



3rd ANNUAL MEETING
of the GERMAN
CRYSTALLOGRAPHIC
SOCIETY (DGK)

PROGRAMME

27–30 MARCH 2023
FRANKFURT am MAIN

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Max-von-Laue-Straße 9 | 60439 Frankfurt am Main (Germany)

Date

27–30 March 2023

Conference website

www.dgk-conference.de

Organiser

German Crystallographic Society (DGK)



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Institute for pharmaceutical chemistry, Goethe University, Frankfurt am Main, Germany

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Institute of Inorganic and Analytical Chemistry, Goethe University, Frankfurt am Main, Germany

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Crystallography and mineralogy, Goethe University, Frankfurt am Main, Germany

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Dear colleagues,

It is an honor and a great pleasure to invite you on behalf of the organizing committee to the 31st Annual Conference of the German Crystallographic Society (Deutsche Gesellschaft für Kristallographie, DGK), which will take place at the Riedberg Campus of the Goethe University of Frankfurt am Main.

We believe that after the long break caused by the Corona pandemic the crystallographic community will be eager to meet again in order to reconnect and to foster new interactions and collaboration. We closely collaborated with the working groups of the DGK to organize a balanced program that covers all areas of crystallography. The meeting this year will comprise 20 microsymposia, two poster sessions and six plenary lectures.

We are particularly glad that we have been able to attract a number of distinguished scientists that have accepted our invitation for a plenary lecture. We hope that you will all enjoy this meeting and we particularly encourage the young crystallographers to participate in the scientific discussions.

Kind regards

Prof. Dr. Stefan Knapp
Goethe University, Institute of Pharmaceutical Chemistry

Prof. Dr. Martin U. Schmidt
Goethe University, Institute of Inorganic and Analytical Chemistry

Prof. Dr. Björn Winkler
Goethe University, Institute of Geosciences

PROGRAMME OVERVIEW | MONDAY, 27 MARCH

Lecture hall OSZ H3	Lecture hall OSZ H4	Lecture hall OSZ H5	Lecture hall OSZ H6	Seminar room OSZ S4
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09.00–12.30
DGK Board meeting
p. 10

13.00–13.30			
Opening			
13.30–14.30			
Plenary lecture I Hartmut Michel p. 10			
14.30–14.45 Coffee break and industrial exhibition			
14.45–16.15			
Organic molecules and coordination compounds p. 10	Crystallography in materials sciences I p. 11	Crystal physics p. 12	Bio-crystallogra- phy II: Signaling, macromolecular interactions and new structures p. 13
16.15–16.45 Coffee break and industrial exhibition			
16.45–17.45			
Plenary lecture II Yasar Krysiak p. 14			
17.45–18.15			
Special lecture: Max-von-Laue Award p. 14			
18.15–19.15			
DGK Honour evening p. 14			
19.15–20.45			
Welcome reception at the Industrial exhibition p. 50			

PROGRAMME OVERVIEW | TUESDAY, 28 MARCH

Lecture hall OSZ H3	Lecture hall OSZ H4	Lecture hall OSZ H5	Lecture hall OSZ H6
09.00–10.30			
Bio-crystallography I: Hit finding and design of small molecule inhibitors p. 15	Instrumentation and technological development p. 16	Micro- and nano-crystalline materials (powder diffraction, disordered material) I p. 17	
10.30–11.00 Coffee break and industrial exhibition			
11.00–12.00			
Plenary lecture III Elena Bykova p. 17			
12.00–13.30			
DGK General assembly p. 17	12.30–13.30 Bruker AXS GmbH p. 18	12.30–13.30 Lunch break	
13.30–13.45			
Special lecture IUCR 2029 p. 18			
13.45–14.15 Coffee break and industrial exhibition			
14.15–15.15			
Plenary lecture IV Juan Manuel García-Ruiz p. 18			
15.15–16.45			
Bio-crystallography III: New structures and mechanisms p. 19	Extreme/non-ambient and high-pressure conditions I p. 20	Crystallography in art and heritage + Teaching p. 21	Young crystallographers: Lightning talks p.21
16.45–18.45			
Poster session I p. 34			
18.45–20.15			
Get together Young crystallographers p. 51			

PROGRAMME OVERVIEW | WEDNESDAY, 29 MARCH

Lecture hall OSZ H3	Lecture hall OSZ H4	Lecture hall OSZ H5	Lecture hall OSZ H6
09.00–10.30			
Bio-crystallography IV: Structure-based design p. 23	Complex, aperiodic and disordered structures p. 24	Extreme/non-ambient and high-pressure conditions II p. 25	Computational methods p. 26
10.30–11.00 Coffee break and industrial exhibition			
11.00–12.00			
Plenary lecture V Jordi Benet-Buchholz p. 27			
12.00–12.30 Coffee break and industrial exhibition			
12.30–13.30			
Rigaku Europe SE p. 27	12.30–13.30 Lunch break		
13.30–14.30			
Plenary lecture VI Daren Fearon p. 27			
14.30–16.00			
Bio-Crystallography V: Synchrotrons and new technologies p. 28	Inorganic crystal structures I p. 29	Theoretical crystallography p. 30	Micro- and nano- crystalline materials (powder diffraction, disordered material) II p. 31
16.00–18.00			
Poster session II p. 43			
19.00–23.00			
Social evening at Schuch's Restaurant p. 50			

PROGRAMME OVERVIEW | THURSDAY, 30 MARCH

Lecture hall OSZ H4	Lecture hall OSZ H5	Seminar room
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09.00–10.00	
Plenary lecture VII Julia Dshemuchadse p. 32	
10.00–10.30 Coffee break and industrial exhibition	
10.30–12.00	
Electron crystallography and microscopy p. 32	Crystallography in materials sciences II p. 33
12.00–12.30	
Closing	

13.30–15.45
Chemical crystallography – Joint symposium of DGK and GDCh p. 33

Sessions	DGK Honour evening
Poster session	DGK General assembly
Plenary lecture	Industrial symposium
Meetings	Social programme

09.00–12.30

DGK Board meeting

Seminar room – OSZ S4

13.00–13.30

Opening ceremony

Lecture hall – OSZ H3

13.30–14.30

Plenary lecture I

Lecture hall – OSZ H3

Chair

Stefan Knapp (Frankfurt am Main/DE)

13.30

Photosynthesis and Cellular Respiration – Structures and Conclusions

PT-1

Hartmut Michel (Frankfurt am Main/DE)

14.45–16.15

Organic molecules and coordination compounds

Lecture hall – OSZ H3

Chairs

Beatrice Cula (Berlin/DE), Alexander Pöthig (Garching/DE)

14.45

OP-001

Structure determination from unindexed powder data?

The challenging case of leuko-pterine

Martin U. Schmidt (Frankfurt am Main/DE)

Federica Bravetti (Frankfurt am Main/DE, Turin/IT), Lukas Tapmeyer

Kathrin Skorodumov, Edith Alig, Stefan Habermehl

Robert Hühn (Frankfurt am Main/DE), Simone Bordignon, Angelo Galli

Carlo Nervi, Michele R. Chierotti (Turin/IT)

15.00

OP-002

High-quality X-ray powder diffraction data for structure determination

Maciej Grzywa (Neu-Isenburg/DE)

15.15

OP-003

The link between structure and properties for future targeted design of Luminescent complexes

Laura Christina Folkers (Darmstadt/DE), Claus Feldmann (Karlsruhe/DE)

15.30

OP-004

Irradiation by X-Rays heals and kills the crystal of giant supramolecule

Eugenia Peresypkina (Regensburg/DE), Berthold Stöger (Vienna/AT)

Alexander Virovets (Frankfurt am Main/DE)

15.45

OP-005

Heterobimetallic Coordination Polymers with

Dithiocarbamatocarboxylate (DTCC) Ligands

Phil Liebing (Jena/DE)

16.00

OP-006

How can robots help to crystallize small molecules?

Bernhard Spingler (Zurich/CH)

14.45–16.15

Lecture hall – OSZ H4

Chairs

Crystallography in materials sciences I

Claudia Weidenthaler (Mülheim an der Ruhr/DE)

Thorsten M. Gesing (Bremen/DE)

14.45

OP-007

From stannite- to wurtz-stannite-type structure in the

$\text{Cu}_2\text{Mn}(\text{Ge}_x\text{Sn}_{1-x})\text{S}_4$ solid solution

Susan Schorr (Berlin/DE), David Matzdorff (Berlin/DE)

Maxim Avdeev (Sydney/AU), Galina Gurieva

15.00

OP-008

Systematic study of mechanochemically synthesized perovskite materials

Tobias Rathmann, Sabri Ufuk Arisan

Hilke Petersen (Mülheim an der Ruhr/DE), Martin Etter (Hamburg/DE)

Claudia Weidenthaler (Mülheim an der Ruhr/DE)

15.15

OP-009

NaSICONs: crystal chemistry and properties

Maxim Avdeev (Lucas Heights/AU)

15.30

OP-010

Does the Solvent Matter? – Influence of the solvent in hybrid halide perovskites precursor solution

Ana Palacios Saura, Joachim Breternitz, Armin Hoell

Susan Schorr (Berlin/DE)

15.45

OP-011

Synergic effects of various transition metal cations in cubic anti-perovskites: Structural and electrochemical aspects

Mikhail Gorbunov, Daria Mikhailova (Dresden/DE)

16.00

OP-012

Structural changes in lanthanide bearing monazite under swift heavy ion irradiation

Julien Marquardt (Frankfurt am Main/DE), Theresa Lender (Aachen/DE)

Lkhamsuren Bayarjargal, Eiken Haussühl (Frankfurt am Main/DE)

Christina Trautmann (Darmstadt/DE), Lars Peters (Aachen/DE)

Björn Winkler (Frankfurt am Main/DE)

14.45–16.15

Crystal physics

Lecture hall – OSZ H5

Chairs

Eiken Haussühl (Frankfurt/DE), Sergio Speziale (Potsdam/DE)

14.45

OP-013

Symmetry protected 1D chains in mixed-valence iron oxides
Denis Vasiukov (Lund/SE), Ghanashyam Khanal (Piscataway, NJ/US)
Ilya Kупenko (Münster/DE), Georgios Aprilis (Grenoble/FR)
Xiang Li (Münster/DE), Sergey Ovsyannikov
Stella Chariton (Bayreuth/DE), Valerio Cerantola (Grenoble/FR)
Vasily Potapkin (Bayreuth/DE), Aleksandr Chumakov (Grenoble/FR)
Leonid Dubrovinsky (Bayreuth/DE), Kristjan Haule (Piscataway, NJ/US)
Elizabeth Blackburn (Lund/SE)

15.07

OP-014

Phase transition and twinning in flexible single crystals of caffeine
cocrystal solvate

Somnath Dey, Theresa Lender (Aachen/DE)

Carsten Paulmann (Hamburg/DE), Lars Peters (Aachen/DE)

15.29

OP-015

$\text{Li}(\text{Nb,Ta})\text{O}_3$ – phase diagram and Curie temperature of solid solution
single crystals

Steffen Ganschow, Detlef Klimm, Umar Bashir, Mario Brützm

Klaus Böttcher (Berlin/DE), Felix Bernhardt, Simone Sanna (Gießen/DE)

Matthias Bickermann (Berlin/DE)

