26th ANNUAL MEETING of the GERMAN CRYSTALLOGRAPHIC SOCIETY (DGK)

PROGRAMME

5–8 MARCH 2018
ESSEN

www.dgk-conference.de

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TABLE OF CONTENTS

ORGANISATION AND IMPRINT

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Universität Duisburg-Essen
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Conference website
www.dgk-conference.de

Organiser
German Crystallographic Society (DGK)

Conference chair
Prof. Dr. Matthias Epple
Universität Duisburg-Essen
Anorganische Chemie

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Dear colleagues,

It is a pleasure and an honor to invite you to the 26th Annual Meeting of the German Society of Crystallography to the University of Duisburg-Essen. The venue of the Annual Meeting is Essen in the heart of the Ruhrgebiet that is actually not as grey as some of you might expect. In the contrary, after coal and steel industries have contracted and shifted to more environmentally friendly processes, this area has undergone a remarkable transformation. Notably, in 2010, Essen was the center of the European Capital of Culture, and in 2017, it was the European Green Capital.

Many scientific disciplines rely on crystallography, covering inter alia fields like materials sciences, geosciences, crystal structure determination, and protein crystallography. The University of Duisburg-Essen with its two campi at Duisburg and Essen (and a third campus for the University Hospital) has two central research units with direct relevance to crystallography – Nanosciences, as represented by the Center for Nanointegration Duisburg-Essen (CeNIDE), and biological sciences, as represented by the Center for Biomedical Technology (ZMB). Both have supported the Annual Meeting. In the direct vicinity, there are other major research institutions like the Universities at Bochum and Dortmund and a number of Max-Planck Institutes and Fraunhofer institutes, many of them relying on chemical, physical and biological crystallography.

A number of prominent Plenary Speakers have agreed to give presentations at our Annual Congress. We are glad to welcome you to Essen, to contribute and to participate in an exciting conference in a stimulating environment. We wish you a memorable experience!

Matthias Epple
Inorganic Chemistry, University of Duisburg-Essen
Conference chair 2018

GENERAL INFORMATION

Conference language

The conference language is English.

Opening hours

	Monday	Tuesday	Wednesday	Thursday
Check-in	12.00–18.30	08.00–17.30	08.00–16.00	08.30–14.00
Media check-in	12.00–18.30	08.00–17.30	08.00–16.00	08.30–11.00
Industrial exhibition	12.30–20.00	09.00–19.30	09.00–18.00	09.00–14.00

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 check-in on site.

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 for purchase at the check-in at the conference.

Registration

DGK-Member	170 EUR
Non-Member	200 EUR
Student	80 EUR
Welcome Reception	10 EUR
Conference Dinner	40 EUR

Payment and confirmation of payment

An invoice will be sent to you via e-mail within 14 days. It is a valid invoice which may be submitted to the local tax and revenue office. All fees are due upon receipt of the invoice. Payment transfers must include participant's name and invoice number. Payment is also accepted by credit card (Master-/Eurocard, American Express, VISA). In case you have transferred the registration fee shortly before the start of the conference (up to 10 days prior to conference opening), we ask you to please present your transfer remittance slip onsite.

General terms and conditions

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

Certificates of attendance

Certificates of attendance can be picked up upon request at the check-in on the last conference day.

GENERAL GUIDELINES FOR AUTHORS AND PRESENTERS

Technical information

The presentation should be prepared as PDF, MS Office PowerPoint for Windows or key for Macintosh DVD in the 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 early agreement. However, this is not recommended as 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, reserving time for the discussion. Chairs and moderators may interrupt should you overrun your time limit.

Poster sessions

Your poster must be in English and no larger than DIN A0 portrait format (width 84,1 cm x height 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 44 ff.

Please note that there are two poster sessions:

Poster session I – Posters with an even ID
All posters with an even ID should be mounted on Monday and be removed at the end of the poster session on Tuesday.

Poster session II – Posters with an odd ID
All posters with an odd ID should be mounted on Wednesday in the morning and be removed on Thursday, 8 March by 11.00 at the latest. Posters that have not been removed, will be disposed without further notice.

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

Exhibitors

Anton Paar Germany GmbH (Ostfildern/DE)
Bruker AXS GmbH (Karlsruhe/DE)
DECTRIS Ltd. (Baden-Dättwil/CH)
Dunn Labortechnik GmbH (Asbach/DE)
Excillum AB (Kista/SE)
FIZ Karlsruhe (Eggenstein-Leopoldshafen/DE)
Huber Diffraktionstechnik & AXO Dresden (Rimsting/DE)
Incoatec GmbH (Geesthacht/DE)
Malvern Panalytical GmbH (Kassel/DE)
Oxford Cryosystems (Long Hanborough/GB)
Rigaku Europe (Oxford/GB)
STOE & Cie GmbH (Darmstadt/DE)
Thermo Electron (Karlsruhe) GmbH (Karlsruhe/DE)
Thermo Fisher Scientific (Eindhoven/NL)
XRD Eigenmann GmbH (Schnaitlach-Hormersdorf/DE)

Further sponsors

DFG – Deutsche Forschungsgemeinschaft (Bonn/DE)
Center for Nanointegration Duisburg-Essen, CeNIDE (Essen/DE)
Center for Medical Biotechnology, ZMB (Essen/DE)

Crystal Impact, Dr. H. Putz & Dr. K. Brandenburg GbR (Bonn/DE)
Douglas Instruments Ltd. (Berkshire/GB)
MaTecK GmbH (Jülich/DE)
MDPI AG (Basel/CH)
Protein Data Bank in Europe (Cambridge/GB)
Quantachrome GmbH & Co. KG (Odelzhausen/DE)

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State at printing.

INDUSTRIAL SYMPOSIA

Wednesday, 7 March

Rigaku Europe (Oxford/GB)
12.00–13.00
Room S06 S00 B29

Rigaku Oxford Diffraction will be holding its traditional DGK lunchtime seminar on Wednesday 7th March in Room S06 S00 B29.

A buffet style lunch and beer will be provided.

Speakers will include Dr Mathias Meyer and Dr Fraser White.
Join us to discover the latest developments from Rigaku Oxford diffraction and to get tips for making the most of your instrument.

Thursday, 8 March

Thermo Fisher Scientific (Eindhoven/NL)
10.30–11.00
Room Audimax S04 T01 A01

In 2017 R. Henderson, J. Frank and J. Dubochet have been awarded the Nobel prize in Chemistry for having pioneered cryo electron microscopy (Cryo-EM) and Single Particle Analysis (SPA).
During the last few years Cryo-EM and SPA have grown from techniques able to produce low-resolution structures of protein complexes (a.k.a. blobology) to tools capable of achieving atomic and quasi-atomic resolution for complexes that nobody could solve with any other technique.

This incredible leap forward has made possible by introduction and adoption of new tools, in particular direct electron detectors (DED), ultra-stable cryo-microscope, such as Titan Krios, and the adoption of new SW for automatic data collection and processing.
Cryo-EM benefit of specific advantages, respect to other structural biology techniques such as NMR and X-ray diffraction:

- Crystallization or isotopic labelling is not needed
- Amount of sample required is two orders of magnitude lower
- Different functional conformation of a complex may be sorted out

Cryo-EM has proved to be a very useful technique to be integrated with X-ray and NMR for structure-based drug design.
So it is no surprise that many structural biology groups all over the world are seeking access to this technology in order to find answers to their most relevant biological questions. Nevertheless most new comers to the field are struggling to overcome the adoption barrier that this technique may pose in term of: sample preparation and screening, automatic data acquisition and progressive users training.

In this presentation we will see how the fast pace of cryo-EM growth is going to change the structural biology landscape for the best.
In particular we will discuss the

- Glacios™ Cryo-TEM: A 200kV X-FEG autoloader-provided system capable of automatic screening of multiple grids and reduced footprint.
- The new KriosTM G3i: The latest Krios version with improved automation, increased cryo-performance and higher throughput.
- The new development of mED (Micro electron Diffraction): a technology that holds the promise to solve at high resolution, structures of crystals so small that could be seen at naked eyes. And at 0.1% of the cost of an XFEL.

Lightning Talks of Young Crystallographers (LT1 and LT2)

The "Young Crystallographers" are happy to welcome you to the 4th Lightning Talks at the Annual DGK Meeting. We are looking forward to the two microsymposia where 33 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 at 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 6th Annual Get Together on Thursday. Our program will comprise both a short summary of last year's activities (especially the 2nd LabMeeting in Darmstadt) and 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. Snacks, coffee/tea and soft drinks will be served.

Date	Thursday, 8 March 2018
Time	10.00–11.00
Room	S06 S00 B29

We are looking forward to welcome you!

Melanie and Khai
Chairs of the "Young Crystallographers"

Welcome reception

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, 5 March 2018
Time	18.00–20.00
Fee	10 EUR
Venue	Industrial exhibition area, Foyer of the venue S04

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Social evening

The restaurant “Dampfe” is located in the historic building of the Borbecker-Brewery. From 1895 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, 7 March 2018
Time	19.30–23.00
Fee	40 EUR
Venue	Dampfe – Das Borbecker Brauhaus Heinrich-Brauns-Straße 9–15 l 45355 Essen Distance to the conference venue: 5 km

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Audimax S04 T01 A01	Audimax S04 T01 A02	Room S06 S00 B29	Room S06 S00 B32
			09.00–12.30 DGK Board Meeting
		11.00–12.30 Meeting DGK Wissenschaftskolleg	
13.00–13.30 Opening			
13.30–14.30 Plenary lecture: Sven Lidin p. 18			
14:30–16:00			
Bio-crystallography I: Hot new structures p. 18	Measurements and syntheses under extreme conditions p. 19	New crystal structures I p. 20	New developments in methods and instrumentation in neutron scattering p. 21
Coffee break and industrial exhibition			
16:30–17:00 Special lecture laureate Max-von-Laue Award 2017 p. 21			
17:00–18:00 DGK Ehrenabend p. 21			
18:00–20:00 Welcome reception p. 13			

Audimax S04 T01 A01	Audimax S04 T01 A02	Room S06 S00 B29	Room S06 S00 B32
09:00–10:30			
Bio-crystallography II: Complementation by NMR and EPR p. 22	Crystallography in nanoscience p. 22	Structure-property-relationships p. 23	*In-situ* methods p. 24
Coffee break and industrial exhibition			
11:00–12:00			
Plenary lecture: Holger Dobbeck p. 25			
12:00–13:30			
DGK General Assembly			
13:30–14:30			
Plenary lecture: Leonid Dubrovinsky p. 25			
Coffee break and industrial exhibition			
15:00–15:30	14:30–15:30		
Meeting AK 1	Meeting AK 2 / 19	Meeting AK 6	Meeting AK 20
15:30–17:00			
Bio-crystallography III: Enzymes p. 26	Lightning talks I p. 27	Electron microscopy p. 29	Experimental electron density p. 30
17:00–19:30			
Poster session I			

Audimax S04 T01 A01	Audimax S04 T01 A02	Room S06 S00 B29	Room S06 S00 B32
09:00–10:30			
Bio-crystallography IV: Crystallography in industry p. 31	New crystal structures II p. 31	Spectroscopic methods in crystallography p. 32	Structurally complex materials p. 33
Coffee break and industrial exhibition			
11.00–12.00			
Plenary lecture: Kenneth D.M. Harris p. 33			
		12:00–13:00	12:00–13:00
		Industrial symposium Rigaku Europe p. 10	Meeting AK16
13.00-14.00			
Plenary lecture: Randy Read p. 34			
14:00–15:30			
Bio-crystallography V: Instrumentation and methods p. 34	Lightning talks II p. 35	Developments in molecular crystallography p. 37	Characterization of defects in crystalline materials p. 38
15:30–18:00			
Poster session II p. 44			
19:30–23:00			
Social Evening p. 13			

Audimax S04 T01 A01	Audimax S04 T01 A02	Room S06 S00 B29	Room S06 S00 B32
09:00–10:00			
Plenary lecture: Paulina Dominiak p. 39			
Coffee break and industrial exhibition			
10:30–11:00	10:00–11:00		
Industrial symposium Thermo Fisher Scientific p. 10	Meeting AK7	Get Together Young Crystallographers	Meeting AK13
11:00–12:30			
Bio-crystallography VI: Protein – nucleic acid complexes p. 39	New Crystal structures and properties p. 40	Powder diffraction / PDF p. 41	
12:30–13:30			
Plenary lecture: Erdmann Spiecker p. 42			
13:30–14:00			
Closing			

13.00–13.30 Opening
Audimax S04 T01 A01

13.30–14.30 Plenary lecture
Audimax S04 T01 A01
Chair Thomas Doert (Dresden/DE)

