



Schweizerische Gesellschaft für Kristallographie  
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Swiss Society for Crystallography

Sektion für Kristallwachstum und Kristalltechnologie  
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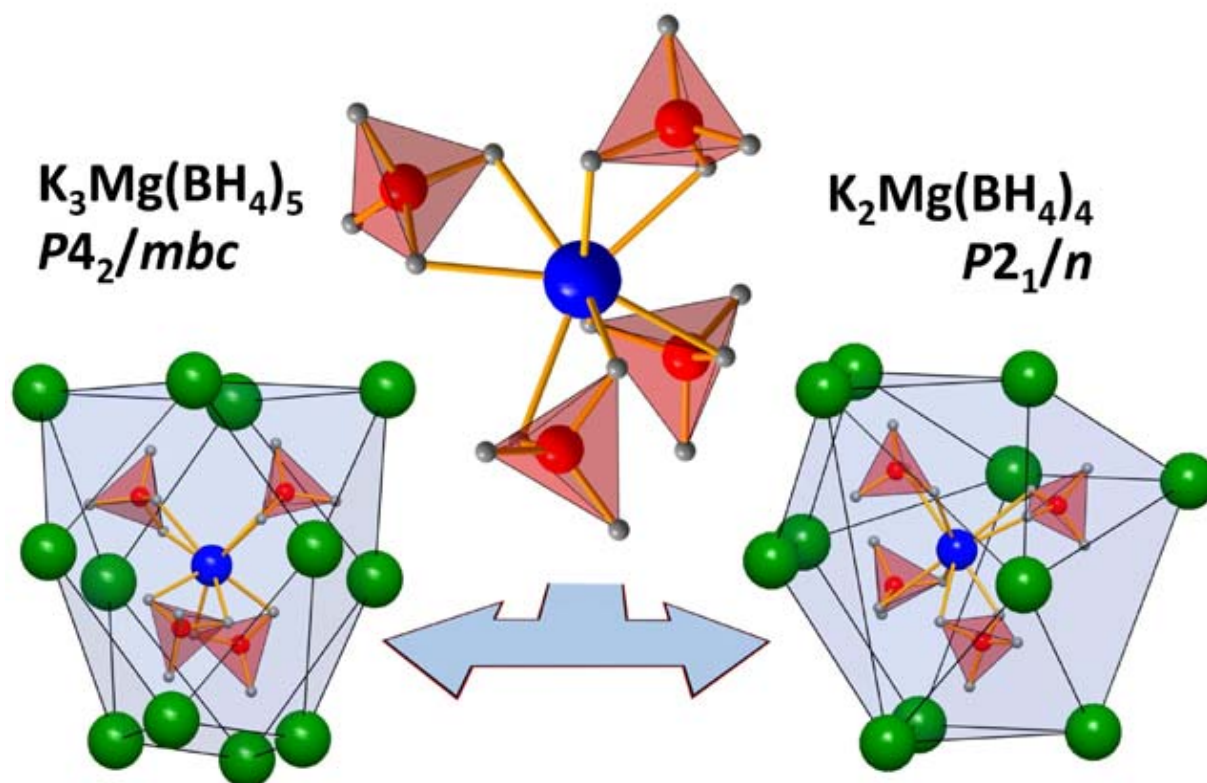
## SGK/SSCr NEWSLETTER

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**In this issue:** SPS-SGK/SSCr joint annual meeting, June 21-22  
Annual Meeting of the SGK/SSCr June 21  
General Assembly of the SGK/SSCr 2012, June 21

**On the Cover:**

Bimetallic borohydrides: Joint methodological efforts and complex systems,  
atoms labels: K green, Mg blue, B red, H grey,  
see report on page 7.

## SGK/SSCr Newsletter No. 86

The President's Page	5
Bimetallic borohydrides: Joint methodological efforts and complex systems	7
Conference Report: International Symposium on Advanced Inorganic Nanomaterials, Namur, Belgium, 2011 (ACIN)	13
News for and from members	15
Welcome of new SGK/SSCr members	15
New personal members, missing Adresses	15
Travel grants for young SGK/SSCr members	15
Globi und die Professorin	16
New website: A preview	16
Electronic IUCr Newsletter	17
Recent publications by our members	18
Proposal of a European Crystallographic School (ECS) with a response from A. Linden and H.-B. Bürgi	20 21
Annual Meeting of the Swiss Physical Society, Zurich, June 21-22	22
Program of the Annual Meeting of the SGK/SSCr, Zurich, June 21	22
Venue and sponsors	23
Program	24
List of posters (June 21-22)	25
Abstracts of oral contributions	26
Abstracts of posters	33
Agenda of the Annual General Assembly 2012, Zurich, HCI J6, June 21	46
Summary SGK/SSCr Finances	47
SGK/SSCr Financial Report 2011	48
Budget 2012	50
Conference Flyers	51
Call for proposals: SLS, SINQ, SMS, ESRF/SNBL, ILL, FRM-II, SNS	53
Calendar of forthcoming meetings	54
Become a member of SGK/SSCr	56
Institutional members and supporting institutions	57



## **Dear members of the Swiss Crystallographic Society,**

This year, on behalf of the 100<sup>th</sup> birthday of Bragg's Law, our Society will try out a new model for our annual meeting: a joint conference with the Swiss Physical Society. The SPS is a larger sister society and belongs also, as we do, to the Platform "Mathematics, Astronomy and Physics" of the Swiss Academy of Sciences SCNat. They proposed a Bragg symposium, which made us discuss to have the annual meeting together in June. This 2-day event will thus also host our annual meeting as well as a session dedicated and organized by us. It will be held in June at ETH Zurich, and I cordially invite you to assist our meeting and session, and to also enjoy the contact with SPS which will also allow us to get in touch with a wider audience.



In August this year, during the ECM in Bergen, our Society will submit a bid for the annual ECA-meeting in order to bring the ECM to Basel in 2016. We hope that this event will come back to Switzerland soon. Many of you have already expressed their wish to help in the organization and we will certainly come back to you.

Finally, my term as president of our Society comes to an end this summer. This means that we will have to elect a new president for the next three years. Also, new members to the board of our Society will have to be elected. This is another important reason to participate in our annual meeting. I would like to seize the occasion and thank the board members who supported me so actively during these past three years, and thank you all for being members of our society.

With my best regards,

Katharina Fromm



## **Bimetallic borohydrides: Joint methodological efforts and complex systems**

Contributed by P. Schouwink and Radovan Černý  
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Complex multi-phase systems containing light and heavy elements as well as different kinds of disorder at the same time are a major challenge to solve unambiguously. Rarely one methodological approach is enough. A purposeful implementation of various mutually complementary experimental techniques is essential to obtain the whole picture. However, in the field of borohydrides, especially theoreticians and experimental X-ray crystallographers have frequently clashed with each other ever since the first report on the structure of  $\text{LiBH}_4$  [1], when it comes to accurate structural descriptions.

A promising energy storage material, different approaches on characterizing as well as synthesizing and tailoring these compounds provide a lot of space where experimentally as well as theoretically oriented researches may be at cross-purposes or in conflict with each other: thermodynamics, kinetics, stable structures and structural evolutions, influence of external parameters, phase equilibria, etc. Surprisingly, there is quite little overlap between results generated by theory and experiment.

Compounds prone to be applicable in hydrogen storage often show some degree of disorder induced by the rotational affinity of the  $\text{BH}_4^-$  tetrahedron. While ab initio calculations have a hard time dealing with disorder it can often be nailed quite well with experimental methods. On the other hand, absolute positions and correct orientations as well as space group ambiguities (H is not easily localizable from diffraction data) may be determined and resolved resorting to density functional theory (DFT), which in spite of its success in structure validation/correction [2-4] remains quite useless for prediction.

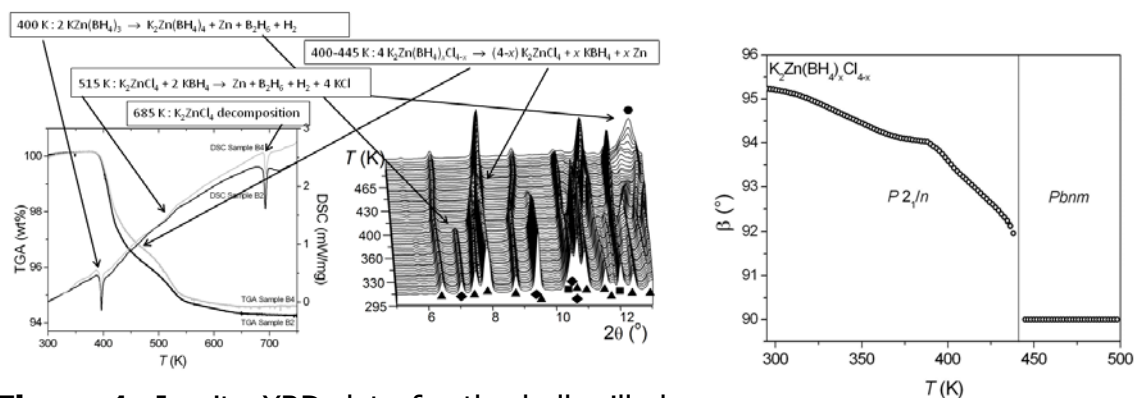
Here we present two case studies of how different techniques, experimental as well as theoretical (DFT), can complement one another. The recently studied complex hydride systems  $\text{KBH}_4 - \text{ZnCl}_2$  [5] and  $\text{KBH}_4 - M(\text{BH}_4)_2$  ( $M = \text{Mg}, \text{Mn}$ ) [6] both provide a comprehensive application of different techniques.

The choice of the synthesis pathway for metal borohydrides is very often the simple mechano-chemical one, i.e. ball milling. While wet chemistry is considered a useful way of obtaining the binary compounds, this is not so straightforward for the bimetallic, or even trimetallic ones, due to the increased number of components and competing phase equilibria of different potentially stable phases in a complex system.

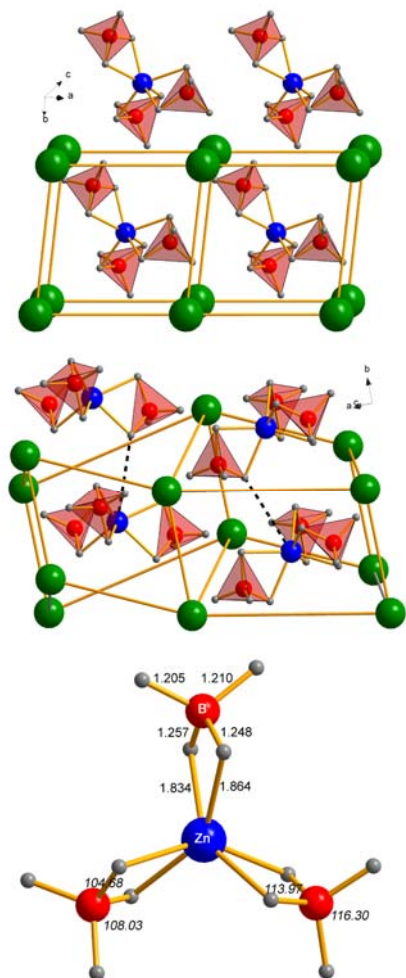
Compounds presented here were obtained by ball-milling, yielding very fine-crystalline powders of about 100 nm grain size. All structures were indexed and solved in direct space using the software FOX [7]. In many cases the ambiguity starts when assigning a space group, often there is no possible way of unambiguously achieving this with XRD when data quality is sub-optimal and patterns are multiphase. Concerning site-disorder, for example, a choice between many SG may be assisted by common sense and crystallographic headaches, but may also be facilitated by building different models, varying in local order and then performing ab initio calculations on these. A lucky situation arises when the model with the lowest free energy coincides with the model favored by common sense. This said, a fact that always counteracts this approach is

that DFT will work well when dealing with 0 K stable structures, ball milling and other synthetic approaches however often yield a phase anywhere in the P-T diagram.

In our first case [5], the system  $\text{KBH}_4 - \text{ZnCl}_2$ , an initially rather hopeless looking data-labyrinth was solved in quite an elegant way, making use of what is sensible and necessary. In situ powder diffraction data as a function of temperature ( $T$ -ramp) are shown in figure 1 for the ball-milled composition  $2\text{KBH}_4 : 1\text{ZnCl}_2$ .



**Figure 1:** In situ XRD data for the ball-milled composition  $2\text{KBH}_4:1\text{ZnCl}_2$  (middle) collected at SNBL ( $\lambda = 0.7035 \text{ \AA}$ ). TGA/DTA plot on the left and the structural evolution of  $\text{K}_2\text{Zn}(\text{BH}_4)_x\text{Cl}_{4-x}$  exemplified by the thermal behavior of the monoclinic angle  $\beta$  on the right. Reaction schemes are shown to correlate the different data sets (symbols see text).



