Young Crystallographers'

10th Anniversary Meeting

at **DESY**

04. – 06. October 2023

Contents

Acknowledgement to supporters

We gratefully acknowledge the support provided by STOE&Cie., Anton Paar, Rigaku, OlexSys, X-Spectrum, Dectris, DESY, and the German Crystallographic Society (DGK) for their generous financial support.

General Information

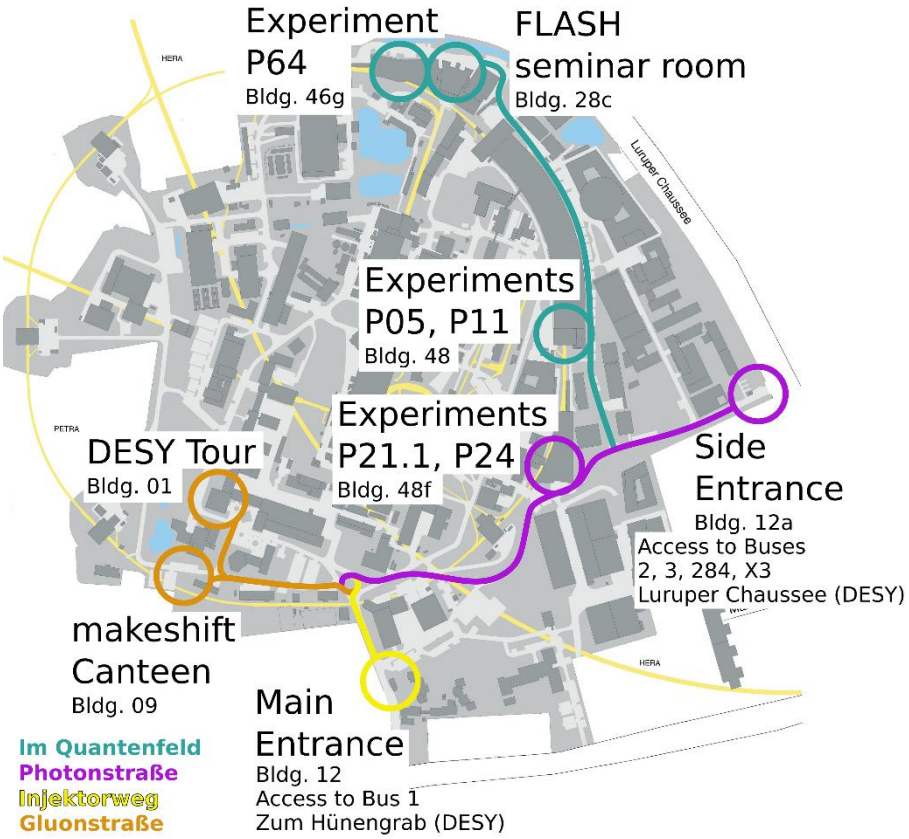
Dates
Wednesday, October 4th 2023 – Friday, October 6th 2023

Expenses
The registration fee of 60 EUR per person covers the costs for one lunch, coffee breaks, BBQ, and lab tour.

Social Evenings
On Monday we will go to the ÜberQuell (St. Pauli Fischmarkt 28-32 20359 Hamburg) – we will go there together after the DESY-tour.

Venue
DESY research campus, seminar room FLASH, building 28c (see map!), 2nd floor, Notkestraße 85, 22607 Hamburg

Map of DESY


Experiment
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makeshift
Canteen
Bldg. 09
Main
Entrance
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Im Quantenfeld
Photonstraße
Injektorweg
Gluonstraße
HERA
PETRA
HERA

Welcome Note

Dear Young Crystallographers,

We are pleased to welcome you to our 10th anniversary meeting at DESY, Hamburg, and we are very proud to celebrate this event together with you at one of the most renowned research facilities in Europe!

This meeting is based on four pillars: networking, knowledge transfer, lightning talks, and social activities. During the conference, you will get in touch with Industry, Academics, and young peers in an open-minded and relaxed atmosphere. You will enjoy exciting crystallographic talks and the unique opportunity to see how life & research works inside one of the largest particle / high-energy physics and photon science research facilities.