13.30 Structure dynamics in crystaline solids
Sven Lidin (Lund/SE)

14.30–16.00 Bio-crystallography I – hot new structures
Audimax S04 T01 A01
Chairs Norbert Sträter (Leipzig/DE), Yves Muller (Erlangen/DE)

14.30
S01-01 A symmetry break in a symmetric homodimer results in crystals with alternating layers of order and disorder
Hartmut Niemann, Willem Bleymüller, Maria Ebbes
Christina Geerds (Bielefeld/DE)

14.45
S01-02 IL-1 family cytokines use distinct molecular mechanisms to signal through their shared co-receptor
Sebastian Günther (Hamburg/DE; BaltimoreMD/US), Daniel Deredge
Amanda L. Bowers (Baltimore, MD/US), Alessandra Luchini (Manassas, VA/US)
Daniel A. Bonsor, Robert Beadenkopf (Baltimore, MD/US)
Lance Liotta (Manassas, VA/US), Patrick L. Wintrode
Eric J. Sundberg (Baltimore, MD/US)

15.00
S01-03 Insight into a synthetic TetR-derived protein – RNA aptamer switch
Florian Grau (Erlangen/DE), Florian Groher, Beatrix Suess (Darmstadt/DE)
Yves Muller (Erlangen/DE)

15.15
S01-04 Structural basis of modulation of host protein synthesis by a virus: the SARS-CoV macrodomain II binds human Paip1
Jian Lei (Lübeck/DE), Yue Ma-Lauer, Albrecht von Brunn (Munich/DE)
Rolf Hilgenfeld (Lübeck/DE)

15.30 S01-05
A family of unconventional deubiquitinases with modular chain specificity determinants
Christian Pichlo, Thomas Hermanns, Ilka Woiwode
Karsten Klopffleisch (Cologne/DE), Katharina F. Witting
Huib Ovaa (Leiden/NL), Ulrich Baumann, Kay Hofmann (Cologne/DE)

15.45 S01-06
Structural basis for antibacterial peptide export by bacterial ABC transporters
Konstantinos Beis (London/GB)

14.30–16.00 Audimax S04 T01 A02
Measurements and syntheses under extreme conditions

Chair
Ulrich Schwarz (Dresden/DE)

14.30 S02-01
The crystal chemistry of calcite-type structure carbonates at extreme conditions
Stella Chariton (Bayreuth/DE), Elena Bykova (Hamburg/DE)
Maxim Bykov (Bayreuth/DE), Valerio Cerantola (Grenoble/FR)
Georgios Aprilis, Catherine McCammon, Leonid Dubrovinsky (Bayreuth/DE)

14.45 S02-02
Pressure-induced spin transitions in garnets at 45-70 GPa
Alexandra Friedrich (Würzburg, Frankfurt a. M./DE), Monika Koch-Müller
Ilias Efthymiopoulos (Potsdam/DE), Wolfgang Morgenroth (Frankfurt a. M./DE)
Joelson Cott (Minneapolis, MN/US), Renata Wentzcovitch (New York, NY/US)

15.00 S02-03
In-situ X-ray diffraction studies on tourmalines at high pressures and temperature
Klaus-Dieter Grevel (Jena/DE), Bernd Marler (Bochum/DE)
Andreas Ertl (Vienna/AT), Christian Lathe (Potsdam/DE)

15.15 S02-04
New insights on the high pressure behaviour of the $GeSe_xTe_{1-x}$ solid solution
Markus Herrmann (Jülich/DE), Ralf Stoffel, Michael Küpers (Aachen/DE)
Mohammed Ait Haddouch (Jülich/DE), Andreas Eich (Aachen/DE)
Konstantin Glazyrin (Hamburg/DE), Andrzej Grzechnik (Aachen/DE)
Karen Friese (Jülich/DE)

15.30
S02-05
A new high-pressure and high-temperature polymorph of $FeCO_3$
Chris-Julian Fruhner, Lkhamsuren Bayarjargal, Dominik Zimmer
Rita Luchitskaia (Frankfurt a. M./DE), Elena Bykova (Hamburg/DE)
Wolfgang Morgenroth, Björn Winkler (Frankfurt a. M./DE)

15.45
S02-06
Using Raman scattering to measure strains in crystals under non-hydrostatic stress conditions
Ross Angel, Mara Murri, Mattia Mazzucchelli (Pavia/IT)
Mauro Prencipe (Torino/IT), Boriana Mihailova (Hamburg/DE)
Matteo Alvaro (Pavia/IT)

14.30–16.00
Room S06 S00 B29
New crystal structures I

Chair
Thomas Doert (Dresden/DE)

14.30
S03-01
Polymorphism and isomerism in coordination compounds – the nemesis of crystal design
Christian Näther, Tristan Neumann, Aleksej Jochim, Carsten Wellm
Inke Jess (Kiel/DE), Michał Rams, Zbigniew Tomkowicz (Krakow/DE)
Luzia S. Germann, Robert E. Dinnebier (Stuttgart/DE)

15.00
S03-02
From giant supramolecules to coordination polymers with supramolecules as nodes
Alexander Virovets, Eugenia Peresypkina, Barbara Krämer
Manfred Scheer (Regensburg/DE)

15.15
S03-03
New data on incorporation of rare-earth elements into uranyl layers: synthesis and crystal structures of novel praseodymium(III) compounds
Sergey Aksenov, Tyler Spano, Madison Turner
Peter Burns (South Bend, IN/US)

15.30
S03-04
High-pressure synthesis of the new binary superconductor lutetium trigermanide $LuGe_3$
Julia-Maria Hübner, Matej Bobnar, Yurii Prots, Ulrich Schwarz (Dresden/DE)

15.45
S03-05
Polyanions with covalent Si-H, Ge-H and Sn-H bonds in Zintl-phase hydrides
Henry Auer, Robin Guehne, Marko Bertmer, Jürgen Haase
Holger Kohlmann (Leipzig/DE)

14.30–16.00 New developments in methods and instrumentation in neutron scattering
Room S06 S00 B32
Chair Astrid Schneidewind (Garching/DE)

14.30 S04-01 Energy Research with Neutrons (ERWIN) and installation of a neutron powder diffraction option at MLZ
Michael Heere (Garching/DE)

14.45 S04-02 Lithium transport in modern solid-state lithium conductors studied by neutron diffraction
Anatoliy Senyshyn (Garching/DE)

15.00 S04-03 Increasing Q-resolution and the science case for neutron Larmor diffraction
Markos Skoulatos (Garching/DE)

15.15 S04-04 Structure analysis with hot neutrons and under extreme conditions on HEIDI
Martin Meven, Andrew Sazonov (Aachen, Garching/DE), Georg Roth
Andrzej Grzechnik (Aachen/DE)

15.30 S04-05 Crystal chirality versus magnetic chirality in $CsCuCl_3$ determined by neutron polarization analysis
Vladimir Hutanu (Garching bei Munich/DE), Y. Kousaka (Okayama/JP)
K. Ohishi, K. Kakurai (Tokai/JP), Georg Roth (Aachen/DE)

15.45 S04-06 Novel type of neutron polarisation analysis with the multianalyser at PUMA
Steffen Schwesig, Oleg Sobolev, Götz Eckold (Göttingen/DE)

16.30–17.00 Special lecture laureate: Max-von-Laue Award 2017
Audimax S04 T01 A01
Chair Thomas Doert (Dresden/DE)

16.30 Serial crystallography using synchrotrons and X-ray free-electron lasers: data processing with CrystFEL
Thomas A. White (Hamburg/DE)

17.00–18.00 DGK Ehrenabend
Audimax S04 T01 A01

18.00–20.00 Welcome reception
Foyer S04 (see page 13)

09.00–10.30 Bio-crystallography II – complementation by NMR and EPR
Audimax S04 T01 A01
Chairs Gregor Hagelüken (Bonn/DE), Janosch Hennig (Heidelberg/DE)

09.00
S05-01
Seeing the width of the conformation ensemble
Gunnar Jeschke (Zurich/CH)

09.30
S05-02
De novo structure prediction of biomolecules using crystallographic and NMR-derived solvent-accessibility data
Christoph Hartlmüller, Christoph Göbl, Johannes Günther (Neuherberg/DE)
Antje Wolter, Jens Wöhnert (Frankfurt a. M./DE)
Michael Sattler (Neuherberg/DE), Tobias Madl (Graz/AT)

09.45
S05-03
Resolution and validation of SAS-based structural model
Anne Tuukkanen (Hamburg/DE; Hinxton/GB)
Gerard J. Kleywegt (Hinxton/GB), Dmitri I. Svergun (Hamburg/DE)

10.00
S05-04
The structure and function of the eukaryotic condensin subunits
Markus Hassler, Marc Kschonsak, Christian Haering (Heidelberg/DE)

10.15
S05-05
Probing protein structure and dynamics by combing X-ray crystallography and EPR spectroscopy of spin labeled protein single crystals
Thomas Risse, Phillipp Consentius, Bernhard Loll, Ulrich Gohlke
Markus C. Wahl, Udo Heinemann (Berlin/DE)

09.00–10.30 Crystallography in nanoscience
Audimax S04 T01 A02
Chair Ullrich Pietsch (Siegen/DE)

09.00
S06-01
Thickness prediction and elastic strain investigation in single GaAs/(In,Ga)As/GaAs core-shell-shell nanowires using in-plane and out-of-plane X-ray diffraction
Ali Al Hassan, Arman Davtyan (Siegen/DE), Hanno Küpers, Ryan B. Lewis
Abbes Tahraoui, Lutz Geelhaar (Berlin/DE), Ullrich Pietsch (Siegen/DE)

09.15
S06-02
Quantum entanglement, Kondo effect, and electronic transport in quantum dots system
Sahib Babaee Tooski (Malayer/IR)

09.30 S06-03
Silver-platinum nanoparticles in the miscibility gap – characterization by X-ray diffraction
Viktoria Grasmik, Kateryna Loza, Oleg Prymak (Essen/DE)
Marc Heggen (Jülich/DE), Matthias Epple (Essen/DE)

09.45 S06-04
Time-resolved *in-situ* X-ray nano-diffraction of a single growing GaAs nanowire by self-catalyzed MBE
Seyed Mohammad Mostafavi Kashani, Jonas Vogel, Arman Davtyan (Siegen/DE)
Ludwig Feigl (Karlsruhe/DE), Danial Bahrami, Julian Jakob (Siegen/DE)
Philipp Schroth (Karlsruhe, Siegen/DE), Tilo Baumbach (Karlsruhe/DE)
Ullrich Pietsch (Siegen/DE)

10.00 S06-05
Fast scanning X-ray diffraction as a strain and orientation microscope at beamline ID01 of the ESRF
Carsten Richter, Gilbert Chahine, Tao Zhou, Marie-Ingrid Richard
Steven Leake (Grenoble/FR), Marvin Zoellner (Frankfurt (Oder)/DE)
Armelle Even, Tobias Schulli (Grenoble/FR)

10.15 S06-06
Nanoscience crystallography at a high brilliance laboratory X-ray diffractometer – from mesoscopic to atomic length scales
Emmanuel Kentzinger, Ulrich Rücker, Asma Qdemat, Thomas Brückel (Jülich/DE)

09.00–10.30 Structure-property-relationships
Room S06 S00 B29
Chair Thomas Schleid (Stuttgart/DE)

09.00 S07-01
Magnetic properties and proton dynamics in phosphatic oxyhydroxides
So Hyun Park (Munich/DE)

09.15 S07-02
Interplay of cation disorder and thermoelastic properties of $MgGa_2O_4$
Christian Hirschle, Jürgen Schreuer (Bochum/DE)
Zbigniew Galazka (Berlin/DE)

09.30 S07-03
Ordering phenomena in rare-earth oxoborates
Marie Münchhalfen, Jürgen Schreuer (Bochum/DE), Christoph Reuther
Jens Götze, Erik Mehner, Hartmut Stöcker (Freiberg/DE)

09.45
S07-04
On the growth mechanism of hetero epitaxial {100} Nickel Titanium shape memory alloy thin films
Sandra Hahn (Chemnitz/DE), Volker Klemm, David Rafaja (Freiberg/DE)
Sandra Kaufmann-Weiß (Karlsruhe/DE), Sebastian Fähler (Dresden/DE)
Martin F.-X. Wagner (Chemnitz/DE)

10.00
S07-05
Synthesis of all-inorganic double perovskite solar absorbers – How to make a theoretician (un)happy
Joachim Breternitz, Susan Schorr (Berlin/DE)