The multiphase puzzle is solved by temperature aided decomposition, identifying the prior reported phase  $\text{K}_2\text{ZnCl}_4$  (triangles) first.  $\text{KZn}(\text{BH}_4)_3$  is indexed and solved shortly after (diamonds), thermal data and diffraction showing exactly the same event. Squares refer to  $\text{K}(\text{BH}_4)_x\text{Cl}_{1-x}$  and circles to the decomposition product  $\text{KCl}$ . A kink in the cell parameter evolution of  $\text{K}_2\text{ZnCl}_4$  (demonstrated on the monoclinic angle in figure 1), showing anomalous negative expansion at higher temperatures prompts to rethink its structure and composition. Irregular behavior in DTA supports this idea. It is correlated with a change in composition in the solid solution  $\text{K}_2\text{Zn}(\text{BH}_4)_x\text{Cl}_{4-x}$ , releasing  $\text{BH}_4^-$  at higher temperatures but initially thought to be a pure ternary chloride, and accompanied finally by a symmetry change  $\text{monocl} \rightarrow \text{orth}$  at  $440^\circ\text{C}$  (figure 1, right), while the monoclinic angle  $\beta$  approaches  $90^\circ$ , and while  $\text{KBH}_4$  is produced to buffer  $\text{BH}_4^-$  release (see reactions in figure 1). Interestingly,  $\text{BH}_4^-$  substitution on the chlorine site suppresses the ferroelectric phase transition reported for  $\text{K}_2\text{ZnCl}_4$ . The  $\text{KBrO}_3$ -derived trigonal  $\text{KZn}(\text{BH}_4)_3$  is brought into context with a compound of identical stoichiometry

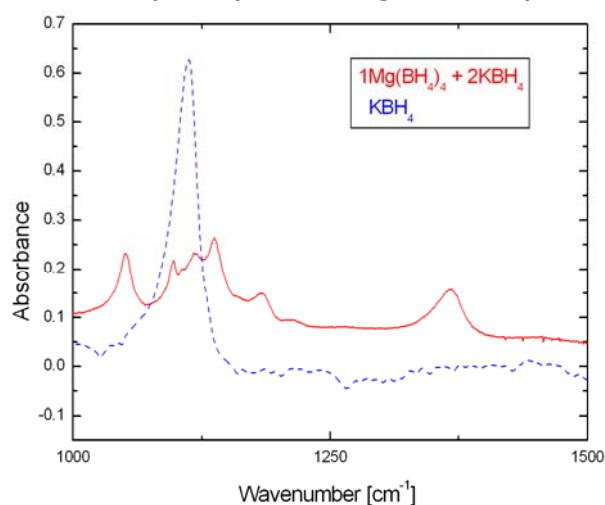
**Figure 2:** Top:  $\text{KZn}(\text{BH}_4)_3$ , middle:  $\text{NaZn}(\text{BH}_4)_3$  and  $[\text{Zn}(\text{BH}_4)_3]^-$  from DFT on  $\text{KZn}(\text{BH}_4)_3$ , bottom.



based on sodium [8,9]. The space groups of both are  $R\bar{3}$  and  $P2_1/c$ , respectively; a comparison is given in figure 2. A slight difference between the two is believed to be responsible for the lower symmetry of the Na-phase. It is evidenced in the higher symmetry of the complex anion  $[\text{Zn}(\text{BH}_4)_3]^-$  in  $\text{KZn}(\text{BH}_4)_3$ , namely  $D_3$  (32) (see figure 2). This is achieved by correlated rotation of all 3  $\text{BH}_4$  groups by  $16^\circ$  (angle between coordinating H-H edge and perpendicular direction to the plane of B atoms, figure 3, bottom) in the latter, while one group stands perpendicular to this plane in  $\text{NaZn}(\text{BH}_4)_3$ . While this is suggested already by semi-rigid body refinements making use of anti-bump restraints, it is unambiguously determined and validated in a quick convergence of a periodic DFT calculation. The rotation of this third  $\text{BH}_4$  group, likely induced by the larger potassium cation, allows the structure to avoid a short H-contact to the next complex anion  $[\text{Zn}(\text{BH}_4)_3]^-$  (dashed lines for  $\text{NaZn}(\text{BH}_4)_3$  in figure 2) and thus to circumvent strong distortion, resulting in a more regular  $\text{K}_8$  cage around the complex anion and a higher symmetry space group. The power of powder diffraction is well manifested here, an elaborate control of anti-bump restraints ensures getting a maximum from basically poor data, potentially biased however. This is where the power of DFT hits in, and allows to confirm the validity of the model.

The second case study [6] concerns the system  $\text{KBH}_4 - M(\text{BH}_4)_2$  ( $M = \text{Mg}, \text{Mn}$ ). The fact that Mg and Mn occur isostructurally here allows to draw some conclusions concerning bonding character and the influence electronegativity may have in isostructural compounds containing complex anions  $[M(\text{BH}_4)_4]^{x-}$ .  $\text{K}_2M(\text{BH}_4)_4$ , a pure borohydride though similar to  $\text{K}_2\text{Zn}(\text{BH}_4)_x\text{Cl}_{4-x}$ , was solved in  $P2_1/n$ , independently from the K-Zn system and assisted in analyzing the latter. Two questions arise here: (1) which is the  $M \dots \text{H}$  coordination scheme with the complex anion and (2) what effect does the difference in size and electronegativity of Mg and Mn have on  $[M(\text{BH}_4)_4]^{2-}$ . XRD alone, unlike neutron powder diffraction, even if done at high brilliance sources, is not capable of answering (1) on its own, due to the fact that even the most reliable and stable refinement is somewhat biased by introduced anti-bump restraints. In this case, the choice was to be made between bidentate, tridentate or 2+1 coordination. Vibrational spectroscopy (IR), sensitive to local order and the symmetry of central atom surroundings, and thus to different B-H stretching and bending schemes, strongly suggested the bidentate case. A molecular calculation was carried out on the  $[\text{Mg}(\text{BH}_4)_4]^{2-}$  cluster yielding the same result. This was then repeated in a periodic calculation, which showed up many interesting limits when performing DFT on this kind of compounds (e.g. necessity of introducing weak interactions, v.d.W., etc.), amongst others it expanded the unit cell in an unconstrained model, however steadily reproducing the  $M \dots \text{H}_2$  coordination scheme. The same was the case for a fixed lattice, also when all  $\text{BH}_4$  groups were inserted in random orientation. Knowing the  $M \dots \text{H}$  coordination scheme is of great importance to understand the compounds properly, and has always been a key parameter in structures containing  $\text{BH}_4$  groups [10]. The hydrogen release mechanism supposedly consists of narrowing of H-B-H angles, thus decreasing H-H distances below a critical value, this process may well be temperature dependent and will also depend on the metal hydrogen coordination scheme in addition to electronegativity of the metal cation. Concerning the ionocovalent bonding character we may tentatively draw an interesting conclusion with regards to  $\text{K}_2M(\text{BH}_4)_4$ .  $\text{Mn}^{2+}$  and  $\text{Mg}^{2+}$  have ionic radii of 80 pm and 71 pm, respectively, in tetrahedral coordination. Given this, we observe an inverse behaviour to what we would expect; not only does the Mn compound show the smaller unit cell volume, 1003.61(15) vs. 1012.66(15)  $\text{\AA}^3$  for Mg, but also on a local scale, i.e. regarding the nearest neighbors surrounding  $M$ ,

the inter-atomic distances are shorter. We assume this to be due to electronic effects, e.g. a higher degree of covalency in bonding due to the more similar electronegativities of Mn and the  $\text{BH}_4^-$  anion. The Pauling electronegativity of Mg and Mn is 1.31 and 1.55, that of  $\text{BH}_4^-$  is higher than 2 according to simple group electronegativities. The average distance  $M\text{-B}$  within the complex anion is 2.503(3) and 2.454(4) Å for Mg and Mn, respectively. While DFT already has its problems with the stable and well characterized  $\text{K}_2\text{M}(\text{BH}_4)_4$  phase, due to the high number of degrees of freedom and a shallow minimum, it is incapable of dealing with a second interesting phase found in this system, namely  $\text{K}_3\text{Mg}(\text{BH}_4)_5$ . This latter is host to pronounced dynamics already at room temperature. Derived from  $\text{Cs}_3\text{CoCl}_5$ , it contains 2 crystallographically distinct boron sites, one of them (B1) pertaining to a complex anion as found in  $\text{K}_2\text{Mg}(\text{BH}_4)_4$ , the other however in an octahedral environment of K, thus forming a  $\text{KBH}_4^-$ , i.e.  $\text{ReO}_3$ -like sublattice. K-B distances within this  $\text{BK}_6$  polyhedron are anisotropic and average ones larger compared to  $\text{KBH}_4$ . An assumed disorder due to this is coherent with a careful inspection of systematic extinctions. The most likely choice of space group is between  $P4_2bc$  and  $P4_2/mbc$ . While the former forces  $\text{B}_2$  in  $\text{BK}_6$  to be displaced off center in direction  $-c$  and  $+c$ , respectively, in adjacent  $\text{BK}_6$  chains parallel  $c$ , the latter allows for a much likelier solution of disordering around an average central position in the octahedron, thus this symmetry is adopted. DFT is at a loss here to validate this concept. However, while one single K-B distance in  $\text{KBH}_4$  leads to an isolated infrared active mode centered around  $1120\text{ cm}^{-1}$  (bending), produced by a  $\text{BH}_4$  group in an isotropic environment, in a lattice with differing K-B distances within a similar environment to  $\text{KBH}_4$  should lead to splitting of this mode, to lower (larger K-B distance) and higher (lower K-B distance) energies, respectively. An IR spectrum shows exactly this situation (figure 3). With raising temperature (IR data not collected yet) 1-dimensional positional disorder is enhanced along the  $c$ -axis. The motion of  $\text{B}_2\text{H}_4$  in turn causes K2 to disorder as well. The maximum extent of this disorder is evidenced in a phase transition to a higher symmetry  $I4/mcm$ , the symmetry of the prototype. This is triggered by reorientation of the complex anion  $[\text{Mg}(\text{BH}_4)_4]^{2-}$  due to close H-H distances of  $\text{BH}_4$  groups approaching one another (figure 4). Only diffraction is capable of detecting this sluggish transition, evidenced by the disappearing of weak reflections extinct by body centering. While symmetry changes, the  $a$ -axis evolves in a nonlinear fashion as a function of temperature, undoubtedly due to the re-orientation of  $[\text{Mg}(\text{BH}_4)_4]^{2-}$ , and thus to repulsive effects (figure 4a). The intensity of this phase post-transition however is so minor in in-situ XRD measurements that it is DTA which helps us to identify the decomposition event. An interesting phase-relationship between both the RT and HT phases brings us back to "common sense" and experience. Amongst the ionic-covalent oxides we find  $\text{Sr}_3\text{SiO}_5$  and  $\text{Ba}_3\text{SiO}_5$ , also derived from  $\text{Cs}_3\text{CoCl}_5$ .

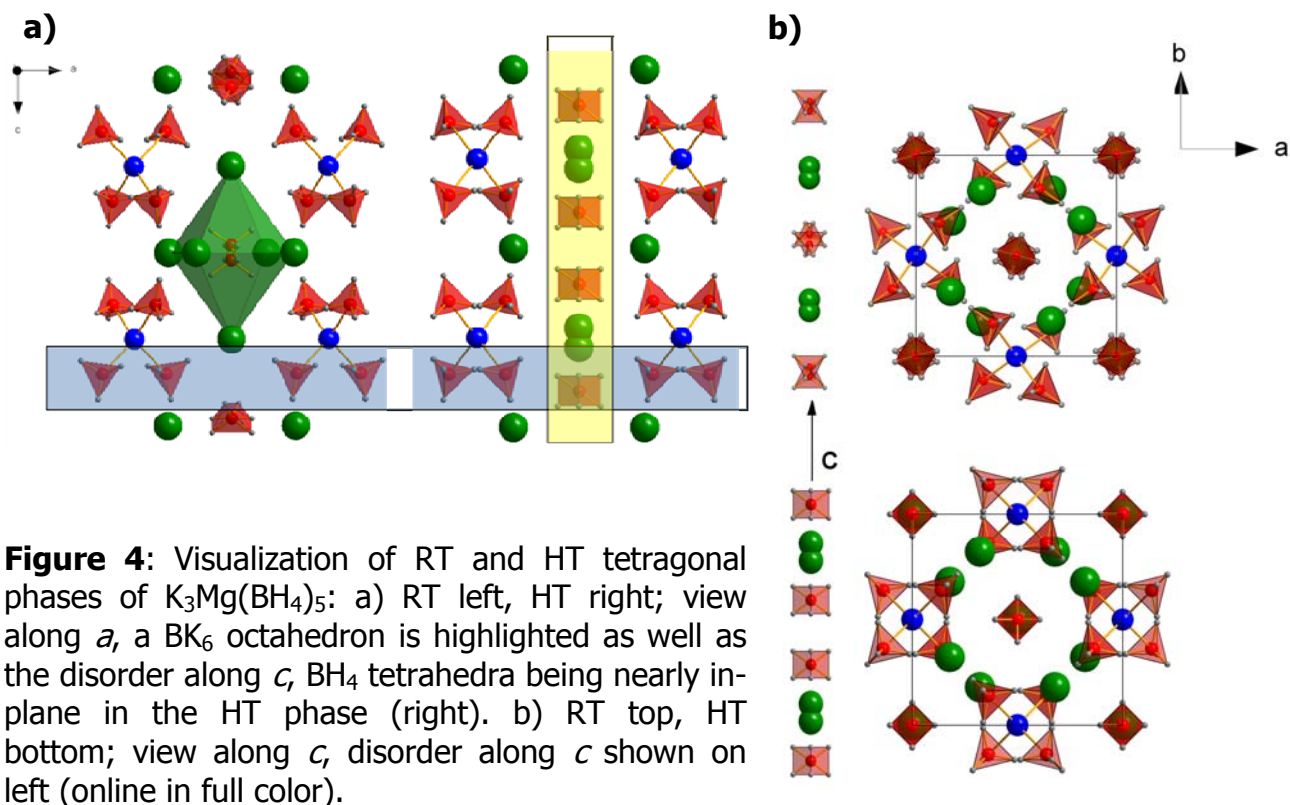


**Figure 3:** Infrared spectra of a mixture 1  $\text{Mg}(\text{BH}_4)_2$  : 2  $\text{KBH}_4$  (red, full line) and  $\text{KBH}_4$  (blue, dashed line). Color on-line version only.

fashion as a function of temperature, undoubtedly due to the re-orientation of  $[\text{Mg}(\text{BH}_4)_4]^{2-}$ , and thus to repulsive effects (figure 4a). The intensity of this phase post-transition however is so minor in in-situ XRD measurements that it is DTA which helps us to identify the decomposition event. An interesting phase-relationship between both the RT and HT phases brings us back to "common sense" and experience. Amongst the ionic-covalent oxides we find  $\text{Sr}_3\text{SiO}_5$  and  $\text{Ba}_3\text{SiO}_5$ , also derived from  $\text{Cs}_3\text{CoCl}_5$ .

