



Schweizerische Gesellschaft für Kristallographie
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Swiss Society for Crystallography

Sektion für Kristallwachstum und Kristalltechnologie
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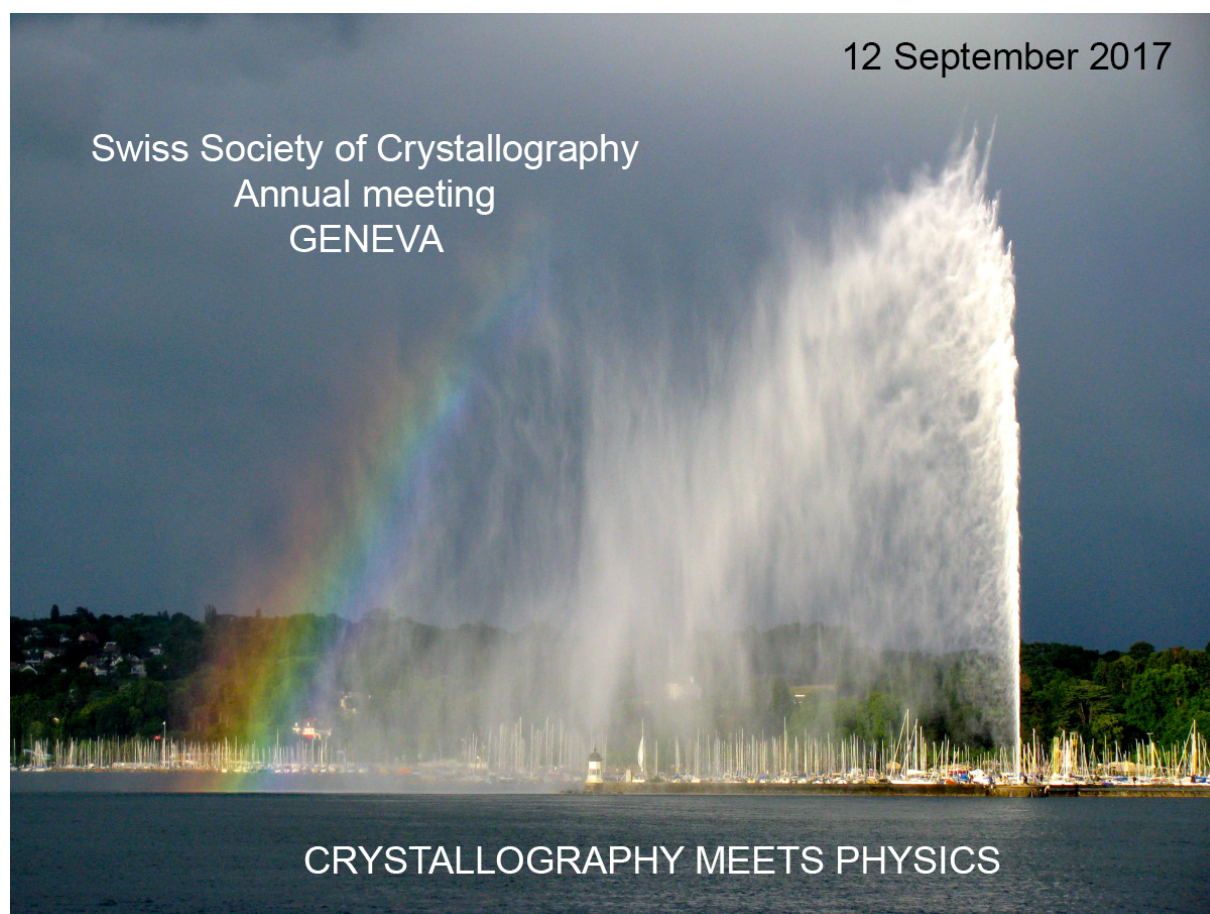
SGK / SSCr NEWSLETTER

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General Assembly of the SGK/SSCr 2017, Sept. 12

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Welcome to the annual meeting of the Swiss Society of Crystallography in Geneva.

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The President's Page



After the hectic 2016, we are back to tradition and on September 12, we will have in Geneva the annual meeting in its standard format of a one day symposium. I thank the colleagues working at the University of Geneva for their efforts in preparing an exciting meeting and I wish you all will be able to join us.

The program of the meeting is provided in this newsletter and I am sure it will be of interest for you.

Very important is also attending our annual assembly held within the congress. The agenda and some important issues are described in details in this newsletter. Please contribute to make the assembly smart and send us your remarks, if any, in advance, so that the discussion can focus only on important points.

During the last period we unfortunately received the sad news of the death of our esteemed colleague Howard Flack (commemorated in the previous newsletter) and this year the traditional Zurich School of Crystallography was organized for the first time without his appealing lectures on chirality. Despite this big loss, the ZSC was a great success, as testified also by the report in this issue of the newsletter. I thank the organizers for their wonderful job and their continuous efforts. I know that the organization of ZSC 2019 has already started and our society appreciate this enormous commitment.

Some of us will attend the IUCr assembly in Hyderabad on 21-28 august, where the Swiss research in crystallography is indeed very well represented with keynote lectures, chairs and lectures within microsymbosia. Many colleagues are also involved in the IUCr commissions, which are important for the organization of meetings and schools in the next triennium. After ECM30, it is so relaxing attending a meeting organized by others and concentrating only on the research activities!

See you in Geneve!

Piero Macchi
(President of the SGK-SSCr)

PROGRAM Swiss Society Annual Meeting 2017, GENEVA

Monday 11th of September:

19:30 – 22:30 Get together dinner, La Perle du Lac, Genève

Tuesday 12th of September:

09:30 – 10:00 Welcome Coffee and Registration

10:00 – 10:10 Opening ceremony

10:10 – 10:50 Dmitry **Chernyshov**, SNBL, Grenoble

Ferroelectrics under electric field probed by synchrotron radiation.

10:50 – 11:10 **Björn Wehinger**, University of Geneva

Secrets of diffuse scattering. How to probe elasticity and magneto-elastic waves using x-rays.

11:10 – 11:30 **Romain Sibille**, PSI, Villigen

Spin liquid in anion-disordered Tb₂Hf₂O₇ – an example of the importance of single-crystal neutron diffraction in physics; presentation of the new instrument ‘Zebra’ at SINQ.

11:30 – 11:40 SSCr PhD prize ceremony

11:40 – 12:10 Prize-winner invited talk

12:10 – 13:50 Lunch and Poster Session

12:50 – 13:50 Assembly of the Swiss Society for Crystallography

13:50 – 14:30 **Jörg Standfuss** PSI, Villigen

Serial Crystallography at Synchrotrons and Free Electron Lasers.

14:30 – 14:50 **Anjani K. Maurya**, Empa, St Gallen

Structural analysis of electrospun fiber membrane by SAXS and WAXS.

14:50 – 15:10 **Paula Corcosa**, University of Fribourg

New Monometallic and Heterobimetallic Complexes of Silver(I), Zinc(II) and Copper(II) with an Amino Acid Derived Ligand as Potential Antimicrobial Agents.

15:10 – 15:40 Coffee Break

15:40 – 16:20 **Marco Gibertini**, EPF Lausanne

Novel 2D materials from high-throughput computational exfoliation of experimentally known compounds.

16:20 – 16:40 **Rebecca Scatena** University of Bern

Electron density and Dielectric properties of highly porous Metal Organic Frameworks.

16:40 – 17:00 **Mehrdad Asgari**, EPFL Sion

In-situ neutron diffraction study of carbon dioxide adsorption on M-BTT frameworks, a series of highly crystalline MOFs.

17:00 – 17:10 Poster award ceremony

17:10 – 17:20 Closing remarks

LIST OF ABSTRACTS (alphabetical order)

In-situ neutron diffraction study of carbon dioxide adsorption on M-BTT frameworks, a series of highly crystalline MOFs

Mehrdad Asgari (1), Pascal Schouwink (1), Sudi Jawahery (2), Berend Smit (1 and 2), Safak Bulut (1), Wendy Queen (1)

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Metal Organic Frameworks (MOFs) are a relatively new class of porous materials that have shown record-breaking surface areas (up to 7000 m²/gr)[1], making them the most porous materials discovered to date and allowing them to adsorb significant amounts of gas. As a result, carbon capture is one of the most important applications for which MOFs have been extensively studied. Considering the large number of potential MOFs that can be accessed, through a combination of numerous metal clusters and organic linkers, determining the relationship between all their structural features (such as pore size and shape and chemical functionalities) and their corresponding carbon dioxide adsorption properties is of utmost importance. In this regard, in-situ characterization can be advantageous. Considering their crystalline nature, MOFs have a nonhomogeneous van der Waals potential energy landscape that dictates how incoming guest molecules arrange themselves on the internal framework surface[2]. This makes diffraction the most direct way to probe static site-specific binding properties.

In this report a comprehensive study of the CO₂ adsorption in several of the metal-substituted M-BTT analogs is carried out. In-situ neutron diffraction studies reveal for the first time, a molecular level view of CO₂ adsorption in this framework family and allow rationalization of the observed CO₂ adsorption isotherms. The experimental results have further been compared with those obtained from DFT simulations and show excellent agreement in all cases regarding CO₂ binding geometries and isosteric heats of CO₂ adsorption. Combining synthesis, characterization, and computation, can render unique insight into CO₂ adsorption processes that will hopefully provide an accelerated search for materials with optimal properties for energetically relevant gas separations.

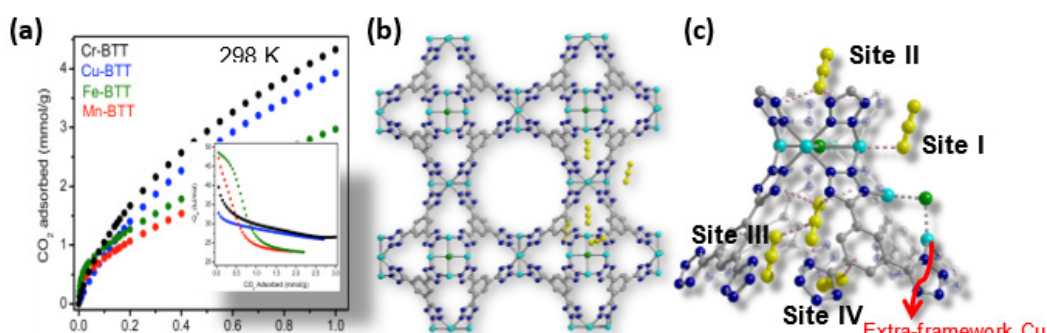


Figure 1-(a) CO₂ adsorption isotherms for M-BTT series at 298 K and isosteric heat of adsorption obtained from variable temperature adsorption data based on Clasius-Clapeyron equation. (b) The schematic figure of M-BTT frameworks with CO₂ adsorption positions. (c) The

[1] Leung, Dennis YC, Giorgio Caramanna, and M. Mercedes Maroto-Valer. Renewable and Sustainable Energy Reviews 39 (2014): 426-443.

[2] Zuluaga, Sebastian, et al. Journal of Physics: Condensed Matter 26.13 (2014): 133002.1.

Evaluation of semiconductor materials and systems quality using HRXRD methods

Zoltán Balogh-Michels, Francesco Pagani, Corsin Battaglia, Arndt Remhof,
Michael Reinke, Patrik Hoffmann, Alex Dommann, Antonia Neels

*Empa, Swiss Federal Institute for Materials Science and Technology,
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The combination of single crystalline materials and/or single crystals with thin layers has enormous industrial usage. Electron microscopy can reveal local defects, but HRXRD gives by its high strain and defect sensitivity the possibility to probe a more subtle deviation from the materials ideal state. High-resolution X-ray diffraction is a highly versatile tool, which combines high reciprocal space resolution with a large investigated volume. Especially useful is the so called in-plane diffraction, in which the diffraction happens on lattice planes perpendicular to the specimen surface. The combination of in-plane and out-of-plane diffraction allows the reconstruction of stresses as well as the identification of crystal symmetries.

In this presentation we are going to show the details of three examples from high resolution investigations:

- Si wafers produced by a low temperature bonding process are object to deformation and strain, in some cases the bending of the wafers up to 0.01° coupled with strain is observed (Fig. 1). [1]
- BaTiO_3 was grown in epitaxial fashion on Si and MgO substrates. In plane investigations revealed tetragonal lattice distortion and the mosaicity for the layer system [2]
- $\text{Li}_4\text{Ti}_5\text{O}_{12}$ was grown epitaxially on SrTiO_3 substrates. Using in plane investigations different domains of orientations became obvious.

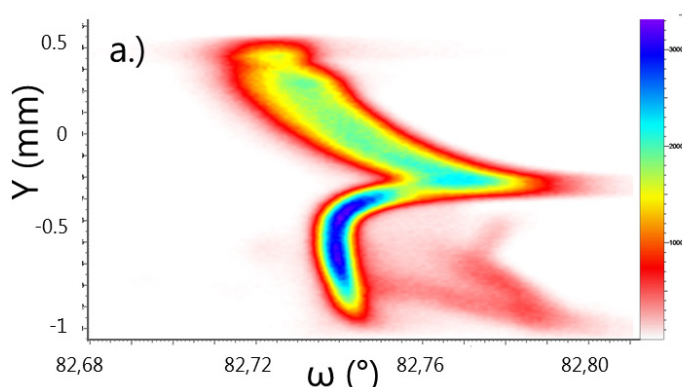


Fig. 1: wafer bending revealed by laterally resolved rocking curves

[1] Z. Balogh-Michels, K. Zweiacker, Y. Zhang, A. Jung, Ch. Flötgen, G. Chahine, A. Dommann, R. Erni, H. von Känel and A. Neels, *Acta. Cryst. A*, 72 (2016) s299-300.

