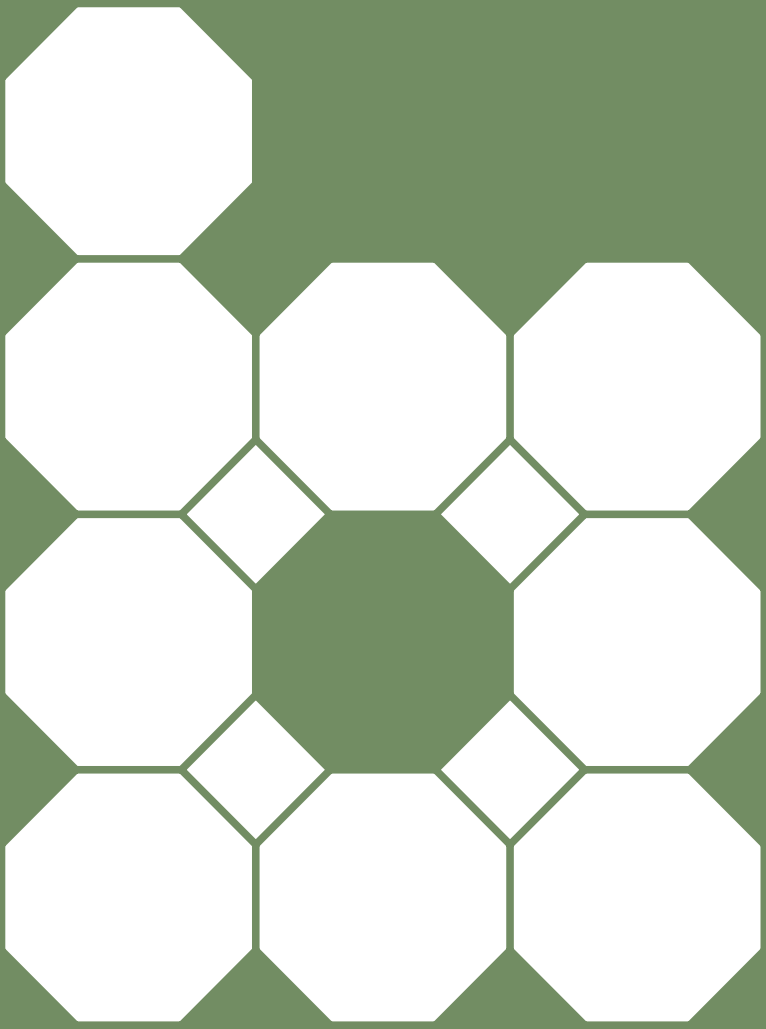
Young Crystallographers

Berlin 2016

21-23 September

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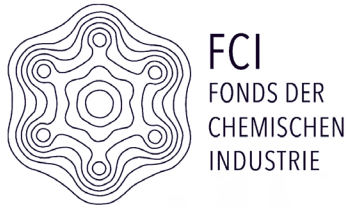
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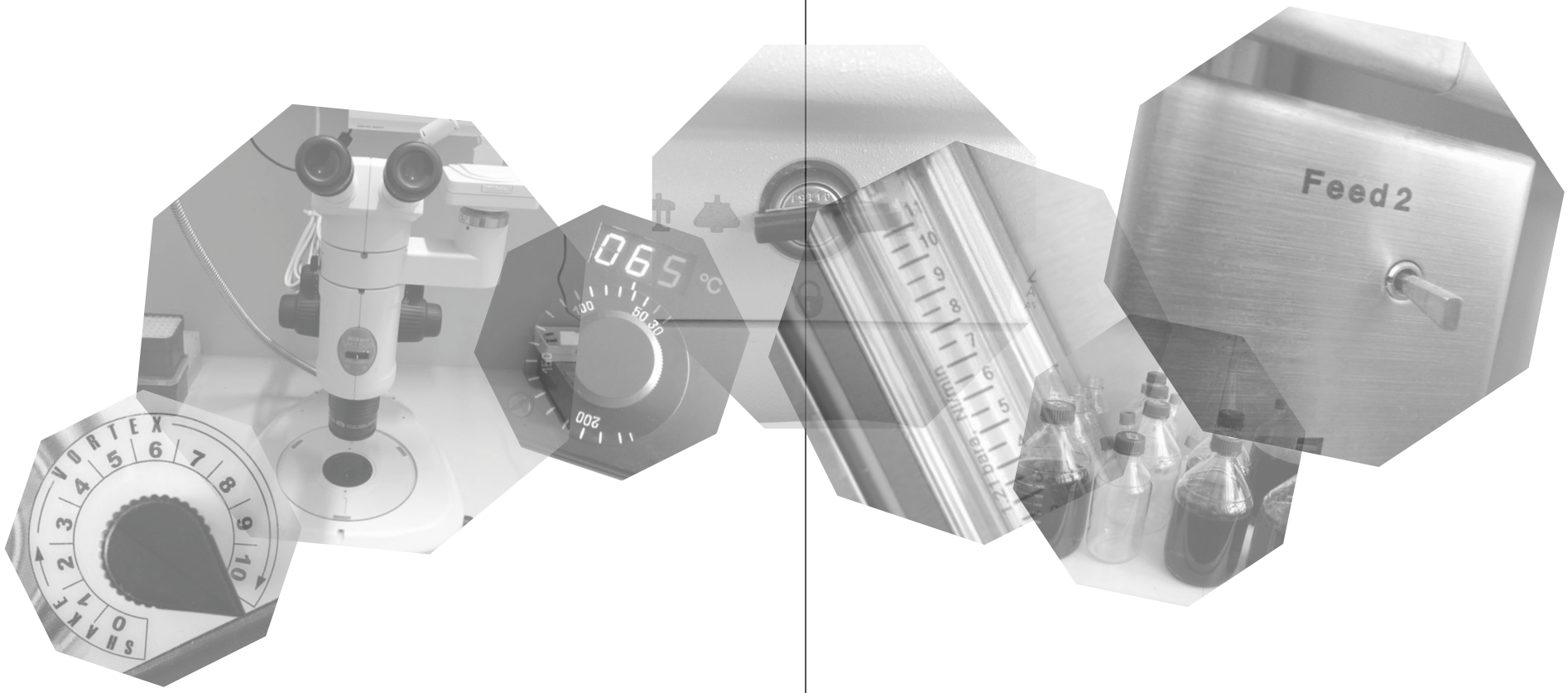