15.51

OP-016

Vibrational circular dichroism of crystals: The interplay of symmetry and
chirality

Sascha Jähnigen (Paris/FR)

14.45–16.15

Lecture hall – OSZ H6

Chair

Bio-crystallography II: Signaling, macromolecular interactions and new structures

Robert Tampé (Frankfurt am Main/DE)

14.45

OP-017

Structural and functional characterization of the eukaryotic chaperone trigger factor

Yvonne Carius (Homburg/DE), Fabian Ries

Felix Willmund (Kaiserlautern/DE), C. Roy D. Lancaster (Homburg/DE)

15.03

OP-018

Crystal structure of a transient MHC I–tapasin–ERp57 editing complex defines chaperone promiscuity in the endoplasmic reticulum

Ines Müller, Christian Winter, Christoph Thomas (Frankfurt am Main/DE)

Robbert Spaapen (Amsterdam/NL), Simon Trowitzsch

Robert Tampé (Frankfurt am Main/DE)

15.21

OP-019

Turning peptides into pyrroloindoline alkaloids: a closer look at crocagin biosynthesis

Sebastian Adam (Saarbrücken/DE), Dazhong Zheng (Glasgow/GB)

Andreas Klein, Carsten Volz (Saarbrücken/DE)

William Mullen (Glasgow/GB), Sally Shirran (St Andrews/GB)

Brian Smith (Glasgow/GB), Olga Kalinina, Rolf Müller (Saarbrücken/DE)

Jesko-Alexander Koehnke (Glasgow/GB)

15.39

OP-020

Pharmacological targeting of the LRRK pathway – the kinase domains and beyond

Sebastian Mathea (Frankfurt am Main/DE)

15.57

OP-021

AI usage in Structural Biology

Andrea Thorn (Hamburg/DE)

16.45–17.45

Lecture hall – OSZ H3

Chair

Plenary lecture II

Reinhard Neder (Erlangen/DE)

16.45

PT-2

Electron Crystallography in the Spotlight of Materials Science

Yasar Krysiak (Hannover/DE)

17.45–18.15

Lecture hall – OSZ H3

Special lecture laureate – Max-von-Laue Award 2023

18.15–19.15

Lecture hall – OSZ H3

DGK Honour evening

19.15–20.45

Foyer

Welcome reception (see page 50)

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09.00–10.30

Lecture hall – OSZ H3

Chairs

Bio-crystallography I: Hit finding and design of small molecule inhibitors

Manfred S. Weiss (Berlin/DE), Stefan Knapp (Frankfurt am Main/DE)

09.00

OP-022

Crystallographic fragment screening: Efficient access to new lead in drug discovery

Gerhard Klebe (Marburg/DE)

09.30

OP-023

How to successfully conduct crystallographic fragment screening at BESSY II

Laila S. Benz, Jan Wollenhaupt, Tatjana Barthel (Berlin/DE)

Elmir Jagudin (Lund/SE), Dirk Wallacher, Thomas Hauss

Thomas Crosskey, Frank Lennartz, J. H. William Scanlan (Berlin/DE)

Andreas Heine (Marburg/DE), Tobias Krojer (Lund/SE), Uwe Mueller

Manfred S. Weiss (Berlin/DE)

09.50

OP-024

DESY's new High-Throughput screening beamline HiPhaX

Wiebke Ewert, Sebastian Günther, Patrick Reinke, Sven Falke

Julia Lieske, Lars Gumprecht, Jan Meyer, Pontus Fischer

Alke Meents (Hamburg/DE)

10.05

OP-025

Torsion angles to map and visualize the conformational space of a protein

Helen Ginn (Didcot/GB)

10.10

OP-026

Fragment-based design of mycobacterial thioredoxin reductase inhibitors: From a fragment screening to novel inhibitors

Friederike Theresa Füsser, Philipp Otten (Münster/DE)

Jan Wollenhaupt, Manfred S. Weiss (Berlin/DE), Anna Junker

Oliver Koch, Daniel Kümmel (Münster/DE)

09.00–10.30

Lecture hall – OSZ H4

Chairs

Instrumentation and technological development

Thomas Hartmann (Frankfurt am Main/DE), Arnt Kern (Karlsruhe/DE)

09.00

OP-027

P24 Beamline: A High-Performance beamline for small molecule chemical crystallography at DESY

Leila Noohinejad, Carsten Paulmann, Martin Tolkiehn (Hamburg/DE)

09.15

OP-028

Diamond hybrid anodes and high-brightness cathodes: An efficient combination for microfocus X-Ray sealed tubes with very high intensities at low power

Jürgen Graf (Geesthacht/DE), Tobias Stürzer, Anna Lübben
Roger Durst (Karlsruhe/DE), Kaan Atak, Paul Radcliffe
Carsten Michaelsen (Geesthacht/DE)

09.30

OP-029

Instrumentation for time-resolved synchrotron X-ray diffraction studies of adsorption-induced switching in crystalline nanoporous solids

Volodymyr Bon (Dresden/DE), Azat Khadiev
Dmitri Novikov (Hamburg/DE), Stefan Kaskel (Dresden/DE)

09.45

OP-030

Science case and concepts of a macromolecular diffractometer for the High Brilliance Neutron Source (HBS)

Zhanwen Ma, Klaus Lieutenant, Jörg Voigt (Jülich/DE)
Tobias E. Schrader (Garching/DE), Thomas Gutberlet
Thomas Brückel (Jülich/DE)

10.00

OP-031

Growth of good quality bulk size trans-Stilbene single crystal for Neutron and gamma detection applications

Rajesh Paulraj, Mohamad Asikali, Lizbeth Alex (Chennai/IN)
Mohit Tyagi (Mumbai/IN), Ramasamy Perumal (Chennai/IN)

10.15

OP-032

Synchrotron will help you: from subtle diffuse scattering to giant supramolecules

Alexander Virovets (Frankfurt am Main/DE)
Eugenia Peresyphkina (Regensburg/DE), Berthold Stöger (Vienna/AT)
Manfred Scheer (Regensburg/DE)

09.00–10.30

Lecture hall – OSZ H5

Chairs

Micro- and nano-crystalline materials (powder diffraction, disordered material) I

Robert E. Dinnebier (Stuttgart/DE), Jürgen Horbach (Düsseldorf/DE)
Ulrich Fotheringham (Mainz/DE)

09.00

OP-033

Democratizing Quality: High Throughput PXRD Total Scattering @
Bernd Hinrichsen (Ludwigshafen/DE)

09.30

OP-034

Microstructural insights into the ordering process of the novel cubic polymorph of low-temperature disordered $\text{Cu}_2\text{ZnSnS}_4$
Sebastian Bette (Stuttgart/DE), Eleonora Isotta
Binayak Mukharjee (Trento/IT), Robert E. Dinnebier (Stuttgart/DE)
Paolo Scardi (Trento/IT)

10.00

OP-035

Local structure evolution of amorphous sodium tantalate prepared by a sol-gel method investigated by *in situ* crystallization studies
Ezgi Onur Sahin (Mülheim an der Ruhr/DE), Siyuan Zhang
Christina Scheu (Düsseldorf/DE)
Claudia Weidenthaler (Mülheim an der Ruhr/DE)

10.15

OP-036

Finding a measure for the quality of pair distribution functions from in-house total scattering data
Konrad Krämer, Thorsten M. Gesing, Lars Robben (Bremen/DE)

11.00–12.00

Lecture hall – OSZ H3

Chair

Plenary lecture III

Björn Winkler (Frankfurt am Main/DE)

11.00

PT-3

High Pressure Chemical Crystallography of Geo- and Technologically Important Materials
Elena Bykova (Bayreuth/DE)

12.00–13.30

Lecture hall – OSZ H3

DGK General assembly

SCIENTIFIC PROGRAMME | TUESDAY, 28 MARCH

12.30–13.30

Lecture hall – OSZ H4

Bruker AXS GmbH – Lunchtime seminar:
Challenging samples – new high efficiency tools

12.30

Pair-Distribution-Function Generation and Refinement in TOPAS
Arnt Kern (Karlsruhe/DE)

12.50

How to reduce electrical power requirements for high-intensity X-ray sources?
Jürgen Graf (Geesthacht/DE)

13.10

New solutions for high energy radiation studies
Tobias Stürzer (Karlsruhe/DE)

13.30–13.45

Lecture hall – OSZ H3

Special lecture

13.30

Informational event on IUCR 2029
Manfred S. Weiss (Berlin/DE)

14.15–15.15

Lecture hall – OSZ H3
Chairs

Plenary lecture IV

Ulrich Schwarz (Dresden/DE), Wulf Depmeier (Kiel/DE)

14.15

PT-4

Exploring the interface of crystals with life, art and mind: a tale of interdisciplinarity
Juan Manuel García-Ruiz (Armillá/ES)

15.15–16.45

Lecture hall – OSZ H3

Chair

Bio-crystallography III: New structures and mechanisms

Wulf Blankenfeldt (Braunschweig/DE)

15.15

OP-037

Characterization of biohybrid superlattices with single crystal diffraction and small-angle X-ray scattering

Tobias Beck (Hamburg/DE)

15.30

OP-038

Structure and Assembly of the Proline Reductase Complex from

Clostridioides difficile

Christian Behlendorf, Wulf Blankenfeldt (Braunschweig/DE)

15.45

OP-039

Virulence factors of *Pseudomonas aeruginosa* – The Phospholipases

Nishika Sabharwal, Ge Yang, Michele Lunelli, Udom Sae-Ueng

Joerg Labhan, Michael Kolbe (Hamburg/DE)

16.00

OP-040

Structural characterization of a cyclic oligonucleotide activated and CRISPR protease triggered antiviral signaling cascade

Niels Schneberger (Bonn/DE), Haotian Chi (St Andrews/GB)

Katja Blumenstock, Stella Arau Jakubzik, Jonas Moecking (Bonn/DE)

Stefano Da Vela (Hamburg/DE), Jonathan Schmid-Burgk (Bonn/DE)

Dmitri Svergun (Hamburg/DE), Matthias Geyer (Bonn/DE)

Malcolm F. White (St Andrews/GB), Christophe Rouillon

Gregor Hagelueken (Bonn/DE)

16.15

OP-041

Structure, dynamics and allosteric modulation of the caseinolytic protease P from *Staphylococcus epidermidis*

Bruno Alves França, Vasundara Srinivasan, Holger Rohde

Christian Betzel (Hamburg/DE)

16.30

OP-042

Sustainable use of metabolites in glutamine amidotransferases multienzyme complexes

Sihyun Sung (Hamburg/DE), Franziska Funke, Sandra Schlee

Jan Philip Wurm, Remco Sprangers, Reinhard Sterner (Regensburg/DE)

Matthias Wilmanns (Hamburg/DE)

15.15–16.45

Lecture hall – OSZ H4

Chairs

Extreme/non-ambient and high-pressure conditions I

Lkhamsuren Bayarjargal (Frankfurt am Main/DE)

Anna Pakhomova (Grenoble/FR)

15.15

OP-043

High pressure chemical crystallography: From mineral physics to material sciences

Leonid Dubrovinsky, Natalia Dubrovinskaia (Bayreuth/DE)

15.45

OP-044

Lawsonite's phase diagram: *In-situ* HP, HT diffraction study

Dmitrii Druzhbin (Grenoble/FR), Anja Rosenthal (Grenoble/FR,

Canberra/AU), Wilson Crichton (Grenoble/FR)