[2] M. Reinke, Y. Kuzminykh, F. Ettes, A. Abel, T. Lagrange, A. Neels, J. Fompeyrine, P. Hoffmann, *Adv. Mater. Interfaces*, 2017, 10.1002/admi.201700116.

Modified Anion Packing of $\text{Na}_2\text{B}_{12}\text{H}_{12}$ in Close to Room Temperature Superionic Conductors

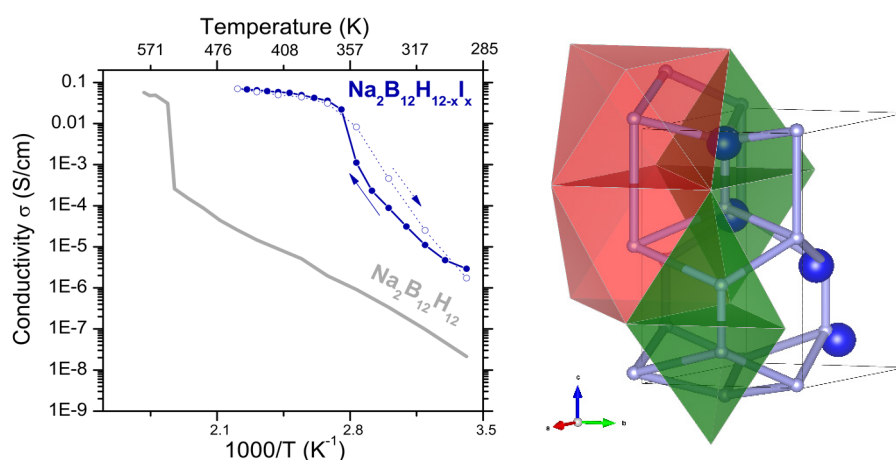
Yolanda Sadikin (1), Pascal Schouwink (2), Matteo Brighi (1), Zbigniew Łodziana (3), Radovan Černý (1)

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(2) EPFL ISIC-GE-VS, Rue de l'Industrie 17, CH-1950, Sion, Switzerland

(3) Polish Academy of Sciences, Institute of Nuclear Physics, ul. Radzikowskiego 152, 31-342 Kraków, Poland

"Three different types of anion packing, i.e., hexagonal close packed (*hcp*), cubic close packed (*ccp*), and body centered cubic (*bcc*), are investigated experimentally and with *ab initio* calculations in the model system $\text{Na}_2\text{B}_{12}\text{H}_{12}$. Solvent free and water assisted mechanical grinding provide polycrystalline samples for temperature-dependent synchrotron radiation X-ray powder diffraction and electrochemical impedance spectroscopy. It is shown that among the common close packed lattices, the *hcp* anionic backbone creates very favorable conditions for three-dimensional ionic conduction pathways, comprised of O–O, T–T, and T–O–T (O for octahedral, T for tetrahedral) cation hops. The *hcp* lattice is stable with respect to *ccp* and *bcc* lattices only at higher volumes per formula unit, which is achieved either by cationic substitution with larger cations or partial substitution of hydrogen by iodine on the *closo*-anion. It is found that the partial cationic substitution of sodium with lithium, potassium, or cesium does not lead to enhanced conductivity due to the obstruction of the conduction pathway by the larger cation located on the octahedral site. Substitution on the *closo*-anion itself shows remarkable positive effects, the ionic conductivity of $\text{Na}_2\text{B}_{12}\text{H}_{12-x}\text{I}_x$ reaching values of close to $10^{-1} \text{ S cm}^{-1}$ at a rather low temperature of 360 K. While the absolute value of σ is comparable to that of $\text{NaCB}_{11}\text{H}_{12}$ ^[1], the temperature at which it is attained is approximately 20 K lower. The activation energy of 140 meV is determined from the Arrhenius relation and among the lowest ever reported for a Na-conducting solid."



- [1] Tang, W. S. *et al.* Unparalleled lithium and sodium superionic conduction in solid electrolytes with large monovalent cage-like anions. *Energy Environ. Sci.* **8**, 3637–3645 (2015).

Reconstruction of the prior parent grains from Electron BackScatter Electron Diffraction (EBSD) maps. From algebra to engineering.

Cyril Cayron

EPFL/IMX/LMTM, Rue de la Maladière 71b, 2000 Neuchâtel, Switzerland

Displacive first or second-order phase transformations, such as those encountered in ferroelectrics, martensitic steels, shape memory alloys etc., generate domains. The orientations of the domains, called orientational variants, are given by the symmetries of the parent and daughter phases and by the orientation relationship; they are algebraically defined by cosets; their number is given by the Lagrange's formula. The misorientations between the variants, called operators, are defined by double-cosets; their number is given by the Burnside's formula. The set of variants and operators is not a group but a groupoid [1,2]. A geometrical illustration of the variants for the case of FCC-BCC martensitic transformation is given in Fig.1a. The groupoid composition table can be used to reconstruct the prior parent grains from EBSD maps [2]. An example is given in the case of a martensitic steel in Fig.1b. It is also possible to map in colours the gradients of orientation relationships in fully transformed materials [4].

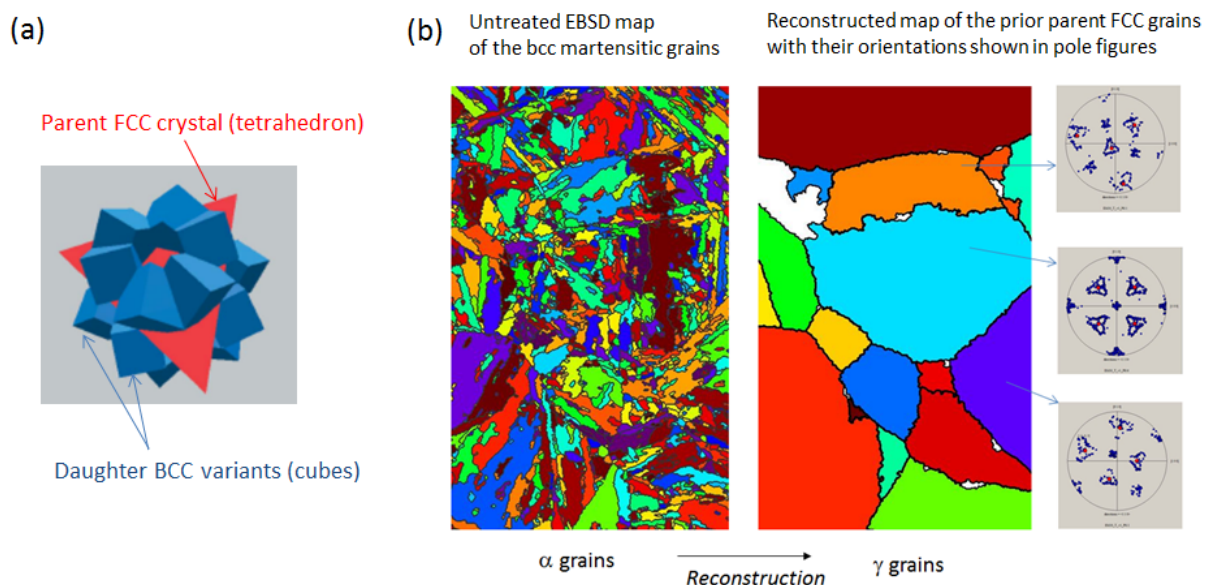


Fig1. Orientational variants. (a) Geometric representation. (b) EBSD reconstruction.

- [1] C. Cayron, *Groupoid of orientational variants*, Acta Cryst. A 62 (2006) 21-40.
- [2] C. Cayron, *GenOVa: a computer program to generate orientational variants*, J. Appl. Cryst. 40 (2007) 1179-1182.
- [3] C. Cayron, *ARPGE: a computer program to automatically reconstruct the parent grains from backscatter diffraction data*, J. Appl. Cryst. (2007) 1183-1188.
- [4] C. Cayron, *EBSD imaging of orientation relationships and variant groupings in different martensitic alloys and Widmanstätten iron meteorites*, Mater. Charac. 94 (2014) 93-110.

Anion Disorder in $K_3BH_4B_{12}H_{12}$ and its Effect on Cation Mobility

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(2) Polish Academy of Sciences, Institute of Nuclear Physics, Kraków, Poland

(3) Institute of Metal Physics, Ural Division of the Russian Academy of Sciences, Ekaterinburg, Russia

Mixed anion borohydride – *closo*-borane of potassium, $K_3BH_4B_{12}H_{12}$, has been synthesized using mechanochemistry and characterized by combination of temperature dependent Synchrotron Radiation X-ray Powder Diffraction, solid state Nuclear Magnetic Resonance, Thermal Analysis, Electrochemical Impedance Spectroscopy, Topology Analysis and *ab initio* solid state calculations [1]. At RT the compound crystallizes in the monoclinic superstructure ($P2_1/c$) of the cubic anti-perovskite prototype. At 565 K it transforms by first order phase transition into a rhombohedral ($R-3m$) deformation of the cubic prototype, which further transforms at 680 K by a second order phase transition into a cubic ($P2_1$) anti-perovskite structure. The first phase transition is related to the repulsive homopolar H-H contacts between BH_4^- and $B_{12}H_{12}^{2-}$ anions which are released at bigger cell volumes, and the orientation of BH_4^- anion becomes disordered. The second phase transition is related to orientational disorder of the $B_{12}H_{12}^{2-}$ anion at bigger cell volumes. The parameters of reorientational motion (activation energies and jump rates) for both BH_4^- and $B_{12}H_{12}^{2-}$ anions in the monoclinic phase were found from the nuclear spin-lattice relaxation measurements. The effect of orientation disorder of both anions on mobility of cations was studied as a case example for the whole family of complex hydrides based on borohydride or *closo*-borane anions, important solid-state electrolytes. While the dynamics of smaller BH_4^- anion does not have any measurable effect on K^+ mobility, the dynamics and orientation disorder of bigger $B_{12}H_{12}^{2-}$ is promoting the K^+ mobility, which would otherwise be limited by a small radius of conducting channels even in the cubic anti-perovskite structure.

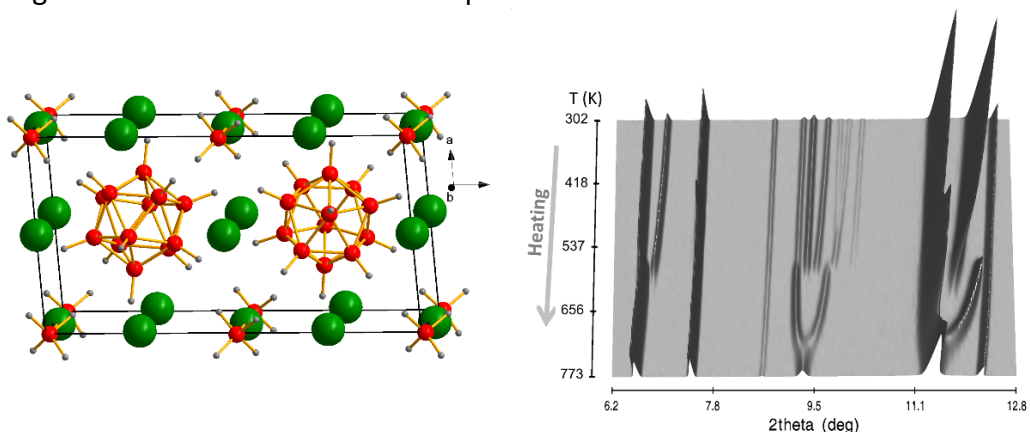


Figure : Crystal structure of monoclinic polymorph of $K_3BH_4B_{12}H_{12}$ (left). Variable temperature SR-XPD data (T -ramp) of the water assisted ball milled $KBH_4:K_2B_{12}H_{12}$ mixture ; heating (4 K/min) between RT and 773 K (right).

[1] *J. Phys. Chem. C.* (2017), 121, 5503-5514

News from the X04SA Materials Science beamline of the SLS

Antonio Cervellino and Nicola Casati

Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen, Switzerland

There are several new opportunities for research and sophisticated experiments in the realm of X-ray powder diffraction at the the X04SA Materials Science beamline of the SLS. As first, to the pre-existing Mythen II detector (120° with 0.0036° resolution) we added recently a 2-D Pilatus 6M for situations where the higher speed (but smaller 2θ range) and the twodimensionality of the pattern are essential. Secondly, easier access for simple experiments. For a few capillaries to be simply measured in standard conditions, the new MesQuik access channel (<https://www.psi.ch/sls/ms/pdmesquik>) is there. A short scientific proposal is needed and the review process is accelerated, aiming to deliver the data within 10 weeks from submission. Samples are mailed in and measured at one of three energies (12.4 - 17.5 - 22.0 keV) in a standard way. Finally, many new devices allow for a number of new scientific opportunities, as

- a new in-situ ball-milling device, capable of following mechano-chemical reactions of powders with a time-resolution on the scale of seconds. A new double-profile chamber, with a thin planar section that is accessible only to the powder, guarantees an unprecedented angular resolution and low background for this type of devices.
- a novel high-pressure liquid jet device, shooting a liquid horizontally through the beam, in perfect Debye-Scherrer geometry. The reacting liquids can be mixed just before ejection (or with a controlled delay) from up to 4 components, with as many high-pressure pumps, flow-meters and thermal baths. The liquid jet is collected in a stirred cuvette where additional data (as pH) can be taken. The jet is rocksteady oscillation free; its diameter (0.05-0.5 mm) is selected by choosing the nozzle.
- a new liquid drop 68 kHz ultrasound levitator, capable of statically holding a 0.5-2 mm liquid drop perfectly immobile under the beam. The device, just tested, will be completed with an enclosure for humidity control and a larger non-scattering exit window for a better angular range. The drop is manually injected in place using a precision calibrated syringe.

