PROGRAMME

22nd Annual Conference of the German Crystallographic Society (DGK)

17–20 March 2014
BERLIN

Principal Editor:
T.F. Kuech

Editorial Board:
R.S. Feigelson
K. Nakajima
G.B. Stringfellow

Aims and Scope

The journal offers a common reference and publication source for workers engaged in research on the experimental and theoretical aspects of crystal growth and its applications, e.g. in devices. Experimental and theoretical contributions are published in the following fields: theory of nucleation and growth, molecular kinetics and transport phenomena, crystallization in viscous media such as polymers and glasses; crystal growth of metals, minerals, semiconductors, superconductors, magnetics, inorganic, organic and biological substances in bulk or as thin films; molecular beam epitaxy, chemical vapor deposition, growth of III-V and II-VI and other semiconductors; characterization of single crystals by physical and chemical methods; apparatus, instrumentation and techniques for crystal growth, and purification methods; multilayer heterostructures and their characterisation with an emphasis on crystal growth and epitaxial aspects of electronic materials. A special feature of the journal is the periodic inclusion of proceedings of symposia and conferences on relevant aspects of crystal growth.

For more information: **www.journals.elsevier.com/journal-of-crystal-growth**

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Organisation and Imprint

Conference organiser
Deutsche Gesellschaft für Kristallographie (DGK)

Conference chair
Prof. Susan Schorr
Helmholtz-Zentrum Berlin für Materialien und Energie (HZB)
and Freie Universität Berlin
Hahn-Meitner-Platz 1, 14109 Berlin

Local organising committee
Holger Dobbek (Humboldt-Universität zu Berlin)
Udo Heinemann (Max-Delbrück-Centrum für Molekulare Medizin)
Martin Lerch (Technische Universität Berlin)
Beate Paulus (Freie Universität Berlin)
Manfred Reehuis (HZB)
Susan Schorr (HZB/Freie Universität Berlin)
Manfred S. Weiss (HZB)

Conference website
www.dgk-conference.de

Conference organisation and Industrial exhibition
Conventus Congressmanagement & Marketing GmbH
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Design/Layout
Layout	www.krea.tif-design.de
Print	www.siblog.de
Circulation	550
Editorial Deadline	26 February 2014

Dear colleagues,

It is a great pleasure to invite you all on behalf of the local organizing committee to the 22nd Annual Conference of the German Crystallographic Society (DGK) to the capital of Germany, Berlin. The conference venue is the prestigious Henry-Ford Bau of the "Freie Universität Berlin".

The scope of this 22nd DGK annual meeting is to show the diversity of crystallography as an interdisciplinary science. We are very glad that a number of renowned scientists, representing all different fields of crystallography, have accepted our invitation for a plenary lecture.

The year 2014 is a very special one – the International Year of Crystallography proclaimed by the UN. We are very proud to host the DGK annual meeting just in that year. To celebrate this occasion with us on the day before the conference, we invite you to a special symposium "IYCr2014 celebration" followed by a IYCr2014 party.

It is our intention to offer researchers, feeling home within the interdisciplinary field of crystallography, an inspiring scientific platform. We especially welcome young scientists who participate in the conference and in the activities of the „Young Crystallographers" group.

Let us together make the 22nd Annual Conference of the DGK in the International Year of Crystallography a memorable one!

See you in Berlin in March 2014!

Susan Schorr

Prof. Susan Schorr
Conference Chair

General Information

Venue and date (for GPS)

Henry-Ford-Bau, Freie Universität Berlin
Garystraße 35 • 14195 Berlin-Dahlem
17–20 March 2014

Registration

DGK-Member	170 EUR
DGK Non-Member	200 EUR
Student*	80 EUR
IYCr Party, 17 March 2014	10 EUR
Social Evening, 19 March 2014	40 EUR

*Confirmation required

Payment/Confirmation of payment

An invoice or confirmation of registration will be sent to you via postal or electronic mail within 14 days after online or paper registration. This invoice is a valid invoice which may be submitted to the local tax and revenue office. All fees are due upon receipt of invoice/ registration confirmation. Payment transfers must include participant's name and invoice number. Payment is also accepted by credit card (Master/Eurocard, American Express, VISA). Should you transfer your invoice amount within 10 days before the start of the event, please present your transfer remittance slip at the check-in desk as proof of payment.

Accommodation

We have allocated a contingent of rooms at different hotels. Further information can be found on www.dgk-conference.de. Please note: Conventus GmbH acts as an intermediary party and assumes no liability for reservations made. Changes and cancellations have to be addressed to the respective hotel directly.

Travel by train

Good for the environment. Convenient for you. Travel by train from 99 EUR to the congresses and events of Conventus 2014.

The price for your congress event ticket for round trip* is:

- 1st class 159 EUR
- 2nd class 99 EUR

Your ticket price for international calls will be furnished upon request.

This offer is valid for all events of Conventus Congressmanagement & Marketing GmbH in 2014.

Please call our service number **+49 (0)1805 31 11 53**** to book your ticket and quote **„Conventus"** as reference. Please have your credit card at hand.

Your price advantages compared to the regular price *:**

for example on the track From ↔ to (and return)			1st class 159 EUR Regular fair	1st class 159 EUR Savings	2nd class 99 EUR Regular fair	2nd class 99 EUR Savings
Frankfurt a. M.	↔	Berlin	398 EUR	239 EUR	246 EUR	147 EUR
Munich	↔	Berlin	441 EUR	282 EUR	260 EUR	161 EUR

Conventus Congressmanagement & Marketing GmbH and Deutsche Bahn wish you a pleasant journey!

* Changes and reimbursement before the first day of validity are 15 EUR excluded from the first day of validity onwards. Passengers restrict themselves to a particular train and travel times. For a supplement of 30 EUR in 2nd class resp. 20 EUR in 1st class full flexible tickets are also available.

** The booking line is available from Monday to Saturday 08^{00}–21^{00}. Calls will be charged at 0.20 EUR per minute, the expenses from cell phones max. 0.60 EUR per minute.

*** Prices are subject to change.

General Information

Publishing of abstracts

All abstracts will be published in a printed abstract volume (provided with an ISBN). The volume is available on demand via registration.

Poster awards

The three best posters will be awarded with 300 EUR, 200 EUR and 100 EUR for the 1st, 2nd and 3rd price, respectively. The award ceremony will be held during the social evening. The winners will be informed with a button on their posters.

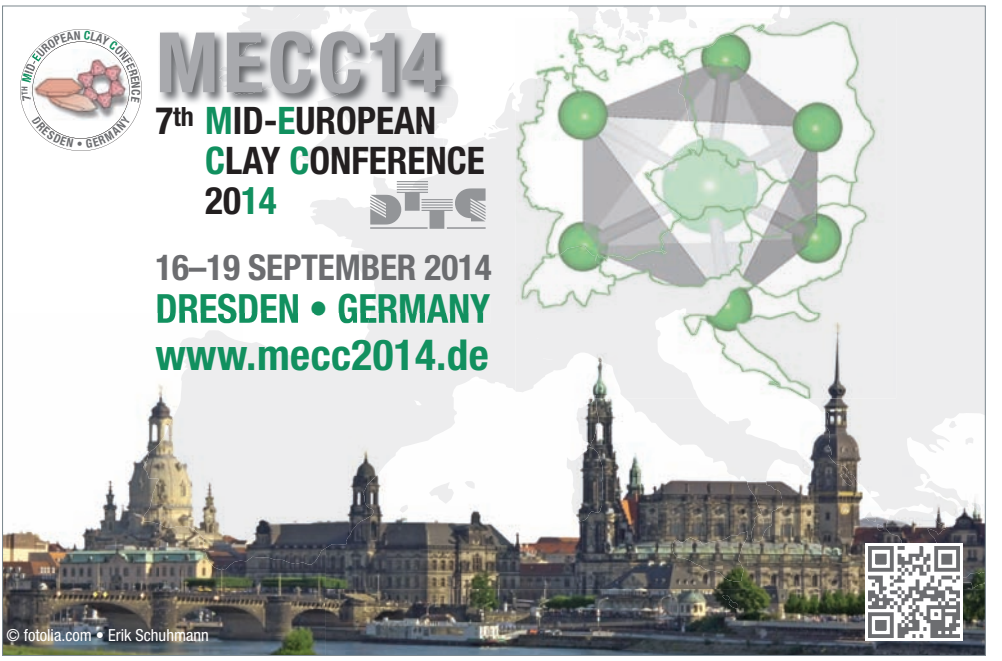
Opening hours	Mon 17 March	Tue 18 March	Wed 19 March	Thu 20 March
Check In	13^{00}–19^{00}	08^{00}–19^{00}	08^{00}–18^{30}	08^{00}–16^{30}
Media Check In	13^{00}–19^{00}	08^{00}–18^{30}	08^{00}–18^{00}	08^{00}–16^{30}
Trade Exhibition	16^{30}–20^{00}	10^{00}–18^{00}	10^{30}–17^{30}	10^{30}–16^{30}

Internet

WLAN will be provided free of charge. Please use the access data:
network: conference • password: 2hhxkkb7

Restaurants nearby the conference venue:

- Café Bistro Aux Delices Normands, Berliner Straße 49, Distance: 100 m
- Wok Way – Asiatisches Bistro, Garystraße 45, Distance: 100 m
- Cafeteria FU Wirtschaftswissenschaften, Garystraße 21, Distance: 200 m
- Cafeteria Otto-Suhr-Institut, Ihnenstraße 21, Distance: 260 m



Submitting your presentation/technical information

Please prepare your presentation in 4:3 aspect ratio. A presentation notebook with a PDF reader and MS Office PowerPoint 2007 will be provided. The use of personal notebooks is possible upon agreement. However, it may interrupt the flow of the programme in the lecture hall. Please provide an adapter for VGA if necessary. A notebook, presenter and laser pointer are available at the speaker's podium in the lecture hall. A technical supervisor will help you.

Speakers preparation

Please submit your presentation at the media check-in (seminar room 2) no later than 90 minutes before the presentation begins. You may view and/or edit your presentation. For submission, please use a USB flash drive.

Poster sessions

Posters should be no larger than DIN A0 portrait format (84.1 cm x 118.9 cm). Poster boards are 120 cm x 150 cm. They are only to be used with the designated pins. Poster boards will be numbered. You will find your poster number in the programme book on page 42 ff. Poster should be removed

Exhibitors, Sponsors and Media Cooperation

We would like to thank the following companies for their support:

Lunch symposium
Agilent Technologies GmbH (Waldbronn/DE)

Sponsor lanyards and name badges
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Media cooperation
Wissenschaftliche Verlagsgesellschaft Stuttgart (Stuttgart/DE)
Naturwissenschaftliche Rundschau
Elsevier (Amsterdam/NL)
Journal of Crystal Growth

Exhibitors
1 ChemPur Feinchemikalien und Forschungsbedarf GmbH (Karlsruhe/DE)
2 Budzylek GbR (Neuss/DE)
3 FIZ Karlsruhe (Eggenstein-Leopoldshafen/DE)
4 Agilent Technologies GmbH (Waldbronn/DE)
5 MK Versuchsanlagen (Mücke/DE)
6 Bruker AXS GmbH (Karlsruhe/DE)
7 INCOATEC GmbH (Geesthacht/DE)
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9 Xenocs SA (Sassenage/FR)
10 Stoe & Cie GmbH (Darmstadt/DE)
11 PANalytical GmbH (Kassel/DE)
12 Oxford Cryosystems Ltd (Long Hangborough/GB)
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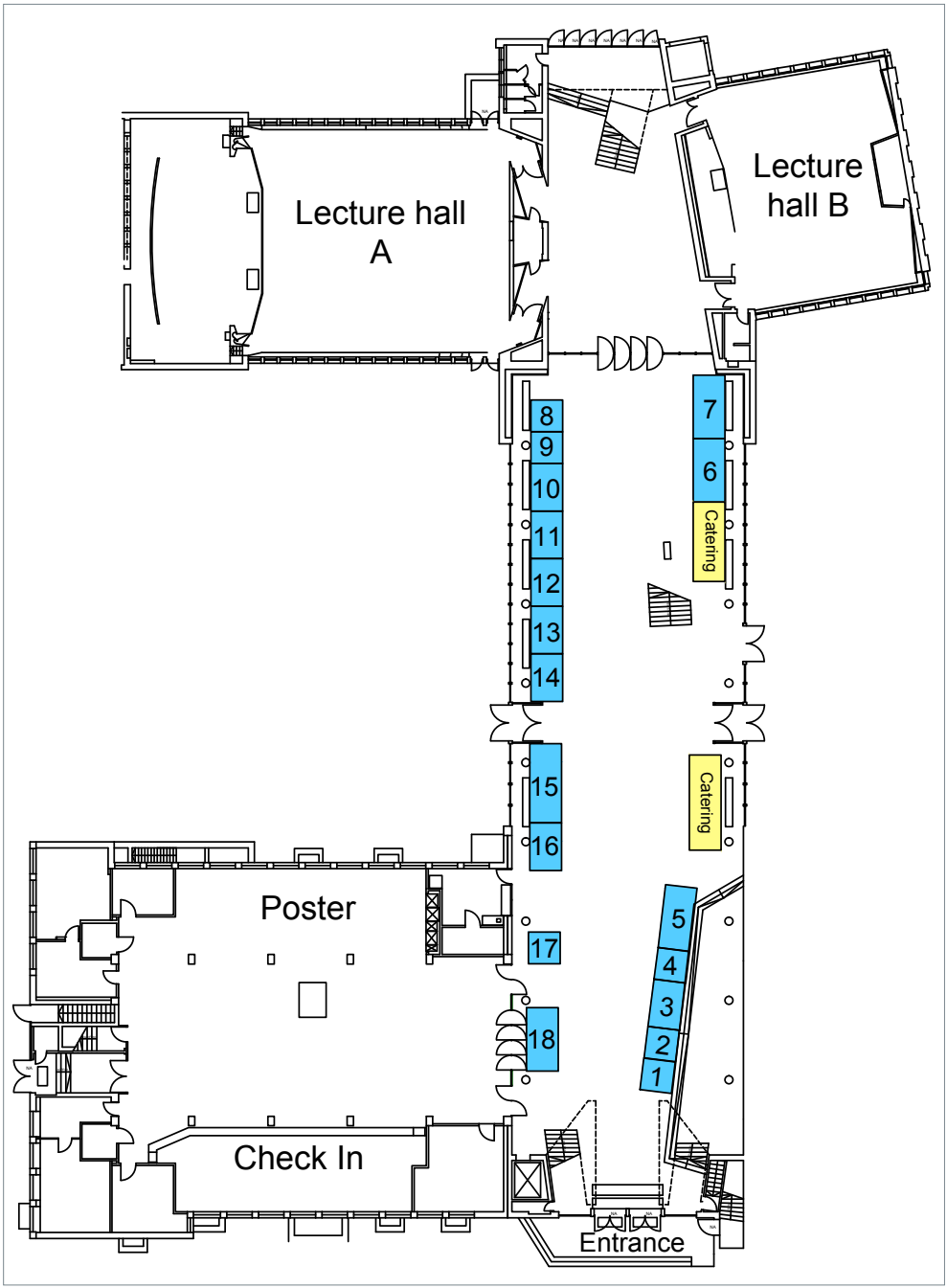
16 Dectris Ltd. (Baden/CH)
17 Verlag Walter de Gruyter GmbH (Berlin/DE)
18 International Union of Crystallography (Chester/GB)

state at printing



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Tuesday, 18 March 2014, 13^{15}–14^{15}, Lecture hall B

Agilent Technologie

Agilent Technologies (Waldbronn/DE)

Advances in Data Quality in Area Detector Diffraction Experiments.
Mathias Meyer (Wroclaw/PL)

The data quality of single crystal diffraction experiments depends on several factors: a) The diffractometer and the area detector hardware, b) the sample, c) the experimental procedure/strategy and d) the data reduction approach and software.

