium there are five lectures, two invited lectures of 30 minutes and three 20 minute lectures selected from the abstracts.

- 17:00 – 19:00 **Opening Session**
*Chairs: K. M. Fromm (Fribourg, CH)
P. Macchi (Berne, CH)*
- 17:00 **Welcome by Congress Chair**
K. M. Fromm (Fribourg, CH)
- 17:10 **Greetings from the authorities**
*M. Dell’Ambrogio, State Secretary,
State Department of Education, Research and
Innovation (Berne, CH)
H.-P. Wessels, Representative of Basel-City (Basel,
CH)*
- 17:35 **Musical welcome by Solodurum (alporner blower
trio)**
- 17:45 **Welcome words**
*M. Tanner, President of the Swiss Academy of
Sciences (Berne, CH)
P. Macchi, President of the Swiss Society of
Crystallography (Berne, CH)
J. Mesot, Director of the Paul Scherrer Institute
(Villigen, CH)
A. Bacchi, President of the European
Crystallographic Association (Parma, IT)*
- 18:15 **Musical performance by Solodurum (alporner
blower trio)**
- 18:20 **9th Max Perutz Prize of the European
Crystallographic Association**
*U. Heinemann, (Max Delbrück Center for Molecular
Medicine, Berlin, DE)*
- 18:25 **On the fascinating way from abstract superspace
theory to the practical structure analysis of
modulated and composite crystals**
*V. Patrick (Institute of Physics of the Czech
Academy of Sciences, Prague, CZ), winner of the
9th Max Perutz Prize*

*Followed by Welcome Reception within the
industrial exhibition*

Sydney

08:30 – 09:30

Plenary Lecture Ada Yonath

Chair: M. Hennig (leadXpro AG, Villigen, CH)

Crystallography & Ribosomes, Antibiotics Resistance, Parasites, the Microbiome, Environmental issues, Origin of Life and More
A. Yonath (Weizmann Institute, Jerusalem, IS)

Rio

09:40 – 10:00

Commercial Presentation hosted by NanoTemper Technologies GmbH

Easy and Rapid Analysis of Protein Stability, Quality and Aggregation by nanoDSF
T. Pflüger (NanoTemper Technologies GmbH, Munich, DE)

09:30 – 10:00

Coffee break

Focus Area 1 (SIG 1)

Sydney

10:00 – 12:00

MS 7 Protein & glycobiology structure determination

Chairs: J. Agirre (York Structural Biology Laboratory, UK)

G. Sulzenbacher (CNRS, Marseille, FR)

10:00 MS7-01

Structures of lytic polysaccharide monooxygenases and their interaction with polysaccharide substrates

L. Lo Leggio (Department of Chemistry, University of Copenhagen, DK)

10:30 MS7-02

Membrane Enzymes: the Structural basis of Phosphatidylinositol Mannosides Biosynthesis in Mycobacteria

M. Guerin (IKERBASQUE, Basque Foundation for Science, Bilbao, ES)

11:00 MS7-03

Structural studies of medically-interesting protease inhibitors and lectins that belong to the β -trefoil family

A. Wlodawer (Center for Cancer Research, National Cancer Institute, Frederick, MD, US)

11:20 MS7-04

Structure-function characterization reveals catalytic diversity in the galactose oxidase family
S. Urresti (Department of Chemistry, (University of York, UK)

11:40 MS7-05

Structure of the factor H-sialic acid complex links sialic acid recognition to atypical hemolytic uremic syndrome and reveals a novel conformation of the GM1 glycan

B. Blaum (Interfaculty Institute of Biochemistry, University of Tübingen, DE)

Focus Area 4 (SIG 7, 13)

Singapore

10:00 – 12:00

MS 36 Crystallography in solid state reactions and catalysis

Chairs: K. Bučar (University College London, UK)

F. Lahoz (University of Zaragoza, ES)

- 10:00 MS36-01 **Designing single-crystal-to-single-crystal Diels–Alder reactions: the role of nonbonded interactions**
D. Leventis (Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, ZA)
- 10:30 MS36-02 **The Emergence of Medicinal Mechanochemistry**
T. Friscic (McGill University, Montreal, CA)
- 11:00 MS36-03 **Last advances in *in situ* monitoring of mechanochemical reactions by X-ray diffraction**
V. Ban (Paul Scherrer Institute, Villigen, CH)
- 11:20 MS36-04 **Hindered reduction of NiO on Al containing carriers studied by *in situ***
L. Lundegaard (Haldor Topsøe A/S, Lyngby, DK)
- 11:40 MS36-05 ***In situ* diffraction studies during transition metal catalysis**
C. Weidenthaler (Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, DE)

Focus Area 3 (SIG 2, 3, 4)

Darwin

10:00 – 12:00

MS 23 Charge and spin density of materials at extreme conditions

Chairs: N. Casati (Paul Scherrer Institute, Villigen, CH)

P. Guionneau (CNRS, Univ. Bordeaux, FR)

- 10:00 MS23-01 **Anagostic Interactions under Pressure: Attractive or Repulsive?**
W. Scherer (Universität Augsburg, DE)
- 10:30 MS23-02 **Charge Density Studies of Switchable Molecular Materials at Extreme Conditions: What; How & Why?**
H. Shepherd (University of Kent, UK)
- 11:00 MS23-03 **Copper-pyrazine magnetic polymers under high pressure**
A. Lanza (Laboratory of Synchrotron Radiation, Paul Scherrer Institute, CH)
- 11:20 MS23-04 **Hydrogen maleate salts: Precise and accurate determination of the hydrogen atom position in short hydrogen bonds using X-ray diffraction at extremely low temperatures**
S. Grabowsky (Universität Bremen, DE)
- 11:40 MS23-05 **Charge density of the semiquinone radical anion**
K. Molčanov (Rudjer Bošković Institute, HR)

		Focus Area 4 (SIG 7, 13)	Boston 3
10:00 – 12:00		MS 31 Crystal energy landscapes: computation and uses	
		<i>Chairs: M. Neumann (Avant Garde Materials Simulation Deutschland GmbH, Freiburg, DE) A. Reilly (The Cambridge Crystallographic Data Centre, UK)</i>	
10:00	MS31-01	Computed Crystal Energy Landscapes: A First Step towards Digital Drug Product Design?	<i>S. Reutzel-Edens (Lilly Research Laboratories, US)</i>
10:30	MS31-02	Accurate and Affordable Lattice Energy Calculations: A Solved Problem?	<i>A. Tkatchenko (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, DE)</i>
11:00	MS31-03	Organic crystal polymorphism: A benchmark for dispersion corrected mean field electronic structure methods	<i>J.G. Brandenburg (Department of Chemistry, University College London, UK)</i>
11:20	MS31-04	Generation of crystal structure landscapes using known crystal structures	<i>G. Shields (Cambridge Crystallographic Data Centre, UK)</i>
11:40	MS31-05	<i>Ab initio</i> ³⁵ Cl solid state NMR-based crystallography of active pharmaceutical ingredients.	<i>A. Pulido (School of Chemistry, University of Southampton, Southampton, UK)</i>
		Focus Area 1 (SIG 1)	Rio
10:00 – 12:00		MS 12 Biophysical characterization and crystallization	
		<i>Chairs: R. Meijers (European Molecular Biology Laboratory, Hamburg, DE) B. Byrne (Imperial Collage London, UK)</i>	
10:00	MS12-01	The magnesium transporter A, a bacterial P-type ATPase dependent on cardiolipin and selectively sensitive to free magnesium <i>in vitro</i>	<i>J.P. Morth (Centre for Molecular Medicine, Nordic EMBL Partnership, University of Oslo, NO)</i>
10:30	MS12-02	New Pipelines for Automated High Throughput Ligand Screening	<i>I. Cornaciu (EMBL Grenoble, FR)</i>
11:00	MS12-03	DNA Structure and Dynamics – A Combinational Approach	<i>J. Hall (Department of Chemistry, University of Reading, UK)</i>

11:20 MS12-04 **Racemic DNA Crystallography: advantages and applications**
P. Mandal (Université de Bordeaux, CBMN (UMR5248), Pessac, FR)

11:40 MS12-05 **An all-in-one lanthanide complex to overcome the two major bottlenecks in protein crystallography.**
S. Engilberge (Institut de Biologie Structurale, Grenoble, FR)

Focus Area 5 (SIG 6, 8, 9)

Osaka

10:00 – 12:00

MS 39 X-Ray diffraction on the μ s to ps time scale

*Chairs: M. Wulff (European Synchrotron Radiation Facility, Grenoble, FR)
S. Gorfman (University of Siegen, DE)*

10:00 MS39-01 **Time-resolved X-ray microdiffraction for ferroelectric heterostructures**
J.Y. Jo (Gwangji Institute of Science and Technology, KR)

10:30 MS39-02 **Laser driven acoustic vibrations in nanowires studied by time-resolved GIXD.**
D. Khakhulin (European XFEL GmbH and the Hamburg Centre for Ultrafast Imaging, DE)

11:00 MS39-03 **Simulations of single-pulse Laue diffraction from proteins with radiation from synchrotron and XFEL sources**
V. Kabanova (European Synchrotron, Grenoble, FR)

11:20 MS39-04 **Time-resolved photocrystallography on a laboratory diffractometer on the millisecond time scale**
D. Schaniel (Université de Lorraine, Vandoeuvre-Nancy, FR)

11:40 MS39-05 **X-ray study of femtosecond structural dynamics of the charge-density wave compound 1T-TaS₂**
S. Ravy (Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Université Paris-Saclay, Orsay, FR)

Focus Area 2 (SIG 5, 11, 12)

Samarkand

10:00 – 12:00

MS 15 Minerals and materials

*Chairs: F. Hatert (University of Liège, BE)
R. Nilica (RHI-AG Technical Center Leoben, Vienna, AT)*

10:00 MS15-01 **How crystallography can assist process mineralogy – two metallurgical examples**
V. Kahlenberg (University of Innsbruck, Institute of Mineralogy and Petrography, AT)

- 10:30 MS15-02 Crystal chemistry of layered Pb hydroxocarbonate minerals
O. Siidra (Saint-Petersburg State University, RU)
- 11:00 MS15-03 Phase diagrams of $Ba_2M^{2+}Te^{6+}O_6$: insight into the interplay between crystal structure and magnetic dimensionality
A. Gibbs (ISIS Pulsed Neutron and Muon Source, Rutherford Appleton Laboratory, Harwell Oxford, UK)
- 11:20 MS15-04 Crystal structure and polymorphism of $NaSrVO_4$: the first $A'B''X^VO_4$ larnite related structure from X-ray powder data
G. Nenert (PANalytical B. V., EA Almelo, NL)
- 11:40 MS15-05 Ordering phenomena in minerals: the Verwey phase of natural magnetite
G. Perversi (Centre for Science at Extreme Conditions and School of Chemistry, University of Edinburgh, UK)
- Sydney
- 12:30 – 13:30 **Commercial User Workshop hosted by Dectris**
- Sydney
- 14:00 – 16:00 **MS 10 H-bonding & weak interactions in crystals: neutrons and X-rays**
*Chairs: B. Zakharov (Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, RU)
A. Thompson (University of Oxford, UK)*
- 14:00 MS10-01 Nanoscale hydrogen bound network revealed by neutron scattering
H. Bordallo (The Niels Bohr Institute - University of Copenhagen, DK)
- 14:30 MS10-02 Molecular Interactions in Pharmaceutical Compounds
K. Edkins (School of Medicine, Pharmacy and Health, Durham University, UK)
- 15:00 MS10-03 High resolution neutron and X-ray diffraction RT studies of an H-FABP – Oleic acid complex: study of the internal water cluster and the ligand binding by a transferred multipolar electron density distribution
A. Podjamy (IGBMC, CNRS, INSERM, Uds, Illkirch, FR)
- 15:20 MS10-04 Targeting transthyretin amyloidosis: Joint neutron and X-ray diffraction analysis of a pathogenic protein
A.W. Yee (Life Sciences group, Institut Laue-Langevin, Grenoble, FR)

