



21st Annual Conference of the German Crystallographic Society

19–22 March

Freiberg (Sachsen)

From Symmetry to Function



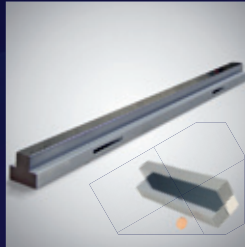
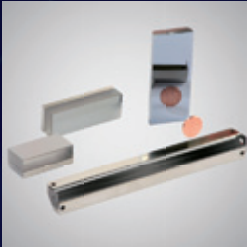
PROGRAMME



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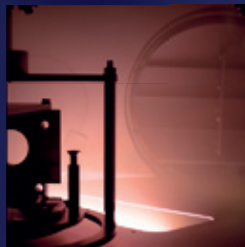
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for Cu, Mo, Ag, Cr and Co



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Conference Organiser

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

Conference Chair

Prof. Dirk C. Meyer

TU Bergakademie Freiberg, Institut für Experimentelle Physik

Leipziger Straße 23

09599 Freiberg (DE)

Local Organising Committee

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Claudia Funke

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Juliane Hanzig

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Edwin Kroke

Tilman Leisegang

Dirk C. Meyer

David Rafaja

Ulrike Wunderwald

Matthias Zschornak

Scientific Committee

DGK Executive Board

DGK Working Group Chairs

Former Conference Chairs

All speakers of the DGK working groups, the members of the DGK board and distinguished DGK members and former conference presidents were invited to participate in the abstract reviewing process and the constitution of the scientific programme.

Conference Organisation

Conventus Congressmanagement & Marketing GmbH

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Editorial Deadline

05 March 2013

Dear Colleagues,

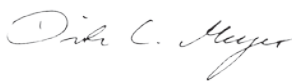
It is a great honour and pleasure for me to invite you all on behalf of the local organizing committee to the 21st Annual Conference of the German Crystallographic Society (DGK) in Freiberg at the beginning of spring 2013. Our venue is located in the center of the Free State of Saxony.



The scope of this 21st DGK annual meeting in Freiberg is to cover the whole innovation chain from fundamental research via applied crystallography science to application. Accordingly we have invited plenary speakers representing relevant fields of modern crystallography as well as representatives of the local industries, which are successful global players. In particular we are proud, that Prof. Dan Shechtman, Nobel Prize Laureate of 2011, has accepted our invitation to give a public lecture at this conference. It is our aim to provide all of you and especially the scientific sections of our society an accessible and inspiring scientific platform. In particular we would like to encourage young crystallographers to interact and participate in the development of the DGK. For this purpose a dedicated 'young crystallographer' session will be part of the programme.

We are looking forward to your attendance and contributions from all fields of crystallography.

Kind regards



Prof. Dirk C. Meyer
Conference Chair

DGK Working Group Meetings

We will provide the following seminar rooms for the usual meetings.

Seminar room 1116 (Julius-Weisbach-Bau)

Seminar room 1105 (Ledebur-Bau)

Seminar room 1085 (Erich-Rammeler-Bau)

If you are planning to hold an assembly, please send an email to felix.angermueller@conventus.de or coordinate this onsite. The Arbeitskreis-Meetings will be announced at the info board next to the check-in.

Special Industrial Symposium

With the Industrial Symposium we present a forum for the commercial aspects of crystallography. We have invited Directors of the three global acting companies which produce semiconductor wafers at their local sites in Freiberg. In their talks Dr. Neuhaus (SolarWorld Innovations); Dr. Mühe (Siltronic AG) and Dr. Eichler (Freiberger Compound Materials GmbH) will present the companies profile and give an impression of the challenges of today's market.

Dan Shechtman received the Nobel Prize in Chemistry in 2011 for the discovery of quasicrystals. He proved for the first time the existence of aperiodic crystalline structures in the system Al-Mn in 1982 and published his observations in 1984.

Following his PhD studies at the Technion – Israel Institute of Technology in Haifa, which he finished in 1972, he spent three years as NRC Fellow at the Aerospace Research Laboratory at Wright Patterson Air Force Base in Ohio. Since 1975 he was a member of the department of materials engineering at the Technion in Israel. The work which made him famous originates from the time of his sabbatical at the Johns Hopkins University, Baltimore, during the years 1981–1983. Studying Al-Mn alloys in the transmission electron microscope, he observed for the first time 10-fold symmetric diffraction patterns. Until that time, it was believed that only structures consisting of 3-dimensionally periodic lattices can give rise to sharp interference patterns. These structures can possess 2-, 3-, 4- or 6-fold symmetries but never 5- or 10-fold symmetries. Since his discovery contradicted all common sense and science, it took him as long as 2 years to confirm and verify his results. Dan Shechtman showed in his work that structures with periodicity in higher dimensional space really exist in nature and yield indeed their own characteristic footprints in diffraction patterns.

In 1984 Dan Shechtman returned as Associate Professor to the Department of Materials Engineering at Technion and became Full Professor in 1986. Since 1998 he is Distinguished Professor of the Philip Tobias Chair for Materials Science at the Technion.

Symposium Young Crystallographers

The DGK board explicitly addresses the young generation of crystallographers and wishes to support the young scientist in defining their own platform of communication, networking and commutation of experiences.

Hence, the young members of the DGK are invited and encouraged to establish their dedicated Arbeitskreis during this conference.

The constitution of an Arbeitskreis Young Crystallographers should also be aimed at an advertisement of crystallographic science to the community of young scientists and, in gaining new members, keeping the DGK young.

To constitute this platform during the conference, a Young Crystallographers Symposium will be organized. Ms Sibylle Gemming (Helmholtz-Zentrum Dresden-Rossendorf/TU Chemnitz) will mentor this meeting and will further act as linker between the young crystallographers and the DGK board. Additionally, during this Symposium Ms Aline Bergert (e-learning center, TU Bergakademie Freiberg) will present some possibilities of organizing web-based social networks.

If the participants agree on the spot on a suitable and convenient concept, Ms Bergert will assist them in the spontaneous setup of a web-based platform.

A special issue of the journal Crystal Research and Technology (CRAT) will comprehend the scientific outcome of the conference according to the motto “from symmetry to function”. This issue will be dedicated to mirror the current state of crystallography in 2013 and specifically to the linkage between fundamental research, functionality and application. In collaboration with the editors of the journal, Dirk C. Meyer and Barbara Abendroth, both of the TU Bergakademie Freiberg, will be the guest editors of this special issue. All plenary speakers are invited to submit a paper of their presentation. Further, speakers of the DGK Arbeitskreise and the session chairmen are invited to suggest one or more selected contributions out of the community. These papers should reflect, similar to the scope of the conference, not only a distinguished research but also should illuminate the connection of fundamental crystallographic research to application or potential applications in the respective fields of research.

A book is coming home

The university library of the TU Bergakademie Freiberg owns a number of unique collections including manuscripts, rare and precious prints, scientific remains and autographs, engineering drawings, maps and coins.

Dr. Wolfgang Hönle, member of the DGK and for a long time co-editor of the journal “Zeitschrift der Kristallographie” is a collector of rare books. Some decades ago he bought a historic book about basics of physics and chemistry from 1832 in an antiquarian bookshop. It was written by Karl Wilhelm Gottlob Kastner (1783–1857), a German chemist and the academic teacher of Justus von Liebig (1803–1873). The book was formerly a part of the library of the Bergakademie. For unknown reasons, it was withdrawn from the inventory in 1971. On the occasion of the annual DGK Meeting in Freiberg, Dr. Hönle will return the book to the university library which is very grateful for his donation.

Installation of a bronze relief in commemoration of the discovery of indium and germanium by scientists of the Bergakademie Freiberg

The bronze relief to be installed in the entrance area of castle Freudenstein displays the two elements indium and germanium to commemorate their discovery by Clemens Winkler, Ferdinand Reich and Theodor Richter at the Bergakademie Freiberg.

The 150th anniversary of the discovery of indium by Ferdinand Reich (1799–1882) and Hieronymus Theodor Richter (1824–1898) in the year 1863 is the occasion for installing the bronze relief.

Today, Indium is an important resource for semiconductor industry since it is necessary for the production of transparent electrodes using indium tin oxide. The discovery of Germanium by Clemens Winkler (183–1904) dates back to the year 1886. Nowadays, applications of the element semiconductor germanium are found in high-frequency devices, different detectors and optical elements.

Being a central place within Freiberg, the installation of the relief on the Schlossplatz symbolizes the present importance of these two elements for the semiconductor industry and Freiberg. Also, the Schlossplatz reflects the close connection between Freiberg and the university since it will be the center of the future “science corridor”.

Venue and Date (for GPS)

Neue Mensa
Agricolastraße 10a
09599 Freiberg (DE)
19–22 March 2013

Conference Website

www.dgk-conference.de

Registration

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

DGK-Member	150 EUR
DGK Non-Member	180 EUR
Student*	70 EUR
Get Together, 19 March 2013	10 EUR
Social Evening, 21 March 2013	30 EUR

*Confirmation required

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 before 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 respective hotel directly.

Good for the environment. Convenient for you. Travel by train from 99 EUR to to the congresses and events of Conventus 2013.



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			Regular fair	Savings	Regular fair	Savings
Hamburg	↔	Freiberg	332 EUR	173 EUR	216 EUR	117 EUR
Frankfurt a. M.	↔	Freiberg	284 EUR	125 EUR	199 EUR	100 EUR
München	↔	Freiberg	288 EUR	129 EUR	178 EUR	97 EUR
Berlin	↔	Freiberg	204 EUR	45 EUR	107 EUR	8 EUR

Conventus Congressmanagement & Marketing GmbH and Deutsche Bahn wish you a pleasant journey!

* 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 30 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.



- 1 Venue Neue Mensa
- 2 Social Evening at Tivoli
- 3 Terra Mineralia
- 4 St. Mary's Church
- 5 Reiche Zeche

Publishing of Abstracts

The abstracts will be published in a printed supplement of the journal “Zeitschrift für Kristallographie” (Oldenbourg Verlag). You can order this booklet online and onsite for 50 EUR. Please note that the supplements will be sent to you after the conference.

Poster Awards

All posters will be rated according to scientific basis and visual appearance. The best posters will be awarded. The poster prices are sponsored by Jena Bioscience GmbH and Oldenbourg Verlag.



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 at the foyer in the ground floor.

Media Check-In

The media check-in is located in seminar room 2, 1st floor.

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

	19 March	20 March	21 March	22 March
Industrial Exhibition	16 ³⁰ –19 ³⁰	10 ⁰⁰ –17 ¹⁵	10 ⁰⁰ –17 ¹⁵	09 ³⁰ –10 ³⁰
Poster Exhibition	–	10 ³⁰ –18 ¹⁵	09 ⁰⁰ –18 ⁰⁰	–
Check-In	13 ³⁰ –19 ⁰⁰	08 ⁰⁰ –18 ³⁰	08 ⁰⁰ –18 ³⁰	08 ⁰⁰ –13 ⁰⁰
Media Check-In	15 ⁰⁰ –19 ⁰⁰	08 ³⁰ –18 ³⁰	08 ³⁰ –18 ⁰⁰	08 ³⁰ –11 ⁰⁰

Internet

There are computers with internet access available at media check-in (seminar room 2). Additionally Wi-Fi will be provided. The name of the network is “gast”. The password is “days2013”.

Catering

During the breaks, snacks and beverages will be provided for free of charge, except for the lunch breaks. Lunch will be sold at costs.

Service for Handicapped Persons

The premises are suitable for the handicapped.

Restaurants nearby the conference venue:

Restaurant Schwanenschlößchen
Meißner Ring 33 • 09599 Freiberg
Phone +49 (0)3731 21 65 33
Distance from the conference venue: 0,5 km

Hotel Kreller
Fischerstraße 5 • 09599 Freiberg
Phone +49 (0)3731 359 00
Distance from the conference venue: 1,3 km

Stadtwirtschaft Freiberg
Burgstraße 18 • 09599 Freiberg
Phone +49 (0)3731 69 24 69
Distance from the conference venue: 1,0 km

Hotel am Obermarkt
Waisenhausstraße 2 • 09599 Freiberg
Phone +49 (0)3731 263 70
Distance from the conference venue: 1,1 km

Pizzeria Little Cesar
Meißner Gasse 5 • 09599 Freiberg
Phone +49 (0)3731 24 82 35
Distance from the conference venue: 0,9 km

Kartoffelhaus Am Schüppchenberg
Berggasse 7 • 09599 Freiberg
Phone +49 (0)3731 35 56 00
Distance from the conference venue: 1,3 km

Pfeffersack historische Gastwirtschaft
Kirchgasse 15 • 09599 Freiberg
Phone +49 (0)3731 45 86 76
Distance from the conference venue: 0,9 km

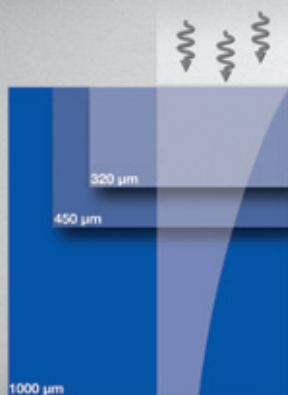
Gaststätte Ratskeller
Obermarkt 16 • 09599 Freiberg
Phone +49 (0)3731 221 51
Distance from the conference venue: 1,1 km

HIGH-ENERGY SENSORS

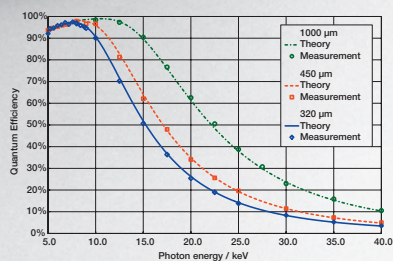
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Photon energy	Sensor thickness (μm)		
	320	450	1000
5.4 keV (Cr)	94 %	94 %	94 %
8.0 keV (Cu)	97 %	98 %	98 %
12.4 keV (1 Å)	72 %	84 %	98 %
17.5 keV (Mo)	37 %	47 %	76 %
22.2 keV (Ag)	20 %	27 %	50 %



sales@dectris.com | www.dectris.com

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Submitting Your Presentation/Technical Information

Please prepare your presentation in 4:3 aspect ratio.