The talk will highlight key aspects of each of these factors.
The hardware revolves around the notions of absolute detectivity, overhead, readout speed, minimizing systematic errors and diffractometer access. Advances in area detector technology and data collection approaches will be presented. Agilent's new CCD camera generation S2 with Smart Sensitivity Control will be put in context of existing CCD detectors.
The sample choice, mounting, protection environment is controlled within reason by the user. The experimental procedure comprises the choice of wavelength, the geometric strategy, the mode of scan and detector operation and the decision on absolute detectivity vs. redundancy. Agilent's CrysAlisPro software implements the 4^{th} generation of strategy software with new features for data quality.

The data reduction software has to be optimized at extracting consistently area detector data not only under good conditions, but also under real life flaws of the practical experimental procedure. Especially twinned samples represent a challenge. The new data reduction approach for twins significantly improves the data quality of small molecule and protein twins.

Food and beverages will be served.

IYCr Party & Welcome Reception

Come together for drinks and snacks after the conference day to enjoy this evening and celebrate the International Year of Crystallography 2014. Allow yourself interesting conversations with colleagues, old friends, exhibitors and meet new acquaintances.

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Date	Monday, 17 March 2014
Venue	Industrial exhibition area
Time	18^{00}–20^{00}
Fee	10 EUR

Berlin City Tour by bus

If you want to get a quick overview of the most important sights of Berlin, a bus-tour would be the perfect choice. Between the famous street "Kurfürstendamm" and "Alexanderplatz" you will get to know all sights in the Berlin city center. You can leave the bus at least once to take a walk around some sights like the "Brandenburger Tor".

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Date	Tuesday, 18 March 2014
Time	15^{00}–17^{30}
Fee	20 EUR
Language	German
Meeting point	Check-In
min.	20 participants
max.	36 participants

Booking is possible until 13 March 2014 at the latest!

Berlin City Tour by foot

Discover the world-famous and most inspiring places of Berlin. With this tour you can get a great insight into Berlin's historical and present times. The "Brandenburger Tor", remains of the Berlin Wall, the Holocaust Monument and many other interesting buildings and places will be visited. The tour ends at the "Brandenburger Tor".

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Date	Wednesday, 19 March 2014
Time	14^{00}–16^{00}
Fee	10 EUR
Language	German
Meeting point	Checkpoint Charlie • Friedrichstraße 43–45 • 10117 Berlin
min.	10 participants
max.	20 participants

Booking is possible until 13 March 2014 at the latest!

Social Evening at Restaurant "Nolle"

The restaurant "Nolle" is located in the heart of Berlin, directly under the historic S-Bahn arch (S and U-Bahnhof Friedrichstraße) and offers an impressive original atmosphere of a typical 1920s restaurant, giving a perfect ambience for our Berlin dinner. "Nolle" is where the first beer palace, "Der Franziskaner", was opened a hundred years ago. It is a place of traditional hospitality, showing Berlin as it was in the past and as it continues to be in the present. Join us for a unique evening, only a few steps away from the most famous sights of Berlin and enjoy this atmosphere after a long conference day!

© Restaurant Nolle

Date	Wednesday, 19 March 2014
Time	20^{00}–23^{00}
Fee	40 EUR
Address	Restaurant "Nolle" • Georgenstraße • S-Bahnbogen 203 • Berlin

A bus shuttle to Restaurant Nolle will be provided. It starts 19^{15} at the Henry-Ford-Bau and also stops at the SeminarisCampus Hotel at 19^{25}. Around the restaurant are less parking places available.

At 23^{00} the bus shuttle will return to the SeminarisCampus Hotel and to the Henry-Ford-Bau.

Berlin Wall bike tour

Don't miss the possibility of a guided bike tour through Berlin and discover the history of the Berlin Wall along its former course. The tour leads you to the memorial site and remains of the Wall. You will also see one of the last watchtowers, Checkpoint Charlie and many other famous historical sights. The tour ends at the "Fernsehturm".

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Date	Thursday, 20 March 2014
Time	14^{00}–16^{00}
Fee	25 EUR incl. bike
Language	German
Meeting point:	bike rental at the 'Fernsehturm' • Panoramastraße 1a 10178 Berlin
min.	7 participants
max.	15 participants

Booking is possible until 13 March 2014 at the latest!

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- Acquisition and maintenance (ongoing service) of industry partners
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IYCr 2014 Celebration – a special symposium to celebrate the International Year of Crystallography

Round Table Speakers

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14^{30}–16^{45} IYCr 2014 Celebration

Lecture hall A

Chairs Sine Larsen (Copenhagen/DK), Susan Schorr (Berlin/DE)

14^{30} Opening
Susan Schorr (Berlin/DE)

14^{35} Musical intermezzo

14^{40} Crystallography: Past – Present – Future
Sine Larsen (Copenhagen/DK)

Crystallographers at work:

15^{10} Growth of Si- and Ge-Nanocrystals
Torsten Boeck (Berlin/DE)

15^{25} Crystallography in science management
Yvonne Tomm (Berlin/DE)

15^{40} Macromolecular crystallography and drug discovery
Ursula Egner (Berlin/DE)

15^{55} Crystallography in public relations
Michael Tovar (Berlin/DE)

16^{10} Discussion

16^{40} Musical closing

16^{45} Coffee break

17^{00}–18^{00} DGK Ehrenabend

Lecture hall A Preisverleihungen

Vortrag des Laue-Preisträgers
Detection of pressure-induced phase transitions using second harmonic generation
Lkhamsuren Bayarjargal (Frankfurt a. M./DE)

18^{00}–20^{00} IYCr Party & Welcome Reception (see page 13)

09^{00}–09^{30} Conference opening
Lecture hall A Susan Schorr (Berlin/DE)

09^{30}–10^{30} Plenary lecture
Lecture hall A Metal nanoparticles in energy catalysis; the role of structure and
P01 dynamics
Robert Schlögl (Berlin/DE)
Chair Thorsten Ressler (Berlin/DE)

11^{00}–13^{00} MS01 – Crystallography of pharmaceutically active compounds &
Lecture hall A halogen and hydrogen bonds in crystal engineering
Chairs Ullrich Englert (Aachen/DE), Norbert Nagel (Frankfurt a. M./DE)

11^{00} Small-molecule crystallography – applications to pharmaceuticals
MS01–T1 Elena Boldyreva (Novosibirsk/RU)

11^{20} Absolute configuration determination for light atom structures using
MS01–T2 a liquid metal Jet X-ray source with Ga Kα radiation
Jürgen Graf (Geesthacht/DE), Michael Ruf (Suhl, Karlsbad/DE)
Bruce Noll (Madison, WI/US), Severine Freisz, Alexander Gerisch
Holger Ott (Karlsruhe/DE), Birger Dittrich (Goettingen/DE)
Andreas Kleine, Carsten Michaelsen (Geesthacht/DE)

11^{40} Refinement of macromolecular structures against neutron data with
MS01–T3 SHELXL-2013
Tim Gruene, H. W. Hahn, A. V. Luebben (Goettingen/DE)
F. Meilleur (Oak Ridge, TN/US), G. M. Sheldrick (Goettingen/DE)

12^{00} Influence on crystallisation process of amino acids from solution
MS01–T4 Klaus Merz, Anna Kupka, Hermann Gies (Bochum/DE)

12^{20} Crystal Engineering involving ditopic ligands of modified acetylacetones
MS01–T5 Carina Merkens (Aachen/DE), Fangfang Pan (Jyväskylä/FI)
Ulli Englert (Aachen/DE)

12^{40} Pair distribution function analysis of organic compounds – improving
MS01–T6 the modelling of the atomic vibrations
Dragica Podgorski (Frankfurt a. M./DE)
Pavol Juhas, Simon J. L. Billinge (Upton, NY/US)
Martin U. Schmidt (Frankfurt a. M./DE)

11^{00}–13^{00} Lecture hall B	MS02 – Functional materials and technologies for energy conversion and catalysis
Chairs	Martin Lerch (Berlin/DE), Martin Meven (Munich/DE)
11^{00} MS02–T1	Wet chemical synthesis andcharacterisation of $SrTiO_3$-Ruddlesden-Popper-films for photoelectrochemical water splitting Diana Karsch, Doreen Eger, Erik Mehner, Hartmut Stöcker Dirk Meyer (Freiberg/DE)
11^{15} MS02–T2	Cu/SBA-15 catalysts for methanol steam reforming (MSR): increase in intrinsic activity due to redox pretreatment Gregor Koch, Thorsten Ressler (Berlin/DE)
11^{30} MS02–T3	Structure determination of the first example of a metal-interlayer expanded zeolite Hermann Gies (Bochum/DE), Bilge Yilmaz (Iselin, NJ/US) Trees De Baerdemaeker (Leuven/BE), Mathias Feyen Ulrich Müller (Ludwigshafen/DE), Feng-Shou Xiao (Hangzhou/CN) Dirk De Vos (Leuven/BE)
11^{45} MS02–T4	Absorption behavior of H_2 in three-dimensional CAU metal organic framework structure Moritz-Caspar Schlegel, Margarita Russina (Berlin/DE) Norbert Stock (Kiel/DE), Helge Reinsch (Leuven/BE) Daniel Többens (Berlin/DE), Martin Krüger (Kiel/DE)
12^{00} MS02–T5	The hydrogenation of Zintl phases by in situ neutron powder diffraction Holger Kohlmann (Leipzig/DE), Patrick Wenderoth (Saarbrücken/DE)
12^{15} MS02–T6	Chalcopyrite semiconductors – atomic-scale structure and band gap bowing Claudia S. Schnohr, Stefanie Eckner, Helena Kämmer, Tobias Steinbach Martin Gnauck, Andreas Johannes (Jena/DE), Christian A. Kaufmann Christiane Stephan, Susan Schorr (Berlin/DE)
12^{30} MS02–T7	The influence of sodium on the defect characteristics in off stoichiomteric Cu(In, Ga)Se_2 Christiane Stephan, Christian Kaufmann, Dieter Greiner Susan Schorr (Berlin/DE)
12^{45} MS02–T8	In-situ XRD investigation of thin film growth by thermal co-evaporation Götz Schuck, Manfred Kastowsky (Berlin/DE), Gunar Kaune Stefan Hartnauer, Roland Scheer (Halle/Saale/DE)

11^{00}–13^{00} MS03 – Temperature, pressure and field induced processes/phase transitions
Lecture hall D
Chairs Eiken Haussühl, Leonore Wiehl (Frankfurt a. M./DE)

11^{00} EosFit7 – a new program for equation of state analyses and calculations
MS03–T1 Ross Angel (Padua/IT), Javier Gonzalez-Platas (La Laguna, Tenerife/ES)
Matteo Alvaro, Fabrizio Nestola (Padua/IT)

11^{15} Pressure-induced spin transition in henritermierite, a tetragonal Mn^{3+} hydrogarnet
MS03–T2 Alexandra Friedrich, Wolfgang Morgenroth
Björn Winkler (Frankfurt a. M./DE), Alexander Perlov
Victor Milman (Cambridge/GB)

11^{30} The behaviour of SiO_2 under dynamic loading and unloading
MS03–T3 Eva-Regine Carl, Andreas Danilewsky, Ghislain Trullenque
Thomas Kenkmann (Freiburg i. Br/DE), Hanns-Peter Liermann (Hamburg/DE)

11^{45} Pressure-induced first-order phase transitions in ion-conducting anion-excess fluorite KY_3F_{10} studied with single-crystal x-ray diffraction
MS03–T4 Andrzej Grzechnik, Karen Friese (Aachen/DE)

12^{00} Decomposition of SF_6 in the presence of glassy carbon in the laser heated diamond anvil cell
MS03–T5 Nadine Rademacher, Lkhamsuren Bayarjargal, Wolfgang Morgenroth
Alexandra Friedrich, Björn Winkler (Frankfurt a. M./DE)

12^{15} Structure-property relations of orthorhombic $[(CH_3)_3NCH_2COO]_2(CuCl_2)_3 \bullet 2\ H_2O$
MS03–T6 Eiken Haussühl (Frankfurt/DE), Jürgen Schreuer (Bochum/DE)
Leonore Wiehl, Natalia Paulsen (Frankfurt/DE)

12^{30} Cancrinite-group minerals at non-ambient conditions the role of the extraframework population
MS03–T7 Paolo Lotti, Giacomo Diego Gatta (Milano/IT)
Volker Kahlenberg (Innsbruck/AT), Marco Merlini, Nicola Rotiroti (Milano/IT)

12^{45} Comparative elasticity of cordierite – effect of heavy-ion irradiation on the compressibility of H_2O- and CO_2-rich cordierite
MS03–T8 Katharina Sarah Scheidl (Vienna/AT), Martin Schmitt (Innsbruck/AT)
Giacomo Diego Gatta (Milano/IT), Christina Trautmann (Darmstadt/DE)
Bea Schuster (Darmstadt/DE), Ronald Miletich (Vienna/AT)

13^{15}-14^{15} Lecture hall B

Lunch Symposium Agilent Technologies GmbH

Agilent Technologies

Advances in Data Quality in Area Detector Diffraction Experiments.
Mathias Meyer (Wroclaw/PL) (see page 12)

14^{30}–16^{30} Lecture hall A

MS04 – Hot new structures I

Chairs: Thomas Barends (Heidelberg/DE), Hartmut Niemann (Bielefeld/DE)

14^{30} MS04–T1
RNA polymerase I structure and transcription regulation
Christoph Engel (Munich/DE)