New Monometallic and Heterobimetallic Complexes of Silver(I), Zinc(II) and Copper(II) with an Amino Acid Derived Ligand as Potential Antimicrobial Agents

Paula Corcosa, Aurélien Crochet and Katharina M. Fromm

University of Fribourg, Chemin du Musée 9, 1700 Fribourg, Switzerland¹

Over the past years, multiresistant bacteria have gained more and more ground: Once very effective antibacterial drugs cannot prevail anymore over certain bacteria. Thus, scientists are bothering to invent new compounds: Some focusing to create new derivatives of famous antibiotics like Penicilline, others getting back to synthesize complexes with precious or essential metals as they are known since antiquity for their antimicrobial properties. It has not only been an old tradition to throw silver coins in fountains but rather to keep the drinking water free of microbes owing to the antimicrobial activity of this precious metal. Even the ancient Greeks and Romans drank instinctively from silver vessels to keep the liquids fresh or ate from silver plates.[1] It has been found that silver ions damage the DNA of bacteria by interfering with guanine and adenine base pairs[2] and that they induce an overproduction of reactive oxygen species (ROS) such as hydroxyl radicals by disrupting the metabolic pathways of Fenton chemistry.[3,4] Furthermore, it is known that silver ions interact strongly with thiol groups and inhibit or degrade therefore the disulfide bond formation in many proteins and enzymes. This leads finally to the increase of the bacterial membrane permeability.[3] Based on our extensive experience with antimicrobial silver compounds [f.ex. 4,6], and silver resistance of bacteria [4,5], we now present combinations of silver ions with zinc or copper ions in bimetallic complexes with p-amino-L-phenylalanine to create a synergistic antimicrobial effect in order to fight more efficiently against bacteria.

[1] Fromm, K. M. Nat. Chem. 2011, 3, 178.

[2] Arakawa, H.; Neault, J.

F.; Tajmir-Riahi, H. A. Biophys. J. 2001, 81, 1580.

[3] Morones-Ramirez, J. R.; Winkler, J. A.; Spina, C. S.; Collins, J. J. Science Translational Medicine 2013, 5 (190), 1-11.

[4] Eckhardt, S.; Brunetto, P. S.; Gagnon, J.; Priebe, M.; Giese, B.; Fromm, K. M. Chem. Rev. 2013, 113, 4708-4754.

[5] Mirolo, L.; Schmidt, T.; Eckhardt, S.; Meuwly, M.; Fromm, K. M. Chem. Eur. J. 2013, 19, 1754-1761.

[6] Varisco, M.; Khanna, N.; Brunetto, P. S.; Fromm, K. M. ChemMedChem 2014, 9, 1221-1230.

Structural Investigation of the High-Spin→Low-Spin Relaxation Dynamics in the Spin Crossover Compound [Fe(pz)Pt(CN)₄]

Teresa Delgado (1), Cristian Enachechu (2), Antoine Tissot (3), Laure Guénée (4), Andreas Hauser (1) and Céline Besnard* (4)

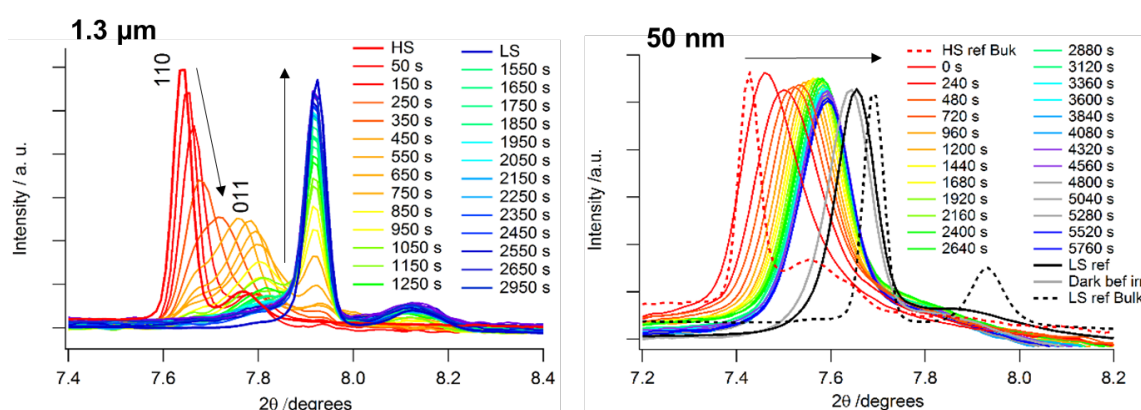
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(8) *Laboratoire de Cristallographie. Université de Genève. 24, Quai Ernest Ansermet, CH-1211 Genève, Switzerland.*

"Spin transitions are associated with large structural changes [1]. The metal-ligand bond lengths difference in iron(II) complexes of ~ 0.2 Å creates elastic interactions between the centres, resulting in cooperative effects that influence the thermal and light-induced spin crossover [2]. Synchrotron X-Ray powder diffraction reveals a quantitative photo-induced LS-to-HS conversion based on Light-Induced Excited Spin State Trapping at 10 K on microcrystalline and nanocrystalline powders of [Fe(pz)Pt(CN)₄] \cdot xH₂O (pz = pyrazine) [3]. Time-resolved measurements evidence that the HS-to-LS relaxation depends on the particle size. For particles above 383 nm, the relaxation proceeds by a two steps mechanism: a random HS to LS conversion at the beginning of the relaxation followed by a nucleation-growth process, whereas by reducing the size to 142 nm and lower no nucleation is observed. Furthermore using a scanning method within the framework of the mechanoelastic model [4], diffraction-like peaks for all the relaxation curves and their dependence with the size have been simulated and explained."



[1] P. Guionneau, Dalton Trans 2014, 43, 382.

[2] P. Gülich, A. Hauser, H. Spiering, Angew. Chem. Int. Ed. 1994, 33, 2024.

[3] T. Delgado, A. Tissot, L. Guénée, C. Besnard, A. Hauser, Chem. Eur. J. 2015, 21, 3664.

[4] C. Enacheanu, A. Hauser, Physical Chemistry Chemical Physics 2016, 18 (30), 20591-20599.

Crystal structure of hydrated and anhydrous Transition Metals *closo*-boranes (TM = Mn, Fe, Co, Ni, Cu)

Emilie Didelot, Yolanda Sadikin, Radovan Černý

DQMP, Laboratory of Crystallography, University of Geneva

Closo-boranes of transition metals (TM) were studied in the framework of boron chemistry, but only very few compounds have been prepared as anhydrous due to synthetic road using water as solvent [1-7]. TM *closo*-boranes are interesting as insertion electrodes for Li- and Na-ion batteries in combination with *closo*-borane solid electrolytes [8, 9]. Indeed, the same chemistry of the electrode and electrolyte provide stable electrode/electrolyte interface.

We have studied TM *closo*-boranes prepared by water assisted mechanosynthesis (ball milling) of the mixture $\text{Na}_2\text{B}_{12}\text{H}_{12} + \text{TMCl}_2$ (TM = Mn, Fe, Co, Ni, Cu). Six crystal structures have been solved from temperature dependent synchrotron radiation X-ray powder diffraction among them four are hydrated and two anhydrous. Two different TM- H_2O complexes were found: An octahedral complex crystallizing in three different deformation variants of complex centred *closo*-borane cube, and a complex containing four water molecules centering also a *closo*-borane cube.

Anhydrous TM *closo*-boranes crystallizes with *bcc* packing of *closo*-boranes with bivalent TM (Co, Ni) disordered on a tetrahedral site (Fig. 1 left), and monovalent Cu^{I} bridging two *closo*-boranes (Fig. 1 right). All three TMs are coordinated by six hydrogens in a distorted octahedral coordination presenting no orientational disorder up to 573 K.

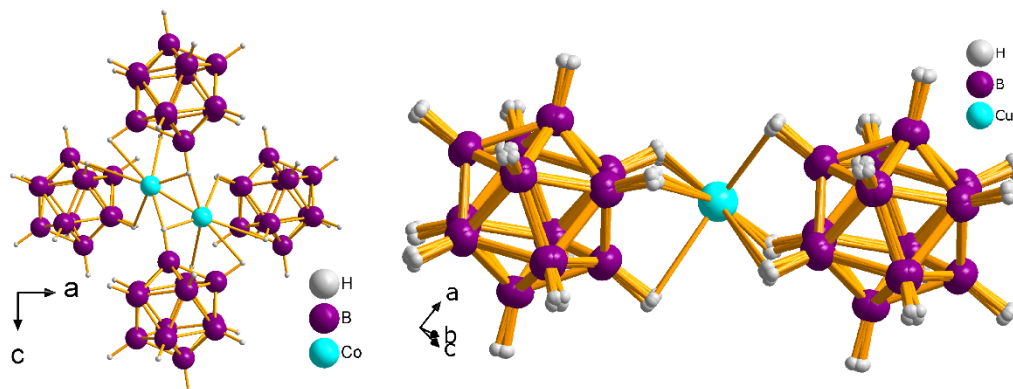


Figure 1: Representation of Co and Cu *closo*-boranes: Co^{II} disordered on a tetrahedral site (left) and Cu^{I} bridging two *closo*-boranes (right).

- [1] Muetterties E.L. et al., *Inorganic Chem.* **1964**, 3, 444-451.
- [2] Paskevicius M. et al. *Nature Comm.* **2017**, submitted.
- [3] Tiritiris et al., *Z. Anorg. Allg. Chem.* **2004**, 630, 1763.
- [4] Tiritiris et al., *Z. Anorg. Allg. Chem.* **2008**, 634, 317-324.
- [5] Nguyen-Duc Van et al., *Z. Anorg. Allg. Chem.* **2015**, 641, 2484-2489.
- [6] Tiritiris et al., *Z. Anorg. Allg. Chem.* **2011**, 637, 682-688.
- [7] Kleeberg F.M. et al. *Z. Anorg. Allg. Chem.* DOI: 10.1002/zaac.201404031
- [8] Udovic T.J. et al. *Chem. Commun.* **2014**, 50, 3750-3752.
- [9] Tang W.-S. Et al. *ACS Energy Lett.* **2016**, 1, 659-664.

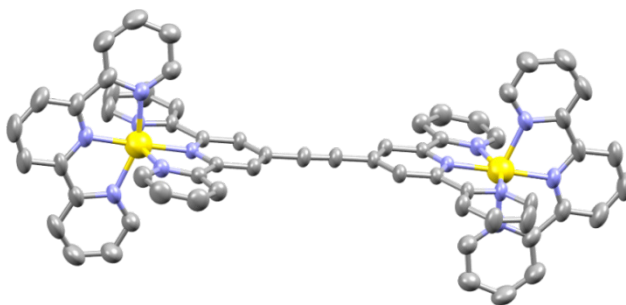
Crystal structures of Cr^{III} bimetallic complexes: a key for unravelling electronic communication

Benjamin Doistau (1), Davood Zare (1), Homayoun Nozary (1), Céline Besnard (2), Laure Guénée (2), Yan Suffren (1), Andreas Hauser (1), Claude Piguet (1)

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Motivated by the recent environmental concerns, energy conversion received increasing interest during the last decades and chemists took advantages of the toolkit of supramolecular chemistry for designing polymetallic architectures working as energy converting devices. The introduction of some metal ions as sensitizers and activators in molecular systems often permitted to observe down-shifting,^[1] sometimes up-conversion phenomena.^[2] Despite the particularly appealing photo-physical features, sensitizers based on Cr^{III} complexes remain underrepresented in multimetallic supramolecular architecture performing energy conversion, while Ru^{II} analogues are widely exploited for this purpose. Since Cr^{III} displays longer excited state lifetimes than Ru^{II},^[3] we decided to overcome the Cr^{III} chemistry complexity in order to permit its use as sensitizer in polypyridine-based architectures. The synthesis and XRD characterization of a family of Cr^{III} bimetallic complexes was performed and the electronic communication through different bridging ligands was studied. Altogether, the crystal structures, the isotropic magnetic coupling constants, the distribution of the Cr^{III} energy levels and the unravelling of intramolecular intermetallic energy transfer rate constants identify the alkyne-bridged back-back bis-terpyrine ligands as the best candidates for exploiting trivalent Cr^{III} in polynuclear organometallic clusters.^[4]



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Bonding in Polyiodides

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Iodine is a halogen and thus, according to classical covalent bonding models, it forms just one bond. Due to its hypervalency, however, it can form chains containing up to 29 atoms, building anionic 3D networks.[1] These polyiodides consist of I^- , I_2 and I_3^- building blocks which combine to chains of varying lengths and motifs. The high structural variability as well as the uncommon bonding situation make polyiodides an interesting topic of research. In order to examine them we pursued two main approaches: First, we studied crystals under high pressure and second, we used quantum crystallography[2] to obtain an experimental wavefunction.