A presentation notebook with a PDF reader and MS Office PowerPoint 2007 will be provided. The use of personal notebooks is possible upon agreement. However, it may interrupt the flow of the programme in the lecture hall. Please provide an adapter for VGA if necessary.

A notebook, presenter and laser pointer are available at the speaker's podium in the lecture hall. A technical supervisor will help you.

Speakers preparation

Please submit your presentation at the media check-in (seminar room 2) no later than 90 minutes before the presentation should begin. You may view and/or edit your presentation.

For submission, please use a USB flash drive, CD or DVD disc which should not be copy-protected.

Poster Sessions

Posters should be no larger than DIN A0 portrait format (84.1 cm x 118.9 cm). Poster boards are 120cm x 150cm. They are only to be used with the designated pins. Poster boards will be numbered. You will find your poster number in the programme book on page 47 ff.



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Systat Software GmbH (Erkrath/DE)

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AXO Dresden GmbH (Dresden/DE)
Bruker AXS (Karlsruhe/DE)
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EFG GmbH (Berlin/DE)
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FIZ Karlsruhe (Eggenstein-Leopoldshafen/DE)
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INCOATEC GmbH (Geesthacht/DE)
International Union of Crystallography (Chester/GB)
Jena Bioscience GmbH (Jena/DE)
MK Versuchsanlagen (Mücke-Merlau/DE)
Oldenbourg Wissenschaftsverlag GmbH (Munich/DE)
Oxford Cryosystems (Long Hanborough/GB)
PANalytical GmbH (Kassel/DE)
Rigaku Europe SE (Ettlingen/DE)
Röntgenlabor Dr. Ermrich (Reinheim/DE)
Stoe & Cie GmbH (Darmstadt/DE)
XENOCSS SA (Sassenage/FR)



Media Cooperations

DIV Deutscher Industrieverlag GmbH (Munich/DE)
„Zeitschrift für Kristallographie“
Elsevier B. V. (Amsterdam/NL)
„Journal of Crystal Growth“
Gesellschaft Deutscher Chemiker e. V. – GDCh (Frankfurt a. M./DE)
„Nachrichten aus der Chemie“
International Union of Crystallography – IUCr (Chester/GB)
„Acta Crystallographica“ • „Journal of Applied Crystallography“ • „Journal of Synchrotron Radiation“
Springer Healthcare Ltd. (London/GB)
„Journal of Chemical Crystallography“
Springer Science + Business Media B. V. (Dordrecht/NL)
„Biogeochemistry“
Cambridge University Press (Cambridge/GB)
„The European Physical Journal – Applied Physics“
Wissenschaftliche Verlagsgesellschaft (Stuttgart/DE)
„Naturwissenschaftliche Rundschau“

State at printing

Wednesday, 20 March 2013, 12¹⁵–13¹⁵, Lecture Hall 1

Bruker AXS (Karlsruhe/DE)



Speakers Björn Hansson, Carsten Michaelsen, Martin Adam, Eric Hovestreydt

Bruker, Incoatec and Excillum are pleased to invite you. Again you can expect 'fresh from the press' information on our products.

This does include exciting results from the recently announced D8 VENTURE with METALJET. We will address new stand-alone options, but also software and hardware upgrades for existing XRD and SC-XRD installations.

The seminar is a perfect opportunity to see familiar faces but also to welcome new members to the family.

Thursday, 21 March 2013, 12¹⁵–13¹⁵, Lecture Hall 1

Agilent Technologies (Waldbronn/DE)

Speaker Mathias Meyer

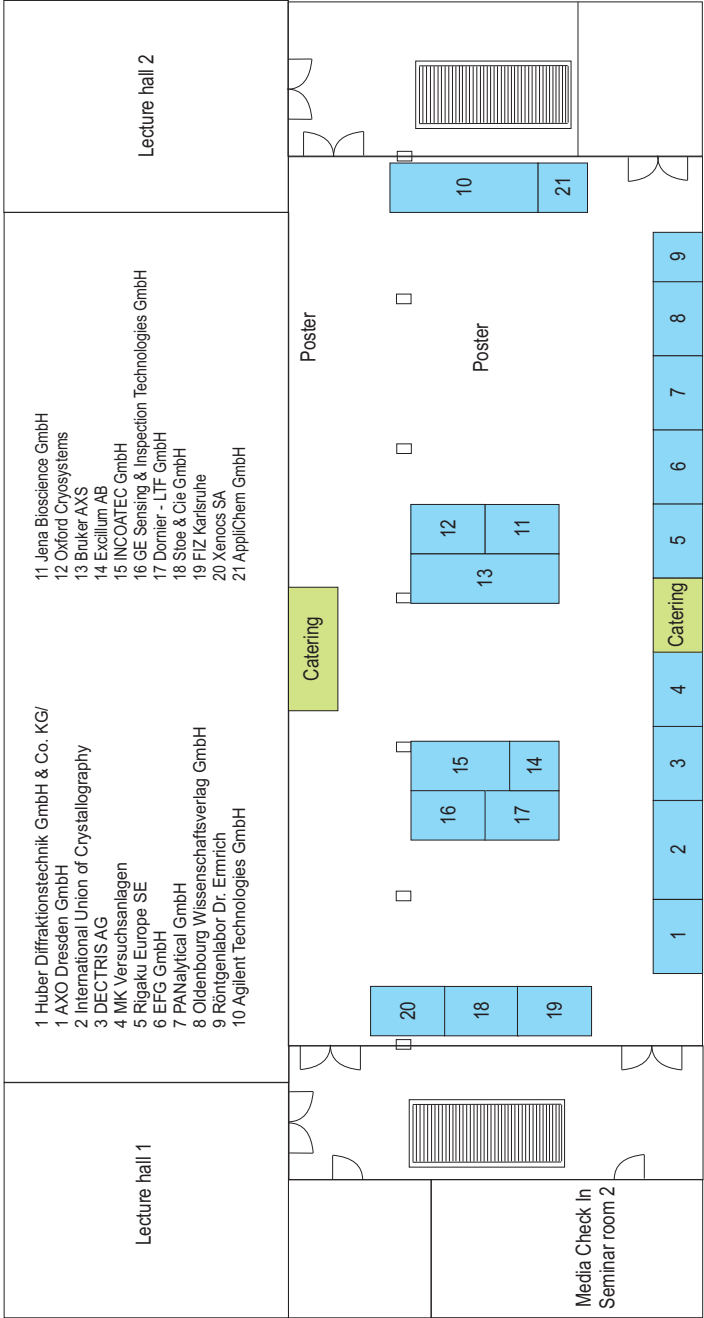


Agilent Technologies

"CrysAlisPro: A Perfect Tool from Crystal to Structure". CrysAlisPro covers all aspects of crystal screening, experiment planning and strategy, data reduction and corrections, processing pipelines for automated structure solution and refinement.

The talk will cover these subjects and highlight new developments in hard- and software. It will also cover the use for non-Agilent diffraction data formats.

Floor Plan



Get Together

Come together for drinks and snacks and enjoy this evening and allow yourself interesting conversations with colleagues, old friends, exhibitors and new acquaintances.

Date	Tuesday, 19 March 2013
Venue	Industrial exhibition area
Time	18 ³⁰ –19 ³⁰
Fee	10 EUR



© fotolia.com/Farina3000

Terra mineralia – Around the world in 90 minutes

This is an entertaining as well as history-charged round tour of the exhibition from A for 'Ausstellungskonzept' (exhibition concept) to Z for 'Zepterquarz' (sceptre quartz). This guide gives an overview of the most beautiful exhibits from every continent, the origin of the exhibition, the changeable past of Freudenstein Castle and the collector's passion. The tour ends at the Terra mineralia.



© Stadtverwaltung Freiberg, 2012

Date	Wednesday, 20 March 2013
Time	15 ⁰⁰ –16 ³⁰
Fee	12 EUR
Language	German
Meeting point	terra mineralia Schloss Freudenstein • Schlossplatz 1 • 09599 Freiberg max. 20 participants
Distance from venue	800 m (by feet 10 minutes)

Descent in shaft 'Reiche Zeche'

The shaft 'Reiche Zeche' with its spacious mining claim provides visitors with the opportunity to explore the history of the Freiberg ore mining, which goes back to the 14th century, via secured vertical and horizontal corridors of a total of 14 km length and depth up to 230 m. This tour will lead us through 2 km of former mining area. The tour ends at the conference venue.



© fotolia.com/Erik Schuhmann

Date	Wednesday, 20 March 2013
Time	14 ¹⁵ –17 ¹⁵
Duration tour	2 h
Fee	30 EUR
Language	German
Meeting point	Check-In max. 20 participants

Guided Tour through St. Mary's Church with the organ 'Silbermannsorgel'

The St. Mary's Church was built towards the end of the 12th century. Since 1537, the Freiberg cathedral is an evangelical lutheran church. The cathedral is famous for its gateway 'Goldene Pforte', the two organs 'Silbermann-Orgeln', the pulpit 'Bergmanns- und Tulpenkanzel', the roman crucifixion, the graves 'Fürstengrablege' and several other historical artifacts. The great organ in the western gallery was built by Gottfried Silbermann between 1711 and 1714. The guided tour contains an audio sample of this great organ. The tour ends at the church.



© fotolia.com/Frederico di Campo

Date	Thursday, 21 March 2013
Time	16 ⁰⁰ –17 ⁰⁰
Fee	10 EUR
Language	German
Meeting point	Freiberger Dom Untermarkt 1 • 09599 Freiberg, Saxony max. 20 participants
Distance from venue	850 m (by feet 11 minutes)

Social Evening at Tivoli Freiberg

Many famous artists have experienced the stage floor of the Tivoli. Take the chance to get in touch with friends and colleagues and have an enjoyable evening in the Concert- and Ballhouse Tivoli in Freiberg.



© Tivoli Freiberg

Date	Thursday, 21 March 2013
Time	20 ⁰⁰ –23 ⁰⁰
Fee	30 EUR
Address	Konzert- und Ballhaus Tivoli Dr.-Külz-Straße 3 • 09599 Freiberg, Saxony
Distance from venue	1 km

Company Tours

In the course of our conference we are offering you to visit the premises of some local manufacturing companies in the field of crystallography.

Get introduced in the processes from the production to the final products and learn about the companies' philosophy and status within an extensive guided tour through the production halls. To reach the companies' sites a shuttle transfer will be available. The tours end at the conference venue.