14^{50} MS04–T2
Structural studies of spliceosomal B-complex proteins
Alexander Ulrich, Tonio Schütze, Martin Seeger, Markus C. Wahl (Berlin/DE)

15^{10} MS04–T3
Structure and function of a novel RNA-binding domain
Markus C. Wahl, Sunbin Liu (Berlin/DE)

15^{30} MS04–T4
Eukaryotic translation initiation factors 3 subunit b (eIF3b) contains a novel nine-bladed WD40 domain
Yi Liu, Piotr Neumann, Bernhard Kuhle, Thomas Monecke
Ralf Ficner (Goettingen/DE)

15^{50} MS04–T5
Specific molecular targeting of oncofetal fibronectin by Anticalins
Andre Schiefner (Freising-Weihenstephan/DE)

16^{10} MS04–T6
Structural insights into PROPPINs, a family of phosphoinositide binding proteins
Karin Kühnel (Goettingen/DE)

14^{30}–16^{30} Lecture hall B Chair	MS05 – Inorganic structural chemistry – synthesis, structure, properties and applications I Thomas Schleid (Stuttgart/DE)
14^{30} MS05–T1	In-situ PDF study on the nucleation of ZnO nanoparticles in ethanolic solution Mirijam Zobel, Reinhard B. Neder (Erlangen/DE)
14^{45} MS05–T2	Twinning structure and phase analysis of tin/ni nanoparticles by high-resolution transmission electron microscopy (HRTEM) I. V. Luzhkova, A. N. Ermakov, A. M. Murzakaev Yu. G. Zainulin (Ekaterinburg/RU)
15^{00} MS05–T3	ICSD Desktop – the new interface to ICSD Stephan Rühl (Eggenstein-Leopoldshafen/DE)
15^{15} MS05–T4	Solid solutions of $CdIn_2Te_4$ and silver indium tellurides – structure and element distribution by resonant X-ray scattering Simon Welzmiller, Felix Hennersdorf (Leipzig/DE) Thorsten Schröder (Munich/DE), Gerald Wagner, Oliver Oeckler (Leipzig/DE)
15^{30} MS05–T5	New insights in the pseudobinary system $(SnSe)_nBi_2Se_3$ Oliver Oeckler, Philipp Urban (Leipzig/DE) Christina Fraunhofer (Munich/DE), Gerald Wagner (Leipzig/DE)
15^{45} MS05–T6	Bridgman-Stockbarger growth and characterization of tin (II) sulfide Frederic Hofherr (Freiburg/DE)
16^{00} MS05–T7	A new compound in the system $Na_{3-x}Ag_xSbS_3$ ($0 \leq x \leq 3$) – crystal structure of Na_2AgSbS_3 Arno Pfitzner Constantin Pompe (Regensburg/DE)
16^{15} MS05–T8	Investigation of sodium insertion into $Fe[Fe(CN)_6]$ and $Fe[Co(CN)_6]$ Siegbert Schmid, Thomas Godfrey, Cameron J. Kepert, Lisa Cameron (Sydney/AU), Juan-Carlos Pérez-Flores Flaviano García-Alvarado, Alois Kuhn (Sydney/AU, Boadilla del Monte/ES)

14^{30}–16^{30} MS06 – Structure-property relations in materials sciences I

Lecture hall D

Chairs Claudia Weidenthaler (Mülheim/DE), Bernd Marler (Bochum/DE)

14^{30} MS06–T1
Hydrogen positions and their effect on exchange couplings of Cu-minerals
Helge Rosner, Stefan Lebernegg (Dresden/DE)
Oleg Janson (Dresden/DE; Tallinn/EE)
Alexander Tsirlin (Tallinn/EE)

14^{45} MS06–T2
Using the concept of natural tilings to identify promising zeolite frameworks for CO_2/N_2 separation – a computational study
Michael Fischer, Robert Bell (London/GB)

15^{00} MS06–T3
In situ powder diffraction meets breaking crystals
Tomce Runcevski, Robert E. Dinnebier (Stuttgart/DE)

15^{15} MS06–T4
In situ X-ray diffraction study of InAlN-based heterostructure during annealing
Lars Grieger, Alexander Kharchenko, Joachim Woitok (Almelo/NL)

15^{30} MS06–T5
Pyroelectricity in strontium titanate single crystals?
Erik Mehner, Juliane Hanzig, Sven Jachalke, Florian Hanzig
Matthias Zschornak, Hartmut Stöcker, Dirk C. Meyer (Freiberg/DE)

15^{45} MS06–T6
Extension of crystal structure prediction to hydrates, organometallic and inorganic compounds
Detlef W. M. Hofmann, Liudmila N. Kuleshova (Pula/IT)

16^{00} MS06–T7
Structural and magnetic phase transitions in antiferromagnetic $PrCaFeO_4$
Navid Qureshi (Cologne/DE), Martin Valldor (Cologne, Dresden/DE)
Lisa Weber (Cologne/DE), Anatoliy Senyshyn (Garching/DE)
Yvan Sidis (Saclay/FR), Markus Braden (Cologne/DE)

16^{15} MS06–T8
Point defects and diffusion in crystalline oxides
Jianmin Shi, Klaus-Dieter Becker (Braunschweig/DE)

18^{00}–19^{00} Plenary lecture

Lecture hall A

P02
New opportunities for X-ray crystallography – fourth generation lightsources and computational advances
Axel Brunger (Stanford, CA/US)

Chairs Manfred Weiss (Berlin/DE), Yves Muller (Erlangen/DE)

0900–1100 Lecture hall A
Chair

MS07 – Synchrotron opportunities and challenging structure determinations I

Manfred Weiss (Berlin/DE)

0900 MS07–T1
Update on the facilities for macromolecular crystallography at BESSYII in Berlin of HZB
Uwe Mueller (Berlin/DE)

0920 MS07–T2
Structural biology beam lines at the ESRF – new developments
Davidvon Stetten (Grenoble/FR)

0940 MS07–T3
New capabilities for Macromolecular X-ray Crystallography at beamline P11 at PETRA III
Alke Meents, Anja Burkhardt, Bernd Reime, Tim Pakendorf
Saravanan Panneerselvam, Nicolas Stuebe, Jan Roever
Jan Meyer, Martin Warmer, Pontus Fischer, Dennis Goeries (Hamburg/DE)

1000 MS07–T4
EMBL Beamlines for macromolecular crystallography at PETRA III
Thomas Schneider, Gleb Bourenkov, Michele Cianci, Johanna Kallio
Guillaume Pompidor, Ivars Karpics, Stefan Fiedler (Hamburg/DE)

1020 MS07–T5
The long-wavelength macromolecular crystallography beamline at diamond light source
Armin Wagner, Vitaliy Mykhaylyk, Ramona Duman (Chilton, Didcot/GB)

1040 MS07–T6
Serial crystallography using synchrotron radiation – novel strategies for macromolecular microcrystallography
Gleb Bourenkov, Cornelius Gati, Marco Klinge, Dominik Oberthür
Dirk Rehders, Michael Heymann, Caroline Seuring, Frsco Stellato
Oleksandr Yevanov, Christian Betzel, Thomas Schneider
Henry Chapman (Hamburg/DE), Lars Redecke (Hamburg/DE)

09^{00}–11^{00} MS08 – Quasicrystals and incommensurate structures

Lecture hall B

Chairs Karen Friese (Juelich/DE), Walter Steurer (Zurich/CH)

09^{00} MS08–T1 Crystal structure and modulation of Λ-Co(sepulchrate)-trinitrate at low temperatures
Andreas Schönleber, Somnath Dey
Sander van Smaalen (Bayreuth/DE), Finn Krebs Larsen (Aarhus/DK)

09^{15} MS08–T2 The 3+1D modulated structure of $InMo_4O_6$, a molybdenum cluster compound hosting In_6 and In_7 oligomers
Peter Schultz, Oliver Oeckler (Leipzig/DE)

09^{30} MS08–T3 (3+2) incommensurately modulated structure of $K_2Sc[Si2O_6]F$
Clivia Hejny, Volker Kahlenberg, Tim Eberhard
Hannes Krüger (Innsbruck/AT)

09^{45} MS08–T4 On the triangle wave function
Carola J. Müller, Sven Lidin (Lund/SE)

10^{00} MS08–T5 Non-crystallographic lattice restrictions in order-disorder structures
Berthold Stöger (Vienna/AT)

10^{15} MS08–T6 Dendritic growth of tenfold twins from an undercooled melt of glass-forming NiZr
Wolfgang Hornfeck, Raphael Kobold, Matthias Kolbe
Dieter Herlach (Cologne/DE)

10^{30} MS08–T7 Quasicrystal and its periodic approximant – do they fit to each other? Epitaxial crystal growth experiments in the Al-Co-Ni system
Birgitta Meisterernst, Lukas Grossmann, Katharina Scheidl
Peter Gille (Munich/DE)

10^{45} MS08–T8 Fulleranes and Frank-Kasper polyhedra in intermetallics
Julia Dshemuchadse, Walter Steurer (Zurich/CH)

09^{00}–11^{00} MS09 – Crystallography in geology – microstructures as indicators of rock forming processes
Lecture hall D
Chairs Rainer Abart (Wien/AT), Claudia Trepmann (Munich/DE)

09^{00} MS09–T1
Rock formation processes constrained by host-inclusion crystallography
Ross Angel, Sula Milani, Paolo Nimis (Padua/IT)
Marco Bruno (Torino/IT), Jeff Harris (Glasgow/GB)
Fabrizio Nestola (Padua/IT)

09^{15} MS09–T2
In-situ monitoring of spinel reaction band formation using synchrotron radiation
Lutz Götze, Susan Schorr, Ralf Milke (Berlin/DE)
Rainer Abart (Vienna/AT), Ralf Dohmen (Bochum/DE)
Richard Wirth (Potsdam/DE)

09^{30} MS09–T3
A perspective on magnesite reactivity
Ulf-NiklasBerninger (Munich/DE; Toulouse/FR)
Guntram Jordan (Munich/DE), Quentin Gautier (Toulouse/FR)
Michael Lindner (Munich/DE), Eric H. Oelkers, Jacques Schott (Toulouse/FR)

09^{45} MS09–T4
Experimental growth of radiaxial-fibrous calcite
Felix Wiethoff, Jürgen Schreuer (Bochum/DE)

10^{00} MS09–T5
Lattice strain across Na-K-interdiffusion fronts in alkali feldspar: an EBSD study
Anne-Kathrin Schäffer (Vienna/AT), Tom Jaepel
Stefan Zaefferer (Düsseldorf/DE), Rainer Abart (Vienna/AT)

10^{15} MS09–T6
Crystal-plastic deformation of zircon from strained natural rocks
Elizaveta Kovaleva, Gerlinde Habler, Urs Klötzli (Vienna/AT)

10^{30} MS09–T7
High-stress crystal-plasticity of quartz and olivine
Claudia Trepmann (Munich/DE)

10^{45} MS09–T8
Torsional deformation of calcite under high confining pressure
Roman Schuster, Rainer Abart, Erhard Schafler
Gerlinde Habler (Vienna/AT)

11^{30}–12^{30} Plenary lecture
Lecture hall A
P03 Enhanced nucleation of the fcc phase during solidification of alloys by 5-fold symmetry icosahedral quasicrystals
Michel Rappaz (Lausanne/CH)
Chair Susan Schorr (Berlin/DE)

14^{00}–16^{00} MS10 – Protein function and regulation
Lecture hall A
Chairs Yves Muller (Erlangen/DE), Hermann Schindelin (Wuerzburg/DE)

14^{00}
MS10–T1 Structural and biochemical analysis of the RNA-binding protein roquin
Anja Schütz, Udo Heinemann (Berlin/DE)

14^{20}
MS10–T2 S-SAD structure determination of the N-terminal domain of human Prp38 reveals a novel folded domain that anchors alternative splice factors to the spliceosome.
Tonio Schütze, Luise Apelt, Gert Weber, Manfred S. Weiss
Ulrich Stelzl, Markus C. Wahl (Berlin/DE)

14^{40}
MS10–T3 Crystal structure of Muskelin's Discoidin and LisH-domain provides the basis to understand the mechanism and impact of its oligomerization
Carolyn Delto (Wuerzburg/DE), Frank Heisler (Hamburg/DE)
Jochen Kuper (Wuerzburg/DE), Matthias Kneussel (Hamburg/DE)
Hermann Schindelin (Wuerzburg/DE)

15^{00}
MS10–T4 Crystal structure of AibA/AibB, a novel decarboxylase in alternative myxobacterial isovalerate biosynthesis
Tobias Bock (Braunschweig/DE), Eva Luxenburger
Rolf Müller (Saarbrücken/DE), Wulf Blankenfeldt (Braunschweig/DE)

15^{20}
MS10–T5 Structural basis for a Kolbe-type decarboxylation catalysed by a glycyl radical enzyme
Berta M. Martins, Brinda Selvaraj (Berlin/DE), Martin Blaser (Marburg/DE)
Mikolaj Feliks, G. Matthias Ullmann (Bayreuth/DE)
Thorsten Selmer (Juelich, Marburg/DE), Wolgang Buckel (Marburg/DE)

15^{40}
MS10–T6 Structural and chemical transformation of the [4Fe$_3$S]-cluster in the oxygen-tolerant [NiFe] hydrogenase of Ralstonia eutropha
Andrea Schmidt, Jacqueline Kalms, Patrick Scheerer (Berlin/DE)

14^{00}–16^{00} Lecture hall B Chair	MS11 – Synchrotron opportunities and challenging structure determinations II Ullrich Pietsch (Siegen/DE)
14^{00} MS11–T1	Mesoscopic relaxations in nanoscale systems – experimental verification by surface X-ray diffraction and x-ray absorption spectroscopy Holger Meyerheim, Valery S. Stepanyuk, Oleg Brovko Jürgen Kirschner (Halle/Saale/DE)
14^{20} MS11–T2	Submicrosecond X-ray crystallography: new technique, challenges and opportunities Semen Gorfman, Michael Ziolkowski, Hyeokmin Choe Mohammad al Taani, Ullrich Pietsch (Siegen/DE)
14^{40} MS11–T3	Coherent diffraction imaging from semiconductor nanowires Arman Davtyan, Andreas Biermanns, Otmar Loffeld Ullrich Pietsch (Siegen/DE)
15^{00} MS11–T4	Temperature-driven growth of ultra-small ZnO nanoparticles Reinhard Neder, Haimantee Chatterjee, Kaustuv Datta (Erlangen/DE)
15^{20} MS11–T5	Combination of TEM and microfocus synchrotron diffraction for the structure determination of micro- and nanocrystalline materials Felix Fahrnbauer (Leipzig/DE), Tobias Rosenthal Alexey Marchuk (Munich/DE), Philipp Urban, Gerald Wagner (Leipzig/DE) Wolfgang Schnick (Munich/DE), Oliver Oeckler (Leipzig/DE)
15^{40} MS11–T6	Synchrotrons, pixel detectors and diffuse scattering – a great team for real structure determination Thomas Weber (Zurich/CH)

