

DGK 2012

100 Years of X-Ray Diffraction

Laue Day and 20th Annual Meeting of the
German Crystallographic Society (DGK)



12–15 March 2012

MUNICH

An international conference commemorating
the discovery of X-Ray diffraction by
Max von Laue, Walter Friedrich and
Paul Knipping at LMU Munich in 1912

PROGRAMME



2x
intensity
Nova Source

Smarter, Faster, Brighter

With double the Cu X-ray intensity, CSD cell check tools and real-time email notifications, the Agilent SuperNova is better than ever. Find out more at

www.agilent.com/chem/smarter



© Agilent Technologies, Inc. 2012

The Measure of Confidence



Agilent Technologies

Organisation and Imprint	4
Welcome Note	6
General Information	
Venue and Date, Conference Website, Registration	7
Arrival, Travel and Parking	8
Cooperation with German Railways	9
City Map	10
Certificate of Attendance, Poster Prizes, Name Tag, Evaluation, Check-In	12
Media Check-In, Industrial Exhibition, Opening Hours	12
General Tips for Authors and Presenters	14
Sponsors and Media Cooperations	16
Exhibitors	17
Social and Cultural Programme	18
Exhibition Plan	20
Programme Overview	
Sunday, 11 March 2012	21
Monday, 12 March 2012	21
Tuesday, 13 March 2012	22
Wednesday, 14 March 2012	23
Thursday, 15 March 2012	24
Overview Plenary Talks	25
Scientific Programme	
Laue Day • Monday, 12 March 2012	26
Tuesday, 13 March 2012	27
Wednesday, 14 March 2012	32
Thursday, 15 March 2012	37
Poster Overview	42
Poster	44
Workshop	
Thursday, 15 March 2012	62
Friday, 16 March 2012	62
Index of Presenting Authors and Chairs	64
General Terms and Conditions	68

Venue and Date

Ludwig-Maximilians-University Munich
Geschwister-Scholl-Platz 1
80539 Munich (DE)
12–15 March 2012

Conference Website

www.dgk-conference.de

Organiser

Deutsche Gesellschaft für Kristallographie (DGK)
www.dgkristall.de

Conference Chair

Prof. Wolfgang W. Schmahl
Ludwig-Maximilians-University Munich
Department of Earth and Environmental Sciences
Theresienstraße 41
80333 Munich (DE)
wolfgang.schmahl@lrz.uni-muenchen.de

Local Organising Committee

Patrick Cramer	Sohyun Park
Peter Gille	Rossitza Pentcheva
Erika Griesshaber	Winfried Petry
Guntram Jordan	Wolfgang W. Schmahl
Martin Meven	Wolfgang Schnick

Conference Organisation

Conventus Congressmanagement & Marketing GmbH
Felix Angermüller
Carl-Pulfrich-Straße 1
07745 Jena (DE)
Phone +49 (0)3641 311 63 01
Fax +49 (0)3641 311 62 41
felix.angermueller@conventus.de
www.conventus.de

Design/Layout

Layout	www.krea.tif-design.de
Circulation	500
Editorial Deadline	1 February 2012

SEIFERT Galaxy XRD L

Anwendungen

- Einkristallorientierungsbestimmung mit Laue-Technik
- Turbinenschaufeln für Flugturbinen und zur Energieerzeugung
- Bestimmung der relativen Kornorientierung



Überlagerung der berechneten Lauepunkte



LAUE-Software

- Automatische Punktsuche im Laue-Bild
- Automatische Orientierungsbestimmung von den gefundenen Lauepunkten
- Berechnung der theoretisch möglichen Lauepunkte auf Basis der gefundenen Lösung
- Überlagerung der berechneten mit den gemessenen Lauepunkten in der Grafik



GE imagination at work

www.ge-mcs.com

E-Mail: xrd.info@ge.com

Dear Colleagues,

It is my great pleasure to welcome you to Munich to the 20th Annual Meeting of the “German Crystallographic Society” and to celebrate the 100th anniversary of the discovery of X-ray diffraction.

No event has shaped the face of the science of crystallography more than the 1912 experiment in Munich by Laue, Friedrich and Knipping. This breakthrough induced a change of momentum in the almost simultaneous work of Ewald, also in Munich at the time, and that of the Braggs in the UK in Leeds, Cambridge, and London. The achievements of 1912–14 finally opened the way to a new and increasingly important scientific discipline: the measurement and understanding of the structural state of materials or pharmaceutical agents and later even of the structure of the molecular foundations of life. This momentum has been conserved for over a century with recent significant achievements still being decorated with the highest awards in science. Even in our annual meeting in 2012, the focus on atomistic scale structure analysis by diffraction methods dominates the contributions to a great extent. As long as the challenges of structure research continue to sprout, the aperture of a “crystallographic society” perhaps does not need to be widened. A healthy and sustainable scientific ecosystem, though, probably relies very much on methodic and topical diversity.

The “Laue Day”, Monday, 12th March, 2012, will analyse historical and future perspectives of diffraction methods. From Tuesday, 13th March, to Thursday, 15th March, the stage is open for the contributed papers and plenary lectures covering methods and results from crystallographic research in biology, chemistry, physics, mineralogy, and materials science. On Friday, 14th March, a workshop on neutron diffraction will take place, which is combined with visits of the *Neutronenquelle Heinz Maier-Leibnitz (FRM-II)* in nearby Garching on Thursday afternoon and on Friday morning.

I thank all the participants and plenary speakers for their exciting contributions and the chairpersons and programme committee members for their activities to create the attractive programme which we are looking forward to.

Yours sincerely



Prof. Dr. Wolfgang W. Schmahl
Conference Chair

Venue and Date (for GPS)

Ludwig-Maximilians-University Munich
 Geschwister-Scholl-Platz 1
 80539 Munich (DE)
 12–15 March 2012

Conference Website

www.dgk-conference.de

Registration

Please register online at www.dgk-conference.de.

Registration Fees

DGK-Member	150 EUR
Non-Member	180 EUR
Student*	90 EUR
Ice Breaker Party, 11 March 2012	10 EUR
Evening Event at “Deutsches Museum”, 12 March 2012	10 EUR
Social Evening, 14 March 2012	20 EUR
Accompanying Person	50 EUR

*Confirmation required

Registration for Accompanying Person

Accompanying person have no access to the lectures and receive no conference documents. The ice breaker party, the evening event at “Deutsches Museum” and the social evening are included.

Payment/Confirmation of Payment

An invoice or confirmation of registration will be sent to you via postal or electronic mail within 14 days after online or paper registration. This invoice is a valid invoice which may be submitted to the local tax and revenue office. All fees are due upon receipt of invoice/registration confirmation. Payment transfers must include participant’s name and invoice number. Payment is also accepted by credit card (Master/Eurocard, American Express, VISA). Should you transfer your invoice amount within 10 days of the start of the event, please present your transfer remittance slip at the check-in desk as proof of payment.

Accommodation

We have allocated a contingent of rooms at different hotels. Further information can be found on the congress homepage at www.dgk-conference.de. Please note: Conventus GmbH acts as an intermediary party and assumes no liability for reservations made. Changes and cancellations have to be addressed to the appropriate hotel directly.

Arrival

By Plane

From the airport you can use the S-Bahn line 1 towards “Ostbahnhof” until the station “Moosach” and then change to line U3 towards “Fürstenried West”. Exit at the station “Universität”. Another way is with the S8 from “Airport” to “Marienplatz” and then you change to line U3 towards “Moosach” or U6 towards “Garching-Forschungszentrum” until “Universität”.

By Car

Since parking lots are very rare in the centre of Munich, it is generally recommended to travel via bus or urban rail network. The nearest car park to the university is ‘Park One GmbH’ at the Türkenstraße 84, 80799 Munich.

The next Park and Ride possibility is Parkplatz Oberwiesenfeld, Moosacher Straße, 80809 Munich, from there you can use U3 towards “Fürstenried West” and get out at “Universität”.

For illustration have a look at the city map.

Environmental Badge

The environmental badge is obligatory for the green zone in Munich also for foreigners! Vehicles without environmental badge may not pass through the green zone, otherwise a penalty of 40 EUR and a penalty point in penal record Flensburg impend, even if the vehicle would be allowed to pass through the zone based on its emission value. This is also valid for all vehicles registered in foreign countries, like cars, trucks and busses, as well as for business travelers and for tourists.

Public Transportation

By Urban Rail Network (from main station). Use S1 (towards “Ostbahnhof”), S2 (towards “Erding”), S3 (towards “Holzkirchen”), S4 (towards “Ebersberg”), S6 (towards “Zorneding”), S7 (towards “Kreuzstraße”) or S8 (towards “Munich Airport”) until station “Marienplatz” from there you can take the line U3 towards “Moosach” and U6 towards “Garching- Forschungszentrum” till the stop “Universität”.

Cooperation with German Railways (DB)

Good for environment. Convenient for you. Travel by train from 99 EUR to the 20th Annual Meeting of the German Crystallographic Society (DGK).



With the offer of Conventus Congressmanagement & Marketing GmbH and Deutsche Bahn you can save money by visiting DGK congress. Get on board and profit from attractive prices and conditions for train travel.

Have a good connection to your venue and to the nature! Compared with a car each journey by train spares the environment two-thirds CO₂ and compared with a plane even respectable 75 percent.

The price for your event ticket for a return trip* to Munich is:

- nationwide uniform fixed price for a specific train (daily) in:
 - 1st class 159 EUR
 - 2nd class 99 EUR
- nationwide uniform fixed price without specific train (Mon-Thu) in:
 - 1st class 189 EUR
 - 2nd class 129 EUR



Your ticket is valid from **10th to 16th March, 2012**.

Please call our service number +49 (0)1805 3111 53** to book your ticket and quote Conventus as reference. Have your credit card ready please.

This special offer is valid for all meetings of Conventus Congressmanagement & Marketing GmbH in 2012.

From ↔ to (and return)			Regular fair	Offer to congress	Savings
Hamburg	↔	Munich	258 EUR	99 EUR	159 EUR
Berlin	↔	Munich	232 EUR	99 EUR	133 EUR
Frankfurt a. M.	↔	Munich	182 EUR	99 EUR	83 EUR
Tübingen	↔	Munich	120 EUR	99 EUR	21 EUR

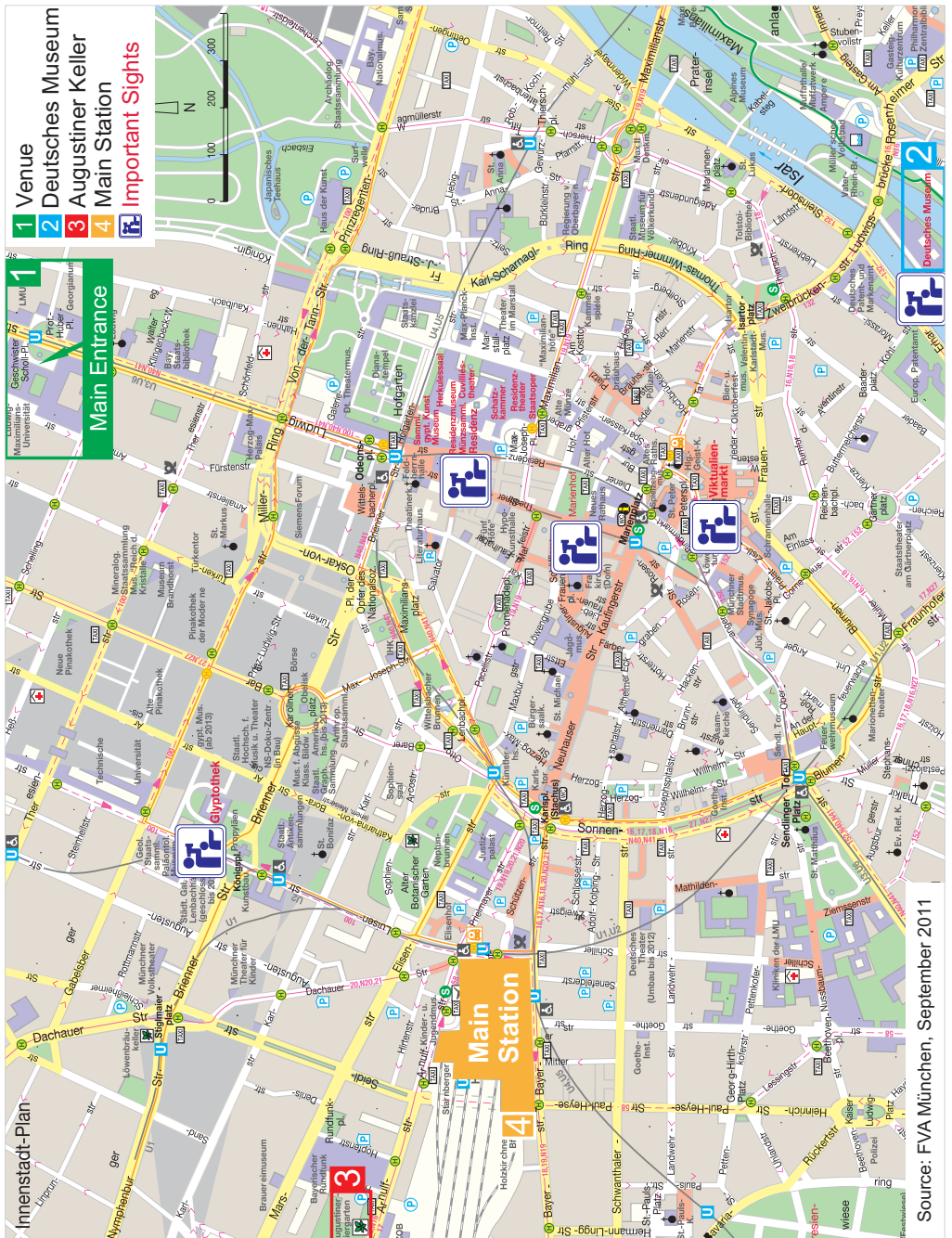
We wish you a pleasant journey with Deutsche Bahn!

* Changes and reimbursement before the first day of validity are 15 EUR excluded from the first day of validity onwards. Passengers restrict themselves to a particular train and travel times. For a supplement of 20 EUR in 2nd class resp. 20 EUR in 1st class full flexible tickets are also available.

** The booking line is available from Monday to Saturday 08⁰⁰–21⁰⁰. Calls will be charged at 0.14 EUR per minute, the expenses from cell phones max. 0.42 EUR per minute.

*** Prices are subject to change.

City Map



Source: FVA München, September 2011

mar μ X

No external cooling water

No routine maintenance

Low running costs

Low cost system



Complete turn-key system
for X-ray crystallography



www.marresearch.com

Certificate of Attendance

Certificates of attendance will be distributed on the last day of the congress at the check-in or upon leaving the additionally certified sessions.

Poster Prizes

All posters will be rated according to scientific basis and visual appearance. The three best posters will be awarded. First place: 300 EUR, second place: 200 EUR and third place: 100 EUR. The poster price is sponsored by Jena Bioscience GmbH.



Name Tag

Attendants and registered accompanying persons will receive a name tag after registration. Admittance to the congress and industrial exhibition is only allowed for those with a name tag. Name tags should be worn at all times.

Evaluation

Please turn in your completed and legible evaluation form to the check-in on the last day. We are always striving to provide high congress quality. This goal can only be reached with your help, your active participation and constructive criticism.

Check-In

The check-in is located in seminar room A011.

Media Check-In

The media check-in is located in seminar room A020.

Industrial Exhibition

There is an accompanying industrial exhibition. The exhibitors are looking forward to welcoming you and to present their comprehensive range of innovative products.

