27th ANNUAL MEETING of the GERMAN CRYSTALLOGRAPHIC SOCIETY (DGK)

PROGRAMME

25–28 MARCH 2019
LEIPZIG

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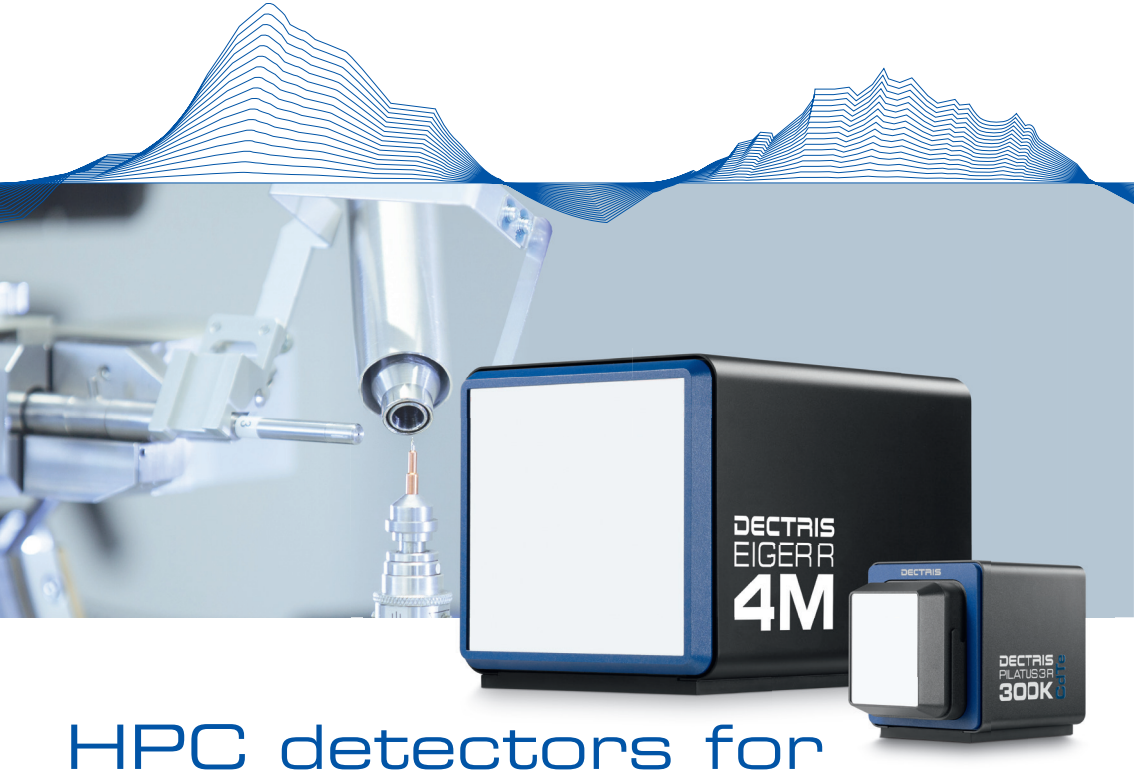

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ORGANISATION AND IMPRINT

Venue
Universität Leipzig | Campus Augustusplatz
Augustusplatz 10 | 04109 Leipzig/DE

Conference website
www.dgk-conference.de

Organiser
German Crystallographic Society (DGK)

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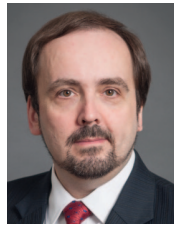
Design and layout

Layout	krea.tif-art UG (haftungsbeschränkt)
Print	printworld.com GmbH
Circulation	500
Editorial Deadline	8 March 2019





Dear colleagues,

It is a pleasure and an honour to welcome you at the 27th Annual Meeting of the German Society for Crystallography held at Leipzig University, 25–28 March 2019. After exactly 20 years, this is the second time Leipzig welcomes crystallographers from all over Germany and many other countries.

The conference venue in the lecture hall building next to the Augusteum at the Augustusplatz is right in the heart of our lively and vibrant city. We hope that you find a little time to visit historical places such as the Nikolaikirche, just a couple of minutes from Augustusplatz. This is where the peaceful revolution in the GDR began, which eventually led to German reunification.

The conference will cover all fields of crystallography and is meant to be a showcase of its multifaceted nature. In good crystallographic tradition, scientists from various disciplines will contribute and ensure a stimulating, interdisciplinary atmosphere.

We are very much honoured that renowned scientists from all over the world and from different fields of crystallography have accepted our invitation for a plenary lecture. The 27th Annual Meeting of the DGK will comprise 20 microsymposia, six plenary lectures and two poster sessions. We hope to provide to all of you an inspiring scientific platform, and we especially encourage young scientists to participate in the conference and in the activities of the “young crystallographers”.

We are looking forward to your attendance and scientific contributions.

Norbert Sträter, Holger Kohlmann and Oliver Oeckler

Monday, 25 March

Lecture hall 9	Lecture hall 8	Lecture hall 10	Lecture hall 11
			09.00–12.30 DGK board meeting
13.00–13.30 Opening			
13.30–14.30 Plenary talk Stefan Zaefferer p. 8			
	14.30–16.00		
	Bio-crystallography I: Signalling, macromolecular interactions & other new structures p. 8	Inorganic crystal structures I p. 9	Micro- and nanocrystalline materials p. 10
16.45–17.15 Laue talk (Paulinum) p. 11			
17.15–18.45 DGK Ehrenabend (Paulinum) p. 11			
18.45–20.30 Welcome reception at the foyer of the Augusteum p. 44			

Tuesday, 26 March

Lecture hall 9	Lecture hall 8	Lecture hall 10	Lecture hall 11
09.00–10.30			
In situ / in operando studies p. 12	Bio-crystallography II: Crystallographic and hybrid methods p. 12	Small molecules at large facilities p. 13	Solid state physics in crystallography p. 14
11.00–12.00 Plenary talk Arwen Pearson p. 14			
12.00–13.30 DGK general assembly			
13.30–14.30 Plenary talk Harald Reichert p. 15			
	14.30–15.30 Thermo Fisher Scientific p. 49	14.30–15.30 Meeting AK 1	14.30–15.30 Meeting AK 20
15.30–17.00			
Inorganic crystal structures II p. 15	Organic molecules and coordination compounds p. 16	Bio-crystallography III: Enzymes p. 17	Young crystallographers: Lightning talks I p. 18
17.00–19.30 Poster session I (even ID's) p. 31			

Wednesday, 27 March

Lecture hall 9	Lecture hall 8	Lecture hall 10	Lecture hall 11
	09.00–10.30		
	Bio-crystallography IV: Structure-based drug design p. 20	Structure-property relationships p. 21	Disordered materials p. 22
11.00–12.00 Plenary talk Xiaodong Zou p. 22			
	12.30–13.30 Rigaku Europe SE p. 49		
13.30–14.30 Plenary talk Holger Stark p. 23			
	14.30–16.00		
	Bio-crystallography V: Instrumentation and methods p. 23	Extreme/non-ambient conditions p. 24	Young crystallographers: Lightning talks II p. 25
16.00–18.30 Poster session II (odd ID's) p. 31			
19.30–23.00 Social evening at Auerbachs Keller p. 44			

Thursday, 28 March

Lecture hall 9	Lecture hall 8	Lecture hall 10	Lecture hall 11
09.00–10.00 Plenary talk Ray Withers p. 28			
	10.00–11.00 Get together young crystallographers p. 46		
	11.00–12.30		
	Instrumentation p. 28	Spectroscopy p. 29	Complex and aperiodic structures p. 30
		12.30–13.00 Closing	

Sessions
Poster session
Plenary talk
Meetings
Industrial symposium
Social programme

13.00–13.30 Opening
Lecture hall 9

13.30–14.30 Plenary lecture
Lecture hall 9
Chair Andreas Leineweber (Freiberg/DE)

13.30 Electron diffraction techniques in scanning electron microscopy: fundamentals and state-of-the-art applications of electron backscatter diffraction (EBSD) and electron channelling contrast imaging (ECCI)
Stefan Zaefferer (Düsseldorf/DE)

14.30–16.00 Bio-crystallography I – Signalling, macromolecular interactions and other new structures
Lecture hall 8
Chair Oliver Daumke (Berlin/DE), Hartmut Niemann (Bielefeld/DE)

14.30 S01-01 Of rats and men – Insight into homologous cytomegalovirus IE1 structures
Johannes Schweininger, Yves A. Muller (Erlangen/DE)

14.45 S01-02 Structural Insights into mitochondrial inner membrane remodeling
Katja Faelber (Berlin/DE), Lea Dietrich (Frankfurt a. M./DE)
Jeff Noel (Berlin/DE), Werner Kühlbrandt (Frankfurt a. M./DE)
Oliver Daumke (Berlin/DE)

15.00 S01-03 A molecular embrace – crystal structure of a DNA repair factor complex
Junqiao Jia, Eva Absmeier (Berlin/DE)
Agnieszka J. Pietrzyk-Brzezinska (Berlin/DE; Lodz/PL)
Markus C. Wahl (Berlin/DE)

15.15 S01-04 Solute binding proteins and their cognate ligands – structure, function and their role in functional annotation
Umesh Yadava (Gorakhpur/IN)

15.30 S01-05 X-ray and cryo-EM structural studies of viral hijacking of the Cullin4-RING ligase ubiquitin-proteasome pathway
Sofia Banchenko, Ferdinand Krupp, Christine Gotthold, Christian Spahn
David Schwefel (Berlin/DE)

15.45 S01-06 Activation mechanism of the receptor tyrosine kinase MET – new crystallographic support for ligand-mediated receptor dimerization
Hartmut Niemann (Bielefeld/DE)

14.30–16.00 Inorganic crystal structures I

Lecture hall 10

Chair Thomas Schleid (Stuttgart/DE)

14.30
S02-01
The $[Ag_2Hg_2]^{4+}$ cluster cation in rudabányaite, a new mineral from the Rudabánya ore deposit
Herta Effenberger (Vienna/AT), S. Szakáll (Miskolc-Egyetemváros/HU)
B. Fehér (Miskolc/HU), T. Váczi (Budapest/HU)
N. Zajzon (Miskolc-Egyetemváros/HU)

14.45
S02-02
The Zintl-Phase hydride $LaGa_2D_{0.71}$
Anton Werwein, Holger Kohlmann, Christopher Benndorf
Marko Bertmer (Leipzig/DE), Alexandra Franz (Berlin/DE)
Oliver Oeckler (Leipzig/DE)

15.00
S02-03
The new trisilicide $BaSi_3$ – high pressure synthesis, crystal structure and chemical bonding
Julia-Maria Hübner, Lev Akselrud, Walter Schnelle, Ulrich Burkhardt
Matej Bobnar, Yurii Prots, Yuri Grin, Ulrich Schwarz (Dresden/DE)

15.15
S02-04
On the crystal structures of long-chain polysulfates
David Jan van Gerven, Stefan Wolf, Mathias S. Wickleder (Cologne/DE)

15.30
S02-05
Crystal structure and thermodynamic behavior of $Bi_6Te_2O_{15}$: the likely structure of the rare mineral pingguite
Gwilherm Nénert, Martin Schreyer (Almelo/NL), Hong Lian
Graeme R. Blake (Groningen/NL)

15.45
S02-06
Chemical preparation, crystallographic characterization and vibrational study of a new condensed phosphate $CaKP_3O_9.H_2O$
Rachida Oubouaza, Malika Tridane, Mustapha Belhabra
Said Belaaouad (Casablanca/MA)