14^{00}–16^{00} Lecture hall D — **MS12 – Inorganic structural chemistry – synthesis, structure, properties and applications II**

Chair: Thomas Doert (Dresden/DE)

14^{00} MS12–T1 — Polymorphism of dolomite-type structures – the C2/c high-pressure form of $BaMg(CO_3)_2$
Thomas Pippinger, Ronald Miletich, Gregor Hofer
Herta Effenberger (Vienna/AT)

14^{15} MS12–T2 — Temperature dependent X-ray diffraction study of the transformation of studtite, $UO_4 . 4 H_2O$, to metastudtite, $UO_4 . 2 H_2O$
Sabrina Labs (Juelich/DE), Johannes D. Bauer
Björn Winkler (Frankfurt a. M./DE), Hildegard Curtius
Dirk Bosbach (Juelich/DE)

14^{30} MS12–T3 — Determination of the nuclear and magnetic structure of $HoNi_2B_2C$ at room temperature and 2.2 K
Karen Friese (Juelich/DE), Vladimir Hutanu, Martin Meven
Andrew Sazonow (Garching/DE), Oksana Zaharko (Villingen/CH)

14^{45} MS12–T4 — Synthesis and characterisation of (La,Pr) monazite solid solution series
Antje Hirsch, Andreas Neumann, Anja Wätjen (Aachen/DE)
Julia Heuser (Juelich/DE), Anja Thust (Frankfurt a. M./DE)
Lars Peters, Georg Roth (Aachen/DE)

15^{00} MS12–T5 — Optimization of crystal and morphological parameters of wet chemical synthesized $LiNbO_3$-films
Doreen Eger, Diana Karsch, Erik Mehner, Hartmut Stöcker
Dirk Meyer (Freiberg/DE)

15^{15} MS12–T6 — Study on the preparation of $NiFe_2O_4$ ceramic nanometer powder and its microstructure
Yihan Liu, Xiaoxu Cheng, Guanglei Song, Jintao Zhang (Shenyang/CN)

15^{30} MS12–T7 — Crystal structures of alkaline earth glycolates and their application as cement admixtures
Ronny Kaden, Herbert Pöllmann (Halle/Saale/DE)

15^{45} MS12–T8 — Introducing the X – |ψ|2 difference electron density in the study of 3-D metal complexes
Birger Dittrich (Hamburg/DE)

17^{30}–18^{30} Plenary lecture
Lecture hall A
P04
Photosystem II – crystal structure and functional studies using serial femtosecond X-ray laser microcrystallography
Wolfram Saenger (Berlin/DE)
Chair
Udo Heinemann (Berlin/DE)

20^{00}–23^{00} Social Evening (see page 14)

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09^{00}–11^{00} MS13 – Therapeutic targets and fragment-based drug discovery

Lecture hall A

Chairs Andreas Heine (Marburg/DE), Michael Hennig (Basel/CH)

09^{00} MS13–T1
X-ray crystallography as gold standard of fragment screening
Johannes Schiebel, Nedyalka Radeva, Ahyoung Park, Helene Köster
Tobias Craan (Marburg/DE), Michael Krug, Monika Ühlein
Manfred Weiss, Karine Sparta (Berlin/DE), Andreas Heine (Marburg/DE)
Uwe Müller (Berlin/DE), Gerhard Klebe (Marburg/DE)

09^{20} MS13–T2
Lead discovery by fragment screening: a new opportunity in industrial drug research
Martina Schäfer (Berlin/DE)

09^{40} MS13–T3
Design of novel aspartic protease inhibitors from fragments exploiting dynamic combinatorial chemistry
Gerhard Klebe, Nedyalka Radeva (Marburg/DE)
Milon Mondal (Groningen/NL), Helene Koester, Ahyoung Park (Marburg/DE)
Constantinos Potamitis, Maria Zervou (Athen/GR)
Anna Hirsch (Groningen/NL)

10^{00} MS13–T4
X-ray structures of human Furin in complex with competitive inhibitors
Sven O. Dahms (Jena/DE), Torsten Steinmetzer (Marburg/DE)
Hans Brandstetter (Salzburg/AT), Manuel E. Than (Jena/DE)

10^{20} MS13–T5
From SARS to MERS – structure-based design of antivirals against middle-east respiratory syndrome coronavirus
Rolf Hilgenfeld, Yibei Xiao, Yuri Kusov, Shyla George, Linlin Zhang
Lili Zhu (Luebeck/DE), Doreen Muth, Marcel A. Müller
Christian Drosten (Bonn/DE), Jian Lei, Qingjun Ma (Luebeck/DE)

10^{40} MS13–T6
Exploring a mycobacterial thiolase – FadA5
Christin Schäfer (Wuerzburg/DE), Rui Lu, Natasha Nesbitt
Nicole Sampson (Stony Brook, NY/US), Caroline Kisker (Wuerzburg/DE)

09^{00}–11^{00} MS14 – Structure-property relations in materials sciences II

Lecture hall B

Chair Bernd Marler (Bochum/DE)

09^{00} MS14–T1
Elastic constants in crystals with point defects considering the example of cluster crystals, a reciprocal space approach
Johannes Häring, Tadeus Ras, Christof Walz, Matthias Fuchs (Konstanz/DE)
Anjan Prasad Gantapara, Marjolein Dijkstra (Utrecht/NL)

09^{15} MS14–T2
In-situ neutron diffraction of monoclinic NiTi B19' revealing components of its elastic-constant-tensor
Peter M. Kadletz (Munich/DE), Markus Hoelzel (Garching/DE)
Wolfgang W. Schmahl (Munich/DE)

09^{30} MS14–T3
Possible piezoelectric materials $CsMZr_{0.5}(MoO_4)_3$ (M = V, Cr, Fe) and $CsCrTi_{0.5}(MoO_4)_3$ – structural considerations
Daria Mikhailova, Angelina Sarapulova (Dresden/DE), Bair Bazarov
Touyana Namsaraeva, Sesegma Dorzhieva, Jibzema Bazarova
Victoria Grossman (Ulan-Ude/RU), Alexander Bush (Moscow/RU)
Iryna Antonyshyn, Marcus Schmidt (Dresden/DE)
Anthony Bell (Hamburg/DE), Michael Knapp
Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE)
Jürgen Eckert (Dresden/DE)

09^{45} MS14–T4
Thermodynamic properties of hexaphenyldisilane from experiment and DFT calculations
Thomas Bernert, Björn Winkler (Frankfurt a. M./DE)
Victor Milman (Cambridge/GB), Lkhamsuren Bayarjargal, Lothar Fink
Matthias Berger, Hans-Wolfram Lerner (Frankfurt a. M./DE)

10^{00} MS14–T5
Coupling of morphologic and crystallographic symmetry in sea urchins
Bernd Maier, Patrick Alexa, Erika Griesshaber (Munich/DE)
Franz Brümmer (Stuttgart/DE), Wolfgang Schmahl (Munich/DE)

10^{15} MS14–T6
Structural and functional characterization of supported vanadium oxide catalysts under propene and propane oxidizing conditions
Juliane Scholz, Thorsten Ressler (Berlin/DE)

10^{30} MS14–T7
Small angle Xray scattering of microcrystalline polymers and beyond
PaninePierre, Galatanu Nicoleta, Manuel Fernadez-Martinez
Frederic Bossan, Sergio Rodrigues (Sassenage/FR)

10^{45} MS14–T8
Evaluation of temperature-dependent X-ray diffraction data using the autocorrelation function
Lars Robben (Bremen/DE), Thorsten M. Gesing (Bremen/DE)

09^{00}–11^{00} MS15 – Charge density for understanding chemical bonding in organic and inorganic structures (dedicated to Prof. Luger)
Lecture hall D
Chair Birger Dittrich (Goettingen/DE)

09^{00} New directions in pseudoatom modeling of X-ray charge densities
MS15–T1 Tibor Koritsanszky (Nashville, TN/US)

09^{30} Low valent silicon – a carbon copy?
MS15–T2 Dietmar Stalke (Goettingen/DE)

10^{00} Charge Density – an experimentalist's view
MS15–T3 Armin Wagner (Oxfordshire/GB)

10^{15} Geometry versus topology – combined AIM, ELI-D and ASF analysis
MS15–T4 of Hapticities and intramolecular H...H contacts in asymmetric Zincocenes
Stefan Mebs, Maren Cilleck (Berlin/DE)

10^{30} Synchrotron data collection in five minutes, automatic model building
MS15–T5 and H-ADP estimation using the invariom database streamlines charge density research of organic molecules
Jens Luebben (Goettingen/DE), Birger Dittrich (Goettingen, Hamburg/DE)
Alke Meents (Hamburg/DE)

10^{45} Is the R-factor resulting from my model refinement adequate?
MS15–T6 Julian Henn (Bayreuth/DE)

11^{30}–12^{30} Plenary lecture
Lecture hall A
P05 Ten years of charge flipping
Chair Lukas Palatinus (Prague/CZ)
Birger Dittrich (Goettingen/DE)

12^{30}–13^{30} Arbeitskreis Junge Kristallographen
Lecture hall D

14^{00}–16^{00}	MS16 – Hot new structures II
Lecture hall A	
Chairs	Thomas Barends (Heidelberg/DE), Hartmut Niemann (Bielefeld/DE)
14^{00}	Moving ions across membranes
MS16–T1	David Wöhlert, Özkan Yildiz, Werner Kühlbrandt (Frankfurt/DE)
14^{20}	Structural basis of substrate specificity of outer membrane channels
MS16–T2	from Acinetobacter baumannii Michael Zahn, Bert van den Berg (Newcastle upon Tyne/GB)
14^{40}	Entrapment of DNA in an intersubunit tunnel system of a single-stranded
MS16–T3	DNA-binding protein Bernhard Loll (Berlin/DE), Homa Ghalei (Berlin, Goettingen/DE) Holger von Moeller, Detlef Eppers (Berlin/DE), Daniel Sohmen Daniel Wilson (Munich/DE), Markus Wahl (Berlin/DE)
15^{00}	Ultra-high affinity chitin binding by LysM domain dimerization in fungal
MS16–T4	effectors prevents host PAMP signaling Jeroen Mesters, Raspudin Saleem-Batcha (Luebeck/DE) Andrea Sánchez-Vallet, Bart Thomma (Wageningen/NL)
15^{20}	Crystal structure of the first bacterial diterpene cyclase and
MS16–T5	structure-based engineering of plasticity residues Ronja Janke (Berlin/DE), Christian Görner, Max Hirte Thomas Brück (Garching/DE), Bernhard Loll (Berlin/DE)
15^{40}	Structure of human α-2,6 sialyltransferase: complex glycans substrate
MS16–T6	specificity and catalysis Markus Rudolph, Bernd Kuhn, Jörg Benz (Basel/CH) Michael Greif, Alfred Engel, Harald Sobek (Penzberg/DE)

14^{00}–15^{45} MS17 – Spectroscopy as supporting method in structure determination

Lecture hall B

Chairs Georg Amthauer (Salzburg/AT), Michael Fechtelkord (Bochum/DE)

14^{00} MS17–T1 Surface-near modifications of $SrTiO_3$ local symmetry due to nitrogen implantation investigated by grazing incidence XANES
Hartmut Stöcker, Matthias Zschornak, Carsten Richter
Dirk Meyer (Freiberg/DE)

14^{15} MS17–T2 Thermogravimetric, temperature dependent infrared and XRD investigations on $NaBO_2 \cdot xH_2O$ system
Zeina Assi, Claus H. Rüscher (Hannover/DE)

14^{30} MS17–T3 Resonant ultrasound spectroscopy – a non-destructive innovative technique to determine all independent elastic moduli
Chandra Shekhar Pandey, Jürgen Schreuer (Bochum/DE)

14^{45} MS17–T4 Mechanisms behind the para- to ferroelectric phase transition in RbH_2PO_4 probed bymeans of purely resonant X-ray diffraction
Carsten Richter, Dimitri Novikov (Hamburg/DE), Elena N. Ovchinnikova
Ksenia Akimokva, Aleksey Oreshko, Vladimir Dmitrienko
M. M. Borisov (Moscow/RU), Matthias Zschornak, Eric Mehner
Dirk C. Meyer (Freiberg/DE), Jörg Strempfer (Hamburg/DE)

15^{00} MS17–T5 High-temperature phase transitions, spectroscopic properties and dimensionality reduction in rubidium thorium molybdate family
Bin Xiao (Juelich/DE), Torsten Gesing (Bremen/DE)
Evgeny Alekseev (Juelich/DE)

15^{15} MS17–T6 Application of a Difference Electron Nanoscope (DEN) – 3D magnetical structures of synthetic fayalite
Werner Lottermoser, Konrad Steiner, Gerhard Scharfetter (Salzburg/AT)
Sven-Ulf Weber (Braunschweig/DE), Michael Grodzicki (Salzburg/AT)
Armin Kirfel (Bonn/DE), Georg Amthauer (Salzburg/AT)

15^{30} MS17–T7 A crystal chemical study using ^{71}Ga MAS NMR of the fast-ion conductor $Li_7La_3Zr_2O_{12}$ doped with Ga
Georg Amthauer, Daniel Rettenwander, Charles A. Geiger (Salzburg/AT)

15^{45}–16^{00} Arbeitskreis Spektroskopie (AK12)
Lecture hall B

14^{00}–15^{25} MS18 – Crystallography in archeometry
Lecture hall D
Chairs Klaus Bente (Leipzig/DE), Christoph Berthold (Tübingen/DE)

14^{00} MS18–T1 Kristallographische Methodenkombination am Beispiel von keltischen Fibelbesatzen
Klaus Bente (Tübingen/DE)

14^{10} MS18–T2 Non destructive chemical imaging of archaeological artifacts with the SLcamα®, an X-ray color camera
Christoph Berthold (Tübingen/DE), Oliver Scharf (Berlin/DE)
Klaus Bente, Klaus G. Nickel (Tübingen/DE), Rainer Wedell
Aniouar Bjeoumikhov (Berlin/DE)

14^{25} MS18–T3 Microstructural analysis of bone apatite in archeological finds by XRD full line profile analysis
Balazs Kocsis (Munich/DE), Anita Toncala (Martinsried/DE)
Melanie Kaliwoda, Bernd Maier (Munich/DE)
Gisela Gruppe (Martinsried/DE), Wolfgang Schmahl (Munich/DE)