10.15
S07-06
Visualisation of crystalline structures in injection molded parts
Yvonne Spörer, Ines Kühnert (Dresden/DE)

09.00–10.30
Room S06 S00 B32
In-situ methods

Chair
Claudia Weidenthaler (Mülheim a. d. Ruhr/DE)
Bernd Hinrichsen (Ludwigshafen/DE)

09.00
S08-01
X-ray perspective on nanomaterials chemistry
Dorota Koziej (Hamburg/DE)

09.30
S08-02
In-situ formation and growth characterization of iron oxide nanoparticles by synchrotron X-ray scattering techniques
Robert Wendt, Eike Gericke, Anna Lang (Berlin/DE)
Dragomir Tatchev (Sofia/BG), Giorgia Greco, Markus Wollgarten
Armin Hoell, Klaus Rademann, Simone Raoux (Berlin/DE)

09.45
S08-03
In-situ observation of nanoparticle size reduction during laser synthesis in liquids
Alexander Letzel, Bilal Gökce (Essen/DE)
Shyjumon Ibrahimkutty (Stuttgart/DE), Andreas Menzel (Villigen/CH)
Anton Plech (Eggenstein-Leopoldshafen/DE), Stephan Barcikowski (Essen/DE)

10.00
S08-04
In-situ/operando powder X-ray diffraction investigations during heterogeneous catalysis of the partial oxidation of acrolein
Barbara Albert, Jörg Steffan, Kathrin Hofmann, Stefan Knoche
Herbert Vogel (Darmstadt/DE)

10.15 New developments using the "*in-situ*" crystallization with a CO_2-laser
S08-05 Jordi Benet-Buchholz, Eduardo C. Escudero-Adán (Tarragona/ES)
Roland Boese (Essen/DE)

11.00–12.00 Plenary lecture
Audimax S04 T01 A01
Chair Hartmut Niemann (Bielefeld/DE)

Carbon oxide activation at biological Ni,Fe centres
Holger Dobbeck (Berlin/DE)

12.00–13.30 General assembly
Audimax S04 T01 A01 Snacks and drinks will be served.

13.30–14.30 Plenary lecture
Audimax S04 T01 A01
Chair Ulrich Schwarz (Dresden/DE)

Crystallography taken to the extreme
Leonid Dubrovinsky (Bayreuth/DE)

15.30–17.00 Bio-crystallography III – enzymes

Audimax S04 T01 A01

Chairs Wulff Blankenfeldt (Braunschweig/DE), Karsten Niefind (Köln/DE)

15.30
S09-01
Structural and functional insight into human O-GlcNAcase
Christian Roth (Berlin/DE; York/GB), Sherry Chan, Wendy A. Offen
Glyn R. Hemsworth (York/GB), Lianne L. Willems, Dustin T. King
Vimal Varghese, Robert Britton, David J. Vocadlo (Burnaby/CA)
Gideon J. Davies (York/GB)

15.45
S09-02
Structural studies on the substrate and cofactor binding mode of FAD-dependent monooxygenases
Julia Kratky, Renato H. Weiße (Leipzig/DE), Thomas Heine
Dirk Tischler (Freiberg/DE), Norbert Sträter (Leipzig/DE)

16.00
S09-03
Structural and mechanistic investigations on AmbDH3 – a bifunctional dehydratase-cyclase domain in ambruticin biosynthesis
Kwang Hoon Sung (Braunschweig/DE)
Gesche Berkhan (Bayreuth, Hannover/DE), Tim Hollmann
Lisa Wagner (Bayreuth/DE), Wulf Blankenfeldt (Braunschweig/DE)
Frank Hahn (Hannover, Bayreuth/DE)

16.15
S09-04
Structural basis of regioselectivity verified by the structure of the tryptophan 6-halogenase thal
Ann-Christin Moritzer, Hannah Minges, Christian Schnepel, Marcel Frese
Norbert Sewald, Hartmut Niemann (Bielefeld/DE)

16.30
S09-05
Snapshots from the catalytic cycle of the α/β-hydrolase-fold esterase CgHle: trapping the tetrahedral transition state with an arsenic compound and an enzyme/substrate complex with an active-site mutant
Karsten Niefind, Christine Tölzer (Cologne/DE)

16.45
S09-06
Structural studies of bottromycin biosynthesis
Jesko-Alexander Köhnke, Asfandyar Sikandar, Sebastian Adam
Laura Franz (Saarbrücken/DE)

15.30–17.00 Lightning talks I

Audimax S04 T01 A02

Chairs Melanie Nentwich (Freiberg/DE), Khai-Nghi Truong (Aachen/DE)

15.35
LT1-01
High pressure properties of Bi_2SiO_5 from synchrotron powder diffraction and first principle calculations
Adrien Girard, Michal Stekiel, Wolfgang Morgenroth (Frankfurt a. M./DE)
Hiroki Taniguchi (Yokohama/JP), Alexei Bosak (Grenoble/FR)
Björn Winkler (Frankfurt a. M./DE)

15.40
LT1-02
A study on the growth, structural, optical, photoluminescence properties of dye doped l-arginine diphosphate single crystals
Reena Ittyachan (Chalakudy/IN)

15.45
LT1-03
Solvent-controlled molecular self-assembly – from alkoxoiron(III) wheels to coordination networks
Khai-Nghi Truong, Hans Gildenast, Helena Crützen, Alexander Nellessen
Justin Lange, Lynn Ferres, Ulli Englert (Aachen/DE)

15.50
LT1-04
Structure and ligand-induced conformational changes of the calcium-sensing receptor
Mandy Geisler, Norbert Sträter (Leipzig/DE)

15.55
LT1-05
In-situ powder diffraction measurements of a high-yield microwave synthesis of silver nanoparticles using synchrotron radiation
Kevin Pappert (Essen/DE), Luzia S. Germann (Stuttgart/DE)
Martin Etter (Hamburg/DE), Robert E. Dinnebier (Stuttgart/DE)
Matthias Epple (Essen/DE)

16.00
LT1-06
Preparation of active kallikrein7 for structural studies on inhibitor binding
Stefanie Hanke, Jan Pippel, David Ulbricht, John T. Heiker
Norbert Sträter (Leipzig/DE)

16.05
LT1-07
Treatment of wastewater by adsorption on raw ore graphite (deposit point 214-area sidi bouothmane-marrakech)
Said Sabir (Casablanca/MA)

16.10
LT1-08
In-situ XRD studies on the hydrogenation of Ti thin films
Zoltán Balogh-Michels (Dübendorf/CH), Efi Hadjixenophontos
Lukas Michalek, Manuel Roussel, Michael Hirscher, Guido Schmitz (Stuttgart/DE)

16.15
LT1-09
Investigation of illuminated manuscripts by micro-diffraction using an aircooled X-ray microfocus source
Bernd Hasse, Jörg Wiesmann (Geesthacht/DE), Frederik Vanmeert
Koen Janssens (Antwerp/BE)

16.20
LT1-10
Flexibility vs. rigidity – linker extension influence on mof formation and porosity
Friedrich Wilhelm Steuber, Debobroto Sensharma, Paul Wix
Lauren Macreadie, Wolfgang Schmitt (Dublin/IE)

16.25
LT1-11
Synthesis and compressibility of iridium borides
Christopher Neun (Frankfurt a. M./DE), Bendikt Petermüller (Innsbruck/AT)
Lkhamsuren Bayarjargal, Wolfgang Morgenroth,
Dominik Zimmer (Frankfurt a. M./DE), Klaus Wurst
Hubert Huppertz (Innsbruck/AT), Björn Winkler (Frankfurt a. M./DE)

16.30
LT1-12
Single crystal structure investigation of $Cu(C_{10}H_{20}O_5)Br_2{\cdot}2H_2O$ and analysis of physical properties
Natalija van Well (Bayreuth/DE, Villigen/CH), Claudio Eisele (Bayreuth/DE)
Alun Biffin (Villigen/CH), Christian Rüegg (Villigen, Geneva/CH)
Sander van Smaalen (Bayreuth/DE)

16.35
LT1-13
An integrative approach to study the conformation of the Yersinia type-III-effector protein YopO and its activation by actin in solution
Gregor Hagelueken (Bonn/DE), Anne Tuukkanen (Hamburg/DE)
Alexander Selsam, Caspar Heubach, Daniel Marx, Fraser Duthie (Bonn/DE)
Dmitri I. Svergun (Hamburg/DE), Olav Schiemann (Bonn/DE)

16.40
LT1-14
Total scattering and pair distribution function characterization of disordered polymer structures
Maxwell Terban (Stuttgart/DE), Bernd Hinrichsen (Ludwigshafen/DE)
Robert E. Dinnebier (Stuttgart/DE)

16.45
LT1-15
Quantitative modeling of combinatorial transcription factor binding reveals DNA-shape mediated cooperativity
Ignacio Ibarra Del Río, Judith Zaugg (Heidelberg/DE)

16.50 LT1-16
All you can diffract – elucidating the commensurately modulated structure of $HfTaO_{4.5}$
Dennis Wiedemann, Tobias Lüdtke (Berlin/DE), Lukáš Palatinus (Prague/CZ)
Martin J. Mühlbauer (Munich/DE), Elena Willinger, Marc Willinger (Berlin/DE)

15.30–17.00 Electron microscopy
Room S06 S00 B29
Chairs Marc Heggen (Jülich/DE), Kateryna Loza (Essen/DE)

15.30 S10-01
Elastic and inelastic contributions in electron diffraction
Tatiana Gorelik (Ulm/DE)

15.45 S10-02
A detailed *in-situ* and *ex-situ* TEM study of the carbonization process of electrospun PAN derived fibres
Roland Schierholz, Daniel Kröger, Martin Gocyla, Hermann Tempel
Hans Kungl, Rüdiger-A. Eichel (Jülich/DE)

16.00 S10-03
Cation disorder in Ca_1-xLixAl_1-xGe_1+xN_3 (x ≈ 0.2) by STEM-HAADF
Lucien Eisenburger (Leipzig, Munich/DE), Jonas Häusler
Wolfgang Schnick (Munich/DE), Oliver Oeckler (Leipzig/DE)

16.15 S10-04
TEM-based analysis of the crystal structure of a Ge-rich layer sandwiched between spintronic Fe_3Si
Holm Kirmse, Bernd Jenichen, Elena Willinger, Xing Huang, Benedikt Haas
Christoph T. Koch (Berlin/DE)

16.30 S10-05
Thermal stability of porous iridium nanoparticles by *in-situ* tem heating
Kateryna Loza, Kevin Pappert (Essen/DE), Marc Heggen (Jülich/DE)
Matthias Epple (Essen/DE)

16.45 S10-06
Transrotational structure with complicated lattice misorientations revealed by TEM for 2 kinds of spherulites growing in amorphous films
Vladimir Kolosov (Ekaterinburg/RU)

15.30–17.00 Experimental electron density
Room S06 S00 B32
Chairs Ullrich Englert (Aachen/DE), Christian Lehmann (Mülheim a. d. Ruhr/DE)

15.30
S11-01
Quantum crystallography – original definition and connections to current research developments
Alessandro Genoni (Metz/FR)

15.52
S11-02
Charge and spin density in position and momentum space, density matrices, wave functions and energies of periodic systems, from theory or experiments: in one word – Quantum Crystallography
Piero Macchi (Bern/CH)

16.15
S11-03
Accurate treatment of hydrogen atoms using quantum crystallographic techniques
Lorraine Andrade Malaspina, Simon Grabowsky (Bremen/DE)

16.30
S11-04
Validation of experimental charge density refinement strategies
Regine Herbst-Irmer (Göttingen/DE), Lennard Krause (Aarhus/DK)
Dietmar Stalke (Göttingen/DE)

16.45
S11-05
The electrostatic potential of dynamic charge densities of α-, γ-boron and boron carbide($B_{13}C_2$)
Christian B. Hübschle, Sander van Smaalen (Bayreuth/DE)

17.00–19.30 Poster session I
Foyer S06
(see page 44)

09.00–10.30 Bio-Crystallography IV – Crystallography in industry
Audimax S04 T01 A01
Chair Martina Schäfer (Berlin/DE)

09.00 S12-01 Crystal structure of GNIP1Aa, a novel insecticidal protein from Chromobacterium piscinae
Jörg Freigang (Monheim/DE), Jelena Zaitseva (Morrisville, NC/US)

09.18 S12-02 Structure of the Malaria vaccine candidate antigen CyRPA and its complex with a parasite invasion inhibitory antibody
Paola Favuzza (Basel/CH; Melbourne/AU), Gerd Pluschke
Markus G. Rudolph (Basel/CH)

09.36 S12-03 GTP cyclohydrolase I – a target for treating inflammatory and neuropathic pain structural biology, biophysics and drug discovery
Herbert Nar (Biberach/DE)