Opening Hours

	12 March	13 March	14 March	15 March
Industrial Exhibition		10 ⁰⁰ –18 ⁰⁰	10 ⁰⁰ –18 ⁰⁰	10 ⁰⁰ –13 ³⁰
Poster Exhibition		12 ⁰⁰ –18 ⁰⁰	08 ⁰⁰ –18 ⁰⁰	
Check-In	08 ⁰⁰ –17 ³⁰	08 ⁰⁰ –18 ⁰⁰	08 ⁰⁰ –18 ⁰⁰	08 ⁰⁰ –13 ³⁰
Media Check-In	08 ⁰⁰ –16 ³⁰	08 ⁰⁰ –18 ⁰⁰	08 ⁰⁰ –18 ⁰⁰	08 ⁰⁰ –13 ³⁰

Internet

There are computers with internet access available at media check-in (A020). Additionally WLAN will be provided. The name of the network is “con”. You do not need any password.

Service for Handicapped Persons

The premises are suitable for the handicapped. The elevator can be reached via entrance “Amalienstraße”.

Restaurants nearby the conference venue:

Atzinger

Schellingstraße 9
80799 Munich
Phone: +49 (0)89 28 28 80

Max Emanuel-Brauerei

Adalbertstraße
80799 Munich
Phone: +49 (0)89 271 51 58

Café Puck

Türkenstraße 33
80799 Munich
Phone: +49 (0)89 280 22 80

Café Altschwabing

Schellingstr. 56
80799 Munich
Phone: +49 (0)89 273 10 22

French Cuisine

Bistro Terrine

Amalienstraße 89
80799 Munich
Phone: +49 (0)89 28 17 80

Thai Cuisine

Kun-Tuk

Amalienstraße 81
80799 Munich
Phone: +49 (0)89 28 37 00

Cadu

Ludwigstraße 24
80539 Munich
Phone: +49 (0)89 28 98 66 00

Bachmaier Hofbräu

Leopoldstraße 50
80802 Munich
Phone: +49 (0)89 38 38 680

Grecian Cuisine

Piatsa

Leopoldstraße 33
80802 Munich
Phone: +49 (0)89 34 80 00

Egger Schwabing

Friedrichstraße 27
80801 Munich
Phone: +49 (0)89 39 85 26

Mexican Cuisine

Little Tortilla

Viktor-Scheffelstraße 23
80803 Munich
Phone: +49 (0)89 39 76 77

Esszimmer

Siegfriedstraße 14
80803 Munich
Phone: +49 (0)89 38 34 69 64

Schwabinger Wassermann

Apianstraße 7
80796 Munich
Phone: +49 (0)89 32 38 80 20

Basic Buffet & Restaurant

Herzogstraße 129
80797 Munich
Phone: +49 (0)89 30 76 56 76

Cafe Münchner Freiheit

Münchner Freiheit 20
80802 Munich
Phone: +49 (0)89 33 00 79 90

Ristorante Vinotheka

Il Grapollo

Adalbertstraße 28
80799 Munich
Phone: +49 (0)89 39 62 41

Presentation Submission

Media check-in is located in seminar room A020.

Time Allotment

We ask you to please follow the following: Please prepare your presentation so that you remain within the time allotment. Chair persons have been advised to avoid delays. Contact your chair person before your session begins and advise of any changes or special wishes.

Presentation Form/Submission of Presentation

PDF and PowerPoint presentations are permitted.

Required technical equipment will be available at the congress.

The use of Macintosh as well as the use of a personal laptop for a presentation is not planned, but possible. For video and audio files please submit AVI, WMV and MPG files only as a separate file.

Please make sure that any required CODEC files for any videos are also submitted.

Your presentation and any additional files should be submitted at least two hours before your presentation time.

Please note: If you use a USB stick to save your files, do not protect it with software.

The projection data of your presentations before and during the whole congress will be recorded and managed centrally. There is a notebook with MS PowerPoint 2007 and a video projector in location.

PILATUS 300K

Now for your
Laboratory



PILATUS hybrid-pixel detectors have revolutionized data acquisition at synchrotron beamlines.

With the advent of the new PILATUS 300K 20Hz, DECTRIS brings all the advantages of the hybrid-pixel technology to your laboratory at unrivaled value.



Meet us at the DECTRIS booth for detailed information

We would like to thank the following companies for their support:

Main Sponsor

INCOATEC GmbH (Geesthacht/DE)



Sponsor Conference Bags

Dectris Ltd. (Baden/CH)

Sponsor Lanyards and Name Badges

Bruker AXS (Karlsruhe/DE)

Sponsor Pads and Pens

Agilent Technologies GmbH (Waldbronn/DE)

Sponsor Poster Prize

Jena Bioscience GmbH (Jena/DE)

Sponsors

Agilent Technologies GmbH (Waldbronn/DE)

Crystal Impact GbR (Bonn/DE)

Dunn Labortechnik / Art Robbins Instruments (Asbach/DE)

GE Sensing & Inspection Technologies GmbH (Ahrensburg/DE)

Marresearch GmbH (Norderstedt/DE)

Mateck GmbH (Jülich/DE)

Oxford Instruments GmbH (Wiesbaden/DE)

Oxford University Press (Oxford/GB)

PANalytical GmbH (Kassel/DE)

Röntgenlabor Dr. Ermrich /Reinheim/DE)

Springer-Verlag GmbH (Heidelberg/DE)

Systat Software GmbH (Erkrath/DE)

Media Cooperations

Cambridge University Press (Cambridge/GB)

"The European Physical Journal – Applied Physics"

Elsevier B. V. (Amsterdam/NL)

"Journal of Crystal Growth"

International Union of Crystallography – IUCr (Chester/GB)

"Acta Crystallographica"

"Journal of Applied Crystallography"

"Journal of Synchrotron Radiation"



Wiley-VCH Verlag GmbH & Co. KGaA (Weinheim/DE)

State at printing

The following exhibitors are looking forward to greeting you and to present you their comprehensive range of innovative products:

Agilent Technologies GmbH (Waldbronn/DE)

AXO Dresden GmbH (Dresden/DE)

Bruker AXS (Karlsruhe/DE)

Dectris Ltd. (Baden/CH)

EFG GmbH (Berlin/DE)

FIZ Karlsruhe GmbH (Eggenstein-Leopoldshafen/DE)

GE Sensing & Inspection Technologies GmbH (Ahrensburg/DE)

Huber Diffractionstechnik GmbH & Co. KG (Rimsting/DE)

INCOATEC GmbH (Geesthacht/DE)

International Union of Crystallography (Chester/GB)

Jena Bioscience GmbH (Jena/DE)

Marresearch GmbH (Norderstedt/DE)

MK Versuchsanlagen (Mücke-Merlau/DE)

Oldenbourg Wissenschaftsverlag GmbH (Munich/DE)

Oxford Cryosystems (Long Hanborough/GB)

Oxford Instruments GmbH (Wiesbaden/DE)

PANalytical GmbH (Kassel/DE)

PHYWE Systeme GmbH & Co. KG (Göttingen/DE)

Rigaku Europe SE (Berlin/DE)

Springer-Verlag GmbH (Heidelberg/DE)

Stoe & Cie GmbH (Darmstadt/DE)

Thermo Fisher Scientific GmbH (Dreieich/DE)

Xenocs SA (Sassenage/FR)

State at printing

Ice Breaker Party

Come together for drinks and snacks prior to the Kick-Off of the conference and break the ice in first conversations with our industrial partners and your colleagues.

Date	Sunday, 11 March 2012
Venue	Foyer conference venue
Start	1800
Fee	10 EUR
Registration required!	



© fotolia.com/Tim Porter

Welcome Reception at Deutsches Museum

In the evening of the dedicated Laue Day we would like to invite you to a further lecture and a Laue-exhibition to the “Deutsches Museum”. Snacks and drinks will be served. For your attendance please register.



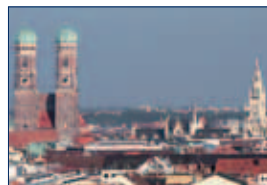
Date	Monday, 12 March 2012
Venue	Deutsches Museum Munich
Start	1900
Fee	10 EUR
distance from venue	2,9 km (by car 6 minutes, by foot 35 minutes)
Address	Museumsinsel 1 80538 Munich

Take U6 (towards “Klinikum Großhadern”) until “Marienplatz”. Go one floor up to S-Bahn. Take any S-Bahn in the direction of “Ostbahnhof”, exit at the next stop: “Isartor” and enjoy the 10 minute walk. The “Deutsches Museum” is signposted from the S-Bahn station “Isartor”. You walk in the direction of your train up the escalator, turn right at the top and go to the street. On the street turn left and head towards the Isar river. Cross the bridge and turn right, walk upstream along the river until you reach entrance of “Deutsches Museum”.

Guided Tour through Munich “Historical City Centre”

Ways in the past and the future.

It all started with the salt. And then? In our search for clues between Petersberg, Altem Hof und Frauenkirche we show how the historical city centre grow over the centuries. We report on markets, beer and brewing traditions, townhouses and the actual life in the city.



historical skyline
© fotolia.com/Thomas Bürgele

Date	Tuesday, 13 March 2012
Start	1400
Duration	1,5 h (Tour ends in the city centre at “Marienplatz”)
Fee	10 EUR
Meeting point	Check-In

Guided Beer Tour

Munich is famous for the "Hofbräuhaus", but there are a lot of more places which have something to do with beer. You will learn something about beer barons, the origin of the "Russsmaß", the purity requirements and something about the beer battles.

It is a fascinating tour across the city- and beer history of Munich and there is also a brewery guided tour with beer tasting included.



Hofbräuhaus
© fotolia.com/oromotion

Date	Wednesday, 14 March 2011
Start	14 ⁰⁰
Duration	1,5 h (Tour ends in the city centre at "Marienplatz")
Fee	18 EUR
Meeting point	Check-In

Social Evening at Augustiner Keller

One of the most popular meeting places for the Munich and guests from all around the world, is the Augustiner Keller. The charm of Bavarian tradition, the freshly drawn Augustiner precious substance from wooden barrels, Bavarian specialties and other delicacies of our cuisine invite you to celebrate in the Augustiner Keller.



Augustiner Keller
© Augustiner-Keller München

Date	Wednesday, 14 March 2012
Start	20 ⁰⁰
Fee	20 EUR
Address	Augustiner Keller Arnulfstraße 52 80335 Munich
Distance from venue	3,2 km (by car 7 minutes, by foot 41 minutes)

Take U3 (towards "Fürstenried West") or U6 (towards "Klinikum Großhadern") until "Marienplatz". From there take S1 (towards "Freising"), S2 (towards "Petershausen"), S3 (towards "Mammendorf"), S4 (towards "Geltendorf"), S6 (towards "Tutzing"), S7 (towards "Wolfratshausen") or S8 (towards "Herrsching") until "Hackerbrücke".

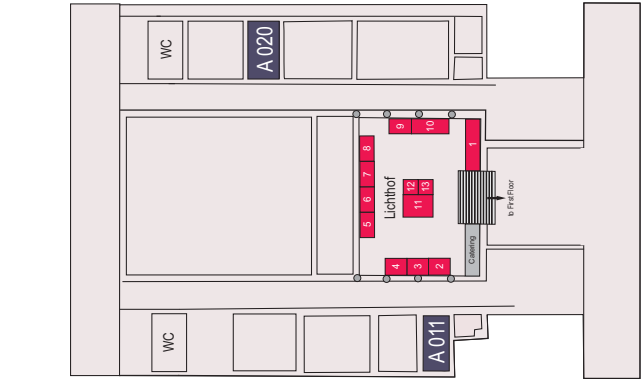
In addition, we recommend visiting the following museums: see page 10

- Alte und Neue Pinakothek
- Glyptothek
- Deutsches Museum
- Staatliches Museum Ägyptischer Kunst

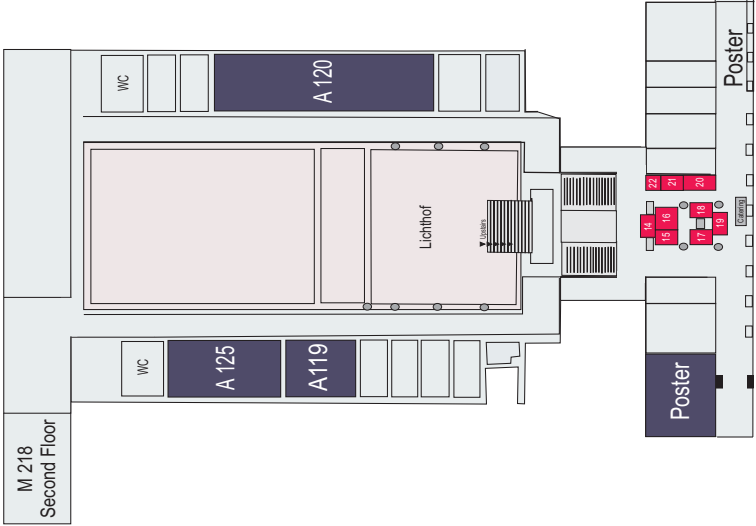


Further touristic offers: www.muenchen.de.

Floor Plan – Ground Floor



Floor Plan – First Floor



Exhibitors

- 1 INCOATEC GmbH
- 2 PANalytical GmbH
- 3 Dectris Ltd.
- 4 Oxford Cryosystems
- 5 International Union of Crystallography
- 6 Stoe & Cie GmbH
- 7 Huber Diffractionstechnik GmbH & Co. KG/
AXO Dresden GmbH
- 8 Agilent Technologies
- 9 PHYWE Systeme GmbH & Co. KG
- 10 Bruker AXS
- 11 GE Sensing & Inspection Technologies GmbH
- 12 Oldenbourg Wissenschaftsverlag
- 13 Oxford Instruments
- 14 Xenocs Sa
- 15 Jena Bioscience GmbH
- 16 Rigaku Europe SE
- 17 FIZ Karlsruhe
- 18 EFG GmbH
- 19 MK-Versuchsanlagen
- 20 Thermo Fisher Scientific GmbH
- 21 Marresearch GmbH
- 22 Springer

Sunday	Seminar room A020	Seminar room A011	
12:00			
13:00	DGK Board Meeting		
14:00		Registration	
15:00			
16:00			
17:00			
18:00	Ice Breaker Party		
19:00			
19:30			
		p. 18	

Monday	Lecture hall M218
09:00	Opening – Welcome Notes by DGK, LMU, TUM, IUCr
09:30	
09:45	
10:00	Michael Eckert
10:15	
10:30	
10:45	Coffee Break
11:00	
11:15	Dieter Schwarzenbach
11:30	
11:45	
12:00	André Authier
12:15	
12:30	
12:45	Lunch Break
13:00	
13:15	
13:30	
13:45	
14:00	Dieter Hoffmann
14:15	
14:30	
14:45	Henning Friis Poulsen
15:00	
15:15	
15:30	Coffee Break
15:45	
16:00	Helmut Dosch
16:15	
16:30	
16:45	Edward N. Baker
17:00	
17:15	
17:30	
18:45	
19:00	Robert Huber (Deutsches Museum)
19:15	
19:30	
19:45	Welcome Reception Deutsches Museum
–	
21:00	

	Lecture hall M218	Lecture hall A125	Lecture hall A120
09:00	MS01 Frontiers in Crystallographic Techniques and Instrumentation I	MS02 Crystallography in Engineering and Technology	MS03 Biocrystallography and Medicine
09:30			
10:00	p. 27	p. 27	p. 28
10:30	Coffee Break		
11:00	Markus Braden		
11:30	p. 28		
12:00	Lunch Break		
12:15			
12:30			
12:45			
13:00			
	Lunch Symposium  p. 29		
13:30	MS04 Electron Microscopy & Diffraction	MS05 Frontiers in Structure Analysis	MS06 Hot New Biomolecular Structures
14:00			
14:30	p. 29	p. 30	p. 30
15:00	Coffee Break		
15:30	Martin Jansen		
16:00	p. 31		
16:30	Poster Session		
17:00			
17:30	p. 31		
18:00	Awards		
18:30	p. 31		
19:00	Laue Price 2011 Lecture		
	p. 31		
19:30			
20:00			

