Leibniz Universität Hannover

D G K

33rd ANNUAL MEETING of the GERMAN CRYSTALLOGRAPHIC SOCIETY (DGK)

PROGRAMME

10–13 MARCH 2025
HANNOVER

www.dgk-conference.de

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ORGANISATION

Venue
Leibniz University Hannover
Welfengarten 1 I 30167 Hannover (Germany)

Date
10–13 March 2025

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German Crystallographic Society (DGK)

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Dear colleagues,

It is our immense pleasure to welcome you to the 33rd Annual Meeting of the German Society for Crystallography (DGK) at the Gottfried Wilhelm Leibniz University Hannover (LUH). The conference will be held at the centrally located Welfenschloss, the main building of our university.

We would like to thank the board of the DGK for trusting us to host this conference, to our office and its staff, as well as to the Conventus team, who supported us in preparing the conference. We are especially grateful to the industrial exhibitors, whose support is essential for this conference.

We would of course also like to express our sincere thanks to all of you, the participants coming from far and wide, as well as our close neighbourhood. We are excited to learn more about the excellent science we have had the pleasure to peruse in your abstracts. The stimulating and interesting ideas from and to all fields of crystallography will provide a great basis for interactions between chemists, physicist, biologists, earth scientists and all material sciences. As a result, and perhaps most importantly, this conference will provide a wonderful opportunity for knowledge transfer between these fields and stimulate new research directions. This breadth of expertise is reflected by our six plenary speakers, who will highlight exhilarating aspects of crystallography.

Topics will be presented in 23 Microsymposia and two poster sessions, including one for young scientists in the form of lightning talks.

So once again, a warm welcome. We are looking forward to your contributions and to an exciting and inspiring conference here at LUH. Thank you for coming to attend and celebrate the 33rd crystallographic conference with us.

The Orga Team
Claus Rüscher, Institute of Earth System Sciences, LUH
Yasar Krysiak, Institute of Inorganic Chemistry, LUH
Armin Feldhoff, Institute of Physical Chemistry and Electrochemistry, LUH
Jesko Köhnke, Institute of Food and one Health, LUH
Hilke Petersen, Institute of Production Engineering and Machine Tools

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17:30-19:30 DGK Honour Evening p. 12					
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DGK General Assembly p. 20				
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Opening & Closing
Poster session
Plenary lecture
Microsymposium
DGK Internal
Industrial symposium
Social programme
Award symposium

13:00–14:15 Opening
Room E001

14:30–15:30 Plenary lecture I
Room E001
Chair Ute Kolb (Mainz/DE)

14:30 tbd
PL-01

16:00–17:15 MS 1 I Functional Materials I
Room E001
Chair Hilke Petersen (Garbsen/DE)

16:00 Thermoelectric Performance Enhancement of Textured Calcium Cobaltite Ceramic Derived from Electrospun Nanoribbons and Spark Plasma Texturing
OP-001 Kristina Kebel, Katharina Kruppa (Hannover/DE), Itzhak Ishay Maor, Anat Karlin (Haifa/IL), Frank Steinbach (Hannover/DE), Gennady Shter (Haifa/IL), Dorothea Stobitzer (Selb/DE), Hilke Petersen, Bernd Breidenstein (Hannover/DE), Meirav Mann-Lahav, Gideon Grader (Haifa/IL), Armin Feldhoff (Hannover/DE)

16:15 Optimized Oxygen Permeation in $La_2NiO_{4+\delta}$ Membranes via Nanorod-Based Crystal Facet Engineering
OP-002 Merle Wellmann, Giamper Escobar Cano, Frank Steinbach (Hannover/DE), Moritz Thiem, Wenji Xie, Anke Weidenkaff, (Darmstadt/DE), Armin Feldhoff (Hannover/DE)

16:30 Novel Hybrid Perovskite Crystal Structures Including Ferrocene as Redox Switch to Reversibly Alter Semiconductor Properties
OP-003 Melina Dahlke, Yasar Krysiak, Sebastian Polarz (Hannover/DE)

16:45 Synthesis and Characterization of Ultrasmall Glutathione Coated Rhenium-Nanoparticles
OP-004 Niklas Kost, Oleg Prymak (Essen/DE), Marc Heggen (Jülich/DE), Kateryna Loza, Matthias Epple (Essen/DE)

17:00 Kesterite Single Crystal Synthesis in Different Salt Flux – Extrinsic Doping Strategies in Monograin Solar Cells
OP-005 Henrik Prell, Galina Gurieva, Susan Schorr (Berlin/DE)

16:00–17:15 MS 2 I Electron diffraction methods
Room F142
Chair Martin Etter (Hamburg/DE), Martin Meven (Garching/DE)

16:00 Serial Precession Electron Diffraction, a Novel and Advantageous Development for Serial Crystallography in a TEM
OP-006 Sergi Plana-Ruiz (Tarragona/ES), Penghan Lu, Govind Ummethala, Rafal E. Dunin-Borkowski (Jülich/DE)

16:15 Unit Cell Parameters Determination From a set of Independent Electron Diffraction Zonal Patterns
OP-007 Tatiana Gorelik (Jülich/DE), Gerhard Miehe (Darmstadt/DE), Fredo Erxleben (Dresden/DE)

16:30 In the Footsteps of Pasteur: Identifying Conglomerate Systems Using State-of-the-Art Electron Diffraction
OP-008 Christian Jandl (Allschwil/CH), Ivo B. Rietveld, Felix Painsecq, Gerard Coquerel (Rouen/FR), Laura Samperisi, Gustavo Santiso-Quinones, Alessia Portieri, Danny Stam (Allschwil/CH)

16:45 An In-Depth Analysis of Modern 3D ED Methods
OP-009 Yann Schmitt, Yasar Krysiak (Hannover/DE), Sergi Plana-Ruiz (Tarragona/ES)

17:00 Correlated Small- and Wide-Angle 3D Electron Diffraction for Structure Analysis of Highly Ordered Nanoparticle-Based Superstructures
OP-010 Elisabeth Fetter, Yann Schmitt, Yasar Krysiak (Hannover/DE)

16:00–17:15 MS 3 I Crystal Chemistry, solid state compounds
Room F107
Chair Thorsten M. Gesing (Bremen/DE), Guido Kreiner (Freiberg/DE)

16:00 The $BeGeN_2$-type: A Story of a Unique Structure
OP-011 Joachim Breternitz (Steinfurt/DE)

16:15 Vacancy Containing Complex Intermetallic Phases Derived from the A2 type (W type)
OP-012 Andreas Leineweber (Freiberg/DE)

16:30 Ternary Ni-Sb-Te Nanoparticles by Co-Reduction in a One-Pot Microwave-Assisted Polyol Process
OP-013 Thomas Doert, Yiran Wang, Eduardo Arturo Carillo Aravena, Michael Ruck, Maria Roslova (Dresden/DE)

16:45
OP-014
Morphotropism in Copper Oxosulfates: Order in $Cs_4Cu_7O_3(SO_4)_6$ vs. Disorder in $Cs_4Cu_7O_3(SO_4)_6[Cu_{0.2}O_{0.2}]$ and Puninite Morphotropic Series
Artem Borisov (Kiel/DE), Oleg Siidra (Saint Petersburg/RU), Dmitri Charkin (Moscow/RU), Ivan Pimshin (Saint Petersburg/RU), Astrid Holzheid (Kiel/DE)

17:00
OP-015
Combinatorial Synthesis: Structure Determination from Complex Mixtures
Martin Schreyer, Gwilherm Nénert (Almelo/NL), Maxim Avdeev (Sydney/AU)

16:00–17:15
Room F128
MS 4 I Teaching of Crystallography

Chair
Reinhard Neder (Erlangen/DE), Robert E. Dinnebier (Stuttgart/DE)

16:00
OP-016
Empowering Biochemistry Students through Hands-On Structural Biology: Teaching and Research Converge
Tatjana Barthel, Frank Lennartz, Thomas Crosskey, Tobias Bock-Bierbaum, Bernhard Loll, Yvette Roske, Uwe Müller, Oliver Daumke, Markus Wahl, Manfred Weiss, Gert Weber (Berlin/DE)

16:15
OP-017
Is my Crystal Structure Solved Correctly?
Alexander Virovets (Frankfurt a. M./DE)

16:30
OP-018
Structure Solution and Refinement by High School Students
Erhard Irmer (Göttingen/DE)

16:45
OP-019
Teaching Crystallography to a Growing Community
Martin Adam, Tobias Stürzer, Jens Luebben (Karlsruhe/DE), Joerg Kaercher, Michael Ruck (Madison, WI/US)

17:00
OP-020
X-ray Schools for Beginners and Advanced X-Ray Diffraction Users at Helmholtz-Zentrum Berlin
Michael Tovar, René Schwiddessen, Daniel M. Többens, Susan Schorr (Berlin/DE)

17:30–19:00
Room E001
DGK Honour Evening

19:00–21:00
Lichthof
Welcome Reception
see page 45

09:00–10:00 Plenary lecture II
Room E001
Chair Claus Rüscher, Armin Feldhoff (Hannover/DE)

09:00 "In-situ, in Air, High Temperature Synchrotron Studies of Ceramics"
PL-02 Waltraud M. Kriven (Urbana, IL/US)

10:30–12:00 MS 5 I Functional Materials II
Room E001
Chair Claudia Weidenthaler (Mülheim a. d. Ruhr/DE)

10:30 Multitechnique Study and Structure Elucidation of two Different Materials with TADF Properties Using Three-Dimensional Electron Diffraction
OP-021 Melanie Appelmann, Ute Kolb, Robert Graf (Mainz/DE)

10:45 Grain Alignment via Magnetic Field to Boost Anisotropic Oxygen Transport in Ruddlesden–Popper Oxide Ceramic Membranes
OP-022 Armin Feldhoff, Giamper Escobar Cano, Zhijun Zhao, Frank Steinbach (Hannover/DE), Bernd Breidenstein, Hilke Petersen (Garbsen/DE), Andreas Graff (Halle (Saale)/DE), Marc Widenmeyer, Anke Weidenkaff (Darmstadt/DE), Motohide Matsuda (Kumamoto/JP)

11:00 Development and Characterization of Reactive Hydro-*closo*-Borates with $[B_nH_n]^{2-}$ Anions (n = 10 and 12): From New Crystal Motifs to High-Energy Materials
OP-023 Rouzbeh Aghaei Hakkak, Thomas Schleid (Stuttgart/DE)

11:15 Residual Stress Measurements of PVD Thin Films – A Comparative Study of Benefits and Flaws of Techniques
OP-024 Hilke Petersen (Garbsen/DE)

11:30 Composition Space Mapping of High-Entropy Perovskites
OP-025 Andrea Kirsch (Copenhagen/DK)