- 15:40 MS10-05 **Bond Formation, Interactions and Reactions in *Peri*-Substituted Naphthalenes.**
J. Wallis (School of Science and Technology, Nottingham Trent University, Clifton Lane, Nottingham, UK)

Focus Area 4 (SIG 7, 13)

Singapore

14:00 – 16:00 **MS 34 Molecular recognition, supramolecular chemistry and crystal engineering**

*Chairs: C.H. Görbitz (University of Oslo, NO)
C. Massera (University of Parma, IT)*

- 14:00 MS34-01 **Sense and flexibility: self-assembly, host-guest chemistry and solid state dynamic behaviour of cyclic peptoids**
C. Tedesco (Università di Salerno, Dipartimento di Chimica e Biologia "A. Zambelli", Fisciano, IT)
- 14:30 MS34-02 **Supramolecular chemistry of the *p*-carboxylatocalix[4]arenes**
S.J. Dalgarno (Heriot-Watt University, Riccarton, Edinburgh, UK)
- 15:00 MS34-03 **Structural Layers in High-Z' Molecular Crystals**
C. Brock (University of Kentucky, US)
- 15:20 MS34-04 **From versatile hydrogen- and halogen-bond acceptors to elastic bending of metal-containing architectures**
M. Dakovic (Department of Chemistry, Faculty of Science, University of Zagreb, HR)
- 15:40 MS34-05 **Mechanisms of Guest Exchange and Selectivity in Host-Guest Systems**
L. Nassimbeni (University of Cape Town, ZA)

Focus Area 3 (SIG 2, 3, 4)

Darwin

14:00 – 16:00 **MS 26 Incommensurate modulated and composite phases**

*Chairs: M. Dusek (Institute of Physics of the Czech Academy of Sciences, Prague, CZ)
A. Abakumov (Skolkovo Institute of Science and Technology, Moscow, RU)*

- 14:00 MS26-01 **Incommensurate charge order and charge-density waves**
S. van Smaalen (University of Bayreuth, Laboratory of Crystallography, DE)
- 14:30 MS26-02 **Incommensurate oxides and sulfides**
B. Stöger (TU Wien, AT)
- 15:00 MS26-03 **Structural phase transitions in the organic-inorganic hybrid perovskites $(C_6H_{11}NH_3)_2[PbX_4]$ (X=I, Br)**
S. Pillet (Laboratoire de Cristallographie, Résonance Magnétique et Modélisations, Institut Jean Barriol, Université de Lorraine, Vandœuvre-lès-Nancy, FR)

- 15:20 MS26-04 Probing the nuclear and magnetic structure of a complex ferromagnetic semiconductor
J. Claridge (University of Liverpool, UK)
- 15:40 MS26-05 Incommensurately modulated crystal structures of Cu_3Si
C. Corrêa (Institute of Physics of the Czech Academy of Sciences, Prague, CZ)
- 14:00 – 16:00 Focus Area 5 (SIG 6, 8, 9) Boston 3
MS 42 Advances in neutron scattering under non-ambient conditions
Chairs: S. Klotz (Pierre and Marie Curie University, Paris, FR)
J. Kulda (TRIPLE AXIS SPECTROMETERS, Grenoble, FR)
- 14:00 MS42-01 The role of oxygen packing in the structural transformations of oxide glasses
A. Zeidler (Physics Department, University of Bath, UK)
- 14:30 MS42-02 Neutron Diffraction Studies of Gas Hydrates
J. Loveday (SUPA, School of Physics and Astronomy and Centre for Science at Extreme Conditions, The University of Edinburgh, UK)
- 15:00 MS42-03 Matrix transformation temperature in boron containing Co-Re alloys for high temperature gas turbine applications
P. Strunz (Nuclear Physics Institute of the CAS, Rež, CZ)
- 15:20 MS42-04 Neutron Total Scattering of Crystalline Materials in the Gigapascal Regime
C. Bull (ISIS Facility, STFC, Rutherford Appleton Lab, UK)
- 15:40 MS42-05 Stroboscopic neutron powder diffraction at HRPT, SINQ
D. Sheptyakov (Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Villigen, CH)
- 14:00 – 16:00 Focus Area 1 (SIG 1) Rio
MS 2 Development of new types of sample preparation (both XFEL & synchrotrons)
Chairs: G. Evans (Diamond Light Source, Harwell, UK)
J. Standfuss (Paul Scherrer Institute, Villigen, CH)
- 14:00 MS2-01 Fundamental Characterization of Liquid-Jet Sample Injectors for XFEL and Synchrotron Use
R.B. Doak (Max-Planck-Institut fuer medizinische Forschung, Heidelberg, DE)

- 14:30 MS2-02 Enabling time-resolved structural studies of biological macromolecules
A. Pearson (Hamburg Centre for Ultrafast Imaging, University of Hamburg, DE)
- 15:00 MS2-03 Macromolecular Crystallography at SwissFEL
I. Martiel (Paul Scherrer Institute, CH)
- 15:20 MS2-04 The newPin project: Towards a new sample holder standard for cryogenic macromolecular x-ray crystallography
G. Papp (European Molecular Biology Laboratory, Grenoble Outstation, FR)
- 15:40 MS2-05 Structure determination of a membrane protein with data collected from micro-crystals in lipidic cubic phase at room temperature in low background CrystalDirect™ crystallization plates.
T. Schneider (European Molecular Biology Laboratory, Hamburg, DE)

General Microsymposia

Osaka

14:00 – 16:00

MS 49 How to...: crystallization for small and large molecules

*Chairs: A. Maloney (The Cambridge Crystallographic Data Centre, UK)
A. Crochet (University of Fribourg, CH)*

- 14:00 MS49-01 Some Tricks for the Single Crystal Growth of Small Molecules
B. Spingler (Department of Chemistry, University of Zurich, CH)
- 14:30 MS49-02 How to... enhance the success of protein crystallization
N. Chayen (Computational and Systems Medicine, Department of Surgery and Cancer, Faculty of Medicine, Imperial College London, UK)
- 15:00 MS49-03 Toward the mitigation of growth rate dispersion through pretreatment of seed crystals
A.K. Rajagopalan (Institute of Process Engineering, ETH Zurich, CH)
- 15:20 MS49-04 Microseed matrix-screening (rMMS): introduction, theory, practice and a new technique for membrane protein crystallization in LCP
P. Shaw Stewart (Douglas Instruments Ltd, UK)
- 15:40 MS49-05 The Highs And Lows Of Extreme Conditions Crystallisation
M. Probert (Newcastle University, UK)

		Focus Area 2 (SIG 5, 11, 12)	Samarkand
14:00 – 16:00		MS 18 Structures of minerals, planetary and carbon materials at earth and planetary conditions	
		<i>Chairs: T. Boffa-Ballaran (University of Bayreuth, DE) M. Merlini (University of Milan, IT)</i>	
14:00	MS18-01	Discovering new materials, minerals and phenomena with evolutionary algorithms	
		<i>A. Oganov (Skolkovo Institute of Science and Technology, Russia, RU)</i>	
14:30	MS18-02	Super-deep diamonds and their mineral inclusions: an overview	
		<i>F. Nestola (Department of Geosciences, University of Padova, IT)</i>	
15:00	MS18-03	Water-rock interactions in carbonaceous chondrites: a meso to nanoscale study of alteration processes in an anoxygenic environment	
		<i>A. Elmaleh (Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (UPMC-CNRS), FR)</i>	
15:20	MS18-04	Structures of meteoritic diamond nanocrystals	
		<i>P. Nemeth (Institute of Materials and Environmental Chemistry, Research Center for Natural Sciences, Hungarian Academy of Sciences, Budapest, HU)</i>	
15:40	MS18-05	Structural trend of alkaline carbonates under high pressure	
		<i>P. Gavryushkin (V.S. Sobolev Institute of Geology and Mineralogy SB RAS, Novosibirsk, RU)</i>	
16:00 – 16:30		Coffee break	
			Sydney
16:30 – 17:30		Keynote Lecture Peter Schurtenberger	
		<i>Chair: A. Stradner (Lund, SE)</i>	
		Colloids in the spotlight – watching crystal-crystal transitions in real time and real space	
		<i>P. Schurtenberger (Lund University, SE)</i>	
			Singapore
16:30 – 17:30		Keynote Lecture Francesca Fabbiani	
		<i>Chair: M. Wörle (Zurich, CH)</i>	
		Exploring crystalline molecular materials at high pressure	
		<i>F. Fabbiani (Georg-August-Universität Göttingen, DE)</i>	

- 17:30 – 19:00 **Poster Session 1**
MS [1, 2, 3, 4, 7, 9, 11, 13, 14, 15, 17, 19, 22, 24, 25, 26, 27, 28, 31, 32, 38, 41, 44, 46, 48]
- Sydney**
- 19:00 – 20:00 **Commercial User Workshop: Progress in Source and Detector Technology for X-ray Crystallography hosted by Bruker**
*Chairs: R. Durst (Bruker, Karlsruhe, DE)
J. Wiesmann (Incoatec, Geesthacht, DE)*
- 19:00 **Welcome to the future: The new D8 2nd Generation**
J. Wiesmann (Incoatec, Geesthacht, DE)
- 19:05 **Microfocus made perfect: I μ S 3.0**
C. Michaelsen (Incoatec, Geesthacht, DE)
- 19:15 **The new PHOTON II, XFEL detector technology in-house**
R. Durst (Bruker, Karlsruhe, DE)
- 19:30 **D8 VENTURE with METALJET and NANOSTAR: One source – two instruments – best results**
V. Smith (Bruker, Karlsruhe, DE)
- 19:40 **Synchrotron data quality in the home laboratory**
M. Adam (Bruker, Karlsruhe, DE)
- 19:50 **Mastering challenging samples**
T. Stürzer (Bruker, Karlsruhe, DE)

Sydney

08:30 – 09:30

Keynote Lecture François Diederich

Chair: B. Giese (Fribourg, CH)

Molecular Recognition in Chemical and Biological Systems: A Multidimensional Approach

F. Diederich (ETH Zurich, CH)

Singapore

08:30 – 09:30

Keynote Lecture Birger Dittrich

Chair: P. Macchi (Berne, CH)

Emphasizing the difference between experimental and theoretical electron density in the solid state: new opportunities from anharmonic thermal motion to excited states

B. Dittrich (Heinrich-Heine University, Düsseldorf, DE)

09:30 – 10:00

Coffee break

Focus Area 1 (SIG 1)

Sydney

10:00 – 12:00

MS 13 Hot structures in biology

Chairs: M. Jaskolski (A. Mickiewicz University, Poznan, PL)

U. Heinemann (Max Delbrück Center for Molecular Medicine, Berlin, DE)

10:00 MS13-01

How Bacteria Make Rocket Fuel: Structure and Mechanism of Hydrazine Synthase

T.R.M. Barends (Max Planck Institute for Medical Research, Heidelberg, DE)

10:30 MS13-02

Challenges at low resolution: crystal structure of the yeast VPS34 complex II.