14.30–16.00	Micro- and nanocrystalline materials (powder diffraction, EM, ...)
Lecture hall 11	
Chairs	Ute Kolb (Mainz/DE), Robert E. Dinnebier (Stuttgart/DE)
14.30 S03-01	Transformation strains to evaluate domain orientations by electron backscatter diffraction Andreas Leineweber, Hanka Becker, Mario J. Kriegel Stefan Martin (Freiberg/DE)
15.00 S03-02	Electron diffraction tomography and X-ray powder diffraction on photoredox catalyst PDI Alexander Bodach (Frankfurt a. M./DE), Haishuang Zhao (Mainz/DE) Nai-Wei Liu, Edith Alig (Frankfurt a. M./DE) Georg Manolikakes (Kaiserslautern, Frankfurt a. M./DE) Lothar Fink (Frankfurt a. M./DE), Ute Kolb (Mainz/DE)
15.15 S03-03	Structure determination of rare-earth vanadium selenide oxides by combination of transmission electron microscopy and microfocused synchrotron radiation Florian Gehlhaar, Christopher Benndorf (Leipzig/DE)
15.30 S03-04	Thermal transformation of amorphous HfO_2 nanoparticles followed by *in-situ* powder diffraction and *in-situ* transmission electron microscopy Oleg Prymak (Essen/DE), Prakash D. Nallathamby (Notre Dame, IN/US) Matthias Epple (Essen/DE), Sergei Rouvimov Ryan K. Roeder (Notre Dame, IN/US)
15.45 S03-05	Simultaneous study of periodic and local-structural features of polycrystalline samples – an upgrade of the powder diffraction and total scattering beamline P02.1 at PETRA III, DESY Michael Wharmby, Martin Etter, Alexander Schökel, Jo-Chi Tseng Mario Wendt, Sergej Wenz (Hamburg/DE)

16.45–17.15 Special lecture laureate – Max-von-Laue Award 2018
Paulinum

16.45 Single-crystal X-ray diffraction in high-pressure science
Elena Bykova (Hamburg/DE)

17.15–18.45 DGK Ehrenabend
Paulinum

18.45–20.30 Welcome reception
Foyer Augusteum
(see page 44)

09.00–10.30 *In situ/in operando* studies
Lecture hall 9
Chair Claudia Weidenthaler (Mülheim a. d. R./DE)

09.00
S04-01 Dynamic observation of gas-solid interactions of porous iridium/iridium dioxide nanoparticles by *in situ* TEM heating in different gaseous environments
Kateryna Loza, Kevin Pappert (Essen/DE), Roland Schierholz
Marc Heggen (Jülich/DE), Matthias Epple (Essen/DE)

09.30
S04-02 *In situ* structural vacancy ordering phenomena observed by *in situ* TEM heating experiments and relation to electrical properties for $Ge_6Sn_2Sb_2Te_{11}$
Torben Dankwort (Kiel/DE), Christine Koch (Bremerhaven/DE)
Anna-Lena Hansen (Kiel/DE), David Johnson (Eugene, OR/US)
Matthias Wuttig (Aachen/DE), Wolfgang Bensch, Lorenz Kienle (Kiel/DE)

09.45
S04-03 Hydrogenation steps to perovskite-type hydride $CaRhH_3$ and *in situ* investigations of its intermediates $CaRh_2H_x$
André Götze, Holger Kohlmann, Jens Möllmer (Leipzig/DE)

10.00
S04-04 Study of proton conductivity on powder samples using XRD
Jiří Plocek (Řež/CZ), David Havlíček (Prague/CZ)

10.15
S04-05 Complementarity of operando XRD and XAS for a deep understanding of $Na_xNi_{0.5}Ti_{0.5}O_2$ as Na-ion battery cathode material
Sebastian Maletti (Dresden/DE), Angelina Sarapulova (Karlsruhe/DE)
Daria Mikhailova (Dresden/DE)

09.00–10.30 Bio-crystallography II – Crystallographic and hybrid methods
Lecture hall 8
Chairs Tobias Beck (Aachen/DE), Arwen Pearson (Hamburg/DE)

09.00
S05-01 Structural basis of ribosomal RNA synthesis
Yongheng Huang, Tarek Hilal, Nelly Said, Bernhard Loll
Markus C. Wahl (Berlin/DE)

09.15
S05-02 Characterization of biohybrid nanomaterials with diffraction methods
Matthias Künzle, Marcel Lach, Tobias Beck (Aachen/DE)

09.30 S05-03
Towards protein structure determination under *predictable* crystallization conditions by host lattice engineering.
Peer Mittl (Zurich/CH)

09.45 S05-04
On the possibility of utilizing the Fourier Shell Correlation for validation of crystal structures
Piotr Neumann, Ralf Ficner (Göttingen/DE)

10.00 S05-05
A crystallographic "superstructure" of a phytochrome photosensory core module reveals pronounced structural flexibility of this protein in the dark state
Patrick Scheerer (Berlin/DE), Soshichiro Nagano (Gießen/DE)
Kristina Zubow (London/GB), Norbert Michael (Berlin/DE)
Katsuhiko Inomata (Kanazawa/JP), Tilman Lamparter
Norbert Krauß (Karlsruhe/DE)

10.15 S05-06
Ligand-induced conformational switch of a VFT domain studied by MST, SAXS and crystal structure analysis
Mandy Geisler, Renato Weiße, Norbert Sträter (Leipzig/DE)

09.00–10.30 Small molecules at large facilities

Lecture hall 10

Chair: Christian W. Lehmann (Mülheim a. d. R./DE)

09.00 S06-01
The Chemical Crystallography Beamline P24 at DESY/Petra III
Nils Nöthling, Richard Goddard (Mülheim a. d. R./DE)

09.30 S06-02
Neutrons know better – characterization of the short intramolecular hydrogen bond in substituted acetylacetones by temperature dependent diffraction
Khai-Nghi Truong (Aachen/DE), Martin Meven (Jülich/DE)
Ullrich Englert (Aachen/DE)

09.45 S06-03
Supramolecular Crystallography Beamline (BL2D-SMC) for the chemical crystallography at Pohang Accelerator Laboratory in Korea.
Dohyun Moon (Pohang, Gyeongbuk/KR)

10.00 S06-04
Giant supramolecules meet synchrotron radiation
Alexander Virovets
Eugenia Peresypkina (Regensburg/DE; Novosibirsk/RU)
Manfred Scheer (Regensburg/DE)

09.00–10.30 Solid state physics in crystallography
Lecture hall 11
Chair Eiken Haussühl (Frankfurt a. M./DE)

09.00 S07-01
Discovery of the wave nature of crystals
Georgi Shpenkov (Bielsko-Biala/PL)

09.15 S07-02
Density functional theory calculations of merohedric twinning in $KLiSO_4$
Hans Grimmer, Bernard Delley (Villigen PSI/CH)

09.30 S07-03
Intrinsic point defects in kesterite-type $Cu_2ZnGeSe_4$ compound semiconductors
Daniel Fritsch, Susan Schorr (Berlin/DE)

09.45 S07-04
Crystal growth and characterization of metal (M^{II})-guanidinium formates $[C(NH_2)_3]M^{II}[(HCOO)_3]$ (M^{II}=Cu, Zn, Mn, Co)
Julia Büscher, Lkhamsuren Bayarjargal, Rita Luchitskaia, Björn Winkler
Eiken Haussühl (Frankfurt a. M./DE)

10.00 S07-05
Effect of thermal annealing on mechanical properties of radiation-damaged allanite-(Ce)
Claudia E. Reissner (Halle a. d. S./DE), Ulrich Bismayer (Hamburg/DE)
Herbert Pöllmann, Tobias Beirau (Halle a. d. S./DE)

10.15 S07-06
Determination of the H_2O content from refractive indices of crystals
Reinhard X. Fischer, Manfred Burianek (Bremen/DE)
Robert D. Shannon (Boulder, CO/US)

11.00–12.00 Plenary lecture
Lecture hall 9
Chair Manfred Weiss (Berlin/DE)

11.00
New tools and infrastructure for time-resolved structural biology
Arwen Pearson (Hamburg/DE)

12.00–13.30 DGK general assembly
Lecture hall 9

13.30–14.30 Plenary lecture
Lecture hall 9
Chair Oliver Oeckler (Leipzig/DE)

13.30 The next generation of synchrotron radiation sources and opportunities for crystallography
Harald Reichert (Grenoble/FR)

14.30–15.30 Industrial symposium – Thermo Fisher Scientific
Lecture hall 8
(see page 49)

15.30–17.00 Inorganic crystal structures II
Lecture hall 9
Chair Caroline Röhr (Freiburg i. Br./DE)

15.30
S08-01
Oxygen's oxidation state at very high pressures
Leonid Dubrovinsky, Egor Koemets, Saiana Khandarkhaeva, Elena Bykova
Maxim Bykov, Natalia Dubrovinskaia (Bayreuth/DE)

15.45
S08-02
High-pressure high-temperature synthesis of transition-metal polynitrides
Maxim Bykov (Bayreuth/DE), Elena Bykova
Georgios Aprilis (Hamburg/DE), Egor Koemets (Bayreuth/DE)
Timofey Fedotenko, Konstantin Glazyrin, Hanns-Peter Liermann
Natalia Dubrovinskaia (Hamburg/DE), Leonid Dubrovinsky (Bayreuth/DE)

16.00
S08-03
Structural distortion and Eu(II) luminescence in perovskite-type $KCaH_{3-x}F_x$ ($0.5 \leq x \leq 3$)
Christian Pflug, Holger Kohlmann (Leipzig/DE)

16.15
S08-04
Is $MAPbI_3$ centrosymmetric? – a crystallographic approach
Joachim Breternitz (Berlin/DE), Sarah Barnett, Harriott Nowell (Didcot/GB)
Frederike Lehmann (Berlin, Potsdam/DE), Susan Schorr (Berlin/DE)

16.30
S08-05
Intergrowth of the β- and δ-Al-Fe-Si intermetallic phase and polytypes of the β phase
Hanka Becker (Freiberg/DE; Trondheim/NO), Tina Bergh
Per E. Vullum (Trondheim/NO), Andreas Leineweber (Freiberg/DE)
Yanjun Li (Trondheim/NO)

16.45
S08-06
Packings of sphere packings – pushing ahead
Marek Petrik (Marburg/DE), Wolfgang Hornfeck (Prague/CZ)

15.30–17.00 Lecture hall 8	Organic molecules and coordination compounds
Chairs	Ullrich Englert (Aachen/DE), Alexander Pöthig (Garching b. München/DE)
15.30 S09-01	Synthesis, crystal structures and thermodynamic relations in polymorphic coordination compounds Christian Näther, Tristan Neumann, Inke Jess (Kiel/DE), Luzia S. Germann Robert E. Dinnebier, Florian Pielnhofer (Stuttgart/DE)
15.45 S09-02	Organometallocavitands as functional pores and building blocks Alexander Pöthig (Garching b. München/DE)
16.00 S09-03	From pentagons to squares – giant supramolecules based on $[Cp^RTa(CO)_2(\eta^4\text{-}P_4)]$ Organometallic Building Block Eugenia Peresypkina, Alexander Virovets (Regensburg/DE; Novosibirsk/RU) Manfred Scheer (Regensburg/DE)
16.15 S09-04	Towards crystal structure solution of organic compounds without prior knowledge of space group and lattice parameters by fit to the pair distribution function Dragica Prill, Carina Schlesinger, Stefan Habermehl (Frankfurt a. M./DE)
16.30 S09-05	IDEAL – Invariom Derived Electron AnaLysis in APEX3 Holger Ott, Jens Lübben (Karlsruhe/DE), Michael Ruf (Madison, WI/US) Christian B. Hübschle (Bayreuth/DE)
16.45 S09-06	Crystalline Sponges by Merck – bringing an exciting new method to a wider audience Carolina von Essen, Clemens Kühn, Anupam Khutia, Kentaro Kawata Wolfgang Hierse (Darmstadt/DE)

