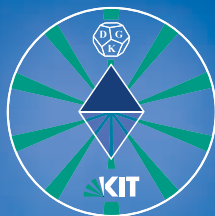


PROGRAMME



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25th ANNUAL MEETING of the GERMAN CRYSTALLOGRAPHIC SOCIETY (DGK)

27–30 MARCH 2017
KARLSRUHE

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Organisation and imprint	4
Welcome note	5
General information	6
General guidelines for authors and presenters	7
Sponsors, exhibitors and media cooperation	8
Industrial symposia	9
Young crystallographers	12
Social and cultural programme	14
Programme overview	
Monday, 27 March	16
Tuesday, 28 March	17
Wednesday, 29 March	18
Thursday, 30 March	19
Scientific programme	
Monday, 27 March	20
Tuesday, 28 March	24
Wednesday, 29 March	32
Thursday, 30 March	39
Poster presentations	46
Index of plenary speakers, presenting authors and chairs	69

ORGANISATION AND IMPRINT

Venue

Karlsruher Institut für Technologie
Audimax (Building 30.95)
Straße am Forum
76131 Karlsruhe/DE

Date

27–30 March 2017

Conference website

www.dgk-conference.de



Organiser

German Crystallographic Society (DGK)

Conference chair

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Institut für Angewandte Materialien (IAM)
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Dear crystallographers,

You are cordially invited on behalf of the local organising and programme committee to the 25th Annual Conference of the German Crystallographic Society (Deutsche Gesellschaft für Kristallographie, DGK), which will take place at the Karlsruhe Institute of Technology (KIT).

The conference venue is the Audimax located at the Forum in the centre of the university's main campus. All aspects of crystallography will be addressed. This year's focus is on the structure-property relationship especially for energy materials. Contributions to this research field can also be compiled in a special issue of "Zeitschrift für Kristallographie" as original papers or reviews. Please indicate with your registration if you want to contribute to this special issue.

Several renowned scientists from different fields of crystallography have accepted our invitation for a plenary lecture. The 25th DGK annual meeting will comprise 17 microsymposia, six plenary lectures and two poster sessions. This conference should provide to all of you an inspiring scientific platform to promote crystallography. In agreement with the aims of the German Crystallographic Society especially young scientists are encouraged to participate in the conference actively, for example in the frame of lightning talks in dedicated sessions.

We are looking forward to your attendance and scientific contributions.



Helmut Ehrenberg
Conference chair



Conference language

The conference language is English.



Opening hours

	Monday	Tuesday	Wednesday	Thursday
Self-/Check-In	12.00–18.30	07.30–17.30	08.00–16.00	08.30–15.00
Media Check-In	12.00–18.30	07.30–17.30	08.00–16.00	08.00–13.30
Industrial Exhibition	13.00–20.00	08.30–19.00	08.30–17.30	09.00–13.30



Name badge

Please wear your name badge during all conference events. Admission to scientific sessions and to the industrial exhibition is restricted to participants wearing their badge. Participants will receive their name badge at the Self-/Check-In.



WiFi access

WiFi is available for free throughout the whole conference area. Please ask at the Check-In for the login data.



Publication of abstracts

All abstracts will be published in a printed supplement of the journal „Zeitschrift für Kristallographie“, Walter de Gruyter. The abstract book is available at the Check-In at the conference.



Session planer

For current detailed information regarding the scientific programme please have a look at our session planer at programm.conventus.de/dgk2017. Compose your individual programme and review it at any time on your way.



General terms and conditions

Please find our general terms and conditions at www.dgk-conference.de.



Registration

All pre-registered delegates who have already paid the registration fee will be receiving a QR code via e-mail prior to the conference. This code needs to be printed out or saved on smartphones. There will be several Self-Check-In counters which can be used to print out your personal name badge. Our staff will be there to assist you. Please be prepared to present a proof of your advanced payment and, if applicable, a proof of your student status. Here you can also pick up your conference materials. On-site registration is also possible and credit card or cash payment will be accepted.

Technical information

The presentation should be prepared as PDF, MS Office PowerPoint for Windows or key for Macintosh DVD in format 4:3.

A presentation notebook with a PDF reader and MS Office PowerPoint 2016 and a laser pointer will be provided in the lecture hall. 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.

Presentation upload at the Media check-in

To guarantee a smooth running programme please upload your presentation at least 2 hours before the start of your talk at the Media Check-In. For submission, please use a USB flash drive, CD or DVD disc that is not protected by any software. Professional staff and equipment will be available for you to arrange your presentation.

Time allocation

Please prepare your presentation for the allotted amount of time. Chairs and moderators may interrupt should you overrun your time limit.

Poster session

Your poster must be in English and no larger than DIN A0 portrait format (84,1 cm x 118,9 cm). Pins will be provided on your poster board. Poster boards will be labelled with your poster number. You can find your poster number in the programme book on page 46ff.

Please note that there are two poster sessions.

Poster session I – Posters with an even ID

All posters with an even ID should be hung by Tuesday 17.30 and be removed, at the latest, by Tuesday 19.30.

Poster session II – Posters with an odd ID

All posters with an odd ID should be hung on Wednesday in the morning and be removed, at the latest, by Wednesday 18.00. Posters that have not been removed, will be considered as waste.

Please note: All posters of the session “Lightning Talks Session 1 (LT1)” will be presented in poster session I on Tuesday and all posters of the session “Lightning Talks Session 2 (LT2)” will be presented in poster session II on Wednesday.

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Oxford Cryosystems Ltd. (Long Hanborough/GB)

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Röntgenlabor Dr. Ermrich (Reinheim/DE)

Thermo Fisher Scientific (Dreieich/DE)

XRD Eigenmann GmbH (Schnaittach-Hormersdorf/DE)

Media cooperation

Wissenschaftliche Verlagsgesellschaft Stuttgart

Naturwissenschaftliche Rundschau

Tuesday, 28 March

Rigaku Europe (Sevenoaks/GB)

11.30–13.00 Room Seminarraum



Rigaku Oxford Diffraction welcomes attendees of the DGK conference in Karlsruhe to our Lunchtime Seminar on Tuesday, 28 March at 11.30 in the Seminarraum. A buffet lunch will be available during the seminar.

Dr. Mathias Meyer, who is the force behind the popular CrysAlisPro software, will be presenting the new developments inside the latest release of the software. He will discuss how it integrates with the current hardware to help you achieve the best from your experiments. There will also be a short introduction from Dr. Joseph Ferrara and Dr. Alexandra Griffin on PX and SMX products respectively.

We encourage you to attend and enjoy your lunch with the Rigaku Oxford Diffraction team.

- | | |
|-------------|---|
| 12.05–12.10 | Dr. Alexandra Griffin – What's new in small molecule crystallography at ROD |
| 12.10–12.15 | Dr. Joseph Ferrara – What's new in macromolecular crystallography at ROD |
| 12.15–12.55 | Dr. Mathias Meyer – CrysAlisPro – latest developments |

Wednesday, 29 March

PANalytical GmbH (Kassel/DE)

11.30–13.00 Room Seminarraum



Speakers

Detlef Opper, PANalytical GmbH (Kassel/DE)

Thorbjörn Schönbeck, PANalytical GmbH (Kassel/DE)

Gwilherm Nénert, PANalytical B.V (Almelo/NL)

From phase identification to structure solution – the latest PANalytical tools

During this lunch seminar, we will present our latest developments and solutions for powder diffraction. Whether this is about monitoring the progress of your chemical synthesis, Rietveld refinement or structure solution from powder data, PANalytical has been making several developments in its product portfolio to help you addressing your challenges.

During this seminar, we will discuss several applications:

- Aeris Benchtop XRD system
- Structure solution from powder data
- In situ and In operando battery applications
- Advanced structural investigations

Thursday, 30 March

FIZ Karlsruhe – Leibniz Institute for Information
Infrastructure (Karlsruhe/DE)

12.00–13.30 Room Seminarraum



The FIZ Karlsruhe ICSD Lunchtime Symposium

Speakers

Dr. Stephan Ruehl (Karlsruhe/DE)

Dr. Dejan Zagorac (Stuttgart/DE)

Falk Meutzner (Freiberg/DE)

Chair

Dr. Helmut Müller (Berlin/DE)

FIZ Karlsruhe is pleased to welcome the attendees of the 25th DGK conference in Karlsruhe to our ICSD Lunchtime Symposium on 30 March. Please enjoy our refreshments, which are offered during the presentation.

For almost 30 years, the ICSD database has been the most important source for inorganic crystal structure data. We will inform you on new developments of the database, demonstrate the implementation of theoretical structures in ICSD, and present an example of how to use ICSD in research.

We are looking forward to meeting you and hope you will enjoy your lunch with FIZ Karlsruhe's ICSD team.

Lightning talks of Young Crystallographers (LT1 and LT2)

The “Young Crystallographers” are happy to welcome you to the 3rd Lightning Talks at the Annual DGK Meeting. We are looking forward to the two microsymposia where 31 young crystallographers introduce their research in 5-minutes appetizer “Lightning Talks”. Instead of an in-session discussion, each contribution is complemented by a poster that will be presented the same day during the poster sessions.

Get-Together of the Young Crystallographers

We would like to welcome all members and interested “young” crystallographers (students, PhD students, postdocs, everybody without tenure) to join our 5th Annual Get Together on Thursday. Our programme will comprise both, a short summary of last year’s activities (especially the 2nd Meeting in Berlin) as well as our ideas for the future. We will elect a new co-chair and there will be plenty of time for general discussions on Young Crystallographers’ matters. Another highlight will be the granting of the “Lightning Talks” prizes. Lunch, coffee/tea and soft drinks will be served.

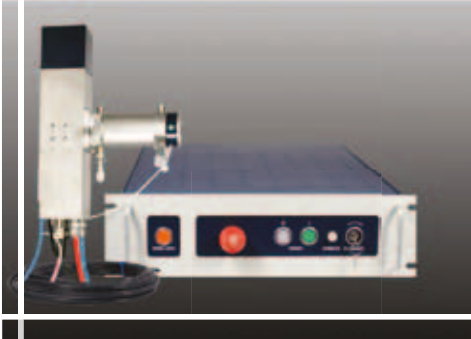
We are looking forward to welcoming you!

Melanie and Carola

Chairs of the “Young Crystallographers”

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Dr. Paul Ulrich Pennartz, European Channel Manager

Phone: + 49 (0) 2403 15051, Email: paul.pennartz@rigaku.com

Welcome reception



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Come together for drinks and snacks after the first conference day to enjoy the evening. Allow yourself interesting conversations with colleagues, old friends, exhibitors and meet new acquaintances.

Date	Monday, 27 March
Time	18.15
Fee	10 EUR
Venue	Industrial exhibition area, foyer of the venue

Social evening



© Hoepfner Burghof

The restaurant Hoepfner Burghof is located in the historic building of the Hoepfner-Brewery and is one of the landmarks of Karlsruhe. From 1899 self-made beer was served in this brewery. Today it offers excellent regional cuisine as well as the traditional home-brewed beer in a rustically and attractive ambience. Enjoy the last evening of the conference with your colleagues in a pleasant atmosphere.

Date	Wednesday, 29 March
Time	19.30
Fee	40 EUR
Venue	Hoepfner Burghof Karlsruhe Haid-und-Neu Straße 18 76131 Karlsruhe/DE
Distance to the conference venue	1 km

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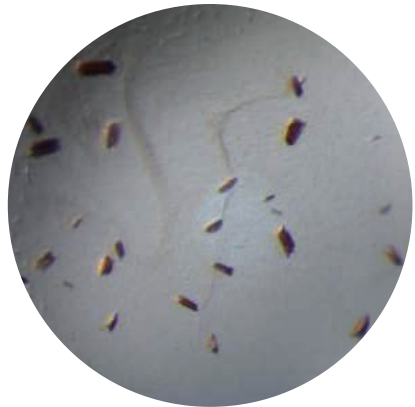
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Crystals

Audimax A	Audimax B	Seminarraum	Meeting Room
			09.00–12.30 DGK Board Meeting
13.15–13.30 Opening			
13.30–14.30 Plenary session Ilme Schlichting p. 20			
14.45–16.15			
MS01 New approaches in structural biology p. 20	MS02 Structural chemistry under non-ambient conditions p. 21	MS03 Materials science p. 22	
Coffee break and industrial exhibition			
16.45–17.15 Special lecture laureate Max-von-Laue Award p. 23			
17.15–18.15 DGK Ehrenabend p. 23			
18.15–20.00 Welcome reception p. 14			

Audimax A	Audimax B	Seminarraum
08.30–10.00		
MS04 Crystal physics p. 24	MS05 Macromolecular machines and switches p. 25	MS06 Materials for energy storage and conversion p. 26
Coffee break and industrial exhibition		
10.30–11.30		
Plenary session Dierk Raabe p. 26		
Lunch break and industrial exhibition		11.30–13.00
		Industrial Symposium Rigaku Europe p. 9
13.00–14.00		
Plenary session Tamir Gonen p. 27		
14.00–16.00		
DGK Mitgliederversammlung DGK General Assembly p. 27		
16.00–17.30		16.00–18.00
LT1 Lightning talks p. 28		MS07 Fragment based ligand screening p. 30
17.30–19.00		
Poster session I – even IDs p. 46		

Audimax A		Audimax B		Seminarraum	
08.30–10.00					
MS08 Phase transitions and dynamic phenomena <					

Audimax A	Audimax B	Seminarraum
09.00–10.30		
MS12 Spectroscopy as supporting tool in crystallography p. 39	MS13 Molecular crystallography at the limits p. 40	MS14 In situ/in operando studies of energy materials p. 41
Coffee break and industrial exhibition		
11.00–12.00		
Plenary session Krzysztof Wozniak p. 41		
Lunch break and industrial exhibition	12.00–13.30	12.00–13.30
	Get-Together of the Young Crystallographers p. 12	Industrial Symposium FIZ Karlsruhe p. 11
13.30–15.00		
MS15 New crystal structures and structure systematics p. 42	MS16 Nanoscience p. 43	MS17 Advances and application of neutron and synchrotron radiation p. 44
15.00–15.30		
Closing		

09.00–12.30 **Board meeting**

Meeting Room

13.15–13.30 **Opening**

Audimax A

13.30–14.30 **Plenary session**

Audimax A

Chair Norbert Krauß (Berlin/DE)

PL1 Protein structure and dynamics using X-ray free-electron lasers
Ilme Schlichting (Heidelberg/DE)