N. Soler (MRC Laboratory of Molecular Biology, Cambridge, UK)

11:00 MS13-03

X-Ray Crystal Structure of a Chromosome

C. Davey (School of Biological Sciences, Nanyang Technological University, 60 Nanyang Drive, SG)

11:20 MS13-04

Zinc dependent 3'-nucleases/nucleotidases from plants, fungi and bacteria – varied roles and specificity

J. Dohnalek (Institute of Biotechnology CAS, Biocev, Vestec, CZ)

11:40 MS13-05

Structure and dynamics of the polymyxin-resistance-associated response regulator PmrA in complex with the promoter DNA

C.-D. Hsiao (Institute of Molecular Biology, Academia Sinica, TW)

Committees

Welcome

Programme Overview

Venue Overview

Exhibition Floor Plan

Scientific Programme

Poster Overview

Social Events

General Information

		Focus Area 1 (SIG 1)	Singapore
10:00 – 12:00		MS 3 Data collection and processing software (XFELS & synchrotrons)	
		<i>Chairs: A. Mancuso (XFEL, Hamburg, DE) T. Schneider (European Molecular Biology Laboratory, Hamburg, DE)</i>	
10:00	MS3-01	MX data analysis developments at Diamond Light Source.	
		<i>G. Evans (Diamond Light Source, Harwell Science and Innovation Campus, Didcot, UK)</i>	
10:30	MS3-02	Hidden treasure in serial femtosecond diffraction	
		<i>A. Barty (CFEL/DESY, DE)</i>	
11:00	MS3-03	Processing XFEL Still Shots and Merging Multi-crystal Data	
		<i>N. Sauter (Lawrence Berkeley National Laboratory, US)</i>	
11:20	MS3-04	Data sets merging in serial crystallography	
		<i>R. Warshamanage (Swiss Light Source, Paul Scherrer Institute, Villigen, CH)</i>	
11:40	MS3-05	Experimental phasing with serial crystallography at XFEL and synchrotron radiation	
		<i>K. Yamashita (RIKEN SPring-8 Center, Advanced Photon Technology Division, Sayo, JP)</i>	

		Focus Area 3 (SIG 2, 3, 4)	Darwin
10:00 – 12:00		MS 27 Dynamical refinement of electron diffraction data	
		<i>Chairs: R. Beanland (University of Warwick, UK) M. Gemmi (Center for Nanotechnology Innovation, Pisa, IT)</i>	
10:00	MS27-01	Structure refinement using precession electron diffraction tomography and dynamical diffraction theory	
		<i>L. Palatinus (Institute of Physics of the CAS, Prague, CZ)</i>	
10:30	MS27-02	Accurate unit cell determination from rotation electron diffraction data	
		<i>W. Wan (Bezelii Center EXSELENT on Porous Materials and Inorganic and Structural Chemistry, Department of Materials and Environmental Chemistry, Stockholm University, SE)</i>	
11:00	MS27-03	Study of partial occupancies and Jahn-Teller distortions in $(\text{Na}, \square)_5[\text{MnO}_2]_{13}$ by XRPD Rietveld and electron diffraction dynamical refinements	
		<i>E. Mugnaioli (Dipartimento di Scienze Fisiche, della Terra e dell'Ambiente, Università degli Studi di Siena, Siena, IT)</i>	

11:20 MS27-04 Localization of hydrogen atoms in organic molecules using dynamical refinement of electron diffraction data

P. Brazda (Institute of Physics of the CAS, CZ)

11:40 MS27-05 Improving rotation electron diffraction data quality by data merging

Y. Wang (Berzelii Center EXSELENT on Porous Materials and Inorganic and Structural Chemistry, Department of Materials and Environmental Chemistry, Stockholm University, SE)

Focus Area 2 (SIG 5, 11, 12)

Rio

10:00 – 12:00

MS 19 Solid state oxygen fuel cell, hydrogen storage & battery materials

*Chairs: B. Frick (Institut Laue-Langevin, Grenoble, FR)
K. Edstroem (Uppsala University, SE)*

10:00 MS19-01 Structure and dehydration mechanism of the proton conducting brownmillerite $\text{Ba}_2\text{In}_2\text{O}_5$

M. Karlsson (Department of Physics, Chalmers University of Technology, SE)

10:30 MS19-02 *In operando* pair distribution function analysis and solid-state NMR studies of antimony anodes for sodium-ion batteries

P. Allan (Diamond Light Source, Diamond House, Harwell Science & Innovation Campus, Didcot, Oxfordshire, UK)

11:00 MS19-03 Quasi-Elastic Neutron Scattering Studies on Solid Electrolytes for all-solid-state Lithium Batteries

D. Blanchard (Department of Energy, Technical University of Denmark (DTU), DK)

11:20 MS19-04 Characterization of cation ordering, oxygen vacancy distribution and proton sites in hexagonal and cubic $\text{BaTi}_{1-x}\text{Sc}_x\text{O}_{3-\delta}$

P. Henry (European Spallation Source ERIC, Lund, SE)

11:40 MS19-05 Lattice dynamics of the ionic superconductor $\text{Li}_4\text{C}_6\text{O}$. Inelastic neutron scattering and Powder Averaged Lattice Dynamics (PALD) investigations.

S. Rols (Institut Laue Langevin, Grenoble, FR)

Focus Area 4 (SIG 7, 13)

Osaka

10:00 – 12:00

MS 35 Simulation of dynamics in molecular compounds

*Chairs: M. Meuwly (University of Basel, CH)
A.O. Madsen (University of Copenhagen, DK)*

10:00 MS35-01 Lattice Vibrations in Molecular Crystals: Polymorphism and Phase Transitions

J. Nyman (University of Southampton, UK)

- 10:30 MS35-02 Diffuse scattering, spectroscopy and *ab initio* density functional theory
M. Gutmann (Rutherford Appleton Laboratory, ISIS Facility, Chilton Didcot, Oxfordshire, UK)
- 11:00 MS35-03 Predicting Urea Crystal Shapes Grown from Solution with Molecular Dynamics Simulations
Z. Bjelobrk (Institute of Process Engineering, ETH Zürich, CH)
- 11:20 MS35-04 Computational dehydration of an organic hydrate using molecular dynamics simulations
A. Larsen (Department of Pharmacy, University of Copenhagen, DK)
- 11:40 MS35-05 The application of tailor-made force fields and molecular dynamics for NMR crystallography
X. Li (Department of Pharmacy, University of Copenhagen, DK)

Focus Area 5 (SIG 6, 8, 9)

Samarkand

10:00 – 12:00 **MS 44 Total scattering: pdf analysis and diffuse scattering in X-Ray, neutron and electron diffraction**

*Chairs: V. Holý (Charles University in Prague, CZ)
C. Giannini (Institute of Crystallography - CNR/IC, Bari, IT)*

- 10:00 MS44-01 Confined liquid structure and chemical kinetics from total neutron scattering
T. Youngs (ISIS Facility, STFC Rutherford Appleton Laboratory, UK)
- 10:30 MS44-02 Correlated disorder in relaxor ferroelectrics
J. Hlinka (Institute of Physics, The Czech Academy of Sciences, Prague, CZ)
- 11:00 MS44-03 Mapping of reciprocal space with ferroelectrics under electric field
D. Chernyshov (Swiss-Norwegian BeamLines at the European Synchrotron Radiation Facility, Grenoble, FR)
- 11:20 MS44-04 Pair Distribution Function calculated from electron diffraction data
T. Gorelik (University of Mainz, DE)
- 11:40 MS44-05 Searching for Ti-clusters in $\text{Mg}_{0.7}\text{Ti}_{0.3}$ thin film
H. Kim (National Institute of Advanced Industrial Science and Technology, Tokyo, JP)

Sydney

12:30 – 13:30 **Commercial User Workshop hosted by Rigaku Oxford Diffraction**

- 12:30 What's New in Chemical Crystallography at Rigaku Oxford Diffraction
A. Griffin (Rigaku Oxford Diffraction, UK)

12:45		CrysAlisPro <i>M. Meyer (Rigaku Oxford Diffraction, Wroclaw, PL)</i>
13:15		What's New in Structural Biology at Rigaku Oxford Diffraction <i>A. Criswell (Rigaku Oxford Diffraction, Houston, US)</i>
		Focus Area 4 (SIG 7, 13) Sydney
14:00 – 16:00		MS 32 Polymorphs, cocrystals, solvates, salts: a jungle for scientists and industries <i>Chairs: M. Schmidt (University of Frankfurt, DE) C. Esterhuysen (University of Stellenbosch, Matieland, ZA)</i>
14:00	MS32-01	Thymine and Orotic Acid – small molecules with unusual hydrates and intriguing solid state phenomena <i>D. Braun (Institute of Pharmacy, University of Innsbruck, AT)</i>
14:30	MS32-02	Selection of Solid State Forms for New Chemical Entities: Challenges, Opportunities and Lessons <i>C. Saal (Merck Group, Darmstadt, DE)</i>
15:00	MS32-03	Pharma: improving and controlling properties. Cocrystals, bio-inspired MOFs and Ionic Liquids. Gabapentine a case study. <i>M.T. Duarte (Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, PT)</i>
15:20	MS32-04	Traversing the solid form jungle using the power of the Cambridge Structural Database <i>N. Feeder (The Cambridge Crystallographic Data Centre, UK)</i>
15:40	MS32-05	In the jungle, the mighty jungle, the crystals grow tonight! <i>U. Werthmann (Boehringer Ingelheim GmbH, DE)</i>
		Focus Area 1 (SIG 1) Singapore
14:00 – 16:00		MS 4 New developments in phasing and refinement <i>Chairs: E. Dodson (York Structural Biology Laboratory, UK) R. Read (University of Cambridge, UK)</i>
14:00	MS4-01	Refinement without a model <i>J. Agirre (York Structural Biology Laboratory, Department of Chemistry, University of York, UK)</i>
14:30	MS4-02	New bulk-solvent models improves model-to-data fit and facilitates map interpretation <i>P. Afonine (Lawrence Berkeley National Laboratory, Berkeley CA, US)</i>

- 15:00 MS4-03 **Fragon – rapid fragment-based molecular replacement**
H. Jenkins (York Structural Biology Laboratory, Department of Chemistry, University of York, UK)
- 15:20 MS4-04 **BORGES_MATRIX: a tool to generate models for ab initio phasing and for structure interpretation.**
M. Sammito (Georg August University of Göttingen, Dept. of Structural Chemistry, DE)
- 15:40 MS4-05 **Substructure determination from SAD data using phase retrieval techniques**
P. Skubak (Faculty of Science, Leiden Institute of Chemistry, Biophysical Structural Chemistry, Leiden, NL)

Focus Area 5 (SIG 6, 8, 9)

Darwin

14:00 – 16:00 **MS 43 Combining x-ray diffraction and other techniques for in situ and operando studies**

*Chairs: F. Fauth (Cells, Barcelona, ES)
H. Ehrenberg (Karlsruhe Institut of Technology, DE)*

- 14:00 MS43-01 **Revealing Secrets of Lithium-Ion Battery Operation by Neutron Scattering**
M. Muehlbauer (Helmholtz-Institute Ulm for Electrochemical Energy Storage HIU Karlsruhe, DE)
- 14:30 MS43-02 **New insight on structural and redox processes involved upon cycling of $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}_3$, an attractive positive electrode material for Na-ion batteries**
T. Broux (CNRS, University of Bordeaux, Bordeaux INP, Pessac, FR)
- 15:00 MS43-03 **In situ analysis of mechanochemical reactions using combined X-ray diffraction and Raman spectroscopy**
F. Emmerling (Bundesanstalt für Materialforschung und -prüfung, DE)
- 15:20 MS43-04 **Operando Study of Ceria Based Solid Oxide Electrochemical Cells**
C. Dejoie (ESRF - The European Synchrotron, Grenoble, FR)
- 15:40 MS43-05 **Combined measurements of atomic displacements, lattice strain and macroscopic polarization in ferroelectrics**
S. Gorfman (University of Siegen, Department of Physics, DE)