15.30–17.00 Lecture hall 10	Bio-crystallography III – Enzymes
Chairs	Wulf Blankenfeldt (Braunschweig/DE), Hermann Schindelin (Würzburg/DE)
15.30 S10-01	Structure-based insights into molybdenum cofactor biosynthesis, transport and insertion Joern Krausze (Braunschweig/DE)
15.45 S10-02	Structural characterization of cold-adapted β-D-galactosidase mechanism Maria Rutkiewicz (Berlin/DE; Lodz/PL), Manfred S. Weiss (Berlin/DE) Anna Bujacz (Lodz/PL)
16.00 S10-03	Elucidation of cd_1 nitrite reductase NirS maturation of Pseudomonas aeruginosa by NirF and NirN with X-ray crystallography Thomas Klünemann (Braunschweig/DE), Arne Preuß Gunhild Layer (Freiburg i. Br./DE), Wulf Blankenfeldt (Braunschweig/DE)
16.15 S10-04	Structure of the c-di-AMP synthesising diadenylate cyclase CdaA Jana Laura Heidemann, Piotr Neumann, Achim Dickmanns Ralf Ficner (Göttingen/DE)
16.30 S10-05	Legumain inhibitory cystatin E transforms to multimers with distinct function Elfriede Dall, Julia Hollerweger, Sven Dahms Hans Brandstetter (Salzburg/AT)
16.45 S10-06	Adaptation of a bacterial multidrug resistance system revealed by the structure and function of AlbA Jesko-Alexander Köhnke (Saarbrücken/DE)

15.30–17.00	Young crystallographers – Lightning talks I
Lecture hall 11	
Chairs	Marius Kremer (Aachen/DE), Linda Hollenbeck (Cologne/DE)
15.30 LT1-01	Investigation of a reversible phase transition at low temperatures and the underlying structure property relations for coordination compounds featuring pyridine-2,6-dicarboxylic acid Marius Kremer, Ullrich Englert (Aachen/DE)
15.35 LT1-02	Modelling in the 20's – prospects and possibilities Stefan Diez, R.B. Neder (Erlangen/DE)
15.40 LT1-03	Template effects on the pressure-dependent behaviour of zeolites: a computational case study of chabazite-type fluoroaluminophosphates Michael Fischer (Bremen/DE)
15.45 LT1-04	Solid state structure of an unusual molecular arene-stabilized bismuth(III)/tungsten(IV) oxidocarboxylate Claudia Maria Bianga, Walter Frank (Düsseldorf/DE)
15.50 LT1-05	Ion beam assisted thin film growth using mass separated low-energy nitrogen ions Michael Mensing, Philipp Schumacher, Christoph Grüner, Sören Herath Andriy Lotnyk, Jürgen W. Gerlach, Bernd Rauschenbach (Leipzig/DE)
15.55 LT1-06	Crystal growth investigations of lithium iridate, Li_2IrO_3 Linda Hollenbeck, Petra Becker (Cologne/DE)
16.00 LT1-07	Crystallographic explorations into uniform distribution theory Wolfgang Hornfeck (Prague/CZ)
16.05 LT1-08	Visual diagnostics for macromolecular X-Ray diffraction – AUSPEX Andrea Thorn (Würzburg/DE)
16.15 LT1-10	And yet it moves – anion diffusion in the inverse perovskites $BaLiX_3$ (X = H, D, F) Dennis Wiedemann, Eva Heppke, Alexandra Franz (Berlin/DE)

16.20
LT1-11
A novel supramolecular bismuth(III) compound derived by hydrolysis of bismuth(III) triflate in acetonitrile
Martha Majewski, Walter Frank (Düsseldorf/DE)

16.25
LT1-12
Stabilizing the cubic phase of the triple cation hybrid perovskite $(FA_{1-x}MAx)_{1-y}Cs_yPbI_3$
Frederike Lehmann (Berlin, Potsdam/DE), Alexandra Franz
Susan Schorr (Berlin/DE)

16.30
LT1-13
Quantitative analysis of electron diffraction patterns from scroll nanotubes
Azat Khadiev (Hamburg/DE), Zufar Khalitov (Kazan/RU)

16.35
LT1-14
A new $BaCa(CO_3)_2$ polymorph
Dominik Spahr, Lkhamsuren Bayarjargal (Frankfurt a. M./DE)
Victor Vinograd (Jülich/DE), Rita Luchitskaia (Frankfurt a. M./DE)
Victor Milman (Cambridge/GB), Björn Winkler (Frankfurt a. M./DE)

16.40
LT1-15
Pressure induced phase transitions of dwornikite
Martin Ende (Vienna/AT), Terhi Kirkkala (Jyväskylä/FI)
Michael Loitzenbauer, Dominik Talla, Ronald Miletich
Manfred Wildner (Vienna/AT)

16.45
LT1-16
Structure analyses of zeolite-sorbate systems
Vincent Stock, Bernd Marler (Bochum/DE)

16.50
LT1-17
Crystal growth, crystal structure, and optical characterization of $CsMTiO_4$ (M = Al, Fe and Ga) crystals with fourfold coordinated titanium Ti^{4+}
Jan D. Groeneveld, Manfred Burianek (Bremen/DE)
Lennart Fischer (Freiburg i. Br./DE), Robert D. Shannon (Boulder, CO/US)
Reinhard X. Fischer (Bremen/DE)

17.00–19.30
Foyer first floor
Poster session I
(see page 31)

09.00–10.30 Bio-crystallography IV – Structure-based drug design

Lecture hall 8

Chairs Stefan Knapp (Frankfurt a. M./DE), Roman Hillig (Berlin/DE)

09.00
S11-01
Rational identification of allosteric regulation sites in biocatalysts: a way to new therapies
Roman Fedorov, Johannes Cramer, Jana Führing
Petra Baruch (Hannover/DE), Julia Lieske (Hannover, Hamburg/DE)
Ole Zeymer, Xiaoyi Zhou, Ohm Prakash, Bjarne Feddersen, Jan Lohöfener
Nicola Steinke, Penelope Kay-Fedorov, Christine Goffinet
Ute Curth (Hannover/DE), Christian Brütting
Hans-Joachim Knölker (Dresden/DE), Françoise Routier
Dietmar Manstein, Rita Gerardy-Schahn (Hannover/DE)

09.15
S11-02
Crystal structures of gephyrin in complex with antimalarial artemisinis: molecular basis for inhibitory neurotransmission regulation by artemisinins
Vikram Kasaragod, Hermann Schindelin (Würzburg/DE)

09.30
S11-03
Structure-based design of broad-spectrum antivirals targeting coronaviruses and enteroviruses
Linlin Zhang (Lübeck/DE), Daizong Lin (Changchun/CN; Lübeck/DE)
Qingjun Ma, Yuri Kusov, Rolf Hilgenfeld (Lübeck/DE)

09.45
S11-04
Crystallographic fragment screening at HZB – workflow for efficient user experiments
Jan Wollenhaupt (Berlin, Marburg/DE), Alexander Metz (Marburg/DE)
Tatjana Barthel, Martin Gerlach, Christian Feiler (Berlin/DE)
Steffen Glöckner (Marburg/DE), Dirk Wallacher (Berlin/DE)
Gerhard Klebe (Marburg/DE), Manfred S. Weiss (Berlin/DE)

10.00
S11-05
Discovery of fragments that stabilize the KRAS-SOS1 interaction
Roman Hillig (Berlin/DE)

10.15
S11-06
Structural biology for antibody design at Roche
Armin Ruf (Basel/CH)

09.00–10.30 Structure-property-relationships

Lecture hall 10

Chair Thomas Doert (Dresden/DE)

09.00
S12-01 Vacancy distributions, optical properties and switching mechanisms in epitaxial $Ge_2Sb_2Te_5$ thin film
Mario Behrens, Andriy Lotnyk, Jürgen W. Gerlach
Bernd Rauschenbach (Leipzig/DE)

09.15
S12-02 Structural complexity in the $Cu_2ZnGeSe_4$ – $Cu_2ZnSiSe_4$ solid solution series
Susan Schorr, Sara Niedenzu, Alexandra Franz, Galina Gurieva (Berlin/DE)

09.30
S12-03 Hexagonal Bariumtitanate stabilized as ultra-thin film on Pt(111): an X-ray diffraction and electron-energy-loss spectroscopy study
Holger Meyerheim, Katayoon Mohseni, Stefan Förster, Eva M. Zollner
Florian Schumann (Halle a. d. S./DE), Roberto Felici (Grenoble/FR)
Wolfram Hergert, Wolf Widdra (Halle a. d. S./DE)

09.45
S12-04 Composition-dependent structural transformations in layered oxides of Rh and Li
Daria Mikhailova, Sebastian Maletti, Steffen Oswald (Dresden/DE)

10.00
S12-05 Data mining force field – crystal properties estimation and screening for polymorphs, cocrystals and salts
Liudmila Kuleshova (Uttenreuth/DE)
Detlef W. M. Hofmann (Uttenreuth/DE; Pula/IT)

10.15
S12-06 Hydrothermal structure degradation mechanisms of porous materials DAY, AlPO-5, SAPO-34 and silica gel investigations on long-term stability of porous materials under hydrothermal stress and discussion of the different decomposition mechanisms
Thomas Herzog (Berlin/DE), Josef-Christian Buhl (Hannover/DE)
Wolfgang Lutz, Wolfgang Wieprecht (Berlin/DE)

09.00–10.30 Disordered materials

Lecture hall 11

Chair Jürgen Horbach (Düsseldorf/DE)

09.00
S13-01
Randomly and domain like occurring planar defects in layered honeycomb materials
Sebastian Bette (Stuttgart/DE), Florian Pielnhofer (Regensburg/DE)
Leo Diehl (Stuttgart, Munich/DE), Bettina, V. Lotsch, Tomohiro Takayama
Hidenori Takagi, Robert E. Dinnebier (Stuttgart/DE)

09.15
S13-02
Cu/Zn disorder in $Cu_2ZnSn(S_{1-x}Se_x)_4$ – the off-stoichiometry influence
Galina Gurieva, Alexandra Franz, Susan Schorr (Berlin/DE)

09.30
S13-03
Combining experimental and computational techniques to understand phase transitions of the nucleobase adenine
Dubravka Sisak Jung (Baden-Dättwil/CH), Ivan Halasz (Zagreb/HR)
David McDonagh, Graham Day (Southampton/GB)

09.45
S13-04
A disorder model for the 1-Bromoadamantane Thiourea host guest inclusion compound
Ella Schmidt (Erlangen/DE), Arkadiy Simonov (Freiburg i. Br./DE)
Reinhard Neder (Erlangen/DE)

10.00
S13-05
Sample size effects on fracture toughness testing of Bulk Metallic Glas (and some insights into Stress Corrosion Cracking of $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$)
David Geissler, Martin Uhlemann, Horst Wendrock (Dresden/DE)
Jens Freudenberger (Dresden, Freiberg/DE), Martina Zimmermann
Annett Gebert (Dresden/DE)