14.45–16.15 **MS01 – New approaches in structural biology**

Audimax A

Chair Thomas Barends (Heidelberg/DE)

14.45
MS01-01 Serial synchrotron crystallography using a high viscosity extrusion injector device on beamline MASSIF-3 at the ESRF
David von Stetten, Max Nanao, Ulrich Zander, Martin Weik
Giorgio Schiro, Jacques-Philippe Colletier, Nicolas Coquelle
Eugenio de la Mora, Joyce Woodhouse (Grenoble/FR)
R. Bruce Doak, Bob Shoeman, Marie Gruenbein
Marco Kloos (Heidelberg/DE), Pascal Theveneau, Fabian Dobias
Sylvain Aumonier, Antoine Royant (Grenoble/FR)
Ilme Schlichting (Heidelberg/DE), Gordon Leonard
Christoph Mueller-Dieckmann (Grenoble/FR)

15.05
MS01-02 Analysing structure and function of TRAP transporters by combining X-ray crystallography and pulsed EPR.

Janin Glaenger, Martin F. Peter (Bonn/DE)
Gavin H. Thomas (York/GB), Gregor Hagelueken (Bonn/DE)

15.25
MS01-03 MeshAndCollect and more – synchrotron serial crystallography at the ESRF

Ulrich Zander (Grenoble/FR)

- 15.45
MS01-04 AUSPEX – a diagnostic tool for graphical X-ray data analysis
Andrea Thorn (Hamburg/DE), James Parkhurst (Didcot, Oxfordshire/GB)
Paul Emsley, Robert A. Nicholls (Cambridge/GB), Melanie Vollmar
Gwyndaf Evans (Didcot, Oxfordshire/GB)
Garib Murshudov (Cambridge/GB)
- 16.05
MS01-05 P11 at PETRA III – a versatile beamline for high-throughput and
serial crystallography
Anja Burkhardt, Saravanan Panneerselvam, Olga Lorbeer
Tim Pakendorf, Bernd Reime, Jan Meyer, Pontus Fischer
Nicolas Stuebe, Philip Roedig, Martin Warmer
Alke Meents (Hamburg/DE)
- 16.10
MS01-06 High-resolution 3D printed injectors for time resolved serial
crystallography
Michael Heymann (Martinsried/DE)
- 14.45–16.15
Audimax B **MS02 – Structural chemistry under non-ambient conditions**
Chairs Ulrich Schwarz (Dresden/DE), Cordula Braun (Darmstadt/DE)
- 14.45
MS02-01 Novel nitrogen-rich iron nitrides synthesized at high-pressure
high-temperature conditions
Maxim Bykov (Bayreuth/DE), Elena Bykova
Georgios Aprilis (Bayreuth, Hamburg/DE)
Konstantin Glazyrin (Hamburg/DE)
Irina Chuvashova (Bayreuth, Hamburg/DE)
Egor Koemets, Leonid Dubrovinsky (Bayreuth/DE)
- 15.00
MS02-02 Synthesis of binary hafnium oxides at high pressures and high
temperatures
Lkhamsuren Bayarjargal, Wolfgang Morgenroth, Nadine Schrodtt
Björn Winkler (Frankfurt a. M./DE), Victor Milman (Cambridge/GB)
Chris Stanek, Blas P. Uberuaga (Los Alamos, CA/US)
- 15.15
MS02-03 High-pressure synthesis and crystal structure of a new
orthorhombic modification of Ir_4B_5
Benedikt Petermueller (Innsbruck/AT), Christopher Neun
Björn Winkler (Frankfurt a. M./DE), Hubert Huppertz (Innsbruck/AT)

- 15.30
MS02-04 The photo-induced and temperature reversible single-crystal-to-single-crystal transformation of a two-dimensional polymer
Gregor Hofer, Florian Grieder, A. Dieter Schlüter
Thomas Weber (Zurich/CH)
- 15.45
MS02-05 Diffusion pathways in ion conductors – making the most of neutron-diffraction data
Dennis Wiedemann (Berlin/DE)
- 16.00
MS02-06 Thermoelectric properties and atom mobility in argyrodite-type $\text{Cu}_8\text{GeSe}_4\text{Te}_2$
Stefan Schwarzmüller, Daniel Souchay, Daniel Günther
Alex Gocke (Leipzig/DE), Iurii Dovgaliuk (Grenoble/FR)
Oliver Oeckler (Leipzig/DE)
- 14.45–16.15
Seminarraum **MS03 – Materials science**
Chairs Manuel Hinterstein (Karlsruhe/DE), Martin Etter (Hamburg/DE)
- 14.45
MS03-01 Structure – property relationship in spincrossover nanocomposites
Dominik Schaniel, Pierrick Durand, Sébastien Pillet
Bertrand Fournier, Khaled Rassoul
El-Eulmi Bendeif (Vandoeuvre les Nancy/FR)
- 15.00
MS03-02 Characterization of domain wall dynamics in lead zirconate titanate using X-ray photon correlation spectroscopy
Semën Gorfman (Freiburg i. Br./DE), Alexei Bokov (Burnaby/CA)
Arman Davtyan (Siegen/DE), Zuo-Guang Ye (Burnaby/CA)
Alexei Zozulya (Hamburg/DE), Ullrich Pietsch (Siegen/DE)
Michael Sprung (Hamburg/DE), Christian Gutt (Siegen/DE)
- 15.15
MS03-03 Correlated three-dimensional imaging of dislocations – insight into the onset of thermal slip in semiconductor wafers
Daniel Hänschke (Eggenstein-Leopoldshafen/DE)
Andreas Danilewsky (Freiburg i. Br./DE)
Elias Hamann (Eggenstein-Leopoldshafen/DE)
Simon Bode (Karlsruhe/DE)
Lukas Helfen (Eggenstein-Leopoldshafen/DE; Grenoble/FR)
Tilo Baumbach (Eggenstein-Leopoldshafen, Karlsruhe/DE)

15.30
MS03-04 Assessment of solid electrolytes by Voronoi-Dirichlet partitioning: crystallographic, energetic, and economic parameters for Na and Al conductors

Falk Meutzner, Wolfram Münchgesang, Tina Nestler

Matthias Zschornak, Robert Schmid (Freiberg/DE)

Artem A. Kabanov (Samara/RU)

Mateo Ureña de Vivanco (Freiberg/DE)

Alexander P. Shevchenko (Samara/RU)

Tilmann Leisegang (Freiberg/DE; Samara/RU)

Vladislav A. Blatov (Samara/RU), Dirk C. Meyer (Freiberg/DE)

15.45
MS03-05 In-situ electric field dependent synchrotron X-ray diffraction study characterizing extrinsic and intrinsic contributions to the electromechanical response of high performance piezoceramic (1-x)PbTiO₃-(x)BiScO₃

Lalitha Kodumudi Venkataraman (Darmstadt/DE)

Dipak Kumar Khatua (Bangalore/IN), Chris M. Fancher

Jacob L.Jones (Raleigh, NC/US), Rajeev Ranjan (Bangalore/IN)

16.00
MS03-06 Simulation of beryllium crystal under hydrogen pressure
Michael Selzer, Daniel Schneider, Britta Nestler (Karlsruhe/DE)

16.45–17.15 **Laue Talk**

Audimax A

Chair

Thomas Doert (Dresden/DE)

16.45 Investigating and understanding drug polymorphism: how high-pressure crystallography can help
Francesca Fabbiani (Göttingen/DE)

17.15–18.15 **Ehrenabend**

Audimax A

18.15–20.00 **Welcome reception** (see page 14)

Foyer

08.30–10.00 **MS04 – Crystal physics**

Audimax A

Chairs Eiken Haussühl (Frankfurt a. M./DE), Jürgen Schreuer (Bochum/DE)

08.30 Strontium titanate in the electric field – pyroelectric, piezoelectric and tetragonal

MS04-01

Hartmut Stöcker, Juliane Hanzig, Erik Mehner, Sven Jachalke
Carsten Richter, Matthias Zschornak (Freiberg/DE)
Behnam Khanbabaee, Semën Gorfman (Siegen/DE)
Dirk C. Meyer (Freiberg/DE)

08.45 Time-resolved reciprocal space mapping of $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ single crystal under an alternating electric field

MS04-02

Hyeokmin Choe (Siegen/DE), Johannes Bieker (Darmstadt/DE)
Ullrich Pietsch (Siegen/DE), Uta Ruett (Hamburg/DE)
Pam A. Thomas (Coventry/GB), Semën Gorfman (Siegen/DE)

09.00 Anelastic relaxation effects in langasite-type crystal species

MS04-03

Christian Hirschle, Jürgen Schreuer (Bochum/DE)

09.15 Mechanical properties of zircon and the effect of radiation damage

MS04-04

Tobias Beirau (Halle (Saale)/DE), William D. Nix (Stanford, CA/US)
Ulrich Bismayer (Hamburg/DE), Lynn A. Boatner (Oak Ridge, TN/US)
Herbert Pöllmann (Halle (Saale)/DE), Rodney C. Ewing (Stanford, CA/US)

09.30 High pressure elastic properties of FeCO_3 and MgCO_3

MS04-05

Michał Stekiel (Frankfurt a. M./DE), Tra Nguyen-Thanh (Grenoble/FR)
Stella Chariton, Catherine McCammon (Bayreuth/DE)
Alexei Bosak (Grenoble/FR), Rita Luchitskaia (Frankfurt a. M./DE)
Keith Refson (Surrey/GB), Victor Milman (Cambridge/GB)
Björn Winkler (Frankfurt a. M./DE)

09.45 New EoS and new methods in the EoSFIT7 program suite

MS04-06

Ross Angel, Matteo Alvaro, Javier Gonzalez-Platas
Fabrizio Nestola (Padova/IT)

08.30–10.00 **MS05 – Macromolecular machines and switches**

Audimax B

Chair

Timm Maier (Basel/CH)

08.30 Molecular structure of hydrazine synthase – an enzyme complex producing rocket fuel

MS05-01

Andreas Dietl (Heidelberg/DE), Christina Ferosi

Wouter J. Maalcke (Nijmegen/NL), Andreas Menzel (Villigen/CH)

Simon de Vries (Delft/NL), Jan T. Keltjens (Nijmegen/NL)

Mike S. M. Jetten (Nijmegen, Delft/NL)

Boran Kartal (Nijmegen/NL; Bremen/DE)

Thomas R. M. Barends (Heidelberg/DE)

09.00 Structural analysis of the Tuberous Sclerosis (TSC) Complex involved in regulation of cellular growth

MS05-02

Reinhard Zech, Patrick Hansmann, Daniel Kümmel (Osnabrück/DE)

09.20 Reaction control in fatty acid megasynthases

MS05-03

Jan Gajewski (Frankfurt a. M./DE), Floris Buelens (Göttingen/DE)

Renata Pavlovic, Manuel Fischer, Eckhard Boles (Frankfurt a. M./DE)

Helmut Grubmüller (Göttingen/DE)

Martin Grininger (Frankfurt a. M./DE)

09.40 The inhibition mechanism of human 20S proteasomes enables next-generation inhibitor design

MS05-04

Fabian Henneberg, Jil Schrader, Ricardo A. Mata

Kai Tittmann (Göttingen/DE), Thomas R. Schneider (Hamburg/DE)

Holger Stark (Göttingen/DE), Gleb Bourenkov (Hamburg/DE)

Ashwin Chari (Göttingen/DE)

08.30–10.00 **MS06 – Materials for energy storage and conversion**

Seminarraum

Chairs

Claudia Weidenthaler (Mülheim a. d. Ruhr/DE)
Susan Schorr (Berlin/DE)

08.30
MS06-01 Comparative analysis of diffraction experiments for lithium insertion materials

William R. Brant (Sydney/AU; Uppsala/SE)
Siegbert Schmid (Sydney/AU)

09.00
MS06-02 Structural characterisation of $(\text{Ag}_{1-x}\text{Cu}_x)_2\text{ZnSnSe}_4$ by neutron diffraction

Galina Gurieva, Alexandra Franz, Susan Schorr (Berlin/DE)

09.20
MS06-03 Investigations on oxygen exchange rate of ion implanted single crystalline strontium titanate for air electrode application

Max Stöber, Charaf Cherkouk, Juliane Walter (Freiberg/DE)
Matthias Schelter, Jens Zosel (Meinsberg/DE)
Slawomir Prucnal (Dresden-Rossendorf/DE), Tilmann Leisegang
Dirk Carl Meyer (Freiberg/DE), Michael Mertig (Meinsberg/DE)

09.40
MS06-04 Crystal structure analysis and in-situ diffraction studies of new complex aluminum hydrides as hydrogen carriers

Claudia Weidenthaler, Thomas Bernert
Michael Felderhoff (Mülheim a. d. Ruhr/DE)

10.30–11.30 **Plenary session**

Audimax A

Chair

Helmut Ehrenberg (Karlsruhe/DE)

PL2 Atomic-scale analysis of energy materials using advanced atomprobe tomography

Dierk Raabe (Düsseldorf/DE)

11.30–13.00 **Industrial Symposium Rigaku Europe** (see also page 9)

11.30–12.30 **Meeting Arbeitskreis 6, 20**
Rooms will be announced on site

13.00–14.00 **Plenary session**

Audimax A

Chair Anton Meinhart (Heidelberg/DE)

PL3 microED opens a new era for biological structure determination
Tamir Gonen (Ashburn, VA/US)

14.00–16.00 **Mitgliederversammlung (General Assembly)**

Audimax A

16.00–17.30 **LT1 – Lightning talks of Young Crystallographers**

Audimax A

Chairs Matthias Zschornak, Hartmut Stöcker (Freiberg/DE)

16.00 The UV-triggered decomposition of 3-(4-pyridyl)-acetylacetone

LT1-01 (P68) Khai-Nghi Truong, Marius Kremer, Ulli Englert (Aachen/DE)

16.05 Structure-property relationships in mullite-type and related compounds

LT1-02 (P25)

Linda Hollenbeck, Timo Rütten, Jürgen Schreuer (Bochum/DE)
Hartmut Schneider (Bremen/DE)

16.10 Understanding of electrochemical mechanism of 4d layered cathode Li_2RuO_3 – in situ synchrotron study combined with electrochemical kinetics

LT1-03 (P48)

Ye Yao (Changchun/CN), Xiaofei Bie (Kyoto/JP), Björn Schwarz
Lars Riekehr, Christoph Dräger
Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE)
Yingjin Wei, Fei Du (Changchun/CN)