	Lecture hall M218	Lecture hall A125	Lecture hall A120		
09:00	MS07 Pressure-, Field-, & Temperature-Induced Processes I p.32	MS08 Spectroscopy p. 32	MS09 Structure of Biological Macromolecular Complexes p. 33		
09:30					
10:00					
10:30	Coffee Break				
11:00	Edgar Weckert p. 34	Lunch Break			
11:30					
12:00					
12:15					
12:30					
12:45					
13:00					
13:30	MS10 Pressure-, Field-, & Temperature-Induced Processes II p. 34	MS11 Aperiodic Crystals p. 35	MS12 Theory & Simulation p. 35		
14:00					
14:30					
15:00	Coffee Break				
15:30	Ilme Schlichting p. 36				
16:00					
16:30	Poster Session p. 36				
17:00					
17:30					
18:00	DGK- Member Meeting p. 36				
18:30					
19:00					
19:30					
20:00 – 00:00					
	Social Evening at the Augustinerkeller p. 19				

	Lecture hall M218	Lecture hall A125	Lecture hall A120
9:00	MS13 Structure & Function – Biomaterials I	MS14 Structural Chemistry & Mineralogy	MS15 Frontiers of Structural Biology Methods
9:30			
10:00	p. 37	p. 37	p. 38
10:30	Coffee Break		
11:00	Fiona Meldrum		
11:30	p. 38		
12:00	Lunch Break		
12:30			
13:00			
13:30	MS16 Structure & Function – Biomaterials II	MS17 Structure & Function – New and Smart Materials	MS18 Frontiers in Crystallographic Techniques and Instrumentation II
14:00			
14:30	p. 38	p. 39	p. 39
15:00	Karl-Peter Hopfner		
15:30	p. 40		
16:00	Closing/Outlook 2013		
	p. 40		

Tuesday, 13 March 2012

- 11⁰⁰–12⁰⁰ **Coupling of charge orbital and magnetic order in transition-metal oxides**
Markus Braden (Cologne/DE)
- 15³⁰–16³⁰ **The energy landscape concept of matter, bridging crystallography and chemistry**
Martin Jansen (Stuttgart/DE)

Wednesday, 14 March 2012

- 11⁰⁰–12⁰⁰ **New light sources for structural studies**
Edgar Weckert (Hamburg/DE)
- 15³⁰–16³⁰ **X-ray free-electron lasers – emerging opportunities for structural biology**
Ilme Schlichting (Heidelberg/DE)

Thursday, 15 March 2012

- 11⁰⁰–12⁰⁰ **Bio-inspired crystallization – challenging single crystal shape and structure**
Fiona Meldrum (Leeds/GB)
- 15⁰⁰–16⁰⁰ **Integrated structural analysis of DNA double-strand break repair**
Karl-Peter Hopfner (Munich/DE)

09 ⁰⁰ Lecture Hall M218	Opening – Welcome Notes Gautam Desiraju (Bangalore/IN) President of the International Union of Crystallography Sine Larsen (Copenhagen/DK) Representative of European Large Scale Facilities for Crystallography
10 ⁰⁰ LT-01	Disputed discovery – the beginnings of X-ray diffraction in crystals in 1912 and it's repercussions Michael Eckert (Munich/DE)
10 ⁴⁵ –11 ¹⁵	Coffee Break
11 ¹⁵ LT-02	Developement of diffraction-based crystallography, from Laue to the present day Dieter Schwarzenbach (Lausanne/CH)
12 ⁰⁰ LT-03	X-ray optics, from Röntgen to Laue, Ewald, Compton, Borrmann and synchrotron radiation André Authier (Peyrat-Le-Chateau/FR)
12 ⁴⁵ –14 ⁰⁰	Lunch Break
14 ⁰⁰ LT08	Max von Laue (1879–1960) – knight without fear or fault Dieter Hoffmann (Berlin/DE)
14 ⁴⁵ LT-04	From multigrain crystallography to 3D movies of polycrystalline materials Henning Friis Poulsen (Lyngby/DK)
15 ³⁰ –16 ⁰⁰	Coffee Break
16 ⁰⁰ LT-05	Laue's gateway to the nanocosmos – the future Helmut Dosch (Hamburg/DE)
16 ⁴⁵ LT-06	Laue's legacy to biology – the impact of X-ray diffraction on our understanding of living systems Edward N. Baker (Auckland/NZ)
19 ⁰⁰ LT-07 Dt. Museum	Beauty and fitness for purpose – architecture of proteins, the building blocks of life Robert Huber (Martinsried/DE)
19 ⁴⁵ –21 ³⁰	Welcome Reception and Laue Exhibition (see page 18)

0900–1030 Lecture hall M218 Chair	MS01: Frontiers in Crystallographic Techniques and Instrumentation I Martin Meven (Garching/DE)
0900 MS01-T01	New strategies and better data with PILATUS detectors Marcus Müller (Baden/CH)
0915 MS01-T02	SINGLE – a programme to control single-crystal diffractometers for high-precision lattice parameter measurements Ross Angel (Padova/IT)
0930 MS01-T03	Utilizing synergetics – coupling μ-XRD² with μ-Raman Christoph Berthold (Tübingen/DE)
0945 MS01-T04	In-house research facility for simultaneous measurements of elastic properties and densities of single crystals at high pressures Alexander Kurnosov (Bayreuth/DE)
1000 MS01-T05	Progress in Laue topography Andreas Danilewsky (Freiburg i. Br./DE)
1015 MS01-T06	Exploring structural properties at the micron and sub-micron scale with focused synchrotron radiation and scanning diffraction techniques Manfred Burghammer (Grenoble/FR)
0900–1030 Lecture hall A125 Chair	MS02: Crystallography in Engineering and Technology Ullrich Pietsch (Siegen/DE)
0900 MS02-T01	On the validity of the Warren model of stacking faults David Rafaja (Freiberg/DE)
0915 MS02-T02	Hydrothermale Synthese von CSH-Phasen (Tobermorit) mit dem Additiv Ca-Format Andrea Hartmann (Hanover/DE)
0930 MS02-T03	Determining glass-content of dental ceramics with high-energy synchrotron radiation Christiane Hartmann (Göttingen/DE)
0945 MS02-T04	Neutron diffraction on ferroelectric ceramics under electric field Markus Hoelzel (Garching/DE)

10 ⁰⁰ MS02-T05	The effect of polyaniline and BaTiO₃ on crystal structure, electric and magnetic properties of nanocrystalline Ni_{1-x}Zn_xFe_{1.5}Cr_{0.5}O₄ Karimat El-Sayed (Cairo/EG)
10 ¹⁵ MS02-T06	Incommensurate magnetic ordering in BiFeO₃-PbTiO₃ composites Anatoliy Senyshyn (Garching/DE)
09 ⁰⁰ –10 ³⁰ Lecture hall A120 Chair	MS03: Biocrystallography and Medicine Caroline Kisker (Würzburg/DE)
09 ⁰⁰ MS03-T01	Structure-based reengineering of designed Armadillo repeat proteins abandoned domain swapping of N-terminal capping repeats Peer Mittl (Zurich/CH)
09 ¹⁵ MS03-T02	A specific binding motif enables SycD-YopD recognition Madeleine Schreiner (Bielefeld/DE)
09 ³⁰ MS03-T03	The crystal structure of death receptpr 6 (DR6) – a potential receptor of the amyloid precursor protein (APP) Miriam Than (Jena/DE)
09 ⁴⁵ MS03-T04	Characterization of glyoxalase I/Bleomycin resistance proteins in pseudomonas aeruginosa PA01 Allegra Vit (Bayreuth/DE)
10 ⁰⁰ MS03-T05	Unwinding the differences of the mammalian PERIOD clock proteins by X-ray crystallography Ira Schmalen (Martinsried/DE)
10 ¹⁵ MS03-T06	Hexokinase flexibility causes oligomer-depended activity Bartholomeus Küttner (Leipzig/DE)
10 ³⁰	Coffee Break and Industrial Exhibition
11 ⁰⁰ –12 ⁰⁰ P-01 Lecture hall M218 Chair	Coupling of charge orbital and magnetic order in transition-metal oxides Markus Braden (Cologne/DE) Helmut Ehrenberg (Karlsruhe/DE)
12 ⁰⁰ –13 ³⁰	Lunch Break and Industrial Exhibition

1215–1315

Lecture hall A120

Chair

Lunch Symposium – 100 Years Laue – 10 Years Incoatec – 1 Year IµS High Brilliance

Till Samtleben – Incoatec GmbH (Geesthacht/DE)



10 years Incoatec, the past, the now and the future

Dr. Carsten Michaelsen – Incoatec GmbH (Geesthacht/DE)

High throughput in Chemical Crystallography from an industrial point of view

Dr. Ina Dix – Novartis (Nürnberg/DE)

The new D8 – latest developments in SC-XRD

Dr. Martin Adam – Bruker AXS (Karlsruhe/DE)

Food and Beverage will be served for registered participants.

1330–1500

Lecture hall M218

Chair

MS04: Electron Microscopy & Diffraction

Christina Scheu (Munich/DE)

1330

MS04–T01

The importance of the correct intensity simulation of EBSD patterns

Gert Nolze (Berlin/DE)

1345

MS04–T02

Accurate band profile analysis in EBSD patterns using frequency space tiling

Farangis Ram (Düsseldorf/DE)

1400

MS04–T03

CryoTEM in materials science – studying biomimetic mineralization

Nico Sommerdijk (Eindhoven/NL)

1415

MS04–T04

Structure elucidation of germanium tin antimony tellurides by TEM and X-ray methods

Tobias Rosenthal (Munich/DE)

1430

MS04–05

Oxygen precipitation in semi conductor silicon wafers studied with X-ray diffraction in an energy dispersive Laue geometry

Alexander Gröschel (Erlangen/DE)

1445

MS04–T06

In-Situ measurement of early stages of oxygen precipitation in silicon by dynamical X-ray diffraction

Johannes Will (Erlangen/DE)

1330–1500	MS05: Frontiers in Structure Analysis – Electron Density and other Precision Studies
Lecture hall A125	
Chairs	Ulli Englert (Aachen/DE), Christian Lehmann (Mülheim/DE)
1330	Electron density contributions to drug development
MS05–T01	Peter Luger (Berlin/DE)
1345	A joint modelisation of X-ray and neutron diffraction data – application to magnetic molecular materials
MS05–T02	Claude Lecomte (Nancy/FR)
1400	Charge density study of alpha-Boron at 100 K
MS05–T03	Swastik Mondal (Bayreuth/DE)
1415	ShelXle – a cute GUI for SHELXL
MS05–T04	Christian B. Hübschle (Göttingen/DE)
1430	Frontiers in structural analysis of high-pressure molecular crystal structures
MS05–T05	Francesca Fabbiani (Göttingen/DE)
1445	Structural investigation of ZnO nanoparticles by pair distribution function (PDF)
MS05–T06	Kaustuv Datta (Erlangen/DE)
1330–1500	MS06: Hot New Biomolecular Structures
Lecture hall A120	
Chair	Karl-Peter Hopfner (Munich/DE)
1330	Convergent evolution of Rubisco activases from green plants and red algae
MS06–T01	Andreas Bracher (Martinsried/DE)
1345	Structural insight into the activation mechanism of toxoplasma gondii nucleoside triphosphate diphosphohydrolases by disulfide reduction
MS06–T02	Ulrike Krug (Leipzig/DE)
1400	Identification of a novel TGF-β-binding site in the structure of the ZP-C domain of murine TGFR-3
MS06–T03	Uschi Diestel (Erlangen/DE)
1415	Structural and functional organization of the Ska complex – a key assembly for stable kinetochore-microtubule attachments
MS06–T04	Arulanandam Arockia Jeyaprakash (Martinsried/DE)

14 ³⁰ MS06-T05	Crystal structure of yeast splicing factor Cwc2 reveals a novel architecture of a multipartite RNA-binding protein Jana Schmitzova (Göttingen/DE)
14 ⁴⁵ MS06-T06	Structural and functional studies of spliceosome catalytic activation Karine Santos (Berlin/DE)
15 ⁰⁰	Coffee Break and Industrial Exhibition
15 ³⁰ –16 ³⁰ P-02 Lecture hall M218 Chair	The energy landscape concept of matter, bridging crystallography and chemistry Martin Jansen (Stuttgart/DE) Wolfgang Schnick (Munich/DE)
16 ³⁰ –18 ⁰⁰	Poster Session (see page 42)
18 ⁰⁰ –19 ⁰⁰ Lecture hall M218	Award Ceremony
19 ⁰⁰ –19 ³⁰ Lecture hall M218	Laue Price 2011 Lecture – Crystallography and crystal chemistry in the diamond anvil cell Alexandra Friedrich (Frankfurt a. M./DE)

0900–1030 Lecture hall M218 Chairs	MS07: Pressure-, Field-, & Temperature-Induced Processes I Eiken Haussühl (Frankfurt a. M./DE), Jürgen Schreuer (Bochum/DE)
0900 MS07–T01	How to use Jana2006 to process high-pressure single-crystal data Andrzej Grzechnik (Bilbao/ES)
0915 MS07–T02	Elasticity of Sm-doped $\text{Y}_3\text{Al}_5\text{O}_{12}$ with an independent absolute pressure scale and its calibration as a primary pressure standard Dmytro Trots (Bayreuth/DE)
0930 MS07–T03	Influence of crystal size and uniaxial stress on the B4 to B1 phase transition pressure in AlN and ZnO nanocrystals investigated with second harmonic generation (SHG) Leonore Wiehl (Frankfurt a. M./DE)
0945 MS07–T04	Crystal structure of α-FeOOH under high-pressure Elena Bykova (Bayreuth/DE)
1000 MS07–T05	High pressure behavior of wadeite $\text{K}_2\text{ZrSi}_3\text{O}_9$ Niklas Niederwieser (Innsbruck/AT)
1015 MS07–T06	Comparative first principles study of pressure induced phase transitions in Mn_2O_3 and MnTiO_3 Carmen Quiroga (Munich/DE)
0900–1030 Lecture hall A125 Chairs	MS08: Spectroscopy Georg Amthauer (Salzburg/AT), Michael Fechtelkord (Bochum/DE)
0900 MS08–T01	Aluminum ordering and clustering in Al-rich synthetic phlogopite – the influence of fluorine investigated by $\{^{19}\text{F}/^1\text{H}\}$ ^{29}Si CPMAS NMR spectroscopy Michael Fechtelkord (Bochum/DE)
0915 MS08–T02	The Automatic Tuning Matching Goniometer (ATMG) probe system – mapping chemical questions using orientation dependent NMR experiments Oliver Pecher (Aachen/DE)