10.15
S13-06
The concentration quenching of $Ba_3Bi_2(BO_3)_4$ occurs at 50 mol.%. (λ_{ex} = 393 nm). The detailed analysis, quantitative characteristics and the role of the Eu^{3+} ions distribution in the crystal strictures $Ba_3Bi_2(BO_3)_4$: Eu^{3+} are given in the presentation
Andrey Shablinskii, Rimma Bubnova, Stanislav Filatov, Ilya Kolesnikov
Alexey Povolotskiy (Saint-Petersburg/RU)

11.00–12.00 Plenary lecture

Lecture hall 9

Chair Ute Kolb (Mainz/DE)

11.00
Development of electron diffraction techniques for ab initio crystal structure determination and phase analysis – from small molecules to proteins
Xiaodong Zou (Stockholm/SE)

12.30–13.30 Industrial symposium – Rigaku Europe SE
Lecture hall 8 (see page 49)

13.30–14.30 Plenary lecture
Lecture hall 9
Chair Norbert Sträter (Leipzig/DE)

13.30 The symbiosis of X-ray crystallography and cryo-EM
Holger Stark (Göttingen/DE)

14.30–16.00 Bio-crystallography V – Instrumentation and methods
Lecture hall 8
Chairs Christoph Müller-Dieckmann (Grenoble/FR), Kay Diederichs (Konstanz/DE)

14.30
S14-01 Assessing heterogeneity of data compared by correlation coefficients: theory and examples
Kay Diederichs (Konstanz/DE)

14.45
S14-02 Efficient data collection methods for time-resolved serial synchrotron crystallography enabled the structural analysis of the full turnover of an enzyme
Eike C. Schulz, Pedram Mehrabi (Hamburg/DE)
Henrike M. Müller-Werkmeister (Potsdam/DE), Raison Dousza
Friedjof Tellkamp (Hamburg/DE), Emil F. Pai (Toronto/CA)
R. J. Dwayne Miller (Hamburg/DE; Toronto/CA)

15.00
S14-03 Improvements in automated data analysis and processing within autoPROC, combined with advanced characterisation, mitigation and visualisation of the anisotropy of diffraction limits using STARANISO
Clemens Vonrhein, Ian Tickle, Claus Flensburg, Peter Keller
Wlodek Paciorek, Andrew Sharff, Gerard Bricogne (Cambridge/GB)

15.15
S14-04 Facilities for macromolecular crystallography at the HZB
Martin Gerlach, Christian Feiler, Ronald Förster, Christine Gless
Thomas Hauß, Huiling He, Michael Hellmig, Alexandra Kastner
Maria Rutkiewicz, Lukas Schmuckermaier, Michael Steffien
Helena Taberman, Piotr Wilk, Jan Wollenhaupt
Manfred S. Weiss (Berlin/DE)

15.30
S14-05 *In crystallo* optical spectroscopy for Structural Biology at the ESRF – the *ic*OS Lab as a tool for time-resolved protein crystallography experiments
Antoine Royant (Grenoble/FR)

15.45
S14-06
Fixed-target serial crystallography using in cellulo grown microcrystals
J. Mia Lahey-Rudolph, Robert Schönherr
Lars Redecke (Lübeck, Hamburg/DE)

14.30–16.00
Lecture hall 10
Extreme/non-ambient conditions

Chairs
Ulrich Schwarz (Dresden/DE), Karen Friese (Jülich/DE)

14.30
S15-01
A new high-pressure polymorph of $ZrSiO_4$ revealed by DFT modelling and Raman spectroscopy
Boriana Mihailova (Hambug/DE), Claudia Stangarone (Pavia/IT; Berlin/DE)
Naemi Waeselmann (Hambug/DE), Ross Angel (Pavia/IT)
Mauro Prencipe (Torino/IT), Matteo Alvaro (Pavia/IT)

14.45
S15-02
Crystalline polymeric carbon dioxide is stable at megabar conditions
Ronald Miletich (Vienna/AT), Kamil Dziubek (Sesto Fiorentino/IT)
Martin Ende (Vienna/AT), Demetrio Scelta
Roberto Bini (Sesto Fiorentino/IT), Mohamed Mezouar
Gaston Garbarino (Grenoble/FR)

15.00
S15-03
Successful quantitative experimental charge density under high pressure: feasibility study
Krzysztof Wozniak, Roman Gajda, Anna Makal, Marcin Stachowicz
Szymon Sutula (Warszawa/PL), Pierre Fertey (Paris/FR)

15.15
S15-04
High pressure suppression of correlation effects in $CaMn_7O_{12}$
Michal Stekiel, Adrien Girard, Dominik Zimmer (Frankfurt a. M./DE)
Konstantin Glazyrin (Hamburg/DE), Javier Ruiz-Fuertes (Santander/ES)
Xinyu Du, Yuan Li (Beijing/CN), Björn Winkler (Frankfurt a. M./DE)

15.30
S15-05
Structural changes in $MgSiO_3$ glass up to 138 Gpa
Clemens Prescher (Hamburg, Cologne/DE)
Vitali Prakapenka (Chicago, IL/US), Johannes Stefanski (Cologne/DE)

15.45
S15-06
Temperature dependence of the crystal structure and magnetic properties of Mn_5Si_3 and $MnFe_4Si_3$ at high pressures
Andreas Eich (Aachen/DE), Paul Hering (Jülich/DE)
Luana Caron (Bielefeld, Dresden/DE)
Hao Deng (Garching b. München, Aachen/DE), Vladimir Hutanu
Martin Meven (Aachen, Garching b. München/DE), Karen Friese (Jülich/DE)
Andrzej Grzechnik (Aachen/DE)

14.30–16.00 Young crystallographers – Lightning talks II

Lecture hall 11

Chairs Marius Kremer (Aachen/DE), Linda Hollenbeck (Cologne/DE)

14.30 LT2-01
Prediction of phase transitions by data mining via temperature-dependent force fields
Detlef W. M. Hofmann (Uttenreuth/DE; Pula/IT)

14.35 LT2-02
Interactions in a two-dimensional Ag^{I} coordination polymer
Steven van Terwingen, Ullrich Englert (Aachen/DE)

14.40 LT2-03
In-situ XRD study on the crystallization of thin HfO_2 films
Zoltán Balogh-Michels (Buchs SG, Dübendorf/CH), Thomas Gischkat
Igor Stevanovic, Andreas Bächli (Buchs/CH), Antonia Neels (Dübendorf/CH)

14.45 LT2-04
Site-symmetry method applied for the study of layer and multilayer materials bythe Bilbao Crystallographic Server
Gemma de la Flor, Danel Orobengoa (Bilbao/ES), Yuri Kitaev
Robert Evarestov (Saint Petersburg/RU), Emre Tasci (Ankara/TR)
Mois Aroyo (Bilbao/ES)

14.50 LT2-05
Crystal structure and de- and rehydration behavior of two new chloride-containing Zeolitic Imidazolate Frameworks
Gianpiero Gallo (Stuttgart/DE), Stephan Glante (Erlangen/DE)
Sebastian Bette (Stuttgart/DE), Martin Hartmann (Erlangen/DE)
Robert E. Dinnebier (Stuttgart/DE)

14.55 LT2-06
Automated orientation imaging and phase mapping in the TEM: prospects for reliable detection of martensite in steels
Jonas Werner, Thomas E. Weirich (Aachen/DE)

15.00 LT2-07
Defect characterization of 4H-SiC with Synchrotron White Beam X-ray topography and high resolution X-ray diffractometry
Melissa Roder (Freiburg i. Br./DE), Peter Wellmann, Matthias Arzig
Johannes Steiner (Erlangen/DE), Andreas Danilewsky (Freiburg i. Br./DE)

15.05 LT2-08
Solving structures with native SAD on laboratory X-ray sources
Andreas Förster, Clemens Schulze-Briese (Baden-Dättwil/CH)
Claudio Klein (Norderstedt/DE)

15.10
LT2-09
Size-dependent structural, spectroscopic and thermoanalytic properties of nano- to poly-crystalline $Bi_2Fe_4O_9$
Andrea Kirsch, M. Mangir Murshed (Bremen/DE)
F. Jochen Litterst (Braunschweig/DE), Thorsten M. Gesing (Bremen/DE)

15.15
LT2-10
New concepts for single-crystal sapphire cells to study solid-gas reactions via *in situ* neutron scattering
Raphael Finger, Holger Kohlmann (Leipzig/DE)

15.20
LT2-11
Local magnetic properties and couplings of $Co_{2-x}Mn_xB$:A^{59}Co and ^{55}Mn zero field NMR study
Patrizia Fritsch, Franziska Hammerath (Dresden/DE), Semih Ener
Maximilian Fries, Ingo Opahle (Budapest/HU)
Eszter Simon (Darmstadt/DE, Budapest/HU)
Sabine Wurmehl (Dresden/DE), Hongbin Zhang (Darmstadt/DE)
Oliver Gutfleisch (Darmstadt, Hanau/DE)

15.25
LT2-12
Analysis of aluminum conductivity in high-valent transition metal oxides with bond-valence-site-energy calculations
Manuel Rothenberger, Dirk C. Meyer (Freiberg/DE), Tilmann Leisegang
Falk Meutzner (Freiberg/DE; Samara/RU), Tina Nestler (Freiberg/DE)

15.30
LT2-13
Symmetry lowering on heating
Maria Krzhizhanovskaya, Rimma Bubnova
Stanislav Filatov (St. Petersburg/RU)

15.35
LT2-14
Synthesis and crystal structure of new alkali-chalcogenido-manganates/indates A_3MnInQ_4
Michael Langenmaier, Julian N. Brantl
Caroline Röhr (Freiburg i. Br./DE)

15.40
LT2-15
Existence or non-existence of iota-alumina?
Stephan Lenz, Hartmut Schneider, Reinhard X. Fischer (Bremen/DE)

15.45
LT2-16
In-situ characterization and thermal decomposition behavior of ammonium-exchanged FAU type zeolites
Ahmed Gadelmawla, Iris Spiess, Johannes Birkenstock
Michael Wendschuh (Bremen/DE), Lennart Fischer (Freiburg i. Br./DE)
Reinhard Fischer (Bremen/DE)

15.50 LT2-17
Texture formation in obliquely deposited metal thin films
Susann Liedtke-Grüner, Christoph Grüner, Andriy Lotnyk
Michael Mensing, Jürgen W. Gerlach, Philipp Schumacher
Bernd Rauschenbach (Leipzig/DE)

16.00–18.30
Foyer first floor
Poster session II
(see page 31)

19.30–23.00
Auerbachs Keller
Social evening
(see page 44)

09.00–10.00 Plenary lecture
Lecture hall 9
Chair Holger Kohlmann (Leipzig/DE)

09.00 Order in 'disorder' – a modulation wave approach to the crystal chemical understanding of structured diffuse scattering
Ray Withers (Canberra/AU)

10.00–11.00 Get together young crystallographers
Lecture hall 8 (see page 46)

11.00–12.30 Instrumentation
Lecture hall 8
Chairs Martin Meven (Aachen/DE), Ullrich Pietsch (Siegen/DE)

11.00 S16-01 Resolving protein structures with electrons – cryo TEM and micro ED with JEOL
Emanuel Katzmann (Freising/DE)

11.15 S16-02 Pushing data quality for laboratory Pair Distribution Function experiments
Mirijam Zobel, Sabrina Thomä, Nils Prinz (Bayreuth/DE)