16.15 Hydrothermal preparation of LFP particles with high crystalline for electrochemistry

LT1-04 (P77)

Guiying Tian, Frieder Scheiba, Helmut Ehrenberg
Kiran Chakravadhanula (Eggenstein-Leopoldshafen/DE)

16.20 High-resolution single-crystal X-ray diffraction investigations of β -Rhombohedral Boron

LT1-05 (P144)

Claudio Eisele (Bayreuth/DE)

16.25 Specificity of the rhodopsin transducin interaction

LT1-06 (P54)

Dennis Kwiatkowski, Nicolas Heyder, Karoline Lê Công
Johanna Tiemann, Peter Hildebrand, Michal Szczepek
Patrick Scheerer (Berlin/DE)

16.30 Materials inspired by nature – synthesis and characterisation of perryite-related compounds $\text{Ni}_{8-x}\text{Fe}_x\text{Si}_3$ with $0 \leq x \leq 8$

LT1-07 (P65)

Simone Gallus (Aachen/DE), Mamuka Chikovani, Jörg Persson
Jörg Voigt, Karen Friese (Jülich/DE)
Anatoliy Senyshyn (Garching/DE), Andrzej Grzechnik (Aachen/DE)

- 16.35
LT1-08 (P24) Elastic properties and phase transitions of pure and Mn-doped åkermanite
Michael Haiduk, Juergen Schreuer (Bochum/DE), Manfred Burianek
Reinhard X. Fischer (Bremen/DE)
- 16.45
LT1-09 (P159) Lab-based x-ray diffractometer for the investigation of low temperature magnetic field-induced phase transitions
Tom Faske, Wolfgang Donner (Darmstadt/DE)
- 16.50
LT1-10 (P184) Synthesis and characterisation of monazite solid solution series
Antje Hirsch (Aachen/DE), Philip Kegler (Jülich/DE), Igor Alencar
Javier Ruiz-Fuertes, Anja Thust
Johannes Bauer (Frankfurt a. M./DE), Charlotte Schausten
Lars Peters, Georg Roth (Aachen/DE)
- 16.55
LT1-11 (P167) Binary protein crystals for the assembly of inorganic nanoparticle superlattices
Matthias Künzle, Marcel Lach, Thomas Eckert
Tobias Beck (Aachen/DE)
- 17.00
LT1-12 (P82) Boehmite (γ -AlOOH) nanoparticles as model system for monitoring particle formation in water based reaction media within the second time scale
Stefan Diez (Erlangen/DE)
- 17.05
LT1-13 (P21) Investigation of inversion domains in HTVPE GaN layers grown on sapphire substrates
Michael Barchuk, Mykhaylo Motylenko, Gleb Lukin, Tom Schneider
Olf Pätzold, David Rafaja (Freiberg/DE)
- 17.10
LT1-14 (P52) In operando X-ray total scattering experiments on Li-oxygen batteries
Andy Fiedler, Frieder Scheiba, Murat Yavuz
Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE)
- 17.15
LT1-15 (P39) X-ray crystallographic fragment screening and hit optimization
Nicole Bertoletti, Florian Braun, Alexander Metz, Lorena Zara
Andreas Heine, Gerhard Klebe
Sandrine Marchais-Oberwinkler (Marburg/DE)

- 17.20
LT1-16 (P98) Maximum vacancy ordering in mullite
Paul Klar, Noelia de la Pinta, Gabriel Alejandro Lopez
Iñigo Etxebarria, Tomasz Breczewski, Gotzon Madariaga (Bilbao/ES)
- 16.00–18.00
Seminarraum **MS07 – Fragment based ligand screening**
Chairs Manfred Weiss (Berlin/DE), Andreas Heine (Marburg/DE)
- 16.00
MS07-01 Addressing protein targets with small molecule fragments and
self-optimized inhibitors by crystallography
Gerhard Klebe (Marburg/DE)
- 16.40
MS07-02 The landscape of EPHA2 inhibition
Denis Kudlinzki (Frankfurt a. M./DE), Stephanie Heinzlmeir (München/DE)
- 17.00
MS07-03 Fragment based screening to target the ubiquitin activating enzyme
for cancer therapy
Mohit Misra (Würzburg/DE)
Franziska Huschmann (Berlin, Marburg/DE)
Maximilian Kuhn, Christoph Sottriffer (Würzburg/DE)
Manfred Weiss (Berlin/DE), Hermann Schindelin (Würzburg/DE)
- 17.20
MS07-04 Unravelling the nature of the druggable pockets by chemical fragments
Apirat Chaikwad (Frankfurt a. M./DE)
- 17.40
MS07-05 Fragment-screening studies on the ectonucleotidase CD73
Emma Rose Scaletti (Leipzig/DE), Franziska Huschmann
Uwe Mueller, Manfred S. Weiss (Berlin/DE)
Norbert Sträter (Leipzig/DE)
- 17.30–19.00 Poster session I – even IDs (see page 46 ff.)



JAHRES TAGUNG



der Deutschen
Gesellschaft für
Biomaterialien



9.–11.
November 2017
Würzburg

SAVE THE DATE

08.30–10.00 **MS08 – Phase transitions and dynamic phenomena**

Audimax A

Chairs Thomas Doert (Dresden/DE), Caroline Röhr (Freiburg i. Br./DE)

08.30 Phase transitions and new structures at low temperature in
MS08-01 $\text{Ba}_{1-x}\text{Sr}_x\text{CuSi}_2\text{O}_6$ spin dimer compounds
Natalija van Well (Villigen/CH), Pascal Puphal (Frankfurt a. M./DE)
Bjoern Wehinger (Villigen, Geneva/CH)
 Mariusz Kubus (Villigen, Bern/CH), Jürg Scheffer (Villigen/CH)
 Sander van Smaalen (Bayreuth/DE)
 Christian Rüegg (Villigen, Geneva/CH)

08.45 Polymorphic phase-transitions of CsGaQ_2 (Q = S, Se)
MS08-02 Daniel Friedrich, Marc Schlosser, Arno Pfitzner (Regensburg/DE)

09.00 Kinetic effects in piezoelectric actuator materials
MS08-03 Manuel Hinterstein, Michael Knapp (Karlsruhe/DE)
 Andrew Studer (Sydney/AU), Martin Etter (Hamburg/DE)
 Alexander Schoekel (Karlsruhe/DE), Hyeokmin Choe
 Semen Gorfman (Siegen/DE), Michael J. Hoffmann (Karlsruhe/DE)

09.15 Zintl phases hydride LnTtHx (Ln = La, Nd) (Tt = Si, Ge, Sn)
MS08-04 Anton Werwein, Henry Auer, Lena Kuske, Holger Kohlmann (Leipzig/DE)

09.30 Temperature-dependent structural changes in a Jacobsen catalyst:
MS08-05 X-ray induced spin-crossover, phase transition or just rotational
 disorder?
Jennifer Ballay (Düsseldorf/DE), Martin Lutz (Utrecht/NL)
 Oliver Janka, Rainer Pöttgen (Münster/DE), Constantin Czekelius
 Birger Dittrich (Düsseldorf/DE)

09.45 Structure and thermal stability of boehmite derived transition aluminas
MS08-06 Martin Rudolph, Mykhaylo Motylenko, Tilo Zienert, Hartmut Stöcker
 David Rafaja (Freiberg/DE)

08.30–10.00 **MS09 – Hot biostructures**

Audimax B

Chairs Anton Meinhart (Heidelberg/DE), Norbert Krauss (Karlsruhe/DE)

08.30 Intra-molecular regulation of nucleotide binding to the

MS09-01

Ski₂-like RNA helicase Brr₂

Eva Absmeier, Karine F. Santos, Markus C. Wahl (Berlin/DE)

08.55

MS09-02

A RecQ helicase in disguise – how the unconventional structure of the human RecQ4 Helicase defines its special position in the RecQ helicase family

Sebastian Kaiser, Florian Sauer, Caroline Kisker (Würzburg/DE)

09.20

MS09-03

Structural studies on ectonucleotidases involved in purinergic signaling

Christoph Döhler, Matthias Zebisch, Norbert Sträter (Leipzig/DE)

09.45

MS09-04

Escherichia coli HrpB – a helicase containing a unique C-terminal region

Agnieszka J. Pietrzyk-Brzezinska, Markus C. Wahl (Berlin/DE)

08.30–10.00

MS10 – Electron crystallography

Seminarraum

Chairs

Hans-Joachim Kleebe (Darmstadt/DE)

Christian Kübel (Karlsruhe/DE)

08.30

MS10-01

Structural characterisation of porous functional materials using a combination of electron diffraction tomography, HRTEM and powder X-ray diffraction

Haishuang Zhao, Bastian Barton (Mainz/DE), Isabel Großkreuz

Hermann Gies (Bochum/DE), Timo Rhauderwiek

Norbert Stock (Kiel/DE), Ute Kolb (Mainz/DE)

08.48

MS10-02

The rotation method in electron crystallography

Tim Gruene (Villigen/CH), Jan Pieter Abrahams (Villigen, Basel/CH)

Eric van Genderen (Villigen/CH), Max Clabbers

Thorsten Blum (Basel/CH)

- 09.06
MS10-03 Crystal structure of a disordered organic pigment determined by electron diffraction
Tatiana E. Gorelik, Christian Czech, Sonja M. Hammer
Martin U. Schmidt (Frankfurt a. M./DE)
- 09.24
MS10-04 TEM investigation of CuMn_2O_4 spinel catalyst upon reduction and subsequent reoxidation
Maximilian Trapp, Mathis M. Müller
Hans-Joachim Kleebe (Darmstadt/DE)
- 09.42
MS10-05 Radial distribution function imaging – a new TEM method to analyze multiphase amorphous materials
Xiaoke Mu (Eggenstein-Leopoldshafen, Ulm/DE)
Di Wang (Eggenstein-Leopoldshafen/DE), Tao Feng (Nanjing/CN)
Christian Kübel (Eggenstein-Leopoldshafen, Ulm/DE)
- 10.30–11.30 **Plenary session**
Audimax A
Chair Ullrich Pietsch (Siegen/DE)
- PL4 Crystallography of epitaxial semiconductor-superconductor hybrid nanocrystals
Peter Krogstrup (Copenhagen/DK)
- 11.30–13.00 **Industrial Symposium Panalytical GmbH** (see also page 10)
Seminarraum

- 13.00–14.00 **Plenary session**
 Audimax A
 Chair Martin Meven (Aachen/DE)
- PL5 Magnetism in quasicrystals and their periodic approximants
Andreas Kreyssig (Ames, IA/US)
- 14.30–16.00 **LT2 – Lightning talks of Young Crystallographers**
 Audimax A
 Chairs Alexander Pöthig (München/DE), Linda Hollenbeck
 Michael Haiduk (Bochum/DE)
- 14.30
 LT2-01 (P4) Spin density of a cAAC-based stable radical from single-crystal X-ray diffraction
Marion Flatken, Birger Dittrich (Düsseldorf/DE)
- 14.35
 LT2-02 (P23) Synthesis, characterization of compounds of earth alkaline rare-earth aluminates
Chimednorov Otgonbayar, Herbert Pöllmann (Halle (Saale)/DE)
- 14.40
 LT2-03 (P83) In-situ time-resolved XRD and RHEED study of the polytypism in GaAs nanowires
Julian Jakob (Eggenstein-Leopoldshafen, Karlsruhe/DE)
 Philipp Schroth (Eggenstein-Leopoldshafen, Siegen/DE)
 Ludwig Feigl (Eggenstein-Leopoldshafen/DE)
 Seyed Mohammad Mostafavi Kashani, Jonas Vogel
 Ullrich Pietsch (Siegen/DE)
 Tilo Baumbach (Eggenstein-Leopoldshafen, Karlsruhe/DE)
- 14.45
 LT2-04 (P96) Modelling Disorder with DSR in ShelXle and Olex2
Daniel Kratzert (Freiburg i. Br./DE)
- 14.50
 LT2-05 (P147) The growth kinetics and the structure of expanded austenite in AISI316L stainless steels characterized by in-situ XRD
Zoltán Balogh-Michels (Dübendorf/CH), Alexander Faeht
 Simon Kleiner, Jean-Martin Rufer (Biel/CH)
 Patrick Markgraf (Egerkingen/CH), Alex Dommann
 Antonia Neels (Dübendorf/CH)

- 14.55
LT2-06 (P55) Structural characterization of fluorescence optimized bacterial phytochromes as optogenetic tool
Luisa Sauthof, Andrea Schmidt, Michal Szczepek, Bilal Qureshi
Tammo Stevens, Maria Fernandez Lopez, Francisco Velazquez Escobar
Norbert Michael (Berlin/DE), Norbert Krauß
Tilman Lamparter (Karlsruhe/DE), Peter Hildebrandt
Patrick Scheerer (Berlin/DE)
- 15.00
LT2-07 (P51) $\text{P2-Na}_{0.66}\text{Co}_{0.95}\text{Ti}_{0.05}\text{O}_2$ – a high performance cathode material for sodium ion batteries
Noha Sabi (Marrakesh, Ben Guerir/MA), Angelina Sarapulova
Sylvio Indris, Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE)
Jones Alami (Ben Guerir/MA)
Ismael Saadoun (Marrakesh, Ben Guerir/MA)
- 15.05
LT2-08 (P64) Synthesis of sphalerite – different ways to obtain chemically pure and doped material
Judith Heinrich, Marcus Schwarz, Gerhard Heide (Freiberg/DE)
- 15.15
LT2-09 (P16) In-situ synchrotron XRPD study of crystallization kinetics of CaCO_3 in liquid microjet
Ahmed Mohammed, Antonio Cervellino, Andrea Testino
Agnese Carino (Villigen/CH)
- 15.20
LT2-10 (P75) In-situ time-resolved X-ray diffraction of a single GaAs nanowire during thermal annealing and at growth conditions
Seyed Mohammad Mostafavi Kashani (Siegen/DE)
Dominik Kriegner (Prague/CZ)
Philipp Schroth (Siegen, Karlsruhe/DE), Jonas Vogel (Siegen/DE)
Ludwig Feigl, Julian Jakob (Karlsruhe/DE), Arman Davtyan
Danial Bahrami (Siegen/DE), Tilo Baumbach (Karlsruhe/DE)
Ullrich Pietsch (Siegen/DE)
- 15.25
LT2-11 (P47) In situ studies of NASICON-type $\text{Ca}_{0.5}\text{Ti}_2(\text{PO}_4)_3$ @carbon for sodium-ion batteries
Qiang Fu, Angelina Sarapulova
Natalia Bramnik (Eggenstein-Leopoldshafen/DE)
Zhixuan Wei Fei Du (Changchun/CN), Michael Knapp
Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE)