16.00

OP-045

The effect of Al on the post-stishovite transition of H₂O-bearing stishovite: Insights from in-situ XRD and ultrasonic interferometry

Anja Rosenthal (Grenoble/FR, Canberra/AU)

Wilson Crichton (Grenoble/FR), Andrew Thomson

John Brodholt (London/GB), Dmitrii Druzhbin (Grenoble/FR)

Robert Myhill (Bristol/GB), Rong Huang (London/GB)

16.15

OP-046

Pressure-induced solid-state amorphization of SnI₄ revisited

Kazuhiro Fuchizaki (Matsuyama/JP)

16.30

OP-047

Swift heavy ion irradiation of nano-structured bismuth pressurized in diamond anvil cells

Christopher Schroeck (Frankfurt am Main, Darmstadt/DE)

Ioannis Tzifas (Darmstadt/DE), Lkhamsuren Bayarjargal (Frankfurt

am Main/DE), Kay-Obbe Voss, Ina Schubert

Michael Wagner (Darmstadt/DE), Wilfried Sigle (Stuttgart/DE)

Isabel Armstrong-Cowell, Maria-Eugenia Toimil-Molares

Christina Trautmann (Darmstadt/DE)

Björn Winkler (Frankfurt am Main/DE)

15.15–16.45

Lecture hall – OSZ H5

Chairs

Crystallography in art and heritage + Teaching

Reinhard Neder (Erlangen /DE), Wulf Depmeier (Kiel/DE)

15.15

OP-048

Teaching crystallographic symmetry online

Mois I. Aroyo (Leioa/ES), Eli Kroumova (Bilbao/ES)

Gemma de la Flor (Karlsruhe/DE)

15.45

OP-049

X-ray powder diffraction in education

Robert E. Dinnebier (Stuttgart/DE), Paolo Scardi (Trento/IT)

16.15

OP-050

Life history reconstruction from tooth enamel of the medieval population in lower Saxony

Jana Storsberg, Kateryna Loza (Essen/DE), Immo Heske (Göttingen/DE)

Matthias Eppe (Essen/DE)

16.30

OP-051

Structural features of traditional background less ornaments of near East and Central Asia. Modern tessellations by Imamaddin Amiraslan Imamaddin Amiraslanov (Baku/AZ)

15.15–16.45

Lecture hall – OSZ H6

Chairs

Young crystallographers: Lightning talks

Constantin Buyer (Stuttgart/DE), Jakob Möbs (Marburg/DE)

15.15

LT-01

Towards an understanding of the OAS-Based innate immune signaling: The role of the positively charged residues in the product release channel

Pavel Kats, Xiaoyi Zhou, Jannik Wiebe, Ole Zeymer, Jan Lohöfener

Nicola Steinke, Petra Baruch (Hannover/DE)

Rune Hartmann (Aarhus/DK), Dietmar J. Manstein

Roman Fedorov (Hannover/DE)

15.21

LT-02

Mono- and heterometallic REE heptafluorobutyrate as single-source precursors for NaLnF₄ thin film deposition

Artem Shevchenko (Stuttgart/DE), Daria Blinnikova (Moscow/RU)

Sebastian Bette (Stuttgart/DE), Andrei Anosov

Dmitry Tsybarenko (Moscow/RU)

15.27

LT-03

High-pressure synthesis of ternary nitrides in Na-W-N system

Natalia Martynova (Cologne/DE), Elena Bykova (Bayreuth/DE)

Timofey Fedotenko (Hamburg/DE), Leonid Dubrovinsky (Bayreuth/DE)

Maxim Bykov (Cologne/DE)

- 15.33
LT-04 Low-Temperature Measurement of the Unexpected Hydrate
 $\text{Cs}_2[\text{B}_{12}\text{H}_{12}] \cdot 2 \text{H}_2\text{O}$
Rouzbeh Aghaei Hakkak, Thomas Schleid (Stuttgart/DE)
- 15.39
LT-05 The Heaviest Lanthanoid-Containing Silver Thiophosphate: $\text{Ag}_3\text{Lu}[\text{PS}_4]_2$
Pia Lena Lange, Thomas Schleid (Stuttgart/DE)
- 15.45
LT-06 Novel binary, ternary and quaternary phases in the Bi-Mn-Pt-I system
Maria Herz, Michael Ruck (Dresden, Würzburg/DE)
- 15.51
LT-07 Survey of zirconium-containing NaSICON-type solid-state Li^+ ion
conductors with the aim of increasing reduction stability by partial
cation substitution
Asmaa Loutati (Jülich/DE)
- 15.57
LT-08 Upgrading the High-Energy Beamline P21.1 at PETRA III (DESY)
Katharina Köhler (Frankfurt am Main/DE), Ann-Christin Dippel
Martin von Zimmermann (Hamburg/DE)
Alessandro Mirone (Grenoble/FR)
Björn Winkler (Frankfurt am Main/DE)
- 16.03
LT-09 Crystalline sponge method for pharmaceutically active ingredients:
A chemical space analysis
Carolina von Essen (Darmstadt/DE)
- 16.09
LT-10 Coordination-Driven insertion of a guest molecule in the pore of a
Copper(I)-Based Metallocavitand
Thomas Pickl, Markus Anneser, Alexander Pöthig (Garching/DE)
- 16.15
LT-11 Refinement of anomalous dispersion correction parameters in X-ray
single-crystal structure determination
Florian Meurer (Regensburg/DE)
- 16.30
LT-12 Hydrothermal Synthesis of Anisotropic Ferrite Microparticles
Luisa Wartner (Hamburg /DE)

18.45–20.15 Get together Young crystallographers (see page 51)

Lecture hall – OSZ H4

09.00–10.30

Lecture hall – OSZ H3

Chairs

Bio-crystallography IV: Structure-based design

Sandra Jacobs (Basel/CH), Martina Schaefer (Berlin/DE)

09.00

OP-052

Structural characterization of WDR5-degrader interfaces and its implications for optimal PROTAC design

Andreas Kraemer (Frankfurt am Main/DE)

09.20

OP-053

Structural elucidation of cathepsin L inhibitors is pushing the concept of dual-target anti-viral drugs

Sven Falke, Julia Lieske, Patrick Reinke

Sebastian Günther (Hamburg/DE), Alexander Herrmann (Munich/DE)

Wiebke Ewert (Hamburg/DE), Jure Loboda, Katarina Karničar

Aleksandra Usenik, Nataša Lindič, Andreja Sekirnik (Ljubljana/SI)

Henry Chapman (Hamburg/DE), Winfried Hinrichs (Greifswald/DE)

Gregor Ebert (Munich/DE), Dusan Turk (Ljubljana/SI)

Alke Meents (Hamburg/DE)

09.50

OP-054

The induced-fit binding mechanism of cell-permeable dichlorophenylpyridine-based furin inhibitors

Sven O. Dahms (Salzburg/AT), Gisela Schnapp, Martin Winter

Frank H. Büttner, Christian Gnam

Alexander Pautsch (Biberach an der Riß/DE)

Hans Brandstetter (Salzburg/AT)

10.10

OP-055

Allosteric inhibition as a new mode of action: A neutralizing antibody targeting the activated form of coagulation factor XI

Martina Schaefer (Berlin/DE)

09.00–10.30

Lecture hall – OSZ H4

Chairs

Complex, aperiodic and disordered structures

Sander van Smaalen (Bayreuth/DE), Somnath Dey (Aachen/DE)

09.00

OP-056

Comparison of the local stabilisation mechanism in Ca- and Y-stabilized zirconia using 3D- Δ PDF-analysis

Ella Mara Schmidt (Bremen/DE)

09.15

OP-057

Successive modulated phases of Rb_2ZnCl_4

Surya Rohith Kotla (Bayreuth/DE), Sitaram Ramakrishnan (Bayreuth/DE, Higashihiroshima/JP), Toms Rekis (Bayreuth/DE, København/DK)

Achim M. Schaller (Bayreuth/DE), Jin-Ke Bao (Bayreuth/DE,

Shanghai/CN), Claudio Eisele (Bayreuth/DE), Leila Noohinejad

Martin Tolkiehn, Carsten Paulmann (Hamburg/DE), Geoffroy de Laitre

Marc de Boissieu (Saint-Martin-d'Hères, Grenoble/FR)

Sander van Smaalen (Bayreuth/DE)

09.30

OP-058

Modulations in Cu-Pb-Sb-Se andorite-type sulfosalt structures

Paul Sicher, Berthold Stöger (Vienna/AT)

09.45

OP-059

Charge density wave phase transition in EuAl_2Ga_2 in magnetic phase transition

Harshit Agarwal, Surya Rohith Kotla (Bayreuth/DE)

Sitaram Ramakrishnan (Higashi-Hiroshima/JP)

Claudio Eisele (Bayreuth/DE), Leila Noohinejad, Martin Tolkiehn

Carsten Paulmann (Hamburg/DE), Biplab Bag (Jharkhand/IN)

Bishal Baran Maity, Shovan Dan, Arumugam Thamizhavel (Mumbai/IN)

Srinivasan Ramakrishnan (Pune/IN), Sander van Smaalen (Bayreuth/DE)

10.00

OP-060

Cr-pincer complexes with two disorder modes: One-dimensional diffuse scattering and what we can learn from it

Berthold Stöger, Daniel Himmelbauer (Vienna/AT)

10.15

OP-061

Potassium-iron orthotellurate hydrate $\text{H}_6\text{K}_3\text{FeTe}_2\text{O}_{12}$, an OD structure featuring 1D diffuse scattering

Tobias Wolflehner, Berthold Stöger (Vienna/AT)

09.00–10.30

Lecture hall – OSZ H5

Chairs

Extreme/non-ambient and high-pressure conditions II

Anna Pakhomova (Grenoble/FR)

Lkhamsuren Bayarjargal (Frankfurt am Main/DE)

09.00

OP-062

Crystal chemical design and high-pressure synthesis of non-dense polynitrides

Maxim Bykov (Cologne/DE), Elena Bykova (Bayreuth/DE)

Alexander Goncharov (Washington, D.C./US)

Leonid Dubrovinsky (Bayreuth/DE)

09.30

OP-063

Cation-substitution in Pyrocarbonates

Dominik Spahr, Jannes König, Lkhamsuren Bayarjargal

Eiken Haussühl (Frankfurt am Main/DE), Victor Milman (Cambridge/GB)

Hanns-Peter Lierman (Hamburg/DE)

Björn Winkler (Frankfurt am Main/DE)

09.45

OP-064

Novel dysprosium carbides synthesised at high pressures

Fariia Iasmin Akbar, Leonid Dubrovinsky, Natalia Dubrovinskaya

Alena Aslandukova, Andrii Aslandukov, Yuqing Yin (Bayreuth/DE)

Timofey Fedotenko (Hamburg/DE), Dominique Laniel (Edinburgh/GB)

10.00

OP-065

Columnar hydrofluorocarbons from pressure-induced polymerization of polycyclic arene-perfluoroarene co-crystals

Alexandra Friedrich (Würzburg/DE), Ines E. Collings (Grenoble/FR)

Kamil F. Dziubek, Samuele Fanetti (Sesto Fiorentino (FI)/IT)

Krzysztof Radacki (Würzburg/DE), Javier Ruiz-Fuertes (Santander/ES)