Siltronic AG

Date	Wednesday, 20 March 2013
Duration	14 ⁴⁰ –17 ¹⁵
Fee	10 EUR
Meeting point	14 ³⁰ at the Check-In max. 20 participants

Deutsche Solar GmbH

Date	Thursday, 21 March 2013
Duration	13 ¹⁰ –15 ⁴⁵
Fee	10 EUR
Meeting point	13 ⁰⁰ at the Check-In max. 20 participants

Freiberger Compound Materials GmbH

Date	Thursday, 21 March 2013
Duration	13 ¹⁰ –15 ⁴⁵
Fee	10 EUR
Meeting point	13 ⁰⁰ at the Check-In max. 20 participants

Prof. Peter van Aken
Max Planck Institute for Intelligent Systems
Stuttgart Center for Electron Microscopy (StEM)
Heisenbergstraße 3 • 70569 Stuttgart (DE)

Prof. Claudia Felser
Max Planck Institute for Chemical Physics of Solids
Inorganic Chemistry
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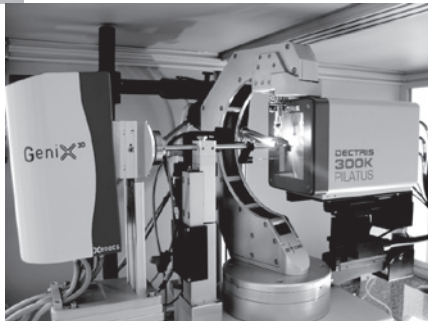
Prof. Susan Schorr
Helmholtz-Zentrum Berlin für Materialien und Energie
Department of Crystallography
Hahn-Meitner-Platz 1 • 14109 Berlin (DE)

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Technion
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Technion City • 32000 Haifa (IL)

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Tuesday 19 March 2013

	Audimax	Lecture Hall 1	Lecture Hall 2
09:00	09:00–14:00		
	DGK Board Meeting Aula, Raum 1.12 Universitätshauptgebäude		
10:00			
11:00			
12:00			
13:00			
	p. 28		
14:00			
15:00	15:00–15:30		
	Conference Opening p. 28		
	15:30–16:30		
16:00	Claudia Felser p. 28		
		Coffee Break and Industrial Exhibition	
17:00	17:00–18:30	17:00–18:30	17:00–18:30
	MS01 Non-ambient Conditions: Pressure, Temperature and Fields at Work I	MS02 General Crystallography: Modelling and Analysis Bridging the Scales I p. 30	MS04 Crystallography in Materials Science: Real Structures I
18:00		MS03 Aperiodic and Modulated Structures: Potential in Higher Dimensions p. 30	p. 31
	p. 28	18:30–19:30	
		Get Together in the Industrial Exhibition	
19:00			
			p. 19
20:00		20:00–21:30	
		Public Lecture Dan Shechtman in the Alten Mensa	p. 31

Wednesday 20 March 2013

	Audimax	Lecture Hall 1	Lecture Hall 2
09:00	09:00–10:00		
	Václav Holý		
	p. 32		
10:00	Coffee Break and Industrial Exhibition		
	10:30–12:00	10:30–12:00	10:30–12:00
	MS05	MS06	MS07
11:00	Non-ambient Conditions: Pressure, Temperature and Fields at Work II	General Crystallography: Modelling and Analysis Bridging the Scales II	Spectroscopy and other Tools for Analysis I
	p. 32	p. 32	p. 34
12:00	Lunch Break		12:00–13:00
		12:15–13:15	Symposium
		Lunchsymposium	Young Crystallographers
		Brucker AXS	p. 35
13:00		p. 35	
	13:30–14:30		
	Peter van Aken		
14:00	p. 35		
	14:30–16:00		
	Poster Session, Coffee Break and Industrial Exhibition		
15:00			p. 35
16:00	16:00–17:00	16:00–17:00	16:00–17:00
	MS08	MS09	MS10
	Non-ambient Conditions: Pressure, Temperature and Fields at Work III	Crystallography in Materials Science: Real Structures II	Spectroscopy and other Tools for Analysis II
	p. 35	p. 36	p. 37
17:00	Coffee Break and Industrial Exhibition		
	17:15–18:15	17:15–18:15	17:15–18:15
	MS08	MS09	MS11
	Non-ambient Conditions: Pressure, Temperature and Fields at Work III	Crystallography in Materials Science: Real Structures II	Along the Innovation Chain: From Minerals and Crystals via Natural Sciences to Functional Materials
18:00	p. 35	p. 36	p. 38
	18:15–19:15		
	DGK Members Meeting		
19:00	p. 38		
	Snack Break at the Foyer Audimax		
	19:30–21:00		
	DGK Ehrenabend		
20:00			
	p. 38		

Programme Overview

Thursday 21 March 2013

	Audimax	Lecture Hall 1	Lecture Hall 2
09:00	09:00–10:00 Keith Moffat p. 39		
10:00	Coffee Break and Industrial Exhibition		
	10:30–12:00	10:30–12:00	10:30–12:00
11:00	MS12 Biocrystallography: Synthesis, Structure and Function I p. 39	MS13 Crystal Physics, Crystal Chemistry: Synthesis and New Crystal Structures I p. 40	MS14 Crystallography: History, Art, Cultural Heritage, Teaching and Public Communication p. 40
12:00	Lunch Break	12:15–13:15 Lunchsymposium Agilent Technologies p. 41	
13:00	13:30–14:30 Rüdiger Kniep p. 41		
14:00		14:30–16:00 Poster Session, Coffee Break and Industrial Exhibition	
15:00			p. 41
16:00	16:00–17:00 MS15 Biocrystallography: Synthesis, Structure and Function II p. 41	16:00–17:00 MS17 Materials for Electronics: Energy and Data Storage through the Eyes of Crystallographers p. 42	16:00–18:15 MS18 Industrial Symposium
17:00	Coffee Break and Industrial Exhibition		
	17:15–18:15	17:15–18:15	
18:00	MS16 Biocrystallography: Biomimetic Materials, Drug Design, Processes and Functions p. 42	MS17 Materials for Electronics: Energy and Data Storage through the Eyes of Crystallographers p. 42	p. 43
19:00			
20:00	20:00–23:00 Social Evening p.20		

Friday 22 March 2013			
	Audimax	Lecture Hall 1	Lecture Hall 2
09:00	09:00–10:00		
	Susan Schorr		
	p. 44		
10:00	Coffee Break and Industrial Exhibition		
	10:30–11:45	10:30–12:30	10:30–12:30
	MS19	MS20	MS21
11:00	Biocrystallography: Biomimetic Materials, Drug Design, Processes and Functions, Others	Crystal Physics, Crystal Chemistry: Synthesis and New Crystal Structures II	Cutting Edge Techniques in Analysis and Preparation
	p. 44		
12:00		p. 46	p. 46
	12:30–13:00		
	Conference Closing		
13:00	p. 47		

09⁰⁰–14⁰⁰ DGK Board Meeting

Aula, Room 1.12 Universitätshauptgebäude, Akademiestraße 6

15⁰⁰ Conference Opening

Audimax

15³⁰ Heusler compounds – From spintronics to topological insulators

Audimax

Speaker

C. Felser (Dresden/DE)

Chair

A. M. Deac (Dresden/DE)

16³⁰–17⁰⁰ Coffee Break and Industrial Exhibition

17⁰⁰–18³⁰ MS01 –Non-ambient Conditions – Pressure, Temperature and Fields at Work I

Audimax

Chair

M. Meven (Garching/DE)

17⁰⁰ Neutrodiffraction at the Swiss Neutron Spallation Source SINQ

MS01–T01

M. Frontzek, D. Cheptiakov, O. Zaharko, S. Van Petegem, J. Gavilano (Villigen-PSI/CH)

17¹⁵ X-ray diffraction investigations under non ambient conditions at the Rossendorf Beamline ROBL

MS01–T02

C. Baetz, J. Grenzer, O. Roshchupkina (Dresden/DE), P. Kidambi, B. Bayer
S. Hofmann, R. Weatherup (Cambridge/GB)

17³⁰ Diamond anvils with a spherical support designed for X-ray and neutron diffraction experiments in DAC

MS01–T03

N. Dubrovinskaia, L. Dubrovinsky (Bayreuth/DE), M. Hanfland (Grenoble/FR)
M. Hofmann (Garching/DE)

17⁴⁵ Oxygen diffusivity in silicon derived from dynamical X-ray diffraction

MS01–T04

J. Will, A. Gröschel, C. Bergmann, A. Magerl (Erlangen/DE)

18⁰⁰ XRD In-situ studies of Crystallization of different TiO₂ thin films

MS01–T05

R. Kuzel, L. Nichtova, A. Kadlecova, Z. Matej, Z. Hubicka, S. Kment
J. Bursik (Prague/CZ)

18¹⁵ Diffusion constants from time-resolved powder diffraction data analysed with a shrinking-core model

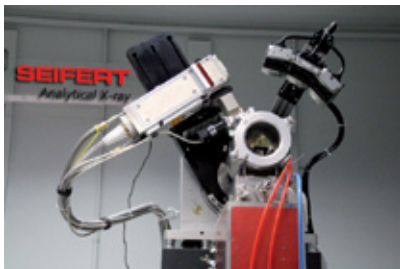
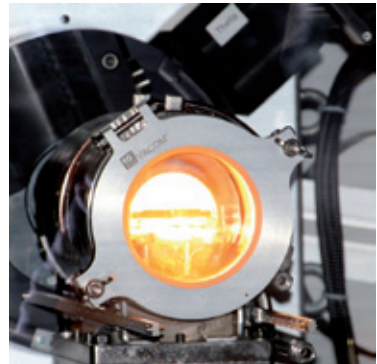
MS01–T06

A. Falenty, M. Jansen, A. N. Salamatina, W. F. Kuhs (Göttingen/DE)

Seifert Sun XRD

Röntgendiffraktometer für schnelle In-situ-Anwendungen (z. B. CIGS PV)

Das Seifert Sun XRD ist speziell entwickelt worden für Echtzeituntersuchungen von Temperaturübergängen in der Metallurgie oder auch der Dünnschichttechnologie wie den CIGS – Cu(In,Ga)Se_2 Systemen in der Fotovoltaik. Im Sekundentakt können Reaktionen unter den unterschiedlichsten Rahmenbedingungen wie Druck, Temperatur und Heizraten an großflächigen Proben untersucht werden.



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17⁰⁰–17⁴⁵

Lecture Hall 1
Chair

MS02 – General Crystallography – Modelling and Analysis Bridging the Scales I

P. Paufler (Dresden/DE)

17⁰⁰

MS02–To1

Struktur und Dynamik von Einzelmolekülen eingebettet in Nanoporen

T. Woike (Dresden/DE)

17¹⁵

MS02–To2

Nucleation of ZnO Nanoparticles – structural changes of precursor and nuclei

M. Zobel, R. Neder (Erlangen/DE)

17³⁰

MS02–To3

Experimental evidence of orbital order for icosahedral B₁₂ cluster in boron-rich solids

S. Mondal, S. van Smaalen, N. Dubrovinskaia, L. Dubrovinski (Bayreuth/DE)

17⁴⁵–18³⁰

Lecture Hall 1
Chair

MS03 – Aperiodic and Modulated Structures – Potential in Higher Dimensions

S. van Smaalen (Bayreuth/DE)

17⁴⁵

MS03–To1

The modulated structure of 1-Adamantanammonium 4-fluorobenzoate

A. Schönleber, S. van Smaalen (Bayreuth/DE), H.-C. Weiss (Leverkusen/DE)

A. J. Kesel (Munich/DE)

18⁰⁰

MS03–02

The theory of proper ferroelectrics with an incommensurate phase in complex compounds with structural defects

B. Gadjiev (Dubna/RU)

18¹⁵

MS03–To3

The crystal structure of modulated 2:1 mullite (Al_{4.8}Si_{1.2}O_{9.6}) revisited

J. Birkenstock (Bremen/DE), V. Petříček (Prague/CZ), B. Pedersen (Garching/DE)

H. Schneider, (Bremen, Cologne/DE), R. X. Fischer (Bremen/DE)

17⁰⁰–18³⁰ MS04 – Crystallography in Materials Science – Real Structures I

Lecture Hall 2

Chair H. Fueß (Darmstadt/DE)

17⁰⁰ MS04–To1 Stacking fault energy obtained from in-situ X-ray diffraction experiments under bending

D. Rafaja, S. Martin, P. Gallardo Martinez (Freiberg/DE)

17¹⁵ MS04–To2 Electric field stabilized polar phase in strontium titanate single crystals at room temperature

J. Hanzig, M. Zschornak, B. Abendroth, F. Hanzig, E. Mehner, H. Stöcker, C. Röder, A. Talkenberger, G. Schreiber, D. Rafaja (Freiberg/DE), S. Gemming (Dresden/DE), D. C. Meyer (Freiberg/DE)

17³⁰ MS04–To3 Multi-temperature high-resolution study of diffuse X-ray scattering in $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$

S. Gorfman (Siegen/DE), D. Keeble, P. Thomas (Coventry/GB)

17⁴⁵ MS04–To4 Quantitative phase analysis in partially stabilised zirconia by combined XRD and EBSD characterisation

S. Martin, D. Rafaja (Freiberg/DE)

18⁰⁰ MS04–To5 Anisotropic 1D domain pattern in NaNbO_3 epitaxial thin films grown on (110) TbScO_3

M. Schmidbauer, A. Duk, J. Schwarzkopf (Berlin/DE)

18¹⁵ MS04–To6 Characterization of dislocations and cracks in freestanding GaN single crystals

I. Ratschinski, H. S. Leipner, F. Heyroth, W. Fränzel (Halle/DE), G. Leibiger, F. Habel (Freiberg/DE)

18³⁰–19³⁰ Get Together in the Industrial Exhibition

20⁰⁰ Quasi-Periodic Materials – Crystal Redefined

Alte Mensa

Speaker D. Shechtman (Haifa/IL)

Chairs W. Schmahl (Munich/DE), D. C. Meyer (Freiberg/DE)

Venue for the Public Lecture of Prof. Dan Shechtman:

Alte Mensa

Petersstraße 5

09599 Freiberg

09⁰⁰

Audimax
Speaker
Chair

Electronic Materials seen by X-rays

V. Holý (Prague/CZ)
D. Rafaja (Freiberg/DE)

10⁰⁰–10³⁰

Coffee Break and Industrial Exhibition

10³⁰–12⁰⁰

Audimax
Chair

MS05 – Non-ambient Conditions – Pressure, Temperature and Fields at Work II

U. Schwarz (Dresden/DE)

10³⁰

MS05–To1

Synthesis and thermal behavior of pauflerite, β -VOSO₄, and it's polymorph modification, α -VOSO₄