- 15.35
LT2-13 (P69) Fostering what is needed tomorrow – facing problems in teaching crystallographic topics
Stefanie Langenstück, Ulli Englert (Aachen/DE)
- 15.40
LT2-14 (P186) Synthesis, compressibility and stability of W7Re13B
Christopher Neun (Frankfurt a. M./DE)
Benedikt Petermüller (Innsbruck/AT), Lkhamsuren Bayarjargal
Wolfgang Morgenroth (Frankfurt a. M./DE)
Hubert Huppertz (Innsbruck/AT), Björn Winkler (Frankfurt a. M./DE)
- 15.45
LT2-15 (P43) A systematic in situ and real-time investigation of mechanochemical formation of pharmaceutical cocrystals
Luzia S. Germann (Stuttgart/DE), Leigh Loots, Cristina Mottilla
Joseph Marrett, Jean-Louis Do (Montreal/CA)
Nicola Casati (Villigen/CH), Robert E. Dinnebier (Stuttgart/DE)
Tomislav Friščić (Montreal/CA)
- 15.50
LT2-16 (P73) Time-resolved in-situ high-resolution X-ray diffraction of growing self-catalysed GaAs nanowires
Philipp Schroth (Siegen, Karlsruhe/DE), Julian Jakob, Martin Köhl
Ludwig Feigl (Karlsruhe/DE), Seyed Mohammad Mostafavi Kashani
Jonas Vogel, Arman Davtyan (Siegen/DE)
Jörg Stempfer (Hamburg/DE), Tilo Baumbach (Karlsruhe/DE)
Ullrich Pietsch (Siegen/DE)

14.30–16.00 **MS11 – Structural biology meets chemistry**

Audimax B

Chairs Wulf Blankenfeldt (Bayreuth/DE), Jesko Köhnke (Saarbrücken/DE)

14.30 The fine-tuned machinery of O₂-tolerant [NiFe] hydrogenase
MS11-01 Andrea Schmidt, Patrick Scheerer, Jacqueline Kalms (Berlin/DE)

14.55 BIODIFF – a neutron diffractometer optimized for crystals with large
MS11-02 unit cells – new developments and recent application examples
Tobias Erich Schrader, Andreas Ostermann (Garching/DE)
Michael Monkenbusch, Bernhard Laatsch (Jülich/DE)
Philipp Jüttner, Winfried Petry (Garching/DE)
Dieter Richter (Garching, Jülich/DE)

15.15 Structural basis for the formation of (2S,4R)-methyl-proline within
MS11-03 the biosynthesis of griselimycins, natural products with
anti-tuberculosis activity
Peer Lukat (Braunschweig/DE)
Yohei Katsuyama (Tokyo/JP; Saarbrücken/DE)
Silke Wenzel (Saarbrücken/DE)
Mark Brönstrup (Braunschweig/DE), Rolf Müller (Saarbrücken/DE)
Wulf Blankenfeldt (Braunschweig/DE)

15.35 Elucidation of photochemical mechanisms by combination of
MS11-04 protein crystallography, spectroscopy and computational chemistry
Tatiana Domratcheva (Heidelberg/DE)

16:00–17:30 Poster session II – odd IDs (see page 46 ff.)

19.30–23.00 **Social evening** (see page 14)

Hoepfner Brauerei

- 09.00–10.30 **MS12 – Spectroscopy as supporting tool in crystallography**
 Audimax A
 Chair Michael Fechtelkord (Bochum/DE)
- 09.00
MS12-01 The First Ni(II) complex of 4-methoxypicolinic acid – synthesis, crystal structure, infrared and UV-Vis spectra – a combined experimental and DFT study
Ömer Tamer (Sakarya/TR)
- 09.15
MS12-02 Crystal structure solution and phase characterization of α/β -Ni(OH)₂-like basic nickel chlorides
Sebastian Bette, Robert E. Dinnebier (Stuttgart/DE)
 Daniela Freyer (Freiberg/DE)
- 09.30
MS12-03 Improving QM/MM and MO/MO computations of displacement parameters in crystal structures and comparison to measured IR spectra for predicting both external and internal modes of vibration
Birger Dittrich, Dennis R. Dombrowski, Christoph A. Sever
 Jens Lübben (Düsseldorf/DE)
- 09.45
MS12-04 Complex substitution in intermetallics
 Volker Peters, Alexander Korthaus (Aachen/DE)
 Oliver Pecher (Dresden, Aachen/DE; Cambridge/GB)
Frank Haarmann (Dresden, Aachen/DE)
- 10.00
MS12-05 Pressure induced phase transition in Eu doped CaCO₃ detected by fluorescence spectroscopy
Chris-Julian Fruhner, Lkhamsuren Bayarjargal, Nadine Schrodtt
 Rita Luchitskaia, Björn Winkler (Frankfurt a. M./DE)
- 10.15
MS12-06 Microfocusing source based beam solution for analytical instruments
Paul Ulrich Pennartz (Eschweiler/DE)

09.00–10.30 **MS13 – Molecular crystallography at the limits**

Audimax B

Chairs Alexander Pöthig (Garching/DE), Astrid Schneidewind (Jülich/DE)

09.00 ab initio ORTEP – fundamentals, function, tentative future

MS13-01 Richard Dronskowski (Aachen/DE)

09.30 Diffuse single crystal scattering corrected for molecular formfactor effects

MS13-02

Ella Schmidt, Reinhard Neder (Erlangen/DE)

09.45 How far can we see? – atomic resolution structure of giant supramolecules

MS13-03

Alexander Virovets, Eugenia Peresypkina

Manfred Scheer (Regensburg/DE; Novosibirsk/RU)

10.00 Caviplexes – complexes of macrocyclic NHC-ligands with defined cavities

MS13-04

Alexander Pöthig (Garching/DE)

10.15 Facilities for macromolecular crystallography at the HZB

MS13-05

Martin Gerlach, Christian Feiler, Ronald Förster, Christine Gless

Niklas Grabicki, Thomas Hauß, Michael Hellmig, Franziska Huschmann

Alexandra Kastner, Piotr Malecki, Karine Röwer

Lukas Schmuckermaier, Michael Steffien, Piotr Wilk

Manfred S. Weiss (Berlin/DE)

- 09.00–10.30 **MS14 – In situ/in operando studies of energy Materials**
 Seminarraum
 Chairs Siegbert Schmid (Sydney/AU), Michael Knapp (Karlsruhe/DE)
- 09.00 In situ diffraction 100
MS14-01 Holger Kohlmann (Leipzig/DE)
- 09.30 Uncommon phase transformation in LiRhO₂ upon Li-extraction
MS14-02 Daria Mikhailova (Karlsruhe/DE), Olesia Karakulina
Dmitry Batuk (Antwerp/BE), Artem Abakumov (Moscow/RU)
Joke Hadermann (Antwerp/BE), Alexander Tsirlin (Augsburg/DE)
Helmut Ehrenberg (Karlsruhe/DE)
- 09.50 Investigating the formation of nanosized Pt-M (M = Ni, Co) alloys by
MS14-03 in-situ pair distribution function analysis
Seyma Ortatatli, Claudia Weidenthaler
Johannes Knossalla (Mülheim a. d. Ruhr/DE)
- 10.10 In-situ diffraction studies during ammonia decomposition with
MS14-04 transition metal catalysts
JoChi Tseng, Claudia Weidenthaler (Mülheim a. d. Ruhr/DE)
- 10.30–11.00 **Meeting Arbeitskreis 12**
Room will be announced on site
- 11.00–12.00 **Plenary session**
 Audimax A
 Chair Ulli Englert (Aachen/DE)
- PL6** A century after the Braggs – on precision and accuracy of single crystal
 X-ray results
Krzysztof Wozniak (Warsaw/PL)
- 12.00–13.30 **Industrial Symposium FIZ Karlsruhe – Leibniz Institute for Information**
 Seminarraum **Infrastructure** (see page 11)

12.00–13.30 **Get Together of the Young Crystallographers (see page 12)**

Audimax B

13.30–15.00 **MS15 – New crystal structures and structure systematics**

Audimax A

Chair Thomas Schleid (Stuttgart/DE)

13.30 [LiAl₂(OH)₆]*X*·*m*H₂O LDH containing different carboxylic anions of various chain sizes

MS15-01

Anton Niksch (Halle (Saale)/DE)

13.48 Crystal structures of organolithium compounds from powder data

MS15-02

Alexander Bodach, René Hebestreit, Lothar Fink, Michael Bolte
Martin U. Schmidt (Frankfurt a. M./DE)

14.06 Hydrothermal synthesis of CoMo₂Sb₂O₁₀ and FeSbO₂F₂

MS15-03

Sk Imran Ali (Stockholm/SE), Reinhard K. Kremer (Stuttgart/DE)
Mats Johnsson (Stockholm/SE)

14.24 Crystal structure and polymorphism of NaSrVO₄ – the first A^IB^{III}X^VO₄ larnite related structure from X-ray powder data

MS15-04

Gwilherm Nenert (Almelo/NL), Paul O’Meara (Cambridge/GB)
Thomas Degen (Almelo/NL)

14.42 Structural crystallography of novel alkali neptunyl selenate and selenite compounds – 2D-sheet selenates and 1D-selenite

MS15-05

Eike M. Langer (Jülich/DE), Olaf Walter (Karlsruhe/DE)
Evgeny V. Alekseev (Jülich, Aachen/DE)

13.30–15.00 **MS16 – Nanoscience**

Audimax B

Chairs Ulli Pietsch (Siegen/DE), Michael Hanke (Berlin/DE)

13.30
MS16-01 Electron tomography as a powerful tool for superstructure crystallography and defect analysis of self-assembled nanoclusters
Christian Kübel (Eggenstein-Leopoldshafen/DE)

14.00
MS16-02 Ferroelectric domains in strained $\text{K}_{0.75}\text{Na}_{0.25}\text{NbO}_3$ epitaxial films grown on (110) TbScO_3 probed by scanning X-ray nanodiffraction
Martin Schmidbauer, Michael Hanke, Albert Kwasniewski
Dorothee Braun, Leonard von Helden (Berlin/DE)
Steven John Leake (Grenoble/FR), Jutta Schwarzkopf (Berlin/DE)

14.15
MS16-03 An algorithm to decorate nanoparticle surfaces
Reinhard Neder (Erlangen/DE)

14.30
MS16-04 Time-resolved in-situ X-ray investigations during growth of $\text{In}_x\text{Ga}_{1-x}\text{As}$ core-shell nanowire structures
Ludwig Feigl (Eggenstein-Leopoldshafen/DE)
Philipp Schroth (Eggenstein-Leopoldshafen, Siegen, Karlsruhe/DE)
Julian Jakob (Eggenstein-Leopoldshafen, Karlsruhe/DE)
Seyed Mohammad Mostafavi Kashani, Jonas Vogel
Arman Davtyan (Siegen/DE), Sonia Francoual, Jörg Stremper
Ullrich Pietsch (Hamburg/DE), Tilo Baumbach (Karlsruhe/DE)

14.45
MS16-05 Structural and compositional analysis of isolated core-shell (In, Ga)N/GaN rods based on nanofocus X-ray diffraction and scanning transmission electron microscopy
Thilo Krause, Michael Hanke, Lars Nicolai, Zongzhe Cheng
Michael Niehle, Achim Trampert (Berlin/DE), Maik Kahnt
Gerald Falkenberg, Christian Schroer (Hamburg/DE)
Jana Hartmann, Hao Zhou, Hergo Wehmann
Andreas Waag (Braunschweig/DE)

- 13.30–15.00 **MS17 – Advances and application of neutron and synchrotron radiation**
Seminarraum
Chairs Martin Meven (Aachen/DE), Astrid Schneidewind (Garching/DE)
- 13.30
MS17-01 Probing structural distortions with high precision – resonant X-ray diffraction with photon energies tuned to destructive interference
Matthias Zschornak (Freiberg/DE)
Carsten Richter (Freiberg, Hamburg/DE), Dmitri V. Novikov (Hamburg/DE)
Erik Mehner, Melanie Nentwich, Juliane Hanzig, Hartmut Stöcker
Tilman Leisegang, Dirk C. Meyer (Freiberg/DE)
Semën Gorfman (Siegen/DE)
- 13.45
MS17-02 High-pressure geophysics using synchrotron radiations
Hans J. Mueller, Frank R. Schilling, Christian Scheffzük
Birgit R. I. Mueller (Karlsruhe/DE)
- 14.00
MS17-03 Feasibility of high-pressure single-crystal neutron diffraction in diamond anvil cells on the diffractometer HEIDI at the Heinz Maier-Leibnitz Zentrum (MLZ) in Garching
Andrzej Grzechnik, Martin Meven (Aachen/DE), Karen Friese (Jülich/DE)
- 14.15
MS17-04 Determination of coordination site disorder in $\text{LiMn}_{2-x}\text{Ti}_x\text{O}_4$ through combined X-ray diffraction and XAS studies
Denissa T. Murphy, Siegbert Schmid (Sydney/AU)
- 14.30
MS17-05 The D19 diffractometer at the ILL – for chemical and protein crystallography
Estelle Mossou (Grenoble/FR)
- 14.45
MS17-06 Analysis of VHCF damage in duplex stainless steel using micro-beam X-ray diffraction and a pnCCD detector
Ali Abboud, Ullrich Pietsch, Benjamin Dönges
Hans-Juergen Christ (Siegen/DE)
- 15.00–15.30 **Closing**
Audimax A

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POSTER OVERVIEW

Advances and application of neutron and synchrotron Radiation	47
Crystal physics	49
Fragment based ligand screening	51
Hot structures	51
In situ/in operando studies of energy materials	52
Macromolecular machines and switches	53
Materials for energy storage and conversion	53
Materials science	54
Molecular crystallography at the limits	54
Nanoscience	55
New approaches in structural biology	57
New crystal structures and structure systematics	58
Phase transitions and dynamic phenomena	63
Spectroscopy as supporting tool in crystallography	64
Structural biology meets chemistry	65
Structural chemistry under non-ambient conditions	65