11:45 Topochemical Reactions: Fluorination and De-Fluorination of Ruddlesden–Popper Type Oxide in the Context of Structural-Optical Properties for the Photocatalytic Application
OP-026 Shama Perween (Stuttgart/DE)

10:30–12:00 Room F142 Chair	MS 6 I Advances and applications of spectrocopy and neutron and synchrotron radiation Holger Kohlmann (Leipzig/DE), Martin Meven (Garching/DE)
10:30 OP-028	The High-Brilliance Neutron Source Project – A Next Generation Neutron Source for Science and Industry Thomas Gutberlet, Paul Zakalek, Karen Friese, Stephan Förster (Jülich/DE), Mirijam Zobel (Aachen/DE), Ulrich Rücker, Jörg Voigt, Eric Mauerhofer, Klaus Lieutenant, Jingjing Li, Johannes Baggemann (Jülich/DE)
10:45 OP-029	Iterative Tomographic Reconstruction of Strain for Polycrystalline Samples Peter Modregger, Felix Wittwer, Ahmar Khaliq (Siegen, Hamburg/DE)
11:00 OP-030	Superstructure Refinement of α-Black Minium from Combined nPDF and sPDF Data within ML-DFT-PDF Analysis. Thorsten M. Gesing, Wilke Dononelli, Lars Robben, M. Mangir Murshed (Bremen/DE)
11:15 OP-031	New Instrumentation at P02.2, PETRA III, DESY Employing Soller Slits for Structural Measurements of Non-Crystalline Materials at Extreme Conditions Christoph Otzen, Giuseppe Cocomazzi (Freiburg i. Br./DE), Mario Wendt, Konstantin Glazyrin (Hamburg/DE), Clemens Prescher (Freiburg i. Br./DE)
11:30 OP-032	Simultaneous XRD and XRF with Sub-Micrometer Spatial Resolution for Defect Determination Ahmar Khaliq, Felix Wittwer, Peter Modregger (Siegen, Hamburg/DE)
11:45 OP-033	Estimation of ^{29}Si, ^{27}Al and ^{19}F Chemical shifts for Muscovites, Trilithionites and Polylithionites using Density Functional Theory (DFT) WIEN2k Calculations and Comparison with Experimental NMR Shifts Michael Fechtelkord (Bochum/DE)
10:30–12:00 Room F107 Chair	MS 7 I Complex and Aperiodic Structures Thomas Doert (Dresden/DE)
10:30 OP-034	Complex Stacking Disorder in Boratriptycene-Type Lewis Superacid Precursors Mischa Wenisch, Alexander Virovets (Frankfurt a. M./DE), Berthold Stöger (Wien/AT)

10:45
OP-035
Phase Diagram of and Quantum Criticality in $Sc(V_{1-x}Cr_x)_6Sn_6$
Michael Merz, Nour Maraytta (Karlsruhe/DE), Xinrun Mi, Xintong Chen (Chongqing/CN), Frédéric Hardy, Liran Wang, Christoph Meingast (Karlsruhe/DE), Aifeng Wang, Yisheng Chai, Mingquan He (Chongqing/CN)

11:00
OP-036
Freezing Na hopping in Zinc-Phosphate Sodalite $|Na_6(H_2O)_8|[ZnPO_4]_6|$
Konrad Krämer, Thorsten M. Gesing, Lars Robben (Bremen/DE)

11:15
OP-037
Ordering Phenomena of Aperiodic Mullite from Refined Superspace Models
Paul Benjamin Klar (Bremen/DE)

11:30
OP-038
Crystal Structure and Anisotropic Magnetic Properties of Incommensurately Modulated $K_{1-x}CrSe_2$ ($x \approx 0.13$)
Felix Eder, Catherine Witteveen, Enrico Giannini, Fabian O. von Rohr (Geneva/CH)

11:45
OP-039
Incommensurate Displacive and Occupational Modulation in Hexakis(Urea-*O*)iron(III) Nitrate
Toms Rekis (Frankfurt a. M./DE)

10:30–12:00
Room F128
MS 8 I Structural biology meets chemistry

Chair
Jesko Köhnke (Hannover/DE), Daniel Kümmel (Münster/DE)

10:30
OP-040
Structural Insights Guiding Further Applications of Flavin-Dependent Halogenases
Simon Bork, Hartmut H. Niemann (Bielefeld/DE)

10:48
OP-041
Crystal Structures of Non-Covalent Protein-Foldamer Hybrid Architectures
Johannes Sigl, Vasily Morozov, Lingfei Wang (München/DE), Eric Merlet, Yann Ferrand (Bordeaux/FR), Celine Douat, Ivan Huc (München/DE)

11:06
OP-042
The Role of Identical Charges in Enzyme Catalysis: Friends or Foes?
Kai Tittmann (Göttingen/DE)

11:24
OP-043
Towards a Comprehensive Understanding of the Structure and Function of the Human Glycogen Debranching Enzyme in its Role in the Glycogen Metabolism
Christian Roth, Ruben Ananian, Malkeet Singh (Berlin/DE)

11:42	Sustainable use of metabolites in glutamine amidotransferases multienzyme complexes
OP-044	Matthias Wilmanns (Hamburg/DE)
12:15–13:15	Industrial symposium I Bruker AXS GmbH
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13:30	Crystal structure evolution tracking using in situ 3D ED and 4D-STEM
PL-03	Joke Hadermann (Antwerp/BE)
15:00–16:30	MS 9 I Crystalline/Non-crystalline/Disordered
Room E001	
Chair	Andrea Kirsch (Copenhagen/DK)
15:00	Powder Diffraction and Pair Distribution Function Studies of Disorder Phenomena in Battery Electrodes
OP-045	Martin Aaskov Karlsen (Hamburg/DE)
15:30	Structural Investigation of Calcium Phosphate Nanoparticles
OP-046	Oleg Prymak, Kathrin Kostka, Kateryna Loza, Matthias Epple (Essen/DE)
15:45	Effect of the Solvent and the Anion Exchange in Hybrid Halide Perovskites Precursor Solutions
OP-047	Ana Palacios Saura (Berlin/DE), Joachim Breternitz (Berlin, Steinfurt/DE), Armin Hoell, Susan Schorr (Berlin/DE)
16:00	Investigation of the Local Structure of Boron Carbide ($B_{13}C_2$) Using the Pair Distribution Function Method (PDF)
OP-048	Anna Piekara, Wojciech Slawinski (Warsaw/PL)
16:15	Introducing Non-Metals in Skutterudite-Type Fe1.76Ni2.24Sb12 to Improve Thermoelectric Properties
OP-049	Paul Sicher, Oliver Oeckler (Leipzig/DE)
15:00–16:30	MS 10 I Phase transitions- Extreme Conditions
Room F142	
Chair	Martin Etter (Hamburg/DE), Ella Schmidt (Bremen/DE)

15:00 OP-050
The Displacive Phase-Transition Anharmonicity Energy Model DEA+G
Thorsten M. Gesing, Lars Robben, M. Mangir Murshed (Bremen/DE)

15:15 OP-051
Pressure Dependence of the SHG intensity of CO_2-V
Tim Harald Reuter, Lkhamsuren Bayarjargal (Frankfurt a. M./DE), Victor Milman (Cambridge/GB), Björn Winkler (Frankfurt a. M./DE)

15:30 OP-052
Shock Wave Treatment of Si-Al-O-N Polytypoids and Formation of Rocksalt-Type Aluminium Oxynitride rs-Al(O,N)
Kevin Keller, Erica Brendler, Thomas Schlothauer (Freiberg/DE)

15:45 OP-053
Squeezing from Di- To Monohydrate: The Enexpected Pressure-Induced Dehydration of CuTeO3·2H2O
Sharif Abdel Azim, Kamil F. Dziubek, Herta S. Effenberger, Dominik Talla, Ronald Miletich (Wien/AT)

16:00 OP-054
Negative Thermal Expansion in Quaternary Chalcogenide Compound Semiconductors
Susan Schorr, Galina Gurieva (Berlin/DE), Maxim Avdeev (Lucas Heights/AU)

16:15 OP-055
Experimental Charge Density Studies of Phase Transition in Calcite under Pressure
Krzysztof Woźniak, Agnieszka Huć, Marcin Stachowicz, Tomasz Poręba, Mohamed Mezouar (Warsaw/PL), Przemyslaw Dera (Honolulu, HI/US)

15:00–16:30 MS 11 I Molecular Crystallography/Framework structures

Room F107
Chair: Alexander Pöthig (Garching/DE)

15:00 OP-056
Crystallization of Molecular Glass: From Amorphous State to new Polymorphic Forms in the API Sodium Naproxen
Dusko Popovic (Kassel/DE), Gwilherm Nénert, Lei Ding (Almelo/NL)

15:15 OP-057
Capillary Crystallisation: A Versatile Tool for Chemical Crystallography
Nils Nöthling (Mülheim a. d. Ruhr/DE)

15:30 OP-058
Comprehensive Investigation on Carbonyl Hypoiodites: The Fragile Nature of a Complex System
Sevval Efe Celik (Bochum, Essen/DE), Klaus Merz (Bochum/DE)

15:45 Polyiodides Trapped in Hydrogen Bonded Frameworks Constructed by Methylxanthinium Cations
OP-059 Guido J. Reiss (Düsseldorf/DE)

16:00 Amplification of Negative Gas Adsorption in a Multivariate Framework
OP-060 Volodymyr Bon, Francesco Walenszus, Stefan Kaskel (Dresden/DE)

16:15 How the Disordering Within a Giant Supramolecule Influences the Intermolecular Interactions and Crystal Packing
OP-061 Eugenia Peresypkina (Frankfurt a. M./DE)

15:00–16:30 MS 12 I Young Crystallographers: Lightning talks
Room F128
Chair Florian Meurer (Regensburg/DE), Anushka Ghosh (Berlin/DE)

15:00 Crystal Structure of gDcL3·6h2o and its Intercalation into Saponite as new Hybrid Material Formation
LT-01 Lenka Krešáková, Juraj Černák, Juraj Kuchár, Martin Orendáč, Róbert Tarasenko, Hryhorii Titikov (Košice/SK), Jana Madejová, Ľuboš Jankovič (Bratislava/SK)

15:05 An in Situ Neutron Diffraction Experiment on the Deuteration of the CrB Type Zintl Phase EuGe
LT-02 Leonhard Yuuta Dorsch (Leipzig/DE), Thomas Hansen (Grenoble/FR), Holger Kohlmann (Leipzig/DE)

15:10 Coordination Complexes of Rare Earth Lons Using C_3-Symmetrical Triaminoguanidinium-Based Ligands
LT-03 Nico Linnartz, Sonja Liu, Iris Oppel (Aachen/DE)