Julio Pellicer-Porres (Borjassot/ES), Michael Hanfland (Grenoble/FR)

Daniel Sieh (Würzburg/DE), Roberto Bini (Sesto Fiorentino (FI)/IT)

Stewart J. Clark (Durham/GB), Todd B. Marder (Würzburg/DE)

10.15

OP-066

Contribution of X-ray crystallography to the full description of molecular switches behavior under pressure at variable temperature

Mathieu Marchivie (Pessac/FR), Elodie Tailleux (Nancy/FR)

Patrick Rosa (Pessac/FR), Jean-Paul Itié (Gif-sur-Yvette/FR)

Baptiste Vignolle, Philippe Guionneau (Pessac/FR)

09.00–10.30

Computational methods

Lecture hall – OSZ H6

Chairs

Gerhard Raabe (Aachen/DE), Martin U. Schmidt (Frankfurt am Main/DE)

09.00

OP-067

The generation of artificial SEM images of nanoparticles by deep neural networks

Jonas Bals, Matthias Epple (Essen/DE)

09.18

OP-068

Compression and data reduction in serial crystallography

Marina Galchenkova, Alexandra Tolstikova, Dominik Oberthür

Janina Sprenger, Wolfgang Brehm, Thomas White, Anton Barty

Henry Chapman, Oleksandr Yefanov (Hamburg/DE)

09.36

OP-069

New tools for sequence assignment validation in cryo-EM and crystal structure models of macromolecules

Grzegorz Chojnowski (Hamburg/DE)

09.54

OP-070

Treatment of core electrons in quantum crystallography

Florian Kleemiss (Regensburg/DE), Norbert Peyerimhoff (Durham/GB)

Michael Bodensteiner (Regensburg/DE)

10.12

OP-071

Multipole model and topological analysis of chemical bonding in β -boron

Claudio Eisele (Bayreuth/DE)

Sitaram Ramakrishnan (Higashi-Hiroshima/JP), Jin-Ke Bao (Shanghai/CN)

Surya Rohith Kotla (Bayreuth/DE), Carsten Paulmann, Leila Noohinejad

Martin Tolkiehn (Hamburg/DE), Sander van Smaalen (Bayreuth/DE)

11.00–12.00

Lecture hall – OSZ H3

Chair

Plenary lecture V

Martin U. Schmidt (Frankfurt am Main/DE)

11.00

PT-5

3D Electron Diffraction in Pharmaceutical Compounds: Can we measure everything?

Jordi Benet Buchholz (Tarragona /ES)

12.30–13.30

Lecture hall – OSZ H3

Rigaku Europe SE – Lunchtime seminar:

CrysAlis Pro updates

12.30

CrysAlis^{Pro}: An update for X-ray and electron diffraction data

Mathias Meyer (Wroclaw/PL)

13.30–14.30

Lecture hall – OSZ H3

Chair

Plenary lecture VI

Stefan Knapp (Frankfurt am Main/DE)

13.30

PT-6

From crystallographic fragment screen to preclinical candidates:

Open science discovery of SARS-CoV-2 antivirals

Daren Fearon (Southampton, NY/US)

14.30–16.00

Lecture hall – OSZ H3

Chairs

Bio-crystallography V: Synchrotrons and new technologies

Johanna Hakanpää (Hamburg/DE), Anja Burkhardt

Tobias Beck (Hamburg/DE)

14.30

OP-072

In cellulo crystallography – Overcoming resolution limits by cell fusion

Juliane Boger, Iris Breidbach, Robert Schönherr, Sophie Nachtschatt

Lars Redecke (Lübeck/DE)

14.45

OP-073

JINXED: Just in time crystallization for easy structure determination of biological macromolecules

Alessandra Henkel, Marina Galchenkova, Julia Maracke

Oleksandr Yefanov, Johanna Hakanpää (Hamburg/DE)

Jeroen R. Mesters (Lübeck/DE), Henry Chapman

Dominik Oberthür (Hamburg/DE)

15.00

OP-074

Microsecond time-resolved pink beam serial crystallography

Sebastian Günther, Alexandra Tolstikova, Marina Galchenkova

Oleksandr Yefanov, Patrick Reinke, Henry Chapman (Hamburg/DE)

Robert Henning (Chicago, IL/US), Matteo Levantino (Grenoble/FR)

Alke Meents (Hamburg/DE)

15.15

OP-075

Facilities for Macromolecular Crystallography at the HZB

Manfred S. Weiss, Laila S. Benz, Tatjana Barthel, Thomas Crosskey

Alexander Dillmann, Ronald Förster, Paula Fröling, Christine Gless

Thomas Hauss, Michael Hellmig, Frank Lennartz, J. H. William Scanlan

Gert Weber, Jan Wollenhaupt, Uwe Mueller (Berlin/DE)

15.30

OP-076

Macromolecular Crystallography at DESY

Johanna Hakanpää, Clemente Borges, Spyros Chatziefthymiou

Andrey Gruzinov, Jialing Song, Helena Taberman, Guillaume Pompidor

Wiebke Ewert, Sebastian Günther, Patrick Reinke, Pontus Fischer

Alke Meents, Jan Meyer (Hamburg/DE)

15.45

OP-077

EMBL@PETRA IV – an Integrated Facility for Structural Biology and Imaging

Selina Storm, Gleb Bourenkov, Liz Duke, Jonas Albers, Clement Blanchet

Michael Agthe, David von Stetten, Enrique Rodriguez Garcia

Stefan Fiedler, Dmitri Svergun, Matthias Wilmanns

Thomas Schneider (Hamburg/DE)

14.30–16.00

Lecture hall – OSZ H4

Chairs

Inorganic crystal structures I

Caroline Röhr (Freiburg im Breisgau/DE), Thomas Doert (Dresden/DE)

14.30

OP-078

In the search of missing binaries: Ternary approaches of alkali metal thallides

Stefanie Gärtner (Regensburg/DE)

14.45

OP-079

Ammonium and alkali metal selenocyanates

Frank Tambornino (Marburg/DE)

15.00

OP-080

Hydrogenation as an instrument for modifying structures and properties of MNi_3 and $LnTiGe$ (M = main-group metal, Ln = lanthanide) intermetallics compounds

Mihai Sturza, André Götze, Holger Kohlmann (Leipzig/DE)

15.15

OP-081

Foreign anion inclusion in $M^{II}_3(Te^{IV}O_3)_2(OH)_2$ (M = Mn, Co, Ni, Mg) phases

Felix Eder, Matthias Weil (Vienna/AT)

15.30

OP-082

Selenium/Tellurium halides with strong SHG-Effects

Maxime Bonnin, Lkhamsuren Bayarjargal, Victor Milman, Björn Winkler
Claus Feldmann (Karlsruhe/DE)

15.45

OP-083

Discovery and characterization of a new aluminium phosphate sulfate mineral

Thomas Witzke, Gwilherm Nénert (Almelo/NL)

14.30–16.00

Lecture hall – OSZ H5

Chairs

Theoretical crystallography

Gerhard Raabe (Aachen/DE), Michael Fischer (Bremen/DE)

14.30

OP-084

Emergent properties under high pressure: Can a finite chain of HCN molecules model a crystal?

Chieh-Min Hsieh, Tim Neudecker (Bremen/DE)

14.48

OP-085

Advances in the parameter space concept for crystal structure determination – Linearization of intensity isosurfaces

Muthu Vallinayagam (Dresden/DE), Melanie Nentwich (Hamburg/DE)

Dirk C. Meyer (Dresden/DE), Karl Fischer (Saarbrücken/DE)

Matthias Zschornak (Dresden/DE)

15.06

OP-086

Pathway for a martensitic quartz-coesite transition

Tim Schaffrinna (Frankfurt am Main/DE)

Victor Milman (Cambridge/GB), Björn Winkler (Frankfurt am Main/DE)

15.24

OP-087

Beyond sphere packings – *Packings* of sphere packings

Marek Petrik (Marburg/DE), Wolfgang Hornfeck (Prague/CZ)

15.42

OP-088

Solving the phase problem in crystallography with artificial intelligence

Toms Rekis, Anders S. Larsen, Anders Ø. Madsen (Copenhagen/DK)

14.30–16.00

Lecture hall – OSZ H6

Chairs

Micro- and nano-crystalline materials (powder diffraction, disordered material) II

Robert E. Dinnebier (Stuttgart/DE), Jürgen Horbach (Düsseldorf/DE)

Ulrich Fotheringham (Mainz/DE)

14.30

OP-089

Challenging characterization of ultrasmall nanoparticles of coin and platinum metals

Oleg Prymak, Oliver Wetzel, Benedikt Kruse, Kateryna Loza (Essen/DE)

Marc Heggen (Jülich/DE), Claudia Weidenthaler (Mülheim an der

Ruhr/DE), Matthias Eppe (Essen/DE)

15.00

OP-090

Synthesis and ultrastructure of ultrasmall monometallic and bimetallic silver-platinum nanoparticles (2 nm)

Natalie Wolff, Kateryna Loza, Oleg Prymak (Essen/DE)

Marc Heggen (Jülich/DE), Torsten Schaller, Felix Niemeyer (Essen/DE)

Claudia Weidenthaler (Mülheim an der Ruhr/DE)

Matthias Eppe (Essen/DE)

15.15

OP-091

A perfect liaison: Combining crystal mapping with PXRD

Johannes Merkelbach, Christian Jandl, Gunther Steinfeld, Danny Stam

Petra Simoncic (Villigen/CH)

15.30

OP-092

Synthesis and characterization of new high-entropy cuprates

Andrea Kirsch, Mathias Tegtmeier, Xenia Bredahl Gjelsten

Kirsten M. Ø. Jensen (Copenhagen/DK)

15.45

OP-093

Sublimation of silver and silver-gold core-shell nanocubes studied by *in-situ* powder diffraction and electron microscopy (SEM, TEM)

Aikaterini Karatzia, Kateryna Loza, Oleg Prymak (Essen/DE)

Marc Heggen (Jülich/DE), Matthias Eppe (Essen/DE)

19.00–23.00

Schuch's Restaurant

Social evening (see page 50)

09.00–10.00

Lecture hall – OSZ H4

Chairs

Plenary lecture VII

Constantin Buyer (Stuttgart/DE), Jakob Möbs (Marburg/DE)

09.00

PT-7

Simulating complex crystal structures and their assembly in hard and soft condensed materials

Julia Dshemuchadse (Ithaca, NY/US)

10.30–12.00

Lecture hall – OSZ H4

Chair

Electron crystallography and microscopy

Ute Kolb (Mainz/DE)

10.30

OP-094

XtalAB Synergy-ED: To cryo, or not to cryo, that is the ED question

Christian J. Schürmann, Khai-Nghi Truong, Robert Bücken

Fraser White (Neu-Isenburg/DE), Tomislav Stolar, Krunoslav Užarević

Luca Grisanti, Ernest Meštrović (Zagreb/HR), Mathias Meyer

Michał Jasnowski (Wrocław/PL), Akihito Yamano, Sho Ito, Eiji Okunishi

Yoshitaka Aoyama (Tokyo/JP), Joseph Ferrara (The Woodlands, TX/US)

10.45

OP-095

Structure determination of Nanocrystalline Metal-Organic frameworks by 3D electron diffraction

Christian Jandl, Johannes Merkelbach, Gunther Steinfeld

Eric Hovestreydt (Villigen/CH)

11.00

OP-096

3D structure determination with 3 MeV relativistic electrons

Ana Carolina Rodrigues, Vincent Hennicke, Max Hachmann

Wolfgang Brehm, Jan Meyer, Letícia de Melo Costa, Karol Bustos

Patrick Reinke, Tim Pakendorf, Hossein Delsim-Hashemi

Miriam Barthelmess, Klaus Fllöttmann, Alke Meents (Hamburg/DE)

11.15

OP-097

3D electron diffraction of perfect crystals is perfect for dynamical refinement

Petr Brazda (Prague/CZ), Paul Klar (Bremen/DE)

Lukas Palatinus (Prague/CZ)

11.30

OP-098

Crystal structure determination from low-resolution electron diffraction data – molecular replacement?