Advances and application of neutron and synchrotron radiation

- P1 Modern CPAD detector technology for higher energy X-rays
Eric Hovestreydt, Martin Adam, Roger Durst (Karlsruhe/DE)
- P2 In-situ synchrotron radiation study of Ag-Sn bilayer growth
Nikolay Zotov, Peter Schützendübe, Paul Rossi, Eric J. Mittemeijer
Shyjumon Ibrahimkutty, Peter Wochner (Stuttgart/DE)
- P3 Temperature-dependent structural and spectroscopic investigations of $(\text{Bi}_{1-x}\text{Fe}_x)\text{FeO}_3$ ($x = 0.17$ and 0.33) using neutron elastic and light inelastic scattering
Andrea Kirsch, M. Mangir Murshed (Bremen/DE), Melanie Kirkham
Ashfia Huq (Oak Ridge, TN/US), Thorsten M. Gesing (Bremen/DE)
- P4 Spin density of a cAAC-based stable radical from single-crystal X-ray diffraction
Marion Flatken, Birger Dittrich (Düsseldorf/DE)
- P5 Practical aspects on the application of δ -recycling to synchrotron through-the-substrate microdiffraction data
Jordi Rius, Anna Crespi (Bellaterra/ES), Oriol Vallcorba (Barcelona/ES)
- P6 Neutron radiography study on temperature and moisture effects on the tensile strength of bentonite moulding sand
Guntram Jordan, Korbinian Schiebel, Wolfgang W. Schmahl (München/DE)
Burkhard Schillinger (Garching/DE), Anders Kaestner (Villigen/CH)
- P7 Enhanced options at the BESSY II beamline KMC-2
Daniel Többens, Götz Schuck, Dirk Wallacher, Nico Grimm, Susan Schorr (Berlin/DE)
- P8 Magnetic structure determination of pyroxenes in the solid solution series $\text{LiFeGe}_2\text{O}_6 - \text{NaFeGe}_2\text{O}_6$
Günther Redhammer, Gerold Tippelt (Salzburg/AT)
Anatoliy Senyshyn (Garching/DE), Georg Roth (Aachen/DE)
- P9 An approach to forward model time-of-flight neutron diffraction data for uniaxial load conditions using the example of sandstone
Simon Breuer, Birgit Müller, Frank Schilling (Karlsruhe/DE)
Christian Scheffzük (Karlsruhe/DE; Dubna/RU)
- P10 The automatized sample changing system at the high resolution powder diffraction beamline P02.1 at PETRA III, DESY
Martin Etter, Jozef Bednarcik, Mario Wendt, Sergej Wenz (Hamburg/DE)

- P11 Transition metal diborides: versatile materials with interesting crystal structures
Kathrin Hofmann, Mehmet Kayhan, Barbara Albert (Darmstadt/DE)
- P12 The neutron time-of-flight diffractometer EPSILON for residual and applied strain analysis on geological samples under uniaxial and triaxial load conditions
Simon Breuer, Christian Scheffzük (Karlsruhe/DE; Dubna/RU), Birgit I.R. Müller Frank R. Schilling (Karlsruhe/DE)
Badmaarag Altangerel (Dubna/RU; Ulaanbaatar/MN)
- P13 Thermal stability of Fe-ion containing oxide materials, studied by *in situ* high-temperature measurements
Angelina Sarapulova, Michael Knapp, Natalia Bramnik, Geethu Balachandran Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE), Olga Chimitova Bair Bazarov, Jibzema Bazarova (Ulan-Ude/RU)
Daria Mikhailova (Eggenstein-Leopoldshafen, Dresden/DE), Yurii Protz Alexander Komarek (Dresden/DE)
- P14 Empirical asymmetry corrections in Rietveld refinements using the Split Pseudo-Voigt function (SPV) and evaluation of Rietveld plots using normalized difference curves
Johannes Birkenstock, Thomas Messner, Reinhard X. Fischer (Bremen/DE)
- P15 Characterisation of photonic crystal fibers using synchrotron radiation
Michael Hagelstein, David Batchelor, Rolf Simon Holger Hessdorfer (Eggenstein-Leopoldshafen/DE), Michael Frosz (Erlangen/DE)
- P16 In-situ synchrotron XRPD study of crystallization kinetics of CaCO_3 in liquid microjet
Ahmed Mohammed, Antonio Cervellino, Andrea Testino Agnese Carino (Villigen/CH)

Crystal physics

- P17** Visualization of Modulation Functions in MoleCoolQt
Christian Hübschle, Sander van Smaalen (Bayreuth/DE)
 Vaclav Petříček (Prague/CZ)
- P18** Anisotropic displacement parameters from electronic-structure theory: how to perform and what to compare
Janine George, Ai Wang, Ruimin Wang, Paul Müller, Ulli Englert
 Richard Dronskowski (Aachen/DE), Volker L. Deringer (Aachen/DE; Cambridge/GB)
- P19** Structure-property relations and structural instabilities in high-temperature piezoelectric materials of the oxoborate-family $RX_2Z_2O(BO_3)_3$
Marie Münchhalfen, Jürgen Schreuer (Bochum/DE), Christoph Reuther
 Jens Götze (Freiberg/DE)
- P20** Orientation relationship of eutectoid FeAl and FeAl₂
Anke Schmitt, Alexander Kauffmann, Sandra Kauffmann-Weiss, Torsten Scherer
 Martin Heilmaier (Karlsruhe/DE)
- P21** Investigation of inversion domains in HTVPE GaN layers grown on sapphire substrates
Michael Barchuk, Mykhaylo Motylenko, Gleb Lukin, Tom Schneider
 Olf Pätzold, David Rafaja (Freiberg/DE)
- P22** Thermoelectric Transport Properties in Magnetically Ordered Crystals
Hans Grimmer (Villigen/CH)
- P23** Synthesis, Characterization of compounds of earth alkaline rare-earth aluminates
Chimednorov Otgonbayar, Herbert Pöllmann (Halle (Saale)/DE)
- P24** Elastic properties and phase transitions of pure and Mn-doped åkermanite
Michael Haiduk, Juergen Schreuer (Bochum/DE), Manfred Burianek
 Reinhard X. Fischer (Bremen/DE)
- P25** Structure-property relationships in mullite-type and related compounds
Linda Hollenbeck, Timo Rütten, Jürgen Schreuer (Bochum/DE)
 Hartmut Schneider (Bremen/DE)
- P26** Influence of substrate potential shape on the diffusion of non-interacting brownian particles
Mehdi Ouahmane, Lehcen Arfa, Lehcen EL Arroum (Casablanca/MA)

- P27 X-ray times-d minus (Td-) diffraction of crystals
Xiangping Gu (Changsha/CN)
- P28 Curie temperature variations in synthetic Al- and Mg-substituted titanomagnetites constrained by thermal history
Sophie-Charlotte Lappe (Aachen/DE), Julie Bowles (Milwaukee, WI/US)
Mike Jackson (Minneapolis, MN/US), Elke Arenholz (Berkeley, CA/US)
- P29 Antimony and arsenic tartrates of divalent cations – crystal growth, crystal structures and vibrational spectroscopy
Ladislav Bohatý, Petra Becker (Köln/DE), Irena Matulková, Ivana Císarová
Ivan Nemec (Prague/CZ)
- P30 Linear optical properties, pyroelectricity and vibrational spectroscopy of polar guanidinium hydrogen phosphite and hydrogen selenite, $\text{Gu}(\text{H}_2\text{PO}_3)$ and $\text{Gu}(\text{HSeO}_3)$
Petra Becker, Ivan Nemec, Irena Matulková, Ivana Císarová (Prague/CZ)
Wolfgang Krumbe (Leichlingen/DE), Lionel Anderson
Ladislav Bohatý (Köln/DE)
- P31 Anelastic relaxation effects in sillenites
Eiken Haussühl (Frankfurt a. M./DE), Jürgen Schreuer (Bochum/DE)
- P33 Crystallography in my life
Heinz Preuß (Hamel/DE)
- P34 Determination of electrostatic magnitudes in a coumarin compound $\text{C}_{17}\text{H}_{13}\text{NO}_3$
Youcef Megrouss, Nourdine Boukabcha, Abdelkader Chouaih
Fodil Hamzaoui (Belaasel/DZ)
- P35 Phase relationship around the Au-Si-Yb 1/1 quasicrystal approximants
Takuya Kurihara (Dresden/DE; Sendai/JP), Tsunetomo Yamada
An Pang Tsai (Sendai/JP), Yurii Prots, Yuri Grin (Dresden/DE)
- P36 Crystal structure and optical properties of triiodides and dibromiodides with methylammonium, formamindinium and guanidinium cations
Michael Daub, Kevin Eble, Harald Hillebrecht (Freiburg i. Br./DE)

Fragment based ligand screening

- P37** The expert system XDSAPP for data processing and fragment-screening
Karine Röwer, Manfred S. Weiss (Berlin/DE), Schiebel Johannes
 Andreas Heine, Gerhard Klebe (Marburg/DE)
 Franziska Huschmann (Berlin, Marburg/DE)
- P38** Highly efficient fragment based lead discovery in the home lab
Vernon Smith, Martin Adam (Karlsruhe/DE), Andreas Heine (Marburg/DE)
- P39** X-ray Crystallographic Fragment Screening and Hit Optimization
Nicole Bertoletti, Florian Braun, Alexander Metz, Lorena Zara
 Andreas Heine, Gerhard Klebe, Sandrine Marchais-Oberwinkler (Marburg/DE)
- P40** Crystallographic fragment-screening (CFS) at the Helmholtz-Zentrum Berlin
 and why CFS should be the first choice
Manfred Weiss (Berlin/DE)
- P41** A hit-validated 96-compound library for efficient coverage of chemical space
 in fragment-based lead discovery
Steffen Glöckner, Alexander Metz, Andreas Heine, Gerhard Klebe (Marburg/DE)

Hot structures

- P42** Pushing back frontiers – synchrotron quality data from the D8 venture
 in-house solution
Vernon Smith, Martin Adam (Karlsruhe/DE), Andrew Doré (Herts/GB)
- P43** A systematic *in situ* and real-time investigation of mechanochemical
 formation of pharmaceutical cocrystals
Luzia S. Germann, Robert E. Dinnebier (Stuttgart/DE), Leigh Loots
 Cristina Mottilla, Joseph Marrett, Jean-Louis Do
 Tomislav Friščić (Montreal/CA), Nicola Casati (Villigen/CH)
- P44** Protein surface engineering enables a detailed view of protein cofactor
 interactions in a bacterial phytochrome
Norbert Krauß (Karlsruhe/DE; London/GB)
 Soshichiro Nagano (Gießen/DE; London/GB), Patrick Scheerer
 Norbert Michael, Kristina Zubow (London/GB)
 Katsuhiko Inomata (Kanazawa/JP), Tilman Lamparter (Karlsruhe/DE)

In situ/in operando studies of energy materials

- P45** Accessing the pyroelectric coefficient – X-ray diffraction, density functional calculation, and electronic measurement
Tilman Leisegang (Freiberg/DE; Samara/RU), Tina Weigel
 Matthias Zschornak, Thomas Behm, Claudia Funke, Sven Jachalke
 Erik Mehner, Hartmut Stöcker, Dirk C. Meyer (Freiberg/DE)
- P46** Infrared spectroscopic study of vibrational modes across the orthorhombic-tetragonal phase transition in methylammonium lead halide single crystals
Götz Schuck, Daniel M. Többsen, Susan Schorr (Berlin/DE)
 Monika Koch-Müller, Ilias Efthymiopoulos (Potsdam/DE)
- P47** *In situ* Studies of NASICON-type $\text{Ca}_{0.5}\text{Ti}_2(\text{PO}_4)_3$ @carbon for sodium-ion batteries
Qiang Fu, Angelina Sarapulova, Natalia Bramnik, Michael Knapp
 Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE), Zhixuan Wie
 Fei Du (Changchun/CN)
- P48** Understanding of electrochemical mechanism of 4d layered cathode Li_2RuO_3 – *in situ* synchrotron study combined with electrochemical kinetics
Ye Yao, Yingjin Wei, Fei Du (Changchun/CN), Xiaofei Bie (Kyoto/JP)
 Björn Schwarz, Lars Riekehr, Christoph Dräger
 Helmut Ehrenberg (Karlsruhe/DE)
- P49** Crystal chemistry of ternary Cu–Li–Sb phases and their structural relations to the Cu–Sb and Li–Sb compounds
Herta Effenberger, Alexander Beutl, Hans Flandorfer (Wien/AT)
- P50** *In-situ* synthesis of ruddlesden-popper (rp) type $\text{La}_2(\text{Co}, \text{Ni})\text{O}_4$: phase changes and reduction/oxidation mechanisms investigated by *in-situ* x-ray powder diffraction
Seyma Ortatati, Jan Ternieden, Claudia Weidenthaler (Mülheim a. d. Ruhr/DE)
- P51** $\text{P2-Na}_{0.66}\text{Co}_{0.95}\text{Ti}_{0.05}\text{O}_2$ – a high performance cathode material for sodium ion batteries
Angelina Sarapulova, Sylvio Indris
 Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE), Noha Sabi, Jones Alami
 Ismael Saadoun (Marrakesh/MA)
- P52** In operando X-ray total scattering experiments on Li-oxygen batteries
Andy Fiedler, Frieder Scheiba, Murat Yavuz
 Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE)

- P53** Investigation of sodium intercalation mechanism in the layered oxide P2 structure by *in situ* synchrotron measurement
Angelina Sarapulova, Sylvio Indris, Natalia Bramnik, Michael Knapp
 Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE)
 Francois Fauth (Barcelona/ES)

Macromolecular machines and switches

- P54** Specificity of the rhodopsin transducin interaction
Dennis Kwiatkowski, Nicolas Heyder, Karoline Lê Công, Johanna Tiemann
 Peter Hildebrand, Michal Szczepek, Patrick Scheerer (Berlin/DE)
- P55** Structural characterization of fluorescence optimized bacterial phytochromes as optogenetic tool
Luisa Sauthof, Andrea Schmidt, Michal Szczepek, Bilal Qureshi
 Tammo Stevens, Maria Fernandez Lopez, Francisco Velazquez Escobar
 Norbert Michael, Peter Hildebrandt, Patrick Scheerer (Berlin/DE)
 Norbert Krauß, Tilmann Lamparter (Karlsruhe/DE)