S. Filatov, R. Bubnova, M. Krzhizhanovskaya (St. Petersburg/RU)

10⁴⁵

MS05–To2

High-pressure crystal structure of Bi₁₂GeO₂₀ sillenite from single-crystal X-ray diffraction and theory

L. Wiehl, A. Friedrich, E. Haussühl, W. Morgenroth, B. Winkler (Frankfurt a. M./DE)

11⁰⁰

MS05–To3

Structures and stabilities of NaLnF₄ and KLnF₄ compounds at ambient and high pressures

K. Frieze (Jülich/DE), A. Grzechnik (Aachen/DE)

11¹⁵

MS05–To4

Compressibility of orthorhombic FeB₄ studied on a single crystal sample

E. Bykova, H. Gou, N. Dubrovinskaia (Bayreuth/DE), M. Merlini
M. Hanfland (Grenoble/FR), L. Dubrovinsky (Bayreuth/DE)

11³⁰

MS05–To5

Single crystal elasticity of Na_{1.07}Mg_{1.58}Al_{4.91}Si_{1.26}O₁₂ NAL phase at high-pressure and temperature

M. G. Pamato, A. Kurnosov, T. Boffa Ballaran, D. M. Trots, D. J. Frost (Bayreuth/DE)

11⁴⁵

MS05–To6

Stability of K₂ThF₆ and K₇Th₆F₃₁ on compression

A. Grzechnik (Aachen/DE), K. Frieze (Jülich/DE)

10³⁰–12⁰⁰

Lecture Hall 1
Chair

MS06 – General Crystallography – Modelling and Analysis Bridging the Scales II

H. Zimmermann (Erlangen/DE)

10³⁰

MS06–To1

Dynamic effects in a neutron diffraction experiment

M. Gutmann, S. Mukhopadhyay, K. Refson (Chilton Didcot/GB)
M. von Zimmermann (Hamburg/DE)

Mehr als **blau**

60 Jahre
Blau Blätter



Die Blauen Blätter

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.

- 1045
MSo6–To2 **Evaluation of site occupancy factors in crystal structure refinements using Boolean satisfiability techniques**
M. Soeken, R. Drechsler, R. X. Fischer (Bremen/DE)
- 1100
MSo6–To3 **Random numbers and their application to the real and dual space description of crystal structures**
W. Hornfeck (Cologne/DE)
- 1115
MSo6–To4 **Structural systematization of the polymorph transitions in crystals – a recent experience**
S. Filatov (Saint Petersburg /RU)
- 1130
MSo6–To5 **Modeling frameworks – from polyhedral conformations and distortions to macroscopic strains**
R. Angel (Padova/IT), N. Ross, J. Zhao, L. Sochalski-Kolbus (Blacksburg, VA/US)
H. Krueger (Innsbruck/AT)
- 1145
MSo6–To6 **Single crystal diffraction from powders – Collecting complete 3D electron diffraction data using the automatic rotation method RED**
S. Hovmöller, W. Wan, X. Zou, J. Sun (Stockholm/SE)
- 1030–1200**
Lecture Hall 2
Chair **MSo7 – Spectroscopy and other Tools for Analysis I**
M. Fechtelkord (Bochum/DE)
- 1030
MSo7–To1 **Spectroscopic methods acting as a supplementary benefit to solve Crystallographic research questions – an overview**
M. Fechtelkord (Bochum/DE)
- 1045
MSo7–To2 **Application of group theory to resonance Raman spectra of relaxor ferroelectrics**
G. de la Flor (Bilbao/ES), A. Rohrbeck, B. Mihailova (Hamburg/DE), E. Tasci
M. Aroyo (Bilbao/ES)
- 1100
MSo7–To3 **Raman spectroscopic Investigations of Monazite-type Ceramics used for Nuclear Waste Conditioning**
J. Heuser, H. Schlenz, C. Babelot, T. Schuppik, S. Schmitz, D. Bosbach (Jülich/DE)
- 1115
MSo7–To4 **Nonlinear deformation in GaN layers due to wafer curvature – simulation and Raman measurements**
C. Röder, F. Beyer, G. Leibiger, F. Habel, M. Abendroth, C. Himcinschi
J. Kortus (Freiberg/DE)

- 11³⁰
MS07–T05 **“Li₇La₃Zr₂O₁₂” garnet doped with Fe – Crystal chemistry and phase stability of a fast Li-Ion conductor**
G. Anthauer, D. Rettenwander, C. A. Geiger (Salzburg/AT)
- 11⁴⁵
MS07–06 **Strontium titanate surface modifications due to Nitrogen implantation investigated by grazing incidence X-ray absorption near-edge spectroscopy**
H. Stöcker, M. Zschornak, B. Abendroth, A. Lehmann, C. Richter
D. C. Meyer (Freiberg/DE)
- 12⁰⁰–13³⁰ Lunch Break
- 12⁰⁰–13⁰⁰ **Symposium Young Crystallographers**
Lecture Hall 2
- 12¹⁵–13¹⁵ **Lunch Symposium – Bruker AXS**
Lecture Hall 1
- 13³⁰
Audimax **Quantitative local strain mapping of semiconductor heterostructures**
Speakers Chair
P. A. van Aken (Stuttgart/DE), V. B. Özöl (Berkeley, CA/US), C. T. Koch (Ulm/DE)
W. Neumann (Berlin/DE)
- 14³⁰–16⁰⁰ **Poster Session**
- 16⁰⁰–18¹⁵ **MS08 – Non-ambient Conditions – Pressure, Temperature and Fields at Work III**
Audimax
Chairs
A. Friedrich (Frankfurt a. M./DE), L. Dubrovinsky (Bayreuth/DE)
- 16⁰⁰
MS08–T01 **Chemically-induced renormalization phenomena in perovskite-type relaxor ferroelectrics under high pressure**
B. Mihailova, N. Waesermann (Hamburg/DE), B. Maier (Munich/DE)
R. Angel (Padova/IT), C. Paulmann (Hamburg/DE), M. Gospodinov (Sofia/BG)
U. Bismayer (Hamburg/DE)
- 16¹⁵
MS08–T02 **Crystalchemistry of silicate perovskite from single crystal X-ray diffraction at multimegabar pressures and high temperatures**
L. Dubrovinsky, E. Bykova, K. Glazyrin, T. Boffa Ballaran, C. McCammon
A. Kantor (Bayreuth/DE), M. Merlini (Grenoble/IT), M. Hanfland (Grenoble/FR)
N. Dubrovinskaia (Bayreuth/DE)
- 16³⁰
MS08–T03 **High-pressure structural behaviour of CaIrO₃ perovskite**
T. Boffa Ballaran, K. Kularatne, A. Kurnosov (Bayreuth/DE), R. G. Trønnes (Oslo/NO)



- 16⁴⁵
MSo8–To4 **Coupling between strain and order parameter – distortion-mode refinement and rarametric refinement of the structural phase transitions in LuF[SeO₃]**
O. V. Magdysyuk, R. E. Dinnebier, C. Lipp, T. Schleid (Stuttgart/DE)
- 17⁰⁰–17¹⁵ Coffee Break and Industrial Exhibition
- 17¹⁵
MSo8–To5 **Detection of the magnetic phase transition of Cr₂O₃ at high pressure using second harmonic generation measurements**
L. Bayarjargal, B. Winkler (Frankfurt a. M./DE)
- 17³⁰
MSo8–To6 **Crystallographic studies of pressure-induced phase transitions in transition-metal oxychlorides**
M. Bykov, E. Bykova, L. Dubrovinsky (Bayreuth/DE), M. Hanfland (Grenoble/FR)
H.-P. Liermann (Hamburg/DE) V. Prakapenka (Chicago, MI/US)
S. van Smaalen (Bayreuth/DE)
- 17⁴⁵
MSo8–To7 **Chemistry of ammonothermal nitride growth**
R. Niewa, S. Zhang, T. Richter (Stuttgart/DE)
- 18⁰⁰
MSo8–To8 **On the the transition mechanism between the pressure-induced zinc-blende-to-NaCl-type phase transition of InAs**
N. Pukallus, H. Sowa, H. Klein (Göttingen/DE)
- 16⁰⁰–18¹⁵
Lecture Hall 1
Chair **MSo9 – Crystallography in Materials Science – Real Structures II**
D. Rafaja (Freiberg/DE)
- 16⁰⁰
MSo9–To1 **Structural characterization of thin epitaxial GaN films prepared by low-energy ion-beam nitridation of Gadroplets**
J. W. Gerlach (Leipzig/DE), T. Höche (Leipzig, Halle/DE), D. Hirsch
B. Rauschenbach (Leipzig/DE)
- 16¹⁵
MSo9–To2 **Local order in intermetallic compounds investigated by *SMARTER* NMR spectroscopy**
F. Haarmann, O. Pecher (Aachen/DE)
- 16³⁰
MSo9–To3 **Real structure of ferritic-pearlitic steels from X-ray diffraction experiments and its effect on the mechanical properties**
D. Simek, M. Motylenko, A. Oswald, R. Schmidtchen, G. Lehmann
D. Rafaja (Freiberg/DE)

- 16⁴⁵
MS09–To4 **Substitutional disorder in intermetallic phases – investigations of chemical bonding by XRD-NMR-QM**
O. Pecher, F. Haarmann (Aachen/DE)
- 17⁰⁰–17¹⁵ Coffee Break and Industrial Exhibition
- 17¹⁵
MS09–To5 **Structural and chemical analysis of shockwave-synthesized superhard γ -Si₃N₄ materials**
A. Köhler, C. Schimpf, T. Schlothauer, M. Schwarz, V. Klemm, G. Heide, E. Kroke
D. Rafaja (Freiberg/DE)
- 17³⁰
MS09–To6 **X-ray grazing incidence diffraction from OTS-SAMs on metal oxides**
H.-G. Steinrück, M. Klimczak, S. Gerth (Erlangen/DE), M. Deutsch (Ramat-Gan/IL)
B. Ocko (Upton, NY/US), A. Magerl (Erlangen/DE)
- 17⁴⁵
MS09–To7 **Effect of dislocation array on morphology and photocatalytic properties of rutile TiO₂ nanostructures**
S. Cha, S. Seo, D.-Y. Lee (Changwon/KR)
- 18⁰⁰
MS09–To8 **X-ray scattering on turbostratic carbon structures**
M. Dopita, M. Emmel, M. Rudolph, A. Salomon, D. Rafaja, C. G. Aneziris (Freiberg/DE)
- 16⁰⁰–16⁴⁵ **MS10 – Spectroscopy and other Tools for Analysis II**
Lecture Hall 2
Chair G. Amthauer (Salzburg/AT)
- 16⁰⁰
MS10–To1 **Neuartige Auswertung von Mikrobeugungsaufnahmen mittels Fokalkurven**
F. Henschel, S. Enghardt, J. Bauch (Dresden/DE)
- 16¹⁵
MS10–To2 **Influence of polarization switching on the Diffraction Anomalous Fine Structure in ultra-thin, ferroelectric barium titanate films**
C. Richter (Freiberg, Hamburg/DE), D. Novikov (Hamburg/DE), M. Zschornak, E. Mehner
D. C. Meyer (Freiberg/DE)
- 16³⁰
MS10–To3 **Application of a Difference Electron Nanoscope (DEN) – correlation between 3D magnetical structures of synthetic fayalite with synchrotron and neutron diffraction and Mössbauer Spectroscopy**
W. Lottermoser, K. Steiner, G. Scharfetter (Salzburg/AT)
S.-U. Weber (Braunschweig/DE), M. Grodzicki (Salzburg/AT), A. Kirfel (Bonn/DE)
G. Amthauer (Salzburg/AT)

- 16⁴⁵
MS10–To4 **A new high-performance small angle X-ray scattering instrument – Rigaku NanoMax™**
P. U. Pennartz, L. Fan, M. Degen, L. Jiang, N. Grupido (Auburn Hills, MI/US)
- 17⁰⁰–17¹⁵ Coffee Break and Industrial Exhibition
- 17¹⁵–18¹⁵
Lecture Hall 2
Chair **MS11 –Along the Innovation Chain – from Minerals and Crystals via Natural Sciences to Functional Materials**
T. Leisegang (Freiberg/DE)
- 17¹⁵
MS11–To1 **Biocalcite architectures – from nanoscale primary particles to functionalized cm-sized multiplex composite crystals**
W. W. Schmahl, E. Grießhaber (Munich/DE), A. Ziegler (Ulm/DE), K. Kelm (Cologne/DE)
G. Jordan, B. Maier (Munich/DE)
- 17³⁰
MS11–To2 **withdrawn**
- 17⁴⁵
MS11–To3 **Growth and characterization of Sn_{1-x}Pb_xS thin films**
S. Lobe, G. Wagner, K. Bente (Leipzig/DE)
- 18⁰⁰
MS11–To4 **On ordering in bixbyite-structured oxide films**
M. Niehle, A. Trampert, X. Kong, O. Bierwagen (Berlin/DE)
- 18¹⁵–19¹⁵
Audimax **DGK Members Meeting** (in german language)
- 19¹⁵–19³⁰ Snack Break at the Foyer Audimax
- 19³⁰–21⁰⁰
Audimax **DGK Ehrenabend** (in german language)
- Preisverleihungen**
Carl-Hermann-Medaille an Emil Makovicky
Will Kleber Gedenkmünze an Helmut Klapper
Max von Laue Preis 2013
- Vorträge**
Max von Laue Preisträger 2012, Tilmann Leisegang
- Die Geowissenschaftlichen Sammlungen der TU Bergakademie Freiberg in Lehre, Forschung und Öffentlichkeit
Gerhard Heide (Direktor der Geowissenschaftlichen Sammlungen Freiberg)
- Musikalische Umrahmung durch das Collegium Musicum der TU Bergakademie