15:15 Unveiling Crystal Packing of 1:1 Co-Crystal of 6-(4*H*-1,2,4-triazol-4-yl) Pyridin-2-Amine and Pyridine-2,6-Diamine: An Energetic Point of View
LT-04 Milica G. Bogdanović (Novi Sad/RS), Maik Wyshusek (Düsseldorf/DE), Iryna Konovalova (Düsseldorf/DE, Kharkiv/UA), Guido J. Reiss (Düsseldorf/DE), Marko V. Rodić (Novi Sad/RS)

15:20 Polynitrides of Main Group Elements Synthesized under Extreme Conditions
LT-05 Lukas Brüning (Frankfurt a. M./DE), Nityasagar Jena (Linkoeping/SE), Elena Bykova, Pascal Jurzick (Frankfurt a. M./DE), Igor A. Abrikosov (Linkoeping/SE), Maxim Bykov (Frankfurt a. M./DE)

15:25 Powder Diffraction Under Pressure, a new Hydrostatic Pressure Diffraction Cell
LT-06 Lukas Sippach (München/DE), Henrique Geraissate, Arne Meyer, Alexander Schoekel, Anita Ehnes (Hamburg/DE), Gregor Kieslich (München/DE)

15:30 Diffuse Scattering in Sanidines
LT-07 Christin Wiggers, Ella Schmidt (Bremen/DE), Daniel A. Chaney (Grenoble/FR)

15:35 Synthesis and Crystal Structure of a High Pressure Polymorph of the Inorganic Pyrocarbonate $Na_2[C_2O_5]$
LT-08 Lena Wedek, Dominik Spahr, Lkhamsuren Bayarjargal, Maxim Bykov (Frankfurt a. M./DE), Victor Milman (Cambridge/GB), Björn Winkler (Frankfurt a. M./DE)

15:40 Formation of Novel Hydrogen-Bearing Iron Oxides FE5O8HX and FE7O11HX through a Thermal Decomposition of goethite FEOOH at High Pressure
LT-09 Valentin Kovalev, Dominik Spahr (Frankfurt a. M./DE), Nico Giordano (Hamburg/DE), Anna Pakhomova (Grenoble/FR), Elena Bykova (Frankfurt a. M./DE)

15:45 The Coordination Number Rule – An Effective Tool for Coordination-Based Prediction and Rationalization of Inorganic Structures?
LT-10 Niklas Langer, Holger Kohlmann (Leipzig/DE)

15:50 Controlled Assemblies of Supramolecular Organometallic Complexes in the Solid-State
LT-11 Julian Zuber, Alexandra Heidecker, Alexander Pöthig (Garching/DE)

15:55 Structural Insights into the Enzymatic Hydrolysis of Polyurethanes with UMG-SP2
LT-12 Parinita Singh (Berlin/DE), Da'san Jaradat (Berlin/DE, Al-Salt/JO), Manfred Weiss, Frank Lennartz, Gert Weber (Berlin/DE)

16:00 Structural Properties, Thermal Expansion and Heat Capacity of Li_2GeO_3 at Low Temperature
LT-13 Denis Werner, Eiken Haussühl, Dominik Spahr, Katharina Köhler, Lkhamsuren Bayarjargal, Lena Wedek, Björn Winkler (Frankfurt a. M./DE)

16:05
LT-14
Controlled Structure and Crystallinity of Electrospun Calcium-Cobaltit Nanofibers for Enhanced Thermoelectric Performance
Itzhak Ishay Maor (Haifa/IL), Katharina Kruppa (Hannover/DE), Adi Rozencweig, Amir Sterzer (Haifa/IL), Frank Steinbach (Hannover/DE), Vadim Beilin (Haifa/IL), Bernd Breidenstein (Hannover/DE), Gennady Shter, Meirav Mann-Lahav (Haifa/IL), Armin Feldhoff (Hannover/DE), Gideon Grader (Haifa/IL)

16:10
LT-15
Structure-Based Discovery of Inhibitors of Itaconic Acid Synthesis by ACOD1 (IRG1)
Mingming Zhao (Braunschweig/DE), Chutao Chen, Frank Pessler (Hannover/DE), Wulf Blankenfeldt, Konrad Büssow (Braunschweig/DE)

16:15
LT-16
Crystallographic and Spectroscopic Study of CO Binding in Dodecameric Tyrosine-Coordinated Heme Protein from *Oligotropha Carboxydovorans*
Anushka Ghosh, Jae-Hun Jeoung, Holger Dobbek, Peter Liebers (Berlin/DE)

16:20
LT-17
The Search for FGE Stabilizing Molecules: From Fragment Screen Hits to Potential Lead(s)
Julia L. Kowal (Bielefeld/DE), Niama Ezzaidi (Southampton/GB), Jan Wollenhaupt (Berlin/DE), Karthikeyan Radhakrishnan, Tatjana Pietrowski, Melanie Löwen, Manisha Thangarasah, Willy Keller, Sarfaraz Alam (Bielefeld/DE), Manfred Weiss (Berlin/DE), Matthias G. J. Baud (Southampton/GB), Hartmut H. Niemann (Bielefeld/DE)

16:25
LT-18
Influence of Ligand Change in the Primary-Coordination Sphere on Metal-Binding of Bimetallic Sulerythrin
Samriddhi Bhattacharya, Jae-Hun Jeoung, Stefan Rünger, Eric Herrmann, Holger Dobbek (Berlin/DE)

16:30-18:00
Lichthof
Poster session I
see page 30

18:15–19:45
Room E001
DGK General Assembly

19:45–20:45
Room F142
Get Together Young Crystallographers
see page 46

09:00–10:00 Plenary lecture IV
Room E001
Chair Ella Schmidt (Bremen/DE)

09:00 Truchet-tile architectures in materials chemistry
PL-04 Andrew Goodwin (Oxford/GB)

10:30–12:00 MS 13 I In situ/operando studies of functional materials
Room E001
Chair Andrea Kirsch (Copenhagen/DK)

10:30 *In situ* X-ray and Neutron Diffraction Studies on Rare-Earth Hydride Oxid es as Photochromic Bulk Materials
OP-062 Marvin Michak, Marie Leinweber, Holger Kohlmann (Leipzig/DE)

10:45 In-situ Monitoring of the Successive Phase Transformation Pathway of NH_3 Decomposition Catalysts by X-ray Powder Diffraction
OP-063 Christos Sidiropoulos, Claudia Weidenthaler (Mülheim a. d. Ruhr/DE)

11:00 Study of Sorption Properties of CALF-20 by *in Situ* X-ray Powder Diffraction
OP-064 Anastasiia Sleptsova, Sebastian Bette, Frank Adams, Robert E. Dinnebier (Stuttgart/DE)

11:15 Sample Cell for I*n-Situ* Measurements of Ferroelectric Polarization and Diffraction at Beamline P24, DESY
OP-065 Preeti Pokhriyal, Heiko-Schulz Ritter, Martin Tolkiehn (Hamburg/DE)

11:30 Peculiarities in Structural Behaviour of Graphite During Anionic Intercalation of PF6-, FSI- and ClO4- at Various Temperatures
OP-066 Mikhail Gorbunov, Daria Mikhailova (Dresden/DE)

11:45 Ammonium Dinitramide- Crystallographic Aspects of the Oxidizers Stability
OP-067 Peter Schultz, Thomas Heintz, Claudia Seidel, Michael Herrmann (Pfinztal/DE)

10:30–12:00 MS 14 I Extreme conditions
Room F142
Chair Susan Schorr (Berlin/DE), Volodymyr Bon (Dresden/DE)

10:30
OP-068 Diverse Geometries of Pyrocarbonate $[C_2O_5]^{2-}$ Units at High Pressures
Dominik Spahr, Lkhamsuren Bayarjargal, Elena Bykova, Maxim Bykov (Frankfurt a. M./DE), Victor Milman (Cambridge/GB), Björn Winkler (Frankfurt a. M./DE)

10:45
OP-069 Stabilization of the $C_2N_5^{7-}$ Anion in Recoverable High-Pressure $Eu_4Fe_{0.9}(C_2N_5)_2$ Pyronitridocarbonate
Fariia Iasmin Akbar, Lukas Brüning (Frankfurt a. M./DE), Uwe Ruschewitz (Köln/DE), Leonid Dubrovinsky (Bayreuth/DE), Maxim Bykov (Frankfurt a. M./DE)

11:00
OP-070 A new Modification of Sm_3Ge_5 Synthesized Under Extreme Conditions and an Unprecedented Intermetallic Suboxide $Sm_{26.25}Ge_{22.75}O_5$
Julia-Maria Hübner, Wilder Carrillo-Cabrera, Thomas Doert, Ulrich Schwarz (Dresden/DE)

11:15
OP-071 High-Pressure Synthesis of an Iron Carbonate, $Fe_2[CO_3]_3$
Lkhamsuren Bayarjargal, Dominik Spahr, Elena Bykova, Yu Wang (Frankfurt a. M./DE), Nico Giordano (Hamburg/DE), Victor Milman (Cambridge/GB), Björn Winkler (Frankfurt a. M./DE)

11:30
OP-072 Cr^{3+}-Containing Carbonates and Cr_2O_3-Pbcn at Extreme Conditions
Yu Wang, Lkhamsuren Bayarjargal, Maxim Bykov, Elena Bykova, Dominik Spahr (Frankfurt a. M./DE), Victor Milman (Cambridge/GB), Konstantin Glazyrin (Hamburg/DE), Björn Winkler (Frankfurt a. M./DE)

11:45
OP-073 Polyamorphism vs. Polymorphism in SnI_4
Kazuhiro Fuchizaki (Matsuyama/JP)

10:30–12:00 MS 15 I New trends in quantum Crystallography
Room F107
Chair Florian Kleemiss (Aachen/DE), Marvin Treger (Hannover/DE)

10:30
OP-074 Current developments of Hirshfeld Atom Refinement
Simon Grabowsky (Bern/CH)

10:45
OP-075 Database-Driven Prediction of Biomolecular Electrostatic and Optoelectronic Properties under Various Conditions
Anna Krawczuk, Raphael Fernandes Ligorio (Göttingen/DE)

11:00 OP-076	Quantum Crystallography as a Chemist's Tool for Chemical Bond Analysis Florian Meurer (Regensburg/DE), Florian Kleemiss (Aachen/DE), Christoph Hennig (Grenoble/FR), Michael Bodensteiner (Regensburg/DE)
11:15 OP-077	What are the Actual Crystal Structure Organisation Principles of Halogen Substituted Anilines from the Energetic Viewpoint? Iryna Konovalova (Düsseldorf/DE)
11:30 OP-078	ORCA Molecular Dynamics Simulation to Predict Temperature Dependent Diffraction Intensities Michael Patzer, Christian W. Lehmann (Mülheim a. d. Ruhr/DE)
11:45 OP-079	Multipole Refinement of a Disordered Structure of a Ni-Li-Olefin Complex Regine Herbst-Irmer (Göttingen/DE)