Tatiana Gorelik (Braunschweig/DE), Peer Lukat

Wulf Blankenfeldt (Braunschweig/DE)

11.45 OP-099	Enhancing the photocatalytic performance of carbon nitrides through controlled local structure modification Diana Piankova, Hannes Zschiesche (Potsdam/DE) Ivo Teixeira (São Carlos/BR), Eric Svensson Cheuk-Wai Tai (Stockholm/SE), <u>Nadezda Tarakina</u> (Potsdam/DE)
10.30–12.00 Lecture hall – OSZ H55 Chair	Crystallography in materials sciences II Elena Bykova (Bayreuth/DE)
10.30 OP-100	Pitfalls in cation and anion mutation of quaternary chalcogenide semi conductors Galina Gurieva, David Matzdorff, Daniel M. Töbrens <u>Susan Schorr</u> (Berlin/DE)
11.00 OP-101	Immediate structural response of halide perovskites under lighting revealed through in-situ X-ray diffraction <u>Joachim Breternitz</u> , Ivo Zizak, Susan Schorr (Berlin/DE)
11.15 OP-102	Pressure-induced depolarization and phase transitions in BaTiO ₃ -based ferro electric solid solutions <u>Tim Harald Reuter</u> , Lkhamsuren Bayarjargal Björn Winkler (Frankfurt am Main/DE)
11.30 OP-103	Crystallography in hydrogen technology: ammonia as hydrogen carrier <u>Claudia Weidenthaler</u> , Simone Gallus (Mülheim an der Ruhr/DE)
11.45 OP-104	Crystallographic structure and point defects vs. efficiency and stability in Cu ₂ ZnSn(S,Se) ₄ monograin solar cells <u>Galina Gurieva</u> (Berlin/DE), Kaia Ernits (Tallin/EE) Nikita Siminel (Chisinau/MD), Alicia Manjon Sanz (Oak Ridge, TN/US) Denis Sheptyakov (Villige/CH), Maxim Avdeev (Sydney/AU) Melanie Kirkham (Oak Ridge, TN/US) Dieter Meissner (Tallin/EE, Tallinn/EE), Susan Schorr (Berlin/DE)
12.00–12.30 Lecture hall – OSZ H4	Closing
13.30–15.45 Seminar room	Chemical crystallography – Joint symposium of DGK and GDCh
13.30	Lectures
15.00	Discussion on the networking of DGK and GDCh

Minerals

- PP-001 Miscibility of AFm-phases and the formation of solid solutions containing sulfate, chloride, carbonate and carboxylate anions
Sebastian Gerhardt, Tiago Kalil Cortinhas Alves, Tobias Beirau
Stefan Stöber (Halle (Saale)/DE)
- PP-002 Comprehensive mineralogical analysis of technogenic soils using spectroscopic methods
Svetlana Ivashevskaya, Gulnara V. Akhmetova (Petrozavodsk/RU)

Spectroscopy

- PP-003 Cation and anion ordering in synthetic lepidolites and lithian muscovites: Influence of the OH/F and Li/Al ratio on the mica formation studied by NMR spectroscopy and X-ray diffraction
Michael Fechtelkord, Lara Sulcek, Bernd Marler (Bochum/DE)

Bio-crystallography I: Signaling, macromolecular interactions and new structures

- PP-004 Investigation of structural requirements for distinct cyclization mechanisms in type III PKS
Marina Kruse, Wulf Blankenfeldt, Ludger Beerhues (Braunschweig/DE)
- PP-005 Towards a structural investigation of MamP, a key player in redox control during magnetosome maturation
Thomas Crosskey, Frank Lennartz, Uwe Müller, Manfred S. Weiss (Berlin/DE)
- PP-006 Crystal structure of 3-Methylguanine
Riccardo Cameli Manzo (Hamburg, Stuttgart/DE), Martin Etter (Hamburg/DE)
- PP-007 High-resolution structure of human nucleoside diphosphate kinase C in complex with different nucleotides
Rezan Amjadi, Theresia Dunzendorfer-Matt (Innsbruck/AT), Santosh Lomada
Thomas Wieland (Mannheim/DE), Sebastiaan Werten
Klaus Scheffzek (Innsbruck/AT)
- PP-008 Comparative structural analyses of the NHL domains from the human E3 ligase TRIM-NHL family
Apirat Chaikuad, Rezart Zhubi, Claudia Tredup
Stefan Knapp (Frankfurt am Main/DE)
- PP-009 Structural characterization of the pyruvate dehydrogenase complex E1 decarboxylation reaction
Alexander Mehr (Göttingen/DE)

- PP-010 Structural and functional studies of legumain-mycocypin complexes
Tasneem Elamin, Naia Santos, Peter Briza, Hans Brandstetter
Elfriede Dall (Salzburg/AT)
- PP-011 SARS-CoV-2 Methyltransferase ligand screening and peptide inhibitors
Viviane Kremling, Janina Sprenger, Dominik Oberthür, Henry Chapman
Oleksandr Yefanov, Marina Galchenkova, Philipp Middendorf, Bjarne Klopprogge
Antonia Kiene, Jerome Carnis, Ivan de Gennaro Aquino, Sven Falke
Christiane Ehrh, Yaiza Fernandez Garcia (Hamburg/DE)
- PP-012 Experimental steps on the way to biotec nacre
Dietmar Blohm (Bremen/DE)

Bio-crystallography II: Other technologies (neutron diffraction, small angle scattering)

- PP-013 The macromolecular neutron single crystal diffractometer BIODIFF for proteins
at the Heinz Maier-Leibnitz Zentrum MLZ
Andreas Ostermann, Tobias E. Schrader (Garching/DE)

Crystallography in art and heritage

- PP-014 Scientific techniques for the identification of mineral pigments of North Russian
icons
Svetlana Ivashevskaya, Irina Nabokova (Petrozavodsk/RU)

Inorganic crystal structures

- PP-015 XRD and DFT studies of new ionic lead compounds $\text{Pb}[\text{ChCN}]_2$ ($\text{Ch} = \text{O}, \text{Se}$)
Alena Shlyaykher, Anna Lea Barba (Marburg/DE)
Aleksandar Zivkovic (Utrecht/NL), Frank Tambornino (Marburg/DE)
- PP-016 $\text{Ba}(\text{BO}_2\text{OH})$ — A monoprotinated monoborate from hydroflux showing intense
second harmonic generation
Yuxi Li, Peter A. Hegarty, Michael Rüsing, Lukas M. Eng
Michael Ruck (Dresden/DE)
- PP-017 Crystal structures of carbonyl (pseudo)halides
Jonathan Pfeiffer, Clemens Trost, Frank Tambornino (Marburg/DE)

POSTER PRESENTATIONS | TUESDAY, 28 MARCH

- PP-018 Crystal structure of $\text{GdSrCa}_3\text{O}[\text{BO}_3]_3$ and $\text{GdSr}_2\text{Ca}_2\text{O}[\text{BO}_3]_3$
Tina Weigel, Erik Mehner, Hartmut Stöcker, Dirk C. Meyer, Jens Götze
Juliane Hanzig (Freiberg/DE)
- PP-019 Two Hg-rich rubidium Ga/In-mercurides with new structure types: $\text{Rb}(\text{Hg}_{1-x}\text{Ga}_x)_7$ and $\text{Rb}_7(\text{Hg}_{1-x}\text{In}_x)_{23}$ ($x=0.1$ each)
Caroline Röhr, Marco Wendorff (Freiburg im Breisgau/DE)
- PP-020 Investigating the Role of the Different Alkali Metals in the Structure Type $\text{K}_{14}\text{Cd}_9\text{Ti}_{21}$
Melissa Janesch, Stefanie Gärtner (Regensburg/DE)
- PP-021 A New Structure of $\text{Pt}(\text{Bi}_x\text{Te}_{1-x})_2$
Yiran Wang, Falk Pabst (Dresden/DE), Anna Isaeva (Amsterdam/NL)
Thomas Doert, Michael Ruck (Dresden/DE)
- PP-022 Structural, optical and vibrational investigations of dolomite-type structures $\text{MSn}(\text{BO}_3)_2$ for $\text{M} = \text{Mn}, \text{Fe}, \text{Co}$ and Ni
Sarah Wittmann, M. Mangir Murshed (Bremen/DE)
Vitaliy Bilovol (Buenos Aires/AR, Krakow/PL), Thorsten M. Gesing (Bremen/DE)
- PP-023 Structural characterization of Cu-tpy-2"nucleotide ternary complexes
Suma Dilipkumar, Nethaji Munirathinam (Bengaluru/IN)
- PP-024 Rim-Brominated Pillarplexes
Julian Zuber, Alexander Pöthig (Garching/DE)
- PP-025 How to carve out the crystal structure of the polyoxometalate $[\text{Ni}(\text{en})_3]_2[\text{V}_{12}\text{As}_8\text{O}_{40}(\text{H}_2\text{O})] \cdot 4\text{H}_2\text{O}$ from synchrotron X-ray powder diffraction data
Sebastian Mangelsen, Maren Rasmussen, Nicole Pienack, Christian Näther
Wolfgang Bensch (Kiel/DE)
- PP-026 Synthesis and characterization of AFm-Phases containing selenite and organic molecules
Tiago Kalil Cortinhas Alves, Sebastian Gehardt, Tobias Beirau
Stefan Stöber (Halle (Saale)/DE)
- PP-027 Synthesis of dimorphic LaFSe and crystal-structure prediction of several more polymorphs of lanthanum fluoride selenide
Constantin Buyer, Hagen Grossholz (Stuttgart/DE), Dejan Zagorac
Jelena Zagorac (Belgrade/RS), J. Christian Schön, Thomas Schleid (Stuttgart/DE)