- 09³⁰
MS08-T03 **A 57Fe Mössbauer study of local structure and cation distribution in mullite-type $\text{Bi}_2\text{Fe}_4\text{O}_9\text{-Bi}_2\text{Mn}_4\text{O}_{10}$ and $\text{Bi}_2\text{Fe}_4\text{O}_9\text{-Bi}_2\text{M}_4\text{O}_9$ (M=Al, Ga) solid solutions**
Sven-Ulf Weber (Braunschweig/DE)
- 09⁴⁵
MS08-T04 **Application of a nanoscope – fayalite 3D difference electron densities from synchrotron diffraction measurements**
Werner Lottermoser (Salzburg/AT)
- 10⁰⁰
MS08-T05 **Ion exchange and adsorption of schwertmannite compared to goethite and lepidocrocite**
Peter M. Kadletz (Munich/DE)
- 10¹⁵
MS08-T06 **Scanning coherent X-ray diffraction microscopy with spatial resolutions down to below 10 nm**
Christian Schroer (Dresden/DE)
- 09⁰⁰–10³⁰
Lecture hall A120
Chair **MS09: Structure of Biological Macromolecular Complexes**
Markus Wahl (Göttingen/DE)
- 09⁰⁰
MS09-T01 **Inhibition of PDZ domain mediated protein-protein interactions**
Yvette Roske (Berlin/DE)
- 09¹⁵
MS09-T02 **Structural and functional investigation of spliceosomal U5 snRNP assembly**
Gert Weber (Berlin/DE)
- 09³⁰
MS09-T03 **Structural studies of a bidirectional transport factor**
Marlene Grünwald (Tübingen/DE)
- 09⁴⁵
MS09-T04 **Why is the mollusc chitin synthase such a complex molecular machine?**
Ingrid Weiss (Saarbrücken/DE)
- 10⁰⁰
MS09-T05 **Insight into the allosteric mechanism of GntR/HutC-type bacterial repressor molecules**
Simon Fillenberg (Erlangen/DE)
- 10¹⁵
MS09-T06 **Structure and Mechanism of Human DNA Polymerase η**
Christian Biertümpfel (Bethesda, MD/US)
- 10³⁰–11⁰⁰ **Coffee Break and Industrial Exhibition**

11 ⁰⁰ –12 ⁰⁰ P-03 Lecture hall M218 Chair	New light sources for structural studies Edgar Weckert (Hamburg/DE) U. Bismayer (Hamburg/DE)
12 ⁰⁰ –13 ³⁰	Lunch Break and Industrial Exhibition
13 ³⁰ –15 ⁰⁰ Lecture hall M218 Chairs	MS10: Pressure-, Field-, & Temperature-Induced Processes II Eiken Haussühl (Frankfurt a. M./DE), Jürgen Schreuer (Bochum/DE)
13 ³⁰ MS10–T01	Crystal structure and magnetic ordering in the metal(III)oxyhalide CrOCl at low temperatures Andreas Schönleber (Bayreuth/DE)
13 ⁴⁵ MS10–T02	Temperature dependence of cation distribution in $(\text{Co}_x\text{Mg}_{1-x})_2\text{SiO}_4$ olivines Jianmin Shi (Braunschweig/DE)
14 ⁰⁰ MS10–T03	Structure-property relationships in silicates – elasticity of natural beryl Chandra Shekhar Pandey (Bochum/DE)
14 ¹⁵ MS10–T04	Atomic scale description of the macroscopic piezo-ferroelectric properties of high performance lead zirconate titanate (PZT) Manuel Hinterstein (Dresden/DE)
14 ³⁰ MS10–T05	Observation of a low-symmetry phase in $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ by high resolution X-ray diffraction and optical birefringence microscopy Semen Gorfman (Siegen/DE)
14 ⁴⁵ MS10–T06	Influence of electric field on temperature-induced local phase transformations in relaxor ferroelectrics studied by polarized raman spectroscopy Bernd Maier (Hamburg/DE)

1330–1500

Lecture hall A125

Chair

MS11: Aperiodic Crystals

Sander van Smaalen (Bayreuth/DE)

1330

MS11-T01

Unravelling the Local ~ 8 Å Structure of Al–Cu–Co quasicrystals by the use of three dimensional pair distribution function analysis

Philippe Schaub (Zurich/CH)

1345

MS11-T02

Standard and non-standard settings of superspace groups

Sander van Smaalen (Bayreuth/DE)

1400

MS11-T03

CuTe – a modulated structure and its electronic origin

Thomas Doert (Dresden/DE)

1415

MS11-T04

Incommensurately modulated structure of nepheline

Karen Frieze (Bilbao/ES)

1430

MS11-T05

From transition kinetics to lock-in mechanisms – manipulating incommensurately modulated structures in Rb-doped K_2ZnCl_4

Karsten Behrendt (Göttingen/DE)

1445

MS11-T06

Phase transitional and critical phenomena in crystallographic superspace

Laurent Guerin (Rennes/FR)

1330–1500

Lecture hall A120

Chairs

MS12: Theory & Simulation

Rossitza Pentcheva (Munich/DE), Gerhard Paul Raabe (Aachen/DE)

1330

MS12-T01

The role of metric parameters in the interpretation of order/disorder (O/D) structures

Berthold Stöger (Vienna/AT)

1345

MS12-T02

Optimising the debye scattering equation for use with polycrystalline materials

Noel Thomas (Höhr-Grenzhausen/DE)

1400

MS12-T03

Rigid bodies and symmetry modes – a great combination

Melanie Müller (Trento/IT)

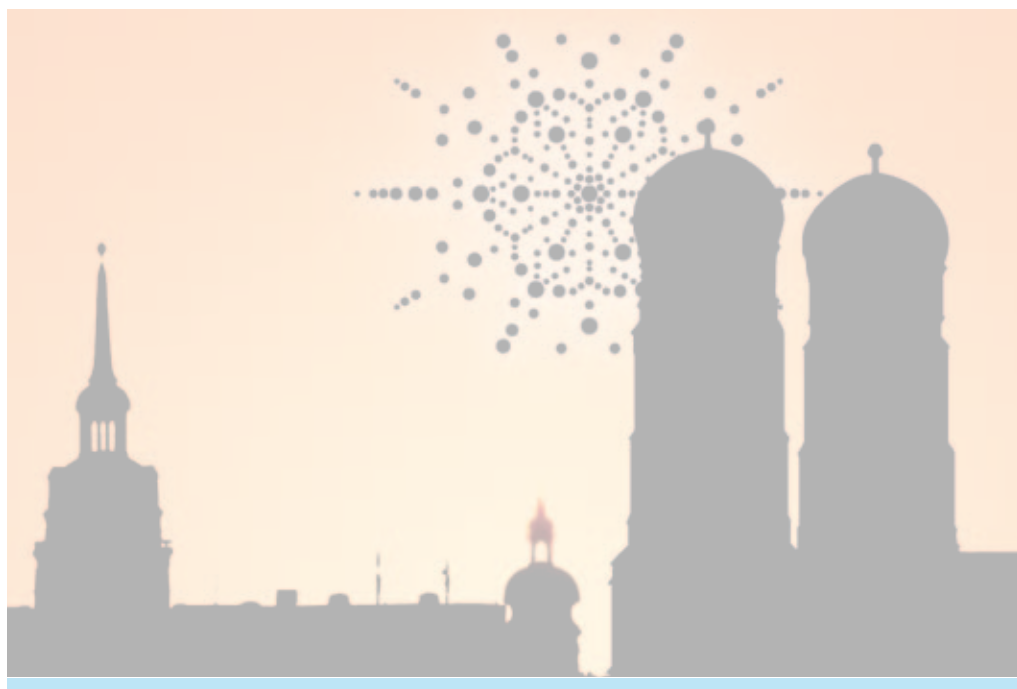
1415

MS1-T04

The bilbao crystallographic server – structure utilities toolbox

Mois Ilia Aroyo (Bilbao/ES)

- 14³⁰
MS12-T05 **Ab initio simulations of lattice stability – an effect of temperature and temperature induced excitations**
Igor Abrikosov (Linköping/SE)
- 14⁴⁵
MS12-T06 **Arsenate adsorption at hydrous FeOOH surfaces – an ab initio study**
Katrin Otte (Munich/DE)
- 15⁰⁰
Coffee Break and Industrial Exhibition
- 15³⁰–16³⁰
P-04 **X-ray free-electron lasers – emerging opportunities for structural biology**
Ilme Schlichting (Heidelberg/DE)
Lecture hall M218
Chair Patrick Cramer (Munich/DE)
- 16³⁰–18⁰⁰
Poster Session (see page 42)
- 18⁰⁰–19³⁰
Lecture hall M218 DGK-Member Meeting
- from 20⁰⁰
Social Evening at the Augustinerkeller (see page 19)

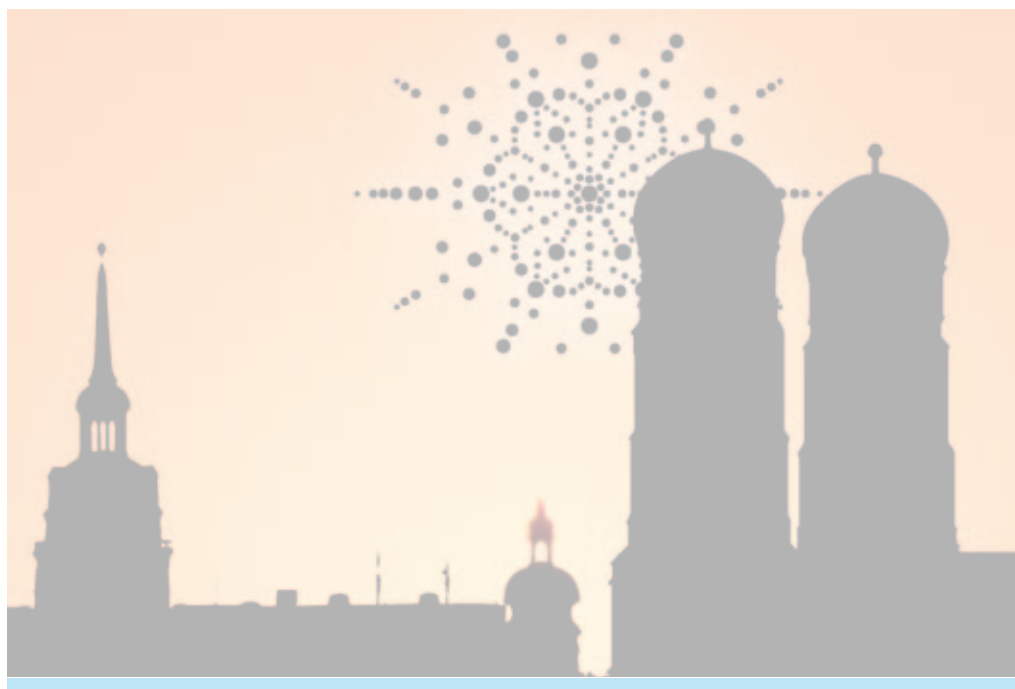


09 ⁰⁰ –10 ³⁰ Lecture hall M218 Chair	MS13: Structure & Function – Biomaterials I Erika Griesshaber (Munich/DE)
09 ⁰⁰ MS13–T01	Organic and inorganic crystals in bioinspired hybrid materials Nico Sommerdijk (Eindhoven/NL)
09 ³⁰ MS13–T02	The effect of physiological saline and soluble matrix proteins of <i>Porcellio scaber</i> ACC deposits on calcium carbonate precipitation Andreas Ziegler (Ulm/DE)
09 ⁴⁵ MS13–T03	Hydroxyapatite-Nanoceramics-Patent – EP 01824443 Ulli Bismayer (Hamburg/DE)
10 ⁰⁰ MS16–T02	Crystallographic, structural and mechanical properties of shark teeth Oleg Prymak (Essen/DE)
09 ⁰⁰ –10 ³⁰ Lecture hall A125 Chairs	MS14: Structural Chemistry & Mineralogy Reinhard Neder (Erlangen/DE), Thomas Schleid (Stuttgart/DE)
09 ⁰⁰ MS14–T01	Structural variability in complex uranyl phosphates and uranyl arsenates of divalent elements Evgeny Alekseev (Jülich/DE)
09 ¹⁵ MS14–T02	Boron in mullites – syntheses, properties and a structural puzzle Hanna Lühns (Bremen/DE)
09 ³⁰ MS14–T03	Combined neutron, X-ray and DFT study of croconic acid Matthias Gutmann (Chilton Didcot/GB)
09 ⁴⁵ MS14–T04	Ionic substitution in meridianiite ($\text{MgSO}_4 \cdot 11\text{H}_2\text{O}$) – solid solutions and novel hydrates Dominic Fortes (London/GB)
10 ⁰⁰ MS14–T05	New methods for the synthesis of ternary rare-earth metal(III) oxoarsenates(III) and (V) with a comparison of the comprehensive crystal structures Sebastian J. Metzger (Stuttgart/DE)
10 ¹⁵ MS14–T06	Time-resolved investigation of crystallisation processes Tanja Gnutzmann (Berlin/DE)

09 ⁰⁰ –10 ³⁰ Lecture hall A120 Chair	MS15: Frontiers of Structural Biology Methods Manfred Weiss (Berlin/DE)
09 ⁰⁰ MS15–T01	EMBL@PETRA3 – an integrated facility for structural biology Thomas R. Schneider (Hamburg/DE)
09 ³⁰ MS15–T02	The new D8 structural biology solutions for macromolecular crystallography: initial results Vernon Smith (Karlsruhe/DE)
09 ⁵⁰ MS15–T03	XDSAPP – a graphical user interface for processing diffraction data using XDS Uwe Mueller (Berlin/DE)
10 ¹⁰ MS15–T04	Localization and orientation of heavy atom cluster compounds using automated molecular replacement Sven Dahms (Jena/DE)
10 ³⁰ –11 ⁰⁰	Coffee Break and Industrial Exhibition
11 ⁰⁰ –12 ⁰⁰ P–05 Lecture hall M218 Chair	Bio-inspired crystallization – challenging single crystal shape and structure Fiona Meldrum (Leeds/GB) Wolfgang W. Schmahl (Munich/DE)
12 ⁰⁰ –13 ³⁰	Lunch Break and Industrial Exhibition
13 ³⁰ –14 ⁴⁵ Lecture hall M218 Chair	MS16: Structure & Function – Biomaterials II Erika Griesshaber (Munich/DE)
13 ³⁰ MS16–T01	Cellulose fibril orientation in primary cell walls of Arabidopsis thaliana (L.) Friederike Saxe (Potsdam/DE)
13 ⁴⁵ MS16–T02	Improved analysis of cellulose microfibril orientation distribution in hardwood by X-ray diffraction Markus Rueggeberg (Potsdam/DE)
14 ⁰⁰ MS16–T03	Characteristics of the aragonite – calcite transition in bivalve shells Klemens Kelm (Cologne/DE)

14 ¹⁵ MS16-T04	Crystallographic assembly of the coccolith elements of <i>Emiliania huxleyi</i> – an electron diffraction study Ramona Hoffmann (Munich/DE)
14 ³⁰ MS16-T05	The nanoscale composite nature of biological materials Patrick Alexa (Munich/DE)
13 ³⁰ –15 ¹⁵ Lecture hall A125 Chair	MS17: Structure & Function – New and Smart Materials Ulrich Bismayer (Hamburg/DE)
13 ³⁰ MS17-T01	The control of material properties by polyhedral tilting Ross Angel (Padova/IT)
13 ⁴⁵ MS17-T02	Structure and properties of the multiferroic BaTiO₃/Fe(001) interface Holger L. Meyerheim (Halle/DE)
14 ⁰⁰ MS17-T03	Structure-property relationships in mullite-type Bi₂M₄O₉ (M = Fe, Ga) and Bi₂Mn₄O₁₀ Jürgen Schreuer (Bochum/DE)
14 ¹⁵ MS17-T04	Structure of disordered Mo-Nb-V-Oxide precursor materials from pair distribution function analysis Reinhard Neder (Erlangen/DE)
14 ³⁰ MS17-T05	Filling vacancies in Ge/Sb/Te materials with lithium Thorsten Schröder (Munich/DE)
14 ⁴⁵ MS17-T06	In situ X-ray characterization and crystallographic investigation of inorganic catalysts for ammonia decomposition Claudia Weidenthaler (Mülheim an der Ruhr/DE)
15 ⁰⁰ MS17-T07	Wasserdesinfektion mittels pyroelektrischen mikro- und nanokristallinen LiNbO₃ und LiTaO₃ Erik Mehner (Freiberg/DE)
13 ³⁰ –15 ⁰⁰ Lecture hall A120 Chair	MS18: Frontiers in Crystallographic Techniques and Instrumentation II Martin Meven (Garching/DE)
13 ³⁰ MS18-T01	Experimental facilities for macromolecular crystallography at diamond light source Ralf Flaig (Didcot/GB)
13 ⁴⁵ MS18-T02	Patterson function solution by δ recycling Jordi Rius (Bellaterra/ES)