09.54 S12-04 Biophysics and structural biology in drug discovery
Roman Hillig (Berlin/DE)

10.12 S12-05 Crystal structure of a thermostable FGF21 variant
Matthias Dreyer (Frankfurt a. M./DE)

09.00–10.30 New crystal structures II
Audimax S04 T01 A02
Chair Christian Näther (Kiel/DE)

09.00 S13-01 New insights in corrosion phenomena of historical art- and craftwork provided by X-ray powder diffraction
Sebastian Bette, Gerhard Eggert, Robert E. Dinnebier (Stuttgart/DE)

09.30 S13-02 Building metal-organic architectures by the design
Marijana Dakovic, Mladen Borovina (Zagreb/HR)
Christer Aakeroy (Manhattan, NY/US), Ivan Kodrin (Zagreb/HR)

09.45 S13-03 Structural characterization of an ultra-high strength Fe-Cr-Ni silicide phase
Sergi Plana-Ruiz (Darmstadt/DE; Barcelona/ES)
Yasar Krysiak (Darmstadt/DE), Lukáš Palatinus (Prague/CZ), David Bowden
Michael Preuss (Manchester/GB), Ute Kolb (Darmstadt, Mainz/DE)

10.00
S13-04
Advantages of chalcogenide bonded metals as basis for potential Alion conducting materials
Falk Meutzner (Freiberg/DE; Samara/RU), Matthias Zschornak
Tina Nestler (Freiberg/DE), Artem A. Kabanov (Samara/RU)
Tilmann Leisegang (Freiberg/DE; Samara/RU), Vladislav A. Blatov (Samara/RU)
Dirk C. Meyer (Freiberg/DE)

10.15
S13-05
Boron allotrope with α-Ga structure synthesized at high pressure and high temperature
Irina Chuvashova (Bayreuth/DE), Elena Bykova (Bayreuth/DE; Argonne, IL/US)
Vitali Prakapenka (Hamburg/DE), Konstantin Glazyrin (Grenoble/FR)
Mohamed Mezouar, Leonid Dubrovinsky (Bayreuth/DE)

09.00–10.30
Room S06 S00 B29
Spectroscopic methods in crystallography

Chair
Michael Fechtelkord (Bochum/DE)

09.00
S14-01
X-ray absorption spectroscopy for crystallography at BESSY II
Daniel M. Többens, Götz Schuck, Ivo Zizak, Susan Schorr (Berlin/DE)

09.15
S14-02
Growth and physicochemical properties of semi-organic NLO crystal picolinium taratrate monohydrate
Sajan Davidson (Mavelikara/IN)

09.30
S14-03
Lattice dynamics of $CaCO_3$ and $MgCO_3$
Michal Stekiel, Adrien Girard (Frankfurt a. M./DE)
Tra Thanh-Nguyen (Grenoble/FR), Wolfgang Morgenroth (Frankfurt a. M./DE)
Alexei Bosak (Grenoble/FR), Björn Winkler (Frankfurt a. M./DE)

09.45
S14-04
Order-disorder phenomena above the Curie temperature in lead titanate
Irina Margaritescu, Kaustuv Datta, Boriana Mihailova (Hamburg/DE)

10.00
S14-05
Characterization spectroscopic infrared and Raman on new type materials sillenite
Hajar Ait Oulahyane, Abdeslam Chagraoui, Leila Loubbidi, Lamia Bourja
Abdenajib Moussaoui, Omar Ait Sidi Ahmed, Abdelmjid Tairi (Casablanca/MA)

10.15
S14-06
Vibrational study, reinvestigation of the crystal structure of $MgHPO_{4.3}H_2O$ and calculated IR frequencies for the PO_{43-} by isotopic substitutions
Mustafa Belhabra, Soufiane Zerraf, Aziz Kheireddine
Malika Tridane (Casablanca/MA), Hicham Moutaabbid (Paris/FR)
Mohammed Moutaabbid, Mohamed Radid, Said Belaaouad (Casablanca/MA)

09.00–10.30 Structurally complex materials
Room S06 S00 B32
Chair Andreas Schönleber (Bayreuth/DE), Sander van Smaalen (Bayreuth/DE)

09.00
S15-01 Two new incommensurately modulated rare earth metal polytellurides
Thomas Doert, Hagen Poddig (Dresden/DE)

09.15
S15-02 Incommensurate modulation of the charge-density wave in CuV_2S_4
Sitaram Ramakrishnan, Ngyuen Hai An, Florian Feulner, Mariia Anurova
Andreas Schönleber, Sander van Smaalen (Bayreuth/DE)

09.30
S15-03 Mullite Al/Si ordering in superspace revealed by DFT
Paul Benjamin Klar, Xabier M. Aretxabaleta, Iñigo Etxebarria
Gotzon Madariaga (Bilbao/ES)

09.45
S15-04 Influence of electric field on the room-temperature local structure of $(1-x)Na_{0.5}Bi_{0.5}TiO_{3-x}BaTiO_3$
Gemma de la Flor (Leioa/ES; Hamburg/DE), Semen Gorfmann (Tel Aviv/IL)
Boriana Mihailova (Hamburg/DE)

10.00
S15-05 Direct observation of polar nanodomains in the incommensurate phase of $(K_{0.92}Rb_{0.08})_2ZnCl_4$ crystals
Claudia Kofahl, Friedrich Güthoff, Götz Eckold (Göttingen/DE)

10.15
S15-06 Influence of microstructure on symmetry determination of piezoceramics
Manuel Hinterstein (Karlsruhe/DE), Henry Ekene Mgbemere (Lagos/NG)
Markus Hoelzel (Garching/DE), Esmaeil Adabifiroozjaei
Charles Sorrell (Sydney/AU), Michael Hoffmann (Karlsruhe/DE)

11.00–12.00 Plenary lecture
Audimax S04 T01 A01
Chair Matthias Epple (Essen/DE)

11.00 New experimental techniques for exploring crystallization pathways and structural properties of solids
Kenneth D. M. Harris (Cardiff/GB)

12.00–13.00 Industrial Symposium Rigaku Europe
Room S06 S00 B29

13.00–14.00 Plenary lecture
Audimax S04 T01 A01
Chair Manfred Weiß (Berlin/DE)

13.00 An unexpected crystallographic insight into renin secretion
Randy Read (Cambridge/GB)

14.00–15.30 Bio-crystallography V – instrumentation and method
Audimax S04 T01 A01
Chair Christoph Müller-Dieckmann (Grenoble/FR), Manfred Weiß (Berlin/DE)

14.00 S16-01 P11 at PETRA III – a versatile beamline for serial and high-throughput crystallography
Anja Burkhardt, Olga Lorbeer, Eva Crosas, Sebastian Günther, Tim Pakendorf Bernd Reime, Jan Meyer, Pontus Fischer, Nicolas Stübe, Martin Warmer Alke Meents (Hamburg/DE)

14.15 S16-02 Facilities for macromolecular crystallography at the Helmholtz Zentrum Berlin
Christian Feiler, Martin Gerlach, Ronald Förster, Christine Gless, Thomas Hauss Michael Hellmig, Franziska Huschmann, Alexandra Kastner, Piotr Malecki Karine Röwer, Lukas Schmuckermaier, Michael Steffien, Piotr Wilk Manfred Weiss (Berlin/DE)

14.30 S16-03 3D printing at the diffraction limit: sample injection for time resolved serial crystallography
Michael Heymann (Martinsried/DE)

14.45 S16-04 EMBL beamlines P13/P14 and associated facilities for macromolecular crystallography at PETRA III – status, results, and future plans
Thomas R. Schneider, Gleb Bourenkov, Guillaume Pompidor, Isabel Bento Johanna Hakanpää, Saravanan Panneerselvam (Hamburg/DE)

15.00 S16-05 Facilities for structural biology at the ESRF – present and future
Gordon Leonard (Grenoble/FR)

15.15 S16-06 Data collection at X-ray free-electron lasers and synchrotrons
Marie Luise Grünbein (Heidelberg/DE)

14.00–15.30 Lightning talks II

Audimax S04 T01 A02

Chairs Melanie Nentwich (Freiberg/DE), Khai-Nghi Truong (Aachen/DE)

14.05
LT2-01 STD-NMR as a tool to identify (and characterize) weakly binding ligands for protein crystallography
Bärbel Blaum (Tübingen/DE)

14.10
LT2-02 $Na_3ZrCo(SiO_4)_2(PO_4)$ as an electrolyte material for sodium-ion batteries
Asmaa Loutati (Casablanca/MA)

14.15
LT2-03 Structure-optimized ProM scaffolds address Ena/VASP as a possible antimetastatic target
Matthias Barone, Matthias Müller (Berlin/DE), Slim Chiha (Cologne/DE)
Udo Heinemann (Berlin/DE), Hans-Günther Schmalz (Cologne/DE)
Ronald Kühne (Berlin/DE)

14.20
LT2-04 High temperature *in-situ* PDF study on TiO_2 nanoparticle growth
Stefan Diez (Erlangen/DE)

14.25
LT2-05 Structural and Raman spectroscopic studies of the two $M_{0.50}SbFe(PO_4)_3$ (M = Mg, Ni) nasicon phases
Hajar Bellefqih (Casablanca/MA)

14.30
LT2-06 Serial synchrotron crystallography at EMBL PETRA III beamline P14
Johanna Hakanpää, Gleb Bourenkov, Ivars Karpics, Guillaume Pompidor
Isabel Bento, Thomas Schneider (Hamburg/DE)

14.35
LT2-07 Phase transition of tetragonal copper sulfide Cu_2S at low temperatures
Dominik Zimmer (Frankfurt a. M./DE), Javier Ruiz-Fuertes (Valencia/ES)
Lkhamsuren Bayarjargal, Eiken Haussühl, Björn Winkler (Frankfurt a. M./DE)
Jun Zhang, ChangQing Jin (Beijing/CN), Victor Milman (Cambridge/GB)
Edith Alig, Lothar Fink (Frankfurt a. M./DE)

14.40
LT2-08 *In-situ* studies of dislocations in GaAs with synchrotron white beam X-ray topography
Patrizia Fritsch (Freiburg i. Br./DE), Merve P. Kabukcuoglu
Simon Haaga (Freiburg i. Br., Karlsruhe/DE), Tilo Baumbach (Karlsruhe/DE)
Andreas N. Danilewsky (Freiburg i. Br./DE)

14.45
LT2-09
Analysis of aluminum conductivitiy in high-valent transition metal oxides with Bond-Valence-Site-Energy calculations
Manuel Rothenberger (Freiberg/DE), Falk Meutzner (Freiberg/DE; Samara/RU)
Tina Nestler (Freiberg/DE), Tilmann Leisegang (Freiberg/DE; Samara/RU)
Dirk C. Meyer (Freiberg/DE)

14.50
LT2-10
Beamline P02.1 – a workhorse for high-resolution powder diffraction and total scattering experiments at PETRA III, DESY
Michael Wharmby, Martin Etter, Jozef Bednarcik, Jo-Chi Tseng, Mario Wendt
Sergej Wenz, Anita Ehnes, Hanns-Peter Liermann, Oliver Seeck (Hamburg/DE)

14.55
LT2-11
Investigations on crystal structures and planar defects of heavily stacking faulted honeycomb iridates
Sebastian Bette, Robert E. Dinnebier, Tomohiro Takayama
Hidenori Takagi (Stuttgart/DE)

15.00
LT2-12
Towards the structure of TRAP transporters with an integrative approach of crystallography and PELDOR
Martin F. Peter, Janin Glaenzer (Bonn/DE), Gavin H. Thomas (York/GB)
Gregor Hagelueken (Bonn/DE)

15.05
LT2-13
New crystal structures of two zirconium metal-organic frameworks
Haishuang Zhao (Mainz/DE), Sebastian Leubner, Timo Rhauderwiek
Norbert Stock (Kiel/DE), Ute Kolb (Mainz/DE)

15.10
LT2-14
In-situ small-angle X-ray scattering (SAXS) and powder X-ray diffraction (PXRD) – complementary tools to investigate the structural behaviour and the composition of mono- and bimetallic nanoparticles
Alexander Rostek, Kateryna Loza, Oleg Prymak (Essen/DE)
Paulo R. A. F. Garcia, Cristiano Luís Pinto Oliveira (São Paulo/BR)
Marc Heggen (Jülich/DE), Matthias Epple (Essen/DE)

15.15
LT2-15
How does the crystal structure influence the final composition of the Au-Fe alloy nanoparticles generated via pulsed laser ablation in liquids?
Anna Tymoczko (Essen/DE), Marius Kamp (Kiel/DE)
Christoph Rehbock (Essen/DE), Ulrich Schürmann (Kiel/DE)
Oleg Prymak (Essen/DE), Lorenz Kienle (Kiel/DE)
Stephan Barcikowski (Essen/DE)