09⁰⁰

Audimax

Speaker

Chair

How do biological macromolecules respond to light? – time-resolved crystallography and protein design

K. Moffat (Chicago, IL/US)

Y. A. Muller (Erlangen/DE)

10⁰⁰–10³⁰

Coffee Break and Industrial Exhibition

10³⁰–12⁰⁰

Audimax

Chair

MS12 – Biocrystallography – Synthesis, Structure and Function I

W. Höffken (Ludwigshafen/DE)

10³⁰

MS12–T01

The bifunctional kinase and Methyltransferase WbdD regulates the polymerization of Lipopolysaccharide O antigen in *Escherichia coli* O9a

G. Hagelueken (Bonn/DE; St Andrews/GB), H. Huang (St Andrews/GB)

B. R. Clarke (Guelph/CA), T. Lebl (St Andrews/GB), C. Whitfield (Guelph/CA)

J.H. Naismith (St Andrews/GB)

10⁴⁵

MS12–T02

Ring-size determination and substrate recognition in the amylomaltase-CA34 complex

C. Roth (Leipzig/DE), T. Maier (Basel/CH), N. Weizenmann (Leipzig/DE), N. Bexten

W. Sängner (Berlin/DE) W. Zimmermann, N. Sträter (Leipzig/DE)

11⁰⁰

MS12–T03

Forward and reverse peptide binding modes and conformational changes of the Hsp70 chaperone DnaK

M. Zahn, N. Berthold, D. Knappe, B. Kieslich, R. Hoffmann, N. Sträter (Leipzig/DE)

11¹⁵

MS12–T04

The nanoscale and composite nature of biological materials

P. Alexa, G. Jordan, E. Griesshaber, W. Schmahl (Munich/DE)

11³⁰

MS12–T05

Composite crystal misorientation and homoepitaxial meso- and microscale co-orientation across matrix membranes in *Mytilus edulis* nacre

B. J. Maier, F. Nindiyasari, E. Griesshaber (Munich/DE)

H. Singh Ubhi (High Wycombe/GB), A. Ziegler (Berlin/DE)

W. Schmahl (Munich/DE)

11⁴⁵

MS12–T06

The intra- and inter-grain crystallographic nano- and microstructure of nacre

E. Griesshaber (Munich/DE), H. S. Ubhi (High Wycombe/GB)

W. Schmahl (Munich/DE)

1030–1200

Lecture Hall 1
Chair

MS13 – Crystal Physics, Crystal Chemistry – Synthesis and New Crystal Structures I

T. Schleid (Stuttgart/DE)

1030

MS13–To1

Structure prediction as a guide in synthesis planning – identification of promising chemical systems for the synthesis of the “5-5” structure type using an *ab initio* minimization structure extrapolation procedure

D. Zagorac, C. J. Schoen, M. Jansen (Stuttgart/DE)

1045

MS13–To2

$M(\text{CH}_3\text{SO}_3)_2(\text{CH}_3\text{SO}_3\text{H})_2$ ($M = \text{Cd}, \text{Zn}, \text{Co}$) – syntheses, crystal structures and thermal decomposition

S. Gagelmann, M. S. Wickleder (Oldenburg/DE)

1100

MS13–To3

$\text{Sr}_3\text{Gd}_2[\text{BO}_3]_4$ – growth, thermal behavior and structure

C. Reuther, H. Schmidt (Freiberg/DE), C. Paulmann (Hamburg/DE), M. Hengst R. Möckel, G. Heide (Freiberg/DE)

1115

MS13–To4

Kristallisationsverhalten von Tobermorit unter Einfluss von $\text{CaCl}_2 \cdot x\text{H}_2\text{O}$

A. Hartmann, D. Schulenberg, J.-C. Buhl (Hanover/DE)

1130

MS13–To5

Growth and characterization of Ce^{3+} doped CaSc_2O_4 single crystal fibers

J. Philippen, C. Gugushev, D. Klimm (Berlin/DE)

1145

MS13–To6

Oxygen-driven competition between structural types in $\text{Sr}_3\text{CoRuO}_{6+x}$ and $\text{Sr}_3\text{CoIrO}_{6+x}$ systems

D. Mikhailova, P. Reichel, A. A. Tsirlin, M. P. Schmidt, L. H. Tjeng (Dresden/DE)

1030–1145

Lecture Hall 2
Chair

MS14 – Crystallography – History, Art, Cultural Heritage, Teaching and Public Communication

W. Deppmeier (Kiel/DE)

1030

MS14–To1

Non-destructive elemental analysis of Mughal silver coins without using X-ray Fluorescence

P. Dasgupta (Kolkata/IN), A. Dutta (Chandarnagore/IN)

1045

MS14–To2

Colouring agents in medieval glazes characterized by $\mu\text{-XRD}^2$ and electron microprobe

R. Gradmann (Würzburg/DE), C. Berthold (Tübingen/DE), J. Badr (Bamberg/DE)
U. Schuessler (Würzburg/DE)

1100

MS14–To3

Warum heißt Bunsenit Bunsenit – Kristallographie und Mineralogie von einst im Licht heutiger Nanoforschung

M. Petrik (Marburg/DE)

- 11¹⁵
MS14–T04 **Making crystallography understandable**
A. Dziwetzki (Freiberg/DE)
- 11³⁰
MS14–T05 **Color-coded cubes – an effective and inexpensive way to display point group symmetries in 3D**
G. Nolze (Berlin/DE)
- 12⁰⁰–13³⁰ Lunch Break
- 12⁴⁵–13⁴⁵ **Lunch Symposium – Agilent Technologies**  **Agilent Technologies**
Lecture Hall1
- 13³⁰
Audimax
Speaker
Chair **Biomimetic Mineralization – Nanocomposite Superstructures as Functional Materials of the Human Body**
R. Kniep (Dresden/DE)
E. Kroke (Freiberg/DE)
- 14³⁰–16⁰⁰ **Poster Session**
- 16⁰⁰–17⁰⁰ **MS15 – Biocrystallography – Synthesis, Structure and Function II**
Audimax
Chair H. Schindelin (Würzburg/DE)
- 16⁰⁰
MS15–T01 **Structural basis of assembly chaperone-mediated snRNP formation**
C. Grimm, J. Pelz, U. Fischer (Würzburg/DE)
- 16¹⁵
MS15–T02 **Structure of the viral effector protein IE1 from cytomegalovirus**
S. Klingl, M. Scherer, T. Stamminger, Y. A. Muller (Erlangen/DE)
- 16³⁰
MS15–T03 **Structure of ADP • AlF₃-Stabilized dark-operative protochlorophyllide oxidoreductase complex**
J. Krausze, C. Lange, J. Moser, D. Heinz (Braunschweig/DE)
- 16⁴⁵
MS15–T04 **Structure of a Helicobacter pylori type IV secretion protein with an unusual RGD motif**
S. Barden, H. Niemann (Bielefeld/DE)
- 17⁰⁰–17¹⁵ Coffee Break and Industrial Exhibition

17⁴⁵–18⁴⁵

Audimax
Chair

MS16 – Biocrystallography – Biomimetic Materials, Drug Design, Processes and Functions

H. Ehrlich (Freiberg/DE)

17¹⁵

MS16–T01

Lattice energy calculation – a quick tool for screening of stability and relative solubility of cocrystals

L. Kuleshova, D. Hofmann (Pula/IT; Uttenreuth/DE)

17³⁰

MS16–T02

Solubility prediction by crystal structure prediction with force fields obtained by data mining on experimental crystal structures

D. W. M. Hofmann, L. N. Kuleshova (Pula/IT; Uttenreuth/DE)

17⁴⁵

MS16–T03

Electron densities of bexarotene and disila-bexarotene from invariom application: a comparative study

P. Luger, M. Weber, C. Hübschle, R. Tacke (Berlin/DE)

18⁰⁰

MS16–T04

Gypsum – cellulose composites with improved material properties Leading to a new low-cost building material

F. Nindiyasari, E. Griesshaber (Munich/DE), T. Zimmermann (Dübendorf/CH)

T. Bechthold (Dornbirn/AT), C. Randow (Berlin/DE), L. Fernandez-Diaz (Madrid/ES)

C. Fleck (Berlin/DE), W. Schmahl (Munich/DE)

16⁰⁰–18⁴⁵

Lecture Hall 1
Chair

MS17 – Materials for Electronics – Energy and Data Storage through the Eyes of Crystallographers

P. Zahn (Dresden/DE)

16⁰⁰

MS17–T01

Microscopic processes in energy and data storage

S. Gemming (Dresden, Chemnitz/DE)

16³⁰

MS17–T02

A high time resolved and flexible synchrotron powder diffraction setup for the *in situ* structural investigation of electrode materials in rechargeable batteries

M. Herklotz (Dresden/DE), F. Scheiba (Karlsruhe, Dresden/DE)

M. Hinterstein (Dresden, Hamburg/DE), A.-C. Dippel (Hamburg/DE)

J. Eckert (Dresden/DE), H. Ehrenberg (Karlsruhe, Dresden/DE)

16⁴⁵

MS17–T03

Structural and magnetic properties of compounds $(\text{Ge}_{1-x}\text{TM}_x\text{Te})_n\text{Sb}_2\text{Te}_3$ (TM=Cr, Mn, Fe)

S. Welzmler, A. Dorn, P. Huth, T. Faske, F. Schleife, B. Kersting

O. Oeckler (Leipzig/DE)

17⁰⁰–17¹⁵

Coffee Break and Industrial Exhibition

- 17¹⁵
MS17–To4 **How Ca/Ba ratio affects the relaxor behavior of $\text{Ca}_x\text{Ba}_{1-x}\text{Nb}_2\text{O}_6$?**
C. S. Pandey, J. Schreuer (Bochum/DE), M. Burianek, M. Mühlberg (Cologne/DE)
- 17³⁰
MS17–To5 **Anatase and rutile formation in atomic layer deposition of TiO_2**
B. Abendroth, S. Rentrop, T. Moebus, R. Strohmeier, F. Hanzig, H. Stöcker
D. C. Meyer (Freiberg/DE)
- 17⁴⁵
MS17–To6 **The $\text{BaTiO}_3(001)\text{--}(2x1)$ reconstruction – structure and magnetism**
H. L. Meyerheim, A. Ernst, K. Mohseni, I. V. Maznichenko, S. Ostanin
F. Klimenta (Halle/DE), N. Jedrecy (Paris/FR), W. Feng, I. Mertig (Halle/DE)
R. Felici (Grenoble/FR), J. Kirschner (Halle/DE)
- 18⁰⁰
MS17–To7 **Residual stress and defect density determination in HVPE grown GaN layers**
M. Barchuk, C. Röder, G. Lukin, J. Kortus, O. Pätzold, D. Rafaja (Freiberg/DE)
- 16⁰⁰–18¹⁵ **MS18 – Special Industrial Symposium**
Lecture Hall 2
Chair U. Wunderwald (Freiberg/DE)
- 16⁰⁰ **Technologietrends in der Silicium Photovoltaik und Anforderungen an den Silicium Wafer**
H. Neuhaus (SolarWorld Innovations GmbH)
- 16⁴⁵ **Siltronic – a leading producer of silicon crystals and wafers**
A. Mühe (Siltronic AG)
- 17³⁰ **Firmenpräsentation Freiburger Compound Materials GmbH**
S. Eichler (Freiburger Compound Materials GmbH)
- 20⁰⁰–23⁰⁰ **Social Evening** (in german language)

09⁰⁰

Audimax
Speaker
Chair

Tetrahedrally Coordinated Compound Semiconductors for Photovoltaic Applications

S. Schorr (Berlin/DE)
W. Neumann (Berlin/DE)

10⁰⁰–10³⁰

Coffee Break and Industrial Exhibition

10³⁰–11⁴⁵

Audimax
Chair

MS19 – Biocrystallography – Others

U. Heinemann (Berlin/DE)

10³⁰

MS19–T01

Synchrotron based fragment screening

U. Mueller, A. Heine, M. Ühlein, M. S. Weiss, G. Klebe (Berlin/DE)

10⁴⁵

MS19–T02

Towards automated high-throughput sample evaluation and diffraction data collection in structural biology at the european synchrotron radiation facility