Welcome Note

Dear participants of the 2nd meeting of the DGK's Young Crystallographers, We are more than happy to welcome you in Berlin!

Here, you will have the chance to present your latest research, ideas, and results. But mainly, this meeting is about meeting your peers – other (PhD) students and postdocs working in the field of crystallography or working with crystallography, but joining groups in chemistry, physics, biology, geology, materials science, etc. Find out more about the different aspects of your field. Get to know new methods and maybe make interesting connections to your project and gain new insights. Learn more about working with or in crystallography in industry. In order to profit from our interactive meeting format, please make sure to pitch your topic for 5 minutes, be present at your poster to discuss your research in more detail, and visit other posters in the remaining time. We are proud to welcome our four invited speakers, who will present general topics of broad interest (page 16). We are grateful for the support from our sponsors and are happy to have their representatives share their experience with us (page 18).

We gratefully acknowledge Christian Lehmann (Mülheim, Germany) for his generous support with the financial planning and organisation. We thank Julia Dshemuchadse (Ann Arbour, US) for keeping the webpage up to date.

We wish you a very pleasant time! Please do not hesitate to ask us or a member of the local organizing team, in case you have any questions.

With best wishes,
Lilith Domnik and Yulia Ilina

Features

During our meeting, we are happy to welcome you at several social activities, which are sponsored and therefore free of additional charge: Our meeting will start with the welcome reception where you will have the possibility to meet other participants while having some beers and snacks. Snacks and drinks will be provided for the coffee breaks and of course during the poster sessions. We will go on an adventure through the “Berlin Underworlds” and take a look at the T.rex “Tristan” in the Natural History Museum. Finally we will end our meeting with our social dinner at the „White Trash“ restaurant. As announced previously, however, there are a few costs that unfortunately we cannot cover. This includes lunch at the university cafeterias or any other place of your choice, local transportation fees and the drinks at the social dinner. Yet, we hope that these costs will be limited and that our offer to support participants through travel grants will help keep your participation costs low.

Schedule

Keynote lectures:
60 min, incl. discussion

Lightning presentations:
5 min, no discussion

Industry presentations:
20 min, discussion at the end of the session

Poster presentations:
All posters (A0 format = 84.1x118.9 cm, portrait) will be displayed throughout the whole event. Please be present at your poster during the session corresponding to your lightning talks. Please take care to adhere to the times given in the schedule unless adjustments are announced during the event.

Wednesday		Thursday		Friday
Arrival and check-in	08:45	Introduction	08:45	
	09:00	Plenary talk *Holger Dobbek*	09:00	Plenary talk *Udo Heinemann*
	09:30		09:30	
	10:00	Lightning talks session 1	10:00	Poster session 2
	10:30		10:30	
	11:00		11:00	
	11:30	Lunch	11:30	Lunch
	12:00		12:00	
	12:30		12:30	
	13:00	Plenary talk *Francesca Fabbiani*	13:00	Guided tour at Natural History Museum
	13:30		13:30	
	14:00	Lightning talks session 2	14:00	
	14:30		14:30	
	15:00		15:00	Plenary talk *Christian Spahn*
	15:30	Poster session 1	15:30	
	16:00		16:00	
	16:30		16:30	
Welcome reception at Orbis Humboldt University Berlin	17:00	Industry talks session	17:00	Closing and lightning talks awards
	17:30		17:30	
	18:00		18:00	
	18:30		18:30	
	19:00	Guided tour at 'Berlin Underworlds'	19:00	Social Dinner at 'White Trash' restaurant Berlin food and live music
	19:30		19:30	
	20:00		20:00	
	20:30		20:30	
	21:00	Dinner at Clärchens Ballhaus	21:00	
	21:30		21:30	
	22:00		22:00	
	22:30		22:30	

Venues

Conference venue:

The meeting will take place on the old historical campus of Humboldt University Berlin (Campus Mitte). It is located within walking distance to the station Friedrichstraße (S5, S7, S75, S1, S2, S25, U6), S-Bahn Brandenburger Tor (S1,S2, S25) and the station Französische Straße (U6).
Central point of destination for Campus Mitte:
Unter den Linden 6
10117 Berlin

If you travel by train, please visit this website in order to find your best connection:
https://www.hu-berlin.de/en/service/contact/how-to-get-to/campus-mitte/train

In case you are going to use public transportation please visit the following website:
https://www.hu-berlin.de/en/service/contact/how-to-get-to/campus-mitte/public-transport

If you are planning to use a bike throughout your stay check this website:
https://www.hu-berlin.de/en/service/contact/how-to-get-to/campus-mitte/bike

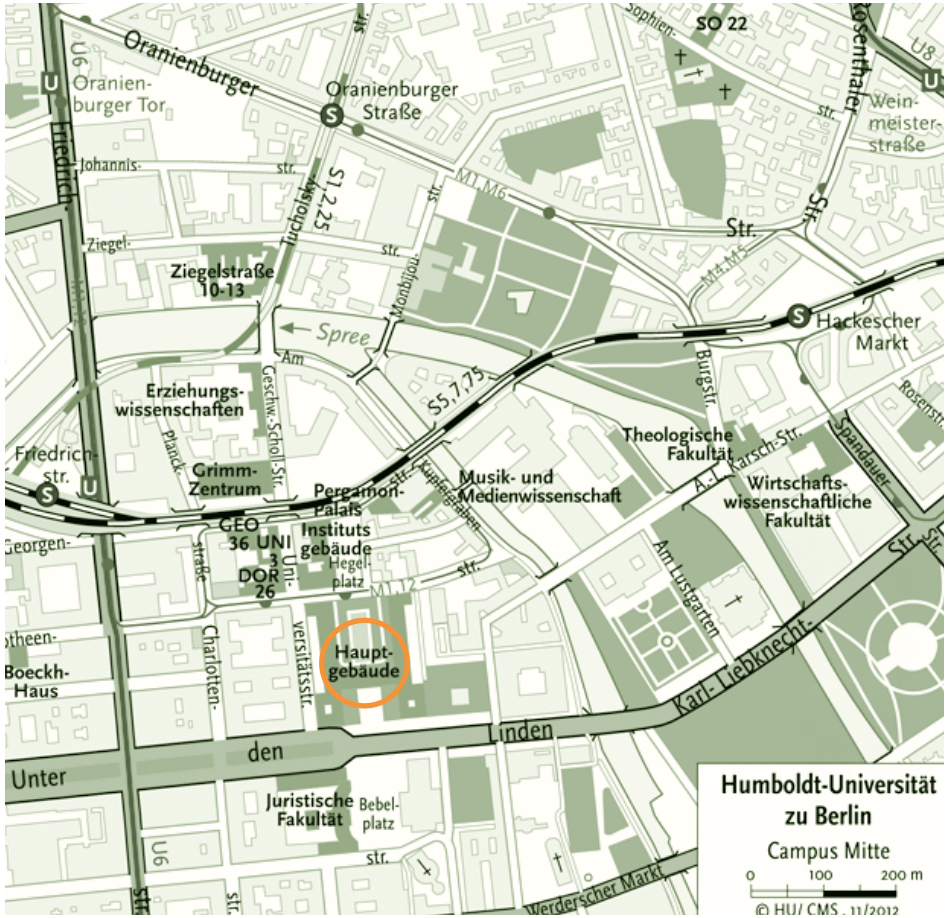
The venue of the scientific program will be in the main building of Humboldt University (Unter den Linden 6, 10099 Berlin). The talks will be held in seminar room 2093 while the posters will be on display in the „Löwenlounge“.

Please keep in mind that in order to use the public transport in Berlin you will have to buy a ticket. For most of your destinations Einzelfahrausweis Berlin AB (single one-way ticket, 2.70 EURO) is good enough. It is valid for 2 hours after stamping and is unidirectional. In case you are travelling from Berlin Schönerfeld you will have to buy a Einzelfahrausweis Berlin ABC (3.30 EURO). The most important rule to observe: you have to stamp your ticket prior to use otherwise you could (and probably would) pay the penalty of 80 EURO (the fact that you are foreigner or do not speak german will not help you). You can stamp you ticket on every S- or U-Bahn platfom. For more information you can visit this useful website:

http://blog.fit2014.org/2014/07/getting-around-in-berlin-heres-your-ticket/

Here you can find the S- and U-Bahn routemaps:

http://www.berliner-verkehr.de/_Netze/2016_r_s_u.jpg



https://www.hu-berlin.de/de/service/kontakt/lage-anfahrt/campus-mitte/standardseite#karte

Welcome reception:

The welcome reception will be held at the Orbis Humboldtianus (the student cafe and meeting point at the HU Campus Mitte) starting from 5 pm until 10 pm. We will use this time to register you for the conference, copy your lightning talk presentation (PDF format), give to you the goodie bag and get to know you in case we haven´t met before while having some beers and snacks. And here ist the address:

International Club „Orbis Humboldtianus“
University main building
Room 3120, 2nd floor (above the Audimax)
Unter den Linden 6
10117 Berlin

FYI: Our plan is to escort you to every social event we have planned for you. In this case you do not need to worry about the way (but the tickets). In case you prefer to go on your own here are the addresses of the meeting points:

Meeting point for guided tour „Berlin Underworlds“
Brunnenstr. 105, southern entrance-hall of the subway station Gesundbrunnen
(exit direction to Humboldthain Park, Brunnenstraße), next to our ticket sales-pavillon

Please be at the meeting point at 7 pm sharp!