15.20
LT2-16
Crystal structure of the human lysosomal mTORC1 scaffold complex
Giridhar Shivalingaiah, Mariana E.G. de Araujo, Andreas Naschberger
Barbara G. Fürnrohr, Taras Stasyk, Theresia Dunzendorfer-Matt
Stefan Lechner, Stefan Welti, Leopold Kremser, Herbert H. Lindner
Martin Offterdinger, Lukas A. Huber, Klaus Scheffzek (Innsbruck/AT)

15.25
LT2-17
Structure determination of 2-(4-(6-Fluoropyridin-3-yl)phenyl)quinoxaline
D. V. Geetha, K. B. Harsha, M. A. Sridhar, K. S. Rangappa (Mysuru, Karnataka/IN)

14.00–15.30
Room S06 S00 B29
Developments in molecular crystallography

Chairs
Ullrich Englert (Aachen/DE), Christian Lehmann (Mülheim a. d. Ruhr/DE)

14.00
S17-01
Modeling bond oriented deformation density in SHELXL
Birger Dittrich, Jens Lübben (Düsseldorf/DE)
Claudia Wandtke (Göttingen/DE), Christian B. Hübschle (Bayreuth/DE)
George M. Sheldrick (Göttingen/DE)

14.30
S17-02
Treating residual density in organic molecules using simplified virtual atoms: a technical note
Alexander Nazarenko (Buffalo, NY/US)

14.45
S17-03
Software development for the P24 “chemical crystallography” beamline at DESY
Marius Kremer (Aachen, Mülheim a. d. Ruhr/DE)
Christian W. Lehmann (Mülheim a. d. Ruhr/DE)

15.00
S17-04
StructureFinder
Daniel Kratzert (Freiburg i. Br./DE)

15.15
S17-05
Structural modulations in elastically bendable co-crystal of caffeine and 4-chloro 3-nitrobenzoic acid under mechanical stress
Somnath Dey, C. Malla Reddy (Mohanpur/IN), Nobuhiro Yasuda (Hyogo/JP)

14.00–15.30 Characterization of defects in crystalline materials
Room S06 S00 B32
Chair Claudia Weidenthaler (Mülheim a. d. Ruhr/DE)
Andreas Danilewsky (Freiburg i. Br./DE)

14.00
S18-01 Semiconductor single crystal growth with reduced defect formation by optimized process parameters
Christiane Frank-Rotsch (Berlin/DE)

14.30
S18-02 Effect of delayed coalescence of nucleation layers on defect structure in HTVPE GaN
Mykhailo Barchuk, Tom Schneider, Gleb Lukin, Olf Pätzold
Christian Röder (Freiberg/DE)
Gernoth Buth (Eggenstein-Leopoldshafen/DE)
Eugene Yakimov (Chernogolovka/RU), David Rafaja (Freiberg/DE)

14.45
S18-03 Characterizing complex molecular disorder using single crystal diffuse scattering
Ella Schmidt, Reinhard B. Neder (Erlangen/DE)

15.00
S18-04 Structural incorporation of Mo^{6+} into akaganéite (β -FeOOH) and its microbial reduction by *Shewanella loihica* PV-4
Ralph Michael Bolanz, Christoph Grauer, Rebecca Cooper (Jena/DE)
Jörg Göttlicher, Ralph Steiniger (Karlsruhe/DE), Stephen Perry (Didcot/GB)
Kirsten Küsel (Jena/DE)

15.15
S18-05 γ-Al_2O_3 – a defect stabilized phase
Martin Rudolph, Mykhaylo Motylenko, David Rafaja (Freiberg/DE)

15.30–18.00 Poster session II
Foyer S06 (see page 44)

19.30–23.00 Social evening
Dampfe – Borbecker Brauhaus
(see page 13)

09.00–10.00 Plenary lecture
Audimax S04 T01 A01
Chair Christian Lehmann (Mülheim a. d. Ruhr/DE)

09.00 Intermolecular interactions from electron density and electrostatic potential perspective
Paulina Dominiak (Warschau/PL)

10.30–11.00 Industrial Symposium Thermo Fisher Scientific
Audimax S04 T01 A01

11.00–12.30 Bio-crystallography VI – protein – nucleic acid complexes
Audimax S04 T01 A01
Chair Markus C. Wahl (Berlin/DE)

11.00 S19-01 The mechanism of negative DNA supercoiling by gyrase – dissecting structure, function and dynamics by single-molecule FRET and X-ray crystallography
Dagmar Klostermeier, Airat Gubaev, Daniela Weidlich
Simon Hartmann (Münster/DE), Markus G. Rudolph (Basel/CH)

11.15 S19-02 Structure and conformational dynamics of type I-Fv CRISPR-Cas mediated DNA interference
Patrick Pausch, Wieland Steinchen, Hanna Müller-Esparza, Daniel Gleditzsch
Florian Altegoer, Lennart Randau, Gert Bange (Marburg/DE)

11.30 S19-03 Canonical and novel non-canonical cold shock-domains of UNR interact with lncRNA roX2 and MLE during roX2 remodelling
Nele Merret Hollmann, Pawel Masiewicz, Lara Jayne Sweetapple
Soeren von Buelow, Pravin Kumar Ankush Jagtap
Janosch Hennig (Heidelberg/DE)

11.45 S19-04 Structural and functional characterization of the spliceosomal protein Prpf39
Francesca De Bortoli, Bernhard Loll, Markus C. Wahl, Florian Heyd (Berlin/DE)

12.00 S19-05 — Crystal structure analysis of a spliceosomal complex of the DEAH-box ATPase Prp2, RNA and ADP-BeF_3
Florian Hamann, Ralf Ficner (Göttingen/DE)

12.15 S19-06 — Building atomic models into electron-microscopy maps with ARP/wARP
Grzegorz Chojnowski (Hamburg/DE), Joana Pereira (Hamburg, Tübingen/DE)
Philipp Heuser, Victor Lamzin (Hamburg/DE)

11.00–12.30 New Crystal structures and properties

Audimax S04 T01 A02

Chair: Joachim Breternitz (Berlin/DE)

11.00 S20-01 — Structure variations within certain rare-earth disilicides
Melanie Nentwich (Freiberg/DE), Matthias Zschornak (Freiberg, Dresden/DE)
Maximilian Sonntag, Roman Gumeniuk (Freiberg/DE)
Sibylle Gemming (Dresden, Chemnitz/DE)
Tilmann Leisegang (Freiberg/DE; Samara/RU), Dirk C. Meyer (Freiberg/DE)

11.15 S20-02 — Hydrothermal synthesis of $M_3Sb_4O_6F_6$ (M = Zn, Fe etc.), $FeSbO_2F_2$ and their characterization
Sk Imran Ali (Tamluk/IN), Mats Johnsson (Stockholm/SE)

11.30 S20-03 — Structural and molecular spectroscopic behaviour of the Mg-Ni kieserite solid solution, $(Mg,Ni)SO_4 \cdot H_2O$, with relevance to icy satellites of Jupiter and Saturn
Dominik Talla, Manfred Wildner (Vienna/AT)

11.45 S20-04 — Structural phase transitions of copper(I) phosphide $Cu_{3-x}P$
Thomas Doert, Alexander Wolff, Jens Hunger (Dresden/DE)

12.00 S20-05 — Crystal, electronic structure, optical and electrical studies of new 2D hybrid perovskite $[(CH_2)n(NH_3)_2]MX_4$; X= Cl, Br; M= Co, Mn; n= 4-9 promising for photovoltaic applications
Seham K Abdel-Aal, Ahmed Seham (Giza/EG)

12.15 S20-06 — Pure gyrotropic phase transitions in the arcanite related materials $PbMGeO_4$ (M = Ba, Sr)
Martin Schreyer, Gwilherm Nénert, Detlef Opper (Almelo/NL)

11.00–12.30 Powder diffraction/PDF

Room S06 S00 B29

Chairs Reinhard Neder (Erlangen/DE), Robert Dinnebier (Stuttgart/DE)

11.00
S21-01
On the robustness of atomic pair distribution function (PDF) models
Simon Billinge (New York, NY/US)

11.30
S21-02
Crystallographic investigation of silver-gold nanoparticles *in-situ*: crystallite size and thermal expansion
Oleg Prymak, Viktoria Grasmik, Kateryna Loza (Essen/DE)
Marc Heggen (Jülich/DE), Matthias Epple (Essen/DE)

11.45
S21-03
New insights into morphotropic phase boundaries of ferroelectric solid solutions from pair distribution function analysis
Kaustuv Datta (Hamburg/DE), Reinhard B. Neder (Erlangen/DE)
Jun Chen (Beijing/CN), Joerg Neuefeind (Oak Ridge, TN/US)
Boriana Mihailova (Hamburg/DE)

12.00
S21-04
Detailed X-ray diffraction and pair distribution function study on the layered compound $CrTe_3$
Anna-Lena Hansen, Bastian Dietl (Kiel/DE), Martin Etter (Hamburg/DE)
Reinhard Kremer (Stuttgart/DE), David C. Johnson (Eugene, OR/US)
Wolfgang Bensch (Kiel/DE)

12.15
S21-05
Crystal structure of coordination polymers solved from X-ray powder diffraction
Luzia S. Germann (Stuttgart/DE), Tristan Neumann, Stefan Suckert (Kiel/DE)
Igor Moudrakovski (Stuttgart/DE), Christian Näther (Kiel/DE)
Robert E. Dinnebier (Stuttgart/DE)

12.30–13.30 Plenary lecture

Audimax S04 T01 A01

Chair Kateryna Loza (Essen/DE)

12.30 The new era of *in-situ* electron microscopy – from qualitative observations to quantitative studies on the nanoscale
Erdmann Spiecker (Erlangen/DE)

13.30–14.00 Closing

Audimax S04 T01 A01

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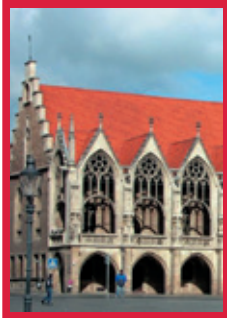

der Deutschen Gesellschaft für Biomaterialien

8. – 10. November 2018 | Braunschweig

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POSTER OVERVIEW

Bio-Crystallography I – Hot new structures

P001 Crystal Structure of the most prominent phospholipase PlaB, a hemolytic virulence factor from Legionella pneumophila
Maurice Diwo (Braunschweig/DE), Wiebke Michel, Katja Kuhle (Wernigerode/DE)
Jörn Krauße (Braunschweig/DE), Antje Flieger (Wernigerode/DE)
Wulf Blankenfeldt (Braunschweig/DE)

P002 Structural and functional analysis of the TSC2 GAP-Domain
Patrick Hansmann (Münster/DE), Stephan Kiontke (Osnabrück/DE)
Daniel Kümmel (Münster/DE)

P003 Structure of the c-di-AMP synthesising diadenylate cyclase CdaA
Jana Laura Heidemann, Piotr Neumann, Achim Dickmanns
Ralf Ficner (Göttingen/DE)

Bio-Crystallography II – Complementation by NMR and EPR

P004 Towards understanding of Hunchback mRNA translation suppression in early embryonic development
Janosch Hennig, Jakub Macosek, Jaelle Foot, Sophie Winter, Pawel Masiewicz
Bernd Simon, Inga Loedige (Heidelberg/DE)

P005 Yeast glucokinase – how small alterations make the difference between glucokinase and hexokinase activity
Renato H. Weiße (Leipzig/DE), Karina Kettner, Thomas Kriegel (Dresden/DE)
Norbert Sträter (Leipzig/DE)

Bio-Crystallography III – Enzymes

P006 Antimetabolite biosynthesis in Pseudomonas aeruginosa
Yafei Xiao (Braunschweig/DE), Chris Calderone (Northfield, IL/US)
Rolf Müller (Saarbrücken, Braunschweig/DE), Wulf Blankenfeldt (Braunschweig/DE)

P007 Towards the structural investigation of an RNA-cleaving deoxyribozyme
Mateusz Mieczkowski (Göttingen/DE)
Claudia Höbartner (Göttingen, Würzburg/DE), Vlad Pena (Göttingen/DE)

P008 Structural insights into phosphoryl transfer mechanism of ADP-dependent glucokinase from Methanocaldococcus jannaschii
Piotr Tokarz, Magdalena Wisniewska (Krakow/PL), Marcin M. Kaminski (Memphis, TN/US)
Grzegorz Dubin, Przemyslaw Grudnik (Krakow/PL)