		Focus Area 2 (SIG 5, 11, 12)	Rio
14:00 – 16:00		MS 20 Materials for energy conversion and harvesting	
		<i>Chairs: M. Hinterstein (Karlsruher Institut für Technologie (KIT), Eggenstein-Leopoldshafen, DE) S. Schmid (The University of Sydney, AU)</i>	
14:00	MS20-01	A structural perception about intrinsic point defects in kesterite type compound semiconductors	
		<i>S. Schorr (Helmholtz-Zentrum Berlin für Materialien und Energie, DE)</i>	
14:30	MS20-02	Application of Total Scattering Methods to the Investigation of Clean Energy Materials	
		<i>L. Malavasi (University of Pavia and INSTM, IT)</i>	
15:00	MS20-03	Interaction of water with (silico) aluminophosphate zeotypes: A comparative investigation using dispersion-corrected DFT	
		<i>M. Fischer (Fachgebiet Kristallographie, FB Geowissenschaften, Universität Bremen, DE)</i>	
15:20	MS20-04	TiO₂ nanocontainers and nanospheres as photocatalysts for CO₂ reduction and photoelectrochemical water splitting: Structural modification.	
		<i>N. Héroult (Departement für Chemie und Biochemie, University of Fribourg, Berne, CH)</i>	
15:40	MS20-05	Structure and magnetocaloric properties of Gadolinium borohydrides	
		<i>P. Schouwink (University of Geneva, CH)</i>	
		Focus Area 3 (SIG 2, 3, 4)	Osaka
14:00 – 16:00		MS 28 New approaches in electron crystallography	
		<i>Chairs: L. Meshi (Ben-Gurion University of the Negev, Beer-Sheva, IL) X. Zou (Stockholm University, SE)</i>	
14:00	MS28-01	When Precession Electron Diffraction Tomography goes dynamical	
		<i>P. Boullay (Laboratoire de Cristallographie et de Sciences des Matériaux (CRISMAT), ENSICAEN, FR)</i>	
14:30	MS28-02	MicroED: Three Dimensional Electron Diffraction of Microscopic Crystals	
		<i>T. Gonen (Group Leader, Howard Hughes Medical Institute, Janelia Research Campus, Ashburn, US)</i>	
15:00	MS28-03	Protein nano-crystallography using optimized quantum area direct electron detectors like the Medipix and Dectris families.	
		<i>E. van Genderen (Paul Scherrer Institute - LBR, CH)</i>	

15:20 MS28-04 **Serial snapshot crystallography using electron diffraction**

S. Smeets (Inorganic and Structural Chemistry Department of Materials and Environmental Chemistry, Stockholm University, SE)

15:40 MS28-05 **Fast electron diffraction tomography on beam sensitive materials at room temperature: pharmaceuticals and zeolites**

M. Gemmi (Center for Nanotechnology Innovation @NEST, Istituto Italiano di Tecnologia, Pisa, IT)

General Microsymposia

Samarkand

14:00 – 16:00

MS 47 Teaching & Education

Chairs: H. Flack (University of Geneva, CH)

H. Stoeckli-Evans (University of Neuchâtel, CH)

14:00 MS47-01 **It is never too early, or too late to start**

E. Boldyreva (Novosibirsk State University, RU)

14:30 MS47-02 **A cross-field perspective on Symmetry & Crystal to introduce Crystallography**

J.-L. Hodeau (Institut Neel, CNRS & Univ. Grenoble Alpes, FR)

15:00 MS47-03 **The power of using 827,948 crystal structures in education**

S. Ward (The Cambridge Crystallographic Data Centre, UK)

15:20 MS47-04 **Improved access to raw diffraction data and its impact on crystallographic education and teaching**

J. Helliwell (School of Chemistry, University of Manchester, UK)

15:40 MS47-05 **The educational and outreach programme of the IUCr**

M. Zema (International Union of Crystallography, Chester, UK)

16:00 – 16:30

Coffee break

Sydney

16:30 – 17:30

Keynote Lecture Sandra W. Jacob

Chair: T. Schirmer (Basel, CH)

Allosteric Kinase Inhibitors

S. W. Jacob (Novartis Pharma AG, Basel, CH)

Singapore

16:30 – 17:30

Keynote Lecture Marcus Neumann

Chair: M. Meuwly (Basel, CH)

Organic crystal structure prediction – from fundamental research to industrial application

M. Neumann (Avant Garde Materials Simulation Deutschland GmbH, Freiburg, DE)

17:30 – 19:00

Poster Session 2

MS [5, 6, 8, 10, 12, 16, 18, 20, 21, 23, 29, 30, 33, 34, 35, 36, 37, 39, 40, 42, 43, 45, 47, 49, 50]

Sydney

19:00 – 20:30

The Bertaut Prize Ceremony and Science Slam

19:00

Science Slam

For the first time, a Science Slam will be held at a ECM-meeting! From all submitted poster abstracts, the Scientific Committee will chose 5-6 highly attractive themes (upon abstract submission, you can chose to be willing to do a science slam if your abstract is chosen) and contact the authors in order to ask them to deliver a 3-minutes presentation of their work. This should be such that a large public can understand it, and entertaining science is very welcome. The winner will be determined by the public with the help of an applaudimeter and will receive a special prize.

19:45

Introduction to the Bertaut-Prize

U. Heinemann (Max Delbrück Center for Molecular Medicine, Berlin, DE)

20:00

Solving problems leads to solving crystal structures

L. Reinhard (Department of Cell and Molecular Biology, Karolinska Institute, SE)

Committees

Welcome

Programme Overview

Venue Overview

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Scientific Programme

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Social Events

General Information

Sydney

08:30 – 09:30

Keynote Lecture Jan Pieter Abrahams

Chair: B. Spingler (Zurich, CH)

Electron nanodiffraction for structural biology

J.P. Abrahams (Biozentrum University of Basel, CH)

Singapore

08:30 – 09:30

Keynote Lecture Simon Parsons

Chair: A. Linden (Zurich, CH)

Understanding the driving forces of phase transitions in molecules

S. Parsons (University of Edinburgh, UK)

09:30 – 10:00

Coffee break

Focus Area 4 (SIG 7, 13)

Sydney

10:00 – 12:00

MS 38 Nanomaterials & graphene

Chairs: M. Woerle (ETH, Zürich, CH)

A. Gil-Mestres (University of Lisbon, PT)

10:00 MS38-01

Shape, Chemical and Crystalline Structure of Nanocrystals and their Impact on the Supercrystal Structure of Colloidal Superlattices

R. Lechner (Institut fuer Physik, Montanuniversitaet Leoben, AT)

10:30 MS38-02

Layered and 2D materials: electronic properties and structural instabilities from first principles

P. Ordejón (Institut Català de Nanociència i Nanotecnologia - ICN2, The Barcelona Institute of Science and Technology and CSIC, ES)

11:00 MS38-03

Preferred orientation of Li⁺ diffusion in nano-LiMnPO₄

N.H. Kwon (University of Fribourg, Chemistry department, Fribourg, CH)

11:20 MS38-04

X-ray studies on polymers and composites: the combination of 2D WAXS, SAXS and X-ray imaging techniques

A. Neels (Center for X-ray Analytics, Empa, Dübendorf, CH)

11:40 MS38-05

Nano- x-ray fluorescence of individual GaAs/InGaAs/GaAs core-shell nanowires grown by molecular beam epitaxy on silicon (111)

A. Al Hassan (Naturwissenschaftlich- Technische Fakultät der Universität Siegen, DE)

		Focus Area 1 (SIG 1)	Singapore
10:00 – 12:00		MS 11 Hybrid approaches and validation (X-ray and electron microscopy)	
		<i>Chairs: F. Rey (Pasteur Institute, FR) M. Botte (leadXpro AG, Villigen, CH)</i>	
10:00	MS11-01	How reliable are atomic models based on cryo-EM reconstructions? Improvements in model fitting and validation.	
		<i>P. Neumann (Department of Molecular Structural Biology, Institute for Microbiology & Genetics GZMB, Georg-August-Universität Göttingen, DE)</i>	
10:30	MS11-02	Cholesteryl esters are a new class of ligands for lipid antigen presentation by CD1c proteins	
		<i>I. Tews (Centre for Biological Sciences, Institute for Life Sciences B85, University of Southampton, UK)</i>	
11:00	MS11-03	Structure of the full-length VEGFR-1 extracellular domain in complex with VEGF-A	
		<i>S. Markovic-Mueller (leadXpro AG, PARK innovAARE, Villigen, CH)</i>	
11:20	MS11-04	Protein-ligand interaction energy for crystallographic model building and validation	
		<i>D. Beshnova (Hamburg Outstation, European Molecular Biology Laboratory, DE)</i>	
11:40	MS11-05	DipSpace and DipCheck: A Distance Geometry-Based Description of Protein Main-Chain Conformation	
		<i>J. Pereira (EMBL Hamburg, DE)</i>	
		Focus Area 2 (SIG 5, 11, 12)	Darwin
10:00 – 12:00		MS 21 Structural disorder and materials' properties at ambient and non-ambient conditions	
		<i>Chairs: D. Chernyshov (Swiss-Norwegian BeamLines at the European Synchrotron Radiation Facility, Grenoble, FR) V. Gavin (European Synchrotron Radiation Facility, Grenoble, FR)</i>	
10:00	MS21-01	Lattice dynamics and elastic properties from thermal diffuse scattering	
		<i>B. Wehinger (Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Villigen, CH)</i>	
10:30	MS21-02	3D Single Crystal Diffuse Scattering – Measurement and Interpretation	
		<i>H.-B. Bürgi (Department of Chemistry and Biochemistry, University of Berne, CH)</i>	

- 11:00 MS21-03 Guest – induced polymorphism and quenching of disorder in the Hofmann spin-crossover compound $\text{Fe}(\text{Pz})\text{Pt}(\text{CN})_4$ studied by *in-situ* powder diffraction.
C. Besnard (Laboratoire de cristallographie, University of Geneva, CH)
- 11:20 MS21-04 Structural disorder in spinel-like nanoparticles probed by total scattering
A. Cervellino (Swiss Light Source, Paul Scherrer Institut, Villigen, CH)
- 11:40 MS21-05 Local order in cadmium cyanide.
A. Simonov (Oxford University, UK)

Focus Area 1 (SIG 1)

Rio

10:00 – 12:00

MS 5 Structural information in drug design

*Chairs: M. Hennig (leadXpro AG, PARK INNOVAARE, Villigen, CH)
V. Mikol (Sanofi, Paris, FR)*

- 10:00 MS5-01 Structural elucidation of ligand binding sites in family B GPCRs and their application in drug discovery
A. Jazayeri (Heptares Therapeutics Ltd, Hertfordshire, UK)
- 10:40 MS5-02 Crystal structures of the human doublecortin C-terminal and N-terminal domains in complex with specific antibodies
A. Ruf (Roche, Pharma Research and Early Development (pRED), Basel, CH)
- 11:00 MS5-03 Combining “dry” co-crystallization with *in situ* diffraction to facilitate ligand screening by X-ray crystallography
G. Labesse (CNRS, Université de Montpellier, Centre de Biochimie Structurale, FR)
- 11:20 MS5-04 Crystal structure of HDAC6: insights into molecular assembly, selective inhibition and microtubule deacetylation
H. Gut (Friedrich Miescher Institute for Biomedical Research, Basel, CH)
- 11:40 MS5-05 Probing nucleotide-induced conformational changes and interaction studies of the GTPase EngA
C. Tomé (Institut de Biologie Structurale, Grenoble, FR)