The best way to get there is first to walk to S-Bahn Friedrichstraße and then take S1 (direction Frohnau or S Oranienburg), S2 (direction Bernau or Buch), S25 (direction S Oranienburg) to S-Bahn Gesundbrunnen.

Here you can find more information about the tour:
http://berliner-unterwelten.de/tour-3.15.1.html

Meeting point for guided tour at the Natural History Museum
The Natural History museum can be reached either by foot (20 to 25 minutes walking, see the map attached) or by the U-Bahn (U6, the terminal station Naturkundemuseum). The guided tour will start at 1 pm sharp, so please plan accordingly.

Meeting point for social dinner at „White Trash“ restaurant
The social dinner will take place in Berlin Treptow. The address of the meeting point:
am Flutgraben 2, 12435 Berlin
If you want to get there by public transport take the U6 Friedrichstraße (direction U Alt-Mariendorf) to the station U Hallesches Tor. Change to U1 line and take the train to the station U Schlesisches Tor (direction S+U Warschauer Str.). The restaurant is approximately 850 m walking distance from the station U Schlesisches Tor.

The dinner will start at 7 pm.

For more information about the restaurant please visit:
http://whitetrashfastfood.com

Keynote Lectures

Keynote Lecture 1

Small molecule activation by metalloenzymes - insights from X-ray crystallography

Holger Dobbek
Humboldt University Berlin
(tba.)

Keynote Lecture 2

High-pressure crystallography on molecular compounds: theory, practice and a personal journey

Francesca Fabbiani
University of Göttingen
(tba.)

Keynote Lecture 3

Structural Basis of Transcriptional and Translational Regulation of Gene Expression

Udo Heinemann
Max Delbrück Center for Molecular Medicine
(tba.)

Keynote Lecture 4

Large scale conformational changes of the ribosome and the mechanism of protein biosynthesis

Christian Spahn
Max Planck Institute for Molecular Genetics
(tba.)

Industry opportunities

STOE - Thomas Hartmann, Sales and Powder
(hartmann@stoe.com)
Shanghaied right away from the lab bench - part III.

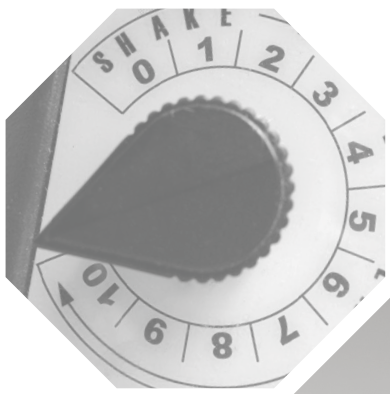
As all university graduates during their years of study, young crystallographers have made contact with supplying companies, public authorities, publishers etc. STOE & Cie GmbH as an example has recruited their scientific staff exclusively from the customers' sites. How will you be getting in?

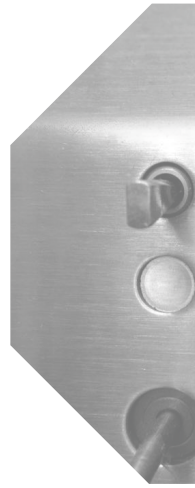
PANalytical - Kristin Gratz, Sales Engineer
(Kristin.Gratz@panalytical.com)
Work as an sales engineer. A job with unexpected challenges

After a short postdoc stay, Kristin started to work as a sales engineer. To date, she worked more than 8 years for PANalytical. She is a sales engineer and project manager, sometimes a teacher, a team leader, a writer, and from time to time also a tour guide...

Dectris – Sascha Grimm (sascha.grimm@dectris.com)
From Physics of Snow to HPC Detectors of DECTRIS - 10 Years of „Detecting the Future"

Sascha holds a master in nanosciences from Basel University and worked as an experimental physicist in Davos before he joined DECTRIS where he primarily works on software integration of detector systems.





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Bruker AXS – Christina Drahten, Application Specialist
(Christina.Drahten@bruker.com)
Young Crystallographers in Industry – what are Application Specialists?

Christina joined our team in Karlsruhe earlier this year as an application specialist for powder diffraction, after working on the high-resolution powder diffraction beamline at the ESRF.

Lightning presentations 1

1 Synthesis, X-ray diffraction, Raman spectroscopy and Investigation of electronic and optical properties of Ba2-xSrxWO5 ceramics

Mohammed ait Haddouch
University Hassan II, Laboratory of chemistry and physics of materials, Casablanca (Morocco)
mohammed.ait.haddouch@gmail.com

We report on the synthesis of Barium Strontium Tungstate Ba2-xSrxWO5 powders with (x = 0; 0.25, 1, 1.75 and 2). The obtained powders were analysed by X-ray diffraction (XRD), Raman spectroscopy and diffuse reflectance spectroscopy. Their electronic structure was investigated by Density functional theory (DFT) calculations.