11.30 S16-03 *In-situ* and *ex-situ* magnetic orientation of microcrystals for single crystal X-ray measurements
Tsunehisa Kimura, Fumiko Kimura, Shu Tsukui, Chiaki Tsuboi (Kyoto/JP)

11.45 S16-04 A new single crystal diffractometer at BM20/ESRF
Christoph Hennig (Grenoble/FR), Atsushi Ikeda-Ohno
Thomas Radoske (Dresden/DE), Andreas Scheinost (Grenoble/FR)

12.00 S16-05 *In-situ* X-Ray diffraction measurements during low energy ion beam nitriding and etching
Darina Manova, Stephan Mändl (Leipzig/DE)

12.15 S16-06 Photon counting with mixed mode detection
Martin Adam, Roger Durst (Karlsruhe/DE)
Joerg Kaercher (Madison, WI/US), Tobias Stuerzer
Bruce Becker (Karlsruhe/DE)

I am interested to participate in the following working groups of the DGK:

(Please here the working group(s) that best match your field of expertise and research)

AK 1	[ ]	Biological Structures
AK 2	[ ]	High Pressure Crystallography
AK 3	[ ]	Electron Microscopy
AK 4	[ ]	Noncrystalline or Partial Crystalline Structures
AK 5	[ ]	Crystal Physics
AK 6	[ ]	Molecule Structures
AK 7	[ ]	Neutron Diffraction
AK 9	[ ]	Theoretical Crystallography
AK 10	[ ]	Microscopy
AK 11	[ ]	Synchrotron Radiation and High Resolution X-ray Diffractometry, Reflectometry and Tomography
AK 12	[ ]	Spectroscopy
AK 13	[ ]	Powder Diffractometry
AK 14	[ ]	Computational Crystallography
AK 15	[ ]	Mineralogical and Technical Crystallography
AK 16	[ ]	Aperiodic Crystals
AK 17	[ ]	Crystallography in Teaching
AK 18	[ ]	Surfaces
AK 19	[ ]	Crystal Chemistry
AK 20	[ ]	Crystallography in Materials Science
AK 21	[ ]	Young Crystallography

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The annual dues

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Send the apllication forms to the Schriftführer der DGK: Dr. Daniel M. Többens, HZB, Abteilung Kristallographie, Hahn-Meitner-Platz 1, D-14109 Berlin-Wannsee, Germany.

An den Vorsitzenden der Deutschen Gesellschaft für Kristallographie e.V. (DGK),
Herr Prof. Dr. Ralf Ficner.

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The annual dues are listed in the following table.

A	Regular Members	40 €	
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11.00–12.30 Spectroscopy

Lecture hall 10

Chair: Michael Fechtelkord (Bochum/DE)

11.00 S17-01
Changes in the cationic and anionic arrangements in the trilithionite: polylithionite system
Lara Sulcek, Nina Becker, Michael Fechtelkord (Bochum/DE)

11.15 S17-02
Fast diffraction and XANES analysis of solid flame reactions at PETRA III
Wolfgang Morgenroth, Dominik Spahr, Jannes Binck, Jianbo Song
Michal Stekiel (Frankfurt a. M./DE), Dmitry Varentsov (Darmstadt/DE)
Norbert Schell (Geesthacht/DE), Vadim Murzin (Wuppertal/DE)
Björn Winkler (Frankfurt a. M./DE)

11.30 S17-03
Element-specific local structure of $Cu_2Zn(Sn,Ge)Se_4$ kesterite alloys
Konrad Ritter (Leipzig, Jena/DE), Cora Preiß (Jena/DE), Galina Gurieva
René Gunder (Berlin/DE), Stefanie Eckner (Jena, Leipzig/DE)
Roman Chernikov, Edmund Welter (Hamburg/DE), Silvana Botti (Jena/DE)
Susan Schorr (Berlin/DE), Claudia Schnohr (Leipzig, Jena/DE)

11.45 S17-04
Lattice dynamics of the $Sb_2Te_{3-x}Se_x$ solid solution from experiment and theory
Markus Herrmann (Jülich/DE), Ralf Stoffel, Michael Küpers (Aachen/DE)
Mohammed Ait Haddouch, Jörg Voigt (Jülich/DE), Doug L. Abernathy
Gabriele Sala, Raphael P. Hermann (Oak Ridge, TN/US)
Richard Dronskowski (Aachen/DE), Karen Friese (Jülich/DE)

12.00 S17-05
A spectroscopic investigation of Eu^{3+} incorporation in $LnPO_4$ (Ln = Tb, $Gd_{1-x}Lu_x$, x = 0.3, 0.5, 0.7) ceramics
Henry Lösch (Dresden/DE), Antje Hirsch (Freiberg/DE)
Jacqueline Holthausen (Hilden/DE), Lars Peters (Aachen/DE)
Bin Xiao (Dresden/DE), Stefan Neumeier (Jülich/DE), Moritz Schmidt
Nina Huittinen (Dresden/DE)

12.15 S17-06
IR-spectroscopic investigation of kieserite–cobaltkieserite solid solutions, Mg1-x*Co*x$SO_4 \cdot H_2O$, under ambient and low temperature conditions with relevance to Mars and icy moons
Dominik Talla, Manfred Wildner (Vienna/AT)

11.00–12.30 Lecture hall 11	Complex and aperiodic structures
Chair	Sander van Smaalen (Bayreuth/DE)
11.00 S18-01	Complex crystal structures of efflorescence phases grown on historic objects Sebastian Bette, Gerhard Eggert, Robert E. Dinnebier (Stuttgart/DE)
11.15 S18-02	Direct observation of polar nanodomains and nucleation processes in the incommensurate Phase using piezo force microscopy Claudia Kofahl, Götz Eckold, Friedrich Güthoff (Göttingen/DE)
11.30 S18-03	Phase transitions of the 3-dimensional charge-density-wave compound CuV_2S_4 Sitaram Ramakrishnan, Andreas Schönleber, Christian B. Hübschle Nguyen Hai An Bui, Florian Feulner, Mariia Anurova (Bayreuth/DE) Dmitry Chernyshov (Grenoble/FR), Natalija van Well, Achim Schaller Toms Rekis, Claudio Eisele (Bayreuth/DE), Martin Tolkiehn (Hamburg/DE) Srinivasan Ramakrishnan (Mumbai/IN), Sander van Smaalen (Bayreuth/DE)
11.45 S18-05	The Sc-Pd system – a new 1/1 Mackay type approximant and alloying of aluminum Tilmann Leisegang (Freiberg/DE; Samara/RU), Pavlo Solokha (Genova/IT) Tatiana G. Akhmetshina, Roman A. Eremin, Albina V. Gurskaya (Samara/RU) Serena De Negri (Genova/IT), Davide M. Proserpio (Samara/RU; Milano/IT) Adriana Saccone (Genova/IT)
12.00 S18-06	From space group to space groupoid – the local symmetry of low-temperature *E*-vanillyl-oxime Berthold Stöger (Vienna/AT)
12.30–13.00 Lecture hall 10	Closing

There are two poster sessions. Posters with an even programme ID will be presented in the poster session I on Tuesday and posters with an odd programme ID will be presented in the poster session II on Wednesday. Authors are asked to be present at their poster during their poster session.

Bio-crystallography I – Signalling, macromolecular interactions and other new structures

P001 Structure-based fragment screening on dynamin GTPase domain
Helena Taberman, Oliver Daumke, Manfred S. Weiss (Berlin/DE)

P002 Engineering chimera constructs to crystallize a complex protein structure
Rezan Amjadi, Theresia Dunzendorfer-Matt, Klaus Scheffzek (Innsbruck/AT)

Bio-crystallography III – Enzymes

P003 Structural studies on the substrate and cofactor binding modes of FAD-dependent monooxygenases
Julia Kratky (Leipzig/DE), Thomas Heine (Freiberg/DE)
Renato H. Weiße (Leipzig/DE), Dirk Tischler (Freiberg/DE), Norbert Sträter (Leipzig/DE)

P004 Substrate specificity determinants of the proprotein convertase furin beyond the S4 pocket
Sven O. Dahms (Salzburg/AT), Kornelia Hardes, Torsten Steinmetzer (Marburg/DE)
Hans Brandstetter (Salzburg/AT), Manuel E. Than (Jena/DE)

Bio-crystallography IV – Structure-based drug design

P005 An approach to improve the solubility of poorly water soluble anti-cancer drug-dasatinib
Mohamed Sheik Tharik Abdul Azeeze (The Nilgiris/IN), Parimaladevi Palanisamy
Vijay Thiruvenkatam, Chinmay Ghoroi (Gandhi Nagar/IN)
S. N. Meyyanathan (The Nilgiris/IN)

P006 Structural studies on inhibitor binding to human kallikrein 7
Stefanie Hanke, Jan Pippel, Catherine A. Tindall, David Ulbricht, John T. Heiker
Norbert Sträter (Leipzig/DE)

P007 Fragment-screening studies on the ectonucleotidase CD73
Norbert Sträter, Philipp Konstantin Richter, Renato Weiße, Susanne Moschütz
Emma R. Scaletti (Leipzig/DE), Alice Douangamath, Jose Brandao-Neto
Renjie Zhang, Frank von Delft (Didcot/GB), Franziska Huschmann, Uwe Müller
Manfred S. Weiss (Berlin/DE)

POSTER PRESENTATIONS

Bio-crystallography V – Instrumentation and methods

P008 P11 at PETRA III – a Versatile Beamline for Serial and High-Throughput Crystallography
Anja Burkhardt, Eva Crosas, Olga Lorbeer, Sebastian Guenther, Tim Pakendorf
Bernd Reime, Jan Meyer, Pontus Fischer, Nicolas Stübe, Martin Warmer
Alke Meents (Hamburg/DE)

P009 Investigation of protein crystals within living insect cells using small-angle X-ray scattering
Robert Schönherr (Lübeck/DE), Cy Jeffries (Hamburg/DE)
Mia Lahey-Rudolph (Lübeck/DE), Clement E. Blanchet
Dmitri I. Svergun (Hamburg/DE), Lars Redecke (Lübeck/DE)

P010 EMBL Beamlines for Macromolecular Crystallography at PETRA III
Thomas Schneider, Gleb Bourenkov, Guillaume Pompidor, Isabel Bento
Johanna Hakanpää, Saravanan Panneerselvam, David von Stetten (Hamburg/DE)

P011 Better data from laser-shaped crystals
Tatjana Barthel (Berlin/DE), Naohiro Matsugaki, Masahide Hikita (Tsukuba/JP)
Manfred S. Weiss (Berlin/DE), Toshiya Senda (Tsukuba/JP)

P012 An all-in-one sample holder for macromolecular X-ray crystallography
Christian Feiler, Dirk Wallacher, Manfred Weiss (Berlin/DE)

Complex and aperiodic structures

P013 $Ir_3Sn_8O_4$ – a cluster compound with incommensurately modulated crystal structure
Malin Lüdicke (Dresden/DE), Tilo Söhnel (Auckland/NZ), Kati Finzel
Thomas Doert (Dresden/DE)

P014 Magneto-elastic phase transitions of the unconventional spin-Peierls compound TiOCl at high pressures and low temperatures
Achim M. Schaller, Maxim Bykov (Bayreuth/DE)
Elena Bykova (Bayreuth, Hamburg/DE), Konstantin Glazyrin (Hamburg/DE)
Sander van Smaalen (Bayreuth/DE)