		General Microsymposia	Osaka
10:00 – 12:00		MS 48 Crystallography in art and cultural heritage	
		<i>Chairs: A. Rafalska-Lasocha (Faculty of Chemistry Jagiellonian University, Krakow, PL) H. Stoeckli-Evans (Institute of Physics, University of Neuchâtel, CH)</i>	
10:00	MS48-01	MAKING GOLD: Recent Developments and New Perspectives	
		<i>A. Zürn (Artist Researcher based in Biel, CH)</i>	
10:30	MS48-02	Micro-XRPD, XRPD tomography and MA-XRPD: three related methods to better understand structural alterations in cultural heritage materials	
		<i>K. Janssens (University of Antwerp, Department of Chemistry, BE)</i>	
11:00	MS48-03	Crystallographic interpretation of mineral decompositions via Rietveld refinement strategy for clustering ancient ceramics	
		<i>M. Emami (Department of conservation and archaeology, Art University of Isfahan, Isfahan, IR)</i>	
11:20	MS48-04	Provenancing of clay-based pigments in paints using quantitative X-ray micro-diffraction analysis	
		<i>P. Bezdicka (Institute of Inorganic Chemistry of the CAS, Husinec-Rez, CZ)</i>	
		Focus Area 5 (SIG 6, 8, 9)	Samarkand
10:00 – 12:00		MS 46 Computational tools for theoretical chemistry in crystallography	
		<i>Chairs: M. Winn (Science and Technology Facilities Council, Swindon, UK) M. Lutz (Utrecht University, NL)</i>	
10:00	MS46-01	Recent Advancements in the Development of X-ray Constrained Wave Function Strategies	
		<i>A. Genoni (CNRS & Université de Lorraine, FR)</i>	
10:30	MS46-02	Synergistic ‘Substrate Activation’ and ‘Oxygen Activation’ in Salicylate Dioxygenase from QM/MM Simulations	
		<i>J. Keastner (University of Stuttgart, Institute for Theoretical Chemistry, DE)</i>	
11:00	MS46-03	Topological collections and knowledge bases for applications in crystal engineering of coordination compounds	
		<i>E. Alexandrov (Samara Center for Theoretical Materials Science, Samara State Aerospace University named after academician S.P. Korolyev (National Research University, RU)</i>	

11:20 MS46-04 **Harnessing the power of the Cambridge Structural Database in your own way: the CSD Python API**
A. Maloney (The Cambridge Crystallographic Data Centre, UK)

11:40 MS46-05 **An Enhanced Hirshfeld Test – Validating Atomic Vibrations in Crystal Structures**
J. Luebben (Heinrich-Heine-University Duesseldorf, DE)

Focus Area 1 (SIG 1)

Sydney

14:00 – 16:00

MS 6 Molecular machines and big complexes

*Chairs: M. Coll (Molecular Biology Institute of Barcelona (IBMB), Barcelona Science Park c/ Baldiri, ES)
C. Müller (European Molecular Biology Laboratory (EMBL), Heidelberg, DE)*

14:00 MS6-01 **Fuzzy Sarcomeric Z-disk Complex: α -Actinin-FATZ**
K. Djjinovic-Carugo (Department of Structural and Computational Biology, Max F. Perutz Laboratories, University of Vienna, AT)

14:30 MS6-02 **Macromolecular machines in genome maintenance**
T. Nicolas (Friedrich Miescher Institute for Biomedical Research Basel, CH)

15:00 MS6-03 **The Architecture of Fully Reducing Polyketide Synthases**
D. Herbst (Department Biozentrum, University of Basel, CH)

15:20 MS6-04 **Crystal structure of the 239 kDa nuclear export complex CRM1 – RanGTP – Snurportin1 – Nup214 – MBP**
R. Ficner (Department of Molecular Structural Biology, Institute for Microbiology and Genetics, GZMB, Georg-August-University Göttingen, DE)

15:40 MS6-05 **Cooperative Motion Analysis of group II chaperonins at single molecule level using nanocrystal and time-resolved diffraction measurement**
H. Sekiguchi (Japan Synchrotron Radiation Research Institute, JP)

		Focus Area 4 (SIG 7, 13)	Singapore
14:00 – 16:00		MS 37 Molecular compounds and MOFs at ambient conditions and under high pressure	
		<i>Chairs: F. Fabbiani (Georg-August-Universität Göttingen, DE) W. Queen (École polytechnique fédérale de Lausanne, Sion, CH)</i>	
14:00	MS37-01	The Effect of Pressure, Guest Uptake and Structural Flexibility on Porous Framework Materials	
		<i>S. Moggach (University of Edinburgh, UK)</i>	
14:30	MS37-02	Role of pressure transmitting media in structural transformations of molecular crystals at high pressures	
		<i>B. Zakharov (Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, RU)</i>	
15:00	MS37-03	Pressure induced chemisorption in isorecticular Metal Organic Frameworks	
		<i>P. Macchi (Department of Chemistry and Biochemistry, University of Bern, CH)</i>	
15:20	MS37-04	High-pressure effects in carbohydrate-based crystals	
		<i>E. Patyk (Department of Materials Chemistry, Adam Mickiewicz University, Poznań, PL)</i>	
15:40	MS37-05	A Series of Highly Stable Isorecticular Lanthanide Metal-Organic Frameworks with Tunable Luminescence Properties Solved by Rotation Electron Diffraction and X-ray Diffraction	
		<i>X. Zou (Department of Materials and Environmental Chemistry, Stockholm University, SE)</i>	
		Focus Area 4 (SIG 7, 13)	Darwin
14:00 – 16:00		MS 30 Hydrogen bonding from theory to applications	
		<i>Chairs: N. Bathori (Cape Peninsula University of Technology, Cape Town, ZA) L. Fábíán (University of East Anglia, Norwich, UK)</i>	
14:00	MS30-01	Crystal Engineering: From Form to Function	
		<i>M. Zaworotko (University of Limerick, IE)</i>	
14:30	MS30-02	Organic Hydrates: Chemistry, H-Bonding & Packing	
		<i>P. Wood (The Cambridge Crystallographic Data Centre, UK)</i>	
15:00	MS30-03	Gold as a hydrogen-bond acceptor	
		<i>C. Esterhuysen (Dept. Chemistry and Polymer Science, University of Stellenbosch, Matieland, ZA)</i>	

15:20 MS30-04 **Supramolecular reactivity in the solid state: Step-wise assembly of ternary cocrystals through hydrogen and halogen bonding**
F. Topić (Department of Chemistry, Nanoscience Center, University of Jyväskylä, FI)

15:40 MS40-05 **Hydrogen-bonded cocrystals of the drug metformin: From molecular interactions analysis to supramolecular synthesis and characterization of Met-bis(DCA), a pharmaceutical cocrystal with enhanced anti-leukemic activity**
P. Gilli (Department of Chemical and Pharmaceutical Sciences and Centre for Structural Diffractometry, University of Ferrara, IT)

Focus Area 2 (SIG 5, 11, 12)

Rio

14:00 – 16:20

MS 14 Biomineralogical crystallography and bioinspired inorganic materials

*Chairs: W. Schmahl (University of Munich, DE)
L. Fernández-Díaz (Institute of Geosciences UCM, CSIC), Madrid, ES)*

14:00 MS14-01 **Learning from Sea Shells – Bio-Inspired Approaches Toward Mesoscale Architectures in Functional Spinel Oxides**
A. Schenk (Institute of Polymer Chemistry, University of Stuttgart, DE)

14:30 MS14-02 **Complex biomimetic self-assembly in simple inorganic precipitation systems**
M. Kellermeier (Material Physics, BASF SE, DE)

15:00 MS14-03 **Biomimetic formation of calcite in intermixed gelatin/agarose hydrogels: Aggregate co-orientation and Mg content**
X. Yin (Department für Geo- und Umweltwissenschaften, Ludwig-Maximilians-Universität, Munich, DE)

15:20 MS14-04 **Polar ordering of macromolecular chains in biomimetic composite materials and natural tissues**
M. Sommer (Department of Chemistry and Biochemistry, University of Bern, Bern, CH)

15:40 MS14-05 **BioMOFs: are we getting alternative carriers for improved drug storage and release?**
S. Quaresma (Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Lisbon, PT)

16:00 MS14-06 **Energy dispersive white beam diffraction: Translating photon energy into the 3rd dimension for one-shot texture analysis**
H. Lichtenegger (Institute of Physics and Materials Science, University of Natural Resources and Life Science, Vienna, AT)

		Focus Area 3 (SIG 2, 3, 4)	Osaka
14:00 – 16:00		MS 22 Beyond multipolar refinement	
		<i>Chairs: A. Genoni (CNRS & Université de Lorraine, FR)</i> <i>S. Grabowsky (Universität Bremen Fachbereich, DE)</i>	
14:00	MS22-01	Quasi-harmonic Treatment of Thermal Effects on Electron Charge and Momentum Densities of Solids from <i>Ab initio</i> Calculations	
		<i>A. Erba (Chemistry Department, University of Torino, Torino IT)</i>	
14:30	MS22-02	Probability densities in different spaces: when multipolar-atom model is just not enough.	
		<i>J.-M. Gillet (Laboratoire SPMS, UMR CNRS 8580, CentraleSupélec, Université Paris-Saclay, FR)</i>	
15:00	MS22-03	Electron Density of a Layered Transition Metal Dichalcogenide	
		<i>H. Kasai (Faculty of Pure and Applied Sciences, TIMS and CiRfSE, University of Tsukuba, JP)</i>	
15:20	MS22-04	Experimental Electron Density of Low-Barrier Hydrogen Bonds in $H_3C_0(CN)_6$	
		<i>K. Tolborg (Center for Materials Crystallography, Department of Chemistry, Aarhus University, DK)</i>	
15:40	MS22-05	Electrostatic Potential of Dynamic Charge Densities	
		<i>C. Hübschle (Laboratory of Crystallography, University of Bayreuth, DE)</i>	
		Focus Area 5 (SIG 6, 8, 9)	Samarkand
14:00 – 16:00		MS 45 Measuring data quality	
		<i>Chairs: P. Evans (Medicinal Research Council, Cambridge, UK)</i> <i>A. Urzhumtsev (Université de Lorraine, Nancy, FR)</i>	
14:00	MS45-01	Processing and data quality in serial femtosecond crystallography	
		<i>T. White (Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, DE)</i>	
14:30	MS45-02	New ways to assess the quality of single and multiple (complete and partial) X-ray diffraction datasets	
		<i>K. Diederichs (Universität Konstanz, DE)</i>	
15:00	MS45-03	Empirical correction for resolution- and temperature-dependent errors caused by factors such as thermal diffuse scattering	
		<i>R. Herbst-Irmer (Institute of Inorganic Chemistry, Georg-August-University Göttingen, DE)</i>	

15:20 MS45-04 Background modelling in the presence of ice rings
J. Parkhurst (Diamond Light Source, UK)

15:40 MS45-05 At home accurate XRD measurements with an hybrid pixel X-ray detector: a comparison with CCD, APS-CMOS commercial detectors and theoretical model
C. Lecomte (Université de Lorraine, FR)