High-pressure structures of tetraethylammonium diiodide triiodide (TEAI) were determined in the range up to 12 GPa. Electrophilic I_2 and nucleophilic I_3^- moieties significantly approach as a function of pressure. This eventually leads to the formation of pentaiodide units at 6.8 GPa, heptaoidides at 7.6 GPa and infinite inorganic polymeric chains at 11.9 GPa. This catenation is anticipated by single crystal - single crystal phase transition at about 5.7 GPa, reducing the lattice symmetry from orthorhombic to monoclinic. The process is reversible; though with a large hysteresis (transition back to orthorhombic system occurs at 1.5 GPa).

The target of traditional methods of X-ray structure refinement is the electron density, which lacks a lot of information compared to a wavefunction as obtained from quantum chemical calculations. A new refinement method, termed X-ray constrained wavefunction refinement[3], allows to combine calculations and fitting to experimental data. Like in traditional quantum chemical calculations a wavefunction is optimized by a variational procedure that minimizes the energy, but an additional restraint requires also the minimization of the difference between observed and calculated structure factors. Thus, a molecular wavefunction is obtained with all the advantages compared to the electron density. The availability of molecular orbitals, for example, allows interpretation in terms of frontier molecular orbital theory. However, these orbitals are not traditional eigenfunctions of the Hamiltonian since they do not come from a pure computational calculation. One of our goals is to investigate their physical meaning by examining the orbital interactions of I_3^- with I_2 in I_5^- polyiodides at different pressures.

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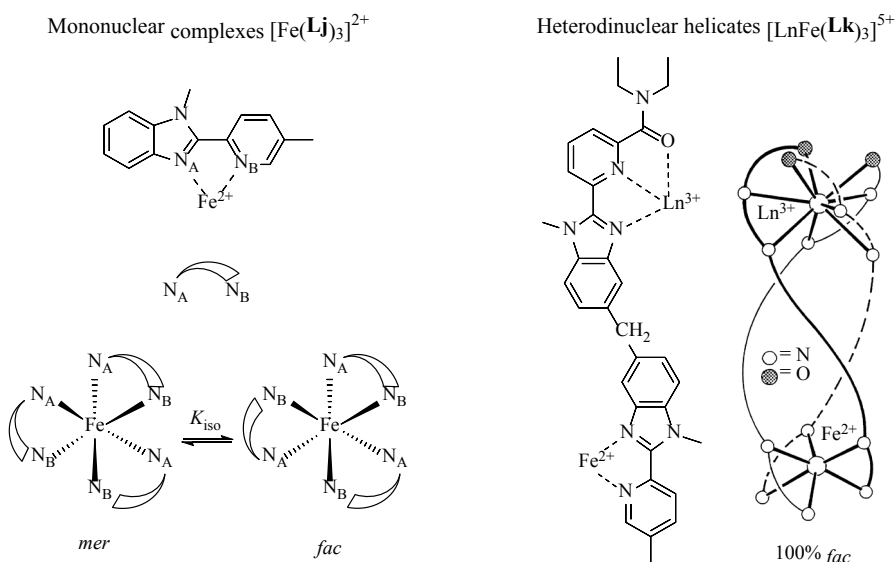
Iron(II) spin crossover in mononuclear and heterodinuclear *d-f* complexes

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Since their discovery, iron(II) spin crossover (SCO) complexes have been extensively studied for their magnetic and optical properties. In those complexes, $3d^6$ iron(II) display a chemical equilibrium between the low spin ($^1A_{1g}$, $S = 0$, diamagnetic) and high spin ($^5T_{2g}$, $S = 2$, paramagnetic) electronic configurations. A subtle balance between ligand-field splitting and spin-pairing energies controls the thermodynamic parameters of the SCO process, which makes these complexes challenging for chemical tuning. In this work, the iron(II) spin transitions occurring in the mononuclear complexes $[\text{Fe}(\text{Lj})_3]^{2+}$ were studied both in solution and in the solid state in order to evaluate the effects of intermolecular packing on the enthalpic and entropic contributions. The use of non-symmetrical didentate ligands results in two structural isomers (meridional and facial, below on the left).¹ The influence of this considerable constraint on SCO spin transitions mainly escaped attention in this well-explored field, this probably because of the very difficult (impossible?) isolation of pure isomers for these labile coordination complexes. Taking advantage of the templating effect brought by trivalent lanthanides in the triple-stranded helicates $[\text{LnFe}(\text{Lk})_3]^{5+}$ (below on the right), this challenge can be approached with the estimation of complete sets of thermodynamic SCO parameters for both meridional and facial isomers.



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Crystal structure and apical oxygen disorder in $\text{Nd}_2\text{NiO}_{4+d}$ investigated by neutron diffraction

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Better understanding of the microscopic origin of oxygen diffusion mechanism in *non-stoichiometric oxides* is essential for future development of intermediate temperature solid oxide fuel cells. In this prospect, mixed ionic and electronic conducting layered rare earth nickelates ($\text{R}_2\text{NiO}_{4+d}$) emerged as promising candidates. Oxygen transport, in these oxides, is driven by *apical oxygen disorder and non-stoichiometry* (1). Oxygen migration is described as an *interstitialcy mechanism* in which excess oxygens diffuses via apical oxygens (2). To further elucidate these points, we have performed single crystal neutron diffraction studies on $\text{Nd}_2\text{NiO}_{4+d}$ system as a function of temperature ($T=2-450$ K) and non-stoichiometry ($d=0.25$ and 0.125). Neutron diffraction studies (HEiDi@MLZ and ZEBRA@SINQ, PSI) reveal the average crystal structure to be orthorhombic ($Fmmm$) and tetragonal ($P4_2/nm$) at room temperature for $d=0.25$ and 0.125 , respectively. No structural transition has been observed in the whole temperature range for both compounds. *Reciprocal space plane mapping* (DMC@SINQ, PSI) shows the evidence of *3d-ordering of excess oxygens* (Fig 1.a) in the whole temperature range. This result confirms the pinning of excess oxygens to the crystal lattice at low temperature. Scattering density studies of the average structure using the *Maximum Entropy Method* for both compounds reveal high displacement amplitudes (Fig. 1. (a), (b)) for apical oxygen atoms toward $[110]$ direction with respect to the high temperature F-symmetry cell *i.e.* toward the nearest interstitial sites. These results confirm the presence of interstitialcy diffusion mechanism in both compounds. However, important differences are also identified for apical oxygen displacements in both compounds due to presence of different structural distortions. For $d=0.25$ compound, all apical oxygens show displacements both in $[110]$ and $[1-10]$ directions whereas in the later compound, only either $[110]$ or $[1-10]$ displacement is

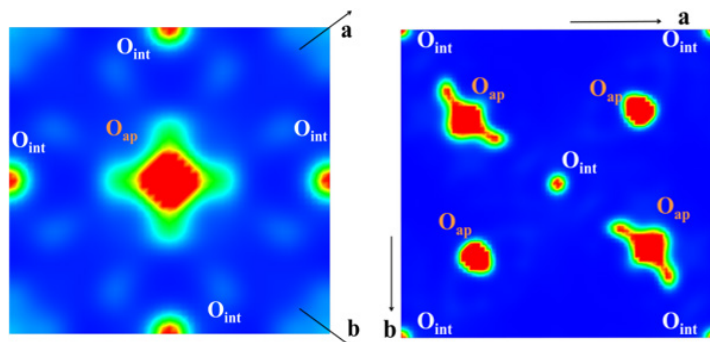


Figure 1. Reconstructed nuclear scattering densities of apical and interstitial oxygens at room temperature for (a) $d=0.25$ (ZEBRA) and (b) $d=0.125$ (HEiDi) compounds obtained from maximum entropy method showing apical oxygen displacement toward $[110]$ directions or toward nearest interstitial sites.

observed. Thus, less number of oxygen migration channels are expected in $d=0.125$ compound. This result possibly explains the lower diffusion coefficient found in less non-stoichiometric samples.

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Structural analysis of electrospun fiber membrane by SAXS and WAXS

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Over the years, electrospinning [1] has been developed as technique to produce the fiber membrane which can be used for different applications such as tissue engineering, biomedical engineering, energy and environmental applications. The structure of the fiber membrane highly depends on the polymer type, the rheological behaviour of electrospinning solution and the environmental conditions. Despite significant advances on understanding the structure and morphology of electrospun membranes by various techniques such as electron microscopy and Differential scanning calorimetry (DSC); their fine structures in nanoscale has not been fully understood.

In our recent studies, we have investigated the structure of electrospun PVDF/hfp based fiber membranes for aligned and non-aligned samples by SAXS and WAXS techniques.

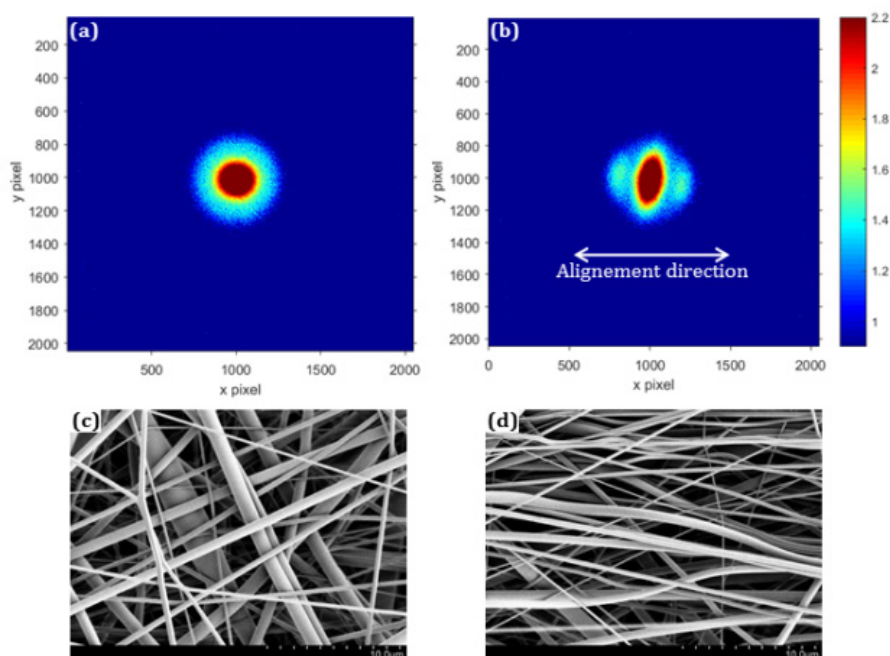


Figure 1. Small angle X-ray scattering patterns from PVDF/hfp; (a) non-aligned, (b) aligned fiber membrane samples. SEM micrographs of PVDF/hfp; (c) non-aligned, (d) aligned samples.

Interpretations of SAXS profiles from membranes are conducted through employment of a model capable of simulating the scattering patterns from fiber membranes over the whole q range [2]. The polymer showed aggregated structures (in both aligned and non-aligned systems) with average correlation length of about 4.2 nm. In addition, non-aligned and aligned membranes represent orthorhombic structure, as understood from WAXS.

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Weak donor-acceptor intermolecular interactions under pressure: the NO₂ ...NO₂ case.

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Weak intermolecular interactions in crystals are crucial in several research fields, particularly in crystal engineering. In some instances, however, their role may be not yet fully understood.[1] High pressure studies can be very useful to increase our knowledge on the many intermolecular interactions in crystals, allowing us to extract valuable information on their compressibility and to clarify their role for crystal packing. Moreover, pressure may prompt these interactions to induce polymorphism or even chemical reactions. Apart from the well known hydrogen bond, also the so-called “halogen”, “chalcogen”, and even “carbon” bond have recently aroused growing interest. At present, however, other kinds of weaker interactions have not been very deeply investigated, and there is a strong need of comparing simultaneously different interactions and establish their hierarchy. A possible unifying scheme classifies them all as electron donor-acceptor interactions within the solid paradigm of frontier molecular orbitals: every interaction is seen as an overlap between the HOMO of the electron donor and the LUMO of the acceptor.[2] In this study, we focused our attention on unusual $\pi^* \leftarrow n$ interactions between NO₂ groups, which can assume several conformation and the nature of which is still controversial.[3]

The crystal structure of 4-amino-4'-nitrobiphenyl was studied at high pressure with XRD experiments and ab initio and periodic-DFT calculations. A previously unreported pressure induced phase transition was observed and it seems to favour the contact between NO₂ groups. High pressure periodic DFT calculations were also performed on other two systems containing several NO₂ ...NO₂ contacts. Finally, to better classify the nature of this unusual interaction, we employed theoretical tools such as pairwise atomic potential energies, modelling of idealized NO₂ ...NO₂ dimeric models, and electron density analysis with Fukui functions.