14^{40} MS18–T4 The Eternal City, but non-eternal coins – dezincification in an ancient roman brass coin
Gerald Eisenblaetter (Leipzig/DE)
Alexandra Franz (Leipzig, Berlin/DE), Nikolay Kardjilov
Stefan Zander (Berlin/DE), Gert Kloess (Leipzig/DE)

14^{55} MS18–T5 Chlorargyrite on attic silver coins
Oliver Baehre, Gert Kloess, Gerald Eisenblätter (Leipzig/DE)

15^{10} MS18–T6 Surface phase analysis on a Classic Kerma tulip beaker
Tom Muenster, Gerald Eisenblaetter (Leipzig/DE)
Alexandra Franz (Berlin/DE), Alexandra Raue, Gert Kloess (Leipzig/DE)

16^{30}–17^{30} Plenary lecture
Lecture hall A
P06
Characterizing intermolecular interactions from the topological analyses of the electrostatic potential and the Laplacian of the electron density
Enrique Espinosa (Nancy/FR)
Chair Ulli Englert (Aachen/DE)

17^{30}–17^{45} Conference Closing
Lecture hall A
Susan Schorr (Berlin/DE)

Posters Overview

Crystallography of pharmaceutically active compounds and halogen and hydrogen bonds in crystal engineering

MS01–P01 Erythromycin A dimethylsulfoxide disolvate 1.43-hydrate
Jürgen Brüning (Frankfurt a. M., Rudolstadt/DE), Tanja K. Trepte
Edith Alig, Jan W. Bats, Martin U. Schmidt (Frankfurt a. M./DE)

MS01–P02 Investigating cyclodextrin complex formation at high pressure
Sofiane Saouane (Goettingen/DE)
Wolfgang Morgenroth (Hamburg, Frankfurt a. M./DE)
Hanns-Peter Liermann (Hamburg/DE)
Francesca P. A. Fabbiani (Goettingen/DE)

MS01–P03 Downsizing material and efforts – Do microfluidic approaches work for small molecules?
Philippe Piechon, Trixie Wagner, Ina Dix (Basel/CH)

MS01–P04 The only hydrogen bond – two ways to build a structure: the role of N-H·O hydrogen bond in crystal structures of N,N-dimethylglycine
Vasily Minkov, Elena Boldyreva, Eugen Kapustin (Novosibirsk/RU)

MS01–P05 A chiral polyiodide with four symmetry independant tyrosinate molecules
Kevin Lamberts, Philipp Handels, Ulli Englert (Aachen/DE)

MS01–P06 The role of detergent in crystal packing upon dehydration of photosystem II crystals
Martin Bommer, Julia Hellmich (Berlin/DE)

Functional materials and technologies for energy conversion and catalysis

MS02–P01 Automated set-up for measurement and evaluation of pyroelectric properties
Sven Jachalke, Erik Mehner, Hartmut Stöcker
Dirk C. Meyer (Freiberg/DE)

MS02–P02 The low-temperature sodium-sulphur secondary battery – materials and structure
Wolfram Münchgesang, Falk Meutzner
Torsten Schucknecht (Freiberg/DE), Michael Kohl
Holger Althues (Dresden/DE), Barbara Abendroth, Tilmann Leisegang
David Rafaja, Dirk C. Meyer (Freiberg/DE)

MS02–P03 Defect separation in strontium titanate single crystals – a concept for electrochemical energy storage
Juliane Hanzig (Freiberg/DE)
Matthias Zschornak (Freiberg, Dresden/DE), Melanie Nentwich
Florian Hanzig, Erik Mehner, Christian Röder, Barbara Abendroth
Tilmann Leisegang, Hartmut Stöcker (Freiberg/DE)
Sibylle Gemming (Dresden/DE), Dirk C. Meyer (Freiberg/DE)

MS02–P04 FEM-simulation of energy conversion and storage concepts based on oxide crystals
Cherkouk Charaf, Zschornak Matthias, Hanzig Juliane
Nentwich Melanie, Meutzner Falk, Urena Mateo, Leisegang Tilmann
Meyer Dirk C. (Freiberg/DE)

MS02–P05 Categorization of electrodes and separators in electrochemical energy storage devices – evaluating new concepts
Falk Meutzner, Tina Nestler, Juliane Hanzig, Matthias Zschornak
Melanie Nentwich, Robert Schmid, Mateo Ureña de Vivanco
Charaf Cherkouk, Bianca Störr, Wolfram Münchgesang
Tilmann Leisegang, Dirk C. Meyer (Freiberg/DE)

MS02–P06 Crystals as the heart of thermal-into-chemical-energy conversion devices
Mateo Ureña de Vivanco, Maximilian Sonntag, Clemens Forman
Matthias Gootz, Erik Mehner, Sven Jachalke, Hartmut Stöcker
Ralph Strohmayer, David Scheithauer, Ibrahim Muritala, Bianca Störr
Matthias Zschornak, Juliane Hanzig, Marco Herrmann, Mandy Koitsch
Robert Pardemann, Tilmann Leisegang, Bernd Meyer
Dirk C. Meyer (Freiberg/DE)

MS02–P07 Comprehensive collection of pyroelectric properties of organic and inorganic materials – database and categorization
Bianca Störr, Robert Schmid, Hartmut Stöcker, Erik Mehner
Sven Jachalke, Juliane Hanzig, Maximilian Sonntag
Tilmann Leisegang, Dirk C. Meyer (Freiberg/DE)

MS02–P08 In situ grazing incidence diffraction in electrochemical catalysis: from theory to experiment
Michael Scherzer, Frank Girgsdies, Malte Behrens
Robert Schlögl (Berlin/DE)

MS02–P09 Magentron sputter deposition and crystallization of $Ba_xSr_{1-x}TiO_3$ thin films
Ralph Strohmeyer, Barbara Abendroth, Hartmut Stöcker
Erik Mehner, Michael Franke, Dirk C. Meyer (Freiberg/DE)

MS02–P10 In situ X-ray diffraction studies on $LiNi_{0.5}Mn_{1.5}O_4$ and also Fe substituted $LiNi_{0.5}Mn_{1.5}O_4$ spinel cathodes during electrochemical cycling
Nilüfer Kiziltas-Yavuz, Aiswarya Bhaskar, Murat Yavuz
Mariyam Susana Dewi Darma, Michael Knapp, Sylvio Indris
Helmut Ehrenberg (Karlsruhe/DE)

MS02–P11 Material concepts for designing an aluminum-ion thin-film battery
Tina Nestler (Freiberg/DE), William Förster
Stefan Braun (Dresden/DE)
Wolfram Münchgesang (Freiberg, Dresden/DE), Falk Meutzner
Juliane Hanzig, Matthias Zschornak, Melanie Nentwich
Robert Schmid, Mateo Ureña de Vivanco, Charaf Cherkouk
Tilmann Leisegang, Dirk Carl Meyer (Freiberg/DE)

MS02–P12 Structural Defects in β–TaON
Martin Lerch, Sevilay Cosgun, Martin Rohloff, Michael Lublow
Thomas Lunkenbein (Berlin/DE), Anatoliy Senyshyn (Munich/DE)
Sönke Müller, Andreas Bartelt, Anna Fischer (Berlin/DE)

MS02–P13 Synthesis and crystal structure of $ScTa_2O_5N$
Martin Lerch, Sevilay Cosgun, Martin Rohloff, Michael Lublow
Anna Fischer (Berlin/DE)

MS02–P14 In situ characterization of mechanically treated MoO_3 and its oxide nitrides as model catalysts for selective propene oxidation
Sven Kühn, Christoph David Feldt, Steven Orthmann, Martin Lerch
Thorsten Ressler (Berlin/DE)

MS02–P15 Skull Melting for growing $Y_{0,2}Zr_{0,2}Ce_{0,6}O_{2-\delta}$ single crystals
Gregor Ulbrich, Martin Lerch (Berlin/DE)

MS02–P16 Microstructural and defect analysis of metal nanoparticles in functional catalysts by diffraction and electron microscopy: The Cu/ZnO catalyst for methanol synthesis
Malte Behrens, Timur Kandemir, Robert Schlögl (Berlin/DE)

MS02–P17 CuZnO nanoparticles supported on nanostructured silica as catalysts for methanol steam reforming (MSR)
Gregor Koch, Katja Pavel, Thorsten Ressler (Berlin/DE)

MS02–P18 Role of V and P in PV_2Mo_{10} supported on silica SBA-15 during oxidation of propene with gas phase oxygen
Rafael Zubrzycki, Thorsten Ressler (Berlin/DE)

MS02–P19 Solid state kinetic investigations of corundum type V_2O_3 under catalytic reaction conditions
Alexander Müller, Dominik Weber, Martin Lerch, Thorsten Ressler (Berlin/DE)

Temperature, pressure and field induced processes/phase transitions

MS03–P01 Parametric Rietveld refinements combined with the new approach of rotational rigid body symmetry modes – investigation of high pressure powder diffraction data
Martin Etter, Robert E. Dinnebier, Melanie Müller (Stuttgart/DE)
Michael Hanfland (Grenoble/FR)

MS03–P02 Structural compression of $Sm_2Ti_2O_7$ and $Er_2Ti_2O_7$ pyrochlores up to 50 GPa from single crystal X-ray diffraction and DFT calculations
Alexandra Friedrich, Wolfgang Morgenroth, Björn Winkler
Eiken Haussühl (Frankfurt a. M./DE), Michael Hanfland (Grenoble/FR)
Victor Milman (Cambridge/GB), Christopher Stanek
Kenneth McClellan (Los Alamos, CA/US)

MS03–P03 Structural, spectroscopic and computational studies on the monoclinic polymorph (form I) of potassium hydrogen disilicate ($KHSi_2O_5$)
Daniela Schmidmair, Volker Kahlenbe, Lukas Perfler (Innsbruck/AT)
Daniel M. Többens (Berlin/DE)

MS03–P04 P21/c to C2/c phase transition in metamict titanite
Tobias Beirau, Boriana Mihailova, Thomas Malcherek
Carsten Paulmann (Hamburg/DE), Lee A. Groat (Vancouver/CA)
Ulrich Bismayer (Hamburg/DE)

MS03–P05 Exploring the water-tert-butylamine system at high pressure
Rubén Granero-García, Frsca P. A. Fabbiani (Goettingen/DE)

MS03–P06 Phase relations between basic copper chlorides of the atacamite group
Thomas Malcherek (Hamburg/DE), Mark Welch (London/GB)
Matthew Sciberras (Sydney/AU), Jochen Schlüter (Hamburg/DE)
Peter Williams (Sydney/AU)

MS03–P07 A new approach to experimental determination of orientation relationships in pressure-induced phase transformations
Nina Pukallus, Helmut Klein, Heidrun Sowa (Goettingen/DE)

MS03–P08 Alternative ways of describing structural phase transitions – the case study of $[Mg(H_20)_6]RbBr_3$
Melanie Müller (Stuttgart/DE; Trento/IT), Robert E. Dinnebier (Stuttgart/DE)
Ann-Christin Dippel (Hamburg/DE), Harold T. Stokes
Branton J. Campbell (Provo, UT/US)

MS03–P09 Switching hydrogen bonds at high pressures in DL-alaninium semi-oxalate monohydrate
Boris Zakharov (Novosibirsk/RU)

MS03–P10 Serine co-crystals under extreme P-T conditions
Sergey Arkhipov, Boris Zakharov, Elena Boldyreva (Novosibirsk/RU)

MS03–P11 In situ diamond anvil cell – Raman spectroscopy and nanoindentation study of the effect of pressure on γ- and δ-polymorphs of chlorpropamide
Alisa Ivanenko, Vasily Minkov, Biljana Jankovic
Elena Boldyreva (Novosibirsk/RU)

Hot new structures

MS04–P01 Better data faster – shutterless data collection using a CMOS detector
Martin Adam, Holger Ott, Severine Freisz (Karlsruhe/DE)
Joerg Kaercher (Karlsruhe/DE; Madison, WI/US), Greg Wachter
Stephen Leo (Madison, WI/US)

MS04–P02 Crystal structure determination of the non-classical 2-norbornyl cation
Frank W. Heinemann, Karsten Meyer (Erlangen/DE)
Franziska Scholz, Ingo Krossing, Daniel Himmel (Freiburg/DE)
Paul von Ragué Schleyer (Athens/GR; Erlangen/DE)

MS04–P03 Crystallisation and preliminary X-ray structure of a bacterial fatty acid synthase
Karthik Paithankar, Mathias Enderle, Martin Grininger (Frankfurt/DE)

MS04–P04 Structure determination by serial femtosecond crystallography
Karol Nass (Heidelberg/DE)

MS04–P05 Kryptoracemate – an example of a very rare class of racemic crystals crystallizing in a Sohnke space group
Beatrice Braun, Reik Laubenstein, Thomas Braun (Berlin/DE)

MS04–P06 New Ce(III)-based metal-organic frameworks – relevant refinement models
Arkady Ellern (Ames, IA/US), Ozan Ayhan, Iurii L. Malaestean
Svetlana G. Baca, Paul Kögerler (Aachen/DE)

MS04–P07 Structural studies on ectonucleotidases involved in purinergic signaling
Christoph Döhler (Leipzig/DE),
Matthias Zebisch (Leipzig/DE; Oxford/GB), Norbert Sträter (Leipzig/DE)

MS04–P08 Improved data quality using the PHOTON 100 detector in shutterless mode
Vernon Smith, Severine Freisz (Karlsruhe/DE)
Matthew Benning (Madison WI/US)

MS04–P09 Solvent effect on crystal structures
Maria Abraham, Iris Oppel (Aachen/DE)

MS04–P10 The autofluorescence characteristics of chalcedony (a crystalline variety of silica) from skates
María Prado Figueroa (Bahía Blanca/AR)

MS04–P11 Crystal structures of the cytosolic 5'-nucleotidase IIIB explain its preference for m7GMP
Thomas Monecke (Goettingen/DE), Juliane Buschmann (Halle/DE)
Piotr Neumann (Goettingen/DE), Elmar Wahle (Halle/DE)
Ralf Ficner (Goettingen/DE)

MS04–P12 Structural changes of Importin β in dependence of divergent crystallization conditions
Marcel Tauchert, Achim Dickmanns, Ralf Ficner (Goettingen/DE)

MS04–P13 Structural analysis of the spliceosomal helicase Prp2 and its intrinsically disordered interaction partner Spp2
Andreas Schmitt, Ralf Ficner (Goettingen/DE)

MS04–P14 Crystal structure of a 3D domain-swapped dimer of the Helicobacter pylori type IV secretion protein CagL
Hartmut Niemann, Stephan Barden, Benjamin Schomburg (Bielefeld/DE)

Inorganic structural chemistry – synthesis, structure, properties and applications