While the Sr compound crystallizes in  $Pncc$ , the Ba-phase is found in  $I4/mcm$ , which corresponds to our HT phase. The difference in symmetry is related to the

different cation size which influences the orientation of  $[\text{SiO}_4]^{4-}$ . This is due to a size effect. Temperature enhanced disorder in  $\text{K}_3\text{Mg}(\text{BH}_4)_5$  may also be rationalized as a temperature-stimulated size effect.



The compound just presented above does not occur in the K-Mn system, it is still unsure if this is due to different reactivities and/or stabilities of reactants or a completely different P-T phase diagram of both systems. While this is the case, there is an additional very interesting phase in the manganese system, not occurring in Mg:  $\text{KMn}(\text{BH}_4)_3$ , which is a borohydride-perovskite (Pv). A lot of effort has been done since in our group and is going on to explore the Pv systems within the borohydrides, being potentially promising for fast-ion conductivity applications. It is assumed that the border for Pv formation due to cation size ratios is K-Mn, Mg is believed to be too small to form a Pv. This is supported by the fact that the first Pv phase is the HT phase in the K-Mn system, inherently subject to lattice expansion and possibly simulating a larger B-cation.

Only a joint methodological effort, hand-in-hand working of crystallographers, chemists and theoreticians can lead to a comprehensive understanding of complex systems such as bimetallic borohydrides, compounds of considerable importance for hydrogen storage and solid state battery applications.

We acknowledge a fruitful collaboration on borohydrides with the groups of the Phys. Chemistry Dpt. of the Geneva University (H. Hagemann, V. D'Anna, L.M. Lawson Daku), of Aarhus University (T. Jensen, D.B. Ravnsbaek, B. Richter, M.B. Ley), of the Catholic University in Louvain (Y. Filinchuk), and of the Inorg. Chem. Inst. in Bratislava (L. Smrčok).

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## Conference report ACIN 2011

International Symposium on Advanced Inorganic Nanomaterials, Namur, Belgium

Contributed by Yvens Chérémond, PhD student in the group of Katharina M. Fromm, Department of Chemistry, University of Fribourg

With support in form of a travel grant by the SSCr, I was able to participate at the International Symposium of Advanced Complex Inorganic Nanomaterials, ACIN 2011 (<http://webapps.fundp.ac.be/acin2011/>), which was held from September 11-14, 2011 in Namur, Belgium. This symposium has been organized by the Laboratory of Inorganic Material Chemistry (CMI) of the Université de Namur (FUNDP) and the Institute of Condensed Matter and Nanoscience (ICMN) at the Université Catholique de Louvain (UCL).

The nano-world has shown interesting properties in several fields like chemistry, catalyst, physics (for their interesting optic), magnetic, as well as mechanics and electrochemical properties. Thus, the aim of this international symposium was to keep up to date the scientific community in new advances and progress in the field of nano-materials. This program has focused on the fundamental and the applied aspect of the field of inorganics, ceramics, hydrides and bio-inspired materials. Another goal of this meeting was to promote the creation of a scientific network by offering several discussion forums in which scientific subject could be debated.

The ACIN 2011 has been organized through four main topics T1-T4, which contained not only new and advanced synthesis methods and architectures but also new applications and interesting properties.

T1: Nano-sized and nano-structured Materials :

Fundamental Aspects, Surface Science Mechanisms, Theoretical Models and Characterization.

T2: Advanced preparation methods :

New precursors, New methods including Sol-Gel processing, New materials, Processing and Shaping.

T3: Templated and Self-assembled (porous) materials including MOFs and hybrid materials.

T4: New Applications and New Properties :

Chemical (catalysis, sensors, gas storage) and Physical (spin crossover, magnetism, optics, conductivity,...) properties and applications in fuel cells, solar cells and batteries.

During the meeting, 6 plenary lectures, 6 keynote lectures, 5 invited lectures, 42 oral presentations and about 300 poster presentations have been given. A committee has been formed for choosing the best poster presentation for each topic.

### Our participation

Our group has given its participation in both an oral and a poster presentation, presented by Dr Nam-Hee Kwon and myself, respectively. The oral presentation title was "Nano-structured manganese-based cathode materials for high power and safe Li-Ion Batteries". My poster, entitled "*Precursors for iron conducting battery oxide materials*" was part of the second poster session. The goal of this poster was to present new hetero-bimetallic Lithium-Iron based aryloxide compounds. Those complexes have been studied in our group for their good volatility properties, as already shown earlier for Li-Co-compounds. Such Li-Co complexes have shown to be good precursors for the

low-temperature synthesis of HT-LiCoO<sub>2</sub> when heating to ca. 450 °C. For the same reason, Li-Iron based aryloxy complexes are still being studied in our lab with a view to discover new and low cost precursors for Li-Fe oxides, or, more generally, Li-metal oxides.

### **Highlights among the presentations**

Several oral and poster presentations have been useful for not only my project but also for projects of other group members. A very exciting talk in the plenary lecture session has been presented by Prof. Clare P. Grey from Cambridge University in this following topic: "Finding improved materials for lithium ion batteries: Challenges for materials chemists". This talk was an excellent overview of the challenges associated with building batteries. The resolution of them will be crucial for the next generation of electrical vehicles and other electronic gadgets. She has presented the development of new diagnostic methods to follow in-situ or ex-situ the working Li-Ion batteries by NMR methods and their applications in the popular paramagnetic cathode and anode materials.

A second particularly interesting talk in the plenary lecture session has given by Prof. Xiao-Ming Chen from the School of Chemistry and Chemical Engineering, Sun Yat-Sen University (Guangzhou, China). The topic was "Porous Metal-Azolate Frameworks (MAFs): Structural Control, Flexibility and Modification". Similarly to the Metal-Organic Frameworks (MOFs), Prof. Chen used metal ions or clusters as nodes and simple azolate ligands like imidazolates and triazolates to construct Metal-Azolate Frameworks (MAFs) which are porous coordination polymers. Simple azolate ligands have high tendency to form insoluble coordination networks in which metal-ligand bonds are very strong and rigid as in zeolite topologies, while the large cages can be expected to have molecular adsorption and storage properties.

For the keynote session, Prof. E. Coronado from the Universidad de Valencia (Spain) presented one of the best talks entitled "Inorganic Nanomaterials for Molecular Spintronics". Prof. Coronado has shown the role of chemistry in molecular nanomagnetism, particularly in molecular spintronics in three examples. In the first example Prof. Coronado talked on design of nanostructured magnetic materials exhibiting magnetic and electric conductivity properties. The second example concerned the electrical addressing of spin-crossover nanoparticles, and the last one on the design of the single molecule magnets using polyoxometalates.

Furthermore, Prof. J. M. Grenèche from the Université du Maine presented a keynote lecture on "Structural and magnetic properties of Fe-based nanostructures and mesoporous materials investigated by Mössbauer spectrometry". G.G. Morgan, under supervision of Prof. M. Albrecht from the University of Fribourg and University College Dublin, has presented an oral lecture on "Surface Ordered Iron(III) Molecular Switches".

### **Conclusions**

This symposium was very useful for scientists, more precisely for PhD students like me who need to keep up to date in the new scientific features. This scientific meeting was also a way to create new or to integrate existing scientist networks for future possible collaborations, which are essential for a vibrant scientific chemistry career. I therefore thank the SSCr for giving me the opportunity to participate in the ACIN 2011.

## **News for and from members**

**We welcome the following new members of the SGK/SSCr:**

### **Personal members**

Mr. Jean-Pierre BROG  
(Department of Chemistry Université de Fribourg, 1700 Fribourg, ph.D. student)

Dr. Pinar ALA BELEN  
(Laboratorium für Kristallographie, ETH Zürich, 8093 Zürich, post-doc)

Stef Smeets  
(Department of Materials, ETH Zürich, 8093 Zürich, ph.D. student)

### **Missing Adresses**

- Evans Shaun Russel, Chemistry and Biochemistry Departement, Bern
- Dan Xie, Laboratory for Crystallography, ETH Zürich
- Sebastian Basso, Laboratoire de Cristallographie, EPF Lausanne

Please report new contact address to the editor. Thanks.

### **Travel grants for young SGK/SSCr members**

The committee will award the grants according to the following rules:

- Preference is given to PhD students
- Proof has to be given that there are no grants available covering the expenses
- A supporting letter by the supervisor of the applicant is necessary
- Applicant **MUST** be a member of our society

If you wish to apply for a travel grant, please send the above mentioned documents to the president of the SGK/SSCr anytime. You should have been member for at least one year before applying for a grant.

Travel grants are good opportunity allowing young scientist to profit from our society in a period with low income. By becoming afterwards a long-term member of our society, you can return this good-will later to the next generation.

Details for applications are given at:

<http://www.sgk-sscr.ch/TravelGrants.pdf>

## Globi und die Professorin

Wer kann schon von sich behaupten, Vorlage für eine Figur in einem Kinderbuch zu sein? Die Ehre fällt der Freiburger Professorin Katharina Fromm zu. Sie stellt im neusten Globi-Buch als (gezeichnete) Person, die im Bereich Chemie tätig ist, ihre Arbeit vor. Das Buch «Chemie mit Globi», das zum Internationalen Jahr der Chemie 2011 erschien, entstand in Zusammenarbeit zwischen der Schweizer Akademie der Naturwissenschaften und dem Globi-Verlag unter Mitarbeit verschiedener Fachleute. Fromm erklärte laut einer Mitteilung der Uni Freiburg, die beschriebenen kindgerechten Experimente machten es zu einem «Lehrbuch, um Neugier zu befriedigen». Kinder lernten dadurch früh, Dinge zu hinterfragen.

Authorized reprint from the Neue Zürcher Zeitung (NZZ, 15. Aug. 2011, Niels Anner)

## New website: Preview

Contributed by C. Bésnard

We are in the process of redesigning the web page of the Swiss Society of Crystallography. Götz Schuck from the German Society of Crystallography has designed a new webpage using WordPress. Wordpress is a widely used Content Management System based on PHP and MySQL. It was chosen because it is both easy to use and powerful.

We are now transferring the content of the old web page into the new one. The current version of the new webpage is available at:

<http://cms.unige.ch/societes/SSCr/>

If you have any comments about the layout of this new web page and any wishes about its content, please contact me, so that we can improve our website.





## Electronic IUCr Newsletter (for WDC members only)

Editors : Judith L. Flippen-Anderson,  
William L. Duax  
Design & Production : Patricia Potter  
Assistant Editor Jane Griffin



Last issue in print

The *IUCr Newsletter* is distributed to 587 libraries and 17,000 crystallographers and other interested individuals in 84 countries. The IUCr also runs Crystallography Online, available at [www.iucr.org](http://www.iucr.org), as a complement to the IUCr print newsletter. Feature articles, meeting announcements and reports, information on research or other items of potential interest to crystallographers should be submitted to the editor at any time. Submission of text by electronic mail and graphics, slides or photographs by express mail is requested. Items will be selected for publication on the basis of suitability, content, style, timeliness, and appeal. The editor reserves the right to edit. Cost of distribution in Algeria, Australia, Colombia, Croatia, Cuba, Czech Republic, India, Italy, Japan, Malaysia, Poland, Portugal, South Africa, Switzerland, Taiwan, The Netherlands, Thailand, and Venezuela is borne by crystallographic associations or institutions or by individual crystallographers in these countries. Address changes or corrections and requests to be added to the mailing list should be addressed to the editorial office.

The newsletter is not available anymore in print and will not be distributed anymore by the SGK/SSCr. We did not transfer the E-Mail list to IUCr for privacy reasons.

If you are listed in the World Directory of Crystallographers (**WDC**, <http://www.iucr.org/people/wdc>), you can apply directly for electronic copies :

Just click all the boxes of the newsletters you like to receive in the future.  
The service is free of charge.

## Recent publications from our members

### Crystal Growth from High-Temperature Solutions

by Dennis Elwell and Hans J. Scheel  
published 1975 by Academic Press, London – New York

is now in parts available as an **electronic version** (December 2011) containing:

- Chapter 11 "Crystal Growth and LPE of High- $T_c$  Superconductors"
- Appendix A "Growth of Striation-free Crystals"
- Appendix B "Epitaxy and the Importance of LPE"

The file is available from the ETH library:

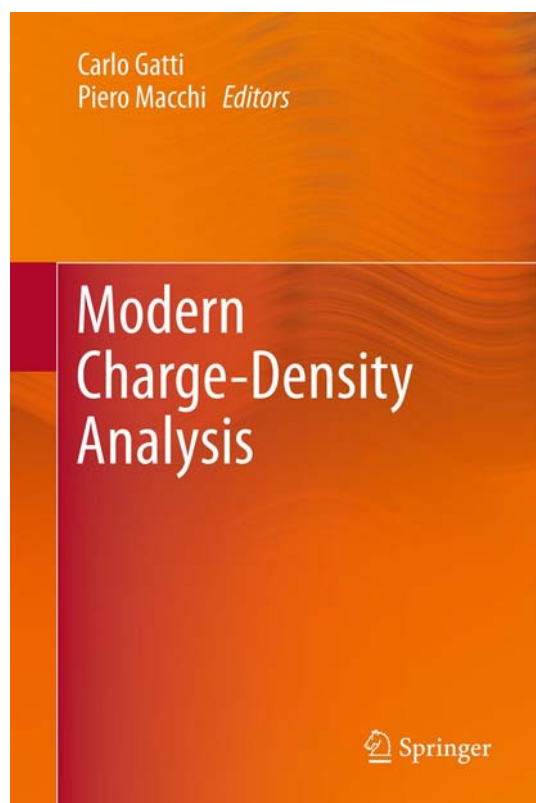
<http://e-collection.library.ethz.ch/view/eth:4822>  
696 pages, file size 224 MB.