- 14⁰⁰
MS18-T03 **Mapping rocking curves of large crystals with high spatial resolution**
Robert Loetzsch (Jena/DE)
- 14¹⁵
MS18-T04 **High-definition X-ray polarimetry**
Berit Marx (Jena/DE)
- 14³⁰
MS18-T05 **High-brilliance X-ray sources for biological crystallography**
Jürgen Graf (Geesthacht/DE)
- 14⁴⁵
MS18-T06 **Yell – program for 3D-PDF diffuse scattering analysis**
Arakadiy Simonov (Zurich/CH)
- 15⁰⁰–16⁰⁰
P-06 **Integrated structural analysis of DNA double-strand break repair**
Lecture hall M218 Karl-Peter Hopfner (Munich/DE)
Chair Udo Heinemann (Berlin/DE)
- 16⁰⁰
Lecture hall M218 **Closing and Outlook 2013**
Wolfgang W. Schmahl (Munich/DE) – Conference Chair 2012
Dirk C. Meyer (Freiberg/DE) – Conference Chair 2013





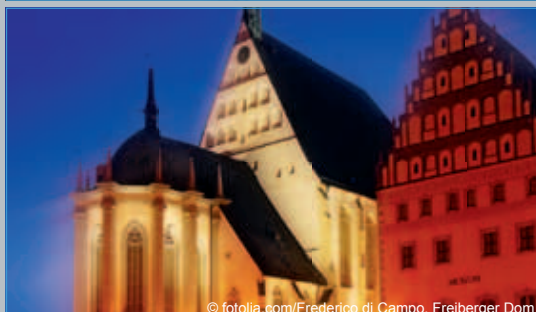
21st Annual Conference of the German Crystallographic Society

19–22 March

2013

Freiberg (Sachsen)

INVITATION



www.dgk-conference.de

		Page
MS01	Frontiers in Crystallographic Techniques and Instrumentation	44
MS02	Crystallography in Engineering and Technology	45
MS03	Biocrystallography and Medicine	47
MS05	Frontiers in Structure Analysis – Electron Density and other Precision Studies	47
MS06	Hot New Biomolecular Structures	48
MS07	Pressure-, Field-, & Temperature-Induced Processes	49
MS08	Spectroscopy	50
MS09	Structure of Biological Macromolecular Complexes	52
MS11	Aperiodic Crystals	52
MS12	Theory & Simulation	53
MS13	Structure & Function – Biomaterials	54
MS14	Structural Chemistry & Mineralogy	54
MS15	Frontiers of Structural Biology Methods	58
MS17	Structure & Function – New and Smart Materials	59
MS19	Preparative Methods for Crystalline Materials	60

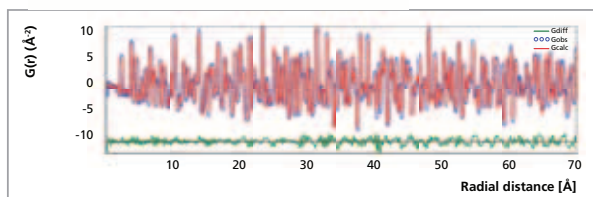
EMPYREAN

The world of X-ray diffraction is no longer flat



The new Empyrean from PANalytical is truly innovative, with cutting-edge technology in every aspect. Empyrean brings the idea of the perfect XRD platform to life.

- The widest range of samples: powders, thin films, nanomaterials, solid objects
- The highest data quality on every sample, no compromises
- Exceptional tube performance
- The highest performance goniometer
- 2nd generation PreFIX for optics and sample platforms
- PIXcel^{3D}: the only detector for 0D, 1D, 2D and even 3D applications
- Unmatched area detector dynamic range, linearity and resolution
- See inside your samples with the world's first 3D detector
- Unique performance in PDF and transmission measurements, using Ag or Mo radiation (see example).



Experimental PDF of silicon (blue dots) compared with a calculated PDF using the known structure of Si (red line).

Cutting-edge
technology.

Ultimate
commitment.

PANalytical GmbH
Nürnberger Straße 113
D-34123 Kassel
T +49 (0)561 5742 0
F +49 (0)561 5742 500
www.panalytical.de
info.de@panalytical.com

The Analytical X-ray Company



PANalytical

MS01	Frontiers in Crystallographic Techniques and Instrumentation
MS01-P01	Neue SAXS/WAXS-Anwendungen auf einem Vielzweck-Röntgenpulverdiffraktometer <u>D. Opper</u> , T. Schönbeck (Kassel/DE)
MS01-P02	Olex2 – a complete package for molecular crystallography <u>H. Puschmann</u> , O. Dolomanov (Durham/GB), L. Bourhis (Paris/FR) Richard Gildea (Berkeley, CA/US)
MS01-P03	Characterisation of matter and on site qualification of materials through X-ray diffraction Giovanni Berti (Pisa/IT)
MS01-P05	High-pressure cooling of virus crystals <u>A. Burkhardt</u> , M. Warmer (Hamburg/DE), A. Wagner (Didcot/GB) D. Stuart (Oxford/GB), R. Reimer, H. Hohenberg, A. Meents (Hamburg/DE)
MS01-P06	A moment in time – 100 Years of X-ray diffraction versus 100 days of PHOTON 100 CMOS detector <u>H. Ott</u> , M. Adam (Karlsruhe/DE), M. Ruf (Madison, WI/US)
MS01-P07	Revised fine-resolution neutron powder diffractometer E9 at BER II/HZB D. M. Többens, M. Tovar, <u>C. Stephan</u> (Berlin/DE), P. Henry (Lund/DK)
MS01-P08	Modular setup for measurement of pyroelectric coefficients and their temperature dependence <u>M. Ackermann</u> , P. Becker, L. Bohatý (Cologne/DE)
MS01-P09	Novel microfocus X-ray sources for high-pressure crystallography <u>T. Samtleben</u> , J. Graf, B. Hasse (Geesthacht/DE), F. Fabbiani (Göttingen/DE) M. Probert (Durham, NC/US), C. Michaelsen (Geesthacht/DE)
MS01-P10	Recent developments of beamline P24 (ChemCryst) at Petra III.14 <u>C. Paulmann</u> , A. Berghäuser, D. Ropers, D. Novikov, U. Bismayer (Hamburg/DE) S. Park, W. Schmahl (Munich/DE), D. Meyer (Freiberg/DE), C. Lehmann (Mülheim/DE) S. van Smaalen (Bayreuth/DE), S. Techert (Göttingen/DE)
MS01-P11	Investigations on specimen fluorescence using Co radiation with point and line X-ray detection systems R. Wenda, <u>T. Kirsch</u> (Nürnberg/DE), D. Götz (Almelo/NL)
MS01-P12	The improved state of STRESS-SPEC for texture characterization <u>W. Gan</u> (Garching/DE), C. Randau (Clausthal-Zellerfeld/DE), M. Hofmann (Garching/DE) N. Al-hamdany, H.-G. Brokmeier (Clausthal-Zellerfeld/DE), M. Müller A. Chreyer (Garching/DE)

- MS01-P13 **The new neutron single crystal diffractometer „BioDiff“ for macromolecular crystallography at the FRM II**
A. Ostermann, T. E. Schrader (Garching/DE), M. Monkenbusch, B. Laatsch (Jülich/DE)
 P. Jüttner, W. Petry, D. Richter (Garching/DE; Jülich/DE)
- MS01-P14 **Proofs of concept of on site X-ray diffraction using robotic technology**
 F. De Marco, G. Berti, M. E. Del Seppia (Pisa/IT)
- MS01-P17 **Molecular excited state-structure determination of metal organic compounds by time resolved X-ray crystallography at beamline P11 at PETRA III**
R. Raghunandan, A. Meents (Hamburg/DE)
- MS01-P18 **Recent software and hardware developments in the SuperNova dual source microfocus diffractometer**
Z. Gál, O. Presly, M. Meyer (Oxfordshire/GB)
- MS02 Crystallography in Engineering and Technology**
- MS02-P01 **Crystallographic description of ϵ -martensite via stacking faults in austenitic TRIP-steels**
S. Martin, D. Rafaja (Freiberg/DE)
- MS02-P02 **Early stages of cement hydration – an in-situ study utilizing high resolution SyXRD**
M.-C. Schlegel, A. Sarfraz, U. Mueller, U. Panne, F. Emmerling (Berlin/DE)
- MS02-P03 **Does K_2CaSiO_4 exist? – a phase-analytical study in the system K_2O - CaO - SiO_2 with implications for the characterization of residual materials**
V. Kahlenberg, E. Arroyabe, R. Tessadri, D. M. Többs (Innsbruck/AT)
- MS02-P04 **Roboter in der Diffraktometrie, keine neue Idee aber sehr effektiv an Stress-Spec**
H.-G. Brokmeier (Göttingen/DE), M. Hofmann, W. Gan, C. Randau (Garching/DE)
 M. Völler (Göttingen/DE), M. Müller (Garching/DE), A. Schreyer (Geesthacht/DE)
 W. Petry (Garching/DE)
- MS02-P05 **Herzenbergite as absorber material in thin-film solar-cells**
 Andreas Stadler (Salzburg/AT)
- MS02-P06 **Crystal structures and compaction behaviour of amine salts of acidic drugs**
C. H. Schwalbe (Cambridge/GB), M. Ramirez, S. David
 B. R. Conway (Birmingham/GB), P. Timmins (Moreton/GB)

- MS02-P07 **Cancrinit-Katoit Kokristallisation beim Recycling von Porenbeton (PB) im System PB-NaOH-NaAlO₂-Na₂CO₃-H₂O**
V. Petrov, A. Hartmann, J.-C. Buhl (Hanover/DE)
- MS02-P08 **Kinetics of dissolution/recrystallization of tobermorite, calcite and quartz from autoclaved aerated concrete (AAC) in NaOH and C₆H₈O₇ solutions**
G. Pawlas, A. Hartmann, V. Petrov, J. C. Buhl (Hanover/DE)
- MS02-P09 **X-ray micro-diffraction analysis of heterogenous concrete samples**
P. Schaub, E. Wieland, R. Dähn, A. Leemann (Villigen/CH)
- MS02-P10 **A statistical method applied to defocussing curves calculation**
B. Aguilar Sanjuan, P. Gomez (Mexico City/MX)
- MS02-P11 **Texture inhomogeneity through the thickness for copper tube**
N. Alhamdany (Garching/DE), H. G. Brokmeier (Clausthal-Zellerfeld/DE)
- MS02-P12 **Influence of mechanical defects on the crystal lattice of silicon**
T. Jauß, A. Danilewsky, J. Wittge, A. Cröll, J. Garagorri (Freiburg/DE), E. Reyes D. Allen (San Sebastian/ES), P. McNally (Dublin/IE)
- MS02-P13 **X-ray diffraction analysis of epitaxial ZnO/a-Al₂O₃ thin film**
N. Anouar (Sfax/TN), D. Schneider (Dresden/DE), H. Fuess (Darmstadt/DE)
M. Ben Ghazlen (Sfax/TN)
- MS02-P14 **Thermal stability and quantification of hydrogen release of NaBH₄ enclosed in aluminosilicate gels**
L. Schomborg, C. Rüschler, J.-C. Buhl (Hanover/DE)
- MS02-P15 **Development of a novel system for building artificial metalloenzymes for enantioselective catalysis**
M. Genz, D. Singer, J. Holldorf, E. Hey-Hawkins, R. Hoffmann, N. Sträter (Leipzig/DE)
- MS02-P16 **Synthesis and crystal structure of CoEu₂Si₃O₁₀**
M. Wierzbicka-Wieczorek (Jena/DE), G. Giester (Vienna/AT)
- MS02-P17 **Crystal structure of hemicarboaluminate cement phase**
T. Runcevski, R. Dinnebier (Stuttgart/DE), H. Pöllmann (Halle/DE)

MS03 Biocrystallography and Medicine

- MS03-P02 **Structural studies of DnaK in complex with proline rich antimicrobial peptides**
M. Zahn, D. Knappe, N. Berthold, R. Hoffmann, N. Sträter (Leipzig/DE)
- MS03-P03 **Pharmaceutical cocrystals as models for the study of drug-receptor interactions**
M. Tutughamiarso, E. Egert (Frankfurt a. M./DE)
- MS03-P04 **Structure determination complicated by tetragonal pseudosymmetry**
S. Barden, H. Niemann (Bielefeld/DE)
- MS03-P05 **Unraveling the function of uncharacterized operons in pseudomonas aeruginosa**
C. Feiler (Bayreuth/DE), D. V. Mavrodi, L. S. Thomashow
W. Blankenfeldt (Pullman, WA/US)

MS05 Frontiers in Structural Analyses – Electron Density and other Precision Studies

- MS05-P01 **Behind the scenes – an insight into the crystal energy landscapes of two new dimeric toluene-2,4-diisocyanate polymorphs**
L. Vella-Zarb, R. Dinnebier (Stuttgart/DE)
- MS05-P02 **From X-ray macro- and microstructure characterization substances and materials to sub-nano and electronic levels**
B. Kodess, P. Kodess (Moscow/RU)
- MS05-P03 **Static and dynamic charge densities of Lysozyme**
J. Netzel, S. van Smaalen (Bayreuth/DE)
- MS05-P04 **A new access to extinction corrections**
A. K. Hüsecken (Dortmund/DE), U. Pietsch (Siegen/DE)
- MS05-P05 **Direct insight into the effect of protonation and deprotonation of an organic molecule – the case of sulfadiazine**
F. Pan, R. Wang, U. Englert (Aachen/DE)
- MS05-P06 **The generalized invariom database**
B. Dittrich, C. Hübschle, K. Pröpper, T. Stolper (Göttingen/DE)

MS06	Hot New Biomolecular Structures
MS06-P01	Crystal structure of nicotiana tabacum malonyltransferase (NtMatI) in complex with its cofactor malonyl-CoA (MLC) C.-J. Liu (New York, NY/US), <u>Babu Manjasetty</u> (Grenoble/FR) X.-H. Yu (New York, NY/US), S. Panjikar (Victoria/AU) M. Chance (Cleveland, OH/US), G. Taguchi (Tokida/JP)
MS06-P02	SiiE – insights into a giant 5559 amino acids adhesin of <i>Salmonella enterica</i> <u>M. Griebel</u>, Y. A. Muller (Erlangen/DE)
MS06-P03	The trans-dienelactone hydrolase from cupriavidus necator – a novel metalloenzyme <u>C. Roth</u> (Leipzig/DE), S. Wegener, M. Schlömann (Freiberg/DE) N. Sträter (Leipzig/DE)
MS06-P04	Crystal structure of the autochaperone region of the <i>Shigella flexneri</i> autotransporter IcsA <u>K. Kühnel</u>, D. Diezmann (Göttingen/DE)
MS06-P05	Structural basis for furaneol formation in strawberry fruits <u>A. Schiefner</u>, Q. Sinz, I. Neumaier, W. Schwab, A. Skerra (Freising-Weihenstephan/DE)
MS06-P06	Structure of a classical MHC class I molecule that binds “non-classical” ligands <u>B. Loll</u>, C. Seng Hee, S. Gao (Berlin/DE), M. M. Miller (Duarte, CA/US) B. Uchanska-Ziegler, O. Daumke, A. Ziegler (Berlin/DE)
MS06-P07	The inhibited conformation of the eukaryotic Rrp44 exonuclease <u>D. Lika Makino</u>, M. Baumgartner, F. Bonneau, E. Conti (Martinsried/DE)
MS06-P08	Crystal structure of intraflagellar transport complex 25/27 E. Lorentzen, <u>S. Bhogaraju</u> (Martinsried/DE)
MS06-P09	Protein kinase domain of CTR1 from arabidopsis thaliana promotes ethylene receptor cross-talk H. Mayerhofer, <u>S. Panneerselvam</u>, J. Mueller-Dieckmann (Hamburg/DE)