Furthermore, you will have the chance to present your latest research, ideas, and results throughout your lightning presentations (short talk and long poster session) as well as in discussion with your fellow Young Crystallographers. The meeting will offer you the chance to ask questions and connect with the experts during the sessions, in the breaks and especially during our Conference Dinner.

Mainly, this meeting is about meeting your peers – students, PhD's, Postdocs and other young scientific employees, working with crystalline materials, from groups all over chemistry, physics, materials science, biology, geology, 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.

In order to profit from our exchange-based 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 happy to welcome Tobias Beck (Universität Hamburg, Germany) and Donatella Loru (DESY, Germany) to give the lectures about different aspects of Hamburg-based crystallography. Furthermore, beamline scientists of five different beamlines show their field of study in live experiments!

We are looking forward to the industry talks of Julian Schmehr (X-Spectrum, Hamburg, Germany) Marius Kremer (Anton Paar, Graz, Österreich), Felix Hennersdorf (Rigaku Oxford Diffraction, Neu-Isenburg, Germany), and Laura Christina Folkers (STOE and Cie GmbH, Darmstadt, Germany).

We are also hoping to see you again in March 2024 for the Annual DGK Meeting in Bayreuth (Germany, https://dgk-conference.de/) where we will organize a dedicated Lightning Session as well as our annually assembly.

So please stay tuned, we will keep you posted: https://dgk-home.de/aks/jkyc/
Please also consider subscribing our newsletter, which will inform you about news, events and opportunities.
We wish you a very pleasant time! Please do not hesitate to ask us if you have any questions.
Best wishes,

Florian & Jakob (Chairs of the Young Crystallographers)

Organizers

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Schedule

The program features two academic talks, four industrial talks, two lightning talk sessions followed by the poster sessions, lab tours as well as experiments and Barbeque.

Academic talks
60 min, incl. discussion

Industrial talks
30 min, incl. discussion

Lightning talks
5 min, no discussion

Please prepare a few slides in PPT(X) or PDF format for your talk. We will provide all the required technique (PC, beamer …). Please, copy your slides on the local computer **before** your lightning talk session.

The focus of your presentation lies on the poster. Lightning talks should only give a short introduction (appetizer) to your recent research.

Poster presentation
All posters (A0 format = 84.1 x 118.9 cm^2, portrait) will be displayed through the whole day. 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.

Program

Wednesday, 4th October 2023

15:30 – 16:00	**Welcome notes**
16:00 – 18:30	**DESY Campus Tour**
19:30 – open	**Dinner**

Thursday, 5th October 2023

09:00 – 12:00	**Experiments at DESY beamlines** (PETRA III)
12:00 – 12:45	**Lunch break**
12:45 – 13:00	**Group Picture**
13:00 – 14:00	**Lightning talks I**
14:00 – 14:30	**Industry talk I** (X-Spectrum)
14:30 – 15:00	**Industry talk II** (STOE&Cie)
15:00 – 16:30	**Poster session I** (with coffee)
16:30 – 17:30	**Academic talk I** (Donatella Loru)
17:30 – 18:00	**Industry talk III** (Rigaku)
18:00 – open	**Conference BBQ**

Friday, 6th October 2022

09:00 – 9:30	**Industry talk IV** (Anton Paar)
9:30 – 10:30	**Lightning talks II**
10:30 – 11:30	**Academic talk II** (Tobias Beck)
11:30 – 13:00	**Poster session II** (with coffee)
13:00 – 13:30	**Closing & Poster Prizes**
13:30 – 15:00	**Break & Transfer**
15:00 – 17:00	**Tour XFEL**

Academic talks

Academic talk I – Structure determination using spectroscopic methods

Dr. Donatello Loru
Center for Free-Electron Laser Science (CFEL)
Gruppe Struktur und Dynamik kalter und kontrollierter Moleküle
Max-Planck-Institut für Struktur und Dynamik der Materie
Hamburg (Germany)

Dr. Donatella Loru works in the group of Melanie Schnell at DESY. The group develops novel spectroscopic methods for structure determination and the understanding of molecular processes. This complements our otherwise very diffraction-focused program.