2 Anelastic relaxation effects in langasite-type crystal species

Christian Hirschle
Ruhr University Bochum, Institute for geology, mineralogy and geophysics, Crystallography
Christian.Hirschle@rub.de

Langasite-type crystal species are among the most important materials for high-temperature piezoelectric applications.However, all langasite-type crystals experience strong ultrasound attenuation at elevated temperatures that is poorly understood and may be caused by anelastic relaxation processes.We investigate the internal friction and the change in the piezoelectric and elastic properties at high temperatures with resonant ultrasound spectroscopy to provide insight into the structural background of the sound attenuation.

3 Cryo-EM Structure of a Tetrameric Cyanobacterial Photosystem I

Dmitry Semchonok
University of Groningen & Electron microscopy
d.o.semchonok@gmail.com

We studied the structure of the thermophilic cyanobacterium Chroococcidiopsis sp. TS-821 by single-particle cryo-electron microscopy. Using in-house equipment (FEI Polara with Gatan GIF 2002), a reconstruction at a resolution of 1.15 nm was obtained, which is sufficient to see the approximate position of the subunits inside PSI by fitting in the known x-ray stricture of Thermosynechococcus elongatus (PSB entry: 1JB0). Higher resolution is necessary to understand from a structural point of view how some cyanobacteria form trimeric and others tetrameric PSI and what it means in terms of regulation and efficiency of energy conversion, for that further improvement to near-atomic resolution is expected to be feasible using a Titan Krios with Falcon-2 or K2 camera, using the frame-collection mode.

4 Can we find aluminium ion conductors? Theoretical Models for the analysis of crystalline solid electrolytes

Falk Meutzner

TU Bergakademie Freiberg, Institute of Experimental Physics
falk.meutzner@gmx.net

By combining different theoretical computational methodologies in a step-wise algorithm, we want to find new potential solid electrolytes for aluminium ions. They focus on geometric and chemical crystallography and have different energetic contributions. Large crystallographic databases are then screened for structures that have not yet been considered for ion conduction.

5 Experimental characterization of the chemical bonds of β-boron based on multipole refinements against high-resolution, single-crystal X-ray diffraction data and maximum maximum entropy calculations

Claudio Eisele
Uni Bayreuth - Laboratory of Crystallography, Prof. dr. Sander van Smaalen
claudio.eisele@uni-bayreuth.de

High-resolution, single-crystal X-ray diffraction data of ß-boron collected at 100 K at Beamline F1, HASYLAB/DESY are analyzed by using the Eval15 suite of programs. By means of multipole refinements and the Maximum Entropy Method of data analysis an electron density map is established which shows the detailed spatial distribution of the valence electron density.

6 Synthesis and characterizations of Nasicon type phosphate Li3CoZr(PO4)3- Evaluation for energetic materials

Asmaa Loutati
Laboratoire de Physico-chimie des matériaux appliquésLPCMA, Faculté des Sciences Ben M'Sik, Casablanca
Loutati.asmaa@gmail.com

Synthesis, structural, optical and magnetic studies of the Nasicon-type phosphate Li-

3CoZr(PO4)3, which represent a promising candidate as an cathode material for the Lithium-ion batteries thanks to their good energetic performance and structural stability.
The electrochemical properties of Li3CoZr(PO4)3 were tested in Lithium cells.

7 Electron microscopic studies of the acetyl coA decarbonylase synthase (ACDS) complex from Archaea

Julia Ilina
Humboldt University Berlin, Structural Biology/Biochemistry
julia.ilina@gmail.com

Despite nearly four decades of extensive spectroscopic and biochemical
studies of the ACDS complex from different organisms, no structure of
the entire complex has been reported so far. Also numerous crystallographic attempts taken in our lab have not shown any positive results yet, suggesting the heterogeneity of the protein of interest. Here we present the preliminary results of the electron microscopic studies of the ACDS complex from the thermophilic archaea.

8 In Situ Powder Diffraction of Complex Oxides for Energy Storage

Kent Griffith
University of Cambridge, Department of Chemistry, Grey Group
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Most high-rate, high-power Li-ion battery materials are nanostructured to minimise diffusion distances. Novel electrode materials with complex structures, beyond the typical layered/spinel/olivine-types, may enable high-rate performance without cost, safety, stability, and scalability issues of nanomaterials. In situ diffraction of structures such as Nb2O5, during electrochemical cycling, provides insight into the (de)lithiation mechanism.

9 Solid State Reactions studied by X-ray Powder Diffraction

Luzia S. Germann
Max Planck Institute for Solid State Research / X-ray Research Facility
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We aim to study different solid state reactions as well as effect on external stimuli by in situ X-ray powder diffraction. This contribution will focus on metal organic frameworks as novel hybrid material class.