10:30–12:00 MS 16 I Structure-based drug discovery
Room F128
Chair Martina Schäfer (Berlin/DE), Roman Federov (Hannover/DE)

10:30 OP-080	Discovery of Innovative Lead Structures through Target-Specific Ligand Screening and In Situ Synthesis Using Protein Crystals Markus Perbandt, Dominik Oberthür, Tobias Beck, Angie Nugraha (Hamburg/DE)
10:48 OP-081	Assembly of Protein Nanocages into Large-Scale Crystalline Structures for Applications in Optical Nanomaterials and Nanomedicine Tobias Beck, Michael Rütten, Laurin Lang, Henrike Wagler (Hamburg/DE)
11:06 OP-082	Exploring LC3/GABARAP Binding Pockets for Degrader Development Adarsh Kumar, Stefan Knapp, Martin Schwalm, Vladimir Rogov (Frankfurt a. M./DE)
11:24 OP-083	Structure-Based Development of Pyocyanin Biosynthesis Inhibitors Against *Pseudomonas Aeruginosa* Marie Thiemann, Moritz Zimmermann, Christina Diederich, Janosch Baumgarten, Conrad Kunick, Wulf Blankenfeldt (Braunschweig/DE)

11:42
OP-084
Molecular Engineering of MjMAT: Manipulating an Enzyme to Accept Large Photocaging Groups
Sonja Titze, Eric Herrmann, Aileen Tekath (Münster/DE), Mehmet Ergüven (München/DE), Nicolas Cornelissen (Münster/DE), Andrea Rentmeister (Münster, München/DE), Daniel Kümmel (Münster/DE)

12:15–13:15
Room E001
Industrial symposium I DECTRIS Ltd.
see page 50

13:30–14:30
Room E001
Plenary lecture V

Chair
Wulf Blankenfeldt (Braunschweig/DE), Hartmut H. Niemann (Bielefeld/DE)

13:30
PL-05
[FeFe] Hydrogenases: from structural insights into the mechanism to new applications in biotechnology
Ingrid Span (Erlangen/DE)

15:00–16:30
Room E001
MS 17 I (Bio)Minerals and storages

Chair
Yasar Krysiak, Claus Rüscher (Hannover/DE)

15:00
OP-085
Geopolymer vs Cement
Waltraud M. Kriven (Urbana, IL/US)

15:30
OP-086
Zirkonium Ceramics as Host Material for Nuclear Waste
Christoph Hennig, Volodymyr Svitlyk, Stephan Weiss, Eleanor Lawrence Bright (Grenoble/FR)

15:45
OP-087
Experimental Investigation of CO_2 and H_2O Absorption and Desorption Behavior of the CALF-20 MOF by *in situ* X-ray Powder Diffraction
Sebastian Bette, Anastasiia Sleptsova, Robert E. Dinnebier (Stuttgart/DE)

16:00
OP-088
The Novel LMU-2 Zeolite Structure and its Transition to Chabazite
Janina Carolin Höner, Andreas Schaate, Yasar Krysiak (Hannover/DE)

16:15
OP-089
Mesocrystal Nanoparticles in the Spotlight of Electrons
Yasar Krysiak (Hannover/DE), Bing-Qiang Lu (Shanghai/CN), Denis Gebauer (Hannover/DE)

15:00–16:30 MS 18 I Computational methods and Artificial Intelligence in Crystallgraphy

Room F142
Chair Anna Krawczuk (Göttingen/DE), Florian Meurer (Regensburg/DE)

15:00 Exploring the Biochemical Impact of the β-Actin G74S Mutation: Structural Insights into Histidine Methylation and Molecular Dynamics Simulations of Actin
OP-090 Anja Marquardt, Dietmar J. Manstein (Hannover/DE)

15:15 Structure Determination by Combining BVS Restricted PDF Modelling and DFT Within an On-The-Fly Trained ML Algorithm
OP-091 Philipp Diephaus, Thorsten M. Gesing, Wilke Dononelli (Bremen/DE)

15:30 Implementation of SALTED Models for Predicting Electron Densities in Single Crystal Structure Refinement
OP-092 Lukas Manuel Seifert (Aachen/DE)

15:45 Implementation of Density Matrix Tight Binding (*PTB*) for Quantum Crystallographic Refinement
OP-093 Ben Ebel, Florian Kleemiss (Aachen/DE)

16:00 Maschine-Learning Assisted Background Removal in Powder Diffraction Pattern
OP-094 Reinhard Neder, Karel Garcia (Erlangen/DE), Ernesto Rams (Erlangen/DE, Havanna/CU)

16:15 Linearization Routines for the Parameter Space Concept to determine Crystal Structures without Fourier Inversion
OP-095 Muthu Vallinayagam (Dresden, Freiberg/DE), Melanie Nentwich (Hamburg/DE), Dirk C. Meyer (Freiberg/DE), Matthias Zschornak (Dresden, Freiberg/DE)

15:00–16:30 MS 19 I Methods in structural biology
Room F107
Chair Johanna Hakanpää (Hamburg/DE), Christian Roth (Berlin/DE)

15:00 Protein Dynamics Revealed by Tuning Relative Humidity
OP-096 Sebastian Günther, Patrick Reinke, Marina Galchenkova, Sven Falke, Pontus Fischer, Sreecidya Thekku Veedu, Jan Meyer, Miriam Barthelmess, Alke Meents (Hamburg/DE)

15:18 Gaining Functional Insights into a Sialic Acid TRAP Transporter through Structure Guided Protein Engineering
OP-097 Philipp Hendricks (Bonn/DE), Martin F. Peter (Copenhagen/DK, Bonn/DE), Yeojin Kim (Bonn, Frankfurt a. M./DE), Jan A. Ruland (Bonn, Mainz/DE), Jan Gerhartz, Jiajun Li, Niels Schneberger, Jan Peter Siebrasse (Bonn/DE), Gavin H. Thomas (York/GB), Ulrich Kubitschek, Gregor Hagelueken (Bonn/DE)

15:36 VHH Antibodies as Auxiliary Tool for Crystallization of Conformationally Flexible Proteins
OP-098 Niels Schneberger, Stephan Menzel, Gregor Hagelueken (Bonn/DE)

15:54 AI-Based Design of Crystallization Chaperones
OP-099 Sophie Binder (Bonn/DE)

16:12 Refinement of ligands with planarity restraints based on conjugation to an aromatic system
OP-100 Norbert Sträter (Leipzig/DE)

15:00–16:00 Lieselotte-Templeton Award Symposium of the Young Crystallographers
Room F128 see page 46

16:30–18:00 Poster session II
Lichthof see page 37

19:00–23:00 Social evening at Restaurant ‘Meiers Lebenslust’
see page 45

09:00–10:00 Plenary lecture VI
Room E001
Chair Jesko Köhnke (Hannover/DE)

09:00 Organic Crystallization Chaperones and Studies on the Origin of Translation
PL-06 Clemens Richert (Stuttgart/DE)

10:15–11:45 MS 20 I Free Topics
Room E001
Chair Clemens Prescher (Freiburg i. Br./DE)

10:15 Hirshfeld Atom Refinement for Spin Density Analysis
OP-101 Daniel Brüx, Ben Ebel, Niklas Pelzer, Florian Kleemiss (Aachen/DE)

10:33 Do we need Synchrotron for Small Molecules?
OP-102 Alexander Virovets, Eugenia Peresypkina (Frankfurt a. M./DE)

10:51 Current Status of the Liquid-Metal-Jet X-ray Source Technology
OP-103 Martin Norrefeldt, Camilla Storaa, Mikael Otendal, Björn A. M. Hansson (Kista/SE)

11:09 Hardware in Synergy: The new PhotonJetMAX-S and UG3
OP-104 Christian J. Schürmann, Jakub Wojciechowski, Christian Göb (Neu-Isenburg/DE), Mathias Meyer, Damian Kucharcyzk, Jaroslaw Blaszczak (Wrocław/PL), Khai-Nghi Truong (Neu-Isenburg/DE), Joseph Ferrara (The Woodlands, TX/US), Fraser White (Neu-Isenburg/DE)

11:27 HTK 1500 High-Temperature Chamber, an environmental heater for non-ambient X-ray diffraction for crystallographic investigations of materials at very high temperatures
OP-105 Barbara Puhr, Marius Kremer, Benedikt Schrode (Graz/AT), Quirin Prasser (Ostfildern/DE)

10:15–11:45 MS 21 I Physical Crystallography
Room F142
Chair Eiken Haussühl (Frankfurt a. M./DE), Marie Münchhalfen (Bochum/DE)

10:15 Correlations between structure and elastic properties of crystals
OP-106 Jürgen Schreuer (Bochum/DE)

10:45 Efficient Soft-Chemical Synthesis of Large van-der-Waals Crystals of the Room-Temperature Ferromagnet 1T-$CrTe_2$
OP-107 Kai D. Röseler, Catherine Witteveen, Céline Besnard (Geneva/CH), Vladimir Pomjakushin (Villingen/CH), Harald O. Jeschke (Okayama/JP), Fabian O. von Rohr (Geneva/CH)

11:00 Crystallographic Challenges of New Compounds Related to the Topological Insulator $Bi_{14}Rh_3I_9$
OP-108 Eduardo Arturo Carillo Aravena (Dresden/DE), Johannes Heßdörfer (Würzburg/DE), Nicolás Pérez (Dresden/DE), Armando Consiglio, Friedrich Reinert, Giorgio Sangiovanni (Würzburg/DE), Michael Ruck (Dresden/DE)

11:15 Single-Crystal Thermoelastic Behavior of Magnetoplumbite Type (Mg, Zr):$SrGa_{12}O_{19}$ and Pr:$SrAl_{12}O_{19}$
OP-109 Marie Münchhalfen, Jürgen Schreuer (Bochum/DE), Christian Rhode, Christo Guguschev (Berlin/DE)

11:30 Molecular Simulation of Host-Guest Nonlinear Optical Materials
OP-110 Nils Marvin Denda, Erik Rohloff, Peter Behrens, Andreas Michael Schneider (Hannover/DE)

10:15–11:45 MS 22 I Software developments for Crystallography
Room F107
Chair Michael Fischer, Paul Klar (Bremen/DE)

10:15 Using Intuitive, Interactive and Colorful Tools for a Straightforward Data Quality Assessment in X-Area
OP-111 Laura Christina Folkers, Friedemann Hahn, Jens Richter (Darmstadt/DE)

10:30 Smart Crystal Alignment Using Deep Learning
OP-112 Anna Lübben, Jens Luebben (Karlsruhe/DE)

10:45 OSCARS: Consolidation of Services in the Photon and Neutron Open Science Cluster
OP-113 Melanie Nentwich (Hamburg/DE), Jordi Bodera (Grenoble/FR), Nicoletta Carboni (Trieste/IT), Patrick Fuhrmann (Hamburg/DE), Andy Götz (Grenoble/FR), A. Paul Millar (Hamburg/DE), Jayesh Wagh (Grenoble/FR)