MS07 Pressure-, Field-, & Temperature-Induced Processes

- MS07-P01 **Thermal stability of metastable fcc-(Ti,Al)N in nanoscaled TiN/AlN multilayers**
U. Ratayski (Freiberg/DE), F. Klimaschin (Freiberg/DE; Moscow/RU), U. Mühle
 D. Rafaja (Freiberg/DE)
- MS07-P02 **Temperatur- und feuchteabhängige Untersuchungen von Kanemit
 (NaHSi₂O₅ * 3 H₂O)**
D. Schmidmair, V. Kahlenberg (Innsbruck/AT), D. Toeblens (Berlin/DE)
 J. De Wit, U. Griesser (Innsbruck/AT)
- MS07-P03 **Partikelwachstum durch 3D-Rotation und Koaleszenz mittels Röntgenpulver-
 beugung in mesoskaligem NiO aufgedeckt**
M. Petrik, B. Harbrecht (Marburg/DE)
- MS07-P04 **Real structure of TSSG grown large Barium hexaferrite single crystals studied by
 white beam X-ray transmission topography**
J. Kräußlich, C. Dubs, O. Wehrhan, P. Görnert (Jena/DE)
- MS07-P05 **High (pressure, temperature) phase diagrams of ZnO and AlN from second
 harmonic generation measurements**
L. Bayarjargal, B. Winkler (Frankfurt a. M./DE)
- MS07-P06 **High resolution X-ray diffraction study of single crystals of lead zirconate titanate**
S. Gorfman (Siegen/DE), D. Keeble (Coventry/GB), M. Glazer (Oxford/GB)
 Z.-G. Ye (Burnaby/CA), P. Thomas (Coventry/GB)
- MS07-P07 **X-ray diffraction and spectroscopic study of selected amino acids and their
 derivatives at extreme conditions – high pressures and low temperatures**
 B. Zakharov, E. Boldyreva, B. Kolesov (Novosibirsk/RU)
- MS07-P08 **Thermal expansion of mullite-type Bi₂Fe₄O₉**
M. M. Murshed (Bremen/DE), H. Krüger (Innsbruck/AT), M. Burianek (Cologne/DE)
 G. Nénert (Grenoble/FR), V. Kahlenberg (Innsbruck/AT), M. Mühlberg (Cologne/DE)
 H. Schneider (Cologne/DE, Bremen/DE), R. Fischer, T. Gesing (Bremen/DE)
- MS07-P09 **High pressure behavior of wadeite K₂ZrSi₃O₉**
N. Niederwieser, C. Hejny (Innsbruck/AT)
- MS07-P10 **The effect of pressure, cooling rate and shear rate on the morphology of isotactic
 polypropylene**
S. Jilg, R. Forstner (Wels/AT)

- MS07-P11 **Experimental determination of orientation relations between the high- and low-pressure phases of InAs**
N. Pukallus, H. Sowa, H. Klein (Göttingen/DE)
- MS07-P12 **Domain redistribution in SrTiO₃ by application of electric fields and mechanical stresses**
J. Sidoruk, J. Leist, H. Gibhardt (Göttingen/DE), K. Hradil (Vienna/AT)
 B. Pedersen, M. Meven (Garching/DE), G. Eckold (Göttingen/DE)
- MS07-P13 **The X-ray study of phase transition in Sc doped TiOCl**
J. Zhang, A. Wölfel, M. Bykov (Bayreuth/DE), R. Kremer (Stuttgart/DE)
 S. van Smaalen (Bayreuth/DE)
- MS07-P14 **Interaction between point defects and higher dimensional defects in SrTiO₃**
J. Hanzig, B. Abendroth, F. Hanzig, H. Stöcker, D. C. Meyer (Freiberg/DE)
- MS07-P15 **Negative thermal expansion in chalcopyrite type multinary semiconductors**
S. Schorr, C. Stephan (Berlin/DE)
- MS07-P16 **Behaviour of alfa-boron at high pressures and temperatures**
N. Dubrovinskaia, G. Parakhonskiy, E. Bykova (Bayreuth/DE)
 M. Hanfland (Grenoble/FR), M. Merlini (Milano/IT), L. Dubrovinsky (Bayreuth/DE)
- MS07-P17 **In situ structural studies at conditions of earth and planetary mantles and cores: techniques and applications**
L. Dubrovinsky, K. Glazyrin, T. Boffa-Ballaran, E. Bykova
 N. Dubrovinskaia (Bayreuth/DE), M. Merlini (Milano/IT), M. Hanfland (Grenoble/FR)
- MS08 Spectroscopy**
- MS08-P01 **Application of a pnCCD in macromolecular crystallography**
S. Send, A. Abboud (Siegen/DE), W. Leitenberger (Potsdam/DE)
 M. S. Weiss (Berlin/DE), R. Hartmann (Munich/DE), L. Strüder (Siegen/DE, Munich/DE)
 U. Pietsch (Siegen/DE)
- MS08-P02 **X-ray diffraction, magnetization, and ⁵⁷Fe Mössbauer spectroscopic characterization of natural single-crystals of chrysoberyl**
 F. J. Litterst, S.-U. Weber (Braunschweig/DE), W. Lottermoser, G. Amthauer (Salzburg/AT)
- MS08-P03 **A table top picosecond pulsed X-ray and laser induced fluorescence spectrometer based on a streak camera system using 2D-photon counting**
N.-P. Pook, A. Adam, J.-C. Fruhner (Clausthal-Zellerfeld/DE), T. Franzl
 U. Denzer (Herrsching/DE)

- MS08-P04 **Annealing behaviour of radiation damaged minerals**
T. Beirau, C. Paulmann, B. Mihailova, U. Bismayer (Hamburg/DE)
- MS08-P05 **Characterisation of Lithium Local Environments in Lithium Cathode Materials by ^6Li and ^7Li MAS NMR Spectroscopy**
J. Kovacevic, M. Fechtelkord (Bochum/DE), D. Mikhailova (Dresden/DE)
H. Ehrenberg (Eggenstein-Leopoldshafen/DE)
- MS08-P06 **Investigation of molecular nature of the conjugated polymer films by resonance soft X-ray reflectivity**
D. Ksenzov, A. Davtyan, F. Schäfers, U. Pietsch, S. Grigorian (Siegen/DE)
- MS08-P07 **Optical spectroscopy on MnWO_4**
L. Dura, H. Gibhardt, J. Leist (Göttingen/DE), L. Bohaty, P. Becker (Cologne/DE)
G. Eckold (Göttingen/DE)
- MS08-P08 **Structure-property relationships in silicates – thermal expansion and elasticity of synthetic emerald**
P. Schröer, J. Schreuer (Bochum/DE)
- MS08-P09 **Structure-property relationships in silicates – thermal expansion and elasticity of natural scapolite**
K. Demtröder, P. Schröer, A. Bürger, J. Kovacevic, J. Schreuer (Bochum/DE)
- MS08-P10 **Electronic structure of single-crystalline $\text{Sr}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ probed by x-ray absorption spectroscopy – strong evidence for isovalent substitution of Fe^{2+} by Co^{2+}**
M. Merz, F. Eilers, T. Wolf, P. Nagel, H. von Löhneysen
S. Schuppler (Eggenstein-Leopoldshafen/DE)
- MS08-P11 **Single crystal dehydration of $\text{NaB}(\text{OH})_4$ -sodalites investigated by Raman depth profiling**
A. Schulz, C. Rüschler, J. Buhl (Hanover/DE)
- MS08-P12 **Thermal decomposition of sodium zincophosphate sodalite examined by autocorrelation analysis of temperature dependent FTIR spectra**
L. Robben, T. M. Gesing (Bremen/DE)

- MS09 Structure of Biological Macromolecular Complexes**
- MS09-P01 Elaboration of new objects belonging to coordination chemistry and molecular magnetism
M. Amel (Lyon/FR), B. Nouredine (Khenchela/DZ), D. Luneau (Lyon/FR)
- MS09-P02 The class C Vps tethering complexes HOPS and CORVET
H. Peters, U. Heinemann (Berlin/DE)
- MS09-P03 The Lin28 cold shock domain acts as an RNA chaperone
F. Mayr, A. Schuetz, U. Heinemann (Berlin/DE)
- MS09-P04 Structural basis of allosteric regulation of eukaryotic phosphofructokinases
M. Kloos (Leipzig/DE)
- MS11 Aperiodic Crystals**
- MS11-P01 Layer disorder in sodium-bismuth-titanate thin films grown by liquid-delivery spin MOCVD
M. Schmidbauer, J. Schwarzkopf, V. Kopp, V. Kaganer, A. Duk, F. Waidick
A. Kwasniewsk, T. Remmele (Berlin/DE)
- MS11-P02 One dimensional liquid-like disorder and phase ordering phase transition in short alkanes/urea inclusion compounds
C. Mariette, L. Guérin, P. Rabiller, B. Toudic, M. D. Hollingsworth (Rennes/FR)
- MS11-P03 The superstructure of trimethyltin hydroxide described in higher-dimensional superspace
S. Dey, A. Schönleber, S. van Smaalen (Bayreuth/DE)
- MS11-P04 Comparison of two structural models, “Superstructure” and “Modulated Structure” for cocrystal of phenazine chloroanilic acid at T=100 K
L. Noohinejad, S. van Smaalen, S. Mondal (Bayreuth/DE)
- MS11-P05 X-ray diffraction study of TiPO_4 structure at low temperatures
M. Bykov, J. Zhang, A. Schönleber, S. van Smaalen (Bayreuth/DE)
J. Law, R. Kremer (Stuttgart/DE), R. Glaum (Bonn/DE)

MS12 Theory & Simulation

- MS12-P01 Simulations of structure, growth and equilibrium form of GdVO_4 crystals
M. Nicolov (Arad/RO)
- MS12-P02 Surface energy calculations of fcc-, bcc- and hcp-metals by application of the bond deficiency model
A. Mutter (Cambridge/GB)
- MS12-P03 3D-PDF analysis of disordered single crystals
T. Weber, A. Simonov (Zurich/CH)
- MS12-P04 CCL – an algorithm for the efficient automatic comparison of clusters
J. C. Schön (Stuttgart/DE), R. Hundt (Bonn/DE), M. Jansen (Stuttgart/DE)
- MS12-P05 A forcefield simulation study – properties of amino acids on the magnetite-(111)-surface
A. Bürger, U. Magdang, H. Gies (Bochum/DE)
- MS12-P06 Molekularmechanische Simulation von Nitraminen mit dem Kraftfeld COMPASS
P. B. Kempa, M. Herrmann (Pfinztal/DE)
- MS12-P07 Calculation of thermodynamic parameters of melts from liquidus-curves
B. Simons (Cologne/DE)
- MS12-P08 Stacking disorder and diffuse scattering in tris(bicyclo[2.1.1]hexeno)benzene evaluated by lattice-energy minimisation
J. Glinnemann, M. U. Schmidt (Frankfurt a. M./DE)
- MS12-P09 Application of the maximum entropy method to X-ray powder diffraction data of ionic conductors
O. V. Magdysyuk, R. E. Dinnebier, M. Jansen (Stuttgart/DE)
- MS12-P10 Structure and IR spectra of $\text{Na}_8[\text{AlSiO}_4]_6(\text{BH}_4)_2$ sodalite – comparison between theoretical predictions and experimental data
M. Marcus, T. Bredow (Bonn/DE), L. Schomborg, C. H. Rücher
J.-C. Buhl (Hanover/DE)
- MS12-P11 Diffraction anomalous fine structure of Ho_2PdSi_3 and $\text{YMn}_{2-x}\text{Fe}_x\text{O}_5$
M. Nentwich, M. Zschornak (Freiberg/DE), C. Richter (Freiberg/DE, Hamburg/DE)
D. C. Meyer (Freiberg/DE)

- MS13 Structure & Function – Biomaterials**
- MS13-P01 **Locally resolved determination of anisotropic properties of human dental enamel**
L. Raue, H. Klein, C. Hartmann (Göttingen/DE)
- MS13-P02 **Rigid structure but mobile unit – crystal engineering as a tool to stabilize the structure – reducing mobility of a side-chain in cysteine containing crystals**
V. Minkov, E. Boldyreva (Novosibirsk/RU)
- MS13-P03 **Structural investigation of isopod cuticle and changes caused by decalcification monitored by sub μ -confocal Raman spectroscopy**
C. Reisecker (Linz/AT), B. Seidl, A. Ziegler (Ulm/DE), S. Hild (Linz/AT)
- MS13-P04 **Eine schwierige Kristallstrukturbestimmung aus Röntgenpulverdaten: Vorzugsorientierung, zwei Chlorid-Ionen auf speziellen Lagen und ein vierfach fehlgeordnetes 2-Butanol**
S. M. Hammer, J. Brüning, N. Nagel, M. U. Schmidt (Frankfurt a. M./DE)
- MS14 Structural Chemistry & Mineralogy**
- MS14-P01 **$K_2Ba_5Si_{12}O_{30}$ – a member of a homologous series among layered potassium barium silicates**
V. Kahlenberg (Innsbruck/AT)
- MS14-P02 **A new thiooxo-rhenate $(Et_4N)_2[(ReO(S_4)_2(\mu_2-S_2)(\mu_2-S))]$ and the reinvestigation of the crystal structure of $(Et_4N)[ReS_4]$**
A. J. Lehner, C. Röhr (Freiburg/DE)
- MS14-P03 **Sillenites – composition, structure, morphology, crystal growth**
T. Melnikova, G. Kuzmicheva, V. Rybakov, N. Bolotina (Moscow/RU)
A. Cousson (Cea, Saclay/FR)
- MS14-P04 **$Ca_xYb_{(1-x)}Ga$ – CrB type and related modulated superstructures**
B. Bauer, C. Röhr (Freiburg i. Br./DE)
- MS14-P05 **Synthesis, crystal structure and 7Li MAS NMR spectroscopy of the new compound $Li_3Zn_{6.9}In_{3.1}$**
V. Mihajlov, C. Röhr (Freiburg i. Br./DE)
- MS14-P06 **Metalide suboxide hydrides $Ba_{21}M_2O_5H_x$**
M. Jehle, (Freiburg/DE), H. Kohlmann (Saarbrücken/DE), H. Scherer
C. Röhr (Freiburg/DE)