For a book review of the 1975-hardcopy, we would like to refer to:  
<http://scripts.iucr.org/cgi-bin/paper?a13027> written by P. Hartmann, Leiden.  
This book itself is unfortunately out-of-print.

## Modern Charge-Density Analysis

C. Gatti and P. Macchi (Editors)

2012, 783 pages, 229 illustrations (181 in color), ISBN 978-90-481-3835-7



This book provides an extensive and up-to-date overview of the interdisciplinary field of charge-density analysis. It is a useful tool both for scientists already working in the field and scientists and PhD students who would like to familiarize themselves with the topic area. It may be of interest to chemists, physicists, crystallographers, materials scientists and biochemists.

*Modern Charge-Density Analysis* focuses on state-of-the-art methods and applications of electron-density analysis. It is a field traditionally associated with understanding chemical bonding and the electrostatic properties of matter. Recently, it has also been related to predictions of properties and responses of materials (having an organic, inorganic or hybrid nature as in modern materials and bio-science, and used for functional devices or biomaterials).

The first part of the book includes theoretical and methodological chapters which provide a wide ranging and up-to-date overview of the physics behind charge-density distribution and the most advanced methods to model and interpret it (from theory or experiment). In the second part, applications in several fields are presented ranging from Biomacromolecules to Energetic Materials. The effects of external stress (e.g. produced by temperature, pressure or photo-excitation) and the resultant electron-density response are analyzed. Implications for chemistry, biology and material science are described with an outlook on future developments. The ever-growing impact of charge-density analysis on modern fields of research including supramolecular chemistry, crystal engineering, complex magnetic materials, molecular reactivity and recognition is strongly featured.

*Modern Charge-Density Analysis* is inherently multidisciplinary and written for chemists, physicists, crystallographers, material scientists, and biochemists alike. It serves as a useful tool for scientists already working in the field by providing them with a unified view of the multifaceted charge-density world. Additionally, this volume facilitates the understanding of scientists and PhD students planning to enter the field by acquainting them with the most significant and promising developments in this arena.

## **European Crystallographic School (ECS) - A proposal to ECA now open for discussion**

Dr. Petra Bombicz, ECA Secretary  
e-mail: bombicz@chemres.hu

The Executive Committee of the European Crystallographic Association has received a proposal from Prof Michele Saviano, President of the Italian Crystallographic Association and Prof Carlo Mealli, Councilor of Italy, on establishing a European Crystallographic School (ECS), to be held annually in a different European country. The initiative has been considered with great interest at the winter meeting of the Executive Committee.

The ECA regularly provides financial support to schools within the ECA region. While still being committed to give regular support to these local initiatives, ECA intends to promote a high level European school that will become a regular event to be hosted each time in a different country. It will be planned to cover each time different aspects of crystallography. It will also be able to exploit a truly international board of renowned teachers, thus helping aggregate future scientists, and serving as a seed for new European scientific networks. The organization of a school at the European level will allow funding from European initiatives, such as the Erasmus Intensive Program. In this way, students or young scientists coming from countries where crystallography is less developed will find excellent opportunities for their advanced education and for starting new contacts and collaborations.

A more detailed description of the proposal on the European Crystallographic School (ECS) and Guidelines for applications to host an ECS, as well as Guidelines for the bidders can be found in the attached file.

The initiative is now open for discussion for a period of two months till 30 May 2012 giving time to discuss it within your National Association and also in the Council of ECA. An electronic voting procedure will take place about the establishment of the European Crystallographic School (ECS) based on the elaborated description and guidelines in the beginning of June 2012. In case of the positive decision of the Council it will allow two other months for preparation of the bid, June -July till the start of the ECM27. The bid presentation and voting on the bids, e.g. the venue of the 1st ECS will take place at the Council Meeting at ECM27 in Bergen. Thus the first ECS may take place in 2014, in the International Year of Crystallography.

The initiative of establishing a European Crystallographic School (ECS) is now **open for discussion till 30th May, 2012**. Please help the evaluation of the project with your and your colleagues' contribution to the discussion.

## **A response to the proposal to establish a European Crystallographic School**

Dear members of the ECA executive committee,

It is with great interest that we learned about the proposal from Prof. Michele Saviano, President of the Italian Crystallographic Association and Prof. Carlo Mealli, Councillor of Italy, on establishing a European Crystallographic School (ECS), to be held annually in a different European country.

Dr. Tony Linden and I would like to comment on this proposal in our capacity as directors of the Zürich School of Crystallography (ZSC), the fifth edition of which will take place at University of Zürich, from June 9 to 22, 2013. We will first summarize the nature of the ZSC, and then express our opinion concerning the proposal.

The ZSC was initiated in 2007 to help compensate for the fact that teaching of elementary and advanced crystallography is increasingly disappearing from the science curricula. The Zürich School of Crystallography fills a niche by offering a course that *allows young researchers in chemistry and physics to investigate crystals of immediate interest in their own research*. The students profit from a combination of theoretical concepts and hands-on experience in all steps of crystal structure analysis, from crystal growth to the interpretation and presentation of results. From our teaching experience over the years, we know that students working on their own problems in hands-on courses are among the most highly motivated.

*Our school* aims to teach the basics and not advanced topics. The audience is limited to 20 people, mainly MSc/PhD students and other *young* researchers. The students are supervised by 10 tutors who lecture on theoretical topics in the mornings and help with the hands-on work in the afternoons. To our knowledge the ratio of two students per tutor is unique among crystallography schools, has contributed significantly to the success of the school and is favourably remarked upon by the participants. Places in the school are now keenly sought after. The 80 chemistry and physics students who have attended our schools are an international lot coming from nearly all European countries, as well as Turkey, The Ukraine, Russia, Nigeria, India, Thailand, Hong Kong, Brazil, Venezuela and the USA. Several of them have begun to appear at the ECMs and IUCr meetings and one now even works for Agilent, thus showing that the school brings young blood into the field.

*Our opinion about the ECS project:* Given the scarcity of crystallographic teaching in science curricula we certainly support the idea of ECA schools, in particular those addressing advanced topics. We feel that ECA schools concentrating on advanced topics would be an ideal complement to our own efforts. Although the format of the biennial ZSC does not fit into the proposed ECS format, we hope that you will consider the ZSC as complementary to the ECA schools, continue to support our school in the future and help to avoid coincidences with respect to contents, dates and the search for external financial support (the next few schools are planned for odd years, starting in 2013 and are usually held in June).

We would be most grateful if you could take the above remarks into account during your deliberations and decisions.

*With best regards,*

*Tony Linden, University of Zurich  
Hans-Beat Bürgi, University of Bern*



## 2012 Meeting of the Swiss Society for Crystallography

### 100 Years of Diffraction: Historical Highlights and a Look Into the Next 100 Years

**June 21-22, 2012 ETH Hönggerberg, Zürich (Campus Science City)**

#### Abstracts and Program

The 2012 annual meeting and general assembly of the SGK/SSCr will be a two-day joint meeting together with the annual meeting of the Swiss Physical Society. All sessions and business of the SGK/SSCr will be conducted on June 21; posters can be displayed for two days.

Sessions will take place in the physics (HPH) and chemistry (HCI) buildings at the ETH Hönggerberg, Zürich.

A buffet lunch will be provided on June 21 for SGK/SSCr participants only and on June 22 for all registered participants. There is an apéro during the poster session on June 21, followed by a grill party (additional registration required).

More details of the SSCr component of the meeting are on the following pages and at:  
<http://www.oci.uzh.ch/group.pages/linden/sgk2012>

Full details, program and registration for the joint meeting are at:  
<http://www.sps.ch/>

An abstract booklet for the full meeting will be distributed at the registration desk.

**Registration deadline: June 1, 2012.** Registration is required so that catering can be arranged. Please register through [www.sps.ch](http://www.sps.ch) and only for the number of days you plan to attend. Late registration will incur a CHF 20 surcharge.

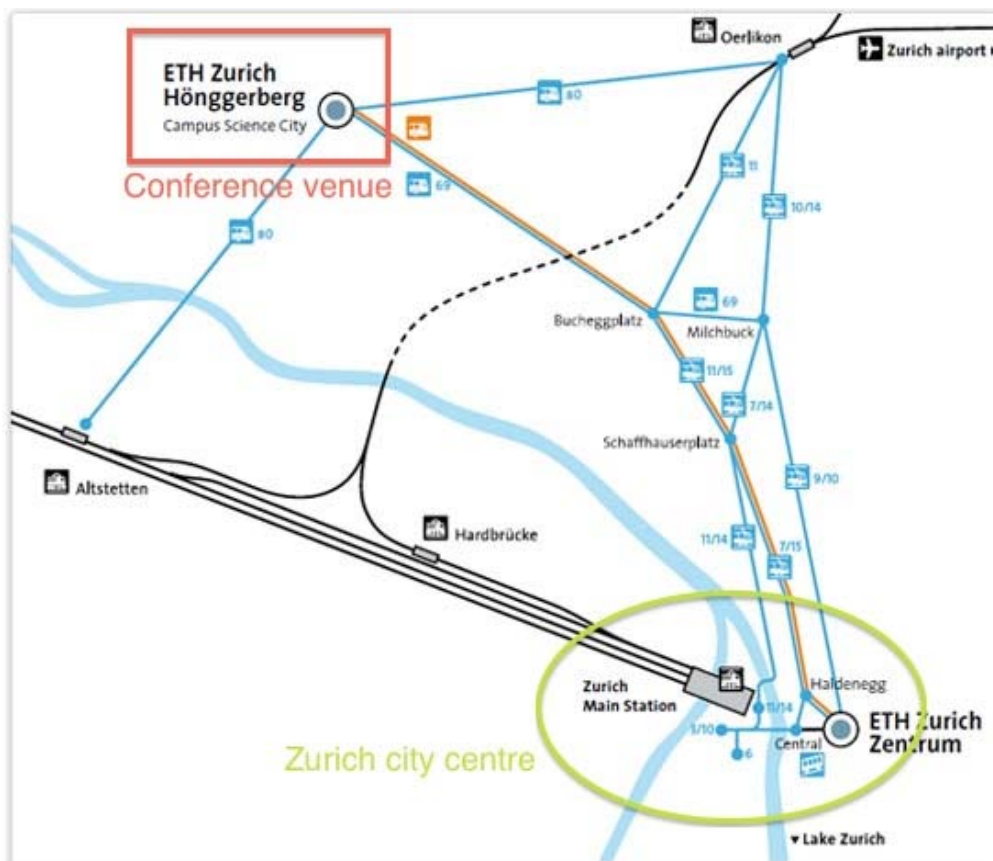
The organizer for the SGK/SSCr activities is Dr. Anthony Linden, Institute of Organic Chemistry, University of Zürich; e-mail: [alinden@oci.uzh.ch](mailto:alinden@oci.uzh.ch)

**Travel:** Parking is available in the underground garage (see the SSCr meeting website for driving directions). However, please use the excellent public transport. Directions and timetables are at:

[http://www.ethz.ch/about/location/hoengg/index\\_EN](http://www.ethz.ch/about/location/hoengg/index_EN)

<http://www.zvv.ch> (Bus Stop: Zürich, ETH Hönggerberg)

Please allow 25-30 minutes to travel from Zürich Hauptbahnhof to the venue.