"Diving into broadband rotational spectroscopy as a gas phase technique for structural investigations"

Broadband rotational spectroscopy stands out as one of the most insightful methods to elucidate gas- phase molecular structures. This technique, which can be applied to study any molecule in the gas phase that has a permanent electric dipole moment, allows for the measurement of the intrinsic properties of the molecules without the influence of solvents, crystals, or matrices, which often alter the conformational preferences. Its exceptional sensitivity to even the subtlest structural alterations in the molecular shape not only makes it particularly well-suited for probing molecules, which can often exhibit complex conformational landscapes, but also allows for discrimination between isotopologues. From the changes in the moments of inertia upon isotopic substitution, the exact position of atoms can be determined using Kraitchman's equations or through a least-squares fit of the internal coordinates. Furthermore, the combination of microwave spectroscopy with supersonic jets enables the study of weakly bound complexes, i.e., complexes stabilized by van der Waals interactions or weak hydrogen bond interactions. The direct comparison with theoretical models offers information about the intra- and intermolecular interactions stabilizing these complexes and can provide insight into processes such as molecular recognition. During this talk, I will present an introductory overview of rotational spectroscopy and I will provide examples to highlight the capabilities of this spectroscopic technique with respect to structural investigations.

Academic talk 2 – Crystalline bio-hybrid materials

Prof. Dr. Tobias Beck (tobias.beck@uni-hamburg.de)
Fachbereich Chemie
Institut für Physikalische Chemie
Universität Hamburg
Hamburg (Germany)

Prof. Dr. Tobias Beck is a research group leader at the University of Hamburg. In the past, he has worked on the crystallography of small molecules and the development of methods for protein crystallography. Now his research is focused on crystalline biohybrid materials based on proteins and nanoparticles.

"Particles, Proteins, Lattices: Construction of Biohybrid Nanomaterials"

Self-assembly is a key tool for construction of functional nanomaterials. We have recently established a novel method for the self-organization of nanoparticles and biomolecular building blocks. Here, protein cages are engineered with opposite surface charge and used as an atomically precise ligand shell for the assembly of inorganic nanoparticles. This approach yields highly ordered nanoparticle superlattices with unprecedented precision. The structure of the matrix can be tuned with external stimuli such as metal ion concentration. In the talk, diffraction methods will be discussed to elucidate the structure of the assemblies. Moreover, the functional properties of the synthesized material will be presented.

Industry talks

Industry talk 1 – "**I**ntroduction to X-ray Detector Technologies"

Julian Schmehr (julian.schmehr@x-spectrum.de)
X-Spectrum GmbH, Hamburg, Germany

A crucial component of any X-ray diffraction experiment is a detector that measures the x-ray photons. In this talk I will give a basic introduction to commonly employed X-ray detector technologies. Focus will be put on hybrid pixel photon counting detectors which have revolutionized synchrotron science. Such devices combine application-specific integrated circuits (ASICs) optimized for measuring x-ray photons with separate semiconductor sensors that directly convert the x-ray photons to an electrical charge. This allows for high detective efficiency over a wide range of X-ray energies, high spatial resolution, and extremely high frame rates. These capabilities have enabled new discoveries in a wide range of applications at synchrotron and XFEL lightsources as well as using laboratory-based x-ray sources, including drug discovery, battery materials research as well as high resolution ptychography imaging.

Industry talk 2 – "What's new at STOE"

Laura Christina Folkers (folkers@stoe.com)
STOE&Cie GmbH, Darmstadt

At STOE we build instruments since 1887, originally for the exterior analysis of crystals and since the 1960ties we are at the pulse of diffraction instruments with our STOE powder X-ray transmission geometry and the first pixel detector system with an open Eulerian cradle for single crystal XRD. Our complete company is located under one roof in Darmstadt, Germany, where research and development, software programming, electrical and mechanical engineering and production takes place. This way we can quickly test new ideas and offer both standard and customized solutions to our customers. Whenever it comes to quality, we accept no compromises. STOE's latest instruments offer you precise profile and Rietveld analyses, as well as ultrafast single crystal diffraction experiments on even the tiniest crystals. With our accessories you can conduct in-operando battery, in-situ heating, pressure, PDF and many more experiments.