- MS14-P07 **Synthesis and crystal structure of the first yttrium(III) bromide oxomolybdate(VI) $\text{YBr}[\text{MoO}_4]$**
I. Hartenbach, H. Henning, T. Schustereit, T. Schleid (Stuttgart/DE)
- MS14-P08 **Derivatives of 2-Aminopyrimidin-4-one – one or two tautomers present in the same crystal**
V. Gerhardt, E. Egert (Frankfurt a. M./DE)
- MS14-P09 **Synthesis and crystal structure of three new K-thioferrates – K_9FeS_7 , K_3FeS_3 and $\text{K}_{1.4}\text{FeS}_2$**
M. Schwarz, C. Röhr (Freiburg i. Br./DE)
- MS14-P10 **Synthesis and crystal structure of the new cesium ruthenate hydrate $\text{Cs}_2[\text{RuO}_3(\text{OH})]_2 \cdot \text{H}_2\text{O}$**
C. Hoch, C. Lenk (Stuttgart/DE)
- MS14-P11 **Crystal structure and phase transition of anhydrous copper(II) acetate, $\text{Cu}(\text{CH}_3\text{COO})_2$ and its relationship to copper(II) acetate monohydrate**
F. Preuschl, M. Wildner (Vienna/AT)
- MS14-P12 **Crystals and quasicrystals**
I. Leban (Ljubljana/SI)
- MS14-P13 **Introducing disorder into CaF_2 -Type $\text{Cs}_2[\text{B}_{12}\text{H}_{12}]$**
C. Hoch, L. W. Zimmermann, T. Schleid (Stuttgart/DE)
- MS14-P14 **Pb_5TeO_8 – a lead-rich oxotellurate(VI) previously reported as “ Pb_3TeO_6 ”**
M. Weil (Vienna/AT)
- MS14-P15 **Crystal structures of proline-derived enamines**
D. A. Bock, C. W. Lehmann, B. List (Mülheim an der Ruhr/DE)
- MS14-P16 **Kristallstrukturbestimmung des Bis-Kuppler-Azopigments P.Y. 155 aus Labor-Röntgenpulverdaten**
J. Brüning, E. Alig (Frankfurt a. M./DE), S. N. Ivashevskaja (Petrozavodsk/RU)
J. van de Streek (Frankfurt a. M./DE; Freiburg i. Br./DE), M. U. Schmidt (Frankfurt a. M./DE)
- MS14-P17 **“Umweganregung” in single crystal neutron diffraction experiments and its impact on the symmetry determination of bismuth metal oxides**
J. Birkenstock (Bremen/DE), E. Rossmannith (Hamburg/DE), G. Nénert (Grenoble/FR)
T. M. Gesing (Bremen/DE), H. Schneider (Cologne/DE), R. X. Fischer (Bremen/DE)
- MS14-P18 **Crystal structures of magnesium chloride hydrates**
H. Schmidt, E. Hennings, W. Voigt (Freiburg/DE)

- MS14-P19 **Low temperature hydrates of sodium salts**
E. Hennings, H. Schmidt, W. Voigt (Freiberg/DE)
- MS14-P20 **Synthesis and crystal structure of 1-(3-cyanopropyl)-3-methylpyridin-1-ium hexachloridoantimonate(V)**
M. Gjikaj, J. Zahlbach (Clausthal-Zellerfeld/DE)
- MS14-P21 **The crystal structure of the hydrated acid $(\text{H}_3\text{O})_2[\text{B}_{12}(\text{OH})_{12}] \cdot 3 \text{H}_2\text{O}$ displaying the dodecahydroxo-closo-dodecaborate anion**
L. W. Zimmermann, T. Schleid (Stuttgart/DE)
- MS14-P22 **Novel amides and amines of gallium – a brief discussion on synthesis and their crystal structures**
S. Zhang, R. Niewa (Stuttgart/DE)
- MS14-P23 **$\text{La}_{10.25}\text{O}_{0.25}\text{N}_{0.75}\text{Se}_{14}$ – the first lanthanum oxide nitride selenide with a stuffed $\text{Pr}_{10}\text{Os}_{14}$ -type structure and subtle interactions of La^{3+} cations**
C. M. Schurz, T. Schleid (Stuttgart/DE)
- MS14-P24 **The first quaternary potassium copper erbium sulfide – KCuEr_2S_4**
M. A. Eberle, T. Schleid (Stuttgart/DE)
- MS14-P25 **The anomalous annealing behaviour of Eifel sanidines – status quo and new approach with neutron diffraction**
J. Kähn, S. Schorr (Berlin/DE)
- MS14-P26 **Practical considerations concerning the efficient use of resonant X-ray scattering for distinguishing elements with similar electron count**
S. Welzmler, P. Urban (Leipzig/DE; Munich/DE), F. Fahnbauer (Munich/DE)
L. Erra (Grenoble/FR), O. Oeckler (Leipzig/DE; Munich/DE)
- MS14-P27 **Synthesis and crystal chemistry of manganese melilites and related phases**
S. Stöber, H. Pöllmann (Halle/DE)
- MS14-P28 **Element distribution and temperature-dependent changes in the crystal structure of $\text{Ge}_2\text{Sb}_2\text{Te}_5$**
P. Urban (Leipzig/DE; Munich/DE), L. Erra (Grenoble/FR), F. Fahnbauer (Munich/DE)
S. Welzmler (Leipzig/DE; Munich/DE), M. Schneider (Munich/DE)
O. Oeckler (Leipzig/DE; Munich/DE)
- MS14-P29 **Crystal structures of ammonium halogenidobismuthates(III)**
W. Frank, S. Schlöots, A. Q. Sachawars, W. Poll, S. Jörgens (Düsseldorf/DE)

- MS14-P30 **Ordered superstructures of $\text{Cu}_x\text{Ta}_{1-y}\text{S}_2$ at low temperatures**
S. I. Ali, S. van Smaalen (Bayreuth/DE), B. Harbrecht, S. Zörb (Marburg/DE)
- MS14-P31 **Structural characterization and discussion of new tetramethylgermane phases from powder data**
 L. Fink, Y. Krysiak, E. Alig, J. Glinnemann, M. Schmidt (Frankfurt a. M./DE)
- MS14-P32 **Structure determination from low-resolution powder diffraction data – crystal structure of the hydrous silicate RUB-52**
H. Gies, B. Marler, R. Wandolski, Z. Li (Bochum/DE)
- MS14-P33 **Anhydrous sodium trifluoroacetate – a 3D coordination polymer with 15 molecules in the asymmetric unit of the crystal structure**
G. Genchev, W. Frank (Düsseldorf/DE)
- MS14-P34 **Average structure of a new hydrous layered TMA-silicate, RUB-55, with silicate layers representing a section of the sodalite as well as octadecasil framework**
B. Marler, A. Grünwald-Lüke, S. Grabowski, H. Gies (Bochum/DE)
- MS14-P35 **Synthesis and crystal structure of AgErS_2 and AgTmS_2**
T. Schleid, S. Strobel, B. Spohn (Stuttgart/DE)
- MS14-P36 **Tm_2TeO_6 – a dimorphic thulium(III) oxotellurate(VI)**
P. Höss, S. Zitzer, T. Schleid (Stuttgart/DE)
- MS14-P37 **Isomorphous gallium substitution in mullite-type $\text{Al}_4\text{B}_2\text{O}_9$**
K. Hoffmann, M. M. Murshed, R. X. Fischer, T. M. Gesing (Bremen/DE)
- MS14-P38 **Crystal structures of short-chain alkali metal alkanesulfonates – anhydrous potassium methanesulfonate, rubidium methanesulfonate hemihydrate and an unusual 13:2 addition compound of potassium ethanesulfonate and potassium bicarbonate**
 W. Frank, J. Volk (Düsseldorf/DE)
- MS14-P39 **Pseudo-symmetry and unusual Cu^{2+}O_5 coordination figures in $\text{Na}_{18}\text{Cu}_3(\text{PO}_4)_8 \cdot 2\text{H}_2\text{O}$ and $\text{Na}_{18}\text{Cu}_3(\text{PO}_4)_8 \cdot 2\text{H}_2\text{O}$**
 H. Effenberger (Vienna/AT)
- MS14-P40 **Dimorphism of Bismuth(II) trifluoroacetate**
V. Verheyen, W. Frank (Düsseldorf/DE)
- MS14-P41 **Crystal structures of two alkaline earth methanesulfonate hydrates**
 T. Trella, V. Verheyen, W. Frank (Düsseldorf/DE)

- MS14-P42 **Complex structures of first uranyl borophosphates, borate phosphate and aluminoborate**
S. Wu (Kiel/DE), S. Wang, J. Diwu (Notre Dame/FR), O. Beermann, W. Depmeier
A. Holzheid (Kiel/DE), T. Malcherek (Hamburg/DE), E. Alekseev (Jülich/DE)
T. Albrecht-Schmitt (Notre Dame/FR)
- MS14-P43 **Morphology and crystal structure of fully hydrated Zeolite Na-A**
R. X. Fischer, M. Šehović (Bremen/DE), W. H. Baur (Western Springs/NZ)
C. Paulmann (Hamburg/DE), T. M. Gesing (Bremen/DE)
- MS15 Frontiers of Structural Biology Methods**
- MS15-P01 **EMBL mx1 beamline for macromolecular crystallography at Petra III @ DESY, Hamburg**
M. Cianci, G. Bourenkov, S. Fiedler, M. Roessle, T. Schneider (Hamburg/DE)
- MS15-P02 **Startup of macromolecular crystallography beamline P14/MX2@Petra III**
G. Bourenkov, M. Cianci, S. Fiedler, T. Schneider (Hamburg/DE)
- MS15-P03 **EMBL@Petra III – the new biosaxs beamline P12**
M. Roessle, S. Fiedler, G. Bourenkov, M. Cianci (Hamburg/DE), V. Haramus
R. Willumeit (Geesthacht/DE), D. Svergun, T. Schneider, M. Wilmanns (Hamburg/DE)
- MS15-P04 **Facilities for macromolecular crystallography at BESSY II -Berlin**
M. Weiss, M. Bommer, R. Förster, M. Hellmig, M. Krug, K. S. Paithankar, M. Steffien
M. Uhlein, U. Mueller (Berlin/DE)

MS17 Structure & Function – New and Smart Materials

- MS17-P01 **Structural and electrochemical studies of the Li-Zn alloys**
I. Chumak (Eggenstein-Leopoldshafen/DE), V. Pavlyuk (Lviv/UA)
 H. Ehrenberg (Eggenstein-Leopoldshafen/DE)
- MS17-P02 **Characterisation of nanocrystalline γ -Fe₂O₃ with synchrotron radiation techniques**
M. Hagelstein, S. Doyle, T. Liu, R. Steininger, D. Szabo
 S. Schlabach (Eggenstein-Leopoldshafen/DE), C. Ferrero, A. Fitch (Grenoble/FR)
 M. Scavini (Milano/IT)
- MS17-P03 **GTECS3D – a new program for graphtheoretical evaluation of extended network structures**
K. Lamberts, C. Merckens, R. Wang, U. Englert, D. Hons, S. Grüter, Y. Guo
 S. Porsche, A. Hamacher, D. Bündgens, T. Kühlen (Aachen/DE)
- MS17-P04 **Bimetallic coordination networks based on Al(acacCN)₃ – a building block between inertness and lability**
C. Merckens, N. Becker, K. Lamberts, U. Englert (Aachen/DE)
- MS17-P05 **Phase-matched spontaneous parametric down-conversion in optically biaxial crystals, example BiB₃O₆**
P. Becker (Cologne/DE), A. Halevy, E. Megidish, L. Dovrat
 H. S. Eisenberg (Jerusalem/IL), L. Bohatý (Cologne/DE)
- MS17-P06 **$\chi^{(3)}$ - nonlinear optical interactions in aragonite**
L. Bohatý (Cologne/DE), A. A. Kaminskii (Moscow/RU), P. Becker (Cologne/DE)
 H. Rhee, O. Lux, H. J. Eichler (Berlin/DE), V. V. Koltashev (Moscow/RU)
 R. Kleinschrodt (Cologne/DE)
- MS17-P07 **Synthesis and characterisation of new compositions with mullite type structure: Bi₂Cr_xM_{4-x}O₉ (M= Al, Ga) and Bi_{2-x}Sb_xAl₄O₉**
 T. Debnath (Dhaka/BD), C. Rüschler (Hanover/DE), A. Hussain (Dhaka/BD)
 L. Schomborg (Hanover/DE)
- MS17-P08 **Structural study of hydrous neodymium acetates**
P. Held, P. Becker, L. Bohatý (Cologne/DE)
- MS17-P09 **High-pressure investigations of spinel-type LiTM₂O₄ (TM = transition metal) cathode materials**
C. Braun, N. K. Yavuz, E. Reitz (Karlsruhe/DE)
 K. Nikolowski (Eggenstein-Leopoldshafen/DE, Dresden/DE)
 J. M. Gallardo-Amores, M. E. Arroyo-de Dompablo (Madrid/ES)
 H. Ehrenberg (Karlsruhe/DE, Eggenstein-Leopoldshafen/DE)

- MS17-P10 **Analysis of photochromic nanoparticles in silica monolith – a total scattering study**
K.-Y. Hsieh, D. Schaniel, E.-E. Bendeif (Vandoeuvre les Nancy/FR)
- MS17-P11 **Ternary and quaternary mixed valence compounds with interesting electrical properties**
 X. Kledi (Tirana/AL), K. Bente, M. Lorenz (Leipzig/DE)
- MS19 Preparative Methods for Crystalline Materials**
- MS19-P01 **The intermediate phase between sodalite and cancrinite – stability investigations of nanocrystals by TIR, STA and hydrothermal leaching**
C. Grader, J.-C. Buhl (Hanover/DE)
- MS19-P02 **Hydrothermal synthesis of eulytite ($\text{Bi}_4(\text{SiO}_4)_3$) crystals**
E. Marina, A. Marin, T. Bublikova, V. Balitsky (Chernogolovka, Moscow Distr./RU)
- MS19-P03 **Synthesis of large single crystal of sugilite**
S. H. Park, J. Heimhilger (Munich/DE)
- MS19-P04 **Neue Einblicke in mehr als 150 Jahre alte anorganisch- organische Hybridmaterialien auf Basis des Elementes Zinn – Synthese und strukturelle Charakterisierung von $[\text{Et}_2\text{Sn}(\text{OH})\text{NO}_3]$**
M. Reichelt, H. Reuter (Osnabrück/DE)
- MS19-P05 **From tin(II) to tin(IV) – one pot synthesis of three coordination compounds with tin in three different oxidation states (II-II/IV-IV) in the presence of fluorine ions and 1,10-phenanthroline**
H. Reuter, S. Schröder, N. Röwekamp-Krugley, M. Imwalle (Osnabrück/DE)
- MS19-P06 **Single crystal growth and characterization of the intermetallic compound InPd**
M. Hahne, P. Gille (Munich/DE)
- MS19-P07 **Characterization of thin films of $\text{Sn}_{1-x}\text{Pb}_x\text{S}$ mixed crystals ($0.0 < x < 0.5$)**
S. Lobe, G. Wagner, R. Kaden (Leipzig/DE), V. Gremenok, V. Lazenka (Minsk/BY)
 K. Bente (Leipzig/DE)
- MS19-P08 **Crystalline rare earth complex synthesis by solvent-drop assisted grinding**
 U. Baisch (Newcastle/GB)



CONVENTUS

- Congressmanagement & Marketing GmbH -

- Relief and support to organizing/scientific committees
- Professionalism
- Dependability and surety (competence)
- Increase profits
- Public relations management
- Attract new participants (attendees)
- Acquisition and maintenance (ongoing service) of industry partners
- Solicit new members



Neutronenstreuung für Kristallographen

Im unmittelbaren Anschluss an die Tagung bietet der Arbeitskreis Neutronenstreuung (AK7) vom 15. bis 16. März am Tagungsort einen Einführungskurs in die Neutronenstreuung speziell für kristallographische Fragestellungen an, der sich an Studenten und Wissenschaftler richtet, die einen Einstieg in dieses Thema suchen. Zu den vorgestellten Techniken gehören Pulver- und Einkristalldiffraktion sowie Kleinwinkelstreuung zur Untersuchung kristalliner und magnetischer Strukturen, inelastische Streumethoden zur Bestimmung struktureller und magnetischer Anregungen, die Analyse diffuser Streuung und Spannungsanalyse. Hierzu werden Beispiele aus der Kristallographie, Physik, Chemie, Biologie und den Materialwissenschaften präsentiert. Daneben werden auch praktische Aspekte wie der Zugang zu diesen Methoden an Großforschungseinrichtungen erörtert. Außerdem haben die Teilnehmer die Möglichkeit, intensiv mit den verschiedenen Experten zu diskutieren und die Experimentiereinrichtungen der Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) in Garching zu besichtigen. Eine Teilnahmegebühr wird nicht erhoben.