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Na₃(CB₁₁H₁₂)(B₁₂H₁₂): a novel fast Na⁺ conductor for solid-state batteries

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Lithium-ion batteries (LIBs) represent the state-of-the-art devices for electrical energy storage, providing power supply to a wide variety of portable electronics. Nowadays LIBs could give substance to the strived conversion of the current car fleet toward a more sustainable hybrid/fully electric mobility. In order to prompt such breakthrough, the on-board energy stored in the battery pack should provide comparable performance with those offered by fossil fuel vehicles. At present, this can be only obtained by using a massive battery pack (600 kg for the Tesla S, for instance). However, safety concerns arise since commercial LIBs are equipped with a flammable liquid electrolyte. Solid-state batteries (SSBs) circumvent this major issue placing a solid electrolyte between the electrodes. Such setup allows achieving superior safety requirements, improved performance (limited self-discharge), higher temperature operational range, more uniform output voltage.¹ Moreover, unlike conventional carbonate mixtures, solid electrolytes (SEs) show a wider voltage window, which noteworthy increase the choice of the positive electrode.² However, such replacement limits the ionic diffusion, especially at room temperature. Therefore, SEs should have good ionic conductivity and low activation energy.³ To date, several solid-state electrolytes were investigated, such as LISICON (Li₁₄ZnGe₄O₁₆), perovskite (Li_{0.5}La_{0.5}TiO₃), garnet (Li₇La₃Zr₂O₁₂), LiPON (Li_{2.88}PO_{3.75}N_{0.14}) structures. They exhibit ionic conductivity between 10⁻³ and 1 mS cm⁻¹ at 25°C and activation energy in the 0.3 – 0.6 eV range.⁴ Besides, ionic conductivity was also investigated in complex hydrides: Matsuo demonstrates increased Li⁺ mobility (10⁻³ mS cm⁻¹) in LiBH₄ after orthorhombic-hexagonal phase transition around 300 K.⁵ Other higher borane systems were studied, highlighting also Na⁺ fast diffusion.^{6,7} The interest in Na⁺ conductivity lies on the possible replacement of current LIB technology with more viable Na-based electric storage systems, thanks to the higher abundance and availability of sodium. On this basis, we investigate Na₃(CB₁₁H₁₂)(B₁₂H₁₂), synthesized via high-energy ball-milling. The structure was solved *ab-initio* from X-ray powder diffraction in the s.g. *Im-3m*. The carborane-borane complex exhibits a Na-conductivity higher than 1 mS cm⁻¹ at 20°C. At 100°C the conductivity increases to 10 mS cm⁻¹, with an activation energy of 136 meV.⁸ It also shows electrochemical stability in the 0-5 V window (vs. Na⁺/Na). Thermal stability has been verified up to 300°C, by *in situ* XRD analysis. The electrochemical behaviour of the new electrolyte is evaluated in solid-state half-cell, toward both negative and positive electrodes, at the temperature of 40 °C. As a preliminary result, Na₃(CB₁₁H₁₂)(B₁₂H₁₂) allows partial Na⁺ de-intercalation from Na₂Fe₂(SO₄)₃, between 3-3.5 V vs. Na⁺/Na.

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Li₄Ti₅O₁₂ thin-film battery anodes and the role of crystallographic orientation on Li-ion conductivity

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Thin-film all-solid-state batteries find applications in smart cards, sensors, and radio-frequency identification tags[1], but also provide a model system for the fundamental study of Li-ion transfer kinetics, defect chemistry[2], and electrochemical stability[3]. Here we investigate the effect of crystallographic orientation on Li transport in Li₄Ti₅O₁₂ thin-films grown by pulsed laser deposition (PLD). Epitaxial phase-pure Li₄Ti₅O₁₂ thin-films were grown on (111) oriented SrTiO₃ substrates and compared to epitaxial Li₄Ti₅O₁₂ thin-films on MgO (100). To avoid lithium deficiency in the films caused by scattering of lithium in the ablation plume and sublimation of lithium once deposited on the substrate, we employ high laser fluence as well as lithium enriched ablation targets. We elucidate the effects of target composition as well as pulsed laser deposition parameters on the final film properties such as structure, phase purity, orientation, compositional profile, Li-ion segregation, and stoichiometry. We show by electron diffraction that epitaxial Li₄Ti₅O₁₂ films grow strained at the interface, but relax to bulk values within a few nanometers away from the interface. From temperature dependent impedance measurements, we find that the activation energy for the epitaxial Li₄Ti₅O₁₂ (111) films (0.73 eV) is lower than for the (100) films (0.78 eV). We discuss strategies and next steps required to integrate epitaxial anode Li₄Ti₅O₁₂ in a thin-film solid-state battery.

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Shedding light into the Semi-Crystalline Biomaterials by Small Angle X-ray Scattering

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Lipids are the main constituents of many biological systems including cell membranes and disease biomarkers such as low density lipoproteins. In recent years, the study of Lipids in the bulk, and at the oil/water interface, has been developed extensively. As the result, the molecular organisation of lipids in nanoscale and formation of various crystalline states have been understood. Despite substantial achievements on understanding of the lipid polymorphism e.g. the crystallisation of medium chain triglycerides (MCT) by various methods such as X-ray diffraction (XRD) and acoustic techniques, the lipids aggregation in semi-crystalline states (or early stages of crystallisation) have not been fully understood, so far.

In this contribution, the existing models for the aggregation of MCTs in liquid state will be reviewed and then, our very recent proposed model based on the analysis of diffuse scattering patterns attained by small angle X-ray scattering (SAXS) studies, will be introduced.

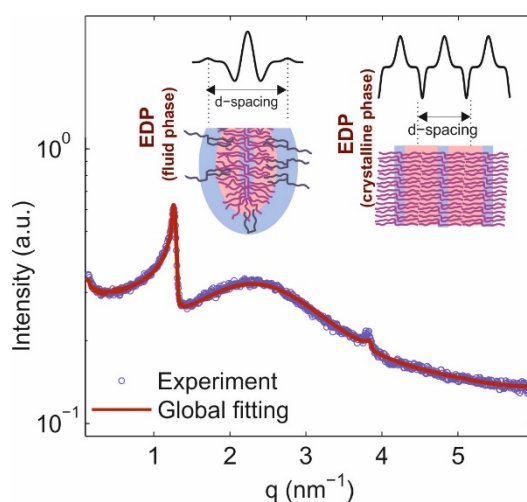


Figure 1. Small angle X-ray scattering pattern from MCTs at liquid crystalline state representing both fluid and crystalline α -phases and the corresponding global analysis demonstrated by the solid line. The insets show the molecular organisation at both phases deduced from the calculated electron density profiles (EDPs).

Electron density and Dielectric properties of highly porous Metal Organic Frameworks

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Porous metal organic frameworks (MOFs) have been identified as the next generation very low dielectric constant (ϵ_r) materials. In fact, the combination of a framework structure and large voids represents a promising route to develop new low- ϵ_r materials, retaining the required thermal stability, high mechanical strength and good adhesion to neighboring layers[1]. Despite the large number of known structures and of designable ones by changing metals, organic linkers, metal-linker ratio, reaction conditions, post-synthetic functionalizations, there is no criterion to select low- ϵ_r candidates, due to the limited knowledge of the structure-property relationship. We have investigated the correlation between the accurate electron density (ED) distribution and the dielectric properties of porous MOFs, given that, the electronic distribution is at the base of systems polarizability. Among the known porous MOFs, $[\text{Cu}_3(\text{BTC})_2]_n$ (BTC=benzene-1,3,5-tricarboxylate) and the isostructural $[\text{Zn}_3(\text{BTC})_2]_n$ have been selected as they combine 69% of porosity, high structural symmetry, good single crystal quality and thermal stability up to 240°C[2]. The determination of ED have been obtained by using high resolution single crystal X-ray diffraction and density functional theory (DFT) calculations. Topological Analysis based on Quantum Theory of Atoms in Molecules (QTAIM) has been applied to characterize the nature of the interactions. We tested different desolvation procedures on single crystal defining its limits and improving the data quality of high resolution X-ray measurements for accurate ED determination. In addition, we adopted virtual desolvation algorithms to remove the contribution of the solvent to the diffraction. This procedure is unprecedented for high resolution data employed in ED modelling. A goal was that of monitoring the effect of the solvent on the electron density distribution, for example by comparing the theoretical simulations against experimental models for crystals with different levels of desolvation. DFT calculations in crystal phase of the static dielectric constant addressed the differences induced by changes on bond strength, coordination geometry, type of the metal ions and voids content. In addition, we recorded by impedance measurements, the frequency dependent dielectric constant behaviors of samples with different degrees of pores desolvation. Eventually, we addressed them to the structural features. From this research, it is clear that ED analysis could bring to a better understanding of the structural features that contribute more to material polarizability.

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Neutron Diffraction Instruments at SINQ Neutron Source

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In this poster, we will present the current status of the suite of neutron diffraction instruments at SINQ spallation neutron source of Paul Scherrer Institut [1]. The to-date experimental parameters, novel developments, and planned upgrades in terms of instrumentation, sample environment, resolution and Q-space for our two powder diffractometers DMC and HRPT, a single crystal diffractometer ZEBRA, and the Time-of-Flight diffractometer POLDI will be discussed.

[1] <https://www.psi.ch/lns-diffraction/neutron-diffraction>

Spin liquid in anion-disordered $\text{Tb}_2\text{Hf}_2\text{O}_7$ – an example of the importance of single-crystal neutron diffraction in physics; presentation of the new instrument ‘Zebra’ at SINQ

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Neutron crystallography plays an important role in physics. The technique allows to solve complex arrangements of magnetic moments as well as to provide useful insights into atomic structures.

In $\text{Tb}_2\text{Hf}_2\text{O}_7$, single-crystal neutron diffraction experiments indicate that correlations typical of a magnetic Coulomb phase develop despite a massive amount of structural disorder around non-Kramers ions [1]. A possible scenario is that the non-magnetic structural disorder transforms this Ising pyrochlore magnet into a quenched random transverse field Ising magnet, inducing quantum fluctuations. The result may be a quantum spin liquid state, which arises from long-range entanglement in the ground state wavefunction.

We take the opportunity here to present the new single-crystal thermal neutron diffractometer, Zebra, which has been built at the Swiss Spallation Neutron Source SINQ at PSI [2]. The instrument enables experiments that can tackle recent scientific challenges in condensed matter physics. Zebra is optimized for small samples and extreme sample environments, which enables to study materials available as small crystals only, or systems with interesting properties emerging at high magnetic fields, high pressures or very low temperatures. New optimized neutron-delivery system and nonmagnetic high-precision sample-positioning system are fully in operation since May 2017. At the current stage of the development of Zebra it is already possible to realize experiments in four-circle geometry or in tilt geometry, using either point or 2D detectors. A second detector unit available by the end of the year, comprising a graphite analyzer, will further the capabilities of the instrument for the measurement of weak diffraction signals.



4-Circle (2K–800 K) and tilt operation mode (0.05–325 K, fields up to 15 T) of Zebra.

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[2] We acknowledge funding from the Swiss National Science Foundation (R'EQUIP/SNF), the support from the University of Fribourg (K. Fromm) as well as the technical support from LDM/AMI@PSI for the design and construction work.

Adenine phase transformations in situ: crystalline, non-crystalline and in between

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Preparation of new polymorphs usually relies on classical crystallization processes, where different crystal forms are prepared by probing the mother liquor. Although this approach to polymorph screening is widely accepted and highly successful, other crystallization processes such as mechanochemical [1,2] and *in situ* screening [3] are also used. The main benefit of these approaches is that they rely on different crystallization mechanisms, thus the wider energy landscape of a solid state can be explored. These screenings, however, are usually carried out either at synchrotron sources, and their transfer to laboratory diffractometers is not straightforward.

This work addresses the identification of new polymorphs by *in situ* temperature-screening in a novel setup of the laboratory STOE STADI diffractometer, operating in transmission mode. The setup involves a suitable temperature chamber (*in situ* oven) and a multimodular MYTHEN2 detector. This enables the complete sets of *in situ* and high-resolution data to be collected in only two steps ($d_{\min} = 0.6 \text{ \AA}$, $2\theta = 74^\circ$).

Target material is adenine, a small molecule exhibiting two polymorphs that are comparably difficult to obtain as pure [4]. Throughout the probed temperature range, several crystalline polymorphs (previously known) and one liquid crystal state of adenine (previously unknown) could be identified and characterized, without having to isolate them from the matrix. Moreover, high temporal and angular resolution of the data allowed for the deeper insight in phase-transition processes to be obtained.

[1] Halasz, I. *et al.* (2013) *Nature Chemistry* **5**(1), 66-73.

[2] Gracin, D. *et al.* (2014) *Angew. Chem. Int. Ed.* **53**, 6193-6197.

[3] Jacques, J.D.M. *et al.* (2005) *Cryst. Growth Des.* **5**(2), 395-397.

[4] Stolar, T. *et al.* (2016) *Cryst. Growth Des.* **16**, 3262-3266.

Porous MOFs and molecular capsules for gas absorption based on anthracene derivatives.