16:00 – 16:30 **Coffee break**

Sydney

16:30 – 17:30

Keynote Lecture Makoto Fujita

Chair: J. Bernstein (New York University, Abu Dhabi, AE)

Crystalline Sponge Method for Absolute Structure Determination

M. Fujita (University of Tokyo, JP)

Singapore

16:30 – 17:30

Keynote Lecture Olivier Thomas

Chair: U. Pietsch (Siegen, DE)

Mechanical properties of nanostructures in the light of synchrotron radiation

O. Thomas (Marseille, FR)

Sydney

17:30 – 18:30

Keynote Lecture Robert von Dreele

Chair: R. Cerny (Geneva, CH)

Structure solution GSAS-II

R. von Dreele (Argonne National Laboratory, US)

Singapore

17:30 – 18:30

Keynote Lecture Petra Fromme

Chair: C. Besnard (Geneva, CH)

Time-resolved femtosecond crystallography opens a new era in Structure Biology

P. Fromme (Arizona State University, Tempe, US)

Sydney

08:30 – 09:30

Keynote Lecture Werner Paulus

Chair: J. Schefer (Villigen, CH)

Transition metal oxides: from structural complexity and topotactic oxygen diffusion pathways to energy applications

W. Paulus (University of Montpellier, Montpellier, FR)

Singapore

08:30 – 09:30

Keynote Lecture Bob Cernik

Chair: A. Dommann (St. Gallen, CH)

X-ray colour diffraction imaging

B. Cernik (The Mill-B10b School of Materials, Manchester, UK)

09:30 – 10:00

Coffee break

Focus Area 1 (SIG 1)

Sydney

10:00 – 12:00

MS 9 Enzyme reactions and dynamics in crystals

Chairs: G. Schneider (Karolinska Institut, Stockholm, SE)

A. Pearson (University of Hamburg, DE)

10:00 MS9-01

Single Crystal Serial Crystallography to Capture Redox Enzyme Catalysis and Dynamics

M. Hough (School of Biological Sciences, University of Essex, Wivenhoe Park, Colchester, UK)

10:30 MS9-02

Time-Resolved Serial Femtosecond Crystallography On Photoswitchable Fluorescent Proteins

M. Weik (Institut de Biologie Structurale, Grenoble, FR)

11:00 MS9-03

Changes in metal coordination are required to regulate activity of bacterial phosphodiesterases, implicated in c-di-GMP regulated biofilm dispersal

A. Hutchin (Centre for Biological Sciences, University of Southampton, UK)

11:20 MS9-04

pH Dependent conformational change of bound maltose observed in the crystal of β -amylase at room temperature.

B. Mikami (Kyoto University, JP)

11:40 MS9-05

Lipidic cubic phase injector is a viable crystal delivery system for time-resolved serial crystallography

P. Nogly (Laboratory for Biomolecular Research, Paul Scherrer Institute, Villigen, CH)

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Focus Area 4 (SIG 7, 13)

Singapore

10:00 – 12:00

MS 33 Hot structures of small molecules

*Chairs: A. Roodt (University of the Free State, Bloemfontein, ZA)
M. Đaković (Ruđer Bošković Institute, Zagreb, HR)*

10:00 MS33-01

How to fill MOFs with different flavours

A. Bacchi (Dipartimento di Chimica, Università di Parma, IT)

10:30 MS33-02

Solid-state transition-metal photoactive materials - tracing structure-property relationships via combined spectroscopic and crystallographic approaches

K. Jarzemska (Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, PL)

11:00 MS33-03

Structural differences in enantiopure and racemate organometallic complexes. Application to $[(\eta^5\text{-C}_5\text{Me}_5)\text{RhCl}(\text{PN})]^n$ complexes

F. Lahoz (Institute for Chemical Synthesis and Homogeneous Catalysis (ISQCH), CSIC – University of Zaragoza, ES)

11:20 MS33-04

Expanding the horizons of sky blue nitrosocarboranes

G. Rosair (Institute of Chemical Sciences, Heriot Watt University, Edinburgh, UK)

11:40 MS33-05

Silolyl-FeCp complexes: is there a way to sila-ferrocene?

P. Bombicz (Institute of Organic Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, HU)

Focus Area 1 (SIG 1)

Darwin

10:00 – 12:00

MS 1 SAXS in Structural Biology

*Chairs: D. Svergun (European Molecular Biology Laboratory, Hamburg, DE)
B. Vestergaard (University of Copenhagen, DK)*

10:00 MS1-01

Disentangling Structural Heterogeneity in Highly Disordered Biomolecular Complexes

P. Bernadó (Centre de Biochimie Structurale, Montpellier, FR)

10:30 MS1-02

Enzyme dynamics visualized by SAXS

D. Albesa-Jové (Structural Biology Unit - CIC bioGUNE, Derio, ES; IKERBASQUE, Basque Foundation for Science, Bilbao, ES)

11:00 MS1-03

From size exclusion to HIS-tags: Increasing sample purity for BioSAXS

M. Brennich (ESRF-The European Synchrotron, Grenoble, FR)

- 11:20 MS1-04 High throughput and time resolved BioSAXS at the P12 beamline of EMBL Hamburg
C. Blanchet (EMBL Hamburg, DE)
- 11:40 MS1-05 Structural insight into host cell surface retention of a 1.5-MDa bacterial ice-binding adhesin
S. Guo (Queen's University, Kingston, CA)
- 10:00 – 12:00 Focus Area 5 (SIG 6, 8, 9) Rio
MS 41 The use of X-ray, electron and neutron scattering in nanoscience
Chairs: J. Stangl (Johannes Kepler University, Linz, AT)
C. Lehmann (Max Planck Institut für Kohlenforschung, Mülheim, DE)
- 10:00 MS41-01 Complementarity of TEM to bulk diffraction techniques for structures at nanoscale
J. Hadermann (University of Antwerp, BE)
- 10:30 MS41-02 X-ray imaging of single nano-structures: from focused beams to coherent imaging and ptychography
V. Favre-Nicolin (ESRF-The European Synchrotron, Grenoble, FR)
- 11:00 MS41-03 Twin domain mapping in topological insulator Bi_2X_3 (X=Se,Te) by scanning XRD and electron backscattering diffraction
D. Kriegner (Charles University in Prague, Faculty of Mathematics and Physics, CZ)
- 11:20 MS41-04 Investigation of layered and porous nanomaterials by diffraction tomography, simulations and HRTEM
Y. Krysiak (Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg University, Mainz, DE)
- 11:40 MS41-05 Strain mapping in Ge microstructures using X-ray white beam Laue microdiffraction
S. Tardif (CEA-INAC, FR)
- 10:00 – 12:00 Focus Area 2 (SIG 5, 11, 12) Osaka
MS 17 Minerals, materials and polymorphs
Chairs: H. Hope (University of Oslo, NO)
E. Nauha (University of Lincoln, UK)
- 10:00 MS17-01 Understanding the polymorphic phase transitions of linear amino acids using *in situ* characterisation
M. Smets (Institute for Molecules and Materials, Radboud University, NL)

- 10:30 MS17-02 Structural studies of M-type ferrites used as template layers for the growth of oriented Y-type ferrites through chemical solution deposition method
R. Kuzel (Charles University in Prague, Faculty of Mathematics and Physics, CZ)
- 11:00 MS17-03 Pore Shape Determination in Mesoporous Ordered Silica Films
G. Popovski (Montanuniversitaet Leoben, AT)
- 11:20 MS17-04 Control of porosity through temperature and pressure
J. Gertenbach (PANalytical BV, Almelo, NL)
- 11:40 MS17-05 Crystallographic reactions in shape memory alloys
O. Adiguzel (Firat University, Department of Physics, TR)

Focus Area 3 (SIG 2, 3, 4)

Samarkand

10:00 – 12:00

MS 25 Quasicrystal and approximant: structure and properties

*Chairs: C. Pay Gomez (Uppsala University, SE)
E. Gaudry (Université de Lorraine, FR)*

- 10:00 MS25-01 Computational Self-Assembly of Complex Crystals
J. Dshemuchadse (Department of Chemical Engineering, University of Michigan, Ann Arbor, US)
- 10:30 MS25-02 Magnetic properties of Au-based Tsai-type approximants
R. Tamura (Department of Materials Science and Technology, Tokyo University of Science, JP)
- 11:00 MS25-03 Atomic structure and phason modes of the Sc-Zn icosahedral quasicrystal
M. de Boissieu (Univ. Grenoble Alpes, SIMAP, FR)
- 11:20 MS25-04 The oxidic two-dimensional quasicrystal and its approximant: X-ray analysis of the atomic structure
H. Meyerheim (Max-Planck-Institut f. Mikrostrukturphysik, DE)
- 11:40 MS25-05 Z-module dislocations in complex intermetallic phases
A. Sirindil (IRCP Chimie-Paristech, FR)

		Focus Area 1 (SIG 1)	Sydney
14:00 – 16:00		MS 8 Membranes and membrane interacting proteins	
		<i>Chairs: H. Remaut (VIB Laboratory of Structural and Molecular Microbiology, Brussel, BE) M. Bublitz (University of Oxford, UK)</i>	
14:00	MS8-01	Gating MscS: Structural basis of mechanosensation and the role of lipids in ion channel regulation	
		<i>C. Pliotas (Biomedical Sciences Research Complex, School of Chemistry, University of St Andrews, St Andrews, UK)</i>	
14:30	MS8-02	The structure and function of calcium activated lipid scramblases and ion channels of the TMEM16 family	
		<i>R. Dutzler (Dept. of Biochemistry, University of Zurich, CH)</i>	
15:00	MS8-03	Crystal Structure of Mitochondrial Respiratory Complex I	
		<i>C. Wirth (Institute for Biochemistry and Molecular Biology, ZBMZ, BIOS Centre for Biological Signalling Studies, University of Freiburg, DE)</i>	
15:20	MS8-04	Architecture and regulation of a redox-driven Na⁺-pump from the pathogen <i>Vibrio cholerae</i>	
		<i>G. Fritz (University of Freiburg, Institute of Neuropathology, DE)</i>	
15:40	MS8-05	Molecular basis of secondary multidrug transport by X-ray crystallography	
		<i>V. Debruycker (Université libre de Bruxelles – Université d'Europe, Brussels, BE)</i>	
		Focus Area 4 (SIG 7, 13)	Singapore
14:00 – 16:00		MS 29 Molecular interactions in crystal packing and molecular assemblies	
		<i>Chairs: D. Braun (University of Innsbruck, AT) K. Rissanen (University of Jvaskyla, FI)</i>	
14:00	MS29-01	The silver bond	
		<i>C.H. Görbitz (Departement of Chemistry, University of Oslo, NO)</i>	
14:30	MS29-02	Molecular interactions and configurational entropy determining the macroscopic polar state of molecular crystals	
		<i>J. Hulliger (University of Bern, Department of Chemistry and Biochemistry, CH)</i>	
15:00	MS29-03	One-dimensional chains in PGM complexes- understanding metallophilic interactions	
		<i>C. Pretorius (University of the Free State, ZA)</i>	

15:20 MS29-04 Insights into molecular spreading and bridging in chromosome condensation from the complex structure of Spo0J and *par*
Y.-J. Sun (National Tsing Hua University, Institute of Bioinformatics and Structural Biology, TW)

15:40 MS29-05 Crystal-Packing and Spin-CrossOver in some Molecular Solids. Trends and new Features.
P. Guionneau (CNRS, Univ. Bordeaux, Pessac, FR)