MS05–P01 Hydrogen selective graphite based membranes
Alexander Schulz, Frank Steinbach, Jürgen Caro (Hannover/DE)

MS05–P02 Simulation of pair distribution function of $CaCO_3$ polymorphs using DISCUS
Marian Happel, Andrea Niedermayr, Hermann Gies (Bochum/DE)

MS05–P03 Detailed studies on hydrogen bonds in various minerals using neutron single crystal diffraction
Martin Meven (Garching/DE), Diego Gatta (Milano/IT)
Andrew Sazonov (Garching/DE)

MS05–P04 Synthesis, structural and optical characterizations of $(Cs,K)_3SmSi_6O_{15}$
Maria Wierzbicka-Wieczorek, Martin Göckeritz (Jena/DE)
Christoph Lenz, Gerald Giester (Vienna/AT)

MS05–P05 Structure properties of the solid-solution $Mn_xZn_{2-x}SiO_4$ ($0 < x < 0.6$)
David Behal (Garching, Munich/DE), So-Hyun Park (Munich/DE)

MS05–P06 $Tl_4Si_5O_{12}$ – a microporous thallium silicate
Volker Kahlenberg, Lukas Perfler (Innsbruck/AT), Peter Blaha (Vienna/AT)

MS05–P07 Analysis of lattice defects in silica zeolites of the structure type MFI
Isabel Großkreuz, Hermann Gies, Bernd Marler (Bochum/DE)

MS05–P08 Untersuchungen der Übergangsreaktion von Tobermorit zu Xonotlit unter dem Einfluss von Additiven und erhöhter Temperatur
Andrea Hartmann, David Schulenberg, J.-Ch. Buhl (Hannover/DE)

MS05–P09 Incorporation of foreign ions in C_2S – synthesis, characterization and hydration
Katharina Pöhler (Halle/Saale/GB)

MS05–P10 Optimierung der Kristallisation von Zeolith Na-A aus Rückständen der Silanproduktion
Andrea Hartmann, Valeriy Petrov, J.-Ch. Buhl (Hannover/DE)
Katrin Rübner, Matthias Lindemann (Berlin/DE)

MS05–P11 Zeolithkristallisation bei simultanem Einsatz SiO_2- und CaO-reicher industrieller Reststoffe und alkalischer Aktivierung
Valeriy Petrov, Andrea Hartmann, Josef-Christian Buhl (Hannover/DE)
K. Rübner
M. Lindemann (Berlin/DE)

MS05–P12 Hydrothermal Synthesis of fine-crystalline eulytite ($Bi_4(SiO_4)_3$) powders in supercritical fluids
Ekaterina Marina, Irina Makhina, Vladimir Balitsky (Chernogolovka/RU)

MS05–P13 The average structure of RUB-12 – a new lithosilicate zeolite
Bernd Marler, Antje Grünewald-Lüke, Hermann Gies (Bochum/DE)

MS05–P14 $Me_2Sn(HPO_3)$, $Et_2Sn[HPO_2(OH)]_2$ und $tBu_2Sn[HPO_2(OH)]_2$ die ersten Diorganozinn(IV)-phosphonate
Hans Reuter, Martin Reichelt (Osnabrück/DE)

MS05–P15 Phase relations in the binary system $Sm_2O_3 – P_2O_5$
Andreas Neumann, Antje Hirsch (Aachen/DE), Julia Heuser (Juelich/DE)
Robin Faust (Aachen/DE), Hartmut Schlenz, Dirk Bosbach (Juelich/DE)
Lars Peters, Georg Roth (Aachen/DE)

MS05–P16 Crystal structure of $CaMg_2P_6O_3N_{10}$
Lukas Neudert, Alexey Marchuk (Munich/DE), Oliver Oeckler (Leipzig/DE)
Wolfgang Schnick (Munich/DE)

MS05–P17 $Ce[AsO_3]$ – Cerium(III) Oxoarsenate(III) with α-$Pb[SeO_3]$-type crystal structure
Florian Ledderboge, Thomas Schleid (Stuttgart/DE)

MS05–P18 (La, Sr, Ce) and (Sm, Ca, Ce) Monazite solid solutions
Andreas Neumann, Antje Hirsch (Aachen/DE), Julia Heuser (Juelich/DE)
Peter Cornel Jung, Jochen Zaddach (Aachen/DE), Hartmut Schlenz
Dirk Bosbach (Juelich/DE), Lars Peters, Georg Roth (Aachen/DE)

MS05–P19 Mechanical and physical properties of monazite-type ceramics $La_{(1-x)}Eu_{(x)}PO_4$
Anja Thust (Frankfurt a. M./DE), Yulia Arinicheva (Juelich/DE)
Eiken Haussühl (Frankfurt a. M./DE), Stefan Neumeier (Juelich/DE)
Lkhamsuren Bayarjargal, Björn Winkler (Frankfurt a. M./DE)

MS05–P20 Thorium arsenates from high temperature solid state reactions
Na Yu, Evgeny Alekseev, Vladislav Klepov (Juelich/DE)

MS05–P21 $CoAs_2O_4$ – synthesis and structural characterisation
Tamara Đorđević, Astrid Wittwer (Vienna/AT)

MS05–P22 New ternary molybdates in the M-Fe(II,III)-Mo-O systems with M=K, Rb
Angelina Sarapulova (Dresden/DE)
Olga Chimitova (Dresden/DE; Ulan-Ude, Russia/RU)
Daria Mikhailova (Dresden/DE), Natalia Kuratieva (Novosibirsk/RU)
Alexander Komarek, Yurii Prots (Dresden/DE)
Helmut Ehrenberg (Eggenstein-Leopoldshafen/DE)

MS05–P23 Synthesis, structure and characterization of $Li_3AsW_7O_{25}$
Pei Zhao, M. Mangir Murshed, Evgeny V. Alekseev
Thorsten M. Gesing (Bremen/DE)

MS05–P24 Four novel organo-templated microporous compounds with DFT: type topology
Tamara Đorđević (Vienna/AT), Ljiljana Karanović, Sabina Šutović
Dejan Poleti (Belgrade/RS)

MS05–P25 Synthesis and crystal structure of new hydrogen carbonate tungstates $Rb_3(HCO_3)(WO_4)$ and $Cs_3(HCO_3)(WO_4)$
Elisabeth Irran, Jorge Higuera-Serrano (Berlin/DE)

MS05–P26 Solvochemical synthesis and structural characterization of the neodymium(III) Fluoride ortho-oxomolybdate(VI) $NdF[MoO_4]$
Tanja Schustereit, Thomas Schleid, Ingo Hartenbach (Stuttgart/DE)

MS05–P27 In-doped multiferroic $MnWO_4$
Ulf Gattermann, So-Hyun Park (Munich/DE)

MS05–P28 New iodine polysulfates syntheses, crystal structures and characterization of $I_2(SO_4)_2(S_2O_7)$, $I_2(SO_4)_2(S_3O_{10})$, and a new modification of $(IO_2)_2(S_2O_7)$
Mathias S. Wickleder, Lisa V. Schindler, Jörn Bruns (Oldenburg/DE)

MS05–P29 Reactions of $B(OH)_3$ with sulfuric acid derivatives – the unprecedented layer structures of $B_2S_2O_9$ and B_6O_9 CH_3SO_3H
Mathias S. Wickleder, Christian Logemann (Oldenburg/DE)

MS05–P30 Syntheses, crystal structures and vibrational spectra of diselenates(VI) $A_2Se_2O_7$ (A = Li, Na, K, Rb, Cs)
Harald Hillebrecht, Michael Daub (Freiburg/DE)

MS05–P31 Synthesis and crystal structure of the scandium(III) fluoride oxoselenate (IV) $ScF[SeO_3]$
Sheng-Chun Chou, Thomas Schleid (Stuttgart/DE)

MS05–P32 On the first boroselenates(VI)
Harald Hillebrecht, Michael Daub (Freiburg/DE)

MS05–P33 $Sc_2Te_3O_9$ – a new crystal structure of the rare-earth metal(III) oxotellurates(IV) with the composition $M_2Te_3O_9$
Sheng-Chun Chou, Thomas Schleid (Stuttgart/DE)

MS05–P34 The high pressure spinel-type Si_3N_4 phase and its capability for oxygen incorporation
Anke Köhler, Christian Schimpf, Volker Klemm, David Rafaja
Thomas Schlothauer, Kevin Keller, Gerhard Heide, Marcus Schwarz
Edwin Kroke (Freiberg/DE)

MS05–P35 Phase transitions of perovskites with the chemical composition $Ca(Ti,Fe,Mn)O_{3-d}$
Stefan Stöber, Herbert Pöllmann (Halle/Saale/DE)

MS05–P36 Tantalum and vanadium substitution in potassium tungsten bronzes
Md. Shahidur Rahman, M. Mangir Murshed, Thorsten M. Gesing (Bremen/DE)

MS05–P37 Synthesis and crystal structure of new mixed metal oxide fluorides with ReO_3-type structure
Suliman Nakhal (Berlin/DE)

MS05–P38 Thermodynamics of oxygen incorporation into bixbyite-type vanadium sesquioxide
Christoph Reimann, Thomas Bredow (Bonn/DE)

MS05–P39 The effects of cooling process on the phases and particle sizes of vanadium slag
Long Li, Wensun Ge, Lian Chen, Yong Chen (Panzhihua/CN)

MS05–P40 Nanoindentation and crystallographic/spectroscopic characterization of Ta_2TiO_7 single-crystals and ceramics
Lukas Perfler, Volker Kahlenberg, Christoph Wikete (Innsbruck/AT)
Reinhard Kaindl (Niklasdorf/AT)

MS05–P41 Crystalline phase formation during the atomic layer deposition of TiO_2
Barbara Abendroth, Solveig Rentrop, Theresa Moebus, Judith Dietel
Hartmut Stöcker, Dirk C. Meyer (Freiberg/DE)

MS05–P42 Synthesis and crystal structure of new mixed metal oxide fluorides AB_2OF_8 (A = Mg, Ti; B = Ti, Zr, Fe)
Suliman Nakhal (Berlin/DE)

MS05–P43 Pressure-induced phase transitions in VOCl
Maxim Bykov, Elena Bykova, Leonid Dubrovinsky (Bayreuth/DE)
Michael Hanfland (Grenoble/FR), Sander van Smaalen (Bayreuth/DE)

MS05–P44 Crystal structures of group 14 element tetrachloridoaluminates
Sascha Schloots, Walter Frank (Düsseldorf/DE)

MS05–P45 Syntheses and crystal structures of $Rb_3Sn_2X_7$ (X = Cl, Br)
Harald Hillebrecht, Gerhard Thiele, Bernd Serr (Freiburg/DE)

MS05–P46 Ho_3OFSe_3 and $Ho_3OF_3Se_2$ – two surprising new structure types for rare-earth metall(III) oxide fluoride selenides
Dirk Zimmermann, Thomas Schleid (Stuttgart/DE)

MS05–P47 Synthesis and crystal structures of the dimorphic holmium(III) fluoride selenide HoFSe
Dirk Zimmermann, Thomas Schleid (Stuttgart/DE)

MS05–P48 $SrCuNdS_3$ – a new compound with two different crystal structures
Marcel Eberle, Sabine Strobel, Thomas Schleid (Stuttgart/DE)

MS05–P49 Crystal structure study of naturally occurring phases $Ag_4Pd_3Te_4$ and $Pd_{14}Ag_2Te_9$
Frantisek Laufek, Anna Vymazalova, Milan Drabek, Jan Drahokoupil
Michal Dusek (Prague/CZ)

MS05–P50 Two new nitride tellurides of dysprosium – Dy_3NTe_3 and $Dy_4N_2Te_3$
Markus Foltin, Falk Lissner, Thomas Schleid (Stuttgart/DE)

MS05–P51 Ln_2NBi (Ln = La – Nd) – the first nitride bismuthides of the Lanthanides
Klaus K. Wolff, Falk Lissner, Jürgen Köhler
Thomas Schleid (Stuttgart/DE)

MS05–P52 Crystallographic peculiarities in the solid solution series $La_{1-x}Ce_xOBiS_2$
Thomas Doert, Eike Ahrens (Dresden/DE)

MS05–P53 Low-temperature route to crystalline Cu_2ZnSnS_4
Anna Ritscher, Martin Lerch (Berlin/DE)

MS05–P54 Microstructure and crystallization behavior of the amorphous thermoelectrics $(GeSe_{3.5})_{88}M_{12}$ (M = Bi, Sb)
Robert Schlegel, Gerald Wagner, Oliver Oeckler (Leipzig/DE)

MS05–P55 X marks the path—diffusion pathways in 3R-Li_xTiS_2 as a function of lithium content
Dennis Wiedemann, Suliman Nakhal (Berlin/DE)
Anatoliy Senyshyn (Munich/DE), Martin Lerch (Berlin/DE)

MS05–P56 The crystal chemistry of $CsAlS_2$
Verena Winkler (Regensburg/DE)

MS05–P57 Synthesis and characterization of $Cs_2Ga_2S_5$ and $Cs_2Ga_2Se_5$
Daniel Friedrich (Regensburg/DE)

MS05–P58 Synthesis and structural characterization of a polar framework of thiogallato-closo-dodecaborate anions containing rare-earth metal(III) cations
Fabian M. Kleeberg, Ronja Stromsky, Lucas W. Zimmermann
Thomas Schleid (Stuttgart/DE)

MS05–P59 Kettenstücke, (Doppel-)Ketten und Supertetraeder – neue Caesiumsulfidoferrate $Cs_8[Fe_4S_{10}]$, $Cs_7[FeS_2]_2[Fe_2S_3]_2$ und $Cs_7[Fe_4S_8]$
Michael Schwarz, Caroline Röhr (Freiburg i. B./DE)

MS05–P60 Hole-doped $Ca_{1-x}Na_xFFeAs$ – a new iron-arsenide based superconductor
Klaus K. Wolff, Larysa Shlyk, Markus Bischoff, Eva Rose, Rainer Niewa
Thomas Schleid (Stuttgart/DE)

MS05–P61 Eine neue Modifikation von $CaGe_2$
Michael Jehle, Julia Steckhan, Caroline Röhr (Freiburg i. Br./DE)

MS05–P62 Intermetallische Phasen des quasibinären Schnitts $SrIn_4$-$SrHg_4$
Caroline Röhr, Marco Wendorff (Freiburg/DE)

MS05–P63 New intermetallics in the system Ta/Ga
Harald Hillebrecht, Agbelenko Koffi, Martin ade (Freiburg/DE)