**SGK/SSCr Meeting Sponsors:**

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Swiss Academy of Sciences  
Akademie der Naturwissenschaften  
Accademia di scienze naturali  
Académie des sciences naturelles



## Program of the SGK/SSCr annual meeting June 21, 2012

From 08.00 Registration / poster hanging (HPH foyer – also June 20, 16.00-19.00)

*Physics Plenaries* (HPH G1)

09.00-09.40 J. Fröhlich, ETHZ: From the QHE to Topological Insulators and on to Cosmic Magnetic Fields - a Unified Perspective

09.40-10.20 T. Giamarchi, Geneva: Quantum physics in one dimension

10.20-10.50 *Coffee break* (HPH foyer)

*SGK/SSCr Plenary - Chair: Gervais Chapuis* (HPH G1)

10.50-11.30 D. Schwarzenbach, EPFL: From Laue's discovery and the Bragg's key to the world of atoms to service crystallography

11.30-11.50 SPS Awards Ceremony (HPH G1)

### **11.50-12.30 SGK/SSCr general assembly (HCI J6)**

12.30-13.30 *Buffet lunch (SGK/SSCr participants only) in front of HCI J6*

*100 Years of Diffraction microsposium - Chairs: Jan Lacki & Anthony Linden* (HCI J6)

13.30-14.00 A.M. Glazer, Clarendon Laboratory, Oxford: The two Braggs

14.00-14.30 J. Lemmerich, Berlin: Max von Laue: the physicist and the upright man

14.30-15.00 L. Falvello, Zaragoza: The origins and development of macromolecular crystallography

15.00-15.30 A.L. Spek, Utrecht: Johannes Martin Bijvoet (1892-1980) and absolute structure

15.30-16.00 *Coffee break* (HPH foyer)

*The Next 100 Years microsposium - Chair: Michael Würle* (HCI J6)

16.00-16.25 B. Patterson, PSI: Novel structural studies with an X-ray Free Electron Laser

16.25-16.50 T. Weber, ETHZ: Investigating disorder as a matter of routine - the next steps

16.50-17.15 P. Willmott, PSI: The Materials Science Beamline upgrade

17.15-17.30 A. Neels, Neuchâtel: High Resolution X-Ray Diffraction applications for microsystems

17.30-17.45 D. Šišák, ETHZ: Powder Charge Flipping – input parameter optimization and solution evaluation

17.45-18.00 F. Gschwind, Max Planck Institute, Stuttgart: Intercluster compounds for nanosized materials

18.00-18.15 J. Schefer, PSI: News from the spallation neutron source SINQ: Diffraction

18.15-18.30 H. Grimmer, PSI: Density functional calculations of polysynthetic Brazil twinning in alpha-quartz

18.30-18.35 Poster prize and closing remarks

18.35-20.15 Poster session and apéro (HPH foyer)

20.15-22.30 *Grill party (registration required)*

**June 22** 12.00-13.30 Poster session continues (HPH foyer)

For the complete program of the Swiss Physical Society on June 21 & 22, see:  
<http://www.sps.ch/>



## List of Posters

- 71 E. Hovestreydt, H. Ott, M. Adam, M. Ruf, A moment in time: 100 years of X-Ray diffraction versus 100 days of PHOTON 100 CMOS detector
- 72 R. Caputo, Ab-initio crystal structure prediction. Metal borohydrides.
- 73 Q. Chen, A. Braun, J. Embs, T. Strässle, V. Pomjakushin, W. Mao, S. Clark, S. Holdsworth, N. Bagdassarov, Pressure modulated proton-phonon coupling and its relevance to ceramic fuel cell proton conductors
- 74 C.-L. Chanez, K. Fromm, Mixed-metal precursors for mixed-metal oxides
- 75 Y. Chérémond, K. Fromm, New penta-coordinate iron(III) aryloxide as initiators for ring-opening polymerization
- 76 L. Guenee, P. Chakraborty, R. Bronisz, C. Besnard, P. Pattison, A. Hauser, Light-induced low-spin structure of the bistable  $[\text{Fe}(\text{bbtr})_3](\text{BF}_4)_2$  compound
- 77 O. Zaharko, M. Pregelj, A. Günther, A. Loidl, V. Tsurkan, Magnetic ground state and 2D behavior in the pseudo-Kagomè layered system  $\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Br}$
- 78 O. Sereda, A. Neels, A. Dommann, P. Hess, A. Mazzalai, P. Mural, XRD investigations on PZT layers for actuator systems
- 79 P. Schouwink, L. Smrcok, R. Cerny, Novel trimetallic borohydrides
- 80 N. Aliouane, M. Christensen, J. Schefer, K. Lefmann, TIPSII hybrid spectrometer at the European Spallation Neutron Source ESS: Probing multiple length scales in one instrument
- 81 R. Sura, M. Ceretti, W. Paulus, J. Schefer, L. Keller, K. Conder, E. Pomjakushina, B. Pederson, Neutron diffraction and Oxygen Isotope Back Exchange studies in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4\pm\delta}$  ( $x = 0, 0.05, 0.15$ ) crystals as a function of temperature
- 82 R. Warshamanage, A. Linden, Our fascination with crystals and crystallography – a 7500 year timeline

## Abstracts for the SGK/SSCr annual meeting June 21, 2012, Zürich

**Plenary 3:** From Laue's discovery and the Bragg's key to the world of atoms to service crystallography

Dieter Schwarzenbach

Cristallographie, IPSB, EPFL, Le Cubotron, 1015 Lausanne, Switzerland

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The X-ray diffraction experiment of Friedrich, Knipping and Laue in 1912 marks the birth of modern crystallography. Laue's discovery was the first experimental demonstration of the periodicity of crystal structures. W.H. and W.L. Bragg used the newly discovered X-ray diffraction to determine crystal structures at atomic resolution, thus propelling crystallography to global importance. Knowledge of the geometrical structure of matter had revolutionary consequences for all branches of the natural sciences. The theoretical foundations of structure determination were available by 1920, the basic theories for the solution of the phase problem in the early 1950s. The success of crystallography as an indispensable analytical tool was then due to the development of diffraction equipment and the advent of computers. The construction of fast area detectors and novel radiation sources, synchrotrons, XFELs, neutron spallation sources and electron microscopes assure for diffraction methods a prominent place modern science.

## Session: 100 Years of Diffraction

### 51: The two Braggs

A. Michael Glazer

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E-mail: glazer@physics.ox.ac.uk

Approximately 100 years ago in Germany, Max Theodor Felix von Laue (1879-1960), Paul Karl Moritz Knipping (1883-1935) and Walter Friedrich (1883-1968) showed that X-rays could be diffracted by crystals. Laue was subsequently awarded the Nobel Prize in Physics in 1914. Following this discovery, the unique partnership, father and son, William Henry Bragg (1862-1942) and William Lawrence Bragg (1890-1971) in England, successfully showed how X-ray diffraction could lend itself to the solution of crystal structures, for which they shared the Nobel Prize in Physics in 1915. And thus was begun the modern era of X-ray crystallography. It is not often appreciated that their description of inorganic crystal structures, such as that of NaCl, were not without controversy and took some time to be accepted, especially by those chemists who resented the idea of physicists infiltrating the field of chemistry. The two Braggs decided to divide up the fields of crystallography into organic crystallography (mainly under WHB) and inorganic crystallography (mainly under WLB) so that each could create his own separate area of research activity. The result has been that in England at least almost all crystallographers trace their crystallographic ancestry from one of these two schools. In this talk, I shall show some hitherto unpublished photographs and discuss the background and careers of these two eminent scientists.

### 52: Max von Laue: the physicist and the upright man

Jost Lemmerich

Retired, Berlin.

After reviewing the beginning of his career and his discovery I shall discuss his professorship in Berlin and then the terrible years 1933-1945. I shall then turn to the role of von Laue as the organizer of modern physics.

### **53:** The origins and development of macromolecular crystallography

Larry Falvello

Department of Inorganic Chemistry, University of Zaragoza, Pedro Cerbuna 12, 50009 Zaragoza, Spain

E-mail: falvello@unizar.es

An overview of the development of macromolecular structure analysis by diffraction methods is given in terms of both the necessary conceptual notions and the technical advances that have permitted this field to attain the productivity that it enjoys at the present time. An understanding of the properties of the crystals themselves has been key. Theoretical and practical developments in the broad areas of diffraction measurement, structure solution, structure development and refinement, and visualization have all been necessary for the success of macromolecular crystallography. The early ideas and practices in these areas are described, and the further development of each up to the present time is briefly surveyed. Comments are offered regarding some of the key figures who have contributed to the advance of this endeavor.

### **54:** Johannes Martin Bijvoet (1892-1980) and absolute structure

Ton Spek

Crystal & Structural Chemistry, Utrecht University, NL, Padualaan 8, 5555 Utrecht, 3584CH, Netherlands

E-mail: A.L.Spek@uu.nl

Bijvoet was a member of the pioneer generation of X-ray crystallography. He was the major founding father of crystallography in the Netherlands. The early results of the diffraction technique were not generally accepted yet by the chemical community when he entered the field. His supervisor as an example did not believe in Bragg's model of rocksalt. In 1928 he was appointed lecturer in crystallography and thermodynamics at the University of Amsterdam. In 1939 he moved to Utrecht as a professor in general chemistry, a position that he held until reaching his retirement age of 70 years in 1962. Bijvoet's name in the form of 'Bijvoet pairs' is now part of the terminology of our subject. They are the basis for the determination of absolute chirality of chemical compounds as detailed in the seminal 1951 Nature paper. This technique will be discussed along with current extensions of its applicability.

## Session: The Next 100 Years

### 61: Novel structural studies with an X-ray Free Electron Laser

Bruce Patterson

SwissFEL Project, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

E-mail: bruce.patterson@psi.ch

A single focused pulse from an X-ray Free Electron Laser (XFEL) deposits approximately  $10^{12}$  Gray (J/kg) in a biological sample – this exceeds by five orders of magnitude the “bio-limit” for protein crystallography and causes the irradiated region ( $100 \times 100 \text{ nm}^2$ ) to undergo, within 50 femtoseconds, destructive “Coulomb explosion”. Of what use is such an X-ray source for crystallography? After a brief description of how an XFEL works, I will in this talk give four examples of novel XFEL applications in the imaging of matter, at or close to the atomic scale: 1) sub-picosecond time-resolved resonant diffraction in correlated electron materials, 2) serial “diffract-and-destroy” protein nano-crystallography, 3) 2D-ptychographic crystallography of membrane proteins, and 4) cross-correlation analysis of scattering by nanostructures in solution. Finally, I will comment on the “holy grail” of XFEL science – structure determination of individual protein molecules. The SwissFEL X-ray laser will go into operation at the PSI in late 2016.

### 62: Investigating disorder as a matter of routine - the next steps

Thomas Weber

Laboratory of Crystallography, ETH Zurich, Wolfgang-Pauli-Str. 10, 8093 Zurich, Switzerland

E-mail: thomas.weber@mat.ethz.ch

After one hundred years of X-ray diffraction, the investigation of average crystal structures is now highly automatized and guided by very efficient software. The contrary is true for the analysis of crystalline disorder. Despite significant experimental progress and availability of programs for analyzing diffuse scattering, a good code editor and efficient compilers are still important tools for solving demanding problems. To overcome this problem we are currently developing two computer programs that allow straightforward applications of advanced disorder modeling techniques. The program YELL, which is based on the 3D-PDF method, provides a quick access to qualitative and quantitative disorder properties, but does not in any case deliver complete real structure models. To extract more information the Monte Carlo simulation program ZODS is developed in parallel. The program allows sophisticated Monte Carlo modeling techniques and supports super-computer architectures to compensate the immense computational demands inherent to Monte Carlo simulations.

### 63: The Materials Science Beamline upgrade

Philip Willmott

Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

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The Materials Science Beamline at the Swiss Light Source, Paul Scherrer Institut, has undergone an upgrade from wiggler- to undulator radiation, resulting in an increase of approximately three orders of magnitude in X-ray brilliance. In this presentation, I will describe the physics behind the design of the new insertion device source and the X-ray optics, which also had to be redesigned. Some initial results from both powder diffraction and surface diffraction will also be presented.

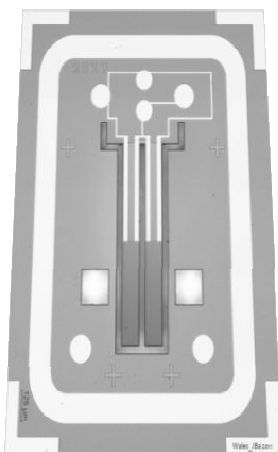
### 64: High Resolution X-Ray Diffraction applications for microsystems

Antonia Neels, Tobias Bandi, Alex Dommann

CSEM, Jaquet Droz 1, 2002 Neuchâtel, Switzerland

E-mail: Antonia.Neels@csem.ch

Microsystems are used in application fields requiring a high reliability such as space and medicine. The aging and failure of microsystems is always connected with the occurrence of defects and their mobility. The mobility of defects will be enhanced by greater stress gradients. Stress gradient and the defects can be easily determined by means of High Resolution X-Ray Diffraction (HRXRD) techniques [1].



Silicon based piezoelectric resonators are developed at CSEM targeting vacuum hermetic packaging technology. In order to support fabrication, HRXRD Rocking Curve (RC) and Reciprocal Space Mapping (RSM) methods are applied. Device strain is studied which influences the application relevant physical parameters such as the resonance frequency and the Q factor in resonators monitoring the vacuum level in the cavity of the microsystem.

Through the combination of functional testing with strain and defect evaluation using HRXRD, a fundamental understanding of the reliability and also aging problems of microsystems is approached.

Figure. Piezoelectric AlN/Si resonator with dimensions of  $1.5 \times 2 \times 1.4 \text{ mm}^3$ .

- [1] A. Neels, A. Dommann, A. Schifferle, O. Papes, E. Mazza, Reliability and Failure in Single Crystal Silicon MEMS Devices, *Microelectronics Reliability*, **2008**, *48*, 1245-1247.

## **65:** Powder Charge Flipping – input parameter optimization and solution evaluation

Dubravka Šišak, Lynne B. McCusker, Christian Baerlocher

Department of Materials Science, ETH Zurich, Wolfgang-Pauli-Str 10, 8093 Zurich, Switzerland

E-mail: dsisak@mat.ethz.ch

A variety of structures have now been solved by the powder charge flipping algorithm in *Superflip*. Its success depends in part on the input parameter values which are generally chosen rather arbitrarily. To understand the effect of the various parameters on structure solution better, a systematic investigation was undertaken. In cases where the data limitations cause the algorithm to fail completely in default mode, this optimization of input parameters coupled with non-random starting phases has succeeded in producing interpretable maps. However, as *Superflip* is an iterative algorithm, many solutions are produced within one run and usually only a few are fully interpretable. As there is no completely reliable criterion for recognizing these solutions, several approaches to solution evaluation have been tested: *Superflip* *R*-values, cluster analysis, entropy calculation and the likelihood function. Work is still in progress, but the results seem to be promising.