Serhii Vasylevskyi and Katharina Fromm

University of Fribourg

The synthesis and study of new functional materials for the adsorption of potentially valuable energetic gases is an extremely demanding area in modern chemistry, since we have global warming issues causing climate change and natural disasters as a result. Therefore, reduction of the amount of CO₂ and CH₄ in the atmosphere is crucial for the green future of our globe.[1-2] Secondly, the high partial pressure of hydrogen can be decreased upon adsorption processes by porous materials which gives the possibility of sorption, storage and transportation of molecular hydrogen.[3] Then the absorbed hydrogen can be easily used as a fuel for industry and for cars due to its green product upon combustion with oxygen.[4] Thus, the synthesis of new materials for such purposes, especially metal organic frameworks (MOFs) is one of the key directions.

At this SSCr meeting we will present new MOFs and coordination compounds of Ni(II), Cu(II) and Zn(II) which have been synthesized with anthracene derived ligands. Their crystal structure was determined by single crystal x-ray diffraction. The complexes show different types of voids: open infinite 1-D channels with diameters ranging from 8 to 20 °Å, as well as 0-D capsules. Estimating the porosity by calculation with the crystallographic program PLATON, the complexes show 37-50 % of porosity. The determination of the sorption capacity by BET for CO₂, CH₄ and H₂ for the Ni-MOF and the capsule compounds of Cu(II) and Zn(II) will complete the study.

- [1]. K. Sumida, D. Rogow, J. Mason, T. McDonald, E. Bloch, Z. Herm, T.-H. Bae, and J. Long, Chem. Rev., 2012, 112, 724781.
- [2]. Z. Zhang, Y. Zhao, Q. Gong, Z. Lib and J. Li, Chem. Commun., 2013, 49, 653-661.
- [3] H.-C. Zhou, J. Long, O. Yaghi, Chem. Rev., 2012, 112, 673674.
- [4]. H. Furukawa and O. Yaghi, J. Am. Chem. Soc. 2009, 131, 88758883.

Characterization of superalloy coatings synthesized by cathodic arc evaporation

K. D. von Allmen (1), X. Maeder (2), J. Ast (2), M. Doebeli (3), M. Gindrat (4), A. Dommann (1), J. Ramm (5), A. Neels (1)

(1) Empa, Swiss Federal Laboratories of Material Science and Technology, Center for X-ray analytics, Überlandstrasse 129, CH-8600 Dübendorf

(2) Empa, Swiss Federal Laboratories of Material Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Feuerwerkerstrasse 39, CH-3602 Thun

(3) ETH Zürich, Labor für Ionenstrahlphysik (LIP), Otto-Stern-Weg 5, CH-8093 Zürich

(4) Oerlikon Surface Solutions AG, Metco Thermisches Beschichten, Rigackerstrasse 16, CH-5610 Wohlen

(5) Oerlikon Surface Solutions AG, Balzers Technology and Service Centre, Iramali 18, LI-9496 Balzers

Thermal barrier coatings (TBC) are used to increase the temperature at which gas turbines can be operated. [1] The bondcoat layer is a crucial part of this multilayer coating and only a few microns thick. It ensures a robust connection between the superalloy substrate and a porous oxide which is applied on top in order to dissipate heat. New methods which allow the preparation of bondcoat layers adapted to specific substrate compositions have been developed by Oerlikon Surface Solutions AG. Bondcoat layers obtained in this new process have been studied with different X-ray diffraction methods from which the phase composition, texture and information about stress have been obtained. Combined with information from electron microscopy and ion beam analysis a complete picture of the growth, the structure and chemical composition of the new bondcoat layers has been obtained. [2]

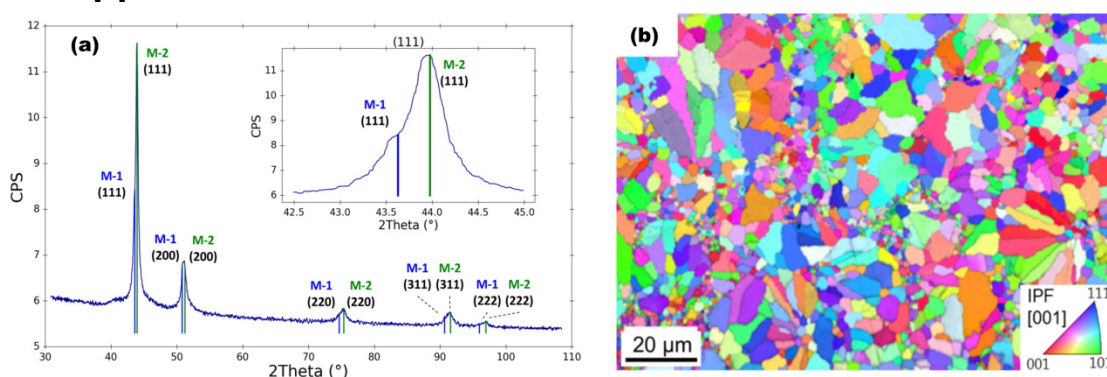


Figure 2 : (a) XRD pattern of a Ni-superalloy bondcoat layer on single crystalline α -Al₂O₃ (b) EBSD map of a Ni-superalloy target from which the coating was prepared.

[1] Clarke, D. R.; Oechsner, M.; Padture, N. P. *MRS Bulletin*, **2012**, 37, 891–898.

[2] J. Ast, M. Döbeli, A. Dommann, X. Maeder, A. Neels, P. Polcik, J. Ramm, K. Rudigier, K. D. von Allmen, B. Widrig, *Surf. Coat. Technol.*, **2017**, in Revision.

Secrets of diffuse scattering. How to probe elasticity and magneto-elastic waves using x-rays.

Björn Wehinger

Department of Quantum Matter Physics, University of Geneva

The first part of my talk focuses on the quantitative analysis of thermal diffuse x-ray scattering (TDS). I will show that high-precision measurements of diffuse scattering intensities together with a rigorous data analysis allow the determination of the full elasticity tensor in a single crystal diffraction experiment [1]. Our approach enables a reliable and model-free determination of the elastic properties and can be performed together with crystal structure investigation in the same experiment.

The second part is about Inelastic X-ray scattering (IXS) with meV energy resolution, which is an ideal tool to study lattice vibrations in crystals. IXS can be also sensitive to other degrees of freedom if strongly coupled to the phonons. One intriguing possibility is when polar phonons couple to spin waves in an ordered magnet. This creates electromagnons, quasiparticles that possess both magnetic and electric dipole moments. In this presentation, I will show, that the strong magnonphonon coupling in the triangular quantum magnet LiCrO₂ enables the measurement of magnetic correlations throughout the Brillouin zone via IXS. Our study reveals intricate details of the magnetoelastic excitation spectrum. We found single particle excitations with momentum dependent lifetime and continuum scattering at low temperature. Moreover, we observed over-damped modes, para-electromagnons, above the Néel temperature [2].

[1] Björn Wehinger, Alessandro Mirone, Michael Krisch and Alexei Bosak, Full Elasticity Tensor from Thermal Diffuse Scattering, *Phys. Rev. Lett.* 118, 035502 (2017).

[2] Sándor Tóth, Björn Wehinger, Katharina Rolfs, Turan Birol, Uwe Stuhr, Hiroshi Takatsu, Kenta Kimura, Tsuyoshi Kimura, Henrik M. Rønnow and Christian Rüegg, Electromagnon dispersion probed by inelastic X-ray scattering in LiCrO₂, *Nat. Comm.* 7, 13547 (2016).



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Swiss Crystallographic Association SGK / SSCr

General Assembly 2017

Tuesday, September 12, 2017, 12:50-13:50

Faculty of Science - University of Geneva, 30, quai Ernest-Ansermet – Geneva

Agenda of the General Assembly 2017

The minutes of our last General Assembly (Basel, Wednesday, August 31, 2016) are published on page 39-45 of the SGK/SSCr newsletter No. 98, July 2017 (this issue), which is also available electronically at <http://www.sgk-sscr.ch/newsletter/>

- 1) Determination of the quorum according to Art. 12/by-laws
- 2) Proposition for acceptance of the minutes of the General Assembly 2016, Basel
- 3)
 - a) Annual report/Jahresbericht / le rapport annuel
 - b) Annual financial statement /Jahresrechnung / les comptes annuels
 - c) Budget for the next year / Aufstellung des Budgets für das kommende Jahr / le budget proposé pour l'année suivanteElections / Wahlen / Élections
- 4)
 - a) definition of a chairperson for the elections
 - b) confirmation of the present board members
 - c) confirmation of the delegates for the Swiss Steering Committee of SNBL: Gervais Chapuis and Radovan Cerny
 - e) election/confirmation of the auditors
- 5) 2018 Meeting and General Assembly: Decision on location/organizer. Proposals are most welcome!
- 6) PhD Prize 2019 (rules, amount)
- 7) Anträge von Mitgliedern
other motions of members

Additional Information:

Year	Entries to SGK/SSCr	Exits from SGK/SSCr
2012	8	8 (since July 2012)
2013	7	15
2014	11	17
2015	23	18*
2016 (as of 06.06)	3	4
2017 (as of 17.07)	10	4

* in 2015, a large number of SGK/SSCr members (>10) have been excluded per decision of the Board because they were not paying the annual fees for more than 3 years, and could not be contacted.

Quorum for final decisions (Art.12, by-laws):

As of 17.07.2017, we have 206 records in our database.

They are grouped as:

- 9 of these are companies (or corporate members),
- 30 are "libraries" (incl. some "quasi-personal" members, from whom we don't expect any fees, but to whom we are regularly sending our Newsletters);
- 167 are personal members (full: 131, students: 32, honorary: 4)

I.e. for the quorum to be able to make decisions, we should have 10% out of 176 corporate and personal members, i.e. at least 18 people.

Board Members:

see last page of this newsletter

Delegates

IUCr: P. Macchi (Bern), Radovan Cerny, Geneva

ECA: J. Schefer (PSI)

IOCG: K. Fromm (Fribourg)

ScNat: P. Macchi (automatically assigned to the acting president)

Revisorenbericht für die Jahresrechnung 2016 der Schweizerischen Gesellschaft für Kristallographie (SGK)

Konten:

UBS	UBS	279-C0291110.0
Credit Suisse	CS	913652-00

Die Unterzeichneten haben Kenntnis genommen von der Jahresrechnung der Schweizerischen Gesellschaft für Kristallographie. Die Rechnungsprüfung betrifft die Periode vom 1. Jan. 2016 bis 31. Dez. 2016. Die Unterzeichneten stellen fest, dass die Abrechnung mit den vorgelegten Belegen übereinstimmt.

Am 31. Dez. 2016 ist der Stand der Konten und der Kasse:

UBS	SFr.	15'669.24
CS	SFr.	18'327.49
Kasse	SFr.	542.10
Summe SGK	SFr.	34'538.83

Die Unterzeichneten beantragen von der Versammlung die Entlastung des Kassierers und der Revisoren für die geprüfte Periode.

Ort / Datum
BERN, 21 Februar 2017

Unterschriften



B. Spingler
(Universität Zürich)



K. Schenk
(EPF Lausanne)

Financial Report

Summary SGK Finances	
Total 31.12.2015	34'713.46
UBS account	15'669.24
CS account	18'327.49
Cash on hand	542.10
Total 31.12.2016	34'538.83
Balance	-174.63

SGK Financial Report 2016	
<u>UBS Account</u>	
	CHF
UBS Balance 31.12.2015	15'892.54
<u>Income:</u>	
Membership dues	
full members (various amounts due to debts)	
82x40 +7x30 +5x70 +9x50 +1x53.85 +1x37 +1x35.50	4'416.35
Students 14x10	140.00
Companies 4x130 +1x390 + 1x390 (for 2017-2019) +1x118 +1x194	1'612.00
Reimbursement ScNat 2015	8'000.00
Interest	2.20
Total Income	14'170.55
<u>Expenses:</u>	
Membership dues to SANW (170 members)	1'190.00
ECM 2016 (Poster prizes)	511.00
Promotion ECM 2016 (Congrex invoice)	9'299.90
ECM Satellite Meeting in Nancy	1'000.00
Powder Diffraction School: PSI Villigen	2'000.00
Travel costs for ECA board meeting, Parma, IT (Fromm)	274.00
General expenses (switch)	8.90
Bank and Post expenses	110.05
Total Expenses	14'393.85
Income – Expenses	-223.30
Starting Balance + Income – Expenses	15'669.24
UBS Balance 31.12.2016	15'669.24

Cash on Hand - 2016

	CHF
Status 31.12.2015	542.10
Total Income	0.00
Total Expenses	0.00
Balance (Income – Expenses)	0.00
Starting Balance + Income – Expenses	542.10
Cash on Hand 31.12.2016	542.10

Credit Suisse (savings account)

	CHF
Status 01.01.2016	18'278.82
Interest (0.385% or 0.100%, resp.)	48.67
Withholding Tax*	-.-
<hr/>	
Balance 31.12.2016	18'327.49
*(only applicable when amount of interest exceeds CHF 200)	

SGK Budget 2018 To be proposed at the SGK assembly 12.09.2017

<u>Credits:</u>	Budgeted
Membership dues	5'000.00
SANW reimbursement for IUCr delegate	1'500.00
SANW master students travel grants	2'000.00
SANW contribution for SGK annual meeting	3'000.00
SANW contribution for PSI School	2'000.00
SANW contribution for PhD prize	1'000.00
Interest (est.)	100.00
<hr/>	
Total Income	14'600.00
 <u>Debits:</u>	
Membership dues to SANW	2'000.00
Annual meeting + poster prize	3'000.00
Travel Grants to Young Scientists	2'000.00
SGK support for PSI School	2'000.00
PhD poster prize	1'500.00
IUCr delegates	2'000.00
ECA national membership dues 2018	250.00
Bank charges	250.00
<hr/>	
Total Expenses	13'000.00
 Income – Expenses	1'600.00