Materials for energy storage and conversion

- P56** Structural and spectroscopic characterizations of layered tungstate hosting as hydrogen storage and conduction material
Niels Lefeld, M. Mangir Murshed, Thorsten M. Gesing (Bremen/DE)
 Patrick Bottke (Oldenburg/DE)
- P57** Crystallographic investigations on $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ solid electrolytes
 Helmut Ehrenberg, Sylvio Indris, Heike Stöffler
 Murat Yavuz (Eggenstein-Leopoldshafen/DE), Andreas Roters
 Meike Schneider (Mainz/DE)
- P58** Investigation on the difference in storage behavior between Na-Ions and Li-Ions battery materials
Asmaa Loutati, Abedsalam El Bouari (Casablanca/MA)
 Orayech Brahim (Miñano Álava/ES)

Materials science

- P59** Influence of heat treatments on low oriented melt-spun poly(3-hydroxybutyrate) fibers
Bernd Michael Liebeck, Pavan Kumar Manvi, Thomas Vad, Thomas Gries
Georg Roth (Aachen/DE), Gunnar Seide (Geelen/NL)
- P60** Cation distribution and point defect concentration in off-stoichiometric $\text{Cu}_2\text{ZnGeSe}_4$ compound semiconductors
René Gunder, Alexandra Franz, Susan Schorr (Berlin/DE)
- P61** Structural trends in chalcopyrite based intermediate band absorber materials
Julien Marquardt, Alexandra Franz, Christiane Stephan, Susan Schorr (Berlin/DE)
- P62** Study of exfoliated molybdenum disulfide (MoS_2)
Munkhbayar Gombosuren, Davaasambuu Jav (Ulaanbaatar/MN)
Palleschi Stefano, Perrozzi Francesco, Ottaviano Luca (L'Aquila/IT)
- P63** Thermal behavior of ADN and ADN-Prills – crystal and micro structure
Michael Herrmann, Paul Bernd Kempa, Ulrich Förter-Barth
Thomas Heintz (Pfinztal/DE)
- P64** Synthesis of sphalerite – different ways to obtain chemically pure and doped material
Judith Heinrich, Marcus Schwarz, Gerhard Heide (Freiberg/DE)
- P65** Materials inspired by nature – synthesis and characterisation of perryite-related compounds $\text{Ni}_{8-x}\text{Fe}_x\text{Si}_3$ with $0 \leq x \leq 8$
Simone Gallus, Andrzej Grzechnik (Aachen/DE), Mamuka Chikovani
Jörg Persson, Jörg Voigt, Karen Friese (Jülich/DE)
Anatoliy Senyshyn (Garching/DE)

Molecular crystallography at the limits

- P66** The XtaLAB mini II – a benchtop diffractometer for undergraduate institutions
Joseph Ferrara, Eric Reinheimer (The Woodlands, TX/US)
- P67** An unconventional view of the molecular structure of a medicinal drug – charge density study of a new solid form of the antiretroviral drug lamivudine (3TC)
Juan Carlos Tenorio (São Carlos/BR; Mülheim a. d. Ruhr/DE)
Javier Ellena (São Carlos/BR), Christian W. Lehmann (Mülheim a. d. Ruhr/DE)
- P68** The UV-triggered decomposition of 3-(4-pyridyl)-acetylacetone
Marius Kremer, Khai-Nghi Truong, Ulli Englert (Aachen/DE)

- P69 Fostering what is needed tomorrow – facing problems in teaching crystallographic topics
Stefanie Langenstück, Ulli Englert (Aachen/DE)

Nanoscience

- P70 Thermal stability and properties of metastable $(\text{Cr,Zr})_2\text{O}_3$
David Rafaja, Christina Wüstefeld, Stefan Bräunig (Freiberg/DE)
 Gintautas Abrasonis, Carsten Baehtz, Matthias Krause
 Sibylle Gemming (Rossendorf/DE), Milan Dopita (Prague/CZ)
- P71 Crystallographic characterization of laser-ablated and polymer-stabilized silver-gold nanoalloys (4 nm)
Oleg Prymak, Jurij Jakobi, Christoph Rehbock, Matthias Epple
 Stephan Barcikowski (Essen/DE)
- P72 Microfluidic synthesis of ultrasmall and nanoalloys in continuous turbulent flow
Ghazal Tofighi, Abhijeet Gaur, Dmitry E. Doronkin, Henning Lichtenberg
 Wu Wang, Thomas Sheppard, Günter Rinke, Jan-Dierk Grunwaldt (Karlsruhe/DE)
- P73 Time-resolved in-situ high-resolution X-ray diffraction of growing self-catalysed GaAs nanowires
Philipp Schroth, Seyed Mohammad Mostafavi Kashani, Jonas Vogel
 Arman Davtyan (Siegen, Karlsruhe/DE), Julian Jakob, Martin Köhl
 Ludwig Feigl, Tilo Baumbach (Karlsruhe/DE), Jörg Stremper (Hamburg/DE)
 Ullrich Pietsch (Siegen/DE)
- P74 Recent developments on incoatec's microfocus source iµs for material science applications
Andreas Stricker, Bernd Hasse, Andreas Kleine, Jürgen Graf
 Carsten Michaelsen (Geesthacht/DE)
- P75 In-situ time-resolved X-ray diffraction of a single GaAs nanowire during thermal annealing and at growth conditions
Seyed Mohammad Mostafavi Kashani, Jonas Vogel, Arman Davtyan
 Danial Bahrami, Ullrich Pietsch (Siegen/DE), Dominik Kriegner (Prague/CZ)
 Philipp Schroth (Siegen, Karlsruhe/DE), Ludwig Feigl, Julian Jakob
 Tilo Baumbach (Karlsruhe/DE)
- P76 Transrotational structure and its features revealed by TEM for 2 kinds of spherulites growing in amorphous films
Vladimir Kolosov (Ekaterinburg/RU)

- P77** Hydrothermal preparation of LFP particles with high crystalline for electrochemistry
Guiying Tian, Frieder Scheiba, Helmut Ehrenberg
 Kiran Chakravadhanula (Eggenstein-Leopoldshafen/DE)
- P78** Sulfur-poly(acrylonitrile) as cathode material for li/s batteries – correlating electrochemical performance and chemical structure
Roland K. Zenn, Martin Frey, Sven Warneke (Böblingen, Stuttgart/DE)
 Kathrin Müller, Robert E. Dinnebier (Stuttgart/DE)
 Andreas Hintennach (Böblingen/DE)
 Michael R. Buchmeiser (Stuttgart, Denkendorf/DE)
- P79** Edta effect on structural and optical properties of Ag_2S nanoparticles
Abdelhafid Souici, Wissam Mouhaou, Salim Ouhenia
 Zahia Chafi (Bejaia/DZ), Nihad Douas, Nassira Keghouche (Constantine/DZ)
- P80** Solving the Hydrogen and Lithium Substructure of Poly(triazine imide)/LiCl by a combination of electron diffraction tomography, nuclear magnetic resonance and X-ray total scattering
Yaşar Krysiak, Ute Kolb (Mainz/DE), Maria B. Mesch, Kilian Bärwinkel
 Jürgen Senker (Bayreuth/DE), Reinhard B. Neder (Erlangen/DE)
- P81** A DEGAS study of the water and hydrogen release from Australian Opal
Kristin Galonska, Gerhard Heide (Freiberg/DE), Paul S. Thomas (Sydney/AU)
 Klaus Heide (Jena/DE)
- P82** Boehmite (γ - $AlOOH$) nanoparticles as model system for monitoring particle formation in water based reaction media within the second time scale
Stefan Diez (Erlangen/DE)
- P83** *In-situ* time-resolved XRD and RHEED study of the polytypism in GaAs nanowires
Julian Jakob, Tilo Baumbach (Eggenstein-Leopoldshafen, Karlsruhe/DE)
 Philipp Schroth (Eggenstein-Leopoldshafen, Siegen/DE)
 Ludwig Feigl (Eggenstein-Leopoldshafen/DE)
 Seyed Mohammad Mostafavi Kashani, Jonas Vogel
 Ullrich Pietsch (Siegen/DE)

New approaches in structural biology

- P84** Optimized sample centering for your best experimental result
Martin Adam, Jaap Toorn (Karlsruhe/DE)
- P85** Binary protein crystals for the construction of nanoparticle superlattices
Tobias Beck (Aachen/DE)
- P86** PROTEUM3 – a new software pipeline for the collection and processing of crystallographic data for structural biology
Tobias Stuerzer, Martin Adam (Karlsruhe/DE)
Joerg Kaercher (Madison, WI/US)
- P87** HKL2MAP – improvement of SAD/MAD phasing results by means of data selection
Fabio Dall’Antonia, Selina Storm, Thomas Schneider (Hamburg/DE)
- P88** Use of cadmium ions for High-throughput experimental phasing
Saravanan Panneerselvam, Anja Burkhardt, Alke Meents (Hamburg/DE)
- P89** ‘Top-hat’ beams for high-quality data collection on the EMBL beamline P14 at PETRA III
Anna Polyakova, Gleb Bourenkov, Ivars Karpics, Stefan Fiedler, Fang Liu
Thomas R. Schneider (Hamburg/DE), Peter Vella, Robert Schnell
Gunter Schneider (Stockholm/SE)
- P90** P13 and P14, the EMBL Beamlines for Macromolecular Crystallography at PETRA III
Thomas R. Schneider, Gleb Bourenkov, Guillaume Pompidor, Isabel Bento
Johanna Kallio, Ivars Karpics, Anna Polyakova, Stefan Fiedler (Hamburg/DE)
Michele Cianci (Ancona/IT)
- P91** A Peltier-cooled microscope stage for protein crystal post-crystallization treatment
Andreas Dietl, Christian Kieser, Thomas R.M. Barends (Heidelberg/DE)

New crystal structures and structure systematics

- P92** Structure and crystal chemistry of calcium salts of substituted acetic acids
Ronny Kaden, Herbert Pöllmann (Halle (Saale)/DE)
- P93** Freehand experiment with rock candy crystals
Heinz Preuß (Hameln/DE)
- P95** A simple way for manually constructing decorated Penrose tilings
Walter Steurer (Zurich/CH)
- P96** Modelling Disorder with DSR in ShelXle and Olex2
Daniel Kratzert (Freiburg i. Br./DE)
- P97** Synthesis and Characterization of a $[\text{Li}_{0+x}\text{Mg}_{2-2x}\text{Al}_{1+x}(\text{OH})_6][\text{Cl}\cdot m\text{H}_2\text{O}]$ ($0 \leq x \leq 1$) solid solution
Anton Niksch (Halle (Saale)/DE)
- P98** Maximum vacancy ordering in mullite
Paul Klar, Noelia de la Pinta, Gabriel Alejandro Lopez, Iñigo Etxebarria
Tomasz Breczewski, Gotzon Madariaga (Bilbao/ES)
- P99** Na_2HfSe_3 – the first ternary sodium hafnium selenide
Falk Lissner, Bettina Hack, Thomas Schleid (Stuttgart/DE)
- P100** Single crystals of the trigonal high-temperature modification of $\text{Cs}_3\text{Bi}_2\text{Cl}_9$
Beate Schulz, Thomas Schleid (Stuttgart/DE)
- P101** Crystal structure and properties of double molybdate $\text{Pr}_2\text{Zr}_3(\text{MoO}_4)_9$
Ingrid Svoboda (Darmstadt/DE), Yunna Tushinova, Bair Bazarov
Olga Chimitova, Jibzema Bazarova (Ulan-Ude/RU), Angelina Sarapulova
Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE)
- P102** Synthesis and characterization of new material, type sillenite $\text{Bi}_{12}\text{TlO}_{20}$
Hajar Ait Oulahyane, Lama Bourja, Leila Loubbidi, Abdenajib Moussaoui
Omar Ait Sidi Ahmed, Abdelmjid Tairi (Casablanca/MA)
Abdeslam Chagraoui, Sylvie Villan (Toulon/FR)
- P103** Pillarplexes – organometallic host-compounds
Philipp Altmann, Alexander Pöthig (Garching/DE)

- P104** Refuting the existence of bicarbonates of higher valent metal ions and crystal structures of new carbonates
Christine Rincke, Horst Schmidt, Wolfgang Voigt (Freiberg/DE)
 Sebastian Bette (Freiberg, Stuttgart/DE), Robert E. Dinnebier (Stuttgart/DE)
- P105** New ruthenates and iridates with garnet-like crystal structures
Hagen Poddig, Jens Hunger, Sirko Kamusella, Thomas Doert (Dresden/DE)
- P106** Bi_xTe family – modular design of topological insulators
Alexander Zeugner, Martin Kaiser, Thomas Doert, Michael Ruck
 Anna Isaeva (Dresden/DE)
- P107** Synthesis and crystal structures of the new ternary borides $\text{Fe}_3\text{Al}_2\text{B}_2$ and $\text{Ru}_9\text{Al}_3\text{B}_8$
Harald Hillebrecht, Sarah Hirt, Felix Hilfinger (Freiburg i. Br./DE)
- P108** Synthesis, crystal structures and properties of the new 2-D hybriide perovskite $\text{C}(\text{NH}_2)_3\text{HC}(\text{NH}_2)_2\text{PbI}_4$
Harald Hillebrecht, Michael Daub (Freiburg i. Br./DE)
- P109** Ordering of ferrocene guest molecule in the pentaphosphaferrocene-based supramolecule
Eugenia Peresyphkina, Alexander Virovets, Manfred Scheer (Regensburg/DE)
- P110** Crystal structure and hydrate water content of synthetic hellyerite, $\text{NiCO}_3 \cdot 5.5 \text{H}_2\text{O}$
Sebastian Bette, Robert E. Dinnebier (Stuttgart/DE), Christine Rincke
 Wolfgang Voigt (Freiberg/DE)
- P111** $\text{SrSc}_2[\text{SeO}_3]_4$ and $\text{BaSc}_2[\text{SeO}_3]_4$ – two alkaline-earth metal oxoselenates(IV) with the smallest rare-earth element
Stefan Greiner, Thomas Schleid (Stuttgart/DE)
- P112** $\text{Li}_7\text{Eu}_3\text{Nb}_2\text{O}_{12}$ with a garnet-related structure containing mixed-valent europium
Daniel Rudolph, Christian Funk, Thomas Schleid (Stuttgart/DE)
- P113** Precious and coinage metal complexes with adamantanecarboxylates
Philipp Schlender, Martin Kaiser, Jens Hunger (Dresden/DE)