POSTER PRESENTATIONS

P009 Control of methylglyoxal synthesis in Bacillus subtilis – structural basis for the regulatory interaction of the methylglyoxal synthase MgsA with the carbon flux regulator Crh
Johannes Arens, Achim Dickmanns, Christopher Zschiedrich, Jan Gundlach
Romina Hofele, Piotr Neumann, Henning Urlaub (Göttingen/DE)
Boris Goerke (Göttingen/DE; Vienna/AT), Jörg Stülke, Ralf Ficner (Göttingen/DE)

P010 Halogenase crystals in space group P32 and in P1 with a non-crystallographic pseudo 32 axis harvested from the same drop
Christiane Widmann, Mohamed Ismail Fouad Ismail (Bielefeld/DE)

P011 Specific allosteric regulation of protozoan sugar-activating nucleotidyltransferases as a new approach to antimicrobial treatments
Ole Zeymer, Johannes Cramer, Jana Führing, Françoise Routier, Anne-Christin Lamerz
Julia Lieske, Petra Baruch (Hannover/DE), Hans-Joachim Knölker (Dresden/DE)
Rita Gerardy-Schahn, Roman Fedorov (Hannover/DE)

Bio-Crystallography IV – Crystallography in industry

P012 Industrial applications at beamline P11 at PETRA III
Eva Crosas, Olga Lorbeer, Sebastian Guenther, Jan Meyer, Pontus Fischer, Bernd Reime
Tim Pakendorf, Nicolas Stübe, Alke Meents, Anja Burkhardt (Hamburg/DE)

Bio-Crystallography V – Instrumentation and methods

P013 Ctrl-D, a tool for diffraction data analysis
Fabio Dall'Antonia, Thomas R. Schneider (Hamburg/DE)

P014 Automating the D8 VENTURE to improve the productivity of home-lab crystallography
Martin Adam, Michael Mrosek, Vernon Smith (Karlsruhe/DE)

P015 Improved home lab productivity without downtime – an old dream comes true
Vernon Smith, Michael Mrosek, Martin Adam (Karlsruhe/DE)

P016 Solving structures with native native SAD on laboratory X-ray sources
Andreas Förster, Clemens Schulze-Briese (Baden-Dättwil/CH)

P017 Shine bright like a diamond – microfocus X-ray sealed tube sources with hybrid diamond anode technology
Jürgen Graf (Geesthacht/DE), Tobias Stürzer, Holger Ott (Karlsruhe/DE)
Paul Radcliffe, Jörg Wiesmann, Carsten Michaelsen (Geesthacht/DE)

P018 Macromolecular neutron diffraction at the FRM II neutron source
Andreas Ostermann, Tobias E. Schrader (Garching/DE)
Michael Monkenbusch, Bernhard Laatsch (Jülich/DE), Philipp Jüttner
Winfried Petry (Garching/DE), Dieter Richter (Jülich/DE)

P019 MX Data collection strategies at EMBL-Hamburg beamlines P13 & P14
Saravanan Panneerselvam, Gleb Bourenkov, Guillaume Pompidor
Johanna Hakanpää, Isabel Bento, Ivars Karpics, Thomas Schneider (Hamburg/DE)

P020 Size and stability analysis in nano-scaled systems
Bastian Arlt (Ostfildern/DE)

P022 Analyzing protein liquid dense clusters – intermediates in the nucleation process: as potential samples for future XFEL experiments
Robin Schubert, Qing-di Cheng, Hsiang-Yu Chung, Shih-Hsuan Chia, Guoqing Chang
Franz X. Kärtner, Markus Perbandt, Christian Betzel (Hamburg/DE)

Bio-Crystallography VI – Protein – nucleic acid complexes

P023 Structural basis of increased Dnmt2 activity by queuine tRNA modification
Sven Johannsson, Piotr Neumann, Alexander Wulf (Göttingen/DE)
Hans-Dieter Gerber (Marburg/DE), Matthias Krull, Ulf Diederichsen
Henning Urlaub, Ralf Ficner (Göttingen/DE)

P024 A conserved structural element in the RNA helicase UPF1 regulates its catalytic activity in an isoform-specific manner
Manjeera Gowravaram (Berlin/DE), Fabien Bonneau (Martinsried/DE)
Vincent Maciej (Berlin/DE), Francesca Fiorini, Joanne Kanaan, Saurabh Raj
Vincent Croquette, Hervé Hir (Paris/FR), Sutapa Chakrabarti (Berlin/DE)

P025 Molecular principles underlying dual RNA specificity in the *Drosophila* SNF protein
Markus C. Wahl, Gert Weber (Berlin/DE), Gregory T. DeKoster (St. Louis, MO/US)
Nicole Holton (Berlin/DE), Kathleen B. Hall (St. Louis, MO/US)

POSTER PRESENTATIONS

Measurements and syntheses under extreme conditions

P026 High pressure lattice dynamics of aragonite and $CaCO_3$ –VII up to 45 GPa
Lkhamsuren Bayarjargal, Chris-Julian Fruhner (Frankfurt a. M./DE), Nadine Schrodt
Björn Winkler (Frankfurt a. M., Wenden-Hünsborn/DE)

P027 High pressure physical properties of lead stannate, Pb_2SnO_4
Wolfgang Morgenroth, Dominik Zimmer, Dominik Spahr, Michał Stękiel
Lkhamsuren Bayarjargal, Björn Winkler (Frankfurt a. M./DE)

P028 Femtosecond diffraction of solid flame reactions at HED at European XFEL
Wolfgang Morgenroth, Lkhamsuren Bayarjargal, Björn Winkler (Frankfurt a. M./DE)
Dmitry Varentsov (Darmstadt/DE), Karen Appel, Ulf Zastrau (Schenefeld/DE)

P029 First evidence of a displacive transformation in $MgSO_4$ H_2O under high pressures
Martin Ende, Johannes Meusburger, Dominik Talla, Ronald Miletich
Manfred Wildner (Vienna/AT)

P030 Hydrogen bonding in natrochalcite under hydrostatic pressure
Martin Ende, Gerald Giester, Ronald Miletich (Vienna/AT)

P031 Synthesis of Co-Cl- and Ni-Cl boracite crystals in hydrothermal solutions
Tatiana Setkova, Vladimir Balitsky, Tatiana Bublikova
Dmitry Khanin (Chernogolovka/RU)

P032 High-pressure behaviour of $SrSO_4$
Dominik Spahr, Michał Stękiel, Lkhamsuren Bayarjargal
Wolfgang Morgenroth (Frankfurt a. M./DE), Victor Milman (Cambridge/GB)
Nadine Schrodt, Björn Winkler (Frankfurt a. M./DE)

P033 High-pressure-high-temperature synthesis, hardness and magnetic properties of the metastable ferromagnet ε -Fe_2MnN
William P. Clark (Stuttgart/DE), Kai Guo (Dresden/DE), Dieter Rau (Stuttgart/DE)
Ulrich Burkhardt, Matej Bobnar, Rodrigo Castillo, Lev Akselrud (Dresden/DE)
Rainer Niewa (Stuttgart/DE), Ulrich Schwarz (Dresden/DE)

New crystal structures

P035 Organic-inorganic hybrid materials from divalent metal cations and expanded N,N'-donor linkers
Mansoureh Zahedi (Tabriz/IR), Ulli Englert (Aachen/DE)

P036 New hybrid electron extraction layer for high-performance bulk heterojunction organic solar cells
Donia Fredj (Mahares/TN)

P037 pinB-$SiMe_2Ph$ – a versatile reagent with diverse structures
Christian Kleeberg (Braunschweig/DE)

P038 $K_7[Fe^{II/III}S_2]_4$ – a new 'reduced' sulfido-ferrate with a commensurate superstructure
Pirmin Stüble, Katharina Köhler, Michael Schwarz, Caroline Röhr (Freiburg i. Br./DE)

P039 New Hg-rich mercurides in the systems K-Hg-In and Rb-Hg-In
Caroline Röhr, Marco Wendorff (Freiburg i. Br./DE)

P040 Synthesis and crystal structure of new alkali-chalcogenido-manganates A_6MnQ_4
Michael Langenmaier, Caroline Röhr (Freiburg i. Br./DE)

P041 Paving the way to new organic-inorganic hybrid perovskites containing derivatives of azobispyridine
Simon Schmitz, Christopher Wallerius, Axel Klein (Cologne/DE)

P042 Functional coordination polymers
Andrzej Kochel (Wroclaw/PL)

P043 Simple and superstructure ternary indium variants of K_2Ga_3
Martha Falk, Caroline Röhr (Freiburg i. Br./DE)

P044 The role of magnesium in zinc-rich ternary phases of the system Ca-Mg-Zn: Systematic experimental, crystallographic and bond theoretical studies
Katharina Köhler, Caroline Röhr (Freiburg i. Br./DE)

P045 Intermediate compounds in $CaREExAl_2\text{-}xO_4$ ($0 \le x \le 2$)
Chimednorov Otgonbayar, Herbert Pöllmann (Halle a. d. S./DE)

POSTER PRESENTATIONS

P046 Reconstruction of individual isomers from disordered average structure
Eugenia Peresypkina, Alexander Virovets (Regensburg/DE), Ivan S. Bushmarinov
Michael G. Medvedev (Moscow/RU), Barbara Krämer, Manfred Scheer (Regensburg/DE)

P047 Layered inorganic-organic hybrid materials – crystal engineering with sodium methanesulfonate and "simple" inorganic halides
Felix Thoelen, Walter Frank (Düsseldorf/DE)

P048 Molecular structures of a pH-dependent, mechanically interlocked switch: organometallic [2]rotaxane vs. organic [3]rotaxane
Alexander Pöthig, Philipp J. Altmann (Munich/DE)

P049 Crystal structure analysis as an essential tool in the characterisation of organometallic compounds – solid state structures of two unusual bismuth-manganese compounds
Claudia Maria Bianga, Walter Frank (Düsseldorf/DE)

P051 Electron-poor ternary representatives of the $BaAl_4$-type structure – a combined crystallographic and bond theoretical study
Carolin Meyer, Matthias Kledt, Caroline Röhr (Freiburg i. Br./DE)

P052 $Sr_4RECl_3[SeO_3]_4$ (*RE* = Y and Yb) – new strontium rare-earth metal(III) chloride oxoselenates(IV) with layer structures
Stefan Greiner, Thomas Schleid (Stuttgart/DE)

P053 The crystal structure of trisodium hexachloroiridate
Martin Etter (Hamburg/DE), Melanie Müller (Duisburg/DE)
Sebastian Bette (Stuttgart/DE)

P054 Higher symmetry at lower temperature – reinvestigation of the historic compound caffeinium triiodide monohydrate
Guido J. Reiss, Martha A. Majewski, Johannes Merkelbach (Düsseldorf/DE)

P055 $Sr_2LnCl_3[SeO_3]_2$ (*Ln* = La — Pr) – strontium lanthanoid(III) chloride oxoselenates(IV) with mixed occupation of the metal positions
Stefan Greiner, Thomas Schleid (Stuttgart/DE)

P056 Cancer treatment by inhibition of nuclear export – crystal structure of a human CRM1-inhibitor complex
Alaa Shaikhqasem, Thomas Monecke, Ralf Ficner (Göttingen/DE)

P057 Structural aspects of the arene solvation of a ternary halide: Comparison of the crystal structures of $[(1,2,4,5\text{-}C_6H_2(CH_3)_4)Ga][AlCl_4]$ and $Ga[AlCl_4]$
Luca Küppers, Walter Frank (Düsseldorf/DE)

P058 Crystal structures of bimetallic molybdenum and tungsten fluoro-alkoxy complexes
Dirk Bockfeld, Celine Bittner, Henrike Ehrhorn, Matthias Tamm (Braunschweig/DE)

P059 $Dy_3O_2Cl[SeO_3]_2$ and $Er_3O_2Cl[SeO_3]_2$ – two non-isotypic lanthanoid oxide chloride oxoselenates(IV)
Sheng-Han Su, Joseph Wontcheu, Thomas Schleid (Stuttgart/DE)

P060 New 2D crystal structures discovered in mixed-valent copper chalcogenide systems
Mihai I. Sturza (Dresden/DE; Argonne, IL/US), Alexander J. E. Rettie, Daniel Bugaris
Fei Han (Argonne, IL/US), Saicharan Aswartham (Dresden/DE)
Duck Young Chung (Argonne, IL/US), Mercouri Kanatzidis (Evanston, Argonne, IL/US)
Bernd Büchner (Dresden/DE)

P061 Single crystals of the new caesium praseodymium selenophosphate $Cs_2PrP_2Se_7$
Beate Schulz, Thomas Schleid (Stuttgart/DE)