Minutes of General Assembly 2016
Wednesday, August 31, 2016
Congress Center Basel, Room Rio, 12:00-14:00
Schweizerische Gesellschaft für Kristallographie

Agenda:

- 1) Determination of the quorum according to Art. 12/by-laws
- 2) Proposition for acceptance of the minutes of the General Assembly 2015, Neuchâtel
- 3)
 - a) Annual report/Jahresbericht / le rapport annuel
 - b) Annual financial statement /Jahresrechnung / les comptes annuels
 - c) Budget for the next year / Aufstellung des Budgets für das kommende Jahr / le budget proposé pour l'année suivante

Elections / Wahlen / Élections
- 4)
 - a) definition of a chairperson for the elections
 - b) confirmation of the present board members
 - c) elections of 3 new board members
(replacement for Petr Leiman, Jürg Schefer, Katharina Fromm).
Already available candidates are: Dr. Antonio Cervellino (SLS, PSI) and Prof. Enrico Gannini (Department Quantum Matter Physics (DQMP), University of Geneva). Further nominations should be communicated to the president prior to the meeting.
Candidates are asked for a short 1-2 minute oral presentation.
 - d) election/confirmation of the auditors and the ECA-delegates
- 5) 2017 Meeting and General Assembly: Decision on location/organizer. Proposals are most welcome!
- 6) PhD Prize 2017 (rules, amount)
- 7) Request from SERI for the administration of SNBL
- 8) Other motions of members

Minutes:

Formalities:

The General Assembly was chaired by Piero Macchi, President, and started at 12.00 h. The Agenda has been published in the Newsletter 96 on 15. July 2016 (Art. 11), point has been added after a request via email.

As keeper of the minutes the secretary Michael Wörle, ETH, was elected unanimously, no abstentions.

Ad 1.

With 40 members being present at this assembly, the necessary quorum of 10% (16) is reached to constitute a quorum (Art. 12). As per 31.08.2016 the SKG has 161 individual and 9 corporate members. A corporate member present is Dubravka Sisak (named according to Art. 14 of the bylaws)

Ad 2.

The minutes of the General Assembly 2015 on 14/09/2015 in Neuchâtel, reported in newsletter 95, have been approved unanimously, no abstentions.

Ad 3 a)

The president expresses thanks to Katharina Fromm and Jürg Schefer for the enormous effort organizing the ECM-30. A detailed report will follow in the next newsletter. Thanks to Michael Wörle for editing the newsletter 95 and 96 (with the collection of the Swiss crystallographic groups) and to Jürg Schefer and the PSI for printing of the newsletter

- The president reports on the meetings of the Swiss Academy of Science (ScNat): MAP meeting (Natural Science Sub-organisation of ScNat). The contribution has been CHF 9300.- for the ECM30.
- ScNat delegate meetings:
 - P. Macchi 23.09.2015
 - P. Macchi 23.3.2016
 - P. Macchi 27.5.2016

Next meeting: 23.9.2016. Budget decision.

- Prof. Aloysio Janner, member since 1969, founder Member of our society and recipient of the Ewald prize 2014, died on 27.01.2016
- Because of the ECM-30 there has been no Annual Meeting of the SGK/SSCr in 2016.
- Given the ECM-30 in Basel, no financial support has necessary for Swiss delegates to ECA (Katharina Fromm, Jürg Schefer) or for PhD/Master students.
- There has been one request of support for other meetings (Abrishamkar Afshin, 500.- CHF to attend the 5th International Conference on Metal-Organic Frameworks & Open Framework Compounds; oral presentation). Accordingly, the budget for supporting PhD/Master-students is not fully used. Afshin Abrishamkar will give his obligatory talk on the next SGK/SSCr-meeting.
- Future events:
 - Oct. 2018:
 - 1) 1-day celebration on the occasion of the 100th anniversary of the death of Paul Scherrer will be organized at PSI, likely October 2018;
 - 2) 8th edition of the Size-Strain conference (PSI) also in October 2018 (Local organizing committee: N. Casati, S. Van Petegem, A. Diaz, A. Cervellino)
Proposal of Katharina Fromm to combine the next annual meeting with either the 1-day celebration or the Size-strain-conference. Decision postponed.

- 3) Swiss-German joint meeting on crystal growth, 8-10th March 2017 in Freiburg (D). Dr. Enrico Giannini is co-organizer and delegate of SGK. Enrico Giannini gives an overview on this joint meeting. The SGK/SSCr got invited by the German Crystallographic Society. The announcement will be issued in October, and more info will be given in the next newsletter.

Ad 3 b)

The president Piero Macchi gives the financial report for 2016.

Summary SGK Finances

	CHF
Total 31.12.2014	37'744.97
UBS account	15'892.54
CS account	18'278.82
Cash on hand	542.10
ScNatCredit (paid on 08.01.2016)	8'000.00
Total 31.12.2015	42'713.46
Balance	4'968.49

UBS Account

	CHF
UBS Balance 31.12.2014	18'910.56
Income:	
Membership dues	CHF
full members (various amounts due to debts)	4'414.00
94x30 +14x60. +1x90 +1x150+2x50 +1x34+ 1x120 + 1x100 + 1x160	
Students 21x10	210.00
Companies 7x130	910.00
Reimbursement Congrex for ECM30 expenses	5'583.43
Interest	2.40
Total Income	11'119.83

Expenses:

	CHF
Membership dues to SANW (206 members)	1'442.00
Promotion ECM 2016 (Flyers PSI)	864.00
Promotion ECM 2016 (Congrex invoice)	2'000.00
IYCr2014 (Rumansch translation)	579.60
Travel costs for ECM committee (Fromm, Schäfer)	1'500.00
Annual Meeting (Neuchatel, CSEM)	3'000.00
Travel Grants (Germann, Finelli, Geschwind)	1'050.00
Travel expenses Simonov (flight and accommodation)	360.00
PhD prize	1000.00

Support for Zurich School of Crystallography	2'000.00
Association to ECA	179.78
Bank transfer cost	20.00
General expenses (switch)	15.50
Bank and Post expenses	126.97
Total Expenses	14'137.85
Income – Expenses	-3'018.02
Starting Balance + Income – Expenses	15'892.54
UBS Balance 31.12.2015	15'892.54

Cash on Hand - 2015

	CHF
Status 31.12.2014	626.90
Income:	
Total Income	0.00
Expenses:	
Post expenses	9.80
DHL expenses (VISA letter for Dr. Simonov)	75.00
Total Expenses	84.80
Balance (Income – Expenses)	-84.80
Starting Balance + Income – Expenses	542.10
Cash on Hand 31.12.2015	542.10

Credit Suisse (savings account)

	CHF
Status 01.01.2015	18'207.51
Interest (1.125% or 1%, resp.)	71.31
Withholding Tax*	-.-
Balance 31.12.2015	18'278.82

- The budget 2015 has been approved by the auditors Kurt Schenk and Bernhard Spingler (Bern, 11.03.2016)
- The budget 2015 was approved unanimously by the delegates, no abstentions.

Ad 3 c)

Budget 2017:

Income:

Membership fees

6'500

ScNat

5'000

Total Income

11'500.00

Expenses:

Membership dues to ScNat

1'200.00

Travel costs for IUCr delegates (Macchi, Cerny)

2'000.00

Annual Meeting

3'000.00

Travel Grants for PhD & Master

2'000.00

PhD prize

1'000.00

Support for Zurich School of Crystallography

2'000.00

Association to ECA

200.00

Bank and Administrative expenses

100.00

Total Expenses

11'500.00

Income – Expenses

-3'018.02

Starting Balance + Income – Expenses

15'892.54

UBS Balance 31.12.2015

15'892.54

The travel costs to attend the next IUCR meeting for the ECA delegates should be separate from the ECA (separate application). The president will ask at ScNat, if there is a possibility for SGK to deduct taxes.

The budget 2017 was approved unanimously by the delegates, no abstentions

Elections:

Ad 4 a)

Chairperson for the election is Piero Macchi (approved unanimously by the delegates, no abstentions)

Ad 4 b)

All present board members are confirmed unanimously:

Piero Macchi (president)

Antonia Neels (vice-president and treasurer)

Michael Wörle (secretary)

Antony Linden

Céline Besnard (website manager)

Ad 4 c)

New Board Members, in replacement of Katharina Fromm, Jürg Schefer and Petr Leman. Candidates proposed by the board members:

Antonio Cervellino (PSI)

Enrico Giannini (University of Geneva), replaces Katharina Fromm

Olha Sereda (CSEM)

All candidates are accepted unanimously by a collective election (no abstentions).

Ad 4 d)

Both auditors were reelected unanimously with no abstentions: Bernhard Spingler and Kurt Schenk

Both ECA delegates were reelected unanimously with no abstentions:

Antony Linden

Katharina Fromm

Ad 5)

Next annual meeting:

Candidate: Univ. Geneva

Celine Besnard, Radovan Cerny, Enrico Giannini

Date: early September 2017, before beginning of the semester

Subject: to come

Ideas:

- Katharina Fromm proposed to contact industry concerning crystal growth.
- SwissFel will have the first measurements in Okt.-Nov- 2017

Ad 6)

PhD prize 2017

Prize money is currently 1'000 CHF, will be increased to CHF 2000.-

Rules:

Thesis defended between June 2015 and May 2017.

Three external (out of Switzerland) referees coordinated by a Swiss delegate (out of the board)

Invitation as speaker at the next annual meeting

Submission deadline is preponed from May to April 30, 2017

Decision June, 30 2017

After discussion it seems desirable to have more time for evaluation, accordingly the submission deadline is 30th April 2017. Further, for submission only the thesis should be required, no publications. An increase of the prize money to CHF 2000.- is accepted unanimously, 0 abstentions.

Ad 7)

Prof. Gervais Chapuis

Request from SERI for the administration of SNBL

Prof. Gervais Chapuis has been invited for explanation of the details and discussion. The Office of the State Secretariat for Education, Research and Innovation (SERI) has changed the way to fund the Swiss Norwegian Beamline. In the past, SERI provided the Swiss financial contribution directly to the Swiss-Norwegian Foundation for Research with X-Rays (SNX foundation, co-chaired by Gervais Chapuis).

However, in the coming years fund raising should be done by one or by a consortium of several Swiss institutions (e.g. PSI, ETH, Universities), respectively, which may wish to entrust the operation of the SNBL to the SNX. SERI would like to interact with the institutions, which are proposed by the community of synchrotron users. Since there is no official association of synchrotron users in Switzerland, the Federal Office of Research believes that this role can be played by the Swiss Crystallographic Association.

The SGK/SSCr is asked to propose to SERI which Swiss institution could play now the role to raise and administrate the funds for SNX/SNBL. The PSI has already

offered to take this role (which actually already had in the past, during the early days of SNBL, before SNX).

Should the SGK/SSCr create a special committee, responsible for the large scale research facilities (like many other associations have) which then should take the corresponding decisions? In case the scheme is approved, a committee of interested persons (not only the board members of course) should be nominated.

- Piero Macchi proposed a committee from the SGK/SSCr collects ideas (not judging quality) and communicates to SGK/SSCr. SGK/SSCr will then communicate to SERI.
- Announcement of Yousef Asadi (IBAKH): PSI is willing to receive the money from SERI and administrate the SNBL.

A votation approved with 31 votes and 9 abstentions that:

- SGK/SSCr establishes a commission
- Gervais Chapuis is chairman of this commission

Minutes written by the Secretary
President
Michael Wörle, 31.08.2016

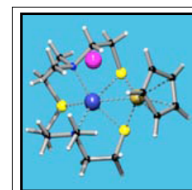
Approved by the
Piero Macchi

Reports of the Zürich School of Crystallography

The Zürich School of Crystallography Bring Your Own Crystals



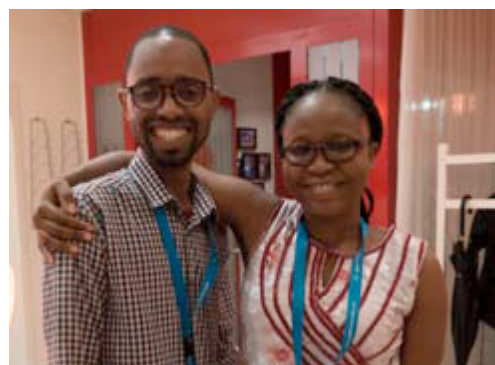
*University of Zürich
June 11 - 22, 2017*



The 7th Zürich School of Crystallography was held, as usual, within the Department of Chemistry at the University of Zürich (UZH). The 20 participants comprised 1 BSc, 1 MSc and 11 PhD students, 2 postdocs, 2 junior and 3 senior academics. They came from 16 countries: Benin, China, Croatia, Finland, Germany, India, Italy, Kazakhstan, Lithuania, Mexico, Russia, Saudi Arabia, Senegal, Switzerland, Thailand, and the United Kingdom. As usual, we had our usual popular 2:1 student:tutor ratio.