11:00 Accelerating Quantum Crystallographic Refinements Using Effective Core Potentials
OP-114 Florian Kleemiss (Aachen/DE), Florian Meurer, Michael Bodensteiner (Regensburg/DE)

11:15
OP-115
Application of Anisotropic Atomic Form Factors in Powder Diffraction
Reinhard Neder, Karel Garcia (Erlangen/DE), Magda Woinska, Wojciech Slawinski (Warsaw/PL)

11:30
OP-116
Uncertainties of Recalculated Bond Lengths and Angles as Implemented in the Crystal Palace Program for Parametric Crystal Structure Analysis
Ross John Angel (Padova/IT), Mattia Mazzucchelli (Lausanne/CH), Lisa Baratelli (Milan/IT), Catherine Fabienne Schweinle (Freiburg i. Br./DE), Javier Gonzalez-Platas (La Laguna/ES), Tonci Balic-Zunic (Copenhagen/DK), Matteo Alvaro (Pavia/IT)

10:15–11:45
Room F128
MS 23 I Structural biology @Synchrotons

Chair
Manfred Weiss (Berlin/DE), Sebastian Günther (Hamburg/DE)

10:15
OP-117
Experiments on the Structural Biology Beamlines Beyond Diffraction and Scattering
Christoph Mueller-Dieckmann (Grenoble/FR)

10:33
OP-119
Project-Based, Rolling Access at MX beamline P11 on PETRA III
Johanna Hakanpää, Spyros D. Chatziefthymiou, Jialing Song, Arka B. Dey, Jan-Peter Kurz, Daniela Unger, Veronica Delsoglio, Guillaume Pompidor, Hans-Christian Wille, Oliver Seeck (Hamburg/DE)

10:51
OP-120
Neutron Diffraction as a Tool for Membrane Biophysics at the Heinz Maier-Leibnitz Zentrum
Christopher Garvey, Markos Skoulatos, Robert Georgii (Garching/DE)

11:09
OP-121
Structural Biology of Bacterial Insecticides Using *in Vivo* Grown Crystals and nanoSFX
Dominik Oberthür (Hamburg/DE), Colin Berry, Lainey Williamson, Hannah Best (Cardiff/GB), Neil Crickmore (Brighton/GB), Marina Galchenkova, Oleksandr Yefanov, Henry Chapman (Hamburg/DE), Robin Schubert, Richard Bean (Schenefeld/DE)

11:27
OP-122
Location and Identification of Light Elements by Long-Wavelength Macromolecular Crystallography
Armin Wagner, Ramona Duman, Christian Orr, Vitaliy Mykhaylyk, Kamel El Omari (Didcot/GB)

11:45–12:15
Room E001
Closing

Young Crystallographers: Lightning talks

PP-001 Band Gap Structure of a RT multiferroic $LiFe_5O_8$ in Tetragonal Distortion from First-Principles Calculations
Yaoshi Cheng, SoHyun PARK (München/DE)

PP-002 Steps of Hydrogen Release of BH_4^- in the Reaction with H_2O in hydro-sodalite / $NaBH_4$-Sodalite Solid Solutions
Lucas Fuchs, Felix Möller, Robin Wassermann, Vanessa Winkler, Claus Rüscher (Hannover/DE)

PP-003 Investigations of De- and Rehaydration Versus CO_2 Sorption and Desorption of Zeolites 13 X, 4A and Hydro Sodalites
Leonie Heim, Lea Landgraf, Luca Pagnocelli, Sophie Khanin, Sandro Sulić, Claus Rüscher, Benedict Hagel (Hannover/DE)

PP-004 Structural Relationships Between CSH-Phases, Alkali-Activated Materials and Geopolymers
Jan Friedling, Hannah Kohne, Niklas Kummer, Niels Stitz, Claus Rüscher (Hannover/DE)

PP-005 Unraveling the Mechanisms of Thermosalient Anisotropic Expansion for Advanced Actuators and Flexible Electronics
Divya I S, Sunil Varughese (Thiruvananthapuram/IN)

PP-091 Structural Relaxation of CSH-binder into a Poly-Siloxo Network through Accelerated Recarbonation
Johanna Hansen, Lena Hielscher, Andreas Hornig, Julia Schubert, Claus Rüscher, Nils Och (Hannover/DE)

PP-092 Crystal Structure of gDcL3·6h2o and its Intercalation into Saponite as new Hybrid Material Formation
Lenka Krešáková, Juraj Černák, Juraj Kuchár, Martin Orendáč, Róbert Tarasenko, Hryhorii Titikov (Košice/SK), Jana Madejová, Ľuboš Jankovič (Bratislava/SK)

PP-093 An in Situ Neutron Diffraction Experiment on the Deuteration of the CrB Type Zintl Phase EuGe
Leonhard Yuuta Dorsch (Leipzig/DE), Thomas Hansen (Grenoble/FR), Holger Kohlmann (Leipzig/DE)

PP-094 Coordination Complexes of Rare Earth Lons Using C3-Symmetrical Triaminoguanidinium-Based Ligands
Nico Linnartz, Sonja Liu, Iris Oppel (Aachen/DE)

PP-095 Unveiling Crystal Packing of 1:1 Co-Crystal of 6-(4H-1,2,4-triazol-4-yl) Pyridin-2-Amine and Pyridine-2,6-Diamine: An Energetic Point of View
Milica G. Bogdanović (Novi Sad/RS), Maik Wyshusek (Düsseldorf/DE), Iryna Konovalova (Düsseldorf/DE, Kharkiv/UA), Guido J. Reiss (Düsseldorf/DE), Marko V. Rodić (Novi Sad/RS)

PP-096 Polynitrides of Main Group Elements Synthesized under Extreme Conditions
Lukas Brüning (Frankfurt a. M./DE), Nityasagar Jena (Linkoeping/SE), Elena Bykova, Pascal Jurzick (Frankfurt a. M./DE), Igor A. Abrikosov (Linkoeping/SE), Maxim Bykov (Frankfurt a. M./DE)

PP-097 Powder Diffraction Under Pressure, a new Hydrostatic Pressure Diffraction Cell
Lukas Sippach (München/DE), Henrique Geraissate, Arne Meyer, Alexander Schoekel, Anita Ehnes (Hamburg/DE), Gregor Kieslich (München/DE)

PP-098 Diffuse Scattering in Sanidines
Christin Wiggers, Ella Schmidt (Bremen/DE), Daniel A. Chaney (Grenoble/FR)

PP-099 Synthesis and Crystal Structure of a High Pressure Polymorph of the Inorganic Pyrocarbonate Na2[C2O5]
Lena Wedek, Dominik Spahr, Lkhamsuren Bayarjargal, Maxim Bykov (Frankfurt a. M./DE), Victor Milman (Cambridge/GB), Björn Winkler (Frankfurt a. M./DE)

PP-100 Formation of Novel Hydrogen-Bearing Iron Oxides FE5O8HX and FE7O11HX through a Thermal Decomposition of goethite FEOOH at High Pressure
Valentin Kovalev, Dominik Spahr (Frankfurt a. M./DE), Nico Giordano (Hamburg/DE), Anna Pakhomova (Grenoble/FR), Elena Bykova (Frankfurt a. M./DE)

PP-101 The Coordination Number Rule – An Effective Tool for Coordination-Based Prediction and Rationalization of Inorganic Structures?
Niklas Langer, Holger Kohlmann (Leipzig/DE)

PP-102 Controlled Assemblies of Supramolecular Organometallic Complexes in the SolidState
Julian Zuber, Alexandra Heidecker, Alexander Pöthig (Garching/DE)

PP-103 Structural Insights into the Enzymatic Hydrolysis of Polyurethanes with UMG-SP2
Parinita Singh (Berlin/DE), Da'san Jaradat (Berlin/DE, Al-Salt/JO), Manfred Weiss, Frank Lennartz, Gert Weber (Berlin/DE)

PP-104 Structural Properties, Thermal Expansion and Heat Capacity of Li2GeO3 at Low Temperature
Denis Werner, Eiken Haussühl, Dominik Spahr, Katharina Köhler, Lkhamsuren Bayarjargal, Lena Wedek, Björn Winkler (Frankfurt a. M./DE)

PP-105 Controlled Structure and Crystallinity of Electrospun CCO Nanofibers for Enhanced Thermoelectric Performance
Itzhak Ishay Maor (Haifa/IL), Katharina Kruppa (Hannover/DE), Adi Rozencweig, Amir Sterzer (Haifa/IL), Frank Steinbach (Hannover/DE), Vadim Beilin (Haifa/IL), Bernd Breidenstein (Hannover/DE), Gennady Shter, Meirav Mann-Lahav (Haifa/IL), Armin Feldhoff (Hannover/DE), Gideon Grader (Haifa/IL)

PP-106 Structure-Based Discovery of Inhibitors of Itaconic Acid Synthesis by ACOD1 (IRG1)
Mingming Zhao (Braunschweig/DE), Chutao Chen, Frank Pessler (Hannover/DE), Wulf Blankenfeldt, Konrad Büssow (Braunschweig/DE)

PP-107 Crystallographic and Spectroscopic Study of CO Binding in Dodecameric Tyrosine-Coordinated Heme Protein from *Oligotropha Carboxydovorans*
Anushka Ghosh, Jae-Hun Jeoung, Holger Dobbek, Peter Liebers (Berlin/DE)

PP-108 The Search for FGE Stabilizing Molecules: From Fragment Screen Hits to Potential Lead(s)
Julia L. Kowal (Bielefeld/DE), Niama Ezzaidi (Southampton/GB), Jan Wollenhaupt (Berlin/DE), Karthikeyan Radhakrishnan, Tatjana Pietrowski, Melanie Löwen, Manisha Thangarasah, Willy Keller, Sarfaraz Alam (Bielefeld/DE), Manfred Weiss (Berlin/DE), Matthias G. J. Baud (Southampton/GB), Hartmut H. Niemann (Bielefeld/DE)

PP-109 Influence of Ligand Change in the Primary-Coordination Sphere on Metal-Binding of Bimetallic Sulerythrin
Samriddhi Bhattacharya, Jae-Hun Jeoung, Stefan Rünger, Eric Herrmann, Holger Dobbek (Berlin/DE)

Teaching of crystallography

PP-006 Powder Diffraction in an Undergraduate Lab Work Course: First Experiences and Lessons Learned
Dirk Bockfeld, Christian Kleeberg, Marc Walter (Braunschweig/DE)

Structure-based drug discovery

PP-007 Serial Fixed-Target Crystallography Reveals Binding of two Inhibitors to a LASV L Protein Domain with Endonuclease Activity
Sven Falke, Sebastian Günther, Patrick Reinke, Marina Galchenkova, Johanna Senst, Philipp Lewe, Yaiza Fernández-García, Susanne Witt, Alke Meents (Hamburg/DE)