P062 Structure varieties of Europium(II) oxoborates – $Eu_2[B_2O_5]$ and EuB_2O_4
Christian Funk, Thomas Schleid (Stuttgart/DE)

P063 Crystal engineering with benzylamines – an inorganic-organic hybrid material containing benzyltrimethylammonium and $[MoOCl_4(H_2O)]$ – anions
Marten Lichte, Felix Thoelen, Walter Frank (Düsseldorf/DE)

P064 $Cs_3Er_7Se_{12}$ and $Cs_3Tm_7Se_{12}$ – two new additions at the far end of the $Cs_3RE_7Se_{12}$ series
Adrian Harald Geyer, Andreas Elbe, Thomas Schleid (Stuttgart/DE)

P065 Redetermination of the crystal structure of tetraethylammonium permanganate at low temperatures with freely refined hydrogen positions
Maurice Conrad, Jörg Bauchert, Thomas Schleid (Stuttgart/DE)

P066 $CsSc_3S_5$ – the first ternary sulfide with $CsEr_3Se_5$-type structure
Constantin Buyer, Dirk D. Zimmermann, Thomas Schleid (Stuttgart/DE)

POSTER PRESENTATIONS

New developments in methods, instrumentation and applications in neutron scattering

P067 FIREPOD – the fine resolution powder diffractometer @ Berlin research reactor BER II
Alexandra Franz, Andreas Hoser, Susan Schorr (Berlin/DE)

Crystallography in nanoscience

P068 Multifunctional nanoparticle superlattices based on engineered protein containers as building blocks
Marcel Lach, Matthias Künzle, Tobias Beck (Aachen/DE)

P069 Synthesis and characterization of rhodium nanoparticles
Mateusz Olejnik, Matthias Epple (Essen/DE)

P070 Synthesis of functionally polymorphic pyroxenes
Dorian Hanaor (Berlin/DE), Mohammed Hussein Assadi (Tsukuba/JP)
Franz Kamutzki, Armando Mandlule, Shyla Basyar (Berlin/DE)

P071 Analysis of Fe stabilized cubic phase $Li7La_3Zr_2O_{12}$ solid electrolytes for solid state Li-ion batteries
Guiying Tian, Frieder Scheiba, Sarapulova Angelina, Zijian Zhao, Andy Fiedler
Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE)

P072 Three dimensional X-ray diffraction imaging of single core-shell-shell nanowires
Arman Davtyan (Siegen/DE), Vncent Favre-Nicolin (Grenoble/FR), Ryan B. Lewis
Hanno Küpers, Lutz Geelhaar (Berlin/DE), Dominik Kriegner (Prague/DE)
Ali Al Hassan, Ullrich Pietsch (Siegen/DE)

Structure-property-relationships

P073 $Cu_2ZnSnSe_4$ – How far does off-stoichiometry go?
Galina Gurieva, Philip Knoll (Berlin/DE), Rafael Ferreira (Berlin/DE; Coimbra/PT)
Susan Schorr (Berlin/DE)

P074 The effect of quenching on the spontaneous electric polarization in relaxor ferroelectric $Sr_{0.52}Ba_{0.48}Nb_2O_6$ (SBN_{52}) and $Ca_{0.28}Ba_{0.72}Nb_2O_6$ (CBN_{28})
Heribert A. Graetsch (Bochum/DE)

P075 Influence of mixed crystal formation on the magnetic properties of thiocyanate coordination Polymers
Carsten Wellm (Kiel/DE, Krakow/PL), Michal Rams (Krakow/DE), Tristan Neumann
Christian Näther (Kiel/DE)

P076 Structural characterization of the $Cu_2ZnGe(S_{1-x}Sex)_4$ solid solution
Sara Niedenzu, Galina Gurieva, Susan Schorr (Berlin/DE)

P077 Structure property relationships in magnetic 1D and 2D $Ni(NCS)_2$ coordination polymers
Aleksej Jochim, Tristan Neumann, Carsten Wellm (Kiel/DE), Michał Rams (Krakow/PL)
Inke Jeß, Christian Näther (Kiel/DE)

P078 Stabilizing the cubic phase of hybrid perovskite $FA_{1-x}MA_xPbI_3$ by incorporation of inorganic atoms
Frederike Lehmann (Berlin, Potsdam/DE), Alexandra Franz, Daniel M. Többens
José Antonio Márquez Prieto, Thomas Unold, Susan Schorr (Berlin/DE)

P079 Structures, thermodynamic relations and magnetism of novel stable and metastable Ni(NCS)2 coordination polymers
Tristan Neumann, Inke Jess (Kiel/DE), Michal Rams (Krakow/PL), Luzia S. Germann
Robert E. Dinnebier (Stuttgart/DE), Christian Näther (Kiel/DE)

P080 Tuning of the intrachain interactions by mixed crystal formation of the anionic ligands in magnetic 1D coordination polymers
Inke Jess, Tristan Neumann (Kiel/DE), Zbigniew Tomkowicz (Krakow/DE)
Michał Rams (Kiel/DE; Krakow/PL), Christian Näther (Kiel/DE)

P081 Structural consequences of synthesis parameters in the semiconductor $ZnGeN_2$
Albina Glibo, Joachim Breternitz, Susan Schorr (Berlin/DE)

P082 Crystal growth, crystal structures, vibrational spectroscopy and optical properties of antimony tartrates of monovalent cations
Ladislav Bohatý, Petra Becker, Peter Held (Cologne/DE), Irena Matulková
Ivana Cisarova, Ivan Nemec (Prague/CZ)

P083 In plane and asymmetric XRD investigation of magnetic thin films
Zoltán Balogh-Michels, Antonia Neels (Dübendorf/CH), Osman ztürk, Baha Sakar
Ali Şems Ahsen (Kocaeli/TR)

P084 The Nature of symmetric and asymmetric liquid crystals based on hydrogen-bonded assemblies
Michael Pfletscher, Sandra Hölscher, Christoph Wölper (Essen/DE)
Markus Mezger (Mainz/DE), Michael Giese (Essen/DE)

POSTER PRESENTATIONS

P086 TomG performs O-methylation in tomaymycin biosynthesis via an on-line tailoring reaction on the NRPS TomA
Jan Pippel (Braunschweig/DE), Alexander von Tesmar
Michael Hoffmann, Antoine Abou Fayad (Braunschweig, Saarbrücken/DE)
Stefan Dausend-Werner (Saarbrücken/DE), Armin Bauer (Frankfurt a. M./DE)
Wulf Blankenfeldt (Braunschweig/DE), Rolf Müller (Saarbrücken, Braunschweig/DE)

P087 Determination of structure-property-relations from single crystal X-ray diffraction data
Tina Weigel, Matthias Zschornak, Thomas Behm, Claudia Funke, Sven Jachalke
Hartmut Stöcker (Freiberg/DE), Tilmann Leisegang (Freiberg/DE; Samara/RU)
Dirk C. Meyer (Freiberg/DE)

P088 Perovskites as potential electrocatalysts for electrochemical oxygen evolution reaction
Seyma Ortatatli, Xiaohui Deng (Mülheim a. d. Ruhr/DE)
Michael Haiduk (Bochum/DE), Harun Tüysüz
Claudia Weidenthaler (Mülheim a. d. Ruhr/DE)

P089 Triclinic pedial sarcosinium hydrogen L-tartrate – crystal growth, pyroelectric and linear optical properties
Petra Becker, Ladislav Bohatý (Cologne/DE)
Lkhamsuren Bayarjargal (Frankfurt a.M./DE), Lionel Andersen (Cologne/DE)

P090 Structure transformation and magnetic properties of iron oxides and hydroxides
Nataliia Dudchenko, Aleksandr Brik, Vitaliy Ponomar (Kyiv/UA)

P092 The thermal expansion behaviour of Mn, Fe, Co and Ni olivines
Peter Schmid-Beurmann, Herbert Kroll, Alexander Sell, Julia Büscher
Robin Dohr (Münster/DE), Armin Kirfel (Bonn/DE)

In-situ methods

P093 *In-situ* crystallisation of sensitive compounds
Christoph Wölper, Stephan Schulz, Dieter Bläser, Stefan Heimann
Benjamin Lyhs (Essen/DE)

P094 *In-situ* synchrotron pair distribution function analysis of amorphous photocatalysts for hydrogen generation
Ezgi Onur Sahin, Gun-hee Moon, Harun Tüysüz (Mülheim a. d. Ruhr/DE)
Candace K. Chan (Tempe, AZ/US), Wolfgang Schmidt
Claudia Weidenthaler (Mülheim a. d. Ruhr/DE)

P095 *In-situ* cryocrystallisation of chiral liquids
Nils Nöthling, Richard Goddard, Christian W. Lehmann (Mülheim a. d. Ruhr/DE)
Rüdiger W. Seidel (Halle a. d. Saale/DE)

P096 *In-situ* analysis of $ZnMn_2O_4$ as High Performance Anode for Lithium-Ion Batteries
Zijian Zhao, Qiang Fu, Angelina Sarapulova, Helmut Ehrenberg
Sonia Dsoke (Eggenstein-Leopoldshafen/DE)

P097 Detecting the structural change and density anomaly in liquid iodides by *in-situ* synchrotron x-ray diffraction and absorption measurements under high pressures
Kazuhiro Fuchizaki (Matsuyama, Kashiwa/JP), Nozomu Hamaya (Tokyo/JP)

P098 Following the effects of micelle expanders on SBA-15 synthesis with *in-situ* SAXS
Francisco Mariano-Neto (Essen/DE; São Paulo/BR), Helena Rasmussen (Aarhus/DK)
Márcia Carvalho de Abreu Fantini, Cristiano Luís Pinto Oliveira (São Paulo/BR)

P099 Low temperature X-ray investigations on silver-based Kesterites
Michael Tovar, Galina Gurieva, Susan Schorr (Berlin/DE)

POSTER PRESENTATIONS

Electron microscopy

P100 *Ab-initio* Calculations of electronic structure of TlInS2
Narmin Ismayilova (Baku/AZ)

P101 Transrotational structure with complicated lattice misorientations revealed by TEM for 2 kinds of spherulites growing in amorphous films
Vladimir Kolosov (Ekaterinburg/RU)

P144 How VPP can make of Cryo-EM an effective tool for drug-design
Max Maletta (Eindhoven/NL)

Experimental electron density

P102 Topological analysis of two [2] catenanes based on Electron Densities from invariom refinements
Peter Luger, Birger Dittrich (Berlin/DE)

P103 Charge density analysis of cobalt(II) phosphate
Helena Keil, Dietmar Stalke, Regine Herbst-Irmer (Göttingen/DE)

P104 Experimental charge density study of alkyllithium compounds
Annika Münch, Dietmar Stalke, Regine Herbst-Irmer (Göttingen/DE), Lena Knauer Carsten Strohmann (Dortmund/DE), Holger Ott (Karlsruhe/DE)

P105 Comparison of different strategies for modelling hydrogen atoms in charge-density analysis
Christian Köhler, Dietmar Stalke, Jens Lübben (Göttingen/DE)
Lennard Krause (Aarhus/DK), Regine Herbst-Irmer (Göttingen/DE)

P106 Halogen bonds involving TFDIB – answers from experimental electron density
Ruimin Wang, Daniel Hartnick, Marius Kremer, Irmgard Karl, Ulli Englert (Aachen/DE)

Spectroscopic methods in crystallography

P107 Substitution and doping in iron pnictides
Michael Merz, Peter Nagel, Meng-Jie Huang, Robert Eder, Thomas Wolf
Stefan Schuppler (Eggenstein-Leopoldshafen/DE)

P108 Application of Raman spectroscopy for identification of anhydrous $CaCl_2$, $KCaCl_3$ and $K_3NaFeCl_6$ in natural inclusions
Svetlana Grishina (Novosibirsk/RU), Peter Kodera (Bratislava/SK)
Lucas Uriarte (Vandoeuvre-lès-Nancy/FR), Alexander Oreshonkov (Krasnoyarsk/RU)
Yana Maximovich (Novosibirsk/RU), Eugenii Roginskii (St. Petersburg/RU)
František imko (Bratislava/SK)

Structurally complex materials

P109 Magnons in the multiferroic phase of cupric oxide
Fabian Ziegler, Steffen Schwesig, Oleg Sobolev, Avishek Maity
Götz Eckold (Göttingen/DE)

P110 Synthesis of alite (impure c3s) & pure c3s, and their structure investigation
Dounia Tlamsamani, Khalid Yamni (Meknès/MA)