- P114** Exploration on structural chemistry and ion-exchange property of uranium borates mixed with oxo-anion $[\text{PO}_4]^{3-}$
Yucheng Hao (Jülich/DE), Evgeny V. Alekseev (Jülich, Aachen/DE)
- P115** ROY – a new approach to co-crystals and the effect of deuteration
Jacqueline Lehnen (Bochum/DE)
- P116** Structural comparison of the matlockite-type pair EuFBr and EuHBr
Daniel Rudolph, Monika Eva Bohem, Thomas Schleid (Stuttgart/DE)
- P117** The Crystal Structure of Tetra-*n*-propylammonium Permanganate
Maurice Conrad, Jörg Bauchert, Thomas Schleid (Stuttgart/DE)
- P118** $\text{Cu}(\text{H}_2\text{O})_4[\text{B}_{10}\text{Cl}_{10}] \cdot 5 \text{H}_2\text{O}$ – crystal structure of a copper(II) decachloro-*closo*-decaborate hydrate with an astonishing coordination feature
Fabian Kleeberg, Thomas Schleid (Stuttgart/DE)
- P119** The crystal structure of the anhydrous cesium thiosulfate $\text{Cs}_2[\text{SO}_3\text{S}]$
Christian Funk, Thomas Schleid (Stuttgart/DE)
- P120** Crystal structure determination of $[\text{NiBr}_2(4\text{-cyp})_2]_n$ and $[\text{NiBr}_2(4\text{-cyp})_1]_n$ by X-ray powder diffraction
Miriam Heine, Lothar Fink, Martin U. Schmidt (Frankfurt a. M./DE)
- P121** A series of coordination polymers employing 2,2''-bipyridine-3,3'',6,6''-tetracarboxylate as a ligand
Andrzej Kochel (Wrocław/PL)
- P122** Amine complexes of mercury(II) halogenides
Cindy Döring (Braunschweig/DE)
- P123** Intermolecular interactions study within two 4-(aminomethyl)benzoic acid proton transfer compounds by means of Hirshfeld surface analysis
Amani Direm (Khenchela/DZ), Angela Altomare, Anna Moliterni (Bari/IT)
 Nourredine Benali-cherif (Khenchela/DZ)
- P124** High temperature Cs_2S_3 and the incommensurate modulated phase $\text{K}_{37}\text{Te}_{28}$: new binary alkali chalcogenides
Pirmin Stüble, Angela Berroth, Fritz Wortelkamp
 Caroline Röhr (Freiburg i. Br./DE)

- P125 Improving your single crystal data collection
Alexandra Griffin (Kent/GB)
- P126 Crystal and electronic structures of alkali triele halogenides of the K_8In_{11} -type structure
Martha Falk, Armin El Addad, Caroline Röhr (Freiburg i. Br./DE)
- P127 The structure of α - and β -moganite
Hans Grimmer, Bernard Delley (Villigen/CH)
- P128 Synthesis and crystal structure of the new sodium tellurido manganate $Na_2Mn_3Te_4$
Michael Langenmaier, Caroline Röhr (Freiburg i. Br./DE)
- P129 Synthesis of copper coordinated bismuth cluster compounds
Maximilian Knies, Martin Kaiser, Ulrike Müller, Thomas Doert (Dresden/DE)
- P130 Triethanolammonium ion conformation and hydrogen bonding
Carl Schwalbe (Cambridge, Birmingham/GB)
- P131 Twinning by Merohedry of 1,3,5-Tribenzyl-4,6-tetrahydrothiazine-2-thione and -selenone
Walter Frank (Düsseldorf/DE)
- P132 Ternary trielides A_3M_5 – a combined synthetic, crystallographic and bond theoretical study
Carolin Meyer, Caroline Röhr (Freiburg i. Br./DE)
- P133 Hydrogen bonds and π - π interactions are structure-directing tools of the 4-aminopyridium cation for the construction of a complex framework
Guido J. Reiss, Martin van Megen, Walter Frank (Düsseldorf/DE)
- P134 The structure of $Br@NaY$, $Na_{45}H_{15}[Si_{139}Al_{53}O_{384}Br_7] \cdot 247 H_2O$, a NaY zeolite impregnated with NaBr
Melanie Müller, Bernd Marler, Aneta Wozniak, Hermann Gies (Bochum/DE)
- P135 Temperature-dependent structure and thermal stability of $[Na_8(MO_4)(H_2O)_2][AlSiO_4]_6$ cancrinites
Hilke Petersen, Lars Robben, Thorsten M. Gesing (Bremen/DE)

- P136** Crystal Engineering of layered hybrid compounds – a layered inorganic-organic hybrid material derived from the “short-chain amphiphile” sodium methanesulfonate and chloroauric acid
Felix Thoelen, Walter Frank (Düsseldorf/DE)
- P137** Synthesis and structural characterization of $\text{Li}_3\text{K}_3\text{Y}_7(\text{BO}_3)_9$
Sebastian Bräuchle, Hubert Huppertz (Innsbruck/AT)
- P138** Synthesis and characterization of a novel ferrite $\text{K}_2\text{Fe}_4\text{O}_7$
Mathias Gogolin, M.Mangir Murshed, Thorsten M. Gesing (Bremen/DE)
- P139** Experimental electron density in bromomalonic aldehyde
Ruimin Wang, Janine George, Richard Dronskowski, Ulli Englert (Aachen/DE)
- P140** Crystal growth of Mn-doped melilites
Manfred Burianek, Patrick Teichmann, Reinhard Fischer (Bremen/DE)
- P141** Structural and magnetic properties of Eu_2TeO_6
Monika Eva Bohem, Björn Blaschkowski, Thomas Schleid (Stuttgart/DE)
- P142** Crystal and magnetic structures of multiferroic melilites: $\text{Ba}_2\text{CoGe}_2\text{O}_7$ versus $\text{Ba}_2\text{MnGe}_2\text{O}_7$
Andrew Sazonov, Vladimir Hutanu, Martin Meven (Garching/DE)
Georg Roth (Aachen/DE)
- P143** Structure of the charge-density wave in CuV_2S_4
Sitaram Ramakrishnan, Andreas Schönleber, Hai An Bui Nyguen Florian Feulner, Mariia Anurova, Sander van Smaalen (Bayreuth/DE)
Dmitry Chernyshov (Grenoble/FR)
- P144** High-Resolution Single-Crystal X-Ray Diffraction Investigations of β -Rhombohedral Boron
Claudio Eisele (Bayreuth/DE)
- P145** Introducing a new tripodal ligand including a hydroxamic acid moiety into coordination chemistry
Dejan Premuzic, Malgorzata Holynska (Marburg/DE)
- P146** Structural relationships between mullite, sillimanite and “sillimullite”
Stephan Lenz, Johannes Birkenstock, Hartmut Schneider Reinhard X. Fischer (Bremen/DE), Lennart A. Fischer (Hannover/DE)

Phase transitions and dynamic phenomena

- P147** The growth kinetics and the structure of expanded austenite in AISI316L stainless steels characterized by in-situ XRD
Zoltán Balogh-Michels, Alex Dommann, Antonia Neels (Dübendorf/CH)
Alexander Faeht, Simon Kleiner, Jean-Martin Rufer (Biel/CH)
Patrick Markgraf (Egerkingen/CH)
- P148** A two dimensional dynamic instability of titanite, CaTiSiO_5
Thomas Malcherek (Hamburg/DE), Michael Fischer (Bremen/DE)
- P149** Thermodynamic and kinetic studies on adsorption of Chromium(VI) onto the olive pomace in the region of Beni Mellal
Aziz Menichi, Abdeslam Chagraoui, Abdelnajib Moussaoui (Casablanca/MA)
- P150** Femtosecond diffraction of solid flame reactions at HED at European XFE
Wolfgang Morgenroth, Lkhamsuren Bayarjargal
Björn Winkler (Frankfurt a. M./DE), Dmitry Varentsov (Darmstadt/DE)
Karen Appel, Ulf Zastrau (Schenefeld/DE)
- P151** Multiferroic Hübnerite with unusual high molybdenum doping studied by X-ray powder diffraction and Raman spectroscopy
Fabian Ziegler, Leonie Marie Gomell, Holger Gibhardt
Götz Eckold (Göttingen/DE)
- P152** Low temperature behaviour of $\text{Sb}_2\text{Se}_{3-x}\text{Te}_x$ mixed crystals
Markus Herrmann, Karen Frieze (Jülich/DE)
Konstantin Glazyrin (Hamburg/DE)
- P153** Structure variations within certain rare earth-disilicides
Melanie Nentwich, Maximilian Sonntag, Roman Gumeniuk
Dirk C. Meyer (Freiberg/DE), Matthias Zschornak (Freiberg, Dresden/DE)
Sibylle Gemming (Dresden/DE)
Tilman Leisegang (Freiberg/DE; Samara/RU)
- P154** Pseudomorphic replacement of calcite by acicular fluorite crystals
Elisabete Trindade Pedrosa (Münster/DE)
Christine Putnis (Perth/AU; Münster/DE)
Andrew Putnis (Münster/DE; Perth/AU)
- P155** High pressure behaviour of Pb_2SnO_4 using Raman spectroscopy
Dominik Spahr, Lkhamsuren Bayarjargal, Wolfgang Morgenroth
Nadine Schrodtt, Rita Luchitskaia, Björn Winkler (Frankfurt a. M./DE)

- P156 Tricritical phase transition in Norsethite
Martin Ende, Ronald Miletich, Herta Effenberger (Wien/AT)
- P157 Zinc oxide phase transitions under non-ambient conditions
Dejan Zagorac, Jelena Zagorac, Milena Rosic, Maria Cebela, Jelena Lukovic
Branko Matovic (Belgrade/RS), J. Christian Schoen (Stuttgart/DE)
- P158 Room temperature aging and tempering of highly nitrogen-supersaturated ferrite
Marius Wetzel, Andreas Leineweber (Freiberg/DE)
- P159 Lab-based x-ray diffractometer for the investigation of low temperature
magnetic field-induced phase transitions
Tom Faske, Wolfgang Donner (Darmstadt/DE)

Spectroscopy as supporting tool in crystallography

- P160 Substitution and doping in iron pnictides
Michael Merz, Peter Schweiss, Peter Nagel, Meng-Jie Huang, Andreas Plog
Robert Eder, Thomas Wolf, Hilbert von Löhneysen
Stefan Schuppler (Eggenstein-Leopoldshafen/DE)
- P161 The First Zn(II) complex of 4-methoxypicolinic acid – synthesis, crystal
structure and IR spectrum
Ömer Tamer, Davut Avci, Yusuf Atalay (Sakarya/TR)
- P162 X-ray diffraction in combination with DFT, vibrational and nuclear magnetic
resonance spectroscopy for the investigation of structures and phase
transitions of molecular and complex aluminium hydrides
Claudia Weidenthaler, Thomas Bernert, Morten Brix Ley, Bodo Zibrowius
Michael Felderhoff (Mülheim a. d. Ruhr/DE), Michael Fischer (Bremen/DE)

Structural biology meets chemistry

- P163** Structure analysis of lignin-based polyurethanes using WAXS
Steffen Witzleben, Katharina Walbrück, Stefanie Klein, Jessica Rumpf
 Margit Schulze (Rheinbach/DE)
- P164** Current status of microfocus X-ray sources for chemical and biological crystallography
Jürgen Graf, Andreas Kleine, Joerg Wiesmann
 Carsten Michaelsen (Geesthacht/DE), Tobias Stuerzer, Severine Freisz
 Holger Ott (Karlsruhe/DE)
- P165** Calcium carbonate biomineralisation
Salim Ouhenia, Daniel Chateigner (Bejaia/DZ)
- P166** A new type of RNA double helix based on U·G and C·A⁺ wobble-base pairing
Udo Heinemann, Ankur Garg (Berlin/DE)
- P167** Binary protein crystals for the assembly of inorganic nanoparticle superlattices
Matthias Künzle, Marcel Lach, Thomas Eckert, Tobias Beck (Aachen/DE)

Structural chemistry under non-ambient conditions

- P168** Crystalline high-pressure phases in the Bi-Co system
Leonore Wiehl, Shrikant Bhat, Iliya Radulov, Konstantin Skokov
 Michael Dürschnabel, Leopoldo Molina-Luna, Sabrina Siculo, Leopold Diop
 Dmitriy Karpenkov, Hans-Joachim Kleebe, Karsten Albe, Ralf Riedel
 Oliver Gutfleisch (Darmstadt/DE), Norimasa Nishiyama (Hamburg/DE)
- P170** Getting the most out of your high pressure experiments
Holger Ott, Martin Adam, Tobias Stuerzer (Karlsruhe/DE)
 Michael Ruf (Madison, WI/US), Juergen Graf (Geesthacht/DE)
- P171** Closer look into close packing: pentacoordinated silicon in high-pressure polymorph of danburite
Anna Pakhomova, Elena Bykova, Konstantin Glazyrin
 Hanns-Peter Liermann (Hamburg/DE), Maxim Bykov
 Leonid Dubrovinsky (Bayreuth/DE), Liudmila Gorelova (Saint-Petersburg/RU)

- P172** Characterization of a new tin borate $\text{Sn}_2\text{B}_3\text{O}_6(\text{OH})$ synthesized under hydrothermal conditions
Sandra Schöneegger, Klaus Wurst, Gunter Heymann, Andreas Schaur
 Hubert Huppertz (Innsbruck/AT), Andreas Saxer
 Dirk Johrendt (Innsbruck/AT; München/DE)
- P173** Electron density investigation of the M-Nitroacetanilide compound via accurate X-ray diffraction data
Nouridine Boukabcha, Youcef Megrouss, Salem Yahiaoui, Abdelkader Chouaih
 Fodil Hamzaoui (Belaasel/DZ)
- P174** Solid solvents – crystal structures of Acetic Anhydride, 2-Methylfuran, Furfural and Furfurylamine
Nils Nöthling, Richard Goddard, Christian W. Lehmann
 Rüdiger Seidel (Mülheim a. d. Ruhr/DE)
- P175** Accurate structures and energetics of neutral-framework zeotypes from dispersion-corrected DFT calculations
Michael Fischer (Bremen/DE), Ross J. Angel (Padova/IT)
- P176** Structural Analysis of hybrid perovskite $\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Br}_x$ solid solution
Frederike Lehmann (Berlin, Potsdam/DE), Alexandra Franz, Daniel M. Töbrens
 Susan Schorr (Berlin/DE)
- P177** Thermal expansion of Co olivine compared with Mn and Fe olivine – an assessment of equations-of-state
Peter Schmid-Beurmann, Herbert Kroll, Alexander Sell
 Julia Büscher (Münster/DE), Armin Kirfel (Bonn/DE)
- P178** Mechanochemical Synthesis of Cubic Li_2TiO_3
Dennis Becker, Robert Haberkorn, Guido Kickelbick (Saarbrücken/DE)
- P179** Lattice Thermal Expansion of $\text{Bi}_2\text{Fe}_4\text{O}_9$, $\text{Bi}_2\text{Fe}_2\text{Mn}_2\text{O}_{10}$ and $\text{Bi}_2\text{Mn}_4\text{O}_{10}$
M. Mangir Murshed (Bremen/DE), Chogondahalli M. N. Kumar
 Ashfia Huq (Oak Ridge, TN/US), Thorsten M. Gesing (Bremen/DE)
- P180** The crystal structure of sodium hexachlororhodate
Martin Etter (Hamburg/DE)