PP-008 Fragment Screening Against the SARS-CoV-2 Macrodomain
Frank Lennartz (Berlin/DE), Christoph Grathwol (Eggenstein-Leopoldshafen/DE), Verena Linhard (Frankfurt a. M./DE), Jan Wollenhaupt (Berlin/DE), Harald Schwalbe (Frankfurt a. M./DE), Nicole Jung (Eggenstein-Leopoldshafen/DE), Weiss Manfred (Berlin/DE)

PP-009 The F2X Facility – Crystallographic Fragment Screening at HZB
Melanie Oelker, Tatjana Barthel, Laila Benz, Frank Lennartz, Uwe Müller, Manfred Weiss (Berlin/DE)

PP-010 In silico Evaluation of Urofascial Syndrome-Related Mutations P140R and N543I in Heparanase 2
Jacqueline Krohn, Dietmar J. Manstein (Hannover/DE)

Structural biology meets chemistry

PP-011 Structural Insights into Dihydrolipoamide Dehydrogenase Intermediate States and Active Site Access Regulation
Fabian Rabe von Pappenheim (Göttingen/DE)

PP-012 Crystallization of the Tryptophan Halogenase Thal to Investigate the Binding of Substrate Peptides
Hendrik Horstmeier, Simon Bork, Nicolai Montua, Hartmut H. Niemann (Bielefeld/DE)

PP-013 Structure-Based Engineering of a Broad-Substrate Polyphosphate Kinase
Hannah Barz, René Rasche, Timo Königsmann (Münster/DE), Rachel Mitton-Fry (Münster/DE, Granville, OH/US), Andrea Rentmeister (Münster, München/DE), Nicolas Cornelissen, Daniel Kümmel (Münster/DE)

Software developments for crystallography

PP-014 A Light-Weight, Python-based GUI for Processing of Macromolecular X-Ray Diffraction Data via Global Phasing"s *autoPROC*[1]
Peer Lukat, Stefan Schmelz, Wulf Blankenfeldt (Braunschweig/DE)

Serial crystallography

PP-015 Standard Sample Preparation and Characterization for Serial Crystallography
Huijong Han, Christina Schmidt, Kristina Lorenzen, Joachim Schulz (Schenefeld/DE)

Porous materials

PP-016 Controlled Crystallization of ZIF Thin Film Stacks with Distinct Order and Adjustable Adsorption Behavior for Photonic Crystal Application
Lukas Steinbach, Nils Christian Keppler, Johanna Fricke, Adrian Hannebauer, Erik Rohloff, Andreas Schaate, Peter Behrens (Hannover/DE)

Non-ambient conditions

PP-017 Synthesis, Structure and Thermal Behavior of Polycrystalline Si-substituted Hydrogrossulars
Artem Shevchenko, Sebastian Bette, Robert E. Dinnebier (Stuttgart/DE)

PP-018 Synthesis and in Situ Synchrotron Diffraction Studies of $BaSiH_6$ at High Pressures and Temperatures
Doreen Cynthia Beyer (Leipzig/DE), Kristina Spektor (Hamburg/DE), Ulrich Häussermann (Stockholm/SE), Holger Kohlmann (Leipzig/DE)

PP-019 Thermal Properties of $SmFeO_3$ and $HoFeO_3$
Iffat Ara Mitu, M. Mangir Murshed, Thorsten M. Gesing (Bremen/DE)

PP-020 The First Transition Metal – BO_4 boracites $M^{3+}M^{2+}{}_2B_7O_{13}(BO(OH)_3)$ (M = Fe, Mn)
Anastasiia Shagova, Leonard Pasqualini, Klaus Wurst, Hubert Huppertz (Innsbruck/AT)

PP-021 Masterful Sample Grilling Starts Here
Martin Adam, Carsten Lenczyk, Tobias Stürzer (Karlsruhe/DE)

PP-022 Novel polymorph of Rhenium Disulfide Stabilized by High-Pressure
Ninel Sharapova, Valentin Kovalev, Dominik Spahr, Fariia Iasmin Akbar (Frankfurt a. M./DE), Anna Pakhomova (Grenoble/FR), Björn Winkler, Elena Bykova (Frankfurt a. M./DE)

PP-023 Multi-Wavelength Pyrometer for Temperature and Optical Properties Diagnostics
Roman Belikov, David Merges (Frankfurt a. M./DE), Dmitry Varentsov, Martin Schanz (Darmstadt/DE), Björn Winkler (Frankfurt a. M./DE)

PP-024 A New High-Pressure Rb_2CO_3 Polymorph
Julia Bungarten, Dominik Spahr, Lkhamsuren Bayarjargal (Frankfurt a. M./DE), Victor Milman (Cambridge/GB), Björn Winkler (Frankfurt a. M./DE)

New trends in quantum crystallography

PP-025 Development of a Reference Database for Chemical Bonding Analysis
Francisca Bartley, Florian Kleemiss (Aachen/DE)

New Crystal structures

PP-026 Hydroflux Synthesis – A Novel Approach for Synthesizing the Rare Earth Vanadium Compound K6[Y(VO4)3]·2H2O
Yuxi Li, Michael Ruck (Dresden/DE)

Electron diffraction method development and instrumentation

PP-027 Testing *PhAI* for Solving Crystal Structures from Electron Diffraction and Powder X-ray Diffraction Data
Toms Rekis (Frankfurt a. M./DE)

PP-028 Custom Systems Powered by MetalJet Bringing Synchrotron Applications to the Lab
Martin Norrefeldt, Camilla Storaa, Till Dreier (Kista/SE), Robert Drake (Oldcastle/CA)

PP-029 First Experiences with the ED-1 Electron Diffractometer
Christian W. Lehmann, Michael Patzer (Mülheim a. d. Ruhr/DE)

Advances and applications of neutron and synchrotron radiation

PP-030 Unravelling Cation Ordering in $Sn_2SbS_2I_3$
Daniel M. Többens (Berlin/DE), Joachim Breternitz (Berlin, Steinfurt/DE), Daniel G. Porter (Didcot/GB), Adair Nicolson (London/GB), Susan Schorr (Berlin/DE)

PP-031 The Method of ASAXS in Material Science and Presentation of Some Analysis Techniques
Armin Hoell, Susan Schorr (Berlin/DE)

PP-032 Chemical Crystallography at PETRA IV
Martin Tolkiehn (Hamburg/DE)

PP-110 Cd Incorporation as a Way to Avoid Cu/Zn Disorder in Kesterites: The Kesterite-Stannite Structural Transition in $Cu_2(Zn_{1-x}Cd_x)SnS_4$
Galina Gurieva (Berlin/DE), Maris Pilvet (Tallinn/EE), Maxim Avdeev (Lucas Heights/AU), Marit Kauk-Kuusik (Tallinn/EE), Susan Schorr (Berlin/DE)

Properties of disordered materials

PP-033 In-house Total Scattering Experiments of Ferrihydrites Adsorbed with NOM or Acetate
Lars Robben (Bremen/DE)

PP-034 Composition Dependence of Lattice Parameters of well Annealed and Cold-Deformed Fe-Ga intermetallics
Guido Kreiner (Freiberg/DE)

Porous materials

PP-035 Synthesis and Properties of Phosphate Enclathrated Cancrinite Single Crystals
Josef-Christian Buhl (Bremen/DE)

PP-036 Solving the Structure of a Novel MOF with Potential Application in Data Storage via Rietveld Refinement
Lukas Moenkeberg (Hannover/DE)

PP-037 Incorporation of Pre-Crosslinked Linkers into UiO-66-type MOFs and their Structural Implications
Tobias Hennig (Hannover/DE)

New Crystal structures

PP-038 Synthesis, Characterization and Structure Property Relations in $(Co_{1-x}Ni_x)Sb_2O_4$
Christopher S. Reuter (Bremen/DE)

PP-039 $[CuCl(o\text{-}van\text{-}en)LnCl(H_2O)_3]Cl{\cdot}CH_3CH_2OH$ (Ln = Eu, Sm, Gd, Nd, Dy): Syntheses by Horizontal Diffusion and Crystal Structure
Andrea Koščíková (Košice/SK)

PP-040 New Series Of Intermetallics $(Sr_3)_{n+2}(M_8)_nM_{18}(Ga)_2$ (M=Li/Ga)
Markus Otteny (Freiburg i. Br./DE)

PP-041 Synthesis, Characterization and in Silico Studies on some Climbazole Derivatives
Ertan Şahin (Erzurum/TR)

Properties of disordered materials

PP-033 In-house Total Scattering Experiments of Ferrihydrites Adsorbed with NOM or Acetate
Lars Robben, Yunru Chen (Bremen/DE)

PP-034 Composition Dependence of Lattice Parameters of well Annealed and Cold-Deformed Fe-Ga intermetallics
Guido Kreiner, Andreas Leineweber (Freiberg/DE)

Porous materials

PP-035 Synthesis and Properties of Phosphate Enclathrated Cancrinite Single Crystals
Josef-Christian Buhl, Thorsten M. Gesing (Bremen/DE)

PP-036 Solving the Structure of a Novel MOF with Potential Application in Data Storage via Rietveld Refinement
Lukas Moenkeberg, Andreas Schaate (Hannover/DE), Dirk Volkmer (Augsburg/DE), Joern Droste (Hannover/DE)

PP-037 Incorporation of P*re-Crosslinked* Linkers into UiO-66-type MOFs and their Structural Implications
Tobias Hennig, Daniel Dyck, Verena Drewes, Erik Rohloff, Andreas Michael Schneider, Andreas Schaate (Hannover/DE)

New Crystal structures

PP-038 Synthesis, Characterization and Structure Property Relations in $(Co_{1-x}Ni_x)Sb_2O_4$
Christopher S. Reuter, M. Mangir Murshed, Thorsten M. Gesing (Bremen/DE)

PP-039 [CuCl(*o-van-en*)LnCl$(H_2O)_3$]Cl·CH_3CH_2OH (Ln = Eu, Sm, Gd, Nd, Dy): Syntheses by Horizontal Diffusion and Crystal Structure
Andrea Koščíková (Košice/SK), Milagros Tomás, Irene Ara, Lawrence Rocco Falvello (Zaragoza/ES), Juraj Černák (Košice/SK)

PP-040 New Series Of Intermetallics $(Sr_3)_{n+2}(M_8)_nM_{18}(Ga)_2$ (M=Li/Ga)
Markus Otteny, Caroline Röhr (Freiburg i. Br./DE)

PP-041 Synthesis, Characterization and in Silico Studies on some Climbazole Derivatives
Ertan Şahin, Ebrar Nur Ozkan, Melek Gokmen Karakaya, Abdullah Menzek (Erzurum/TR)