C. Mueller-Dieckmann (Grenoble/FR)

11⁰⁰

MS19–T03

New tools for biological crystallography – low multiplicity sulfur-SAD phasing in the home lab

S. Freisz (Karlsruhe/DE), M. Benning (Madison, WI/US), V. Smith (Karlsruhe/DE)

11¹⁵

MS19–T04

A generalized mechanism for X-ray radiation damage on the atomic level

D. Heintz, A. Burkhardt, R. Raghunandan (Hamburg/DE), M. Gutmann
A. Wagner (Oxfordshire/GB), M. Nachttegaal (Villigen/CH), E. Weckert
A. Meents (Hamburg/DE)

11³⁰

MS19–T05

Structural and energetic basis of folded protein transport by the FimD usher

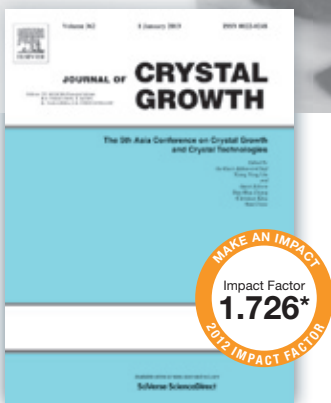
S. Geibel (London/GB), E. Procko (Seattle, WA/US), S.J. Hultgren (St. Louis, MO/US)
D. Baker (Seattle, WA/US), G. Waksman (London/GB)

11⁴⁵

MS19–T06

New sample environment options at the neutron diffractometer “BioDiff”

T. Schrader, A. Ostermann (Garching/DE), M. Monkenbusch, B. Laatsch (Jülich/DE)
P. Jüttner, W. Petry (Garching/DE), D. Richter (Jülich/DE)



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Aims and Scope

The journal offers a common reference and publication source for workers engaged in research on the experimental and theoretical aspects of crystal growth and its applications, e.g. in devices. Experimental and theoretical contributions are published in the following fields: theory of nucleation and growth, molecular kinetics and transport phenomena, crystallization in viscous media such as polymers and glasses; crystal growth of metals, minerals, semiconductors, superconductors, magnetics, inorganic, organic and biological substances in bulk or as thin films; molecular beam epitaxy, chemical vapor deposition, growth of III-V and II-VI and other semiconductors; characterization of single crystals by physical and chemical methods; apparatus, instrumentation and techniques for crystal growth, and purification methods; multilayer heterostructures and their characterisation with an emphasis on crystal growth and epitaxial aspects of electronic materials. A special feature of the journal is the periodic inclusion of proceedings of symposia and conferences on relevant aspects of crystal growth.

For more information: www.journals.elsevier.com/journal-of-crystal-growth

*Thomson Reuters Journal Citation Reports, 2012

Physics



10³⁰–12³⁰

Lecture Hall 1
Chair

MS20 – Crystal Physics, Crystal Chemistry – Synthesis and New Crystal Structures II

T. Doert (Dresden/DE)

10³⁰

MS20–To1

Symmetry and chemistry of complex intermetallics

J. Dshemuchadse, W. Steurer (Zurich/CH)

10⁴⁵

MS20–To2

How complicated can a lillianite homologue become? – the case of jasrouxite

E. Makovicky (Copenhagen/DK), D. Topa (Wien/AT)

11⁰⁰

MS20–To3

Dissolution kinetics of nanocrystals – new insights

M. Petrik, B. Harbrecht (Marburg/DE)

11¹⁵

MS20–To4

Properties and crystal structure of B-mullite

H. Lührs (Bremen/DE), A. Senyshyn (Garching/DE), S. P. King, J. V. Hanna (Coventry/GB)
H. Schneider (Bremen, Cologne/DE), R. X. Fischer (Bremen/DE)

11³⁰

MS20–To5

Structural characterisation of shocked AlN-powders

K. Keller, T. Schlothauer, M. Schwarz, E. Brendler, E. Kroke, G. Heide (Freiberg/DE)

11⁴⁵

MS20–To6

Structural and electrochemical studies of the Li-In alloys

I. Chumak, M. Knapp, H. Ehrenberg (Karlsruhe/DE)

12⁰⁰

MS20–To7

Polymorphism of monomeric nickel acetate with 2-pyridineethanol

M. Trdin, N. Lah, I. Leban (Ljubljana/SI)

12¹⁵

MS20–To8

High temperature elastic properties of a pseudo-single crystal of the nickel-base superalloy CMSX-4

K. Demtröder, H. Buck, P. Wollgramm, G. Eggeler, J. Schreuer (Bochum/DE)

10³⁰–12³⁰

Lecture Hall 2
Chair

MS21 – Cutting Edge Techniques in Analysis and Preparation

C. Paulmann (Hamburg/DE)

10³⁰

MS21–To1

Current status of the Liquid-Metal-Jet X-ray source technology

B. Hansson, O. Hemberg, T. Tuohimaa, M. Otendal, P. Takman (Kista/SE)

10⁴⁵

MS21–To2

Beam conditioning in cutting edge X-ray analytical equipment

J. Graf, A. Kleine, B. Hasse, J. Wiesmann, C. Michaelsen (Geesthacht/DE), J. Lange
C. Ollinger (Karlsruhe/DE)

- 11⁰⁰**
MS21–To3 **A X-ray color camera for spatially resolved XRF and XRD at once and fast chemical mapping of 3-dimensional objects in a laboratory setup**
C. Berthold (Tübingen/DE), O. Scharf (Berlin/DE), K. Bente (Leipzig/DE)
A. Bjeoumikhov (Berlin/DE), I. Ordavo (Munich/DE)
- 11¹⁵**
MS21–To4 **Fast quantitative determination of crystallite size distributions from 2D diffraction data**
M. Chaouachi, S. Neher, S. Stracke, A. Falenty, H. Klein, W. F. Kuhs (Göttingen/DE)
- 11³⁰**
MS21–To5 **Absorb7 and Absorb-GUI for single-crystal absorption corrections under non-ambient conditions**
R. Angel (Padova/IT), J. Gonzalez-Platas (La Laguna/ES)
- 11⁴⁵**
MS21–To6 **A bench top solution for challenging crystal structures**
A. Gerisch, M. Adam (Karlsruhe/DE), R. Glaum (Bonn/DE), M. Ruck (Dresden/DE)
- 12⁰⁰**
MS21–To7 **In-situ characterization of the growth mechanism in the TiN/(Ti,Al)N/AlN multilayers**
U. Ratayski (Freiberg/DE), C. Baehtz (Dresden/DE), D. Rafaja (Freiberg/DE)
- 12¹⁵**
MS21–To8 **Hard X-ray scanning microscopy with diverse contrast mechanisms at Po6, PETRA III**
R. Hoppe (Dresden/DE)
- 12³⁰**
Audimax **Conference Closing**
- 14⁰⁰** **Installation of a bronze relief at the Schlossplatz**

Posters Overview

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PS01

Along the Innovation Chain – From Minerals and Crystals via Natural Sciences to Functional Materials

PS01–P01

Ordered defects in Hydrous Layer Silicates (HLSs) containing Ferrierite-type layers
B. Marler, H. Gies (Bochum/DE)

PS01–P02

Native indium from a quartz-cassiterite-sulfide-paragenesis in the Erzgebirge – an electron microscopy study
M. Trinkl (Bobritzsch, OT Niederbobritzsch/DE), U. Kempe (Freiberg/DE)

PS02

Aperiodic and Modulated Structures – Potential in Higher Dimensions

PS02–P01

Incommensurate phase of the molecular crystal p-C₆F₄Br₂ at T=15 K
L. Noohinejad, S. van Smaalen (Bayreuth/DE)

PS02–P02

The commensurately modulated structure of trimethyltin hydroxide at 220 K
S. Dey, A. Schönleber, S. van Smaalen (Bayreuth/DE)

PS02–P03

Modulated structure of CeCuGa₃
K. Sparta, Y. J. Sohn, G. Roth (Aachen/DE), D. A. Joshi, P. Burger, P. Adelman, D. Ernst T. Wolf, K. Grube, C. Meingast, H. V. Löhneysen (Karlsruhe/DE)

PS02–P04

Local electronic structure studies of Ho₂PdSi₃ using directional anomalous fine structure
M. Nentwich, M. Zschornak (Freiberg/DE), C. Richter (Freiberg, Hamburg/DE)
D. Meyer (Freiberg/DE)

PS03

Biocrystallography I – Synthesis, Structure and Function

PS03–P01

Structural basis of assembly chaperone-mediated snRNP formation
C. Grimm, J. Pelz, U. Fischer (Würzburg/DE)

PS03–P02

Fluorinated boron-dipyromethene (BODIPY) structures for surface analysis
W. Kraus, M. Hecht, T. Fischer, K. Rurack (Berlin/DE)

PS03–P03

P450 BM3 crystal structures reveal the role of the charged surface residue Lys/Arg184 in inversion of enantioselective styrene epoxidation
S. Panneerselvam (Hamburg/DE), A. Shehzad (Aachen/DE), M. Linow (Bremen/DE)
M. Bocla (Aachen/DE), D. Roccatano (Bremen/DE), J. Mueller-Dieckmann
M. Wilmanns (Hamburg/DE), U. Schwaneberg (Aachen/DE)

- PS03-P04 **DegQ-deciphering protein quality control in *Legionella***
W. Robert, H. Scott, A. Schubert, R. Hilgenfeld, G. Hansen (Lübeck/DE)
- PS03-P05 **Conformational polymorphism in Atg8 family proteins**
P. Ma (Grenoble/FR), O. Olubiyi, B. Strodel, O. H. Weiergräber (Jülich/DE)
- PS03-P06 **Studies on FKBP38 activation by Ca²⁺-calmodulin**
M. Michel, A. Stadler, O. H. Weiergräber (Jülich/DE)
- PS03-P07 **Structure of the Fe(II)/2-Oxoglutarate dependent Dioxygenase RdpA in complex with substrate and Co-substrate**
J. Krausze (Braunschweig, Leipzig/DE), R. Müller, N. Sträter (Leipzig/DE)
- PS03-P08 **The hierarchical composite crystal architecture of sea urchin teeth: a crystallographic, chemical and mechanical characterization**
B. J. Maier, A. J. Götz, E. Griesshaber (Munich/DE), J. Deuschle (Stuttgart/DE), R. Abel L. Howard (London/GB), K. T. Fehr, B. Ruthensteiner, W. Schmahl (Munich/DE)
- PS03-P09 **Structural and functional characterization of bacterial MDR-transporters**
P. Simeonov, S. Werner, F. Jaenecke, C. Haupt, K. Bacia, M. Tanabe (Halle/DE)
- PS04 Biocrystallography – Other**
- PS04-P01 **Facilities for macromolecular crystallography at the Helmholtz-Zentrum Berlin**
M. Weiss, M. Bommer, R. Förster, M. Hellmig, M. Krug, S. Pühringer, M. Steffien M. Uhlein, U. Mueller (Berlin/DE)
- PS04-P02 **withdrawn**
- PS04-P03 **Ultraviolet laser radiation damage induced phasing as an efficiently applicable method to solve the crystallographic phase problem of death receptor six (DR6)**
S. Kemmerzell (Jena/DE), M. Krug, U. Mueller (Berlin/DE), M. E. Than (Jena/DE)
- PS04-P04 **Applications with the new, brighter X-ray source from agilent technologies**
Z. Gal (Yarnton/GB)
- PS04-P05 **XDSAPP – a graphical user interface for the convenient processing of diffraction data using XDS**
M. Krug (Berlin/DE)

PS05

Crystal Physics, Crystal Chemistry – Synthesis and New Crystal Structures

PS05–P01

Aminkomplexe des Gold(I)-cyanidsC. Döring, P. G. Jones (Braunschweig/DE)

PS05–P02

Zr₂Fe₁₂As₇ – a new iron arsenide with structural relations to LiFeAsM. Bischoff, L. Shlyk, R. Niewa (Stuttgart/DE)

PS05–P03

The crystal structure of the potassium-trisulphidometallate double salts**K₃[MOS₃]Y (M=Mo, W; =Cl[–], SH[–]) and K₆[WOS₃]₂(S₂O₃) and the first crystal structure of K₂(S₂O₃)**A. J. Lehner, L. V. Schindler, C. Röhr (Freiburg/DE)

PS05–P04

A mononuclear rhenium(III) product obtained in a solvothermal process with catalytic reactionsA. Kochel (Wrocław/PL), M. Hołyńska (Marburg/DE)

PS05–P05

The crystal structure of Cs₁₀Al₆S₁₄V. Winkler, M. Schlosser, A. Pfitzner (Regensburg/DE)

PS05–P06

Series of pentanuclear [Co^{III}₄Ln^{III}] complexes (Ln=La, Sm, Gd) with a tripodal oxime ligandD. Premužić, M. Hołyńska (Marburg/DE)

PS05–P07

Synthesis, characterization and phase transition of Li_{0.4}WO₃ bronzeM. S. Rahman, M. M. Murshed, T. M. Gesing (Bremen/DE)