10 Extending the coordination chemistry of Tris(2-hydroxyiminopropyl)amine: A heptanuclear Fe-complex

Dejan Premužić
AK Hołyńska, Fachbereich Chemie, Philipps-Universität Marburg
dejan.premuzic@googlemail.com

Tris(2-hydroxyiminopropyl)amine is known for his coordination chemistry and possesses the ability to bridge metal centers via oxime group. So far several mononuclear complexes with mainly Ni are known, highest nuclearity was achieved by a heterometallic pentanuclear Co/Ln-complex. Herein we present the heptanuclear Fe-complex with azide as auxiliary ligand.

11 Going paramagnetic: 17O NMR spectroscopy of functional paramagnetic oxides for energy storage, conversion and catalysis

David Halat
Department of Chemistry, University of Cambridge
dh471@cam.ac.uk

Many materials used in battery and fuel cell applications and for chemical looping contain paramagnetic transition metal ions, which limits the utility of NMR spectroscopy as a characterisation tool. We demonstrate new experimental and computational techniques for acquiring and interpreting 17O NMR spectra that provide sensitive insights into the local structure and dynamics of these technologically important phases.

12 Room Temperature Structure of Photosystem II and Substrate Binding Studied by fs X-ray Crystallography

Mohamed Ibrahim
Humboldt University Berlin, Biophysics of Photosynthesis
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The crystal structures of Photosystem II at room temperature were obtained for the illuminated S3-state at 2.8 Å and the dark-adapted S1-state at 3.0 Å resolution. Distinct differences in the overall structure compared to the reported cryogenic temperature structures are observed. There are no major structural changes observed between the dark and illuminated state, which excludes mechanisms that require such large changes in the S3 state.

13 Syntheses, characterization and decomposition of coordination complexes featuring pyrazolyl-substituted acetylacetone and mercury(II) part I

Qianqian Guo
RWTH Aachen, Institute of Inorganic Chemistry
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The pyrazolyl-substituted acetylacetone, H2acacPz, offers O and N donor sites of different Pearson hardnesses. Depending on the stoichiometry between ligand and mercury(II) cations, coordination complexes with various dimensionalities could be derived. Decomposing those mercury compounds with acid leads to the reduction reaction of the ligand forming a layered structure.

14 Syntheses, characterization and decomposition of coordination complexes featuring pyrazolyl-substituted acetylacetone and mercury(II) part II

Khai-Nghi Truong
RWTH Aachen, Institute of Inorganic Chemistry
khai.truong@ac.rwth-aachen.de

The pyrazolyl-substituted acetylacetone, H2acacPz, offers O and N donor sites of different Pearson hardnesses. Depending on the stoichiometry between ligand and mercury(II) cations, coordination complexes with various dimensionalities could be derived. Decomposing those mercury compounds with acid leads to the reduction reaction of the ligand forming a layered structure.

Lightning presentations 2

1 Making the Most of Neutron-Diffraction Data: Lithium Diffusion in Ramsdellite-Like Li2Ti3O7

Dennis Wiedemann
Technische Universität Berlin, Institut für Chemie
dennis.wiedemann@chem.tu-berlin.de

Neutron diffraction at ion conductors allows for in-depth analysis of pathways and associated barriers - if data quality permits it. However, there is a rich method spectrum to extract information also from lower-quality data, comprising, e.g., maximum-entropy reconstruction and topological analyses. A study of ramsdellite-like Li2Ti3O7 shows some of these methods in action.

2 Synthesis, characterisation and thermal properties of adducts of betaine and inorganic copper salts

Marie Münchhalfen
Ruhr University Bochum, Institute for geology, mineralogy and geophysics, crystallography
marie.muenchhalfen@rub.de

Many different structures of trimethylammonioacetate (‘betaine’) with inorganic compounds in different stoichiometric ratios are known, due to its zwitterionic properties. In this work different crystals containing betaine and different copper salts were synthesized. The crystals were investigated regarding their coordination behavior, anion disorder and basic thermal properties.

3 Ena/VASP as possible antimetastatic target addressed by structure-optimized ProM-scaffolds

Matthias Barone
FMP Berlin, AG Kühne, Drug Design
barone@fmp-berlin.de

Ena/VASP is a crucial actin cytoskeleton regulator at the very end of pro-metastatic kinase signalling pathways. We designed modularly built scaffolds (ProMs) that inhibit the challenging proline-rich protein-protein interaction of Ena/VASP and reported an inhibitor that reduces invasion of breast cancer cells by two-thirds. Structure-guided optimization boosted the affinity of the inhibitor against a flat protein surface drastically, while structural simplicity, molecular weight and pharmacological properties were conserved.

4 High throughput DFT screening and experimental characterization of CO2 looping materials

Michael Gaultois
University of Cambridge, Department of Chemistry (Clare Grey)
listerite@gmail.com

Coal fuels more than 40% of global electricity production, and is responsible for over 40% of global CO2 emissions. While we continue to develop alternative and renewable power sources, the capture and sequestration of CO2 from flue gas in fossil fuel power plants and other industrial processes is one viable solution to decrease our CO2 emissions. We have used high-throughput DFT to generate a subset of candidate CO2 capture materials and have prepared and characterized their performance.