PP-042 Different Solvates of a Dehydrobenzo[24]Annulene Derivative Exhibiting Disorder, Modulations and Several Phase Transitions
Christian Kleeberg, Dirk Bockfeld, Mehdi Koohgard, Matthias Tamm (Braunschweig/DE)

PP-043 Synthesis and Characterization of a Series of Novel Schafarzikites $(PbSb)(Fe_{1-x}Cr_x)O_4$
Carla M. Uribe Rincón, Paul Benjamin Klar, Thorsten M. Gesing, M. Mangir Murshed (Bremen/DE)

PP-044 The Unique Crystal Structure of ZnInSbO5
Tobias Wolflehner, Matthias Weil (Wien/AT)

PP-045 Is it Possible to use the Oxidative Dimerization from H-Cysteammonium to H_2-Cystammonium for a Switch Between Lead-Free Ruddlesden-Popper and Dion-Jacobson Phases?
Catherine Fabienne Schweinle, Michael Daub, Harald Hillebrecht (Freiburg i. Br./DE)

PP-046 Four New Oxygen-Rich Phases in the Na-O System Under High Pressure
Junai Lyu, Maxim Bykov, Lukas Brüning, Elena Bykova, Björn Winkler, Fariia Iasmin Akbar (Frankfurt a. M./DE)

PP-047 $Tl_3[CO_3][CB_{11}H_{12}]$: An *anti*-Perovskite-Type Double Salt with Dodecahydro-*closo*-Carbadodecaborate Participation
Alexandra Friedly, Thomas Schleid (Stuttgart/DE)

PP-048 $RbI_4Tm_2Sb_{8.333}O_{14}$: Another Quinary Alkali-Metal Iodide Lanthanoid(III) Oxoantimonate(III) with Halfpipe Structure
Ralf Jules Christian Locke, Kim-Natalie Bozenhardt, Thomas Schleid (Wernau/DE)

PP-049 Conserving Form and Function: Are Identical Active-Site Residues Sufficient to Conserve Product Formation in Terpene Synthases?
Dominik Kolling, Minh Trang Aselmann, Henry Frederik Struwe, Christopher Slotman, Andreas Kirschning, Jesko Köhnke (Hannover/DE)

Mineral storages, hydrogen and CO2 sequestration, reactivities, diffusion, surface activities and physical properties

PP-050 The Effect of the Crystallographic Orientation on Diffusion-Driven Fe-Mg Isotope Fractionation in Olivine
Martin Oeser (Hannover/DE), Ralf Dohmen, Julius Eschenauer (Bochum/DE), Stefan Weyer (Hannover/DE)

Inorganic polymers

PP-051 Mineralogical Evolution of Laterites Soils Transformed to Geopolymer Materials
Sylvain Tome, Claus Rüscher (Hannover/DE)

Industrially relevant materials

PP-052 Hydrothermal Synthesis of ZSM-5 with High Aluminium Content
Sawsan Banjak, Lars Robben, Thorsten M. Gesing (Bremen/DE)

In situ/operando studies of functional materials

PP-053 *In Situ* XRPD Investigations on the Reduction of Iron Oxides by Hydrogen
Michael Häger, Holger Kohlmann (Leipzig/DE)

PP-054 Towards Sustainable Carbonate Synthesis: Mechanochemical Synthesis and In situ X-ray Diffraction Studies
Haritha Das (Mülheim a. d. Ruhr/DE), Volker Kahlenberg, Doris Braun (Innsbruck/AT), Claudia Weidenthaler (Mülheim a. d. Ruhr/DE)

Frontier molecular crystallography

PP-055 Solution and Solid-State Interactions of a Copper(I)-Based Metallocavitand with a Cyclic Guest
Thomas Pickl, Markus Anneser, Alexander Pöthig (Garching/DE)

Free topics

PP-056 Enhancing Methylene Blue Dye Degradation Efficiency through Mn, Co, and Al Doping of Highly Stabilized Organic Ligand-Engineered ZnO Nanoparticles
Reinhard Neder, Imran Ullah (Erlangen/DE), Muhammad Infan (Perak/MY), Inam Din (Peschawar/PK), Humma Parwaz (Bannu/PK), Suriati Sufian (Perak/MY)

Crystalline/non-crystalline materials, relationships

PP-057 Greimas Semiotic Square: Solid-State Compound Classes, Scattering and Implications
Lars Robben (Bremen/DE)

PP-058 MAPLESIRUP – And some Thoughts on the Madelung Part of the Lattice Energy
Günther Thiele (Freiburg i. Br./DE)

PP-059 Comprehensive Structural Analysis of Glutathione-Capped Ultrasmall Metallic and Alloyed Nanoparticles
Kateryna Loza, Natalie Wolff, Oleg Prymak (Essen/DE), Marc Heggen (Jülich/DE), Claudia Weidenthaler (Mülheim a. d. Ruhr/DE), Matthias Epple (Essen/DE)

PP-060 Study of Trisilver Citrate Nucleation and Porous Silver Formation
Dilafruz Allanazarova, Denis Gebauer (Hannover/DE)

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Philip Wiegel, Renat Almeev, Felix Marxer, Francois Holtz (Hannover/DE), Chao Zhang (Xi'an/CN)

PP-062 Unveiling the Spatial Heterogenity of Hydration Reactions in Cementitious Systems With and Without Calcined Clay
Corinna Rozanski, Claus Rüscher (Hannover/DE)

Crystal Chemistry

PP-063 New Aminocarboxylate Ligands
Małgorzta Hołyńska (Noordwijk/NL), Andrzej Kochel (Wrocław/PL)

PP-064 Empty, Filled, Distorted or Compressed? Cd-Containing M_{11} Clusters in Alkali Metal Thallides
Marlene Matt-Willmat, Anthea Weinbrenner, Caroline Röhr (Freiburg i. Br./DE)

PP-065 New Basic Lead Copper Arsenate Minerals- from Layered to Polymerized
Thomas Malcherek, Boriana Mihailova, Jochen Schlüter (Hamburg/DE), Philippe Roth (Zurich/CH), Nicolas Meisser (Lausanne/CH)

PP-066 Dispirotripiperazin (6-6-6 DSTP) Kuaterner Tuzunun Sentezi Için Umut Verici Bir Yön
Mahsa Golmohammadi (Orumiyeh/IR), Tuncay Tunç (Aksaray/TR), Nader Noroozi Pesyan (Orumiyeh/IR), Ertan Şahin (Erzurum/TR)

PP-067 Partitioning of Metals in the Structures of the Solid Solution Series $(Ni,Co,Mg)_3(AsO_4)_2 \cdot 8H_2O$
Juraj Majzlan (Jena/DE), Daniel M. Többens (Berlin/DE)

PP-068 Crystal Chemical Parameters for the Eu(II) Luminescence in Solid-State Metal Hydrides
Arjun Nain, Lukas Millahn, Markus Gebauer, Linda Schmidt, Holger Kohlmann (Leipzig/DE)

PP-069 $RbTm_3S_5$: The First Rubidium Lanthanoid(III) Sulfide with $CsEr_3Se_5$-Type Crystal Structure
Katja Engel, Thomas Schleid (Stuttgart/DE)

PP-070 Synthesis and Crystal Structure of Pyridinium Dodecahydro-*closo*-Dodecahydroborate Dihydrate
Rouzbeh Aghaei Hakkak, Thomas Schleid (Stuttgart/DE)

PP-071 Structural modifications in δ-$(Bi_{1-x}M_x)_2O_3$ phases: influence of M^{3+}-cation Substitution and Compositional Variations
Md. Imran Hossain, M. Mangir Murshed, Thorsten M. Gesing (Bremen/DE)

Charge density distribution from diffraction data

PP-072 Experimental Charge Density Studies of Phase Transition in Natrochalcite under Pressure
Krzysztof Woźniak, Piotr Rejnhard, Roman Gajda, Tomasz Poręba, Mohamed Mezouar (Warsaw/PL), Przemyslaw Dera (Honolulu, HI/US)

Biomineralization/crystallization

PP-073 Analysis of the Early Stages of Silica Formation and the Potential Role in the Prebiotic Chemistry of Life on Earth
Sina Nolte, Denis Gebauer (Hannover/DE)

PP-074 Nucleation Behavior of 2,4-Dihydroxybenzoic Acid
Felix Lücke, Denis Gebauer (Hannover/DE)

Anisotropic physical properties of solids

PP-075 Elastic, Piezoelectric and Dielectric Properties of γ-$LiAlO_2$ Single Crystals as a Function of Temperature
Eiken Haussühl (Frankfurt a. M./DE), Jürgen Schreuer (Bochum/DE), Šarūnas Svirskas (Vilnius/LT), Hartmut Stöcker (Freiberg/DE)

PP-076 Flexible Dynamic Crystals for Conductive and Piezoelectric Applications
Divya I S, Sunil Varughese (Thiruvananthapuram/IN)

Amorphous and crystalline fractions in minerals

PP-077 Transformation Mechanism of Amorphous Calcium Phosphates at Different pH Values
Oliver Jeske, Denis Gebauer (Hannover/DE)

PP-078 Proton Irradiation of Martian Regolith Constituents: A Space Weathering Simulation
Md. Izzuddin Jundullah Hanafi, M. Mangir Murshed, Lars Robben, Erik Klein, Patric Seefeldt, Thorsten M. Gesing (Bremen/DE)

PP-079 Evaluating Rietveld Method in the Determination of Content and Chemical Composition of Inorganic X-ray Amorphous Materials in Soils
Sileola Joseph Akinbodunse, Kristian Ufer, Reiner Dohrmann, Christian Mikutta (Hannover/DE)

Advanced functional materials

PP-080 Synthesis and Characterization of Thermochromic Pyrochlore-Type $Bi_{2-x}Ti_2O_{7-1.5x}$ (x = 0, 0.5)
Roman Paul, Alexander Wollbrink, Thorsten M. Gesing (Bremen/DE)

PP-081 Structural Analysis of Quantum-Crystalline Platinum on SiO_2 Aerogels for On-Chip Catalytic Hydrogen Combustion
Oliver Thueringer, Ana Luiza S. Fiates, Andreas Schander, Raphaell Moreira, Marco Schowalter, Wilke Dononelli, Konrad Krämer, Andreas Rosenauer, Michael J. Vellekoop, Thorsten M. Gesing (Bremen/DE)

PP-082 Anisotropic Platinum-Iridium Nanoparticles: Synthesis and In-Depth Characterization by X-ray Techniques
Rui Guo, Kateryna Loza, Oleg Prymak (Essen/DE), Marc Heggen (Jülich/DE), Cristiano L. P. Oliveira (São Paulo/BR), Matthias Epple (Essen/DE)

PP-084 New Insights into the Mechanisms for Multiferroicity in Rare Earth Orthoferrites
Piotr Fabrykiewicz (Garching, Aachen/DE), Dnyaneshwar Bhosale, Michal Stekiel (Garching/DE), Aleksandr K. Ovsianikov (Aachen/DE), Vladimir Hutanu, Astrid Schneidewind (Garching/DE), Martin Meven (Garching, Aachen/DE)

Advanced computational methods in crystallography (artificial intelligence, materials modelling, ...)