Focus Area 3 (SIG 2, 3, 4)

Darwin

14:00 – 16:00

MS 24 Inorganic and metal-organic magnetic structures

*Chairs: G. Eickerling (University of Augsburg, DE)
D. Schaniel (CRM2 Université de Lorraine Nancy, FR)*

14:00 MS24-01 Elucidating the magnetic behaviour of a unique linear Fe(II)-complex using the electron density
J. Overgaard (Department of Chemistry, Aarhus University, DK)

14:30 MS24-02 Spin, charge and momentum densities of YTiO₃ perovskite
M. Souhassou (CRM2 Université de Lorraine Nanc, FR)

15:00 MS24-03 New antiferromagnets [CuX(py_z)₂](BF₄) with X = Cl and Br.
M. Kubus (Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Villigen, CH)

15:20 MS24-04 Structural and magnetic properties of the low dimensional fluoride β-FeF₃·3H₂O
S. Prugovecki (PANalytical B.V., NL)

15:40 MS24-05 Synthesis and Characterization of Asymmetric Tetranuclear Nickel Chains without Disordered Ligand Phenomenon in Crystallography
L.-H. Tsou (Department of Chemistry, National Taiwan University, Taipei, TW)

Focus Area 2 (SIG 5, 11, 12)

Rio

14:00 – 16:00

MS 16 Structure-property relationships in high pressure crystallography

*Chairs: A. Grzechnik (RWTH Aachen University, DE)
P. Attfield (University of Edinburgh, UK)*

14:00 MS16-01 The large-volume press at ID06 of the ESRF for structure-properties research at extreme conditions
W. Crichton (ESRF, FR)

14:30 MS16-02 New chemistry of hydrogen-rich systems uncovered with the help of extreme conditions
Y. Filinchuk (Université Catholique de Louvain, BE)

- 15:00 MS16-03 **New coordination chemistry and properties revealed by high pressure crystallography**
A. Blake (University of Nottingham, UK)
- 15:20 MS16-04 **Pressure-Tuning of Guest Species and Magnetic Response in Mn- and Fe-based Formate Frameworks**
S. McKellar (EaStCHEM School of Chemistry and the Centre for Science at Extreme Conditions, University of Edinburgh, UK)
- 15:40 MS16-05 **Structural basis for sensitivity to molecular oxygen of oxidases and fluorescent proteins investigated by high pressure crystallography**
B. Lafumat (European Synchrotron Radiation Facility (ESRF), FR)

Focus Area 5 (SIG 6, 8, 9)

Osaka

14:00 – 16:00

MS 40 New detectors for high energy x-ray applications

Chairs: H. Graafsma (DESY Photon Science, Hamburg, DE)
L. Strüder (PNSensor GmbH, Munich, DE)

- 14:00 MS40-01 **Hard X-ray photon counting with “LAMBDA” high-Z detectors**
D. Pennicard (DESY, DE)
- 14:30 MS40-02 **White beam Laue diffraction of polycrystalline materials using 3D energy dispersive detector (pnCCD)**
U. Pietsch (University of Siegen, Department of Physics, DE)
- 15:00 MS40-03 **High-resolution XRD investigation of SiGe/Si heterostructures for novel X-ray detectors**
I. Marozau (CSEM SA, CH)
- 15:20 MS40-04 **PILATUS3 R CdTe large-area detectors for laboratory applications**
M. Müller (DECTRIS Ltd., CH)
- 15:40 MS40-05 **Modern CPAD Detector Technology for Higher Energy X-rays**
H. Ott (Bruker AXS GmbH, Karlsruhe, DE)

General Microsymposia

Samarkand

14:00 – 16:00

MS 50 History of ECA, history of crystallography: contributions to and of crystallography

*Chairs: M. Kaftory (Technion Israel Institute of Technology, Haifa, IL)
P. Paufler (Saxon Academy of Sciences in Leipzig, Dresden, DE)*

14:00 MS50-01

History of crystallography in Switzerland

D. Schwarzenbach (École Polytechnique Fédérale, Lausanne, CH)

14:30 MS50-02

Crystallography in the Courtroom

J. Bernstein (New York University Abu Dhabi, AE)

15:00 MS50-03

Absolute structure

H. Flack (University of Geneva, CH)

15:20 MS50-04

History of Direct Methods: a personal account

D. Viterbo (Università del Piemonte Orientale, DISIT, Alessandria, IT)

15:40 MS50-05

The Artwork of Maurits C. Escher and Crystallography

H. Schenk (University of Amsterdam, NL)

16:00 – 16:30

Coffee break

Sydney

16:30 – 17:30

Keynote Lecture Marek Grzelczak

Chair: H.-B. Bürgi (Zurich, CH)

Self-assembly of nanoparticles through hydrophobic interactions

M. Grzelczak (CIC biomaGUNE, San Sebastian, Ikerbasque, Basque Foundation for Science, ES)

Singapore

16:30 – 17:30

Keynote Lecture Martin Schmidt

Chair: A. Neels (Dübendorf, CH)

New methods for structural investigations of nanocrystalline and amorphous organic compounds

M. Schmidt (University of Frankfurt, DE)

Sydney

17:30 – 18:30

Plenary Lecture Jean-Marie Lehn

Chair: K. M. Fromm (Fribourg, CH)

Self-Organization-driven Supramolecular Chemistry and Adaptive Chemistry

J.-M. Lehn (ISIS, Université de Strasbourg, FR)

18:30 – 19:30

ECM Closing Ceremony and Poster Prizes

Chairs: K. M. Fromm (Fribourg, CH)

P. Macchi (Berne, CH)

Award ceremony of the poster prizes at ECM-30

Invitation to ECS-4

J. Lipkowski (Warsaw, PL)

Invitation to the ECM-31

S. Garcia-Granda (Oviedo, ES)

Closing words of the ECM-30

K. M. Fromm (Fribourg, CH)

P. Macchi (Berne, CH)

A. Bacchi (Parma, IT)

Crystallographic Software Fayre

At the 30th European Crystallographic Meeting in Basel there will be again a Software Fayre, where authors of academic and/or open-source software can present their new developments. The Software Fayre will be held from Monday, 29 August 2016 until Thursday, 1 September 2016 during the lunch break hours (12:00 – 14:00). It will be in lecture room Darwin at the Congress Center Basel.

During the Tutorial Sessions, authors will demonstrate the features of their software on one or more practical examples.

Organiser: Martin Lutz (m.lutz@uu.nl)

Venue: Congress Center Basel, Room Darwin

Programme

Monday, 29 August 2016

Software Fayre

- 12:30 – 13:00 Tutorial Session
"Charge density refinement and intermolecular contacts analysis with MoProSuite package"
(*Christian Jelsch*)
- 13:00 – 13:30 Tutorial Session
"Disordered Structure Refinement DSR"
(*Daniel Kratzert*)

Tuesday, 30 August 2016

Software Fayre

- 12:30 – 13:00 Tutorial Session
"HKL2MAP"
(*Fabio Dall'Antonia*)
- 13:00 – 13:30 Tutorial Session
"SUNBIM: a package for X-ray imaging of nano and biomaterials using SAXS, WAXS, GISAXS and GIWAXS techniques"
(*Dritan Siliqi*)
- 13:30 – 14:00 Tutorial Session
"Topological analysis with ToposPro"
(*Eugeny Alexandrov*)

Special Meetings

Wednesday, 31 August 2016 Software Fayre

- 13:00 – 13:30 Tutorial Session
“MrBUMP”
(Dan Rigden)
- 13:30 – 14:00 Tutorial Session
“AMPLE”
(Dan Rigden)

Thursday, 1 September 2016 Software Fayre

- 12:00 – 12:30 Tutorial Session
“Eval15”
(Martin Lutz)
- 12:30 – 13:00 Tutorial Session
“CrystFEL”
(Thomas White)
- 13:00 – 13:30 Tutorial Session
“OnDA (Online Data Analysis)”
(Valerio Mariani)
- 13:30 – 14:00 Tutorial Session
“ARCIMBOLDO”
(Claudia Millan Nebot)

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Special Meetings

Committee and SIG Meetings

Sunday, 28 August 2016 Committee and SIG Meetings

13:00 – 14:00 ECA Executive Committee Meeting Osaka

Monday, 29 August 2016 Committee and SIG Meetings

12:00 – 13:00 SIG 1 Meeting Singapore
SIG 3 Meeting Samarkand
SIG 7 Meeting Boston 3

12:00 – 14:00 ECA Council 1 Meeting Osaka

13:00 – 14:00 SIG 4 Meeting Samarkand
SIG 5 Meeting Singapore
SIG 9 Meeting Rio

Tuesday, 30 August 2016 Committee and SIG Meetings

12:00 – 13:00 SIG 12 Meeting Rio

12:00 – 14:00 ECM-31 Programme Committee Meeting Osaka

13:00 – 14:00 GIG 3 Meeting Rio

Wednesday, 31 August 2016 Committee and SIG Meetings

12:00 – 13:00 SIG 11 Meeting Sydney
GIG 1 Meeting Osaka

12:00 – 14:00 ECA Council 2 Meeting Samarkand

12:00 – 14:00 General Assembly SGK/SSCr Rio

13:00 – 14:00 SIG 2 Meeting Osaka
SIG 13 Meeting Singapore

Thursday, 1 September 2016 Committee and SIG Meetings

12:00 – 13:00 SIG 6 Meeting Rio

12:00 – 14:00 ECA Executive Committee meets SIGs Osaka

13:00 – 14:00 ECA Council 3 Meeting Singapore
GIG 2 Scientific Committee Meeting Samarkand

Session	Date of Poster Session	Poster Mounting Time	Presentation Time	Poster Removal Time
I	Monday, 29 August 2016	29 August 07:30–10:00	29 August 17:30–19:00	30 August 14:00–15:00
II	Tuesday, 30 August 2016	30 August 15:00–16:30	30 August 17:30–19:00	1 September 16:30–17:30

Poster Session 1

- MS 1
- MS 2
- MS 3
- MS 4
- MS 7
- MS 9
- MS 11
- MS 13
- MS 14
- MS 15
- MS 17
- MS 19
- MS 22
- MS 24
- MS 25
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- MS 28
- MS 31
- MS 32
- MS 38
- MS 41
- MS 44
- MS 46
- MS 48

Poster Session 2

- MS 5
- MS 6
- MS 8
- MS 10
- MS 12
- MS 16
- MS 18
- MS 20
- MS 21
- MS 23
- MS 29
- MS 30
- MS 33
- MS 34
- MS 35
- MS 36
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- MS 39
- MS 40
- MS 42
- MS 43
- MS 45
- MS 47
- MS 49
- MS 50

Instructions for poster presentations

All information about the poster exhibition is available at the poster desk on-site.

Poster Prizes

Participants can apply for the following poster prizes. Application is done simply by hanging sticker(s) of the desired poster prize(s) above your poster. Stickers will be provided at the poster desk on-site.

The ECA will establish a panel of independent judges who will assess the posters, and the poster prizes will be presented at the ECM-30 Closing Ceremony on Thursday, 1 September 2016 at 18:30 in lecture room Sydney.

1. Protein Data Bank in Europe Poster Prize

The best poster submitted by a student and describing macromolecular structure.

2. RCSB Protein Data Bank Poster Prize

The best student poster related to macromolecular crystallography.