P015 $LaTe_{1.8}$ – a new incommensurately modulated structure in the series $RETe_{2-\delta}$
Hagen Poddig, Thomas Doert (Dresden/DE)

P016 The Superspace Piano – a comprehensive introduction to the fundamental concepts of higher-dimensional superspace crystallography based on the simple one-dimensional pattern of black and white keys of a common musical instrument
Paul Benjamin Klar (Prague/CZ)

Disordered materials

P017 Orientionally disorder in monomethyl-quinacridone investigated by Rietveld refinement, pair distribution function analysis and lattice-energy minimizations
Carina Schlesinger, Sonja Hammer, Martin Schmidt (Frankfurt a. M./DE)

P018 A practical approach to generating models for disordered polymers using the x-ray pair distribution function
Maxwell Terban (Stuttgart/DE), Shae Machlus (Tallahassee, FL/US)
Bernd Hinrichsen (Ludwigshafen/DE), Robert E. Dinnebier (Stuttgart/DE)

Extreme/non-ambient conditions

P019 A novel stability field of a high pressure high temperaturepolymorph of dolomite
Jannes Binck (Frankfurt a. M./DE), Stella Chariton (Bayreuth/DE)
Lkhamsuren Bayarjargal (Frankfurt a. M./DE), Leonid Dubrovinsky (Bayreuth/DE)
Björn Winkler (Frankfurt a. M./DE)

P020 High temprature X-ray diffraction tudies of oxygen-deficient $Ca(Mn,Ti)O_{3-\delta}$ perovskites
Stefan Stöber, Herbert Pöllmann (Halle a. d. S./DE)

P021 Temperature-dependent structural investigation of $|Na_8(ReO_4)_2|[AlSiO_4]_6$ sodalite: phase transitions and thermal stability
Hilke Petersen, Lars Robben, Thorsten M. Gesing (Bremen/DE)

P022 Crystal chemistry at multimegabar pressures
Natalia Dubrovinskaia, Leonid Dubrovinsky (Bayreuth/DE)

P023 Is GeI_4's liquid-liquid transition identifiable as a percolation transition of 'bonds'?
Kazuhiro Fuchizaki, Hiroki Naruta (Matsuyama/JP), Takahiro Sakagami (Shizuoka/JP)

P024 Pressure-induced phase transition in Pb_2SnO_4
Dominik Spahr, Michał Stękiel, Dominik Zimmer, Lkhamsuren Bayarjargal
Wolfgang Morgenroth (Frankfurt a. M./DE), Victor Milman (Cambridge/GB)
Björn Winkler (Frankfurt a. M./DE)

P025 The limitations on quasi-harmonic thermal-pressure equations of state from anisotropic thermal pressure
Ross Angel, Gabrielle Zaffiro (Pavia/IT), Claudia Stangarone (Pavia/IT, Berlin/DE)
Boriana Mihailova (Hamburg/DE), Mara Murri, Matteo Alvaro (Pavia/IT)

POSTER PRESENTATIONS

In situ/in operando studies

P026 The thermal behavior of the zincophosphate hydrosodalite between 13 K and 300 K
Lars Robben (Bremen/DE)

P027 *In situ* phase transformation study of calcium sulfates
Laura Ritterbach, Petra Becker (Cologne/DE)

P028 Mechanism of the decomposition of thermoelectric Cu_2Se – *in situ* X-ray diffraction tomography and *ex situ* analyses
Matthias Jakob (Leipzig/DE), Gavin Vaughan (Grenoble/FR)
Oliver Oeckler (Leipzig/DE)

P029 *In situ* XRD of multi-cation doped Mn-spinel, $LiNi_{0.3}Cu_{0.1}Fe_{0.2}Mn_{1.4}O_4$, as 5V cathode material for Li-ion batteries using Ag laboratory source
Michael Knapp, Priyanka Sharma, Susana Darma, Helmut Ehrenberg (Karlsruhe/DE)

P030 Li/O incorporation-induced structural evolution during synthesis of Li-Mn-rich oxides
Weibo Hua, Björn Schwarz, Michael Knapp (Eggenstein-Leopoldshafen/DE)
Martin Etter, Alexander Schökel (Hamburg/DE), Joachim R. Binder, Sylvio Indris
Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE)

P031 Crystallization studies with *in-situ* analytical methods
Thi Yen Nguyen, Julia Stroh, Franziska Emmerling (Berlin/DE)

P032 Effect of amino acids on $CaCO_3$ precipitation
Lydia Amer (Bejaia/DZ)

Inorganic crystal structures

P033 Heteroepitaxial growth of α-, β-, γ- and κ-Ga_2O_3 phases by metal-organic vapor phase epitaxy
Stefan Merker, Volker Gottschalch, Harald Krautscheid (Leipzig/DE)

P034 Investigation into crystal structure and hydrogen-bond network of $Sr[MnO_4]_2 \cdot 3\,H_2O$ at low temperature
Maurice Conrad, Thomas Schleid (Stuttgart/DE)

P035 New Ca/Mg/Zn intermetallics of the intergrowth family of $Ba_2Li_{4.2}Al_{4.8}$ (1a)/Th_6Mn_{23} (1b)/$EuMg_{5+x}$(1c)-type structures
Katharina Köhler, Caroline Röhr (Freiburg i. Br./DE)

P036 The impact of replacements in anion and cation sublattices on optical properties of calcium orthovanadate single crystal
Elizaveta Dunaeva, Liudmila Ivleva, Irina Voronina, Maxim Doroshenko
Alexander Papashvili (Moscow/RU)

P037 New transition metal phosphonates obtained by mechanochemistry
Irina Akhmetova (Berlin/DE), Manuel Wilke (Villigen/CH)
Franziska Emmerling (Berlin/DE)

P038 Hexaaquacopper(II) decachloro-closo-decaborate tetrahydrate: Jahn-Teller distorted octahedra in $Cu(H_2O)_6[B_{10}Cl_{10}] \cdot 4\,H_2O$
Kevin Bareiß, Thomas Schleid (Stuttgart/DE)

P039 Structural diversity of hybrid lead bromide perovskites with pyridine and diazines
Michael Krummer, Michael Daub, Benjamin Zimmermann
Harald Hillebrecht (Freiburg i. Br./DE)

P040 Synthesis and characterization of self-supported SOD-LTN layers for membrane applications
Irma Peschke, Josef-Christian Buhl (Hannover/DE)

P041 Optical properties of SnS_2 synthesized by a facile chemical route
Katia Ihadjaren, Abdelhafid Souici (Bejaia/DZ)

P042 Synthesis and characterization of the hydroxoferrates(III) $A_2Fe_2O_3(OH)_2$ (A = K, Rb, Cs)
Ralf Albrecht, Jens Hunger, Thomas Doert, Michael Ruck (Dresden/DE)

P043 Crystal structure of 2-Ethylanilinium Dihydrogenophosphite $C_8H_{12}NH_2PO_3$
Aziz Kheireddine (Doha/QA), Mustafa Belhabra (Casablanca/MA)
Hamdi Hamdi Ben Yahia (Doha/QA), Said Belaaouad (Casablanca/MA)

P044 Low temperature properties of lead stannate, Pb_2SnO_4
Wolfgang Morgenroth, Dominik Spahr (Frankfurt a. M./DE)
Miguel Avalos-Borja (San Luis Potosí/MX), Martin Tolkiehn
Carsten Paulmann (Hamburg/DE), Björn Winkler (Frankfurt a. M./DE)

P045 Two New Strontium Nitridogermanates – $Sr_4[GeN_4]$ and $Sr_{17}Ge_6N_{14}$
Lukas Link, Yulin Lin, Rainer Niewa (Stuttgart/DE)

P046 New solvate complexes $[Be(Solv)^4]^I{}_2$ of beryllium iodide with polar aprotic solvents
Constantin Hoch, Timotheus Hohl, Torben Sinn (Munich/DE)

POSTER PRESENTATIONS

P047 Synthesis and crystal structure of three new lithium gallides
Jonathan Sappl, Constantin Hoch (Munich/DE)

P048 Crystal structures of $Cs_3VO_4$and $Cs_3VO_4{\cdot}2H_2O$
Constantin Hoch, Cesar Antonio Zegarra Solano (Munich/DE)

P049 Synthesis and characterization of Pt_3Cu_2Sn
Sabrina Schellhase, Wolfgang Morgenroth (Frankfurt a. M./DE)
Erick A. Juarez-Arellano (Tuxtepec, Oaxaca/MX)
Jannes Binck (Frankfurt a. M./DE), Nobumichi Tamura
Camelia Stan (Berkeley, CA/US), Andrei Barkov (Cherepovets/RU)
Björn Winkler (Frankfurt a. M./DE)

P050 An unusual interaction revisited – slipped Sn ^{II} –π-arene bonding in isodurene solvated [SnCl][MCl_4] (M=Al, Ga)
Johannes Merkelbach, Walter Frank (Düsseldorf/DE)

P051 Serendipitous formation of single-crystalline $Mg_2[SiS_4]$
Patrik Djendjur, Thomas Schleid (Stuttgart/DE)

P052 $Nd_7[SbO_6]_3$ – a new ternary rare-earth metal(III) oxoantimonate(V)
Felix C. Goerigk, Thomas Schleid (Stuttgart/DE)

P053 $CsBaInClBr[SeO_3]_2$ – a new halide oxoselenate(IV) containing three different cations
Stefan Greiner, Thomas Schleid (Stuttgart/DE)

P054 Influence of temperature and Fe substitution on the crystal structure of quaternary pavonite-type copper bismuth selenides
Christina Fraunhofer, Stefan Engel, Oliver Oeckler (Leipzig/DE)

P055 Crystal engineering of inorganic-organic hybrid materials – layered double salts derived from sodium ethanesulfonate and “simple” halides
Felix Thoelen, Walter Frank (Düsseldorf/DE)

P056 Crystal structures of M^2+$Zr(SO_4)_3$ with M = Mg, Mn, Co, Ni, Zn and Cd, and their relationship with $Fe_2(SO_4)_3$
Giester Gerald, Talla Dominik, Wildner Manfred (Vienna/AT)

P057 $NaCe_{18}O_9F_{19}Se_9$ – a sodium-containing compound in the Ce_2OF_2Se—$Ce_6O_2F_8Se_3$ system
Constantin Buyer, Sarah Wolf, Thomas Schleid (Stuttgart/DE)

P058 A new ternary structure among alkali metal trielides – structural relations between long-known and new cluster compounds
Martha Falk, Caroline Röhr (Freiburg i. Br./DE)

P059 Investigation of F-containing phases in fluoro-calcium aluminate cements and F-loss during sintering
Sabrina Galluccio, Herbert Pöllmann (Halle a. d. S./DE)

P060 Sr_2H_3Br – an unexpected phase in the SrH_2–$SrBr_2$ system
Daniel Rudolph, Jean-Louis Hoslauer, Thomas Schleid (Stuttgart/DE)

P061 $KSm[P_2Se_6]$ – the structural missing link within the $KRE[P_2Se_6]$ series
Beate Schulz, Thomas Schleid (Stuttgart/DE)

P062 Eu_2ScTaO_6 – the last member of the Eu_2RETaO_6 series
Christian Funk, Eva Brücher, Jürgen Köhler, Thomas Schleid (Stuttgart/DE)

P063 $CsTb_3STe_4$ – The First Quaternary Lanthanoid Chalcogenide with Ordered S^{2-} and Te^{2-} anions
Thomas Schleid, Stephan, P. Meyer, Falk Lissner (Stuttgart/DE)