PS05–P08

Molecular zinc dihydridesT. P. Spaniol, A. Rit, J. Okuda (Aachen/DE)

PS05–P09

A systematic crystal chemical study of alkaline earth rich mixed stannides/germanidesM. Jehle, C. Röhr (Freiburg/DE)

PS05–P10

Growth and morphology of Sillenite crystals synthesized in hydrothermal solutionsE. Marina, A. Marin, I. Mahina (Chernogolovka/RU)

PS05–P11

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- PS05-P21 **$[\text{N}_2\text{C}_6\text{H}_{14}][\text{CuX}_3]\text{-1,4-Diazoniabicyclo[2.2.2]octane trihalocuprate(I), (X=Cl, Br, I):$
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- PS05-P22 **The crystal structure of $\text{Ce}_4\text{Mo}_7\text{O}_{27}$ and its relationship to the structures of $\text{La}_4\text{Mo}_7\text{O}_{27}$ and $\text{Ln}_4\text{Mo}_7\text{O}_{27}$ ($\text{Ln}=\text{Eu, Gd}$)**
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J. Fan, W. Carrillo-Cabrera, Y. Grin (Dresden/DE)

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T. Gruber, R. Nestler, W. Seichter (Freiberg/DE), P. Bombicz (Budapest/HU)
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R. Kaden, H. Pöllmann (Halle a. d. Saale/DE)
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A. Bieniok, U. Brendel, P. Sereni, M. Musso (Salzburg/AT)
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L. Robben, T. M. Gesing (Bremen/DE)
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K. Hofmann, E.-M. Felix, G. Bruhn, B. Albert (Darmstadt/DE)
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M. Wildner, G. E. Büchel, L. Filak, C. Petautschnig, G. Giester (Wien/AT)
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A. Neumann, H. Curtius, M. Klinkenberg, G. Kaiser, D. Bosbach (Jülich/DE)
- PS05-P34 **Tetrapropylammonium Tetrathiorhenate(VII) $(\text{C}_3\text{H}_7)_4\text{N}[\text{ReS}_4]$: a new n-Alkylammonium Thioperrhenate with an ordered crystal structure**
K. K. Wolff, I. Grau, T. Schleid (Stuttgart/DE)
- PS05-P35 **The $[\text{Pt}(\text{S}_2\text{O}_7)_3]^{2-}$ -anion**
J. Bruns, H. Bültel, M. Wickleder (Oldenburg/DE)
- PS05-P36 **Growth and characterization of $(\text{Bi}_{0.5}\text{Na}_{0.5})_{1-x}\text{Ba}_x\text{TiO}_3$ single crystals**
M. Woll, M. Burianek (Cologne/DE), D. Klimm (Berlin/DE), S. Gorfman (Siegen/DE), M. Mühlberg (Cologne/DE)

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M. Eberle, T. Schleid (Stuttgart/DE)
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 L. Wang, I. Spiess, H. Lühns (Bremen/DE), W. H. Baur (Illinois, IL/US)
 R. X. Fischer (Bremen/DE)
- PS05-P39 **$\text{NaLa}_6\text{O}_3\text{F}_9\text{S}_2$ – a chemical extension of the formula type $M_3\text{OF}_5\text{S}$ ($M=\text{Nd, Sm, Gd-Ho}$)**
D. D. Zimmermann, T. Schleid (Stuttgart/DE)
- PS05-P40 **Synthesis and characterization of mullite-type $(\text{Al}_{1-x}\text{Ga}_x)_4\text{B}_2\text{O}_9$**
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 H. Schneider (Cologne/DE), T. M. Gesing (Bremen/DE)
- PS05-P41 **Synthesis and crystal structure of body-centered gallogermanate chloride/hydrate sodalite**
I. Poltz (Hanover, Bremen/DE), L. Robben (Bremen/DE)
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- PS05-P42 **New coordination polymers with aniline-2,5-disulfonic acid and 2,3,5,6-tetrachloro-1,4-benzenedisulfonic acid**
M. Gudenschwager, M. S. Wickleder, J. Christoffers
 T. W. T. Muesmann (Oldenburg/DE)
- PS05-P43 **Applying a novel ligand class – synthesis and structures of metal complexes with ‘normal’ 1,2,3-Triazolylidene Ligands**
A. Pöthig, L.-A. Schaper, X. Wei, F. E. Kühn, W. A. Herrmann (Garching/DE)
- PS05-P44 **$\text{U}_2\text{Pte}_2\text{O}$ – ein neues Pniktidchalkogenid des Urans mit P_{24} -Einheiten**
 K. Stolz, U. Schwarz, T. Doert (Dresden/DE)
- PS05-P45 **Anisotropy study of the magnetoelectric properties of $\text{LiFeSi}_2\text{O}_6$**
M. Ackermann, T. Lorenz, P. Becker, L. Bohatý (Cologne/DE)
- PS05-P46 **Temperaturabhängige Kristallstrukturuntersuchung an $\text{TlFe}_{2-x}\text{Se}_2$ ($x \approx 0,4$)**
 E. Ahrens, T. Doert, M. Ruck (Dresden/DE)
- PS05-P47 **Towards anhydrous rare earth triflates syntheses, crystal structures and characterization of $\text{RE}(\text{CF}_3\text{SO}_3)_3(\text{H}_2\text{O})_3$ ($\text{RE}=\text{Eu-Lu,Y}$) and $(\text{NO})[\text{Sm}_2(\text{CF}_3\text{SO}_3)_7(\text{H}_2\text{O})_3]$**
 J. Bruns, A. Weiz, M. Wickleder (Oldenburg/DE)

- PS05-P48 **Fe²⁺-linking by novel polysulfonate anions**
C. Zitzer, M. Wickleder, J. Christoffers, T. Muesmann (Oldenburg/DE)
- PS05-P49 **Kokristallisation und Kristallmorphologie der Zeolithe LTA und X (FAU) bei der Hydrothermalsynthese silikatreicher Gele**
V. Petrov, T. Koglin, J.-C. Buhl (Hanover/DE)
- PS05-P50 **Pyroelectric properties of the monoclinic rare earth nitrates $A_2Ln(NO_3)_5 \cdot 4H_2O$**
M. Ackermann, L. Andersen, P. Becker, L. Bohaty (Cologne/DE)
- PS05-P51 **On the dehydration mechanism of NaB(OH)₄-sodalites investigated by micro-Raman spectroscopy**
A. Schulz, C. H. Rüschler, J.-C. Buhl (Hanover/DE)
- PS05-P52 **X⁽³⁾-nonlinear optical effects in topaz, Al₂(F_{1-x}(OH)_x)₂SiO₄**
A. A. Kaminskii (Moscow/RU), O. Lux, H. Rhee, H.-J. Eichler (Berlin/DE)
L. Bohatý, P. Becker (Cologne/DE)
- PS05-P53 **Kokristallisation und Kristallmorphologie von Zeolith (LTA) und Sodalith (SOD) bei der Hydrothermalsynthese aluminiumreicher Gele und Einfluss der Alkalinität auf den Kristallisationsablauf.**
V. Petrov, P. Törber, J.-C. Buhl (Hanover/DE)
- PS05-P54 **Metastability of metamict titanite and thermal behaviour of its elastic properties**
U. Bismayer, C. Paulmann, T. Beirau, B. Mihailova, T. Malcherek, P. Guglielmi
G. Schneider (Hamburg/DE), L. Groat (Vancouver/CA), E.K.H. Salje (Cambridge/GB)
- PS05-P55 **Kristallisationsprozesse in stark alkalischen Aufschlusslösungen von Aschen aus der Verbrennung von Schlämmen der Altpapieraufbereitung**
A. Hartmann, V. Petrov, J.-C. Buhl (Hanover/DE), K. Rübner (Berlin/DE)
- PS05-P56 **Kristallographische Untersuchungen zu Zinn(II)-Thiocyanat und seinen Komplexen**
H. Reuter, F. Ye, P. Harpel (Osnabrück/DE)
- PS05-P57 **2,2'-Bipyridin Komplexe von Diethylzinn(IV)-Verbindungen**
H. Reuter, I. Mastall (Osnabrück/DE)
- PS05-P58 **Neue ternäre Barium-Triel-Mercuride**
C. Röhr, M. Wendorff (Freiburg/DE)
- PS05-P59 **1,4-Dithian-1,4-dioxid als potentiell zweizähniger Komplexlignand gegenüber anorganischen und organischen Zinnverbindungen**
H. Reuter, S. Budau (Osnabrück/DE)

- PS05-P60 **Synthesis and crystal structure of $\text{Ba}_3\text{B}_6\text{Si}_2\text{O}_{16}$**
M. Krzhizhanovskaya, L. Gorelova, R. Bubnova, S. Filatov (St. Petersburg/RU)
- PS05-P61 **$\beta\text{-LiSbS}_2$ is $\text{Li}_{1.250}\text{Sb}_{0.917}\text{S}_2$ – synthesis, crystal structure and impedance spectroscopy**
S. Huber, C. De Giorgi, A. Pfitzner (Regensburg/DE)
- PS05-P62 **New sodium ion conducting Chalcogenides – structure analyses and impedance measurements of Na_3SbQ_3 -(Q=S, Se)**
C. Pompe, A. Pfitzner (Regensburg/DE)
- PS05-P63 **Investigation of microscopic origin of piezoelectric effect in $\text{Bi}_{12}\text{SiO}_{20}$ single crystals**
S. Gorfman, M. Zhao, A. Huesecken (Siegen/DE), M. Burianek, M. Mühlberg
U. Pietsch (Cologne/DE)
- PS05-P64 **Detailed studies on silicates using neutron diffraction**
M. Meven (Aachen/DE), G. D. Gatta (Milan/IT)
- PS05-P65 **MTEX for texture, fabric, and anisotropic properties**
H. Schaeben, F. Bachmann (Freiberg/DE), R. Hielscher (Chemnitz/DE)
D. Mainprice (Montpellier/FR)
- PS05-P66 **Determination of Niobium precipitations in micro alloyed steels**
I. Janßen, H. Klein (Göttingen/DE), C. Klinkenberg (Düsseldorf/DE)
- PS05-P67 **Structural characterization of $\text{Cu}_2\text{ZnSn}(\text{S}, \text{Se})_4$ thin films**
S. Schorr, G. Gurieva (Berlin/DE), L. I. Bruc, D. A. Sherban (Chisinau/MD)
T. Unold (Berlin/DE)
- PS05-P68 **Structural investigations of the $\text{MgO-MgCl}_2\text{-H}_2\text{O-CO}_2$ system – the Sorel Cement Phases**
R. Dinnebier, T. Runcevski (Stuttgart/DE)
- PS05-P69 **Oxygen content in SrFeO_3 obtained from Neutron and X-ray powder diffraction modeled by distribution functions**
M. Etter, A. Wedig, D. Samuelis, R. Merkle (Stuttgart/DE), A. Senyshyn (Munich/DE)
J. Maier, R. E. Dinnebier (Stuttgart/DE)
- PS05-P70 **Double-crystal-diffraction measurements of oxygen clusters in single-crystalline silicon**
C. Bergmann, J. Will, A. Gröschel, M. Weisser, A. Magerl (Erlangen/DE)

- PS05-P71 **Investigation of grain boundaries in multi-crystalline silicon**
E.-R. Carl, A. N. Danilewsky (Freiburg/DE), T. Geiger, E. Meißner (Erlangen/DE)
- PS05-P72 **Effect of domains on a multiferroic mineral, huebnerte (MnWO₄)**
S. Park (Munich/DE), D. Behal (Garching/DE), U. Gattermann (Munich/DE)
B. Pedersen (Garching/DE), C. Paulmann (Hamburg/DE)
- PS05-P73 **Crystal structure of 5Mg(OH)₂-MgSO₄·7H₂O – a new magnesium oxysulfate Cement Phase**
T. Runcevski (Stuttgart/DE), W. Chengyou, Y. Hongfa, Y. Bo (Xining/CN)
R. Dinnebier (Stuttgart/DE)
- PS05-P74 **Optical characterization of the protonation and deprotonation of pyroelectric single crystals**
T. Köhler, E. Mehner, J. Hanzig, H. Stöcker, D. C. Meyer (Freiberg/DE)
- PS05-P75 **Lattice controlled corrosion marks in pyrite single crystals of weathered ore veins of the polymetallic sulfide deposit of Freiberg**
F. Haubrich, A. Kluge (Freiberg/DE)
- PS05-P76 **Structure and thermal behaviour of a new ZnII squarate complex, [Zn(HC₄O₄)₂(OH₂)₄]**
F. Dumitru, M.-D. Serb (Bucharest/RO), B. Braun (Berlin/DE)
- PS05-P77 **Very short intermolecular hydrogen bonds in a tren:hydrogen succinate salt**
F. Dumitru, M.-D. Serb (Bucharest/RO)
- PS06 Cutting edge Techniques in Analysis and Preparation**
- PS06-P01 **X-ray powder diffraction analysis of disordered dioctahedral Si-Al layer silicates by the Rietveld method and a recursive method for modeling stacking faults**
K. Ufer (Hanover/DE), R. Kleeberg (Freiberg/DE)
- PS06-P02 **New abilities and performance of neutron powder diffraction at Eg**
A. Franz, D. M. Többens, M. Tovar (Berlin/DE)
- PS06-P03 **DIFFaX-Analyses of faulted phases like Ni(OH)₂ with a MATLABM-based software tool**
B. Priehs, J. Birkenstock (Bremen/DE)