- P181** Novel High-pressure polymorph of NiAs-Type FeN
William Peter Clark, Rainer Niewa (Stuttgart/DE), Simon Steinberg
 Richard Dronskowski (Aachen/DE), Catherine McCammon, Maxim Bykov
 Leonid Dubrovinsky (Bayreuth/DE), Ilya Kупenko (Grenoble/FR)
 Lev G. Akselrud, Ulrich Schwarz (Dresden/DE)
- P182** High-Pressure Synthesis of the Rare-Earth Metal(III) Hydroxide
Ortho-Oxidotungstates(VI) $RE(OH)[WO_4]$ ($RE = Dy, Ho$)
Katharina V. Dorn, Thomas Schleid, Ingo Hartenbach (Stuttgart/DE)
- P183** *In-situ* HT-PXRD studies of $Ca(Fe,Mn,Ti)O_{3-\delta}$ perovskites – phase transitions and
 interplay between octahedral tilting and distortion
Achim M. Schaller, Stefan Stöber, Herbert Pöllmann (Halle (Saale)/DE)
- P184** Synthesis and characterisation of monazite solid solution series
Antje Hirsch, Charlotte Schausten, Lars Peters, Georg Roth (Aachen/DE)
 Philip Kegler (Jülich/DE), Igor Alencar, Javier Ruiz-Fuertes, Anja Thust
 Johannes Bauer (Frankfurt a. M./DE)
- P185** High-pressure X-ray diffraction studies on cuprous sulfides
Dominik Zimmer, Wolfgang Morgenroth, Lkhamsuren Bayarjargal, E. Haussühl
 Björn Winkler (Frankfurt a. M./DE), Javier Ruiz-Fuertes
 David Santamaría-Pérez (València/ES), Jin Zhang (Beijing/CN)
 Claus Mühle (Stuttgart/DE), Changqing Jin (Beijing/CN)
- P186** Synthesis, compressibility and stability of $W_7Re_{13}B$
Christopher Neun, Björn Winkler, Lkhamsuren Bayarjargal
 Wolfgang Morgenroth (Frankfurt a. M./DE), Benedikt Petermüller
 Hubert Huppertz (Innsbruck/AT)

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CONGRESSMANAGEMENT

INDEX OF PLENARY SPEAKERS, PRESENTING AUTHORS AND CHAIRS

A

Abboud, A.
Absmeier, E.
Adam, M.
Ait Oulahyane, H.
Ali, S.
Altmann, P.
Angel, A.

44
33
57
58
42
58
24

F

Fabbiani, F.
Falk, M.
Faske, T.
Fechtelkord, M.
Feigl, L.
Ferrara, J.
Fiedler, A.
Fischer, M.
Flatken, M.
Frank, W.
Friedrich, D.
Fruhner, C.-J.
Fu, Q.
Funk, C.

64
41
47, 66
Herrmann, M.
Herrmann, M.
Heymann, M.
Hillebrecht, H.
Hinterstein, M.
Hirsch, A.
Hirschle, H.
Hofer, G.
Hofmann, D.
Hofmann, K.
Hollenbeck, L.
Hovestreydt, E.
Hübschle, C.

36, 54
25
63
54
21
59
32
29, 67
24
22
65
48
28, 49
47
49

B

Ballay, J.
Balogh-Michels, Z.
Barchuk, M.
Barends, T.
Bayarjargal, L.
Beck, T.
Becker, D.
Becker, P.
Beirau, B.
Bertoletti, N.
Bette, S.
Birkenstock, J.
Blankenfeldt, W.
Bodach, A.
Bohatý, L.
Bohem, M. E.
Boukabcha, N.
Bräuchle, S.
Braun, C.
Breuer, S.
Burianek, M.
Burkhardt, A.
Bykov, M.

32
35, 63
29, 49
20
21
57
66
50
24
29, 51
39, 59
48
38
42
50
62
66
62
21
47, 48
62
21
21

G

Gallus, S.
Galonska, K.
George, J.
Gerlach, M.
Germann, L. S.
Gesing, T. M.
Glöckner, S.
Gogolin, M.
Gombosuren, M.
Gonen, T.
Gorelik, T. E.
Gorfman, S.
Graf, J.
Greiner, S.
Griffin, A.
Grimmer, H.
Grininger, M.
Gruene, T.
Grzechnik, A.
Gu, X.
Gunder, R.
Gurieva, G.

J

39
36, 52
60

K

Kaden, R.
Kaiser, S.
Klar, P.
Klebe, G.
Kleebe, H.-J.
Kleeberg, F.
Knapp, M.
Knies, M.
Kochel, A.
Kodumudi Venka-
taraman, L.
Kohlmann, H.
Köhnke, J.
Kolosov, V.
Kratzert, D.
Krauß, N.
Krauss, N.
Kremer, M.
Kreyssig, A.
Krogstrup, P.
Krysiak, Y.
Kübel, C.
Kudlinzki, D.
Kümmel, D.
Künzle, M.
Kwiatkowski, D.

35, 56
47
58
33
30, 58
30
33
60
41
61
60
23
41
38
55
35, 58
51
33
28, 54
35
34
56
43
30
25
29, 65
28, 53

C

Chaikuad, A.
Choe, C.
Clark, W. P.
Conrad, M.

30
24
67
60

D

Dall'Antonia, F.
Daub, M.
Dietl, A.
Diez, S.
Direm, A.
Dittrich, B.
Doert, T.
Domratheva, T.
Döring, C.
Dorn, K. V.
Dronskowski, R.

57
50
57
29, 56
60
39
23, 32
38
60
67
40

H

Haarmann, F.
Hagelstein, M.
Hagelueken, G.
Haiduk, M.
Hanke, M.
Hänschke, D.
Hao, Y.
Haussühl, E.
Heine, A.
Heine, M.
Heinemann, U.

39
48
20
29, 49
43
22
60
50
30
60
65

39
29, 65
28, 53
61
37, 55
42
50
53
66
60

E

Effenberger, H.
Ehrenberg, H.
Eisele, C.

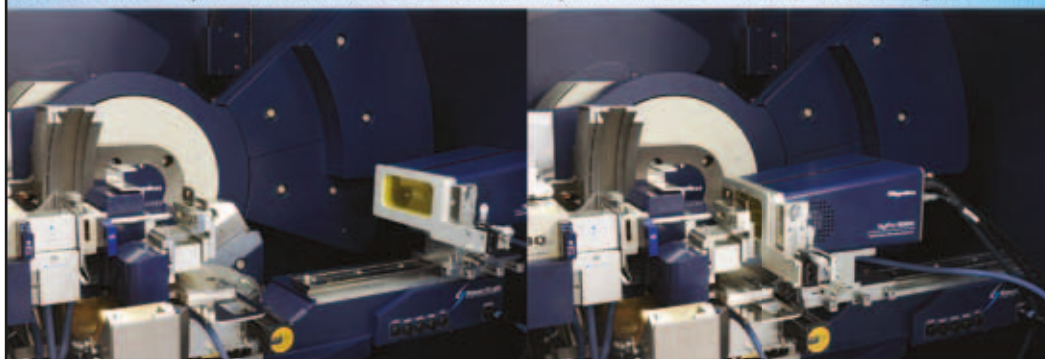
52
26
28, 62

INDEX OF PLENARY SPEAKERS, PRESENTING AUTHORS AND CHAIRS

Leisegang, T.	52	Pietrzyk-Brzezinska, A. J.	33	Steurer, W.	58
Lenz, S.	62	Pietsch, U.	34, 43	Stöber, M.	26
Liebeck, B. M.	54	Poddig, H.	59	Stöcker, S.	24, 28
Lissner, F.	58	Polyakova, A.	57	Stöcker, H.	24, 28
Loutati, L.	53	Pöthig, A.	40	Stöffler, H.	53
Lukat, P.	38	Premuzic, D.	62	Sträter, N.	33
		Preuß, H.	50, 58	Stricker, A.	55
		Prymak, O.	55	Stüble, P.	60
M				Stuerzer, T.	57
Maier, T.	25			Svoboda, I.	58
Malcherek, T.	63	R			
Marquardt, J.	54	Raabe, D.	26		
Megrouss, Y.	50	Rafaja, D.	55	T	
Meinhart, A.	27, 33	Ramakrishnan, S.	62	Tamer, O.	39, 64
Menichi, A.	63	Redhammer, G.	47	Tenorio, J. C.	54
Merz, M.	64	Reiss, G. J.	61	Thielen, F.	62
Meutzner, F.	11, 23	Rincke, C.	59	Thorn, A.	21
Meven, M.	35, 44	Rius, J.	47	Tian, G.	28, 56
Meyer, C.	61	Röhr, C.	32	Többens, D.	47
Meyer, M.	9	Röwer, K.	51	Trapp, M.	34
Mikhailova, D.	41	Rudolph, M.	32	Trindade Pedrosa, E.	63
Misra, M.	30	Ruehl, S.	11	Tseng, J.	41
Mohammed, A.	36, 48				
Morgenroth, W.	63	S		V	
Mossou, E.	44	Sarapulova, A.	36, 48, 52, 53	van Well, N.	32
Mostafavi Kashani, S. M.	36, 55	Sauthof, L.	36, 53	Virovets, A.	40
Mu, X.	34	Sazonov, A.	62	von Stetten, D.	20
Mueller, H.	44	Scaletti, E. R.	30		
Müller, H.	11	Schaller, A. M.	67	W	
Müller, M.	61	Schaniel, D.	22	Wang, R.	62
Münchhaffen, M.	49	Schleid, T.	42	Weidenthaler, C.	41, 64
Murshed, M.	66	Schlender, P.	59	Weiss, M.	51
		Schlichting, I.	20	Werwein, A.	32
N		Schmid, S.	44	Wetzel, M.	64
Neder, R.	43	Schmidbauer, M.	43	Wiedemann, D.	22
Nenert, G.	10, 42	Schmid-Beurmann, P.	66	Wiehl, L.	65
		Schmidt, A.	38	Witzleben, S.	65
Nentwich, M.	63	Schmidt, E.	40	Wozniak, K.	41
Neun, C.	37, 67	Schmitt, A.	49		
Niksch, A.	42, 58	Schneider, T. R.	57	Y	
Nöthling, N.	66	Schneidewind, A.	40, 44	Yao, Y.	28, 52
		Schönbeck, T.	10		
O		Schöneegger, S.	66	Z	
Oppel, D.	10	Schorr, S.	26	Zagorac, D.	11, 64
Ortatatli, S.	41, 52	Schrader, T. E.	38	Zander, U.	20
Otgonbayar, C.	35, 49	Schreuer, J.	24	Zenn, R. K.	56
Ott, H.	65	Schroth, P.	37, 55	Zeugner, A.	59
Ouahmane, M.	49	Schuck, G.	52	Zhao, H.	33
Ouhenia, O.	65	Schulz, B.	58	Ziegler, F.	63
		Schwalbe, C.	61	Zimmer, D.	67
P		Schwarz, U.	21	Zotov, N.	47
Pakhomova, A.	65	Schwarz Müller, S.	22	Zschornak, M.	44
Panneerselvam, S.	57	Selzer, M.	23		
Pennartz, P. U.	39	Smith, V.	51		
Peresypkina, E.	59	Souici, A.	56		
Petermueller, P.	21	Spahr, D.	63		
Petersen, H.	61	Stekiel, S.	24		

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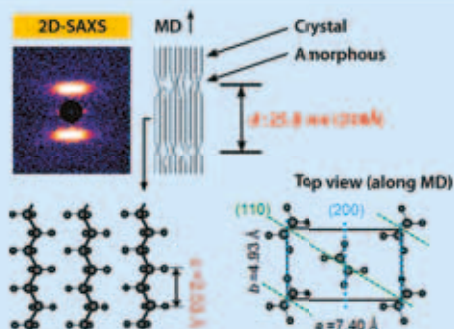
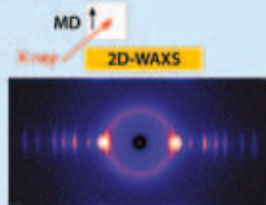
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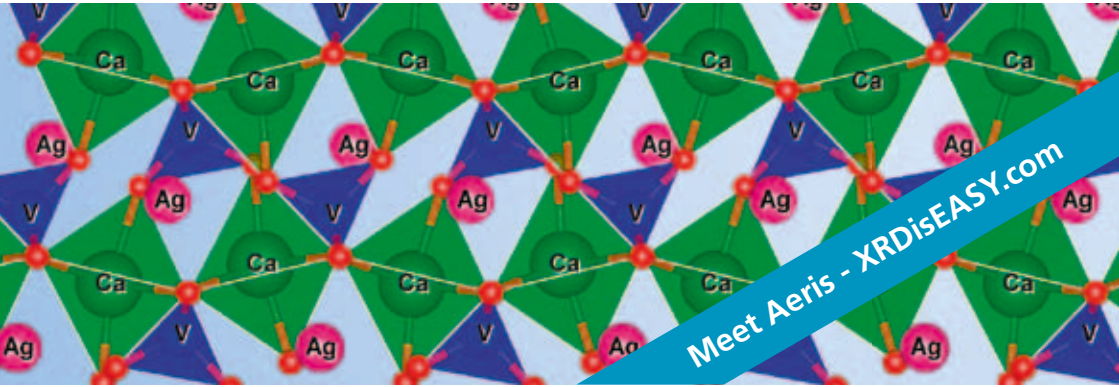
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