P064 Structural characterization of barium (imido-)nitridophosphate networks
Daniel Günther (Leipzig/DE), Sebastian Wendl, Lucien Eisenburger
Wolfgang Schnick (Munich/DE), Oliver Oeckler (Leipzig/DE)

P065 The crystal structure of $CaSiH_{\approx 4/3}$ revisited
Henry Auer, Holger Kohlmann (Leipzig/DE)

P066 Crystal chemistry of alkali nona-stannid cluster compounds – novelties from binary and novel ternary Ga-containing phases
Caroline Röhr, Bernard Lehmann (Freiburg i. Br./DE)

P067 Experimental characterisation of chemical bonding in elemental boron phases
Claudio Eisele (Bayreuth/DE), Somnath Dey, Swastik Mondal (Kolkata/IN)
Carsten Paulmann (Hamburg/DE), Sander van Smaalen (Bayreuth/DE)

P068 $A_3PCr_4O_{16}$ (A = K, Cs) with supertetrahedral $[PCr_4O_{16}]^{3-}$ units – rather orthoposphates with $[PO_4]^{3-}$ tetrahedra and CrO_3 adducts than quate
Harald Hillebrecht, Michael Daub (Freiburg i. Br./DE)

P070 Two novel mixed alkali praseodymium orthoborates – K1.319(8)Li1.681(8) Pr2(BO3)3 and K2LiPr(BO3)2
Pengyun Chen, Mathias Gogolin, M. Murshed, Thorsten M. Gesing (Bremen/DE)

POSTER PRESENTATIONS

P071 Structural diversity of 5-ammonium valeric acid lead iodides through incorporation of methylammonium or solvent
Michael Daub, Harald Hillebrecht (Freiburg i. Br./DE)

P072 Observation of a polymorph of trisodium hexachlororhodate on dehydration
Martin Etter (Hamburg/DE)

P073 Rationalisation of the chemical composition and crystal structure in zinc germanium oxide nitrides
Zhenyu Wang, Joachim Breternitz, Susan Schorr (Berlin/DE)

P074 Neutron laue diffractometer for ambient and non-ambient single crystal analysis
Michael Tovar, Wallacher Dirk, Nico Grimm, Andreas Hoser (Berlin/DE)
Armand Budzianowski, Damian Rusinek (Otwock/PL), Damian Paliwoda (Warsaw/PL)
Susan Schorr (Berlin/DE)

Instrumentation

P075 Shine bright like a diamond – microfocus X-ray sealed tube sources with diamond hybrid anode technology
Jürgen Graf (Geesthacht/DE), Tobias Stürzer, Holger Ott (Karlsruhe/DE)
Matthew Benning (Madison/US), Durst Roger (Geesthacht, Karlsruhe/DE)
Paul Radcliffe, Jenss Schmidt-May, Carsten Michaelsen (Geesthacht/DE)

P076 Method for determination of the anisotropic rotational diffusion constant of microcrystals dispersed in viscous liquid medium
Fumiko Kimura, Shigeru Horii, Itsuki Arimoto, Toshiya Doi (Kyoto/JP)
Masato Yoshimura (Hsinchu/TW), Masahisa Wada (Kyoto/JP; Yongin-si/KR)
Tsunehisa Kimura (Kyoto/JP)

P077 Advanced anomalous diffraction capabilities at KMC-2 (BESSY II)
Daniel M. Többens, Ivo Zizak, Susan Schorr (Berlin/DE)

P078 Sample environment chamber for the manipulation of temperature and electric field for synchrotron measurements
Melanie Nentwich, Tina Weigel (Freiberg/DE)
Matthias Zschornak (Freiberg, Dresden/DE), Carsten Richter (Grenoble/FR)
Erik Mehner, Hartmut Stöcker, Dirk C. Meyer (Freiberg/DE)

P079 Extreme condition single crystal diffraction with hot neutrons on HEiDi at MLZ
Martin Meven (Aachen/DE), Andrzej Grzechnik (Aachen/DE), Hao Deng
Rajesh Dutta (Aachen/DE), Karen Friese (Jülich/DE)

P080 First single crystal diffraction experiments on the Ga- and In- MetalJet
Nils Nöthling, Christian W. Lehmann (Mülheim a. d. R./DE)

P081 Prediction of possible uranium compounds in drinking waters
Norov Tegshbayar, Oyuntsetseg Bolormaa, Khaniyat TSookhuu (Ulaanbaatar/MN)

P082 Numerical simulation of coherent phasing method for macromolecular electron crystallography
Krishna Khakurel (Prague/CZ)

P083 The new chemical crystallography beamline P24 at DESY
Martin Tolkiehn (Hamburg/DE)

P129 *In situ* and nano X-ray diffraction beamline at PETRA III – research possibilities and first results
Azat Khadiev, Raphael Grifone, Jana Raabe, Dmitri Novikov (Hamburg/DE)

Micro- and nanocrystalline materials (powder diffraction, EM, ...)

P084 Combinatorial search for new alternative fuel cell electro-catalyst support materials
Klaus Stöwe, Aline Clausing, Daniel Reichert, Thomas Schwarz (Chemnitz/DE)
Maximilian Weber (Saarbrücken/DE)

P085 Cellular automata models for intra-cage reactions in sodalites
Lars Robben (Bremen/DE)

P086 Synthesis and characterisation of ultra-small monometallic and bimetallic noble metal nanoparticles (Ag, Au, Pt, AgPt, AgAu)
Oliver Wetzel, Matthias Epple, Kateryna Loza, Marc Heggen (Essen/DE)

P087 XPS investigations on quartzite surfaces of natural rock samples for proof of Al exposure
Klaus-Jürgen Hünger, Mario Kositz, Matti Danneberg (Cottbus/DE)
Joerg Radnik (Berlin/DE)

P088 Crystal structure of kaňkite, $FeAsO_4 \cdot 3.5H_2O$, and its dehydration product $Fe_2(AsO_4)(HAsO_4)(OH)(H_2O)_3$
Juraj Majzlan (Jena/DE), Jakub Plášil, Lukáš Palatinus, Gwladys Steciuk (Praha/CZ)

P089 Heterocyclic ligands for water sorption in metal –organic frameworks – a structural study using the rietveld method
Michael Wharmby (Hamburg/DE), Helge Reinsch, Dirk Lenzen (Kiel/DE)
Mohammad Wahiduzzaman, Guillaume Maurin (Montpellier/DE)
Norbert Stock (Kiel/DE)

POSTER PRESENTATIONS

P090 New tricks for an old dog – the powder diffraction and total scattering beamline P02.1 at PETRA III, DESY
Michael Wharmby, Martin Etter, Alexander Schökel, Jo-Chi Tseng, Mario Wendt
Sergej Wenz (Hamburg/DE)

Organic molecules and coordination compounds

P091 2D Framework[Cu^{II}(2,3′-2′,3-bpdc)H_2O]n – synthesis, structure and photoluminescence properties
Andrzej Kochel, Kamil Twaróg (Wrocław/PL), Małgorzta Hołyńska (Marburg/DE)

P092 Bulk crystallized hydrazone ligand vs. its layered crystallized Zn(II) complex
Leila Noohinejad, Seyed. A. Hosseini-Yazdi (Tabriz/IR), Natalija van Well
Sander van Smaalen (Bayreuth/DE)

P093 Single-source precursors for ternary aluminates
Sebastian Kuesel, Harald Krautscheid (Leipzig/DE)

P094 New 2D networks with a direct fluorine-metal bond – MF(CH_3COO) (M: Sr, Ba, Pb)
Steffen Breitfeld, Gudrun Scholz, Franziska Emmerling
Erhard Kemnitz (Berlin/DE)

P095 Rational design of proton-electron transfer system based on nickel dithiolene complexes with pyrazine skeletons
Yojiro Kimura, Mikihiro Hayashi, Yukihiro Yoshida, Hiroshi Kitagawa (Kyoto/JP)

P096 An experimental and theoretical approach to control salt vs. co-crystal vs. hybrid formation – crystal engineering of an E/Z-butenedioic acid/phthalazine system
Analia Ivanna Chamorro Orue, Carsten Schauerte, Roland Boese
Klaus Merz (Bochum/DE)

P097 Synthesis and structure of the donor-free potassium silanide K[$SiPh_3$]
Lothar Fink, Edith Alig, Isabelle Georg, Inge Sänger, Matthias Wagner
Hans-Wolfram Lerner (Frankfurt a. M./DE)

P098 Crystal Engineering of inorganic-organic hybrid materials with heterobifunctional organic building blocks – interplay of hydrogen bonding and π-system interactions of short chained α,ω-ammoniophenylalkanes?
Marten Lichte, Felix Freese, Walter Frank (Düsseldorf/DE)

P099 *In situ* crystallization and crystal structure determinations of some 2-thiophenes
Richard Goddard, Nils Nöthling, Christian W. Lehmann (Mülheim a. d. R./DE)

P100 A pyrazole-containing copper coordination framework – an investigation into ist Hirshfeld surface analysis, magnetic behavior and biological activity
Amani Direm (Khenchela/DZ), Mohammed S. M. Abdelbaky (Oviedo/ES)
Olufunso Abosede (Bayelsa State/NG), Santiago García-Granda (Oviedo/ES)

Small molecules at large facilities

P101 StructureFinder
Daniel Kratzert (Freiburg i. Br./DE)

P102 The crystal structures of α- and β-nitrogen trifluoride
Sergei Ivlev, Matthias Conrad (Marburg/DE)
Markus Hoelzel (Garching b. München/DE), Antti Karttunen (Aalto/FI)
Florian Kraus (Marburg/DE)

Solid state physics in crystallography

P103 Magneto-electronic structure of $REFe_2$ (RE = Ho and Er) intermetallic compounds: ab initio study
Bentouaf Ali (Hay Ennasr/DZ)

P104 Role of particle size distribution and packing density in the SHG powder measurements
Lkhamsuren Bayarjargal (Frankfurt a. M./DE)

P105 Insulator-half metallic transition by the tetragonal distortion – a first-principles study of strain-induced perovskite $RbMnF_3$
Norovsambuu Tuvjargal, Namsrai Tsogbadrakh, Chun Feng
Jav Davaasambuu (Ulaanbaatar/MN)

P106 Phase formation study and crystal growth of cesium cobalt halogenides $Cs_2Co(Cl_{1-x}Brx)_4$ and $Cs_3Co(Cl_{1-x}Brx)_5$ with $0 \leq x \leq 1$
Matous Kloda, Ivana Cisarova, Ivan Nemec (Prague/CZ), Thomas Lorenz
Oliver Breunig, Petra Becker, Ladislav Bohatý (Cologne/DE)

P107 Energy harvesting with PVDF foils
Sandra Jankus, Hartmut Stöcker, Juliane Hanzig, Erik Mehner, Sven Jachalke
Dirk C. Meyer (Freiberg/DE)

P108 Water splitting by pyroelectric single crystals
Thomas Köhler (Freiberg, Dresden/DE), Wolfram Münchgesang
Erik Mehner (Freiberg/DE), Tilmann Leisegang (Samara/RU; Freiberg/DE)
Hartmut Stöcker, Dirk Carl Meyer (Freiberg/DE)

P109 Influence of chloride substitution on the rotational dynamics of methylammonium in $MAPbI_{3-x}C_{Ix}$ perovskites
Götz Schuck (Berlin/DE), Frederike Lehmann (Berlin, Potsdam/DE)
Jacques Ollivier, Hannu Mutka (Grenoble/FR), Susan Schorr (Berlin/DE)