## **66:** Intercluster compounds for nanosized materials

Fabienne Gschwind, Martin Jansen

Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

E-mail: f.gschwind@fkf.mpg.de

The term “intercluster compound” refers to assemblies that are constituted of at least two different, large building blocks, e.g. clusters, complexes, organic molecules. A few intercluster compounds already exist and it has been possible to determine their crystal structures by single crystal X-ray diffraction. These results deliver insights into the arrangement of large building units in the solid-state material and the underlying intermolecular forces. These first results show that intercluster compounds are very promising for the study of structural and physical properties of nanosized particles. They also open a wide range for new applications as for instance the study of quantum effects and of orbital bands. Since only a few compounds have been studied, there is a huge potential for new discovery in this field. We would like to present new approaches and new building blocks for the synthesis of intercluster compounds.

## **67:** News from the spallation neutron source SINQ: Diffraction

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We present news from SINQ, especially the three diffraction instruments (single crystal diffractometer, TriCS, and the two powder diffractometers, HRPT and DMC) operated by the neutron diffraction group and give an outlook on the future instrumentation envisaged at SINQ and our engagement on the new spallation source ESS in Lund. Together with the excellent sample environment ranging from high pressure, high field, very low and very high temperatures, computer controlled (low-temperature) sample changer to specialties such as in-situ measurements under hydrogen, and the present flux (4 times higher than in 1996), SINQ has a very good potential going into the next decade by upgrading the instrumentation and the guide system.

## **68:** Density functional calculations of polysynthetic Brazil twinning in alpha-quartz

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Polysynthetic Brazil twinning in alpha-quartz, which occurs commonly in amethyst, is interpreted in the literature as having its composition planes parallel to one of the faces of the major rhombohedron  $r$ . It is shown that, instead, the composition planes are parallel to one of the faces of the minor rhombohedron  $z$ . The proposed translation 0.4547  $a$  between neighbouring lamellae leads to binding-distances and binding-angles across the composition plane that differ less from their bulk values than for the translation 0.5  $a$  proposed in the literature. Density functional calculations show that the energy of the unrelaxed polysynthetic twin is lower for the proposed translation. They also show that relaxation increases the thickness of the polytwin by 4 pm per composition plane.



## Abstracts of Posters

**71:** A moment in time: 100 years of X-Ray diffraction versus 100 days of PHOTON 100 CMOS detector

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Very recently, the first commercial CMOS active pixel sensor for X-ray crystallography, the PHOTON 100, became available. The PHOTON 100 offers a number of features which make it the superior solution:

- Large 100 cm<sup>2</sup> active area
- High quantum gain, high sensitivity
- Available for Cu, Mo, Ag radiation
- Excellent signal-to-noise
- 3 year detector warranty
- Air cooled

The PHOTON 100 is available with the user-friendly D8 QUEST and D8 VENTURE, featuring the latest generation of the I<sub>μ</sub>S (Incoatec Microfocus Source), focusing monochromators (TRIUMPH), and modern rotating anodes (Turbo X-ray Source). After a short historic overview on X-ray detectors with a focus on the technique used in CMOS based detectors, we will present results obtained on the D8 QUEST and D8 VENTURE. The structures presented will include results from weakly diffracting crystals and crystals exhibiting aperiodicity. Furthermore, high quality data for charge density investigations will be discussed.

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Ab-initio crystal structure prediction is still one of the most challenging and interesting issues in condensed matter science. The first difficult task is the determination of the irreducible descriptors required to search for the global minima among different conformational geometries, a system can adopt when visiting the many local minima of the potential energy surface. I present the possibility of a complete ab-initio approach, starting with the most stable molecular arrangement and then building, from the local optimized geometry, periodic lattice models. The case study is represented by the prediction of the crystal structures of  $MBH_x$ , in particular  $M = Li$ , and  $x \in (0,4)$  [1-3].

- [1] A. Tekin, R. Caputo, A. Züttel, First-principles determination of the ground-state structure of  $LiBH_4$ , *Phys. Rev. Lett.*, **2010**, *104*, 215501.
- [2] R. Caputo, A. Züttel, First-principles study of the paths of the decomposition reaction of  $LiBH_4$ , *Mol. Phys.*, **2010**, *108*, 1263.
- [3] R. Caputo, A. Tekin, Ab-initio crystal structure prediction. A case study:  $NaBH_4$ , *J. Solid State Chemistry*, **2011**, *184*, 1622.

**73:** Pressure modulated proton-phonon coupling and its relevance to ceramic fuel cell proton conductors

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<sup>4</sup> Advanced Light Source LBNL, 1 Cyclotron Road MS 2-400, Berkeley, CA 94720, USA

<sup>5</sup> Mechanics for Modelling and Simulation, EMPA, Überlandstrasse 129, 8600 Dübendorf, Switzerland

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Ceramic proton conductors are believed to be promising solid electrolyte materials for intermediate temperature solid oxide fuel cells at 400°C to 500°C. The common understanding in the solid state ionics community is that solid ceramic electrolyte layers must be "dense". The technical reason behind this requirement is that no gases shall diffuse through the electrolyte. "Tight" or "sealed" would be the more appropriate term. Our systematic experimental studies on proton conductivity with quasielastic neutron scattering, X-ray diffraction, impedance spectroscopy and Raman spectroscopy in-situ and operando at high temperature and high pressure prove directly that superprotonic behaviour and high compressive strain (densification upon pressure) are incompatible states. Whereas extrapolation towards tensile strain suggests that in particular epitaxial strained ceramic films may be the better proton conductors with significantly lower proton diffusion activation energy. The crystallographically specific proton-phonon coupling provides pathways to design electrolyte film assemblies with particularly fast proton conduction routes.

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Heterometallic compounds can be used in different applications, for instance as precursors for photo-electronic devices or mixed-metal oxides in high-T<sub>c</sub> superconductors. A synthetic strategy to obtain mixed-metal oxides is to use decomposition techniques on multi-metallic complexes. Since the organic ligand is decomposed during the synthesis of the desired metal oxide, it is proposed that simple ligand systems, which can be easily and cost-effectively prepared on a multi-gram scale, are used. The preorganization of the metal ions in the complex may give large advantages for the thermal decomposition. The oxide can be obtained under milder conditions (atmospheric pressure and temperatures lower than 500 °C) [1] and new oxide materials can be synthesized.

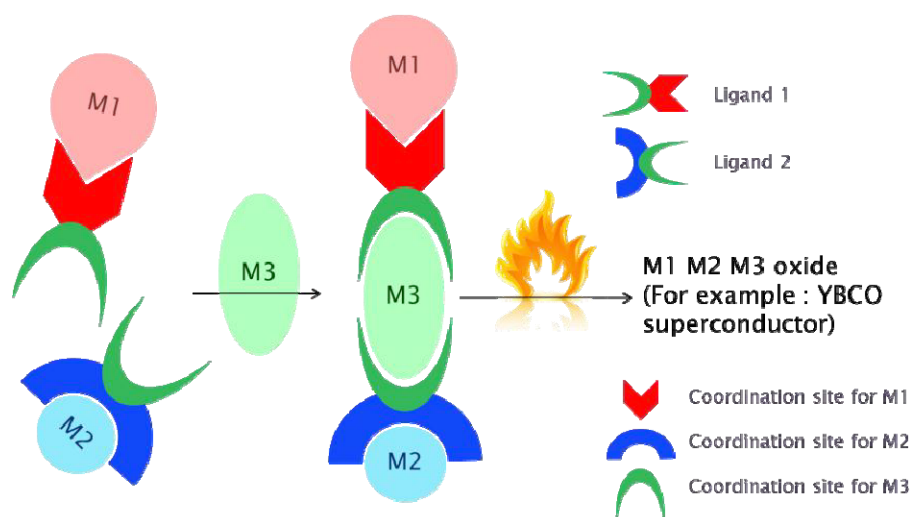


Figure 1. Concept of the project.

[1] F. Gschwind, O. Sereda, K. M. Fromm, *Inorg. Chem.*, **2009**, *48* (22), 10535-10547.

**75:** New penta-coordinate iron(III) aryloxide as initiators for ring-opening polymerization

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In addition to the development of new energy-producing processes, finding new energy-saving procedures offers a promising solution to meet our energy needs in the future. Indeed, catalysis is one of the key technologies for energy saving. A wide variety of metal alkoxides/aryloxides[1] has been used as initiators and catalysts for ring-opening polymerization (ROP). Due to the use of cyclic esters in the tailoring synthesis of biodegradable and bioresorbable materials, interest in the development of well-defined initiators and catalysts has increased. Iron-based catalysts offer many advantages, such as their abundance, their low toxicity and their biocompatibility[1]. For this purpose, the authors will present their first results on a new and cheap hetero-bimetallic Li-Fe based aryloxide complex [2] as an initiator for ring-opening polymerization(ROP) of lactide.

[1] M. Ouchi, T. Terashima, M. Sawamoto, *Chem. Rev.* **2009**, 4963-5050.

[2] Y. Chérémond, A. Crochet, K. M. Fromm, *Eur. J. Inorg. Chem.* **2012**, DOI:10.1002/ejic.201101054.

**76:** Light-induced low-spin structure of the bistable  $[\text{Fe}(\text{bbtr})_3](\text{BF}_4)_2$  compound

Laure Guenee,<sup>1</sup> Pradip Chakraborty,<sup>2</sup> Robert Bronisz,<sup>3</sup> Celine Besnard,<sup>1</sup> Phil Pattison,<sup>4</sup> Andreas Hauser<sup>2</sup>

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In the covalently linked 2D coordination network  $\{[\text{Fe}(\text{bbtr})_3](\text{BF}_4)_2\}$ ?, bbtr = 1,4-di(1,2,3-triazol-1-yl)butane, the iron(II) stay in the high-spin (HS) state down to 10 K. They can, however, be quantitatively converted to the low-spin (LS) state by irradiating into the near IR spin allowed 5dd band and back again by irradiating into the visible 1dd band. At 60 K, upon irradiation at 830 nm, the light-induced LS population also triggers a crystallographic phase transition from space group P-3 to P-1 accompanied by a doubling of the *c* parameter and a splitting of the crystal into different domains. This transition is reversible and the crystal totally recovers either by heating or irradiating at 472 nm. The compound shows true light induced bistability below 100 K, thus having the potential for persistent bidirectional optical switching at elevated temperatures.

**77:** Magnetic ground state and 2D behavior in the pseudo-Kagomè layered system  $\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Br}$

Oksana Zaharko,<sup>1</sup> Matej Pregelj,<sup>2</sup> Axel Günther,<sup>3</sup> Alois Loidl,<sup>3</sup> Vladimir Tsurkan<sup>3</sup>

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Anisotropic magnetic properties of a layered Kagomè-like system  $\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Br}$  have been studied by bulk magnetization and magnetic susceptibility measurements as well as powder and single crystal neutron diffraction. At  $T_N = 27.4$  K the system develops an alternating antiferromagnetic order of (ab) layers, which individually exhibit canted ferrimagnetic moment arrangement, resulting from the competing ferro- and antiferro-magnetic intralayer exchange interactions. A magnetic field  $B_c \sim 0.8$  T applied along the easy c-axis (perpendicular to the layers) triggers a metamagnetic transition, when every second layer flips, i.e., resulting in a ferrimagnetic structure. Significantly higher fields are required to rotate the ferromagnetic component towards the b-axis ( $\sim 7$  T) or towards the c-axis ( $\sim 15$  T). Finally, the estimates of the exchange coupling constants and features indicative of the XY character of this quasi 2D system are presented.

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Piezoelectric actuators are widely used in sensors, mechanical actuation and ultrasonic transducers [1]. Currently, the development of thin piezoelectric multilayer stacks for miniature actuators is a subject of high interest in micro fluidics, micro robotics, and medical devices. To date, PZT ( $\text{Pb}(\text{Zr},\text{Ti})\text{O}_3$ ) thin films are the best candidates to accomplish efficient structures [2]. Since a strong piezoelectric effect is a lattice effect, the investigation of the crystalline quality is a key task to advance in microstructure improvements. X-ray diffraction has been known as a powerful tool to characterize crystalline properties. In this contribution we present a film texture study on recently developed PZT thin films grown by sputter deposition.

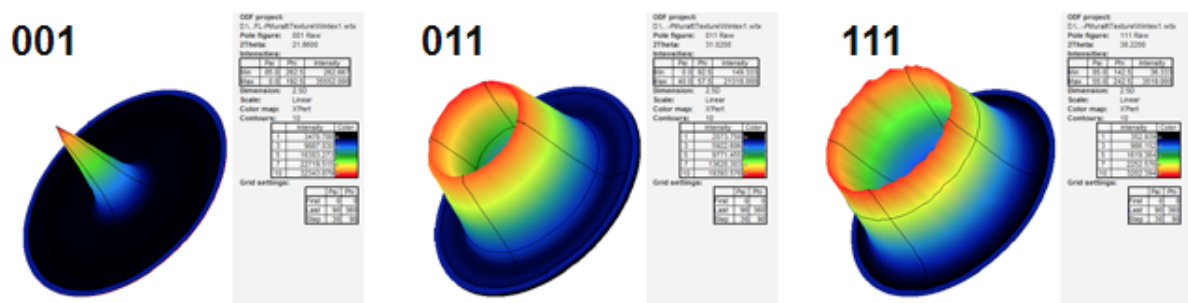


Figure 1. Pole figures showing the high degree of texturing of a PZT thin film with columnar microstructure. The preferred orientation direction is (001).

- [1] C. Y. K. Chee, L. Tong, G. P. Steven, A review on the modeling of piezoelectric sensors and actuators incorporated in intelligent structures, *J. Intell. Mater. Syst. Struct.* 9 (1998) 3–19.
- [2] P. Muralt, Recent Progress in Materials Issues for Piezoelectric MEMS, *J. Am. Ceram. Soc.* 91 (2008) 1385-1396.