- PP-028** Structural and spectroscopic investigation of mechanically induced defective forsterite (Mg_2SiO_4) to describe martian regolith
Muchammad Izzuddin Jundullah Hanafi, M. Mangir Murshed, Lars Robben Wilke Dononelli (Bremen/DE), Andrea Kirsch (Copenhagen/DK)
 Thorsten M. Gesing (Bremen/DE)
- PP-029** Structural characterization of the lone electron pair effect on the $(\text{Pb}_{1-x}\text{Sr}_x)\text{MnBO}_4$ mullite-type phases
Carla M. Uribe Rincón, M. Mangir Murshed, Thorsten M. Gesing (Bremen/DE)
- PP-030** $\text{RbEr}_2\text{S}[\text{S}_2][\text{AsS}_2(\text{S}_2)]$: A Rubidium-Containing Erbium Thioarsenate(III) with a new type of complex anion
Katja Engel, Pia Lena Lange, Thomas Schleid (Stuttgart/DE)
- PP-031** Complete structural and magnetic phase diagram of orthorhombic mixed spinel series $\text{Ni}_{1-x}\text{Cu}_x\text{Cr}_2\text{O}_4$
Michael Tovar, Manfred Reehuis, Norbert Stüßer, Bastian Klemke
 Daniel M. Többsens, Susan Schorr (Berlin/DE)
- PP-032** A nitridosilicatephosphate with amphibole structure
Monika Pointner, Wolfgang Schnick (Munich/DE), Oliver Oeckler (Leipzig/DE)
- PP-033** Ternary Alkali Metal Thallides ATl ($A=\text{Rb}$ and K or Cs)
Vanessa Schwinghammer, Stefanie Gärtner (Regensburg/DE)
- PP-034** Synthesis, characterization and structure-property relations in $\text{Pb}_2(\text{Pb}_{1-x}\text{Sn}_x)\text{O}_4$
Christopher S. Reuter, M. Mangir Murshed, Thorsten M. Gesing (Bremen/DE)

Instrumentation and technological development

- PP-035** Status of the Powder Diffraction and Total Scattering Beamline P02.1 at PETRA III, DESY
Martin Etter, Volodymyr Baran, Henrik Jeppesen, Alba San José Méndez
 Alexander Schökel, Tim Schoof, Mario Wendt, Sergej Wenz (Hamburg/DE)
- PP-036** Higher harmonics in X-rays: Effects, evaluation, 'extinction'
Melanie Nentwich, Dmitri Novikov (Hamburg/DE)
- PP-037** New challenges in non-ambient XRD – New solutions from Anton Paar
Barbara Pühr, Marius Kremer, Andrew O.F. Jones, Timo Müller, Benedikt Schrode
 Praveen Vir (Graz/AT)

- PP-038 The multipurpose powder X-ray diffractometer from Anton Paar
Andrew O. F. Jones, Marius Kremer, Timo Müller, Barbara Pühr
Benedikt Schrode (Graz/AT), Kevin Turke (Ostfildern/DE)
- PP-039 Area detector prototype for the hot dingle crystal diffractometer HEiDi
Martin Meven (Garching, Jülich/DE), Ralf Engels (Jülich/DE)
Muni Poli (Garching, Jülich/DE), Karen Frieze, Andrzej Grzechnik (Jülich/DE)
- PP-040 The new PHOTON III HE detector – Unbeatable sensitivity for short wavelength
crystallography
Tobias Stürzer, Carsten Lenczyk, Ali Abboud, Martin Adam
Roger Durst (Karlsruhe/DE)

Micro- and nano-crystalline materials (powder diffraction, disordered material)

- PP-041 Structural changes of ZrS_2 and HfS_2 during sodium uptake
Lina Liers, Sebastian Mangelsen, Malte Behrens (Kiel/DE)
- PP-042 In-house pair distribution function analysis: Sample dependent data collection
strategies
Konrad Krämer, Thorsten M. Gesing, Lars Robben (Bremen/DE)
- PP-043 Using the plate screener XtalCheck-S for high-throughput screening of powder
samples
Christian J. Schürmann (Neu-Isenburg/DE), Pierre Le Magueres, Mark Del Campo
Joseph Ferrara (The Woodlands, TX/US), Jakub Wojciechowski (Neu-Isenburg/DE)
- PP-044 Combined Rietveld refinement on X-ray and neutron powder diffraction data:
Half or full occupancy of Mg in complex rare-earth perovskite $\text{La}_2(\text{Al}_{1/2}\text{MgTa}_{1/2})\text{O}_6$
Yoo Jung Sohn (Jülich/DE), Volodymyr Baran (Garching, Hamburg/DE)
Ralph Gilles (Garching/DE), Georg Roth (Aachen/DE), Robert Vaßen (Jülich/DE)
- PP-045 Structure and Composition of Size-Tunable Ni–Cu Core–Shell Nanoparticles as
analyzed by ASAXS
Armin Hoell, Maria Heilmann, Robert Wendt, Carsten Prinz, Ralf Bienert
Jörg Radnik, Ana Guilherme Buzanich, Franziska Emmerling (Berlin/DE)
- PP-046 Magnesian Malachite – How much magnesium can we fit in malachite?
Sebastian Mangelsen (Kiel/DE), Nils Prinz (Aachen/DE)
Gereon Behrendt (Berlin/DE), Mirijam Zobel (Aachen/DE)
Malte Behrens (Kiel/DE)

Neutron scattering

- PP-047 Exchange interactions in the iron subsystem in rare-earth orthoferites $RFeO_3$ ($R=Ho, Tb$)
Aleksandr K. Ovsianikov (Aachen/DE), Piotr Fabrykiewicz (Aachen, Garching/DE)
Igor A. Zobkalo (Gatchina/RU), Wolfgang Schmidt (Grenoble/FR)
Avishek Maity (Garching/DE), Kirill A. Shaykhutdinov (Krasnoyarsk/RU)
Martin Meven (Aachen, Garching/DE), Georg Roth (Aachen/DE)

Organic molecules and coordination compounds

- PP-048 Coordination polymers obtained from Berghof reactor
Andrzej Kochel (Wrocław/PL), Małgorzata Holyńska (Wrocław/PL, Marburg/DE)
- PP-049 Absolute structure determination of a chiral silyl ether by the crystalline sponge method
Nils Nöthling, Monika M. Lindner (Mülheim an der Ruhr/DE)
- PP-050 Structural systematics of benzamides and carboxamides
John Gallagher, Islam Osman (Dublin/IE)
- PP-051 Leucopterin, the white pigment in the wings of butterflies: crystal structure analysis by combination of powder and single-crystal diffraction with solid-state NMR and DFT-D optimisations
Federica Bravetti (Turin/IT, Frankfurt am Main/DE)
Lukas Tapmeyer (Mannheim/DE), Kathrin Skorodumov, Edith Alig
Stefan Habermehl, Robert Hühn (Frankfurt am Main/DE), Simone Bordignon
Angelo Gallo, Carlo Nervi, Michele R. Chierotti (Turin/IT)
Martin U. Schmidt (Frankfurt am Main/DE)
- PP-052 Crystal structure of a propyl 4-((1-(2-methyl-4-nitrophenyl)-1H-1,2,3-triazol-4-yl) methoxy) benzoate-copper-di-chloro complex
Muminjon Hakimov (Namangan/UZ), Akmaljon Tojiboev
Ilhomjon Ortikov (Tashkent/UZ)
- PP-053 Tracking the annealing-induced segregation and ordering of thermoplastic polymer chains by total scattering
Maxwell Terban (Stuttgart/DE), Elmar Pöselt (Lemförde/DE)
Marc Malfois (Barcelona/ES), Bernd Hinrichsen (Ludwigshafen/DE)
Robert E. Dinnebier (Stuttgart/DE)

- PP-054 Obtaining and analysing organic crystals and co-crystals
Mirela Nicolov (Timisoara/RO)
- PP-055 Polymorphism in toxic medications: exploring the crystal chemistry of lead and cadmium naproxen
Gwilherm Nénert (Almelo/NL)

Young crystallographers

- PP-056 Pillarplex rotaxanes with α,ω -Dicarboxylic acids
Alexandra Heidecker, Alexander Pöthig (Garching/DE)
- PP-057 A series of four isostructural copper halogenido pentelates with interesting optical properties
Jakob Möbs (Marburg/DE), Rylee James (Tempe, AZ/US), Paula Epure Johanna Heine (Marburg/DE)
- PP-058 Experimental and theoretical study of solid solutions in the system $\text{Nd}_3\text{Ga}_5\text{O}_{12} - \text{Gd}_3\text{Ga}_5\text{O}_{12}$
Sofia Tovstopyat, Nikolay Eremin, Maximilian Nickolsky (Moscow/RU)
- PP-059 Preparation and characterization of apremilast multicomponent solid systems
Yelizaveta Naumkina (Prague/CZ, Tomsk/RU), Jan Čejka (Prague/CZ)
Elena Korotkova (Tomsk/RU)
- PP-060 Towards an understanding of the OAS-Based innate immune signaling: The role of the positively charged residues in the product release channel
Pavel Kats, Xiaoyi Zhou, Jannik Wiebe, Ole Zeymer, Jan Lohöfener, Nicola Steinke Petra Baruch (Hannover/DE), Rune Hartmann (Aarhus/DK), Dietmar J. Manstein Roman Fedorov (Hannover/DE)
- PP-061 Mono- and heterometallic REE heptafluorobutyrate as single-source precursors for NaLnF_4 thin film deposition
Artem Shevchenko (Stuttgart/DE), Daria Blinnikova (Moscow/RU)
Sebastian Bette (Stuttgart/DE), Andrei Anosov
Dmitry Tsybarenko (Moscow/RU)
- PP-062 High-pressure synthesis of ternary nitrides in Na-W-N system
Natalia Martynova (Cologne/DE), Elena Bykova (Bayreuth/DE)
Timofey Fedotenko (Hamburg/DE), Leonid Dubrovinsky (Bayreuth/DE)
Maxim Bykov (Cologne/DE)
- PP-063 Low-Temperature Measurement of the Unexpected Hydrate $\text{Cs}_2[\text{B}_{12}\text{H}_{12}] \cdot 2 \text{H}_2\text{O}$
Rouzbeh Aghaei Hakkak, Thomas Schleid (Stuttgart/DE)

- PP-064 The Heaviest Lanthanoid-Containing Silver Thiophosphate: $\text{Ag}_3\text{Lu}[\text{PS}_4]_2$
Pia Lena Lange, Thomas Schleid (Stuttgart/DE)
- PP-065 Novel binary, ternary and quaternary phases in the Bi-Mn-Pt-I system
Maria Herz, Michael Ruck (Dresden, Würzburg/DE)
- PP-066 Survey of zirconium-containing NaSICON-type solid-state Li^+ ion conductors with the aim of increasing reduction stability by partial cation substitution
Asmaa Loutati (Jülich/DE)
- PP-067 Upgrading the High-Energy Beamline P21.1 at PETRA III (DESY)
Katharina Köhler (Frankfurt am Main/DE), Ann-Christin Dippel
Martin von Zimmermann (Hamburg/DE), Alessandro Mirone (Grenoble/FR)
Björn Winkler (Frankfurt am Main/DE)
- PP-068 Crystalline sponge method for pharmaceutically active ingredients: A chemical space analysis
Carolina von Essen (Darmstadt/DE)
- PP-069 Coordination-Driven insertion of a guest molecule in the pore of a Copper(I)-Based Metallocavitand
Thomas Pickl, Markus Anneser, Alexander Pöthig (Garching/DE)

Bio-crystallography III: Structure-based design

- PP-070 Crystallographic studies of MST3 kinase inhibitor complexes reveal unique ligand-induced structural variations
Dimitrios-Ilias Balourdas, Marcel Rak, Jennifer Amrhein, Joshua Gerninghaus
Thomas Hanke, Andreas Christian Joerger, Stefan Knapp (Frankfurt am Main/DE)
- PP-071 Structural basis of p53 inactivation by cavity-creating cancer mutations and its implications for the development of mutant p53 reactivators
Andreas Christian Joerger (Frankfurt am Main/DE)
- PP-072 Structural and biophysical studies on drug-resistant mutations of the SARS-CoV-2 main protease
Rolf Hilgenfeld, Judith Röske, Kaixuan Zhang (Lübeck/DE)
Ute Curth (Hannover/DE), Xinyuanyuan Sun, Haifa El Kilani (Lübeck/DE)