PP-086 Crystallography and Calphad – Bridging the Gap Using Novel XML-Databases
Alexander Walnsch, Florian Tang, Cassie Früh, Moritz to Baben (Herzogenrath/DE)

PP-087 First Principles Modeling of Novel Organometallic Lead Bromide Phases
Marvin Treger, Melina Dahlke, Yasar Krysiak, Sebastian Polarz, Carolin König (Hannover/DE)

PP-088 Modeling Studies for Selective and Sensitive Metal-Organic Framework Split-Ring-Resonator-Based Chemical Sensors
Erik Rohloff, Tobias Hennig, Andreas Schaate, Stefan Zimmermann, Andreas Michael Schneider (Hannover/DE)

PP-089 Computational Insights into Crystal Structure and Phase Transitions of Acrylonitrile
Michael Fischer (Bremen/DE)

PP-090 Ab Initio Calculations on Electronic Properties of Trans-4-(trifluoromethyl) Cinnamic Acid
Natsagdorj Naranbilegt, Namsrai Tsogbadrakh, Khongorzul Batchuluun (Ulaanbaatar/MN), Tobias Schrader (Garching/DE), Jav Davaasambuu (Ulaanbaatar/MN)

Welcome reception

Come together with your colleagues for the welcome reception and get in the spirit of the 33rd Annual Meeting of the German Crystallographic Society.

Date	Monday, 10 March
Time	18:30–20:30
Fee	included in the conference fee, accompanying person 25 EUR
Location	Industrial exhibition

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Social evening

At the end of the third day of the congress in the restaurant 'Meiers Lebenslust', review the congress experiences so far and enjoy an entertaining evening with good food, music and interesting conversations.

Date	Wednesday, 12 March
Time	19:00–23:00
Fee	65 EUR
Location	Restaurant "Meiers Lebenslust" Osterstraße 64 I 30159 Hannover

All participants may arrange transport themselves.

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Young Crystallographers at DGK 2025 – Join Us!

The Young Crystallographers (DGKYC) warmly invite you to three engaging sessions dedicated to early-career researchers in the dynamic and interdisciplinary field of crystallography. Whether you are presenting, networking or simply curious to learn more, these sessions offer an exciting platform to exchange ideas and connect with peers.

Microsymposium 12: Lightning Talks

We kick off with 18 fast-paced lightning talks, where young crystallographers will present their research in concise, 5-minute snapshots. These presentations serve as an introduction to their work and provide a springboard for deeper discussions at their respective posters. Get ready for a rapid-fire tour of the latest developments all around crystallography!

Date	Tuesday, 11 March
Time	15:00–16:30
Room	Room F128

Get Together of the Young Crystallographers (for young Crystallographers only)

What would a DGK meeting be without a dedicated Young Crystallographers networking event? Join us for an interactive session where we will update you on DGKYC activities, elect a new Co-Chair, and share exciting news about upcoming initiatives. After the formalities, enjoy the opportunity to meet fellow young crystallographers over drinks and snacks in a relaxed setting.

Date	Tuesday, 11 March
Time	19:45–20:45
Location	Room F142

Lieselotte-Templeton Awards Session

We are honored to host a special session featuring the three recipients of the prestigious Lieselotte-Templeton Prize 2025. Each awardee will share key insights from their prize-winning thesis, offering a deeper dive into groundbreaking contributions to the field. This session is a must-attend for those looking for inspiration from some of the brightest young minds in crystallography.

Date	Wednesday, 12 March
Time	15:00–16:00
Location	Room F128

We look forward to welcoming you to one, two, or all three of these sessions—see you there!

For the Young Crystallographers,
Florian Meurer and Anushka Ghosh

Tuesday, 11 March

AK 6 Chemical Crystallography
Room E001 08:15–08:50

AK 7 Physical Crystallography
Room F142 08:15–08:50

AK 8 Mineralogical Crystallography
Room F107 08:15–08:50

AK 9 Materials Science
Room F128 08:15–08:50

Wednesday, 12 March

AK 1 Young Crystallographers
Room F142 The meeting of AK 1 will take place during the Get Together at 19:45–20:45.

AK 2 Teaching of crystallography
Room E001 08:15–08:50

AK 3 Experimental Methods
Room F142 08:15–08:50

AK 4 Theoretical methods
Room F107 08:15–08:50

AK 5 Biological Crystallography
Room F128 08:15–08:50

Conference language

The conference language is English.

Opening hours

	Monday	Tuesday	Wednesday	Thursday
Check-in	13:00–19:00	08:30–18:00	08:30–18:00	08:30–13:00
Industrial exhibition	12:30–21:30	09:30–20:15	09:30–18:00	09:30–12:15

Name badge

Participants will receive their name badge at the check-in on site. 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.

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 will be sent automatically after the conference to the e-mail address used for registration.

Internet

A wireless network will be available throughout the whole building and will be free of charge.

Access data

Network name (SSID):	eduroam
User name:	luh071001@uni-hannover.de
Password:	gH8D4fk8

Catering

All participants and exhibitors will be provided with snacks, coffee and tea in the industrial exhibition. Lunch will be provided on a self-pay basis by the Main Mensa (Callinstraße 23) and by the Cafeteria “Sprengelstube” (below the Lichthof). Please note that only card payment (EC, Visa and MasterCard) is possible. It is not possible to pay in cash at the counters. Water dispensers will be available at the conference venue.

General Assembly 2025

The DGK General assembly will take place on Tuesday, 11 March in Room E001 at 18:15–19:45. We kindly invite all members to attend!

Poster awards

From all the posters accepted, the three best posters will be honoured with prize money of EUR 200 and two prizes of EUR 150. The award ceremony will take place during the social evening on Wednesday, 12 March.

Main sponsors

Bruker AXS GmbH (Karlsruhe/DE)

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MaTecK Material-Technologie & Kristalle GmbH (Juelich/DE)

Media cooperations

Journal of Chemical Crystallography
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Tuesday, 11 March

12:15–13:15 Bruker AXS GmbH (Karlsruhe/DE)
Room E001 Breaking News from X-ray Diffraction

D6 PHASER- All-in-One Benchtop XRD
Michael Evans (Karlsruhe/DE)

Beyond SC-XRD- A texture measurement on the D8 QUEST
Martin Adam (Karlsruhe/DE)

PHOTON IV- Unrivaled Data Quality
Tobias Dunaj (Karlsruhe/DE)

Masterful Grilling Starts Here
Carsten Lenczyk (Karlsruhe/DE)

Wednesday, 12 March

12:15–13:15 DECTRIS Ltd. (Baden-Daettwill/CH)
Room E001 DECTRIS CLOUD – The Open Collaboration Platform for Scientific Data
Max Burian (Villigen/CH)

DECTRIS invites you to their lunch symposium and provides lunch boxes for all participants of the symposium.

DECTRIS CLOUD

Join Our Symposium!

Max Burian

DECTRIS CLOUD - the Open Collaboration Platform for Scientific Data

Wednesday, March 12th, 12:15

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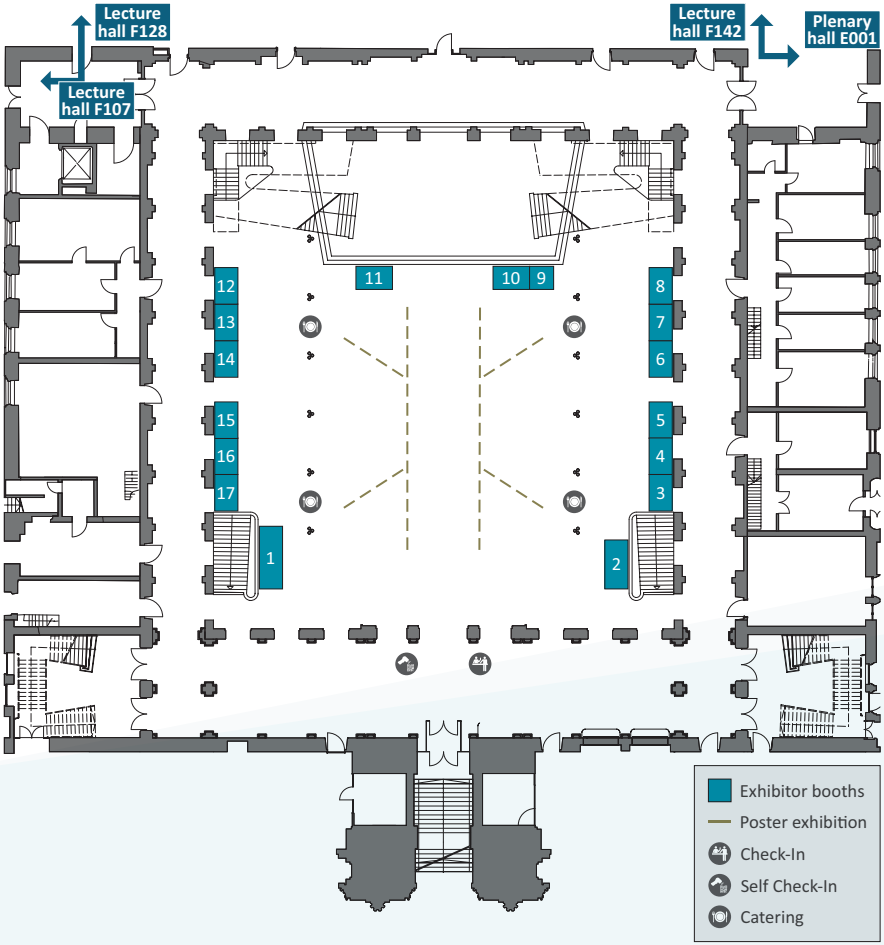

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5	Rigaku Europe SE
6	FIZ Karlsruhe
7	XRD Eigenmann GmbH
8	Anton Paar Germany GmbH
9	Clinisciences

No.	Company
10	IUCr 2029
11	German Crystallographic Society (DGK)
12	Xenocs SAS
13	Malvern Panalytical GmbH
14	Excillium AB
15	Formulatrix Inc.
16	STOE & Cie GmbH
17	Oxford Cryosystems Ltd.

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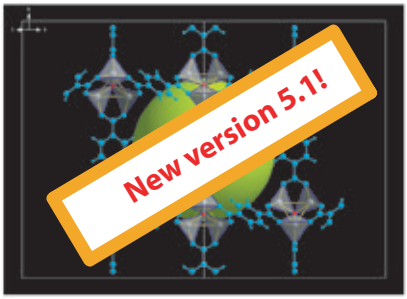

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