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The fascinating diversity in the Crystal Chemistry of novel compounds based on the  $[\text{BH}_4]^-$  group continues to proliferate. In this study we contribute with the structural characterization and classification of recently found novel quaternary borohydrides,  $\text{Li}(\text{Li}_2\text{M})\text{Zn}_5(\text{BH}_4)_{15}$  ( $\text{M}=\text{Mg}, \text{Mn}$ ) and  $\text{LiKMg}(\text{BH}_4)_4$ , which are brought into a crystal-chemical context and compared to ionic-covalent compounds such as oxides or sulfides. It is shown that the symbiosis between Synchrotron Powder Diffraction and Spectroscopical methods provide excellent and reliable results in complicated cases when applied in conjunction with DFT-calculations. The ongoing reports of structural similarities between borohydrides and oxides, sulphides or halides as well as new frameworks observed exclusively among the former directly evidence their structural flexibility, which provides a means of structural compliance with respect to the "tuning" of structural parameters such as site symmetry, mixing and occupancies which in turn directly influence their physical properties, e.g.  $\text{Li}^+$  conductivity and hydrogen release temperature.

**80:** TIPSI hybrid spectrometer at the European Spallation Neutron Source ESS:  
Probing multiple length scales in one instrument

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Ongoing improvements in material performances are led by the incorporation of advanced ceramics and polymers into heterogeneous systems. Their performances usually depend on the interplay between properties defined by the atomic, nano/mesoscopic and microscopic structure of these new materials. Traditionally such structural information has been probed by separate experiments such as wide angle diffraction techniques (atomic scale,  $0.3 \text{ \AA}^{-1} \leq Q \leq 50 \text{ \AA}^{-1}$ ), small angle diffraction (nano/meso,  $0.002 \text{ \AA}^{-1} \leq Q \leq 0.1 \text{ \AA}^{-1}$ ) and direct space imaging (sub-micronic to millimeter scale). The proposed hybrid instrument TIPSI to be built at the European Spallation Neutron Source, ESS, in Lund is designed to obtain a coherent multi-length scale picture of these materials. The idea is to collect simultaneously neutron powder diffraction (probed length  $\zeta \sim 0.01\text{-}5 \text{ nm}$ ), small angle neutron scattering ( $\zeta \sim 1\text{-}1000 \text{ nm}$ ) and neutron imaging ( $\zeta \sim 0.01\text{-}100 \text{ mm}$ ), giving a huge advantage especially for in situ-measurements. The design of such an instrument will be presented using simulation tools.

**81:** Neutron diffraction and Oxygen Isotope Back Exchange studies in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4\pm\delta}$  ( $x = 0, 0.05, 0.15$ ) crystals as a function of temperature

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E. Pomjakushina,<sup>4</sup> B. Pederson<sup>5</sup>

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The understanding of oxygen ion conduction in solids at moderate temperatures is a key issue for the development of oxygen membranes in solid oxide fuel cells [1] or for oxygen sensors. The  $\text{K}_2\text{NiF}_4$  structure [2], *e.g.*  $\text{La}_2\text{MO}_{4\pm\delta}$  ( $\text{M}=\text{Co}, \text{Cu}, \text{Ni}$ ) will undergo oxygen intercalation at ambient temperature. The Oxygen Isotope Back Exchange (OIBE) experiments are done in order to investigate the effect of strontium on the oxygen diffusion in as grown single crystals of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4\pm\delta}$  ( $x = 0, 0.05, 0.15$ ). From  $^{18}\text{O}/^{16}\text{O}$  isotope exchange between 40 °C to 1000 °C free oxygen mobility can be realized for  $x = 0, 0.05$  below 500 °C but is depressed for  $x = 0.10$  and  $0.15$ . This gives evidence that low temperature oxygen mobility can be suppressed by replacing La with Sr. We have also reinvestigated the structural phase transitions of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4\pm\delta}$  ( $x = 0, 0.05, 0.15$ ) crystals on RESI@FRMII and TriCS@SINQ from room temperature to 480 °C. A reversible structural phase transition from the orthorhombic system to the tetragonal system in  $\text{La}_2\text{CuO}_{4\pm\delta}$  and  $\text{La}_{1.95}\text{Sr}_{0.05}\text{CuO}_{4\pm\delta}$  is observed.

[1] Z. P. Shao, S. M. Haile, *Nature*, 431 (2004) 170.

[2] P. Rudolf, W. Paulus, R. Schöllhorn, *Adv. Mater.* 3 (1991) 438.

## **82:** Our fascination with crystals and crystallography – a 7500 year timeline

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Crystals have fascinated people for millennia. The Egyptian Queen Zer (5500 BC) had Turquoise jewellery. The Greeks and Romans studied naturally occurring crystals. Scientists from the 17th–19th centuries classified crystals and mused over their composition, physical properties, shapes and internal arrangement. The concepts of symmetry and space groups were derived well before the discovery of X-ray diffraction. Modern crystallography developed rapidly following the seminal experiments of von Laue and his co-workers in 1912 and the Braggs in 1913 and is a key cornerstone of science today. In the last 100 years, many Nobel Prizes have been awarded to people involved with the development of crystallography or its use as a crucial tool in the investigation of the structure of materials, chemical compounds and biological systems. This poster will present a timeline depicting some of the important milestones in the study of crystals and the development of crystallography over the ages.

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The Measure of Confidence



# Agenda of the SGK/SSCr General Assembly 2011

June 21, 2012, 11.50-12.30, ETH Hönggerberg, lecture hall HCI J6.

The minutes of our last General Assembly (2010) are published on page 12 and 13 of the SGK/SSCr newsletter No. 81, Dec. 2010, available at <http://www.sgk-sscr.ch/Newsletters/SGK-News-81.pdf>.

- 1) Feststellung der Beschlussfähigkeit gemäss Art. 12/by-laws
- 2) Antrag auf Genehmigung der Minutes General Assembly 2010, Bern

a) Jahresbericht  
le rapport annuel

b) Jahresrechnung  
les comptes annuels

c) Aufstellung des Budgets für das kommende Jahr/  
le budget proposé pour l'année suivante

d) Festsetzung des jährlichen Mitgliederbeitrages/  
le montant de la cotisation annuelle

*Antrag des Vorstandes : wie bisher (CHF 30/regular und CHF 10/students)*

e) Wahlen/Elections:

- 1) confirmation of the present board members
- 2) elections of 3 new board members  
(replacement Prof. Steurer and Prof. Schiltz and 1 new board member)  
suggestions have to be made 1 week prior to the assembly to our  
president, [Katharina.fromm@unifr.ch](mailto:Katharina.fromm@unifr.ch)  
**Candidates are asked for a short 1-2 minute oral presentation.**
- 3) election of a new president  
election/confirmation of a new-vice-president  
election/confirmation of a new secretary
- 4) election/confirmation of the auditors
- 5) Delegates to ECA and IUCR

f) Antrag auf Statutenänderung von Artikel 6 (siehe unten)

- g) 1) Information on the bid for ECM-30 in 2016 (Basel)
- 2) Anträge von Mitgliedern  
other motions of members

## Additional information to the Agenda:

- e1,e2 The term of Katharina Fromm is ending in 2012 (3 years, Art. 16iii).  
Katharina Fromm, Jürg Schefer, Piero Macchi, Céline Besnard and Michael Hennig are willing to remain in the board.  
Marc Schiltz moved to Luxemburg taking over a new position as head of the Luxemburg Science Foundation and requested for an end of his term.
- f) The board is suggesting a change of the by-laws (Art. 6). The goal is to limit the financial responsibility of the members to the annual fees due by the member.  
*Link to our by-laws: [http://www.sgk-sscr.ch/Statuts\\_SSCr.html](http://www.sgk-sscr.ch/Statuts_SSCr.html)*

### Art. 6 (present status)

Die persönlichen Mitglieder entrichten einen jährlichen, durch die Mitgliederversammlung bestimmten, Mitgliedsbeitrag. Jahresbeiträge sind zu Beginn des laufenden Jahres fällig. Das Vereinsjahr ist das Kalenderjahr.

### Art 6 (new, if accepted)

Die persönlichen Mitglieder entrichten einen Jahresbeitrag, der durch die Mitgliederversammlung festgelegt und zu Beginn des laufenden Jahres fällig ist. Das Vereinsjahr ist das Kalenderjahr. Der momentane Mitgliedbeitrag beträgt CHF 30 für ordentliche Mitglieder und CHF 10 für Studenten und Doktoranden. Eine persönliche Haftung der Mitglieder für die Verbindlichkeiten der Gesellschaft besteht nicht.

Quorum for final decisions (Art.12, by-laws):  
≥ 10%, out of 168 members = 17 members  
(April 2, 2012: 152 regular, 16 students =168)

## Summary SGK/SSCr Finances

	<b>CHF</b>
<b>Total 31.12.2010</b>	<b>37'013.80</b>
UBS account	19'210.48
CS account	17'871.51
Cash on hand	1'519.40
<hr/>	
<b>Total 31.12.2011</b>	<b>38'601.39</b>
<b>net income over the year</b>	<b>1'587.59</b>

# SGK/SSCr Financial Report 2011

## UBS Account

CHF

**Status 1.1.2011**

**17'747.36**

### Credits:

Membership dues 114x30.- (full member) 10x10.- (students) 9x130.- (companies)	4'915.50
SANW reimbursement for Annual Meeting 2010	3'000.00
SANW for ECA delegate 2011 IUCr	1'000.00
SANW funds for young scientists travel grants	1'000.00
Sponsorships for the meeting	1'400.00
Tax return	262.26
Interest	<u>61.95</u>
<b>Total Income</b>	<b>11'639.71</b>

### Debits:

Membership dues to SANW (173 members)	1'162.00
Annual meeting 2011 (Bern)	3'201.75
Poster Prize annual meeting	565.46
Travel Grant to young scientist (A. Chimpri)	500.00
Travel Grant to young scientist (Y. Cheremond)	500.00
Travel Grant IUCr delegate P. Macchi	1'000.00
Support Zurich School	2'000.00
Support special day Ada Yonath	1'000.00
ECA dues (national membership SGK)	157.28
Bank charges	<u>90.10</u>
<b>Total Expenses</b>	<b>10'176.59</b>

**Income – Expenses**

**1'463.12**

**Starting Balance + Income – Expenses**

**19'210.48**

**UBS Balance 1.1.2012**

**19'210.48**



## Cash on Hand - 2011

	<b>CHF</b>
<b>Status 1.1.2011</b>	<b>1566.40</b>
<b><u>Credits:</u></b>	
3 memberships (Macchi, Rosch, Bensch)	90.00
	<hr/>
<b>Total Income</b>	<b>90.00</b>
<b><u>Debits:</u></b>	
Fee for internet page of SGK	17.00
Meeting SGK2011	120.00
	<hr/>
<b>Total Expenses</b>	<b>137.00</b>
<b>Income – Expenses</b>	<b>-47.00</b>
<b>Starting Balance + Income – Expenses</b>	<b>1519.40</b>
<b>Cash on Hand 1.1.2012</b>	<b>1519.40</b>

## Status of other Accounts

### Credit Suisse (savings account)

	CHF
<b>Status 1.1.11</b>	<b>17'700.04</b>
Interest (1.125% or 1%, resp.)	171.47
Withholding Tax*	-.-
<b>Balance 31.12.11</b>	<b>17'871.51</b>

\*(only applicable when amount of interest exceeds CHF 200)

### **SGK/SSCr Budget 2012 (proposal)**

<u>Credits:</u>	<b>Budgeted</b>
Membership dues (148-regular, 9 comanies, 19 Students)	6'000.00
SANW reimbursement for Annual Meeting 2012	2'500.00
SANW Poster prize annual meeting 2012	500.00
SANW reimbursement for ECA delegate 2012	3'000.00
SANW young scientists travel grants	1'500.00
Interest (est.)	250.00
<b>Total Income</b>	<b>13'750.00</b>
<u>Debits:</u>	
Membership dues to SANW (167 members)	1'200.00
Annual meeting	3'000.00
Travel Grant for ECA delegate (2012)	3'000.00
Travel Grants to Young Scientists	1'500.00
SGK support for PSI School	2'000.00
Workshop at EPFL	1'000.00
ECA national membership dues 2011 (150€)	200.00
Bank charges	200.00
<b>Total Expenses</b>	<b>12'100.00</b>
<b>Income – Expenses</b>	<b>1'650.00</b>

# WORKSHOP ON CRYSTAL ENGINEERING IN SUPRAMOLECULAR CHEMISTRY

**23.-25.07.2012**

**Dept of Chemistry, Chemin du Musée 9,  
Uni Fribourg, 1700 Fribourg**

Max. N° of Participants: 30    Participants from CUSO Universities: free, lodging + food included  
Participants from outside: 800,- CHF (includes lodging + food)

## **Programme:**

### **Monday, 23rd of July 2012**

9h-12h30:        Lectures with coffee break  
12h30-14h:       Lunch & Discussions  
14h-18h30:       Lectures & Exercises & Coffee Break  
18h30-20h:       Poster session & Cheese & Wine

### **Tuesday, 24th of July 2012**

9-12h30:        Lectures with coffee break  
12h30-14h:       Lunch & Discussions  
14h-18h:        Hands on Crystallization Techniques & Hands on X-ray measurements  
19h                BBQ Mixer

### **Wednesday, 25th of July 2012**

9-12h30:        Lectures with coffee break  
12h30-14h:       Lunch and Discussions  
14-18h:         Hands on X-ray measurements & Hands on Crystallization Techniques.