- PS06-P04 **Analysis of 2D diffraction data for the fast determination of crystallite size distributions**
S. Neher, M. Chaouachi, H. Klein, W. F. Kuhs (Göttingen/DE)
- PS06-P05 **Neutron radiography – a quantitative tool to study dehydration of bentonite bonded molding sand**
G. Jordan, C. Eulenkamp (Munich/DE), E. Calzada, B. Schillinger
 M. Hoelzel (Garching/DE), W. Schmahl (Munich/DE)
- PS06-P06 **Complete characterization MOFs using CCD and CMOS detector based SC-XRD systems**
A. Gerisch, M. Adam (Karlsruhe/DE), I. Eryazici, O.K. Farha (Evanston, IL/US)
 E. Hovestreydt, H. Ott, M. Ruf (Karlsruhe/DE), A. A. Sarjeant (Evanston, IL/US)
 K. Yoza (Karlsruhe/DE)
- PS06-P07 **withdrawn**
- PS06-P08 **Serial femtosecond X-ray crystallography of in vivo crystallized proteins opens new routes in structural biology**
L. Redecke (Hamburg, Lübeck/DE), K. Nass, D. P. DePonte (Hamburg/DE)
 D. Rehders (Hamburg, Lübeck/DE), T. A. White, A. Barty, F. Stellato, M. Duszenko
 H. N. Chapman, C. Betzel (Hamburg/DE)
- PS06-P09 **High-efficiency laboratory GISAXS instrument and its applications**
P. U. Pennartz, L. Fan, M. Degen, L. Jiang, N. Grupido (Auburn Hills, MI/US)
- PS06-P10 **The new Kappa-diffractometer at beamline P24 (ChemCryst, Petralia.14, Hasylab/Desy)**
C. Paulmann, A. Berghäuser, D. Ropers, U. Bismayer (Hamburg/DE)
- PS06-P11 **Multi-purpose X-ray diffractometer platform with versatile SAXS / WAXS options**
J. Bolze (Almelo/NL), V. Kogan (Enschede/DE), D. Beckers, P. Munk, M. Fransen (Almelo/NL)
- PS07 General Crystallography – Modelling and Analysis Bridging the Scales**
- PS07-01 **Investigation of the structure of nano-sized Na_nCl_n ($n=4, 8, 12, 16$) clusters using global optimization**
J. Zagorac (Stuttgart/DE; Belgrade/RS), C. J. Schoen, M. Jansen (Stuttgart/DE)
- PS07-02 **Mosaic structure of single crystals – investigation of mosaicity and anisotropy of pyrite**
A. K. Hüsecken (Dortmund/DE), S. Gorfman, U. Pietsch (Siegen/DE)

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F. Pan, U. Englert (Aachen/DE)
- PS07-04 **Computational adsorption experiments by comparison – molecular dynamic simulations for the (100)-FeS₂-H₂O interface with materials Studio 5.0**
S. Meis (Bochum/DE), U. Magdans (Aachen/DE), H. Gies (Bochum/DE)
- PS07-05 **The symmetry and electronic structure of a new, predicted carbon phase**
T. Weißbach, S. Bahmann, J. Kortus (Freiburg/DE)
- PS07-06 **Extent and relevance of stacking disorder in “cubic ice”**
W. F. Kuhs, C. Sippel, T. Hansen, A. Falenty (Göttingen/DE)
- PS07-07 **Structure determination from X-ray powder diffraction data – a systematic survey of a new global optimization algorithm**
G. Roth, J. M. Simons (Aachen/DE)
- PS07-08 **Structural analysis of *Yersinia enterocolitica* pyruvate kinase PykF**
W. Li (Braunschweig/DE), J. Hofmann, C. Marschall, G. Wilharm (Wernigerode/DE)
D. Heinz, J. Krause (Braunschweig/DE)
- PS07-09 **Sequential proton ordering as a mechanism for the low-temperature phase transitions in (NH₄)₃H(SO₄)₂ – single-crystal neutron diffraction studies**
Y. J. Sohn, K. Sparta (Aachen/DE), M. Meven (Aachen, Garching/DE), G. Roth
G. Heger (Aachen/DE)
- PS07-10 **Inhibition of magnesite growth kinetics by acute kink-blocking**
U.-N. Berninger, Q. Gautier (Toulouse/FR), G. Jordan (Munich/DE)
J. Schott (Toulouse/FR)
- PS07-11 **ShelXle – a graphical user interface for SHELXL**
C. Hübschle (Göttingen/DE), B. Dittrich (Göttingen, Hamburg/DE)
G. Sheldrick (Göttingen/DE)
- PS07-12 **DRAWxtl 5.6**
M. Kroeker (Freiburg/DE), B. Toby (Argonne, IL/US), L. Finger (Washington, D.C./US)
- PS07-13 **Role of XRD/XRF Reference materials and values benchmarks on macro and micro scales**
G. Berti, F. de Marco, M. E. Del Seppia (Pisa/IT)

- PS07-14 **Crystallography of bis(nitrilotriacetato)zirconates with divalent cations**
P. Held (Cologne/DE), M. Fridrichová (Prague/CZ), L. Bohatý (Cologne/DE)
- PS07-15 **The collection of crystal models of Abraham Gottlob Werner**
B. Heide, A. Massanek, G. Heide (Freiberg/DE)
- PS08 Materials for Electronics – Energy and Data Storage through the Eyes of Crystallographers**
- PS08-P01 **Benzylidene-Oxazolones – Photoreactivity in the crystal state**
T. Runcevski (Stuttgart/DE), M. Cejuela, M. Blanco-Lomas, D. Sampedro (La Rioja/ES)
R. Dinnebier (Stuttgart/DE)
- PS08-P02 **Production and characterization of LLTO thin films**
J. Derr, J. Birkenstock, F. Andre (Bremen/DE)
- PS08-P03 **Photo chromatic sensors of multinary mixed valence inorganic micro needles**
K. Xhaxhiu (Tirana/AL), C. Kvarnström, P. Damlin (Turku/FI), R. Schmidt-Grund
K. Bente (Leipzig/DE)
- PS09 Non-ambient Conditions – Pressure, Temperature and Fields at Work**
- PS09-P01 **Unexpected low temperature behaviour of Piroxicam Monohydrate**
K. Fücke (Würzburg/DE), A. J. Edwards (Lucas Heights/AU), M. R. Probert
S. E. Tallentire, J. A. K. Howard, J. W. Steed (Durham/GB)
- PS09-P02 **Polarized Raman spectroscopy on multiferroic MnWO_4 under an applied electric field**
M. Adrian, H. Gibhardt, J. Leist (Göttingen/DE), L. Bohatý, P. Becker (Cologne/DE)
G. Eckold (Göttingen/DE)
- PS09-P03 **Intermediates during Ammono-basic crystal growth of GaN**
S. Zhang, R. Niewa (Stuttgart/DE)
- PS09-P04 **High-pressure high-temperature phase diagram of TaN**
A. Friedrich, W. Morgenroth, L. Bayarjargal, N. Rademacher
F. Schröder (Frankfurt a. M./DE), E. A. Juárez-Arellano (Tuxtepec/MX), J. Biehler
J. D. Bauer, B. Winkler (Frankfurt a. M./DE)

- PS09-P05 **High-pressure polymorphs of spinel-type LiMn_2O_4 as cathode materials for lithium-ion batteries**
C. Braun (Dresden, Karlsruhe/DE), N. Kiziltas Yavuz (Karlsruhe/DE)
K. Nikolowski (Leopoldshafen/DE), J. Gallardo-Amores
M.E. Arroyo-de Dompablo (Madrid/ES), H. Ehrenberg (Leopoldshafen, Karlsruhe/DE)
- PS09-P06 **The nanoscale structure of Pb-based relaxor ferroelectrics as revealed by in situ temperature-dependent Raman spectroscopy under an external electric field**
T. Steilmann (Hamburg/DE), B. Maier (Munich/DE), M. Gospodinov (Sofia/BG)
U. Bismayer, B. Mihailova (Hamburg/DE)
- PS09-P07 **Time-resolved X-ray diffraction study of elastic vibrations in piezoelectric crystals generated by alternating electric field**
M. Al Taani, S. Gorfman, M. Ziolkowski, S. Heidbrink, U. Pietsch (Siegen/DE)
- PS09-P08 **Lattice thermal expansion modeling of mullite-type PbFeBO_4**
T. M. Gesing (Bremen/DE), D. Hansmann (Mar del Plata/AR)
G. Nénert (Grenoble/FR), M. M. Murshed (Bremen/DE)
- PS09-P09 **Thermal excitation of superionic Li-mobility – interatomic potentials from (an)-harmonic temperature factors of Li_2Te**
J. Schneider, T. Schröder, M. Hölzel (Munich/DE), O. Oeckler (Leipzig/DE)
W. Schmahl (Munich/DE)
- PS09-P10 **Measurement of pyroelectric properties and ferroelectric to paraelectric phase transition**
S. Jachalke, E. Mehner, H. Stöcker, D. C. Meyer (Freiberg/DE)
- PS09-P11 **Low temperature structural phase transitions of Fe_{1+y}Te**
C. Koz, S. Roessler, A. A. Tsirlin, S. Wirth, U. Schwarz (Dresden/DE)
- PS09-P12 **A polymorphic transition induced by hydrostatic compression of the a-polymorph of chlorpropamide in saturated ethanol solution, accompanied by twinning**
T. N. Drebuschak, Y. V. Seryotkin, E. V. Boldyreva (Novosibirsk/RU)
- PS09-P13 **Crystal and Magnetic Structures of Multiferroic $\text{Ba}_2\text{CoGe}_2\text{O}_7$**
A. Sazonov, V. Hutanu, M. Meven (Aachen, Garching/DE), G. Roth (Aachen/DE)
H. Murakawa, Y. Tokura (Tokyo/JP), I. Kézsmárki (Budapest/HU), Náfrádi (Stuttgart/DE)
A. Gukasov (Gif-sur-Yvette/FR), D. Chernyshov (Grenoble/FR)

PS10 Spectroscopy and other Tools for Analysis

- PS10-P01 **A simple innovative method for X-ray absorption reduction in high temperature powder X-ray diffractometry**
K. Xhaxhiu (Tirana/AL), M. Schlosser (Regensburg/DE), H.-J. Deiseroth (Siegen/DE)
K. Bente (Leipzig/DE)
- PS10-P02 **High-resolution imaging with chemical contrast by using hard X-ray Ptychography**
J. Reinhardt (Dresden/DE)
- PS10-P03 **Pressure-induced structural changes in metamict zircon**
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- PS10-P04 **The effect of chemical variations on the nanoscale structure of relaxor ferroelectrics studied by resonance Raman spectroscopy**
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M. I. Aroyo (Bilbao/ES), M. M. Gospodinov (Sofia/BG), U. Bismayer
B. Mihailova (Hamburg/DE)
- PS10-P05 **Composition profiles across the metal-Nb₂O₅-metal stacks for resistive switching as studied by EDX and EELS**
F. Hanzig, J. Veselý, M. Motylenko, A. Leuteritz (Freiberg/DE), H. Mähne
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- PS10-P06 **On site X-ray diffraction – a new approach for not destructive testing methods**
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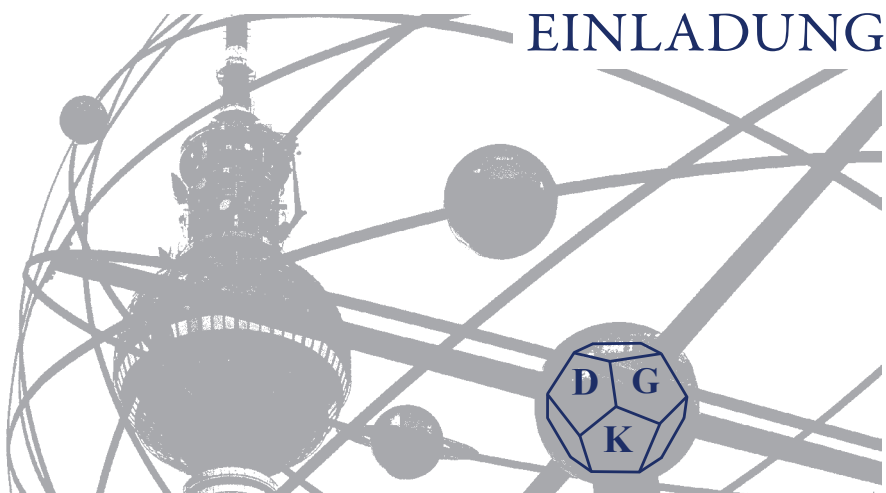
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