Industry talk 3 – "Rigaku Advances in X-ray and Electron Crystallography"

Felix Hennersdorf (felix.hennersdorf@rigaku.com)
Rigaku Oxford Diffraction, Neu-Isenburg (Germany)

The latest range of Rigaku Oxford Diffraction instrument configurations will be summarised, and illustrated with a number of particular example applications. The XtaLAB Synergy-ED is a new and fully integrated electron diffractometer, creating a seamless workflow from data collection to structure determination of three-dimensional molecular structures. The XtaLAB Synergy-ED is the result of an innovative collaboration to synergistically combine our core technologies: Rigaku's high-speed, high-sensitivity photon-counting detector (HyPix-ED) and state-of-the-art instrument control and single crystal analysis software platform (CrysAlisPro for ED), and JEOL's long-term expertise and market leadership in designing and producing transmission electron microscopes. Furthermore, our X-ray diffraction instruments will be presented. The XtaLAB Synergy platform with microfocus or rotating anode sources on one side and a series of Hybrid Photon Counting (HPC) X-ray area detectors on the other side of the four-circle goniometer allows for versatile configurations perfectly adapted to the researcher's needs. These systems can be further equipped with the sample changing robot (XtaLAB Synergy Flow), an Intelligent Gonoimeter Head (IGH) for automated crystal centering, the plate scanning device XtalCheck-S or a high pressure unit.

Industry talk 4 – What is hot and what is not? Tips and tricks for in-situ XRD at non-ambient temperatures

Marius Kremer (marius.kremer@anton-paar.com)
Anton Paar GmbH, Graz (Österreich)

Non-ambient X-ray diffraction (NA-XRD) is an essential characterization method for structural investigation of materials. The most popular parameter for NA-XRD is temperature, with a wide range of hardware solutions available to cover a wide range of temperatures, combined with other parameters such as pressure, gas atmosphere or humidity. While these state-of-the-art solutions are usually designed to be user friendly, efficient and precise, there are certain limitations when it comes to temperature accuracy, heating and cooling rates and temperature stability, just to name a few. This presentation will help to understand and overcome these limitations, while offering tips and tricks on how to get the most out of your high- and low temperature XRD measurements. In addition, some

hints on the integration of non-ambient hardware in a diffractometer, and how a good diffractometer can make your non-ambient experiments easier and more efficient, are presented.

Lightning Presentations

1. Probing octahedral tilts in ferroelectric oxide superlattices with three-dimensional diffuse X-ray scattering

Joohee Bang (joohee.bang@mat.ethz.ch)
ETH Zurich

We perform qualitative and quantitative analysis of octahedral tilts in ferroelectric oxide superlattices via a comprehensive reciprocal space investigation. We collected a complete three-dimensional diffuse X-ray scattering data analyzed with three-dimensional delta pair distribution function (3D-ΔPDF) method [4], which allowed us to acquire direct information about the local atomic pair distribution in the superlattice structures. This work will not only contribute to gaining useful insights on structural local order arising in correlation with the ferroelectric properties, but also lay ground-work for developing a non-disruptive solid-state characterization technique for analyzing local structures of complex oxide heterostructures with atomic-scale resolution.

2. Crystal Engineering, Hirshfeld Surface Analysis and Electrostatic Properties of Co-crystal of Antipyrine with Aromatoc Acid

Nadia Bashir (nadia.bashir557@gmail.com)
The Islamia University of Bahawalpur, Pakistan

Experimental charge density distribution of co-crystal of antioyrine with salicylic acid was analyzed based upon multipole modelling of X-ray diffraction data collected at room temperature. The structure dislpays very strong classical hydrogen bonds as well as other non-covalent interactions. This co-crystal enhance analgesic properties and solubility of API of drug.

3. Mechanistic diversity of an evolved protein form Pseudomonas aeruginosa for a brode substrate class of alpha Keto acid elucidated by Crystallography analysis

Gourab Basu Choudhury (bc89gourab@gmail.com)
CSIR-Indian Institute of Chemical Biology

Pseudomonas aeruginosa genome has 2 annotated Ketopantoate reductase of which one, named as PanE2, is inactive towards its actual substrate Ketopantoate. Crystal structure of the native and several ligand bound complexes provide the

evidence of its active site evolution towards different α-keto acid molecules. Also, it helps finding the most potent molecule against which the protein showed maximum activity.