MS05–P64 Alkaline-earth metal amides as mineralizers for ammonothermal GaN crystal growth – $Ba[Ga(NH_2)_4]_2$ as intermediate
Jan Hertrampf, Shiyu Zhang (Stuttgart/DE),Nicolas S. A. Alt
Eberhard Schlücker (Erlangen/DE), Rainer Niewa (Stuttgart/DE)

MS05–P65 Crystal structure of hexaphenyldisilane $Si_2(C_6H_5)_6$
Lothar Fink, Thomas Bernert, Jürgen Glinnemann, Edith Alig
Matthias Berger, Martin U. Schmidt (Frankfurt/DE)

MS05–P66 Crystal structures of new Cu(II) coordination polymers from X-ray powder data
Haishuang Zhao, Lothar Fink, Yasar Krysiak, Jurgen Glinnemann
Edith Alig, Martin U. Schmidt (Frankfurt a. M./DE)

MS05–P67 Crystal structure of lead(II) methanesulfonate monohydrate
Thomas Trella, Walter Frank (Düsseldorf/DE)

MS05–P68 Crystal structure of 4-Aminopyridin-1-ium Hydrogen (9-Phospho-nononyl)phosphonate
Martin van Megen, Guido Johannes Reiß, Walter Frank (Düsseldorf/DE)

MS05–P69 Crystal structures of two transition metal methanesulfonate hydrates
Thomas Trella, Walter Frank (Düsseldorf/DE)

MS05–P70 Dinuclear transition metal complexes with pyrazolato-bridged imidazolium-based ligands
Stefan A. Reindl, Alexander Pöthig, Fritz E. Kühn
Wolfgang A. Herrmann (Garching/DE)

MS05–P71 Synthesis and crystal structure of $Sr_2Cl_2[C_2O_4]$ 6 H_2O
Harald Henning, Thomas Schleid (Stuttgart/DE)

MS05–P72 The crystal structure of 4,4'-bipyridinium-pentachlorooxomolybdate(V)
Jan van Megen, Walter Frank (Düsseldorf/DE)

MS05–P73 A comparative study of long chain alkaline earth metal carboxylates
Julia Volk, Walter Frank (Düsseldorf/DE)

MS05–P74 Unusual tetraazaadamantane ligand in a series of manganese(IV) dimers with varying bridging ligands
Dejan Premužić, Małgorzata Hołyńska (Marburg/DE)

MS05–P75 A new isomer of the classical $[Mn^{III}_6]$ SMMs
Malgorzata Holynska (Marburg/DE)

MS05–P76 Synthesis and characterisation of oxygenated magnsium phthalocyanine
Jan Janczak, Ryszard Kubiak (Wroclaw/PL)

MS05–P77 Square-planar organoplatinum complexes – crystal structures of three pharmaceutically relevant compounds
William Raven, Ulli Englert, Irmgard Kalf, Pol Hermes (Aachen/DE)

Structure-property relations in materials sciences

MS06–P01 New Mn(II) coordination polymers employing 2,2'-bipyridine-3,3',6,6'-tetracarboxylate as a ligand
Andrzej Kochel (Wrocław/PL), Małgorzata Hołyńska (Marburg/DE)

MS06–P02 Neutron diffraction studies of pressure effects on crystal and magnetic structure of $La_{0.5}Ba_{0.5}CoO_{2.8}$
Vadim Sikolenko (Berlin/DE), Igor Troyanchuk (Minsk/BY)
Daniel Többens (Berlin/DE), Clemens Ritter, Thomas Hansen (Grenoble/FR)
Vadim Efimov (Dubna/RU), Susan Schorr (Berlin/DE)

MS06–P03 Polarized optical absorption spectra and crystal field superposition model calculations of the multiferroic compound Co_3TeO_6
Manfred Wildner, Dominik Reichartzeder (Vienna/AT)

MS06–P04 Temperature-dependent behavior of $|Na_8(NO_2)_2|[AlSiO_4]_6$ in air and carbondioxide
Malik Šehović, Lars Robben, Thorsten M. Gesing (Bremen/DE)

MS06–P05 The Influence of boron on the crystal structure and properties of mullite – investigations at ambient, high-pressure, and high-temperature conditions
Hanna Lührs, Reinhard X. Fischer, Hartmut Schneider (Bremen/DE)
Scott P. King, John V. Hanna (Coventry/GB), Patricia E. Kalita
Kristina Lipinska (Las Vegas, TX/US), Stefan Söllradl (Garching/DE)
Jürgen Konzett (Innsbruck/AT)

MS06–P06 Characterization of the hydrides in Mg-Dy alloy using synchrotron radiation
Yuanding Huang, Lei Yang, Karl Ulrich Kainer, Norbert Hort
Weimin Gan (Geesthacht/DE)

MS06–P07 Thermal expansion across phase-transitions
Thorsten M. Gesing, M. Mangir Murshed, Lars Robben (Bremen/DE)

MS06–P08 A ^{57}Fe mössbauer study of local structure and cation distribution in Mullite-type $Bi_2(Fe_xMn_{1-x})_4O_{10}$ and $Bi_2(Fe_xM_{1-x})_4O_9$, M=Al, Ga, Mn
Sven-Ulf Weber (Braunschweig/GH), Thorsten Gesing (Bremen/DE)
Michael Lufaso (Jacksonville, FL/US)
Hartmut Schneider (Cologne/DE), Fred-Jochen Litterst
Klaus-Dieter Becker (Braunschweig/DE)

MS06–P09 Stimulated Raman scattering in lead carbonate crystals – $PbCO_3$ (cerussite) and $Pb_2CO_3Cl_2$ (phosgenite)
Petra Becker-Bohatý (Cologne/DE)
Alexander A. Kaminskii (Moscow/RU), Hanjo Rhee
André Kaltenbach, Oliver Lux, Hans-Joachim Eichler (Berlin/DE)
Ladislav Bohatý (Cologne/DE)

MS06–P10 Efficient $\chi^{(2)}$- and $\chi^{(3)}$-nonlinear optical processes in single crystals of guanylurea(1+) hydrogen phosphite (GUHP)
Ladislav Bohatý (Cologne/DE), Alexander A. Kaminskii (Moscow/RU)
Hanjo Rhee, Oliver Lux, André Kaltenbach
Hans-Joachim Eichler (Berlin/DE), Ivan Nemec
Michaela Fridrichová (Prague/CZ), Petra Becker-Bohatý (Cologne/DE)

MS06–P11 Multiferroic and linear magnetoelectric properties of erythrosiderite-type and related compounds $A_2[FeCl_5(H_2O)]$ with A = NH4, K, Rb, Cs
Matthias Ackermann, Daniel Brüning, Thomas Lorenz, Petra Becker
Ladislav Bohatý (Cologne/DE)

MS06–P12 Crystal structures of Pigment Red 57:1 ($C_{18}H_{12}CaN_2O_6S$ n H_2O) determined by X-ray powder diffraction
Sonja M. Hammer, Sándor L. Bekö, Martin U. Schmidt (Frankfurt/DE)

MS06–P13 Structural and magnetic characterization of the diluted ferromagnet $Sn_xFe_{4-x}N$ ($0 < x \leq 1$)
Tanja Scholz (Aachen/DE), Anne Houben (Juelich/DE)
Andreas Houben, Richard Dronskowski (Aachen/DE)

MS06–P14 DFT investigations on different magnetic configurations of $PbFeBO_4$
Mangir Murshed (Bremen/DE), Cecilia Mendive (Mar del Plata/AR)
Mariano Curti (Mar del Plata AR), Thorsten Gesing (Bremen/DE)

MS06–P15 Magnetic ordering in the system $Cu_{1-x}Ni_xCr_2O_4$ studied by neutron powder diffraction
Manfred Reehuis, Michael Tovar, Daniel Többens (Berlin/DE)

MS06–P16 A treatment for theoretical determination of defocusing curves and its application for the adjustment of an Eulerian goniometer
Jesus Palacios Gomez (MX City/MX)

MS06–P17 Investigation of precipitation behavior in micro-alloyed steels
Imke Janßen, Helmut Klein, Christian Klinkenberg (Düsseldorf/DE)

MS06–P18 Microstructural analysis and compositional examination of $Cu(In,Ga)Se_2$ thin films by grazing incidence X-ray diffraction
René Gunder, Julien Marquardt, Susan Schorr (Berlin/DE)

MS06–P19 Phase content analysis of off-stoichiometric Cu_2ZnSnS_4 (CZTS)
Kai Neldner, Susan Schorr (Berlin/DE)

MS06–P20 Chemical and structural characterization of off-stoichiometric $Cu_2ZnSnSe_4$
Laura Elisa Valle Rios, Susan Schorr (Berlin/DE)

MS06–P21 Structural and microstructural characterisation of $Cu_2ZnSn(S_{1-x}Se_x)_4$ thin films
Galina Gurieva (Berlin/DE), Mirjana Dimitrievska (Barcelona/ES)
R Günder (Berlin/DE), H Xie, V. Izquierdo-Roca, A. Pérez-Rodríguez
E. Saucedo (Barcelona/ES), Susan Schorr (Berlin/DE)

MS06–P22 Electrophretic deposition of yttria partially stabiloized zirconia on plasma spraying thermal barrier coating
Mohammed Al-Tameemi, Sami Alrubaiye, Hussan Hussan (Baghdad/IQ)

MS06–P23 Structural changes of strontium barium niobate $Sr_{0.53}Ba_{0.47}Nb_2O_6$ (SBN53) at the relaxor ferroelectric transition
Heribert A. Graetsch (Bochum/DE)

MS06–P24 Comparison of neutron and NMR spectroscopic data for chalcopyrite $CuFeS_2$
Ramil Gainov (Berlin/DE), V. A. Golovanevskiy (Perth/AU)
V. V. Klekovkina, A. V. Dooglav, I. N. Penkov
R. R. Khassanov (Kazan/RU), M. Russina (Berlin/DE)

MS06–P25 Use of a single crystal diffractometer for polycrystalline sample characterization
Zoltan Gal (Yarnton/GB)

Synchrotron opportunities and challenging structure determinations

MS07–P01 Data collection options for challenging samples at the Macromolecular Crystallography beamlines at diamond light source
Ralf Flaig (Chilton, Didcot/GB)

MS07–P02 Phasing strategies with HKL2MAP and SITCOM
Fabio Dall\'Antonia, Thomas Schneider (Hamburg/DE)

MS07–P03 A systematic study of acyclic (L-Ala)n-OH peptides combining diffuse scattering, inelastic neutron scattering and DFT
Matthias Gutmann, Sanghamitra Mukhopadyay
Armin Wagner (Chilton Didcot, Oxfordshire/GB)
Martin von Zimmermann (Hamburg/DE), Leigh Connor (Chilton Didcot/GB)
Alke Meents, Anja Burkhardt, Olof Gutowski (Hamburg/DE)

MS07–P04 The annealing behaviour of Eifel sanidine – comparing results from neutron & X-ray diffraction experiments
Johannes Kaehn, Daniel Többens, Manfred Reehuis
Jens-Uwe Hoffmann, Susan Schorr (Berlin/DE)

MS07–P05 Room temperature macromolecular serial crystallography using synchrotron radiation
Dominik Oberthuer (Hamburg/DE), Francesco Stellato, Mengning Liang
Richard Bean, Oleksandr Yefanov,Cornelius Gati, Anton Barty
Anja Burkhardt,Pontus Fischer,Lorenzo Galli, Richard Kirian, Jan Meyee
Saravanan Panneerselvam, Chun Hong Yoon, Thomas A. White
Alke Meents, Henry N. Chapman (Hamburg/DE)

MS07–P06 Generating stereochemical restraints for SHELXL with Grade
Julian Holstein, Oliver Smart, Gerard Bricogne (Cambridge/GB)

MS07–P07 Microstructural and mechanical characterization of cold-drawn pearlitic steel wires using synchrotron X-ray diffraction
Soundès Djaziri, Yujiao Li (Düsseldorf/DE), Shoji Goto (Akita/JP)
Hauke Springer, Gerhard Dehm (Düsseldorf/DE)

MS07–P08 Structural biology using in vivo grown protein crystals
Lars Redecke, Marco Klinge, Cornelius Gati, Gleb Bourenkov (Hamburg/DE)
Robert Schönherr (Luebeck/DE), Karol Nass, Dirk Rehders Dominik Oberthür
Frsco Stellato (Hamburg/DE), Björn Philip Sommer (Hamburg, Tübingen/DE)
Thomas A. White, Anton Barty, Thomas S. Schneider (Hamburg/DE)
Jose Martinez-Costas (Santiago de Compostela/ES)
Rainer Duden (Luebeck/DE), Michael Duszenko (Tübingen/DE)
Henry N. Chapman, Christian Betzel (Hamburg/DE)

MS07–P09 The AGIPD photon detector for the serial femtosecond crystallography apparatus at the european XFEL
Stephan Stern, Steffen Raabe, Hamidreza Dadgostar
Sunil Ananthaneni, Mengning Liang, Patrik Vagovic, Henry N. Chapman
Leonard Chavas, Adrian P. Mancuso, Andrew A. Aquila, Gannon Borchers
Nadja Reimers, Klaus Giewekemeyer, Chun Hong Yoon, Julian Becker
Florian Pithan, Annette Delfs, Helmut Hirsemann, Sergej Smoljanin
Heinz Graafsma (Hamburg/DE), Dominic Greiffenberg, Bernd Schmitt
Xintian Shi (Villingen/CH)

MS07–P10 Capabilities of the Extreme Conditions Beamline at PETRA III, DESY
Wolfgang Morgenroth, Hanns-Peter Liermann, Zuzana Konôpková
Konstantin Glazyrin, Emma McBride, Andre Rothkirch. Mario Wendt
Anita Ehnes (Hamburg/DE)

MS07–P11 Structure Determination of Ho_2PdSi_3
Melanie Nentwich, Matthias Zschornak (Freiberg/DE)
Carsten Richter (Freiberg, Hamburg/DE), Dirk C. Meyer (Freiberg/DE)

MS07–P12 CrystFEL – software for crystallography using FEL sources
Thomas White (Hamburg/DE)

MS07–P13 The serial femtosecond crystallography user's consortia project at the European XFEL
Patrik Vagovic, Leonard Chavas, Stephan Stern, Steffen Raabe
Hamidreza Dadgostar, Sunil Ananthaneni, Mengning Liang
Henry N. Chapman, Adrian P. Mancuso, Andrew Aquila
Gannon Borchers, Nadja Reimers, Klaus Giewekemeyer
Chun Hong Yoon, Julian Becker, Florian Pithan, Annette Delfs
Helmut Hirsemann, Sergei Smoljanin, Heinz Graafsma (Hamburg/DE)
Dominik Greifenberg, Berndt Schmitt, Xintian Shi (Villigen/CH)