3. 3 CCDC Poster Prizes for Younger Scientists

Original research in the field of chemical crystallography or the application of crystallographic information to structural chemistry. This definition shall include advances in instrumental, experimental, theoretical or computational techniques that contribute to this field. Candidates for CCDC Poster Prizes shall not be more than 35 years of age on 1st January of the year in which the Meeting is held, and should normally be the first named author on the poster.

4. SIG 4 Electron Crystallography Poster Prize sponsored by Calidris

Poster about Electron Crystallography.

5. SIG 4 Electron Crystallography Poster Prize sponsored by NanoMEGAS

Poster about Electron Crystallography.

6. SIG 6 Jacek Grochowski Poster Prize sponsored by SRS Daresbury Laboratory and the University of Manchester

This Prize is given in memory of Professor Jacek Grochowski who was greatly involved in SIG 6 and in ECA and is open to all relevant contributions in the domains of instrumentation and experimental techniques.

7. IUCr Journals Poster Prizes

The IUCr Executive Committee is pleased to continue the series of IUCr Journals awards to be presented at meetings of the Regional Associates. A prize will be awarded to the best poster from a graduate or undergraduate student in each of the following three categories: structural biology, chemistry and applied crystallography, and will consist of an IUCr Journals open-access voucher, a copy of A Little Dictionary of Crystallography and a certificate.

8. Oxford Cryosystems Low Temperature Prize

Any crystallographic study with an emphasis on temperature effects.

9. FEBS Journal Poster Prize

Crystallography in Biochemistry

10. Structural Dynamics Poster Prize sponsored by The AIP Publishing/ACA Journal Structural Dynamics

For excellence in research on dynamics of molecular, protein and materials structure, enabled by the emerging new instruments (e.g. XFELs, electron sources, etc.) and new experimental and theoretical methodologies. It is open to students (graduate and undergraduate) and post-docs.

11. Garland Science Poster Prize

Poster must display electron density as primary evidence for any ligand or part of the structure discussed and important for the story.

12. Swiss Crystallographic Association Poster Prizes for Young Scientists

The Swiss Society of Crystallography is pleased to announce 5 prizes for the best posters presented at ECM-30. Applications from all poster presenters are welcome, in particular from younger scientists.

13. SIG12 Poster Prize “Crystallography of Functional Materials” sponsored by STOE & Cie. GmbH (Darmstadt, Germany)

Any student before completing a PhD.

Opening Ceremony & Welcome Reception

The Opening Ceremony will be held on Sunday, 28 August 2016 from 17:00 until 19:00 in lecture room Sydney in the Congress Center Basel, followed by a Welcome Reception.

Young Crystallographers Mixer

The Young Crystallographers Mixer for students will be held on Monday, 29 August 2016 from 20:30 onwards at the Bar Rouge. Pre-registration is required.

The Mixer is open to delegates who qualify for membership of the European Young Crystallographers Group. This includes not only students but postdoctoral fellows and other younger scientists up to an age limit of 35 years. 1 free drink per participant, snacks and DJ entertainment will be provided.

Address: Bar Rouge, Messeplatz 10, Basel, Switzerland

Science Slam and Bertaut Prize Ceremony

The first ever ECM-Science Slam will be held on Tuesday, 30 August at 19:00 in lecture room Sydney where 5-6 participants will present their research in an entertaining 3-minutes talk. The Bertaut Prize Ceremony will take place immediately afterwards in the same room.

ECM-30 Conference Dinner

The official ECM-30 Conference Dinner will take place on Wednesday, 31 August 2016 from 19:00 onwards at Switzerland's oldest and largest zoo. Basel Zoo has been mentioned by the Forbes magazine in 2015 as one of the best zoos worldwide with regards to contribution to wildlife.

Before the dinner (from 18:00 – 19:00), you have the possibility to join one of the tours through the different areas of the zoo (vivarium, etosha house, bird's house, monkeys etc.). The dinner will take place in the recently renovated restaurant of the Basel Zoo, in the middle of the animal compounds, with view on different animal compounds.

Address: Zoo Basel, Binningerstrasse 40, Basel, Switzerland

Phone: +41 58 206 28 20 (Congress Secretariat)

Tram line 10, tram stop "Zoo"

Last trams back to Messeplatz: 23:12 / 23:27 / 23:57

Registration: Pre-registration is required

Fee: CHF 90.- per person



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Tours story of pharma industry in Basel

Roche

Monday, 29 August 2016, 14:00 – approx. 15:30

Tuesday, 30 August 2016, 10:00 – approx. 11:30

Wednesday, 31 August 2016, 14:00 – approx. 15:30

The tour at the Roche site gives an insight into the history of the company, the main drug molecules discovered and developed. In addition a number of buildings at the campus are visited and architectural aspects as well as future site development plans.

Registration: Pre-registration is required

Fee: Free of charge (included in congress registration)

Meeting Point: Main Entry Roche Campus, Grenzacherstrasse 214,
Bau 74, Basel, Switzerland

Novartis

Tuesday, 30 August 2016, 15:50 – approx. 18:15

The new Novartis Campus, a place of knowledge, innovation and encounter. First-class architecture and outstanding design are creating a modern and highly original workplace in the heart of the city. The tour will give you a first impression.

Registration: Pre-registration is required

Fee: Free of charge (included in congress registration)

Meeting Point: Main Entry Novartis Campus, Fabrikstrasse 2,
Main Entrance, Basel, Switzerland

Historical evening walk through Basel

Tuesday, 30 August 2016, 19:30 – approx. 21:00

You will follow on the traces of the famous Basel mathematicians, Euler and Bernoulli. This non-traditional historic tour through Basel will lead you to places which are not necessarily found in the classical city guides, and you will learn about Basel of the 18th century.

Registration: Pre-registration is required

Fee: Free of charge (included in congress registration)

Meeting Point: Münsterplatz, Basel, Switzerland

For detailed instructions how to get there please contact the secretariat on-site.

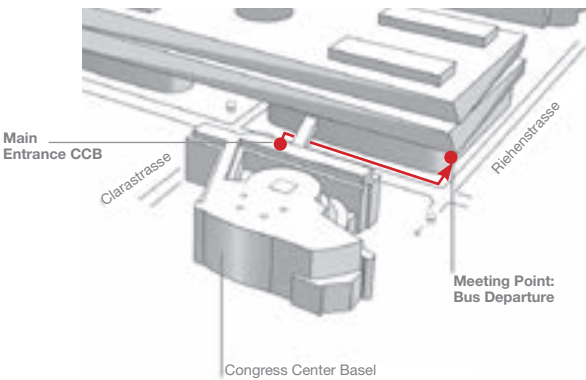
Visit of Free Electron Laser SwissFEL

Excursion to the construction site of the SwissFEL. The Paul Scherrer Institute is constructing a new scientific large-scale facility – the SwissFEL X-ray free-electron laser. This will provide new opportunities for cutting-edge Swiss research. The SwissFEL is scheduled to go into operation at the end of 2016.

Number of participants is limited to 90 and they will be accepted on a first-come-first-served basis. Applicants are kindly asked to book their own accommodation in Basel. Registration fee does not include lunch at the PSI.

Preliminary programme of the excursion:

- 09:00 Departure from Basel by bus (see plan below)
- 10:15 – 10:30 Arrival at PSI (Educational Center OSGA)
- 10:30 – 10:50 Welcome address (OSGA)
- 10:50 – 13:00 Excursions on the SwissFEL site
- 13:00 – 14:00 Lunch at the OASE restaurant (self-service, not included)
- 14:00 – 14:20 Possibility to attend the PSI visitors' center PSI-Forum
- 14:30 Departure of the bus back to Basel
- ~ 16:00 Arrival to Basel



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Abstract Publication

All accepted abstracts (incl. Late Breaking abstracts) are published on the ECM-30 website and online in the journal *Acta Crystallographica Section A*.

ATM

An ATM is located outside the Congress Center on the left hand of the main entrance. VISA and MasterCard are accepted.

Badges

Access to all scientific sessions is only possible with your personal badge. Please always wear your badge! CHF 30.- will be charged for replacement of a lost badge.

Cloakroom

A cloakroom is available on the ground floor during the secretariat opening hours and can be used free of charge. Please note that the cloakroom is unguarded and on your own risk. The Congress Center Basel / Messe Schweiz does not take any responsibilities for lost items.

Coffee & Lunch Breaks

Lunch is served between 12:00 – 13:00 in the exhibition area on the 2nd floor from Monday – Thursday free of charge. Coffee is available from Monday to Thursday in the mornings from 09:30 – 10:00 and in the afternoons from 16:00 – 16:30.

Exhibition (Foyer CCB, 2nd floor) Opening Hours

Sunday, 28 August 2016	17:00 – 21:00
Monday, 29 August 2016	08:00 – 19:00
Tuesday, 30 August 2016	08:00 – 19:00
Wednesday, 31 August 2016	08:00 – 18:45
Thursday, 1 September 2016	08:00 – 19:00

Insurance

The meeting organizer cannot accept liability for personal injuries sustained, or for loss or damage of property, either during, or as a result of the meeting. Please check the validity of your insurance.

Internet Corner

Internet terminals are located in the exhibition area and are available to all congress participants during the opening hours of the exhibition. An attendee list (names and provenance) can be viewed at the internet terminals.

Parking

Parking Messe Basel, Riehenstr. (open 24 hours), CHF 50/day (use public transportation instead). No tickets are sold at the secretariat.

Registration / Secretariat Opening Hours

Sunday, 28 August 2016	16:00 – 19:30
Monday, 29 August 2016	07:30 – 18:00
Tuesday, 30 August 2016	08:00 – 19:30
Wednesday, 31 August 2016	08:00 – 18:45
Thursday, 1 September 2016	08:00 – 19:30

Responsibility

The participant acknowledges that she / he has no right to lodge damage claims against the organisers should the holding of the congress be hindered or prevented by unexpected political or economical events or generally by “force majeure”, or should the non-appearance of speakers or other reasons necessitate programme changes. With her / his registration, the participant accepts this proviso.

Speakers Service Centre (SSC)

The SSC is located close to all lecture halls. All speakers are kindly asked to hand in their PowerPoint presentation at the SSC at least 1 hour before the start of the session.

Venue

The conference takes place at the Congress Center Basel.

Messeplatz 21
4058 Basel / Switzerland
Phone: +41 58 206 28 20

WLAN

Free wireless-LAN is available throughout the whole congress center.



**24th Congress and General Assembly
of the International Union of Crystallography
Hyderabad International Convention Centre
21 - 28 August 2017, Hyderabad, India**

www.iucr2017.org



Plenary Speakers

- Susumu Kitagawa
- John Spence
- Giacomo Chiari

Keynote Speakers

- Simon J.L. Billinge
- Michael Groll
- Massimo Nespolo
- Janet Smith
- Vladislav Blatov
- John Helliwell
- Sakura Pascarelli
- Dietmar Stalke
- Dario Braga
- Richard Henderson
- Vanessa Peterson
- Sriram Subramaniam
- David Bryce
- Jurg Hulliger
- Ingrid J. Pickering
- Dmitri Svergun
- Jean Marc Castera
- Dmitry Khalyavin
- Giuseppe Resnati
- Nigel Unwin
- Neil Champness
- Matteo Leoni
- Robin Rogers
- Hao Wu
- Henry Chapman
- Ron Lifshitz
- Bernhard Rupp
- Vittal Yachandra
- Jon Eggert
- Hartmut Luecke
- Leonid Sazanov
- Jim De Yoreo
- Song Gao
- Wladek Minor
- Adriana Serquis
- Jihong Yu
- Juri Grin
- Ashwini Nangia
- Toshiyuki Shimizu
- Xiaodong Zou