4. First-principles calculations for defects: Color centers in NaCl

Yaoshi Cheng (yaoshi.cheng@campus.lmu.de)
Department für Geo- und Umweltwissenschaften LMU

Color center is a kind of point defects which could be induced by radiation. For researching the effects of anion vacancy in NaCl, I focus on the properties of F-centre states using Density Functional Theory, like atomic positions, DOS, and vibration modes, etc.

5. Ferroelectric Domain Switching in $K_xNa_{1-x}NbO_3$ Thin Films

Marilia de Oliveira Guimaraes (marilia.guimaraes@ikz-berlin.de)
Leibniz-Institut für Kristallzüchtung

$K_xNa_{1-x}NbO_3$ epitaxially grown ferroelectric thin films on rare-scandate substrates have different domain configuration depending on the imposed strain. This ongoing work aims to determine and improve the ferroelectric properties, such as remnant polarization and switching voltage, of $K_xNa_{1-x}NbO_3/DyScO_3$ films with a Mc monoclinic ferroelectric phase. For this purpose, standard macroscopic electrical measurements are performed, as well as electrical measurements in the microscopic level by means of conductive atomic force microscopy (c-AFM) and piezo-response force microscopy (PFM).

6. Structural and Magnetic Properties of Uranium-Hafnium Alloys and Their Hydrides

Shanmukh Veera Venkata Devanaboina (dsvvudaykumar@gmail.com)
Department of Condensed Matter Physics, Charles University

Hydrogenation of γ-Uranium (γ-U) phase alloyed by Zirconium (Zr) forms a single stable phase of α-UH3 hydride with 20% of Zr. To investigate whether Hafnium (Hf) supports the stabilization of bcc α-UH_3 phase similar to Zr, we synthesized $U_{1-x}Hf_x$ alloys with x = 0.10, 0.15, 0.30, 0.40 by arc melting and hydrogenated them by exposure to high pressure of H_2 gas. XRD analysis revealed that β-UH_3 is the dominant phase for 10 at% of Hf, but it is gradually reduced with increasing Hf concentration up to 40 at%, where α-UH_3 exists as a majority phase.

7. Synthesis and Characterization of Sulfido Silicates

Irina Savova Dimitrova (idimitrova@zedat.fu-berlin.de)
Freie Universität Berlin

Inspired by the family of lithium superionic conductors and the sodium ion conductors based on the *A*-Si-S (*A* = Li, Na) systems, we extend the search for solid state electrolytes for all-solid-state batteries to further members of the *A*-Si-S (*A* = Li, Na, K, Rb, Cs) compound class. As only five ternary alkali metal sulfido silicates have been reported so far, the initial focus lies on the synthesis and characterization of new compounds of this class. Herein we present the synthesis and characterization of four new ternary alkali metal sulfido silicates.

8. Structural and optical properties of $Sr_{3-x}Pb_xFe_2TeO_9$ (x = 1.50, 1.88 and 2.17)

Abdelhadi El Hachmi (abdelhadi.elhachimi@uit.ac.ma)
Hassan 1st University & Ibn Tofail University

$Sr_{3-x}Pb_xFe_2TeO_9$ (x = 1.50, 1.88 and 2.17) were synthesized in polycrystalline form via the solid–state reaction route in air, and were studied at room temperature using XRD and UV–Vis spectroscopy techniques [1,2]. The crystal structures were resolved by the Rietveld refinement method; x = 1.50 and 1.88 adopt a tetragonal phase (s.g. I4/mmm) while x = 2.17 adopts a hexagonal phase (s.g. R–3m). The direct bandgap energy (Eg) of ~ 1.89 eV for x = 1.50, ~ 1.87 eV for x = 1.88 and ~ 1.74 eV for x = 2.17 was estimated from the Tauc plots of (αhυ)2 vs. photon energy. The Urbach energy (EU) was determined from the plots of logarithmic absorption coefficient versus hυ. Plots of the incident photon energy dependence of optical parameters such as refractive index, extinction coefficient, real and imaginary parts of the dielectric function, dielectric loss, real and imaginary parts of the complex optical conductivity, linear and nonlinear optical susceptibilities, real and imaginary parts of the electric modulus, real and imaginary parts of the impedance were performed by means of UV–Vis spectrophotometer experiments. As well, the estimated values of the single oscillator energy, dispersion energy, static refractive index and high–frequency dielectric constant were obtained from the linear portion of the (n2 –1)–1 vs. (hυ)2 plots using the Wemple–DiDomenico model.