**Speakers:** Dario Braga and Fabrizia Grepioni, University of Bologna, Italy. Both are leading experts of the field.

Theme 1. crystal engineering background / historical

Theme 2. molecular crystals, intermolecular interactions, H-bonds, halogen bonds etc.

Theme 3. coordination networks, principles, etc.

Theme 4. preparative methods, making crystals, mechanical methods

Theme 5. crystal forms, general, polymorphs, solvates, co-crystals etc

Theme 6. crystal polymorphism, historical background, intellectual property issues

Theme 7. hydrates, co-crystals

Theme 8. chirality in crystals

Theme 9. industrial applications (MOF, pigments, supramolecular gels, pharmaceuticals)

Theme 10. solid-state reactivity (reactions in solid, photocyclizations, reactions with gases).

**Applications (motivation letter + poster abstract)** should be sent by May 31st, 2012 to [katharina.fromm@unifr.ch](mailto:katharina.fromm@unifr.ch) and will be treated on a first come, first served basis.



# AIC International School 2012

## 10<sup>th</sup> Paolo Giordano Orsini School

structure, microstructure, nanostructure

exploiting the potential of powder diffraction techniques

Trento, 15-20 september 2012



### topics

X-ray Powder Diffraction, Structure Solution and Refinement, Line Profile Analysis, Quantitative Phase Analysis, Electron Diffraction and Precession Techniques

### practicals

Structure Solution and Refinement, Quantitative Phase Analysis, Line Profile Analysis

### lecturers

C. Giacovazzo, P. Fornasini, R. Berisio, J. Evans, I.R. Evans, R. Rizzi, A.F. Gualtieri, G. Artioli, M. Leoni, P. Scardi, M. Milanese, M. Gemmi, S. Gialanella

<http://2012.aicschool.org> [info@aicschool.org](mailto:info@aicschool.org)

sponsored by



### scientific committee

M. Milanese (Uni PMN) & M. Leoni (Uni TN) *chairs*, R. Berisio (CNR-IBB), P. Fornasini (Uni TN), S. Gialanella (Uni TN), A.F. Gualtieri (Uni MoRe), A. Moliterni (CNR-IC), P. Scardi (Uni TN), M. Zema (Uni PV)

### organizing committee

*AIC Commission on Teaching*: R. Berisio (CNR-IBB), M. Milanese (Uni PMN), A. Moliterni (CNR-IC), M. Zema (Uni PV).  
*M. Leoni (Uni TN) & P. Scardi (Uni TN) chairs of local organization*, C.L. Azanza Ricardo (Uni TN) *secretariat*, G. Croce (Uni PMN) *webmaster*, P. Fornasini (Uni TN), S. Gialanella (Uni TN)

## Calls for proposals

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

<b>Facility</b>	<b>Deadline(s)</b>	<b>Link</b>
<b>SLS: Swiss Light Source</b> All except PX lines Protein beam lines (PX)	March 15, Sept. 15 Feb. 15, June 15, Oct. 15	<a href="http://www.psi.ch/useroffice">www.psi.ch /useroffice</a>
<b>SINQ: Swiss Spallation Neutron Source</b> All instruments (regular calls)	May 15, Nov. 15	<a href="http://www.psi.ch/useroffice">www.psi.ch /useroffice</a>
<b>SINQ/SLS</b> Joint powder instrument (MS/HRPT)	Feb. 15, 2013	<a href="http://www.psi.ch/useroffice">www.psi.ch /useroffice</a>
<b>SμS: Swiss Muon Source</b> All instruments	Dec. 5	<a href="http://www.psi.ch/useroffice">www.psi.ch /useroffice</a>
<b>ESRF: European Synchrotron</b> All instruments, long term proposals	Jan. 15	<a href="http://www.esrf.eu">www.esrf.eu</a>
All instruments, short term proposals	March 1, Sept. 1	<a href="http://www.esrf.eu">www.esrf.eu</a>
<b>SNBL: Swiss Norwegian Beam Line</b>	March 1, Sept. 1	<a href="http://www.esrf.eu/UsersAndScience/Experiments/CRG/BM01/">www.esrf.eu/ UsersAndScience/ Experiments/ CRG/BM01/</a>
<b>ILL: Institut Laue Langevin</b> All instruments	Feb. 15, Sept. 15	<a href="http://www.ill.eu">www.ill.eu</a>
<b>FRM II: Heinz Maier-Leibnitz</b> All instruments	July 20, 2012	<a href="http://user.frm2.tum.de">user.frm2.tum.de</a>
<b>SNS Spallation Neutron Source</b> Oak Ridge	Sept. 5, 2012	<a href="http://neutrons.ornl.gov">neutrons.ornl.gov</a>

## Calendar of forthcoming meetings

(Please mail missing information on meetings of interest to [Jurg.Schefer@psi.ch](mailto:Jurg.Schefer@psi.ch))

			Abstract Deadline
<b>2012</b>			
April 19-20	Berlin Germany	Science and Scientists ESS: Future Science at ESS <a href="http://ess-scandinavia.eu/">http://ess-scandinavia.eu/</a>	
May 7-10	Rigi Kulm CH	4 <sup>th</sup> MaMaSELF Status Meeting <a href="http://diffraction.web.psi.ch/mamaself-rigi-ch.htm">http://diffraction.web.psi.ch/mamaself-rigi-ch.htm</a>	May 1, 2012
May 10-13	Bad Honnef	Free-Electron Laesers: From Fundamentals to Applications <a href="http://www.hzdr.de/heraeus503">http://www.hzdr.de/heraeus503</a>	expired
June 17-20	Glasgow GB	Fourth European Conference on Crystal Growth (ECCG4), <a href="http://northernnetworkingevents.createsend4.com">http://northernnetworkingevents.createsend4.com</a>	Feb. 24, 2012
June 18-22	Moscow Russia	ISMAM, Int. Symposium on Metastable, Amorphous and Nanostructured Materials, <a href="http://ismanam.ru/">http://ismanam.ru/</a>	March 20, 2012
June 19-23	Como Italy	Insubria International Summer School, Crystallography for Health and Biosciences, <a href="http://scienze-como.uninsubria.it/iiss2012/IISS2012.htm">http://scienze-como.uninsubria.it/iiss2012/IISS2012.htm</a>	March 1, 2012
June 21-22	Zürich CH	SGK/SSCr Annual Meeting 2012, 100 Years of Diffraction Joint Meeting with the Swiss Physical Society <a href="http://www.oci.uzh.ch/group.pages/linden/sgk2012/">http://www.oci.uzh.ch/group.pages/linden/sgk2012/</a>	March 15, 2012
June 24-26	Washington DC, USA	2012 American Conference on Neutron Scattering <a href="http://www.mrs.org/acns-2012/">http://www.mrs.org/acns-2012/</a>	April 2, 2012
June 26-29	Luzern CH	10 <sup>th</sup> European Solid Oxygen Fuel Cells Forum <a href="http://www.efcf.com">http://www.efcf.com</a>	Nov. 30, 2011
July 4-6	Zürich CH	Combined Diffraction-Spectroscopy Workshop CSX2012, <a href="http://www.psi.ch/csx2012">http://www.psi.ch/csx2012</a>	June 11, 2012
July 15-18	Hamburg Germany	Science at FEL's: SRI 2012 Satellite Meeting <a href="http://science-at-fels-2012.desy.de/">http://science-at-fels-2012.desy.de/</a>	April 30, 2012
July 15-20	Hokkai-do Japan	17 <sup>th</sup> Sagamore conference on charge spin and momentum density, <a href="http://rsc.riken.jp/sagamore/home/">http://rsc.riken.jp/sagamore/home/</a>	to be announced
23.-25. July	Fribourg CH	Workshop on Crystal Engineering in Supramolecular Chemistry Katharina.fromm@unibr.ch	May 1, 2012
Aug. 7-11	Bergen Norway	ECM-27 <a href="http://ecm27.ecanews.org">http://ecm27.ecanews.org</a>	May 14, 2012
Aug 27-Sept.1	Brasov Rumania	Int. Summer School on Crystal Growth and Photovoltaic Materials, <a href="http://rocam.unibuc.ro/intschool/index.html">http://rocam.unibuc.ro/intschool/index.html</a>	May 1, 2012
Sept. 2-9	Cairns Australia	7th International Conference on Aperiodic Crystals <a href="http://rsc.anu.edu.au/~perri/Aperiodic">http://rsc.anu.edu.au/~perri/Aperiodic</a>	March 18, 2012
Sept. 15-20	High Tatras Slovakia	6 <sup>th</sup> European Charge Density Meeting <a href="http://ecdm6.stuba.sk/?page=home">http://ecdm6.stuba.sk/?page=home</a>	June/July 2012
Sept. 15-20	Trento Italy	AIC International School joined with "Paolo Giordano Orsini" School: Structure, Microstructure, Nanostructure <a href="http://2012.aicschool.org/">http://2012.aicschool.org/</a>	open
Sept. 25-27	Darmstadt Germany	MSE "Materials Science and Engineering <a href="http://www.mse-congress.de">www.mse-congress.de</a>	Feb. 17, 2012
Oct. 28-31	Taipei Taiwan	The 7 <sup>th</sup> International Workshop on Modeling in Crystal growth (IWMCG-7), <a href="http://iwmcg7.ntu.edu.tw/">http://iwmcg7.ntu.edu.tw/</a>	April 30, 2012
Nov. 18-23	Sydney Australia	SAS'2012: International Small Angle Scattering Conference <a href="http://www.sas2012.com/">http://www.sas2012.com/</a>	May 2012
Nov. 19-22	Prague Czech Rep.	Polymorphism and Crystallization <a href="https://www.scientificupdate.co.uk/conferences/conferences-schedule/register/89-Polymorphism-and-Crystallization.html">https://www.scientificupdate.co.uk/conferences/conferences-schedule/register/89-Polymorphism-and-Crystallization.html</a>	May 18, 2012
Nov. 26-27	Villigen CH	PSI Powder Diffraction School <a href="http://www.psi.ch/events/">http://www.psi.ch/events/</a>	to be announced

**Abstract Deadline****2013**

March 10-15	Regens- burg, DE	DPG-Frühjahrestagung, Condensed Matter Research <a href="http://www.dpg-physik.de/veranstaltungen">http://www.dpg-physik.de/veranstaltungen</a>	
March 19-22	Freiberg DE	21. Jahrestagung der Deutschen Gesellsch. für Kristallographie, <a href="http://www.dgk-conference.de">http://www.dgk-conference.de</a>	to be announced
April 14-19	Washington DC, USA	ARRS 2013 – Meeting of the American Roentgen Ray Society	to be announced
June 9-22	Zurich CH	The Zurich School of Crystallography 2013 <a href="http://www.oci.uzh.ch/group.pages/linden/zsc">http://www.oci.uzh.ch/group.pages/linden/zsc</a>	Jan. 15, 2013
July 2-7	Diablererts CH	Gordon research conference on Electron Distribution and Chemical Bonding, <a href="http://www.grc.org/programs.aspx?year=2013&amp;program=elecdist">http://www.grc.org/programs.aspx?year=2013&amp;program=elecdist</a>	
July 7-12	Moscow Russia	17 <sup>th</sup> International Zeolithe Conference <a href="http://www.izc17.com">http://www.izc17.com</a>	to be announced
Aug. 25-29	Warwick UK	European Crystallographic Association, ECM-28 <a href="http://ecm28.org">http://ecm28.org</a>	

to be announced

**2014**

August	Montreal Canada	IUCr-2014, 23 <sup>rd</sup> General Assembly and Congress of IUCr <a href="http://www.iucr.org/iucr/cong/iucr-xxiii">http://www.iucr.org/iucr/cong/iucr-xxiii</a>	to be announced
to be decided	Villigen CH	PSI Powder Diffraction Summer School	to be announced

**2015**

To be fixed	Rovinj Croatia	ECM-29 2015	to be announced
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**2016**

to be decided	To be decided	European Crystallographic Association, ECM-30 <a href="http://ecm30.org">http://ecm30.org</a>	to be announced
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**2017**

to be decided	Hyderabad India	IUCr-2017, 24 <sup>th</sup> General Assembly and Congress of IUCr <a href="http://www.iucr.org/iucr/cong/iucr-xxiii">http://www.iucr.org/iucr/cong/iucr-xxiii</a>	to be announced
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## Become a member of SGK/SSCr

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

Presently, the yearly membership fee is sfr. 30 (sfr. 10 for students).

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

<b>Name</b>	
<b>Given name</b>	
<b>Title</b>	
<b>Institution</b>	
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<b>Box/building</b>	
<b>ZIP Code</b>	
<b>Town</b>	
<b>Country</b>	
<b>Phone office</b>	+ ( )
<b>Fax office</b>	+ ( )
<b>Phone private</b>	+ ( )
<b>Mobile phone</b>	+ ( )
<b>E-Mail</b>	@
<b>Interest</b>	
<b>Membership subsection crystal growth</b>	Yes ( ) No ( )
<b>Birth date</b>	Day: Month: Year:
<b>Language(s)</b>	
<b>Major research interests</b>	
<b>Highest degree received</b>	
<b>from university</b>	
<b>Present position</b>	

Date: ..... Place: .....  
Signature: .....

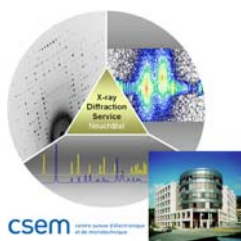
**FAX the completed form to: Dr. Radovan Cerny, 022 379.6108**  
**or use our online application form at <http://www.sgk-sscr.ch>**



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**Società Svizzera di Cristallografia**  
**Societad Svizera per Cristallografia**

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**Prof. Dr. Katharina Fromm**

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