P111 The phonon density of states (PDOS) and the crystal growth of deuterated bis-2-phenylethylamine-$CuCl_4$, -$MnCl_4$ ($(PEA)_2CuCl_4$, $(PEA)_2MnCl_4$) and their mixed crystals
Marek Schomber, Holger Gibhardt (Göttingen/DE), Jitae Park (Munich/DE)
In-Hwan Oh (Daejeon/KR), Wiebke Lohstroh (Munich/DE), Götz Eckold (Göttingen/DE)

P112 Jump rate and jump length in a triple well potential
Mehdi Ouahmane, Lehcen Arfa, Lehcen Elarroum (Casablanca/MA)

P113 Cyclic coordination compounds “donuts” and their host-guest-complexes with fullerenes
Christian Göb, Lisa Sturm, Toshimitsu Sato, Iris Oppel (Aachen/DE)

P114 Comparisons of the microstructure from two bivalve shells – *Pinctada martensii* and Anodonta cynea
Jianhan He (Hamburg/DE), Erika Griesshaber, Wolfgang W. Schmahl (Munich/DE)
Ulrich Bismayer (Hamburg/DE)

P115 Diaquabis(1,10-phenanthroline)zinc(II) dinitrate, a modulated structure
Andreas Schönleber (Bayreuth/DE), Seik Weng Ng (Semenyih/MY)

POSTER PRESENTATIONS

Developments in molecular crystallography

P116 Pressure effect on the arene-perfluoroarene interaction
Alexandra Friedrich, Krzysztof Radacki (Würzburg/DE)
Javier Ruiz-Fuertes (Valencia, Santander/ES), Ines E. Collings (Grenoble/FR)
Daniel Sieh, Marder B. Todd (Würzburg/DE)

P117 The new chemical crystallography beamline P24 at PETRA III (PEX-E), DESY
Carsten Paulmann, Martin Tolkiehn, Ulrich Bismayer, Heiko Schulz-Ritter
Andreas Berghäuser (Hamburg/DE)

Characterization of defects in crystalline materials

P118 Radiation-damaged pyrochlore
Ulrich Bismayer, Peter Zietlow (Hamburg/DE), Tobias Beirau (Halle a. d. Saale/DE)
Jochen Schlüter, Carsten Paulmann (Hamburg/DE), Lee A. Groat (Vancouver/CA)

P119 CuGaS2:Mn chalcopyrite as intermediate band absorber material
Julien Marquardt, Sergiu Levcenco, Alexandra Franz, Christiane Stephan-Scherb
Susan Schorr (Berlin/DE)

P120 Extension of X-ray diffraction laminography – a 4D imaging method for the investigation of defect dynamics in crystalline materials
Simon Bode, Daniel Hänschke, Elias Hamann (Eggenstein-Leopoldshafen/DE)
Merve P. Kabukcuoglu (Eggenstein-Leopoldshafen, Freiburg i. Br./DE)
Simon Haaga (Freiburg i. Br., Eggenstein-Leopoldshafen/DE)
Lukas Helfen (Grenoble/FR; Eggenstein-Leopoldshafen/DE)
Andreas N. Danilewsky (Freiburg i. Br./DE)
Tilo Baumbach (Eggenstein-Leopoldshafen/DE)

P121 Defect and strain characterization of 4H-SiC
Melissa Roder (Freiburg i. Br./DE), Peter Wellmann (Erlangen/DE)
Andreas N. Danilewsky (Freiburg i. Br./DE)

P122 3d imaging of crystalline defects in highly absorbing semiconductor materials with X-Ray diffraction laminography (XDL) on the example of GaAs wafers
Simon Haaga (Freiburg i. Br., Karlsruhe/DE), Daniel Hänschke
Elias Hamann (Karlsruhe/DE), Merve P. Kabukcuoglu (Freiburg i. Br., Karlsruhe/DE)
Simon Bode (Karlsruhe/DE), Lukas Helfen (Karlsruhe/DE; Grenoble/FR)
Tilo Baumbach (Karlsruhe/DE), Andreas N. Danilewsky (Freiburg i. Br./DE)

P123 4D Investigation of the dislocation propagation and their interaction depending on thermal stress by means of X-ray diffraction laminography
Merve P. Kabukcuoglu (Freiburg i. Br., Eggenstein-Leopoldshafen/DE)
Daniel Hänschke, Elias Hamann, Simon Bode (Eggenstein-Leopoldshafen/DE)
Simon Haaga (Eggenstein-Leopoldshafen, Freiburg i. Br./DE)
Lukas Helfen (Eggenstein-Leopoldshafen/DE; Grenoble/FR)
Tilo Baumbach (Eggenstein-Leopoldshafen/DE), Andreas N. Danilewsky (Freiburg i. Br./DE)

Powder diffraction/PDF

P124 Structural effects of Ni-incorporation into malachite
Justus Heese, Andreas Hüttner, Malte Behrens (Essen/DE)

P125 Crystal structure of $La_{0.7}Ca_{0.3}Mn_{0.5}Fe_{0.5}O_3$
Sakin Jabarov (Dubna/RU; Baku/AZ)

P126 *In-situ* X-ray diffraction during the crystallization of sulfidic solid electrolytes
Helmut Ehrenberg, Heike Stöffler, Murat Yavuz, Sylvio Indris (Eggenstein-Leopoldshafen/DE)

P128 Structure determination of cesium heteropolyacids with Keggin anions: $Cs_{2.3}H_{0.7}[PMo_{12}O_{40}]$
Kathrin Hofmann, Barbara Albert, Jörg Steffan, Nadine Dürr, Krasimir Kantchev
Herbert Vogel (Darmstadt/DE)

P129 High temperature XRD and PDF studies of Li-argyrodite Li_6PS_5Cl
Ruth Giesecke (Renningen, Karlsruhe/DE), Murat Yavuz, Sylvio Indris (Karlsruhe/DE)
Thomas Hupfer (Renningen/DE), Helmut Ehrenberg (Karlsruhe/DE)

POSTER PRESENTATIONS

Other topics

P130 Comparison of structures applying the tools available in the Bilbao Crystallographic Server
Gemma de la Flor (Leioa/ES; Hamburg/DE), Danel Orobengoa (Leioa/ES)
Emre Tasci (Ankara/TR), Juan Manuel Perez-Mato, Mois I. Aroyo (Leioa/ES)

P131 Study and characterization of dispersion aggregates of platinum in the active surface of the electrodes of the proton exchange membrane fuel cell by X-ray diffraction
Zineb Hbilate, Youssef Naimi, Driss Takky (Casablanca/MA)

P132 Elaboration and electrical properties of metal phosphate glasses
Fatima ezzahraa Dardar (Casablanca/MA), Michael Gross (Winston Salem, NC/US)
Saida Krimi (Casablanca/MA), Michel Couzi (Bordeaux/FR)
Abdessadek Lachgar (Winston Salem, NC/US), Abdelaziz El Jazouli (Casablanca/MA)

P133 Directional solidification and characterization of Fe – 4.25%C eutectic alloy
Małgorzata Trepczynska-Lent (Bydgoszcz/PL)

P134 The discovery of a molecule-like (without nucleus) structure of atoms
Georgi Shpenkov (Bielsko-Biala/PL)

P135 X-ray optics for optimized performance between 10 eV and 40 keV
Paul Ulrich Pennartz (Eschweiler/DE)

P136 Pump-probe setups for the ultrafast measurements of optical properties in ZnSe
Jav Davaasambuu, Ts. Baatarchuluun, P. Munkhbaatar, Ts. Khos-Ochir, N. Tuvjargal
G. Munkhbayar (Ulaanbaatar/MN), O. Tegus (Hohhot/CN)

P137 The Crystal Structure of *β*-Boron
Claudio Eisele (Bayreuth/DE), Swastik Mondal (Kolkata/IN)
Somnath Dey (Bayreuth/DE), Irina Chuvashova (Villetaneuse/FR)
Carsten Paulmann (Hamburg/DE), Sander van Smaalen (Bayreuth/DE)

P138 Systematic errors in least-squares refinements against diffraction data
Julian Henn (Bayreuth/DE)

P139 Valorization of waste from the wood industry (sawdust) and their use as adsorbent material – physicochemical characterization, modeling and optimization adsorption using response surface methodology (RSM)
Salamat Asmaa (Settat/MA)

P140 The crystal structure transformation In $La_{0.8}K_{0.6}Ca_{1.6}Mn_2O_7$ double layered perovskite manganite
C. Gökhan Nlü (Denizli/TR), Atakan Tekgül (Bursa/TR), Mehmet Acet
Michael Farle (Duisburg/DE)

P141 Crystallography in the context of the energy transition – the battery of tomorrow
Tilmann Leisegang, Falk Meutzner (Freiberg/DE; Samara/RU)
Tina Nestler (Freiberg/DE), Matthias Zschornak (Dresden/DE)
Robert Schmid (Freiberg/DE), Artem A. Kabanov, Roman A. Eremin
Vladislav A. Blatov (Samara/RU), Dirk C. Meyer (Freiberg/DE)

P142 The generation of growth dislocations by inclusions and growth-face damages: an experimental study
Helmut Klapper (Bonn, Aachen/DE), G. Neuroth (Bonn/DE)

P143 Evaluation of the removal capacity of waste water by the adsorption phenomenon on a rock of moroccan origin
Amira Am, M'hammed El Kouali, Mohammed Talbi
Fatima Ouzidan (Casablanca/MA)

INDEX OF PLENARY SPEAKERS, PRESENTING AUTHORS AND CHAIRS

INDEX OF PLENARY SPEAKERS , PRESENTING AUTHORS AND CHAIRS

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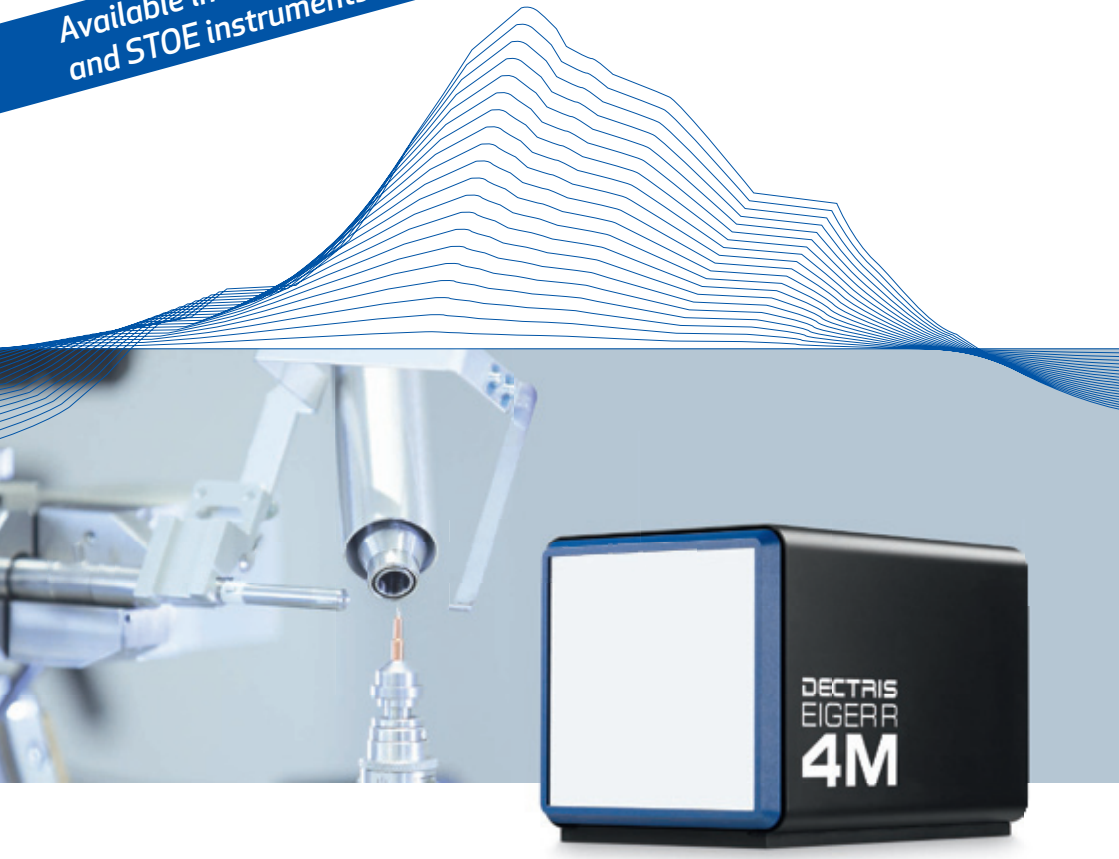

"Having excellent data collection equipment in the lab is crucial when each experiment yields information on what should follow. This practice is not feasible on a synchrotron where we have access only every two to three weeks." *Alexander Wlodawer, National Cancer Institute, USA*

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