[1] A. El Hachmi & B. Manoun, Int. J. Mater. Res., 114 (2023), 100-111.
[2] A. El Hachmi, F. El Bachraoui, S. Louihi et al., J. Inorg. Organomet. Polym. Mater., 30 (2020), 1990-2006.

9. Structure determination of nanocrystalline organic compounds by a global fit to th PDF

Robert Hühn (huehn@chemie.uni-frankfurt.de)
Goethe Universität Frankfurt am Main

The pair distribution function (PDF) gives the close range ordering of atoms. It is also possible to solve a crystal structure based on the PDF. In my master thesis I managed to solve the crystal structure of known organic pigments based on crystals sizes down to 10 nm.

10. Crystallization control possibilities of para-aminobenzoic acid using crystallization additives

Artjoms Jermakovs (art.jer12@gmail.com)
University of Latvia

In this study, para-aminobenzoic acid (pABA) was used as a model substance to investigate the additive crystallization control approach. The crystallization of pABA was explored under different conditions by performing evaporation and cooling crystallization from different solvents. Polyacrylic acid has shown the potential to form a metastable form by cooling crystallization.

11. Synthesis and (crystallographic) characterization of ultrasmall rhodium-glutathione-nanoparticles

Niklas Kost, Kateryna Loza and Matthias Epple (niklas.kost@uni-due.de)
Universität Duisburg-Essen, Institut für Anorganische Chemie

Ultra-small elemental rhodium particles with sizes down to 3 nm are of interest due to their large specific surface area, as they are chemically stable under many reaction conditions and can therefore be of catalytic interest for many reactions. Typical wet chemical syntheses rely on the reduction of the corresponding rhodium cations with suitable reducing agents, followed by colloidal stabilization by a suitable ligand. However, these nanoparticles tend to oxidize, and therefore a more detailed investigation of the oxidation state of these nanoparticles, for example by crystallographic methods, is very important.

12. Crystal structure analysis and refinement of polyoxometalate data sets with partial occupation of metal positions

Jan-Christian Raabe (janchristian.raabe@uni-hamburg.de)
Technische und Makromolekulare Chemie Universität Hamburg

In polyoxometallate chemistry, single framework metal atoms are often substituted by various foreign metal atoms. Single crystal structure analysis often fails to identify a clear substitution pattern because the foreign metal atoms are statistically distributed over all metal positions. Through this contribution, a strategy is presented to reliably model and refine the partial occupation of metal positions.

13. Electron density studies on cobalt complexes

Katharina Rachuy (k.rachuy@stud.uni-goettingen.de)
University of Göttingen, inorganic department

Various cobalt complexes are investigated by high resolution X-ray diffraction in combination with the multipole model. The aim was to obtain d-orbital populations and bond densities.

14. Binary to ternary drug-drug molecular adducts of antihypertensive drug, Ketanserin (KTS) with advanced physicochemical property

Smruti Rekha Rout (hiamsmruti@gmail.com)
Mumbai-Indian Oil Odisha Campus, Institute of Chemical Technology

Focusing on a reliable supramolecular synthons approach, novel molecular salts of the antihypertensive medication ketanserin (KTS) with aromatic carboxylic acid derivatives (benzoic acid (BA), 2-hydoxybenzoic acid (2-HBA), 2,5-dihydroxybenzoic acid (2,5-DHBA)) are reported. Binary salts of KTS with respective salt former were obtained by solvent-assisted grinding followed by solution crystallization.

15. $RE_3Fe_3Sb_7$ – Crystal structures and competing magnetic interactions

Manuel Schulze (manuel.schulze1@tu-dresden.de)
TUD Dresden University of Technology, Chair of Inorganic Chemistry II

The compounds $RE_3TM_3Sb_7$ host rare earth-metal RE and transition metal ions TM in triangular arrangements so that the interplay of 3d and 4f electrons is the origin for exotic magnetic behaviour, like spontaneous negative magnetisation (e.g.