5 Improvement of model quality by rejection of non-isomorphous frames using CC1/2

Greta Assmann
Universtät Konstanz, Department of Biology, Bioinformatics and Biophysics; Group of Prof. Dr. Kay Diederichs
greta.assmann@uni-konstanz.de

Evaluation of crystallographic SBGD reference data sets (Meyer P. et al, 2016) demonstrates that applying the method (Assmann G. et al. 2016) to single frames of a data set easily detects non-isomorphous frames, which can occur because of radiation damage e. g. Rejection of these single frames improved data statistics and comparison with the previously published model showed an improved correlation of observed and calculated intensities. Therfore correctly predicts non-isomorphism and the agreement of data and model.

6 Crystallographic characterization and determination of physical properties of Sanidine from Madagascar

Michael Haiduk
Crystallography, Ruhr Universität Bochum
m.haiduk@gmx.de

Lattice parameters have been determined by X-Ray powder and Single Crystal Diffraction, Density by buoyancy, X-Ray and geometric method, the chemical compostion by X-Ray fluorescence analysis and the thermal stabilty and heat capacity by Difference thermal analysis and Differential scanning calorimetry. Elastic constants have been determined by resonant ultrasound spectroscopy and the thermal expansion coefficients by dilatometer. Correlations between the physical properties and the structure of the Sanidine are discussed.

7 CODH Isozymes same structure – different activities

Lilith Domnik
Humboldt University Berlin, Structural Biology/Biochemistry
lilith.domnik@hu-berlin.de

Carbon monoxide dehydrogenases(CODHs) catalyze the reversible reduction of CO_2 to CO using two electrons and two protons. So far five different CODHs have been identified in Carboxydothermus hydrogenoformans. We investigated and compared CODH-II and CODH-IV. They are structurally similar, but show different activities.

8 Toward a High Temperature V6O13 Based Lithium-Ion Battery

Wei Meng, University of Cambridge
mengwei.v@gmail.com

V6O13 is a promising Li-ion battery cathode material for application in the high temperature oil field environment. The material exhibits a high capacity, and the voltage profile contains several plateaus due to complex and still unresolved transformations. The mechanisms behind the transformations that take place during these voltage plateaus are central to understanding and improving battery performance. In this study we present in situ X-ray diffraction data that highlight an asymmetric six-step discharge and five-step charge process. The LixV6O13 unit cell expands sequentially in c, b, and a directions during discharge and reversely shrinks back during charge. This result sheds light on the high specific capacity of V6O13 and lays the foundation for this material to be used as a cathode for secondary lithium batteries both at ambient and

9 High-speed fixed-target serial femtosecond crystallography

Philip Roedig
DESY
philip.roedig@desy.de

In macromolecular crystallography at X-ray free electrons lasers, common Serial Femtosecond X-ray Crystallography (SFX) experiments using liquid jets for sample delivery suffer from high sample consumption and very low hitrates typically below 10 %. By fast rasterscanning of our self-developed sample holder for macromolecular crystals, we can perform time-efficient SFX experiments with highly improved hit rates of more than 90 %. The method is demonstrated with experimental data from virus and protein crystals measured at LCLS, highlighting the ultra-low sample consumption of the presented method.

10 Structure review of the R2TSi3 family

Melanie Nentwich
Experimentelle Physik, Technische Universität Freiberg
Melanie.Nentwich@physik.tu-freiberg.de

The present work gives a review of the R2TSi3 compounds, with R is an alkaline eath metal, lanthanoide or actinoide and T is atransition metal or Si. Many different structure types arise within these compounds exhibiting different Si/T orderings. We correlate structure types to different atomic parameters concerning electronic structure and atomic size.

11 Calculation of pNMR shifts for paramagnetic periodic solids and surfaces using CP2K, with applications to Li-ion battery materials

Arobendo Mondal
Technical University Berlin
arobendo@gmail.com

- Development and application of modern pNMR theory for priodic solids
- Using supercell models for simulating the bulk properties more accurately
- Using the CP2K code for practical applications, explaining and supporting the experimental results

12 Experimental charge density for hydrogen bond in Hexaaquanickel(II)-3-carboxy-4-hydroxybenzenesulfonate monohydrate.

Ai Wang
RWTH Aachen Inorganic Institute
ai.wang@ac.rwth-aachen.de

There is a few high quality data of hexa-aqua-transition metal complexes in CSD data base. The charge density study of Hexaaquanickel(II)-3-carboxy-4-hydroxybenzenesulfonate monohydrate provides a new prospect to understanding different kinds of Hydrogen bond and how the central metal influence the hydrogen atoms orientation of water molecules.

13 New preparative route for ferromagnetic dinuclear triple carboxylato-bridged Cu(II) complexes and their Applications

Olufunso O. Abosede
Federal University Otuoke, Department of Chemistry. Bioinorganic Research Group
abosedeoo@fuotuoke.edu.ng

A new efficient route for the synthesis of ferromagnetic dinuclear triply-bridged copper (II) complexes of polypyridyl ligands containing carboxylato bridges has been serendipitously discovered. Details of the synthesis, characterization and applications of these complexes will be presented and discussed.