Bio-crystallography IV: Synchrotrons and high throughput methods

PP-073 High energy, high resolution large unit cell X-ray crystallography on the P14@PetraIII Beamline
UmaLakshmi Dakshinamoorthy (Göttingen/DE)

PP-074 Structural and functional insight into a secreted, N-glycosylated Protein—Human zonulin in celiac disease towards drug discovery
Jialing Song, Spyros Chatziefthymiou, Andrey Gruzinov, Guillaume Pompidor
Helena Taberman, Ronald Maitschke-Rajasekharan, Philipp Lewe, Susanne Witt
Tengchuan Jin, Johanna Hakanpää (Hamburg/DE)

Complex, aperiodic and disordered structures

- PP-075** With a pinch of zinc: Solving the disorder problem in 'NaCd₂': Syntheses and crystal structures of Na₄₇(Cd_{1-x}Zn_x)₁₀₂ (x=0.088) and Na₈(Cd_{1-x}Zn_x)₁₇ (x=0.124)
Inga Junker, Katharina Köhler, Caroline Röhr (Freiburg im Breisgau/DE)
- PP-076** Incommensurate structures and radiation damage in Rb₂V₃O₈ and K₂V₃O₈ fresnoites
Andrzej Grzechnik (Jülich, Aachen/DE), Vaclav Petricek (Prague/CZ)
Dmitry Chernyshov, Charles McMonagle (Grenoble/FR)
Tobias Geise (Aachen/DE), Hend Shahed (Jülich/DE)
Karen Frieze (Aachen, Jülich/DE)
- PP-077** Sr₁₃Cd₅₉: The corrected composition and crystal structure of a complex binary cadmide (and most likely many other isotypic intermetallics)
Markus Otteny, Marco Wendorff, Caroline Röhr (Freiburg im Breisgau/DE)

Computational methods

- PP-078** Elucidating host-guest interactions in UV filter-zeolite composites by combining IR spectroscopy and DFT calculations
Michael Fischer (Bremen/DE), Riccardo Fantini, Mattia Sisti (Modena/IT)
Lorenzo Mino (Turin/IT)
- PP-079** Ferroelectric phase transition in barium titanate: An ab-initio- molecular dynamics approach
Christian Ludt, Matthias Zschornak (Freiberg/DE)

Electron crystallography and microscopy

- PP-080** Structures of Vitamin D derivatives by electron diffraction
Krzysztof Woźniak, Kunal Kumar Jha, Michal Chodkiewicz, Monika Wanat
Barbara Gruza, Andrzej Kutner, Tomasz Góral, Paulina Dominiak (Warsaw/PL)
- PP-081** On the cutting edge of electron diffraction quality
Eric Hovestreydt, Johannes Merkelbach, Christian Jandl, Gunther Steinfeld
Danny Stam (Villigen/CH)
- PP-082** Thermal conversion of platinum-group metals by in situ transmission electron microscopy
Kateryna Loza, Aikaterini Karatzia (Essen/DE), Marc Heggen (Jülich/DE)
Matthias Eppler (Essen/DE)

- PP-083 ANTEMA: An Automated Nanoparticle Transmission Electron Micrograph Analysis based on machine learning procedures
Nina Gumbiowski, Kateryna Loza (Essen/DE), Marc Heggen (Jülich/DE)
Matthias Eppele (Essen/DE)

Extreme/non-ambient and high-pressure conditions

- PP-084 In-situ investigation of solid phase evolution during lyophilization of mannitol-based antibody formulations using an XRPD climate chamber
Stefan Weber, Markus Börner, Vanessa Seiler, Madeleine Witting
Norbert Nagel (Ludwigshafen/DE)
- PP-085 New insights in the mechanical phase transition of anatase to rutile (TiO₂) from *in situ* synchrotron investigations
Hilke Petersen, Claudia Weidenthaler (Mülheim an der Ruhr/DE)
- PP-086 Influence of CO₂ on the stability of siderite (FeCO₃) at high pressures and temperatures
Lkhamsuren Bayarjargal, Dominik Spahr, Jannes König
Björn Winkler (Frankfurt am Main/DE)
- PP-087 NanoExtrem: Nano-focus end-station with double-sided CO₂ laser heating for X-ray diffraction, fluorescence and imaging experiments at ID27@ESRF
Wolfgang Morgenroth (Potsdam/DE), Mohamed Mezouar, Gastón Garbarino
Anna Pakhomova, Björn Wehinger (Grenoble/FR), Markus Herrmann
Maximilian Schulze, Sandro Jahn (Cologne/DE), Lélia Libon
Max Wilke (Potsdam/DE)
- PP-088 Mineralogy of large ocean worlds: *In situ* high-pressure studies of hydrates
Anna Pakhomova (Grenoble/FR), Baptiste Journaux (Seattle, WA/US)
Ines E. Collings (Villigen/CH), Sylvain Petitgirard (Zurich/CH)
Tiziana Boffa Ballaran (Bayreuth/DE)
- PP-089 Liquid sulfur density and viscosity measurements by proton radiography
Roman Belikov, David Merges (Frankfurt am Main/DE), Dmitry Varentsov
Karin Weyrich (Darmstadt/DE), Martin Schanz
Fesseha Mariam (Los Alamos, NM/US), Roman Gavrilin, Alexei Skobliakov
Aiush Khurchiev (Moscow/RU), Dmitry Nikolaev (Chernogolovka/RU)
Alexander Müller-Münster, Gustav Schmidt
Björn Winkler (Frankfurt am Main/DE)
- PP-090 Next generation MetalJet sources enabling 10µm high brightness high energy beams for high pressure diffraction application
Julius Hållstedt, Shichao Hu, Geethanjali Gopakumar, Emil Espes (Kista/SE)

- PP-091 How reliable are energies of phonon DOS determined from thermal expansion data?
Ross John Angel (Padova/IT), Giulia Novelli, Simon Parsons (Edinburgh/GB)
 Matteo Alvaro (Pavia/IT)
- PP-092 Investigation of structural modifications under extreme conditions
Ioannis Tzifas, Kay-Obbe Voss (Darmstadt/DE), Maik Lang (Knoxville, TN/US)
 Maria-Eugenia Toimil-Molares (Darmstadt/DE)
 Christopher Schroeck (Darmstadt, Frankfurt am Main/DE)
 Christina Trautmann (Darmstadt/DE)
- PP-093 High temperature behavior of Mn-bearing, Bi-rich hingganite-(Y) from the Jaguarçu Pegmatite, Brasil
Anastasiia Shagova, Liudmila Gorelova, Oleg Vereshchagin (St Petersburg/RU)
 Anatoly Kasatkin (Moscow/RU)
- PP-094 Synthesis, structure and properties of of BaCO₃(hR5)-type PbCO₃
Wilson Crichton (Grenoble/FR), Lkhamsuren Bayarjargal (Frankfurt am Main/DE)
 Victor Milman (Cambridge/GB), Björn Winkler (Frankfurt am Main/DE)

Solid state physics in crystallography

- PP-095 Negative thermal expansion, thermodynamic properties, temperature-dependent Raman scattering and crystal growth of large single crystals of metal-organic framework structures
Eiken Haussühl, Lkhamsuren Bayarjargal, Dominik Spahr, Julia Büscher
 Rita Luchitskaia, Björn Winkler (Frankfurt am Main/DE)
- PP-096 Mineral-like copper oxyvanadates with different dimensions of OCu₄ complexes
Victoria Ginga (Leipzig/DE, St Petersburg/RU), Oleg Siidra (St Petersburg/RU)
 Alexander Tsirlin (Leipzig/DE)

Crystallography in materials sciences

- PP-097 Investigation of by-products of processed spodumene mineral concentrates to lithium hydroxide
Julia Woskowski, Stefan Stöber, Andreas Neumann, Hans Roggendorf
 Ralf Wehrspohn (Halle (Saale)/DE)
- PP-098 Advancements in anomalous diffraction for cation order determination at beamline KMC-2
Daniel M. Többens, David Matzdorff, Yvonne Tomm, Galina Gurieva
 Susan Schorr (Berlin/DE)

- PP-099** The polar guanidinium tartrates $[C(NH_2)_3]_2(L-C_4H_4O_6) \cdot H_2O$ and $[C(NH_2)_3]_2(L-C_4H_4O_6)$: Crystal growth, crystal structures and phase relations
Ivana Cisarová, Irena Matulková, Ivan Nemeč (Prague/CZ), Christoph Grams Joachim Hemberger, Petra Becker, Ladislav Bohatý (Cologne/DE)
- PP-100** Multi-polymorphic tailor-made thin-film titania phases as reference system for photocatalytic persistent organic pollutant degradation
Oliver Thueringer, Alexander Wollbrink, Thorsten M. Gesing (Bremen/DE)
- PP-101** Expanding the family of mineral-like anhydrous alkali copper sulfate framework structures: new phases, topological analysis and evaluation of ion migration potentialities
Artem Borisov (Kiel/DE), Oleg Siidra (St Petersburg/RU)
Vadim Kovrugin (Bordeaux/FR), Andrey Golov (Vitoria-Gasteiz/ES)
Astrid Holzheid, Wulf Depmeier (Kiel/DE)
- PP-102** On the ordered structure of mechanochemically prepared $MAPbCl_3$
Götz Schuck, Daniel M. Többsens, Susan Schorr (Berlin/DE)
- PP-103** The effect of a magnetic field on the precipitation of calcium carbonate Polymorphs
Salim Ouhenia, Lydia Amer (Bejaia/DZ), Daniel Chateigner (Bejaia/DZ, Caen/FR)
Imad Belabbas (Bejaia/DZ)
- PP-104** Crystal growth and characterization of the 12L-Perovskite $Ba_4MlIr_3O_{12}$ with $M = Eu^{III}, Ce^{IV}$ and Nb^V
Henrik Schilling, Petra Becker (Cologne/DE)
- PP-105** Crystal structure of Pigment Yellow 75 from laboratory X-ray powder diffraction data
Svetlana Ivashevskaya (Petrozavodsk/RU)
Martin U. Schmidt (Frankfurt am Main/DE)
- PP-106** High-pressure polymorph of pyrene
Wenju Zhou, Yuqing Yin, Andrii Aslandukov, Leonid Dubrovinsky
Natalia Dubrovinskaia (Bayreuth/DE)
- PP-107** Synthesis and spectroscopic characterization of $(Bi_{1-x}M_x)_2O_3$ ($M = Y, Gd, Er, Tb, Yb$)
Md. Imran Hossain, M. Mangir Murshed, Thorsten M. Gesing (Bremen/DE)
- PP-108** Magnetic, electric and toroidal polarisation modes describing the physical properties of crystals- $NdFeO_3$ case
Piotr Fabrykiewicz (Aachen, Garching/DE), Radosław Przeniosło
Izabela Sosnowska (Warsaw/PL)