All of the participants were very enthusiastic and maintained their eagerness and dedication throughout the School. Everyone mixed well and chatted eagerly together and with the tutors over the meals and during the breaks. Some were just getting their feet wet in the field of crystallography, while others were more experienced, but all came away having learned something new and feeling better equipped to tackle structure determination on their own.



We were very impressed by two young scientists from Africa (Benin & Senegal), who were not only talented and keen to learn, but also eager to take their knowledge home in order to spread the word about crystallography in their region. These participants came highly recommended by Claude Lecomte and significant bursary support, donated by the IUCr, CCDC, and UNESCO was provided in order to facilitate their attendance.

The central goal of the School is to equip each participant with enough knowledge of the theory and practice of X-ray diffraction and single-crystal small-molecule structure

determination so that they can competently determine their own structures when they return to their home laboratory. With this in mind, the practical sessions and example structures are designed to allow the participants to see behind the button-pushing, to



learn about the actual procedures going on when various operations are performed, and to interpret whether or not the results obtained are appropriate. We successfully used the Olex2 software once again this year and found it to be quite suitable in the School environment. The ever expanding range of 2 special tools and option in the program for easily handling special modelling issues, such as disorder, are very useful. The daily schedule alternated lecture blocks and practical work so that the participants could readily associate the theory with the practical aspects. The practical work included access to five diffractometers at the UZH and ETH Zürich campuses and a

fully equipped computer classroom. The diffractometers included the modern Bruker Photon 100 and the newest Rigaku Oxford Diffraction Synergy instruments which are impressive in terms of speed, the availability of two radiation wavelengths and detector sensitivity.

We increased the number of real-case example data sets from two to three and some of the special features within Olex2 were demonstrated with three additional data sets. The participants then worked on a data set collected from one of the samples they had provided. The ease of use of Olex2 allows us to demonstrate more aspects of structure solution and refinement in a shorter time. On the final day, each participant sat a two-hour written exam either to obtain ECTS credit points or to self-test their knowledge. Each day concluded with a short discussion where participants can express their feelings about their experience that day. This year we shortened the School by two days by dropping the scientific excursion and the ten minute participant presentations. We had been concerned

that the participants were worrying too much about preparing their presentations from



midway through the School, rather than concentrating on the material we were trying to teach. While giving a short presentation is good experience, we think that it is not essential for the aim of the School. A side benefit of the shorter School is the reduced subsistence costs. We concluded that this change was beneficial and will repeat the shorter format for the next School planned for June 2019. The questionnaire filled in by the

participants provided overwhelmingly positive feedback. The perennial criticism is the intensity of the School. Participants often wish for more breaks so they can digest the content better. To do so would add accommodation costs and require more time from our team of dedicated tutors, so we feel people have to accept that it is an intense block course, unlike a semester course. Each participant received a certificate and a copy of "Crystal Structure Refinement, A Crystallographer's Guide to SHELXL" by Peter Müller, kindly donated by the IUCr and OUP.

The personal impressions of one of the participants are given below. We are very grateful for the generosity of the sponsors and supporters: Department of Chemistry of the University of Zürich, Swiss Society of Crystallography, Cambridge Crystallographic Data Centre, European Crystallographic Association, International Union of Crystallography, Oxford University Press, Rigaku Oxford Diffraction, Dectris Ltd, Oxford Cryosystems, Hotel Coronado, Zürich, the Chemistry Platform of the Swiss Academy of Sciences, and MiTeGen.

Tony Linden, Hans-Beat Bürgi, School Directors

The Zürich School of Crystallography 2017 – Report from a participant

The Zurich crystallography school exceeded all of my expectations in terms of the quality of tutors, lectures, layout and venue. I was very impressed with the university, hotel and the convenience of the hotel being just a short walk through the park, which provided a nice place to relax in when we were able to.

Having a background in powder diffraction, I had previously not been happy with my grasp of some of the concepts of crystallography. These very difficult concepts were explained clearly and in several ways to us by the tutors. I feel so lucky to have been given the opportunity to learn from such experienced crystallographers, and having one tutor per pair of participants was incredibly beneficial to us. They all went above and beyond, very eager to answer questions at any time and spend time with participants - even late in the evening! Since crystallography is used in so many areas of science, I was concerned about having many topics that weren't relevant. This was not the case and I ended up really learning a lot from the less relevant talks. My other main concern was about the intensity of the course, of which I was warned, however with so many breaks throughout the day and a carefully planned schedule alternating between lectures and practical sessions this wasn't a problem.

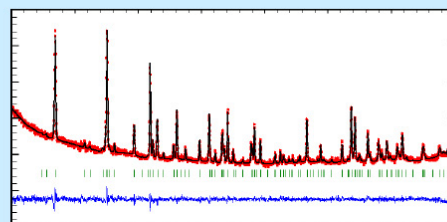
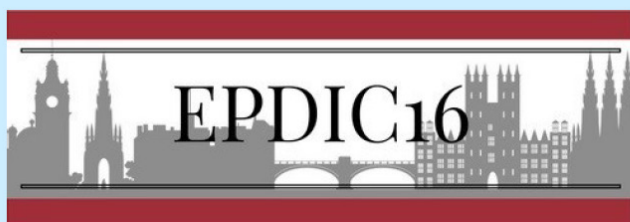
The organisers clearly spent a lot of time working out the best way to arrange everything, and this made a huge difference. The practical sessions were invaluable, especially being able to measure our own crystals on the instruments we use in our home institutions and then actually analyse this data. All the practical exercises were

incredibly useful and taught us how to handle a variety of different challenges that we are likely to face. It was so enjoyable to interact with the tutors and other participants, I appreciated having a mixture of people from such different backgrounds to learn from and socialise with. Zurich is a beautiful place and we were lucky to have a day off to explore the city. From this course I feel like I have gained knowledge of the theory of crystallography as well as all the practical aspects I need to go forward, including how to measure and solve crystal structures, which I would not have had the opportunity to learn elsewhere. This is vital for my current position as well as future career, as being taught correctly and thoroughly now will enable me to use this and pass on this knowledge in the future. The course also gave me a greater appreciation of crystallography than I had previously, and has inspired me to consider new career paths within this area. I highly recommend this course for anyone wanting to gain a proper understanding of crystallography and learn from the best of the best!

Emily Reynolds, University of Oxford, UK

Meetings, Conferences, Workshops, Schools, Courses

16th European Powder Diffraction Conference



16th European Powder Diffraction Conference



**1 - 4 July 2018 John McIntyre Conference Centre
University of Edinburgh, Edinburgh, UK**

<http://epdic16.efconference.co.uk/>



ECM31 in Oviedo



The **31st European Crystallographic Meeting**, ECM31, will take place in the Palace of Exhibition and Congresses (PEC) in Oviedo, Spain, from 22-27 August 2018.

ECM31 is setting up an attractive programme covering the latest advances in crystallography and related sciences to attract young and senior scientists as well as companies and general public.

One extensive agenda for accompanying people will be offered, with special attention to babies and children, with a specific programme of baby-care and children activities during the conference. Asturias, and the city of Oviedo in particular, is a cultural, active and organized region of open minded, hospitable and altruist citizens. Asturias may be easily reached by air, train or car.

The PEC has a spectacular urban design and offers a modern, functional and versatile infrastructure with all facilities. For all these reasons, ECM31 will be an effervescent and fruitful scientific, social and commercial meeting with many learning opportunities in every current aspect of crystallography.

<http://ecm31.ecanews.org>



<http://ecm31.ecanews.org/en/>

INTERNATIONAL SCHOOL OF CRYSTALLOGRAPHY

52nd Course: QUANTUM CRYSTALLOGRAPHY

ERICE-SICILY: 1 – 10 JUNE 2018

Sponsored by the: • European Crystallographic Association • International Union of Crystallography
• Italian Ministry of Education, University and Scientific Research • Sicilian Regional Government

PROGRAMME AND LECTURERS

X-ray constrained wave functions

• D. JAYATILAKA, University of Western Australia, AU

Atomic polarizabilities and dielectric properties of crystals

• P. MACCHI, University of Bern, CH

Crystal orbital theoretical calculations

• B. CIVALLERI, University of Turin, IT

Electron charge and spin density

• N. CLAISER, University of Lorraine, FR

Chemical Bonding in solids

• J. CONTRERAS, Sorbonne University, FR

Electron charge and spin density

• M. DEUTSCHE, University of Lorraine, FR

X-ray constrained wave functions

• B. DITTRICH, University of Düsseldorf, DE

Femto-second X-ray diffraction

• T. ELSAESSER, Max Born Institute, Berlin, DE

Properties from periodic wave functions

• A. ERBA, University of Turin, IT

X-ray constrained molecular orbitals

• A. GENONI, CNRS, FR

Calculations of electronic structures in crystals

• P. GIANNOZZI, University of Udine, IT

Experimental atomic forces in crystals

• F. GIESSIBL, University of Regensburg, DE

Electron density in momentum space

• J. M. GILLET, Ecole Centrale Paris, FR

Hirshfeld atom refinement

• S. GRABOWSKI, University of Bremen, DE

Charge density in biomolecules

• B. GUILLOT, University of Lorraine, FR

Dynamics in crystals

• A. MADSEN, University of Copenhagen, DK

Quantum crystallography

• L. MASSA, City University of New York, NY, US

Quantum chemistry in protein crystals

• K. MERZ, Michigan State University, MI, US

Electron density from electron diffraction

• P. NAKASHIMA, Monash University, AU

Dispersion corrected DFT methods for solids

• M. NEUMANN, Avangarde, DE

Accurate X-ray diffraction measurements

• J. OVERGAARD, University of Aarhus, DK

Experimental quantum chemistry

• M. RAHM, Chalmers University, SE

Quantum crystallography and crystal engineering

• M. SPACKMAN, University of Western Australia, AU

Bonding and properties in metal organic solids

• W. SCHERER, University of Augsburg, DE

QM/MM approaches in bioinorganic chemistry

• U. RYDE, Lund University, SE

More Info: <http://crystalalice.org/2018/>

German-Austrian Conference on Crystal Growth

German-Austrian Conference on Crystal Growth



13-16 Februar, 2018
Vienna, Austria

For further information about the conference, please contact to the responsible persons:

- Dr. Wolfram Miller Email: wolfram.miller@ikz-berlin.de Tel.: +49 761 4588 5636
- Dr. Andrey Prokofiev E-mail: andrey.prokofiev@tuwien.ac.at Tel.: +43 1 58801 13113

Calls for proposals

Beside normal proposals, most facilities allow urgent beam time requests. Please check directly with the facility.

Facility	Deadline(s)	Link
SLS: Swiss Light Source All except PX lines Protein crystallography beamlines (PX)	15.03. and 15.09. 15.04. and 15.10.	www.psi.ch/useroffice/
SINQ: Swiss Spallation Neutron Source All instruments (regular calls)	20.02.2018 (no beam in 2019 due to guide upgrade)	www.psi.ch/useroffice/
SINQ/SLS Joint x+n proposals (MS/HRPT)	15.02.2018	www.psi.ch/useroffice/
SpS: Swiss Muon Source All instruments	31.12. and 10.06	www.psi.ch/useroffice/
ESRF: European Synchrotron long term proposals short term proposals	15. Jan. 2018 10.10.2017	www.esrf.eu/ UsersAndScience/
ILL: Institut Laue Langevin All instruments	14. Sept. 2017	www.ill.eu/
FRM II: Heinz Maier-Leibnitz All instruments Rapid access program	08.09.2017 28.07.2017	www.mlz-garching.de/user- office/ www.mlz-garching.de/user- office/
SNS Spallation Neutron Source Oak Ridge	11.10.2017	neutrons.ornl.gov

Calendar of forthcoming meetings

(Please mail the missing information on meetings of interest to woerle@inorg.chem.ethz.ch)

Application Deadline

2017

Aug. 21-28	Hyderabad, India	The XXIV Congress & General Assembly of the International Union of Crystallography (IUCr-2017) http://www.iucr2017.org	31.05. (early bird)
Sept 12	Geneva	Annual SGK/SSCr-Meeting http://www.sgk-sscr.ch/en/geneva2017/	

2018

Aug. 21-29	Oviedo, Spain	31 th Meeting of the European Crystallographic Association http://ecm31.ecanews.org/en/index.php	20.07.2018
June 1-10	Erice, Italy	Erice International School on Quantum Crystallography	30.09.2017
July 1-4	Edinburgh, UK	16 th European Powder Diffraction Conference	To be announced

2019

Aug.	Vienna, Austria	32 th Meeting of the European Crystallographic Association http://ecm32.ecanews.org/	to be announced

Become a member of SGK/SSCr

If you are working in the field of crystallography, you might be interested in becoming a member of our society. For more information as well as online registration, please go to our website (<http://www.sgk-sscr.ch>).

Presently, the yearly membership fee is CHF 40 (CHF 10 for students).

SGK/SSCr is a member of the Swiss Academy of Science.



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Accademia di scienze naturali
Académie des sciences naturelles



(If you would like to see your logo here, please contact our treasurer, Dr. Antonia Neels)



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Société Suisse de Cristallographie
Società Svizzera di Cristallografia
Societad Svizera per Cristallografia

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