14 Crystallographic characterization and determination of physical properties of Sandine from Madagascar

Linda Hollenbeck
Crystallography, Ruhr Universität Bochum
linda.hollenbeck@rub.de

Lattice parameters have been determined by X-Ray powder and Single Crystal Diffraction, Density by buoyancy, X-Ray and geometric method, the chemical compostion by X-Ray fluorescence analysis and the thermal stability and heat capacity by Difference thermal analysis and Differential scanning calorimetry. Elastic constants have been determined by resonant ultrasound spectroscopy and the thermal expansion coefficients by dilatometer. Correlations between the physical properties and the structure of the Sanidine are discussed.

15 In situ NMR on Li- and Na-ion battery materials

Oliver Pecher
Department of Chemistry, University of Cambridge
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We are developing and exploring the use of a new Automatic Tuning Matching Cycler (ATMC) in situ NMR probe system to track the formation of intermediate phases and investigate electrolyte decomposition during battery cycling.

Organizers

Lilith Domnik
Humboldt University Berlin, Institute for Biology, Structural Biology/Biochemistry

Julia Ilina
Humboldt University Berlin, Institute for Biology, Structural Biology/Biochemistry

Oliver Pecher
Department of Chemistry, University of Cambridge (UK)

Ulli Englert
RWTH Aachen University, Institute for Inorganic Chemistry

Local Berlin Team

Mohamed Ibrahim
Humboldt University Berlin, Institute for Biology, Biophysics of Photosynthesis

Rana Ali
Humboldt University Berlin, Institute for Biology, Biophysics of Photosynthesis

Co-chairs of the DGK's "Young Crystallographers"

Carola Müller
Lund University, Department of Physical Chemistry, Sweden

Melanie Nentwich
TU Bergakademie Freiberg , Institute for Experimental Physics

List of Participants

Mohammed ait Haddouch	Casablanca (Morocco)	S&P I
Dennis Wiedemann	Berlin (Germany)	S&P I
Asmaa Loutati	Casablanca (Morocco)	S&P I
Michael Haiduk	Bochum (Germany)	S&P I
Linda Hollenbeck	Bochum (Germany)	S&P I
Ai Wang	Aachen (Germany)	S&P I
Christian Hirschle	Bochum (Germany)	S&P II
Marie Münchhalfen	Bochum (Germany)	S&P II
Qianqian Guo	Aachen (Germany)	S&P II
Khai-Nghi Truong	Aachen (Germany)	S&P II
Dejan Premužić	Marburg (Germany)	S&P II
Melanie Nentwich	Freiberg (Germany)	S&P II
Dmitry Semchonok	Groningen (Netherlands)	BS
Matthias Barone	FMP Berlin (Germany)	BS
Julia Ilina	Berlin (Germany)	BS
Lilith Domnik	Berlin (Germany)	BS
Mohamed Ibrahim	Berlin (Germany)	BS
Falk Meutzner	Freiburg (Germany)	ESM
Michael Gaultois	Cambridge (United Kingdom)	ESM
Kent Griffith	Cambridge (United Kingdom)	ESM
Wei Meng	Cambridge (United Kingdom)	ESM
David Halat	Cambridge (United Kingdom)	ESM
Oliver Pecher	Cambridge (United Kingdom)	ESM
Arobendo Mondal	Berlin (Germany)	ESM
Claudio Eisele	Bayreuth (Germany)	M&P
Greta Assmann	Konstanz (Germany)	M&P
Luzia S. Germann	Stuttgart (Germany)	M&P
Philip Roedig	Hamburg DESY (Germany)	M&P
Olufunso O. Abosede	Otuoke (Nigeria)	M&P

Structures and Properties	S&P I
Structures and Properties	S&P II
Methods and Processes	M&P
Biological structures	BS
Energy Storage Materials	ESM

Wednesday		Thursday		Friday
	08:45	Introduction	08:45	
	09:00	Plenary talk *Holger Dobbek*	09:00	Plenary talk *Udo Heinemann*
	09:30		09:30	
	10:00	Lightning talks session 1	10:00	Poster session 2
	10:30		10:30	
	11:00		11:00	
	11:30	Lunch	11:30	Lunch
	12:00		12:00	
	12:30		12:30	
	13:00	Plenary talk *Francesca Fabbiani*	13:00	Guided tour at Natural History Museum
	13:30		13:30	
	14:00	Lightning talks session 2	14:00	
	14:30		14:30	
	15:00		15:00	Plenary talk *Christian Spahn*
	15:30	Poster session 1	15:30	
	16:00		16:00	
	16:30		16:30	
	17:00	Industry talks session	17:00	Closing and lightning talks awards
	17:30		17:30	
	18:00		18:00	
	18:30		18:30	
	19:00	Guided tour at 'Berlin Underworlds'	19:00	Social Dinner at 'White Trash' restaurant Berlin food and live music
	19:30		19:30	
	20:00		20:00	
	20:30		20:30	
	21:00	Dinner at Clärchens Ballhaus	21:00	
	21:30		21:30	
	22:00		22:00	
	22:30		22:30	
Arrival and check-in				
Welcome reception at Orbis Humboldt University Berlin				