Spectroscopy

P110 Characterization of the simulation liquids sorption by the packaging material: polyethylene-vinyl acetate
Rachid Atmani, M'hammed El Kouali
Mohammed Talbi, Abdalhak El Brouzi (Casablanca/MA)

P111 Solid State NMR investigations of cation and anion ordering in the system Lithian muscovite – trilithionite
Michael Fechtelkord, Nina Becker, Lara Sulcek (Bochum/DE)

P112 Effects of temperature and pressure on the optical and vibrational properties of thermoelectric SnSe
Ilias Efthimiopoulos (Potsdam/DE), Matthias Berg, Annika Bande, Ljiljiana Puskar
Eglof Ritter (Berlin/DE), Wei Xu (Beijing/CN), Augusto Marcelli
Michele Ortolani (Rome/IT), Martin Harms, Jan Müller, Sergio Speziale
Monika Koch-Müller (Potsdam/DE), Yong Liu, Li-Dong Zhao (Beijing/CN)
Ulrich Schade (Berlin/DE; Beijing/CN)

P113 Changes of the properties of biogenic and synthetic hydroxylapatite under the influence of external factors deduced by magnetic resonance
Valentyn Radchuk, Oleksandr Brik, Natalia Dudchenko (Kyiv/UA)

P114 Characterization spectroscopic infrared and Raman of new type materials sillenite
Hajar Ait Oulahyane (Casablanca/MA)

Structure-property-relationships

P115 Tetragonal mixed system $Cs_2CuCl_{4-x}Br_x$
Natalija van Well (Bayreuth/DE; Villigen/CH), Denis Sheptyakov
Emmanuel Canêvet (Villigen/CH), Claudio Eisele, Sitaram Ramakrishnan (Bayreuth/DE)
Tian Shang, Marisa Medarde (Villigen/CH), Antonio Cervellino (Villigen/DE)
Markos Skoulatos, Robert Georgii (Garching b. München/DE)
Christian Rüegg (Villigen, Geneva/CH), Sander van Smaalen (Bayreuth/DE)

P116 Synthesis and luminescent properties of Sm^{3+} and Dy^{3+} doped earth alkaline borates MB_2O_4 (M = Ca, Sr, Ba)
Chimednorov Otgonbayar, Herbert Pöllmann (Halle a. d. S./DE)

P117 Quantification of stress conditions in quartzite by using RAMAN spectroscopy
Klaus-Jürgen Hünger, Matti Danneberg (Cottbus/DE)
Steven Herold, Joerg Acker (Cottbus, Senftenberg/DE)

P118 Bond lengths in alumino-silicate halide sodalites from 13 K to the decomposition
Marius Wolpmann, Lars Robben, Thorsten M. Gesing (Bremen/DE)

P119 Understanding on microstructure properties of additive manufacturing Ti-based alloy composite used as biomedical implants
Jo-Chi Tseng (Hamburg/DE), Wei Chang, Kuan-Ying Tseng (Hsin-Chu/TW)
Shao-Ju Shih (Taipei/TW), Nien-Ti Tsou (Hsin-Chu/TW), Pei-Yi Tsai
Chih-Chieh Huang (Zhudong/TW), Wei-Chin Huang, E-wen Huang (Hsin-Chu/TW)

P120 Curie temperature studies of synthetic titanomagnetite single crystals
Sophie-Charlotte Lappe, Marten Isenberg (Aachen/DE)

P121 $FAPbBr_3$ – about the influence of deuteration – a temperature dependent neutron diffraction study
Alexandra Franz, Daniel Többens, Frederike Lehmann, Martin Kärgell
Susan Schorr (Berlin/DE)

P122 Investigations on copper iodide as a thermoelectric material
Tobias Stollenwerk, Oliver Oeckler (Leipzig/DE)

P123 Comparative study on the axial negative thermal expansion of linear α- and zig-zag chain backboned β-$PbAlBO_4$
Mathias Gogolin, Mohammed Mangir Murshed, Thorsten M. Gesing (Bremen/DE)

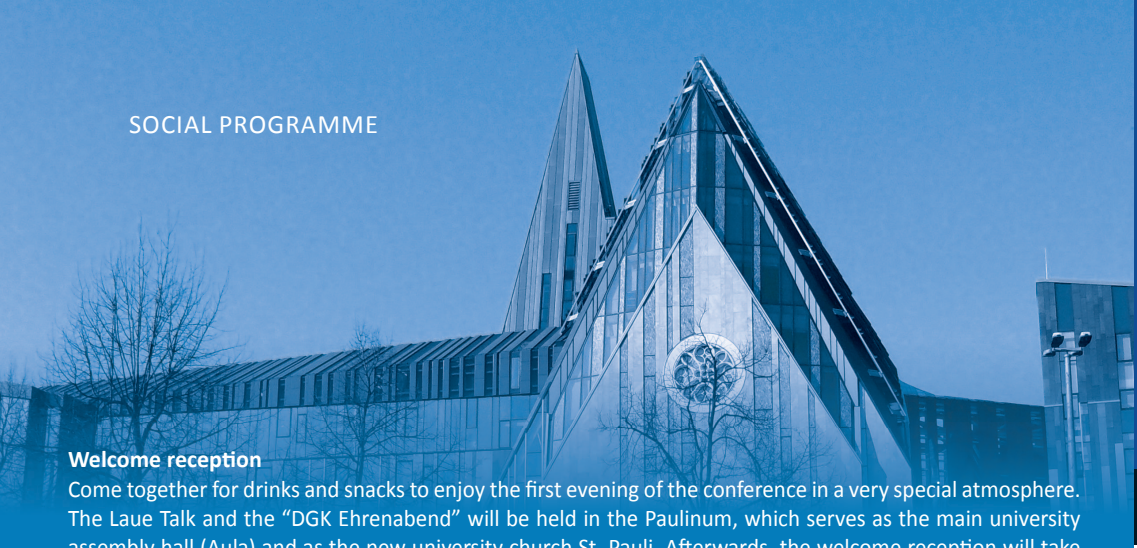
P124 Synthesis and characterization of $(Bi_{1-x}Rx)_2Mn_4O_{10}$ (R = Nd, Sm and Eu) for x = 0.0 – 1.0
Kowsik Ghosh, Thorsten M. Gesing, M. Mangir Murshed (Bremen/DE)

P125 Ferroelectricity, ionic conductivity and structural paths for large cations migration in $Ca_{10.5-x}\,Pb_x(VO_4)_7$ single crystals, x = 1.9, 3.5, 4.9
Dina Deyneko, Darya Petrova, Bogdan Lazoryak, Sergey Aksenov (Moscow/RU)

Late poster

P126 MetalJet source enabling advanced protein crystallography
Emil Espes, Julius Hållstedt

P127 Recent developments in BIO-SAXS using MetalJet X-ray source
Julius Hållstedt, Emil Espes



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 Paulinum, which serves as the main university assembly hall (Aula) and as the new university church St. Pauli. Afterwards, the welcome reception will take place in the foyer of the Augusteum in front of the entrance of the Paulinum. Allow yourself interesting conversations with colleagues and old friends in this impressive building.

Date	Monday, 25 March
Time	18.45–20.30
Fee	included in the conference fee, registration required
Venue	Foyer Augusteum

Social evening

We would like to invite you to the social evening of the conference in "Auerbachs Keller", an old wine cellar and the second eldest restaurant in Leipzig. If the name sounds familiar to you, then perhaps this is due to Johann Wolfgang von Goethe's literary work "Faust I" in which "Auerbachs Keller" was immortalized. Goethe was a great friend and a frequent guest of "Auerbachs Keller" during his studies in Leipzig. Don't miss the opportunity to enjoy a convivial evening in this world-famous and historic location with delicious food and drinks!

Date	Wednesday, 27 March
Time	19.30–23.00, admission from 19.00
Fee	45 EUR
Venue	Auerbachs Keller Leipzig Grimmaische Straße 2–4 I 04109 Leipzig
Distance to the conference venue	350 m

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Topics

- Organic and inorganic structure determination
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Lightning talks of young crystallographers

The "young crystallographers" are happy to welcome you to the 5th Lightning talks at the 27th Annual Meeting of the DGK. This year, we are looking forward to our two microsymposia where 34 young crystallographers will introduce their research in 5-minutes appetizer "Lightning talks". Each contribution is complemented by a poster that will be presented and discussed in the poster sessions afterwards.

Lightning talks I (see page 18)
Date Tuesday, 26 March
Time 15.30–17.00
Room Lecture hall 11

Lightning talks II (see page 25)
Date Wednesday, 27 March
Time 14.30–16.00
Room Lecture hall 11

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. We will give a brief summary of last year's activities (especially our 3rd Meeting in Aachen) 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 Thursday, 28 March
Time 10.00–11.00
Room Lecture hall 8

We are looking forward to welcoming you!

Khai, Linda and Michael
Chairs of the "young crystallographers"

Conference language

The conference language is English.

Opening hours

	Monday	Tuesday	Wednesday	Thursday
Check-in	12.00–17.00	08.00–17.30	08.00–16.00	08.30–13.30
Industrial exhibition	12.30–16.45	09.00–19.30	09.00–18.30	09.00–13.30

Name badge

Please wear your name badge during all conference events. Admission to scientific sessions, the social programme and to the industrial exhibition is restricted to participants wearing their badge. Participants will receive their name badge at the check-in on site.

Publication of abstracts

All abstracts will be published in a printed supplement of the journal "Zeitschrift für Kristallographie", Walter de Gruyter. The abstract book is available for purchase at the check-in.

Certificates of attendance

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

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Walter de Gruyter GmbH
“Zeitschrift für Kristallographie – New Crystal Structures”
“Zeitschrift für Kristallographie – Crystalline Materials”

State at printing

Tuesday, 26 March

Thermo Fisher Scientific (Eindhoven/NL)
14.30–15.30
Lecture hall 8

Micro-ED: A new chapter in structure determination of small molecules and macro-molecules

During the last few years cryo electron microscopy (cryo-EM) and Single Particle Analysis (SPA) have grown from techniques able to produce low-resolution structures of protein complexes (aka blobology) to tools capable of achieving atomic resolution for complexes that nobody could ever solve. This change of paradigm, that lead among other things to the Nobel prize in Chemistry in 2017, goes under the name or resolution revolution.
In the last year another technique has risen to prominence in field of cryo-electron microscopy: micro-ED. It consist in collecting tilt series in diffraction mode of quickly rotating microcrystal in an electron microscope. Micro-ED holds the promise to produce very quickly high-resolution structure of macro-molecules and small molecules out of crystals in the nanometer range or crystalline precipitate. In this presentation we will show the revolutionary potential of microED1,2,3 and we will illustrate which equipment do you need to be successful with both well-established SPA application, and innovative microED technology.
1. IUCrJ Volume 6, Part 2, March 2019
2. Acta Crystallogr D Struct Biol. (2018), 74, 506-518
3. Proc Natl Acad Sci U S A. (2018) 115, 9569-9573

Wednesday, 27 March

Rigaku Europe SE (Oxford/GB)
12.30–13.30
Lecture hall 8

Rigaku Europe SE will be holding its traditional DGK lunchtime seminar on Wednesday, 27 March in Lecture Hall 8. A buffet style lunch and beer will be provided. Speakers will include Dr Mathias Meyer and Dr Peter Emmermann. Join us to discover the latest developments from Rigaku and to get tips for making the most of your instrument.

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