PP-109 $\text{Na}_2\text{Ca}_3\text{Si}_2\text{O}_8$ or $\gamma\text{-Na}_2\text{Ca}_6\text{Si}_4\text{O}_{15}$? A hybrid approach combining 3D single-crystal electron and powder X-ray diffraction for solving a 50-year-old problem
Volker Kahlenberg, Hannes Krüger, Jonathan Vinke (Innsbruck/AT)
Sho Ito (Tokyo/JP), Christian J. Schürmann (Neu-Isenburg/DE)

PP-110 Electron Diffraction – The Swiss knife among the analytical equipment for solid state characterization for pharmaceuticals
Danny Stam (Villigen/CH), Gustavo Santiso-Quinones (Villigen, Basel/CH)
Carsten Schauerte (Bochum/DE), Mihaela Pop (Cluj-Napoca/RO)
Johannes Merkelbach, Christian Jandl, Gunther Steinfeld (Villigen/CH)

PP-111 On the development of MagStREXS: A software to study magnetic structures
Pablo Bereciartua (Hamburg/DE), Juan Rodríguez-Carvajal (Grenoble/FR)
Sonia Francoual (Hamburg/DE)

Inorganic crystal structures

PP-112 Methylxanthine/Halogen System: An energetic point of view study
Irina S. Konovalova (Düsseldorf/DE, Kharkiv/UA), Maik Wyshusek
Guido Johannes Reiss (Düsseldorf/DE)

PP-113 Oxoscandates with scandium in tetrahedral coordination
Irina Zaytseva, Constantin Hoch (Munich/DE)

PP-114 $\text{TmSb}_2\text{O}_4\text{Br}$: The first Tetragonal Lanthanoid Oxoantimonate Bromide without mixed-cation occupation
Ralf Jules Christian Locke, Thomas Schleid (Stuttgart/DE)

PP-115 $(\text{NH}_4)_4(\text{SO}_4)[\text{CB}_{11}\text{H}_{12}]_2$: A New Double Salt with Carbaborate Anions Crystallizing in a Monoclinic Variety of the *anti*- K_2NiF_4 -Type Structure
Alexandra Friedly, Thomas Schleid (Stuttgart/DE)

PP-116 The new alkaline metal mercuride oxides $\text{Cs}_8\text{Hg}_8\text{O}$ and $\text{Rb}_8\text{Hg}_8\text{O}$
Lukas Nusser, Constantin Hoch (Munich/DE)

PP-117 Dialuminate $\text{A}_6[\text{Al}_2\text{Q}_6]$ (A=K, Rb, Cs; Q=S, Se, Te) mit $[\text{Al}_2\text{Q}_6]^{6-}$ -Tetraederdimeren
Michael Schwarz, Vincent Daiber, Caroline Röhr (Freiburg im Breisgau/DE)

PP-118 Synthesis and characterization of zinc/zirconium co-substituted ferrites
Yanina Mariella Dreer, Rainer Niewa (Stuttgart/DE)

PP-119 News from the detector front – Ag(I)/Bi(III)-based bromides as alternatives
Catherine Fabienne Schweinle, Simay Sahsuvar, Harald Hillebrecht
Michael Fiederle (Freiburg im Breisgau/DE)

POSTER PRESENTATIONS | WEDNESDAY, 29 MARCH

- PP-120 Low valent copper clusters as decomposition products of Copper(I) Boryl complexes
Christian Kleeberg, Wiebke Drescher, Corinna Borner (Braunschweig/DE)
- PP-121 Formation and properties of mullite-type photocatalysts for the degradation of persistent organic pollutions
Selina Schuh, Alexander Wollbrink, Thorsten M. Gesing (Bremen/DE)
- PP-122 Re-investigation of the crystal structure of $\text{CuSn}(\text{OH})_6$ by x-ray and neutron powder diffraction
Ellen Häußler, Anton A. Kulbakov, Darren C. Peets, Dmytro S. Inosov
Thomas Doert (Dresden/DE)
- PP-123 New rare iodate selenites with potential for non-linear optical properties
Kevin Eble, Harald Hillebrecht (Freiburg im Breisgau/DE)
- PP-124 Investigation on the crystal structure and phase transition of $\text{K}_{9.6}\text{Ca}_{1.2}\text{Si}_{12}\text{O}_{30}$ at elevated temperatures
Hang Liu, Volker Kahlenberg, Hannes Krüger (Innsbruck/AT)
Edgar Dachs (Salzburg/AT)
- PP-125 Vacancy-ordered perovskite variants: $\text{A}_3\text{As}_2\text{X}_9$ ($\text{A} = \text{Rb}, \text{Cs}, \text{CH}_3\text{NH}_3$; $\text{X} = \text{Cl-I}$) and $\text{Cs}_4\text{As}_2\text{CuCl}_{12}$
Michael Daub, Harald Hillebrecht (Freiburg im Breisgau/DE)
- PP-126 Structural and magnetic properties of $\text{Sr}_3\text{Fe}_{2+x}\text{Mo}_{1-x}\text{O}_{9-3x/2}$ ($x = 0.45, 0.60$, and 1)
Abdelhadi El Hachmi, Said El Ouahbi, Bouchaib Manoun
Hassan Lassri (Settat/MA)
- PP-127 Richardsite $\text{Zn}_2\text{CuGaS}_4$ – a mixed crystal of Sphalerite and Gallite
Yvonne Tomm, Daniel Abou-Ras, Galina Gurieva, Susan Schorr (Berlin/DE)
- PP-128 Accurate crystal structures of ices from X-ray and electron diffractions with Hirshfeld atom refinement
Krzysztof Woźniak, Michał Chodkiewicz, Roman Gajda (Warsaw/PL)
- PP-129 Structural features of interaction 4-aminopyridine with layered semiconductors
Aysel Rahimli, Imamaddin Amiraslanov (Baku/AZ)

Late poster

- PP-130 Sodium-ion solid electrolytes – computational search and experimental validation
Tilmann Leisegang, K. Uhlemann, S. Kachariya, M. Momeni (Freiburg/DE)

From an Idea to a Published Issue

Every year, *Elements* publishes six thematic issues on subjects related to the general disciplines of mineralogy, geochemistry, and petrology. The editorial team looks for topics that

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- represent established but progressing fields
- would be of interest to a broad cross-section of readers
- have not been adequately represented by *Elements* before or have advanced considerably since the topic was previously covered

Each proposal is carefully evaluated by our editorial team for thematic scope, content, and authorship. Feedback is then provided to the proposers.

Elements

An International Magazine of Mineralogy, Geochemistry, and Petrology

Once a proposal is accepted and included in the *Elements* lineup, the fun really begins! Over the subsequent 15–20 months, timelines and deadlines are set, authors are invited by the guest editors to write articles, and articles go through several stages of review (by external reviewers, by the guest and principal editors, and by the *Elements* editorial team). At the end of this process, the issue goes to press and is shipped to our over 16,000 readers.

The journey from an idea to a published magazine involves many steps. The goal? A lineup of well-written thematic issues that readily conveys the exciting aspects of mineralogy, petrology, and geochemistry.

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Would you like to read about a certain topic in *Elements*?
Do you think your research area would make a great thematic issue?

Submit a thematic proposal!

The next submission deadline is **August 25, 2023**.

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We look forward to receiving your proposal!



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SOCIAL PROGRAMME

Welcome reception

Come together for drinks and snacks to enjoy the first evening of the conference in a very special atmosphere. The Laue Talk and the “DGK-Ehrenabend” will be held in the plenary hall. Afterwards, the welcome reception will take place in the foyer of Otto-Stern-Zentrum in the Industrial exhibition. Allow yourself interesting conversations with colleagues, old friends and meet new acquaintances.

Date	Monday, 27 March
Time	19.00–20.45
Fee	included in the conference fee, registration required
Venue	Industrial exhibition



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Social evening

We would like to invite you to the social evening of the conference at “Schuch’s Restaurant”, a rustic guest house on the outskirts of Frankfurt. The original cider pub still dedicates itself to creative apple cuisine and is now being run by the 5th generation. Don’t miss this highlight of the conference. Enjoy the evening in a place with an exciting history.

Date	Wednesday, 29 March
Time	19.00–23.00
Fee	60 EUR
Venue	Schuch’s Restaurant, Alt Praunheim 11 60488 Frankfurt am Main



© Schuch's Restaurant

Lightning talks of Young crystallographers

The “Young crystallographers” are happy to welcome you to the traditional Lightning Talks at the Annual DGK Meeting. This year, we are looking forward to a microsymposium where 10 young crystallographers will introduce their research in 6-minute appetizer “Lightning talks”. Each contribution is complemented by a poster that will be presented and discussed in the poster session afterwards. Furthermore, we are especially happy to have this year’s awardees of the Lieselotte Templeton Prize present their winning research projects.

Date	28 March
Time	15.15–16.45
Room	Lecture hall – OSZ H6

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 Get together on Thursday evening. We will give a brief summary of last year’s activities (especially our 2nd joint meeting with the Young Crystal Growers in Freiberg) and will talk about the upcoming year. We will elect a new co-chair, and will have plenty of time for general discussions on Young crystallographers’ topics. Another highlight will be the granting of the “Lightning talks” poster prizes. Snacks, coffee/tea and soft drinks will be served.

Date	28 March
Time	18.45–20.15
Room	Lecture hall – OSZ H6

We are looking forward to welcoming you!

Constantin Buyer and Jakob Möbs
Chairs of the “Young Crystallographers”

Upcoming events

“Young Crystallographers – 10th Anniversary Meeting at DESY”

Date	4–6 Oktober
Place	DESY Hamburg

GENERAL INFORMATION



Conference language

The conference language is English.



Opening hours

	Monday	Tuesday	Wednesday	Thursday
Check-in	12.00–19.30	08.30–19.00	08.30–18.00	08.30–13.00
Industrial exhibition	13.00–21.00	08.30–20.30	08.30–18.00	08.30–12.30



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 check-in on site.



Publication of abstracts

All abstracts will be published in the abstract book and will be available on the conference homepage.



Certificates of attendance

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



Poster awards

From all accepted posters the three best posters will be awarded with a prize money of 300 EUR, 200 EUR and 100 EUR.

The award ceremony will take place during the social evening on Wednesday, 29 March.

Main sponsors

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Elements – An International Magazine of Mineralogy, Geochemistry and Petrology

Walter de Gruyter GmbH

Tuesday, 28 March

Bruker AXS GmbH (Karlsruhe/DE)

12.30–13.30

Lecture hall – OSZ H4



You are cordially invited to our lunchtime reception:

Challenging samples – new high efficiency tools

Agenda:

Pair-Distribution-Function Generation and Refinement in TOPAS (Arnt Kern)

How to reduce electrical power requirements for high-intensity X-ray sources? (Juergen Graf)

New solutions for high energy radiation studies (Tobias Stuerzer)

Each talk is planned for approximately 15 min. After several years of remote meetings, this seminar is a perfect opportunity to welcome new members to the family but also to see familiar faces.

A small lunch box will be made available during the reception. Please, pick-up your personal ticket at our stand no. 7 on Monday to secure your seat.

Wednesday, 29 March

Rigaku Europe SE (Oxford/GB)

12.30–13.30

Lecture hall – OSZ H3



Lunch cones will be provided. The speaker will be Dr Mathias Meyer. Join us to learn more about the latest developments from Rigaku and get tips on how to get the most out of your unit.

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