MS07–P14 Time-resolved X-ray diffraction study of $Sr_{0.5}Ba_{0.5}Nb_2O_6$ under external electric field
Semën Gorfman, Hyeokmin Choe (Siegen/DE), Jan Dec (Katowice/PL)
Michael Ziolkowski, Ullrich Pietsch (Siegen/DE)
Tadeusz Łukasiewicz (Warsaw/PL)

MS07–P15 EMBL P13 beamline for macromolecular crystallography at PETRA III @DESY, Hamburg, DE
Michele Cianci , Gleb Bourenkov, Johanna Kallio, Guillaume Pompidor
Stefan Fiedler, Thomas Schneider (Hamburg/DE)

MS07–P16 Macromolecular neutron diffraction at the FRM II neutron source
Andreas Ostermann, Tobias E. Schrader (Garching/DE)
Michael Monkenbusch, Bernhard Laatsch (Juelich/DE)
Philipp Jüttner, Winfried Petry (Garching/DE)
Dieter Richter (Juelich/DE)

MS07–P17 X-ray crystallography with microcrystals on a patterned silicon chip
Philip Roedig, Olga Lorbeer (Hamburg/DE), Ismo Vartiainen
Christian David (Villigen/CH), Edgar Weckert
Alke Meents (Hamburg/DE)

MS07–P18 Solvent exchange in protein crystals at cryogenic temperatures
Anja Burkhardt, Martin Warmer (Hamburg/DE)
Armin Wagner (Didcot/GB), Rudolph Reimer, Heinrich Hohenberg
Alke Meents (Hamburg/DE)

MS07–P19 Engineering of the mechanics for the SFX sample delivery system
Sunil Kumar Ananthaneni, Leonard Chavas (Hamburg/DE)

MS07–P20 A spectroscopic comparison of AOS thin films and TCO single crystals
Jörg Haeberle (Cottbus/DE), Diana Gaspar
Pedro Barquinha (Caparica/PT), Stephan Machul, Christoph Janowitz
Zbigniew Galazka (Berlin/DE), Dieter Schmeißer (Cottbus/DE)

MS07–P21 X-ray optics
Paul Ulrich Pennartz, L. Jiang, B. Verman
N. Grupido (Auburn Hills, MI/US), P. Oberta (Prague/CZ)

MS07–P22 High-efficiency SAXS/GISAXS/WAXS instrument for the laboratory: Rigaku S-MAX 3000™
Paul Ulrich Pennartz, M. Degen, N. Grupido (Auburn Hills, MI/US)

MS07–P23 POWHOW – the proposed bispectral neutron powder diffractometer at the European Spallation Source
Werner Schweika, N. Violini, K. Friese (Juelich/DE), K. Lieutenant
D. Nekrassov, C. Zendler (Berlin/DE), A. Houben, P. Jacobs (Aachen/DE)
P. Henry (Lund/SE)

Quasicrystals and incommensurate structures

MS08–P01 Modulated structure of Λ-Co(III) sepulchrate trinitrate in the second low temperature phase
Somnath Dey, Andreas Schönleber
Sander van Smaalen (Bayreuth/DE)
Finn Krebs Larsen (Aarhus/DK)

MS08–P02 Physical properties of incommensurate phase with multifractal distribution of defects
Bahruz Gadjiev (Dubna/RU)

MS08–P03 Structure refinements of Al_3BC and Al_3BC_3 – super structure versus modulation
Harald Hillebrecht (Freiburg/DE), Peter Schultz (Leipzig/DE)

MS08–P04 Cell organelles with crystalloid inclusions and applicability in practice
Antonella Chesca (Brasov/RO)

Crystallography in geology – microstructures as indicators of rock forming processes

MS09–P01 Multiferroic crystals
Jonas Stein, T. Cronert (Cologne/DE), J. Leist (Goettingen/DE)
K. Schmalzl (Juelich/DE), A. Nugroho (Bandung/ID)
A. Komarek (Dresden/DE), G. Eckold (Goettingen/DE)
M. Braden (Cologne/DE)

MS09–P02 Microstructural studies of in situ heated and deformed pure and silica gel-doped polycrystalline salt samples for long-term lithospheric rheology and radioactive waste disposal
Caterina Tommaseo (Berlin/DE)

Protein function and regulation

MS10–P01 Dynamic and conformational variability of the bacterial type-I fatty acid synthase Type-I
Mathias Enderle, Martin Grininger, Luciano Ciccarelli (Frankfurt/DE)

MS10–P02 Structural and functional analysis of the spliceosomal RNA helicase Brr2
Eva Absmeier, Christian Becke, Eva Absmeier, Karine Santos
Markus Wahl (Berlin/DE)

MS10–P03 Analysis of counter-ion effects in nonaqueous enzymology of subtilisin
Michele Cianci (Hamburg/DE), Diana Lousa (Lisboa/PT)
Bartlomiej Tomaszewski (Glasgow/GB)
António M. Baptista, Cláudio M. Soares (Lisboa/PT)
John R. Helliwell (Manchester/GB), Peter J Halling (Glasgow/GB)

MS10–P04 Enthalpic cost of water removal from a hydrophobic glucose binding cavity on HK620 tailspike protein
Ulrich Gohlke (Berlin/DE), Nina Broeker (Golm/DE)
Udo Heinemann (Berlin/DE), Robert Seckler, Stefanie Barbirz (Golm/DE)

MS10–P05 The class C Vps tethering complexes HOPS and CORVET
Heide Behrmann (Berlin/DE), Christian Ungermann (Osnabrück/DE)
Udo Heinemann (Berlin/DE)

MS10–P06 APP-E1 in a new crystal form
Sandra Hoefgen, Sven O. Dahms, Manuel E. Than (Jena/DE)

MS10–P07 Structural basis of exosome-independent RNA 3'-5' degradation
Qianqian Ming, Udo Heinemann (Berlin/DE)

MS10–P08 Structural studies of Terminal Uridylyl Transferases
Ankur Garg, Udo Heinemann (Berlin/DE)

MS10–P09 Structural basis of endoplasmic reticulum-associated degradation of misfolded proteins (ERAD)
Sofia Banchenko, Udo Heinemann (Berlin/DE)

MS10–P10 Crystallographic insights into a cobalt (III) sepulchrate based alternative cofactor system of P450 BM3 monooxygenase
Saravanan Panneerslevam (Hamburg/DE)
Aamir Shehzad (Aachen/DE), Jochen Mueller-Dieckmann
Matthias Wilmanns (Hamburg/DE), Marco Bocola
Ulrich Schwaneberg (Aachen/DE)

MS10–P11 Differential expression of activated protein kinase C receptor (LACK), alpha tubulin and protein disulfide isomerase in sensitive and resistant field isolates of Leishmania tropica by 2-Dimentional electrophoresis and Mass-spectrometry
Homa Hajjaran, Behrouz Vaziri, Mehdi Mohebali, Elham Kazemi-Rad
Ramtin Hadighi (Tehran/IR)

MS10–P12 Structural Investigation of a macromolecular complex formed by the AAA+ ATPase AtCDC48, the UBX adaptor protein PUX1 and the SNARE SYP31
Saša Petrović, Udo Heinemann (Berlin/DE)

MS10–P13 Structural basis for methyl group transfer and acetyl-CoA synthesis in carboxydothermus hydrogenoformans
Sebastian Götzl, Sandra Hennig, Jae-Hun Jeoung, Christian Teutloff
Robert Bittl, Holger Dobbek (Berlin/DE)

MS10–P14 Structure of the ubiquitin activating enzyme loaded with two ubiquitin molecules
Antje Schaefer, Hermann Schindelin (Wuerzburg/DE)

MS10–P15 Exploring substrate and product channels in CO dehydrogenase ii of carboxydothermus hydrogenoformans
Lilith Domnik, Jae-Hun Jeoung, Jochen Fesseler
Holger Dobbek (Berlin/DE)

MS10–P16 Tales from the cloud atlas: structural insights into enzymatic CO_x-transformation
Jochen Fesseler, Jae-Hun Jeoung, Holger Dobbek (Berlin/DE)

MS10–P17 Enzymology with multiple copies in the asymmetric unit – trapping reaction intermediates from a single crystal of homogentisate 1,2-dioxygenase
Jae-Hun Jeoung, Martin Bommer, Holger Dobbek (Berlin/DE)

MS10–P18 The world of CO dehydrogenases
Yulia Dendra, Jochen Fesseler, Jae-Hun Jeoung (Berlin/DE)

MS10–P19 Transportmechanism of the bacterial ABC-transporter MsbA
André Müller (Bochum/DE)

MS10–P20 Design, structure and function of a novel ligand-binding globulin
Karin Schmidt (Erlangen/DE)

MS10–P21 O_2-tolerant [NiFe] hydrogenase of Ralstonia eutropha:
important amino acids in enzyme reactivation
Jacqueline Kalms, Andrea Schmidt, Patrick Scheerer (Berlin/DE)

MS10–P22 Macrodomains of middle-east respiratory syndrome coronavirus
Jian Lei, Rolf Hilgenfeld, QingJun Ma, Jeroen R. Mesters (Luebeck/DE)

MS10–P23 Structural characterization of gephyrin by AFM and SAXS reveals a
mixture of compact and extended states
Bodo Sander (Wuerzburg/DE), Giancarlo Tria
Alexander Shkumatov (Hamburg/DE), Eun-Young Kim (New York, NY/US)
Jörg Günter Grossmann (Liverpool/GB), Ingrid Tessmer (Wuerzburg/DE)
Dmitri Svergun (Hamburg/DE), Hermann Schindelin (Wuerzburg/DE)

MS10–P24 Insights into the ATP-dependent reductive activation of the
corrinoid/iron-sulfur protein of carboxydothermus hydrogenoformans
Sandra Elisabeth Hennig, Sebastian Götzl, Jae-Hun Jeoung
Martin Bommer, Friedhelm Lendzian, Peter Hildebrandt
Holger Dobbek (Berlin/DE)

Therapeutic targets and fragment-based drug discovery

MS13–P01 Automatic data processing using XDSAPP v1.0
Karine Sparta, Uwe Müller, Manfred S.Weiss
Udo Heinemann (Berlin/DE)

MS13–P02 Fragment-screening by X-ray crystallography at the MX-beamlines of
the Helmholtz-Zentrum Berlin
Manfred Weiss, Monika Ühlein, Uwe Mueller
Janina Linnik (Berlin/DE), Andreas Heine
Gerhard Klebe (Marburg/DE)

MS13–P03 Application of structure-based drug design to target histone demethylase enzymes.
David Carter, Edgar Specker, Jessica Przygodda, Martin Neuenschwander
Carola Seyffarth, Jens von Kries, Udo Heinemann, Ulrich Gohlke (Berlin/DE)

MS13–P04 Synthetic PhzB product analogues as inhibitors of a key step in phenazine biosynthesis
Christina Diederich (Braunschweig/DE), Jakob Pletz
Rolf Breinbauer (Graz/AT), Wulf Blankenfeldt (Braunschweig/DE)

MS13–P05 Crystals in renal diseases
Antonella Chesca (Brasov/RO)

MS13–P06 Small-molecule inhibitors of protein-protein interactions – application to Ena/VASP proteins
Yvette Roske, Matthias Barone, Robert Opitz, Ronald Kühne (Berlin/DE)

MS13–P07 Structure-based drug design targeting the main protease of human coronavirus NL63
Linlin Zhang (Luebeck/DE), Daizong Lin (Luebeck/DE; Shanghai/CN)
Qingjun Ma, Yibei Xiao (Luebeck/DE), Hong Liu (Shanghai/CN)
Rolf Hilgenfeld (Luebeck/DE; Shanghai/CN)

Charge density for understanding chemical bonding in organic and inorganic structures (dedicated to Prof. Luger)

MS15-P01 A Bis(ylidic) or a delocalized π-system? – charge density study of the first mixed-valent tetraphosphete
Verena Breuers, Christian W. Lehmann (Düsseldorf/DE)

MS15-P02 Peri-substituted (Ace) Naphthylphosphinoboranes – regular vs. frustrated lewis pairs evaluated by structural parameters and real space bonding indicators
Jens Beckmann (Bremen/DE), Stefan Mebs (Berlin/DE)
Emanuel Hupf (Bremen/DE)

MS15-P03 Visualization tools development started at Peter Luger's group
Christian Hübschle (Bayreuth/DE), Birger Dittrich (Hamburg/DE)
Sander van Smaalen (Bayreuth/DE)

MS15-P04 Point charges for force-field parametrization from the invariom database
Claudia M. Orben (Goettingen/DE), Birger Dittrich (Hamburg/DE)

MS15-P05 Efficient data collection with software and hardware features from Agilent Technologies
Zoltan Gal (Yarnton/GB)

Spectroscopy as supporting method in structure determination

MS17-P01 Crystallograhic orientation of hydrogen defects in lithium niobate and lithium tantalate
Thomas Köhler, Erik Mehner, Juliane Hanzig, Günther Gärtner
Hartmut Stöcker, Dirk C. Meyer (Freiberg/DE)

MS17-P02 XRD and ^{29}Si NMR study of metamict minerals
Peter Zietlow, Tobias Beirau, Michael Fechtelkord (Hamburg/DE)
Lee A. Groat (Vancouver/CA), Carsten D. Paulmann Carsten
Ulrich Bismayer (Hamburg/DE)

MS17-P03 Impact of temperature and barometric pressure fluctuations on X-ray beam intensities
Tina Weigel, Marco Herrmann, Matthias Zschornak
Tilmann Leisegang, Dirk C. Meyer (Freiberg/DE)

MS17-P04 IR and ^{11}B MAS NMR investigations on $H_{4-x}B(OH)_x$ species in the sodalite cage
Lars Schomborg, Claus Henning Rüscher, Josef-Christian Buhl (Hannover/DE
Michael Fechtelkord (Bochum/DE)

MS17-P05 The morpholog and ultra – structure of a new 2 – methoxyethanol utilizing Pseudomonas sp.
Frederick Osaro Ekhaise (Benin City/NG)

Crystallography in archeometry

MS18–P01 Collections of crystal models at TU Berlin
Susanne Franziska Herting-Agthe (Berlin/DE)

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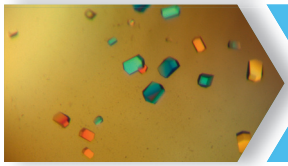

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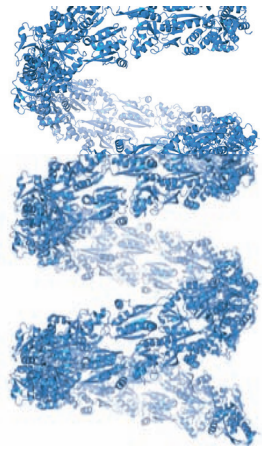

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