Donnerstag, 15. März 2012

13³⁰ Anreise Garching Forschungszentrum
(Personalausweis ist notwendig)

Treffpunkt Forschungs-Neutronenquelle
Heinz Maier-Leibnitz
Lichtenbergstraße 1
85748 Garching

14⁰⁰ Begrüßung und Führung am FRM II

16³⁰ Ende der Führung

Freitag, 16. März 2012, HS A125

09⁰⁰ Pulvermethoden – Kristallstruktur

09⁴⁵ Pulvermethoden – Magnetismus

10³⁰ Kaffeepause

11⁰⁰ Einkristalldiffraktion – Kristallstruktur

11⁴⁵ Einkristalldiffraktion – Magnetismus

12³⁰ Mittagspause

14⁰⁰ Spektroskopie – Phononen/Magnonen

14⁴⁵ Diffuse Streuung

15³⁰ Kaffeepause

16⁰⁰ Materialwissenschaften

16⁴⁵ Biologie – Weiche Materie

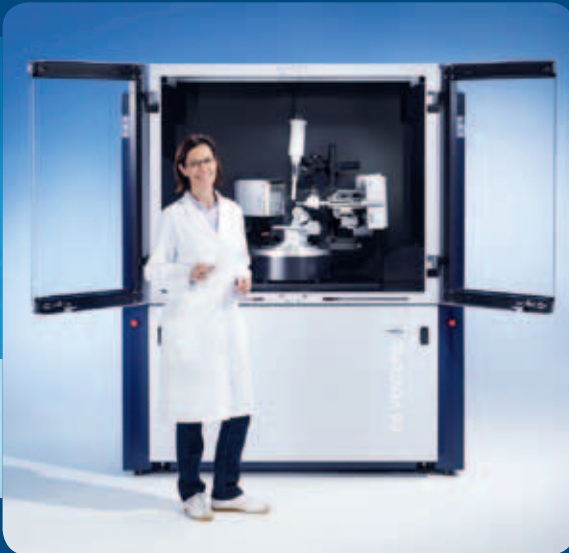
17³⁰ Ende der Veranstaltung



FRM II
Forschungs-Neutronenquelle
Heinz Maier-Leibnitz



Three Wishes Granted...



The new D8 VENTURE with PHOTON 100

- High Performance
- Low Maintenance
- Brightest Microfocus

The D8 VENTURE is the perfect answer to all your questions in single crystal X-ray structure determination. The D8 VENTURE features excellent sample access and visibility. The patented doors either can be opened in a sliding-door-mode or as swinging doors. In addition to single source configurations the D8 VENTURE accommodates dual wavelength configurations. Based on the principles of DAVINCI.DESIGN it is engineered with high modularity from best-in-class components.

www.bruker.com

Innovation with Integrity

SC-XRD

A		C	
Abrikosov, I.	36	Chumak, I.	59
Ackermann, M.	44	Cianci, M.	58
Adam, M.	29	Cramner, P.	36
Alekseev, E.	37		
Alexa, P.	39	D	
Alhamdany, N.	46	Dahms, S.	38
Ali, S. I.	57	Danilewsky, A.	27
Amel, M.	52	Data, K.	30
Amthauer, G.	32	Davtyan, A.	51
Angel, R.	27, 39	Demtröder, K.	51
Anouar, N.	46	Dey, S.	52
Aroyo, M. I.	35	Diestel, U.	30
Authier, A.	26	Dittrich B.	47
		Dix, I.	29
B		Doert, T.	35
Baisch, U.	60	Dosch, H.	26
Baker, E. N.	26	Dubrovinskaia, N.	50
Barden, S.	47	Dubrovinsky, L.	50
Bauer, B.	54		
Bayarjargal, L.	49	E	
Becker, P.	59	Eberle, M. A.	56
Behrendt, K.	35	Eckert, M.	26
Beirau, T.	51	Effenberger, H.	57
Berthold, C.	27	Ehrenberg, H.	28
Berti, G.	44, 45	El-Sayed, K.	28
Bhogaraju, S.	48	Englert, U.	30
Biertümpfel, C.	33		
Birkenstock, J.	55	F	
Bismayer, U.	34, 37, 39	Fabbiani, F.	30
Bock, D. A.	55	Fechtelkord, M.	32
Bohatý, L.	59	Feiler, C.	47
Boldyhyreva, E. S.	49, 54	Fillenberg, S.	33
Bourenkov, G.	58	Fischer, R. X.	58
Bracher, A.	30	Flaig, R.	39
Braden, M.	25, 28	Fortes, D.	37
Braun, C.	59	Friedrich, A.	31
Brokmeier, H.-G.	45, 46	Friese, K.	35
Brüning, J.	55		
Bürger, A.	53	G	
Burghammer, M.	27	Gan, W.	44
Burkhardt, A.	44	Gäl, Z.	45
Bykov, M.	52	Genchev, G.	57
Bykova, E.	32	Genz, M.	46
		Gerhardt, V.	55
		Gibhardt, H.	51
		Gies, H.	57
		Glinnemann, J.	53
		Gnutzmann, T.	37
		Gomez, P.	46
		Gorfman, S.	34, 49
		Grader, C.	60
		Graf, J.	40
		Griesshaber, E.	37, 38
		Grießl, M.	48
		Gröschel, A.	29
		Grünwald, M.	33
		Grzechnik, A.	32
		Guerin, L.	35
		Gutmann, M.	37
		H	
		Hagelstein, M.	59
		Hahne, M.	60
		Hammer, S.	54
		Hanzig, J.	50
		Hartenbach, I.	55
		Hartmann, A.	27
		Hartmann, C.	27
		Haussühl, E.	32, 34
		Heinemann, U.	40
		Held, P.	59
		Hennings, E.	56
		Hinterstein, M.	34
		Hoch, C.	55
		Hoelzel, M.	27
		Hoffmann, R.	39, 47
		Hoffmann, K.	57
		Hopfner, K.-P.	25, 30, 40
		Höss, P.	57
		Hsieh, K.-Y.	60
		Huber, R.	26
		Hübschle, C. B.	30
		Hüsecken, A. K.	47

J

Jansen, M.	25, 31
Jauß, T.	46
Jehle, M.	54
Jeyaprakash, A. A.	30
Jilg, S.	49

K

Kadletz, P. M.	33
Kahlenberg, V.	45, 54
Kähn, J.	56
Kelm, K.	38
Kempa, P. B.	53
Kisker, C.	28
Kloos, M.	52
Kodess, B.	47
Kovacevic, J.	51
Kräußlich, J.	49
Krug, U.	30
Kühnel, K.	48
Kurnosov, A.	27
Küttner, B.	28

L

Lamberts, K.	59
Leban, I.	55
Lecomte, C.	30
Lehmann, C.	30
Lehner, A. J.	54
Lobe, S.	60
Loetzsch, R.	40
Loll, B.	48
Lottermoser, W.	33
Luger, P.	30
Lühns, H.	37

M

Magdysyuk, O. V.	53
Maier, B.	34
Makino, D. L.	48
Manjasetty, B.	48
Marcus, M.	53
Mariette, C.	52
Marina, E.	60

Marler, B.	57
Martin, S.	45
Marx, B.	40
Mayr, F.	52
Mehner, E.	39
Meldrum, F.	25, 38
Melnikova, T.	54
Merkens, C.	59
Merz, M.	51
Metzger, S. J.	37
Meven, M.	27, 39
Meyerheim, H. L.	39
Mihajlov, V.	54
Mittl, P.	28
Mondal, S.	30
Mueller, U.	38
Müller, M.	27, 35
Murshed, M. M.	49
Mutter, A.	53

N

Neder, R.	37, 39
Nentwich, M.	53
Netzel, J.	47
Nicolov, M.	53
Niederwieser, N.	32, 49
Nolze, G.	29
Noohinejad, L.	52

O

Oppen, D.	44
Ostermann, A.	45
Ott, H.	44
Otte, K.	36

Peters, H.	52
Petrik, M.	49
Petrov, V.	46
Pietsch, U.	27
Pook, N.-P.	50
Poulsen, H.F.	26
Prymak, O.	37
Pukallus, N.	50
Puschmann, H.	44

Q

Quiroga, C.	32
-------------	----

R

Raabe, G.P.	35
Rafaja, D.	27
Raghunandan, R.	45
Ram, F.	29
Ratayski, U.	49
Raue, L.	54
Reichelt, M.	60
Reisecker, C.	54
Reuter, H.	60
Rius, J.	39
Robben, L.	51
Roessle, M.	58
Rosenthal, T.	29
Roske, Y.	33
Roth, C.	48
Rueggeberg, M.	38
Runcevski, T.	46
Russo, L.	45

S

Samtleben, T.	29, 44
Santos, K.	31
Saxe, F.	38
Schaub, P.	35, 46
Scheu, C.	29
Schiefner, A.	48
Schlegel, M.-C.	45
Schleid, T.	57
Schlichting, I.	25, 36

U

Schloots, S.	56	Urban, P.	56
van Smaalen, S.	35		
Schmahl, W. W.	38		
Schmalen, I.	28		
Schmidbauer, M.	52		
Schmidmair, D.	49		
Schmidt, H.	55		
Schmitzova, J.	31		
Schneider, T. R.	38		
Schnick, W.	31		
Schomborg, L.	46		
Schön, J. C.	53		
Schönleber, A.	34		
Schorr, S.	50		
Schreiner, M.	28		
Schreuer, J.	39		
Schröder, T.	39		
Schroer, C.	33		
Schröer, P.	51		
Schulz, A.	51		
Schurz, C. M.	56		
Schwalbe, C. H.	45		
Schwarz, M.	55		
Schwarzenbach, D.	26		
Send, S.	50		
Senyshyn, A.	28		
Shi, J.	34		
Sidoruk, J.	50		
Simonov, A.	40		
Simons, B.	53		
Smith, V.	38		
Sommerdijk, N.	29, 37		
Stadler, A.	45		
Stephan, C.	44		
Stöber, S.	56		
Stöger, B.	35		

V

Vella-Zarb, L.	47
Verheyen, V.	57
Vit, A.	28
Volk, J.	57

W

Wahl, M.	33
Weber, S.-U.	33, 50
Weber, G.	33
Weber, T.	53
Weckert, E.	25, 34
Weidenthaler, C.	39
Weil, M.	55
Weiss, I.	33
Weiss, M.	38, 58
Welzmler, S.	56
Wildner, M.	55
Wiehl, L.	32
Wierzbicka-Wieczorek, M.	46
Will, J.	29
Wu, S.	58

Z

Zahlbach, J.	56
Zahn, M.	47
Zhang, J.	50
Zhang, S.	56
Ziegler, A.	37
Zimmermann, L. W.	55

T

Than, M.	28
Thomas, N.	35
Trots, D.	32
Tutughmiarso, M.	47

Mehr als blau



Die Zeitschrift

In den *Nachrichten aus der Chemie* machen Wissenschaftler auf das hohe Potenzial ihrer Forschungsergebnisse aufmerksam, denn Spitzenforschung ist zu wertvoll, um nach jahrelanger intensiver Arbeit nur in Primärjournalen publiziert zu werden.

Registration and Confirmation

Registration is subject to capacity limitations. Registration must include the name of any accompanying person to ensure their inclusion into the planning of the social programme. Upon receipt of registration invoice or confirmation, registration is considered official and effectual. This document is a valid VAT invoice which may be submitted to the local tax and revenue office for tax purposes.

Invoicing and Due Date for Fees

Fees for the scientific programme of the event, the social evening and the social programme will be charged in the name and on behalf of the company Conventus inclusive the statutory VAT rate of 19% (as of 2010). All fees are due upon receipt of the registration invoice or confirmation form. Transfer payments must include the name of the participant and the invoice number, otherwise they will not be accepted. All major credit cards are accepted.

Scope of Services

Event fees includes participation in the scientific programme only. Additional fees for the social programme will apply. Included in this fee are programme book, abstract CD, name tags and a certificate of attendance. These items are generally handed out at the venue.

Cancellations, Changes, Refunds

Cancellations can be made in written form only but is not possible anymore. A cancellation fee of 25 EUR will apply. The same terms apply for cancellations of the social programme, however no cancellation fee will be charged. Any cancellations after this date or no-shows at the event are not eligible for a refund and the full fee in accordance to the registration invoice or confirmation will be due. Any changes in booking, after booking confirmation has been issued, will result in a handling fee of 15 EUR. Any requested additions to existing reservations or reservations made during the event on-site will be processed according to availability.

Event Cancellation, Refunds

There is limited capacity for all events. For certain events a minimum number of participants is required. If the minimum number of participants is not reached, the organiser reserves the right to cancel all or parts of the event on a short-term notice. In this case, all paid fees will be fully refunded.

Force Majeure, Disclaimer

The organiser is responsible for all changes to individual parts of the event. Claims for damages are excluded if the staging of the event or individual components are hampered or prevented by unexpected political or economic events or generally by force majeure or by the cancellation of speakers or if similar changes are required.

Hotel Reservations, Disclaimer

Conventus acts as an intermediary for hotel reservations and therefore assumes no liability for reservations. Changes and cancellations have to be addressed to the according hotels directly. The cancellation terms of the individual hotels apply.

Limitation of Liability

Conventus acts as an intermediary for the programme offered by the organiser and, therefore, assumes no liability whatsoever for the event. Any liability for services and possible problems with the services lies exclusively with the provider of services. Participation in activities of the social programme is exclusively at one's own risk.

Conventus assumes liability for death or injury to body or health, provided there has been negligence or an intentional breach of duties by the event organiser, its legal representatives, or vicarious agents.

In the event of any other damage, the liability of Conventus, its legal representatives and its vicarious agents is limited to deliberate and gross negligent conduct, provided that no essential contractual obligations have been breached.

Applicable Law, Place of Performance and Jurisdiction

The laws of the Federal Republic of Germany apply excluding the *U.N. Convention on Contracts for the International Sale of Goods* (CISG).

To the extent allowed by law, Jena is the place of performance and jurisdiction for all claims.

Use and Storage of Data

Information provided by you will be solely used for the purposes of contractual performance and/or the sending of event invitations from Conventus Congress Management & Marketing GmbH. Your information will not be provided to third parties unless you have provided written consent. You have the right to request information at any time about your saved data without giving reason. Information can also be edited, delete or blocked at any time. You may withdraw your consent to use your personal information by contacting direktmarketing@conventus.de or by postal mail at: Conventus Congressmanagement & Marketing GmbH, Attn: Marketing, Carl-Pulfrich-Straße 1, 07745 Jena. Our online form is also available at www.conventus.de/mailling.

24 February 2010

Introducing AZtec®

A-Z technology for nanoanalysis

innovative
fast
integrated



The most powerful,
most flexible
materials characterisation
system
you'll ever see

email: AZtec@oxinst.com

www.oxford-instruments.com/AZtec

facebook.com/oxinst • twitter.com/oxinst • youtube.com/oxinst



The Business of Science®

I μ S High Brilliance



- for Cu, Mo & Ag
- up to 60% more intensity
- component recognition
- improved safety features
- fully compliant with Machinery Directive 2006/42/EC