$Pr_3Fe_3Sb_7$). Large needle-shaped single crystals of *RE* = Pr, Nd, Sm and *TM* = Fe can be obtained by reacting the elements in a Bi flux followed by hot-centrifugation. The aim of this work is to prepare single crystals of further representatives by substitution of the *RE*, *TM* and pnictogen ions *Pn* (e.g. *RE* = La, Ce, Eu, Gd, Tb and *TM* = Mn, Fe, Co and *Pn* = As, Sb) to examine the interplay between different magnetic contributions and to study the physical properties of the new materials.

16. Crystal structure analysis of multilayer nanographenes

Kazutaka Shoyama (kazutaka.shoyama@uni-wuerzburg.de)
TUD Dresden University of Technology, Chair of Inorganic Chemistry II

Multilayer nanographenes show distinctive photophysical properties due to interlayer interactions. Crystal structure of such complexes has a large unit cell, which leads to an unsatisfactory resolution of diffraction data for small molecule crystallography. Here we discuss some tips for refining such data set that might not be common for small molecule crystallography.

17. Disorder in the layered tellurides *TtPn*2Te4 (*Tt* = Ge, Sn, Pb; *Pn* = As, Sb, Bi) and $(PbS)_nBi_2S_{2+x}Te_{1-x}$

Lennart Staab, Peter Schultz, Lucien Eisenburger, Oliver Oeckler
(lennart.staab@uni-leipzig.de)
Universität Leipzig

Occupational disorder in tetradymite-type layered chalcogenides has been systematically investigated by optimized syntheses and high-quality single crystal diffraction data (many from DESY, beamline P24), including the application of resonant scattering. In addition, atomic-resolution EDX mapping and STEM-HAADF imaging have been used to study cation and anion disorder.

18. Growth of heavily doped n-type germanium ingots

Aravind Subramanian (aravind.subramanian@ikz-berlin.de)
Leibniz Institut für Kristallzüchtung

Heavily doped Ge (HDGe) ingots are useful for detectors in the Mid- and Far-infrared wavelengths. Substrates for such applications are currently produced using epitaxial methods. This work addresses the various challenges present during the bulk growth of HD-Ge crystals. Furthermore, the micro-structure of the grown Czochralski p-type HD-Ge crystals is discussed.

19. Co-crystal structures of multilayer nanographene and helicenes

Yvonne Wagenhäuser (yvonne.vonhausen@uni-wuerzburg.de)
Universität Würzburg

The photophysical properties of nanographenes (and other organic molecules with extended pi-faces) are highly dependent on intermolecular interactions and the packing arrangement with other molecules. Therefore, crystal structure analysis is a quintessential tool to investigate structure-properties relationships of these functional materials. Here we show an example of a co-crystal of a flexible nanographene with helicenes and point out some important aspects for the structure analysis of such multilayer organic complexes.

20. Crystallography of the Keggin polyoxometalate structure

Zainab Yusufzadeh (zainab.yusufzadeh@uni-hamburg.de)
Technische und Makromolekulare Chemie

In the Keggin structure, determined by single crystal structure analysis, different bond types are observed at the molecular level, all of which differ in their bond lengths. The occurrence of the different bond types can be explained by fundamental concepts of coordination chemistry. Furthermore, this contribution presents a type of disorder that can occur during the crystallization of a Keggin structure and a concept for successful modeling.

Become a member in the Deutsche Gesellschaft für Kristallographie (DGK) or of the Young Crystallographers

You can become a member of the Young Crystallographers instantly and free of charge! Simply write an email to the secretary Jan Philipp Wöhrle (info.dgkyc@gmail.com) or sign in with the QR-code in order to be included into the list of members.

For the recommended additional membership in the DGK, please download and send the application form to the secretary of the board of DGK. You can find the application form under the following website:

https://dgk-home.de/intern/mitglieder/mitgliedschaft/

The annual dues for undergraduate and PhD students (up to age 31) amount to 10 €. Regular members need to pay 35 €.

The 31th annual meeting of the German Crystallographic Society (DGK) will be in Frankfurt, Germany (27.-30.03.2023). Come and visit this conference!

The Young Crystallographers are the most active working group in the DGK. Stay tuned and visit our website - **https://dgk-home.de/aks/jkyc/**!!!
We post INFOS on upcoming meetings, workshops, grants, awards, events, etc. Have also a look at our BLOG and our social media platforms: