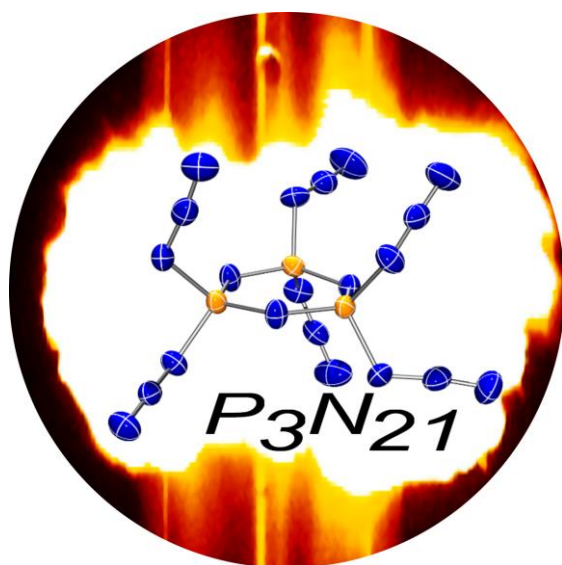




Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie
Swiss Society for Crystallography

Sektion für Kristallwachstum und Kristalltechnologie
Section de Croissance et Technologie des Cristaux



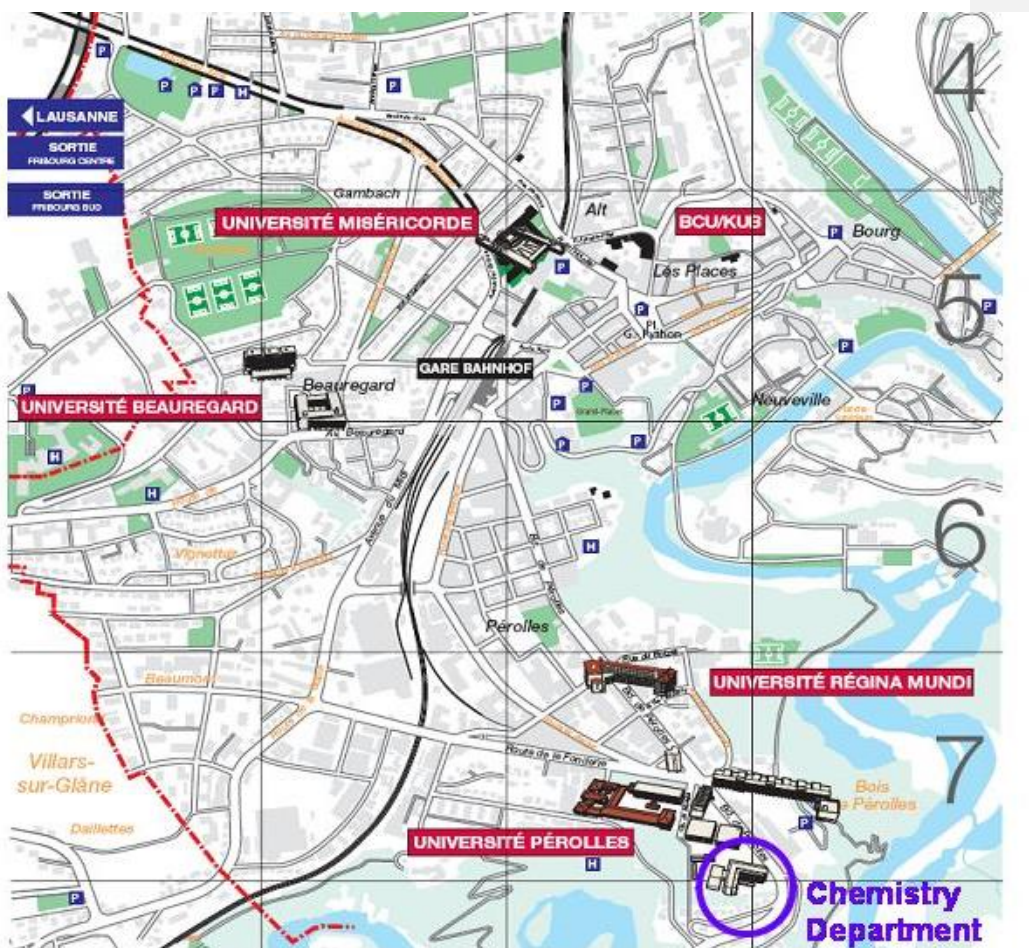
SGK/SSCr NEWSLETTER

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No. 78

Aug. 2009

In this issue: Abstracts and Program of the Annual Meeting in Fribourg, Sept. 8, 2009
Agenda of the Annual Assembly 2009



Map for the Annual Meeting Sept. 8, 2009 in Fribourg (conference site: 15 minutes walking distance from the main station or buses 1, 3 and 7 direction Marly, Péroilles or Cliniques)

On the Cover:

Towards elucidating the exotic chemical reactivity of matter under extreme conditions, for example P_3N_{21} . A dedicated talk will be given by M. Göbel at the annual meeting in Fribourg, abstract page 16-17.

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Lewy-Bertaut Price 2009

Laudatio in Honor of our member, Dr. Lukáš Palatinus, winner of the second edition of the Lewy-Bertaut prize of the European Crystallographic Association ECA and the European Neutron Scattering Association ENSA.

Contributed by G. Chapuis and M. Dusek

Our SGK/SSCr-member, Dr. Lukáš Palatinus (born on 12 June 1977 in Ústí nad Orlicí, Czech Republic) is the lucky winner of the 2nd Erwin Felix Lewy Bertaut prize. He received this distinction for his outstanding contributions to the solution of crystal structures from diffraction data, especially for providing a solution to the phase problem of aperiodic crystals.

Lukáš is an expert in the structure analysis of aperiodic structures, well known among crystallographers as the author of the program Superflip for solving structures of arbitrary dimensions by the charge flipping method. He obtained his Ph.D. at the Laboratory of Crystallography at the University of Bayreuth (Germany) under the supervision of Prof. Sander van Smaalen. During this period, his research resulted in a substantial contribution to the Maximum Entropy Method (MEM) applied to diffraction data of both periodic and aperiodic crystals. Since 2005, Lukáš is pursuing his research at the EPFL in Lausanne in the Laboratory of Crystallography headed by Prof. Gervais Chapuis. In the past several years Lukáš greatly contributed to the development of the method of charge-flipping for solving both periodic and aperiodic crystal structures from diffraction data.

In 2004, G. Oszlányi and A. Sütö published an article describing a new method of charge-flipping for the solution of periodic crystal structures from diffraction data [Acta Cryst. A **60**, 134 (2004)]. Lukáš immediately realized the potential of this method and extended it to aperiodic crystals by applying the charge-flipping algorithm to the generalized electron density in superspace [L. Palatinus, Acta Cryst. A **60**, 604 (2004)]. An initial implementation of this algorithm was made by Lukáš as part of the software BayMEM-a program package for the application of the MEM of which Lukáš then was one of the main authors. One year later, Lukáš developed the computer program Superflip, for the solution of both periodic and aperiodic crystals structures from diffraction data by the method of charge-flipping. Superflip is one of most successful computer programs for charge flipping. The publication on Superflip [L. Palatinus and G. Chapuis, J. Appl. Cryst. **40**, 786 (2007)] has been cited already 23 times by March 2009, *i.e.* within the first 18 months following its publication.

In classical crystallography, charge-flipping has evolved to a powerful alternative to direct methods for the structure solution. Nevertheless several different, well-established procedures exist for the same purpose. On the other hand, in the field of aperiodic crystallography, charge flipping represents a unique tool for *ab-initio* structure solution allowing aperiodic structures to be solved directly, without any *a priori* knowledge about symmetry, average structure, chemical composition or the nature of the modulations. Other methods based on the refinement of modulations from small arbitrary displacements or direct methods require the knowledge of the average structure. Often, these methods fail to lead to a solution. The importance of the work of Lukáš was to provide the first systematic method of structure determination of aperiodic crystals, which has the potential to become the method of choice for solving structures of aperiodic crystals.

In collaboration with Ch. Baerlocher and L. McCusker, ETH Zurich, Lukáš also participated to the extension of the charge-flipping method to powder diffraction data. For this technique, the specific problem is due to the overlap of reflections in powder diffraction patterns. A further contribution of Lukáš was the development and implementation of a method to determine the space group symmetry from the structure usually solved in space group $P1$. This method has the potential to become a real alternative to the traditional procedure based on intensity statistics, especially in cases where the statistics of the diffraction pattern is not fully accessible, as *e.g.* for incomplete data sets, data sets with many weak reflections, electron diffraction data, or powder diffraction data.

Within a short period following his PhD, Lukáš has had a high impact in the field of crystallography, including aperiodic structures. We are particularly happy to congratulate Lukáš for his well-deserved prize. Moreover, we are also particularly proud that the 2nd edition of the prize is attributed for the second time to a scientist working in Switzerland.

PROGRAM OF THE ANNUAL MEETING OF THE SWISS SOCIETY OF CRYSTALLOGRAPHY

September 8th, 2009 (Dinner: Sept 7, 2009)

Organizer: Katharina Fromm, Fribourg
Big Lecture Hall, Department of Chemistry, Chemin du Musée 9, 1700 Fribourg



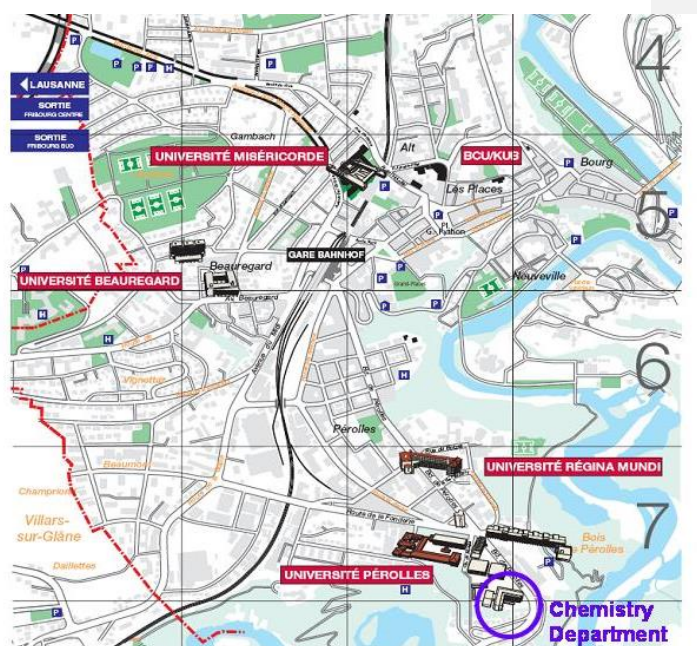
Conference Registration:

Please register at <http://www.unifr.ch/crystallography>
(free of charge, in order to optimize our organisation)

Conference Dinner:

Sept. 7, 2009, 19h (day before the meeting, Restaurant L'Homme Sauvage)
Please contact Katharina Fromm for reservations.

Sponsors:



Program of the Annual Meeting 2009

Big Lecture Hall, Department of Chemistry, Chemin du Musée 9, 1700 Fribourg

Last updates: <http://www.chem.unifr.ch/kf/event/fr/program>

8h30 – 9h00	Registration + Poster hanging
9h00 – 9h05	Welcome (W. Steurer, K. Fromm)
9h05 – 9h50	Prof. Hubert Huppertz, University of Innsbruck, Austria <i>"New aspects in the chemistry of borates"</i>
9h50 – 10h15	Prof. Klaus Yvon, University of Geneva, Switzerland <i>"Hydrogen induced metal-insulator transitions in metal – hydrogen systems"</i>
<hr/>	
10h15 – 10h35	Coffee Break / Posters
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10h35 – 11h20	Prof. Dietmar Stalke, University of Göttingen, Germany <i>"Charge density based ligand design"</i>
11h20 – 11h55	Poster Appetizers
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11h45 – 14h00	Business Lunch + Poster Session
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14h00 – 14h45	Prof. Sander van Smaalen, University of Bayreuth, Germany <i>"Periodic and aperiodic crystals analysed by the Maximum Entropy Method."</i>
14h45 – 15h10	Prof. Bernard Grobéty, University of Fribourg, Switzerland <i>"Kinetics of chrysotile breakdown"</i>
15h10 – 15h35	Prof. Antonia Neels, CSEM, Switzerland <i>"Engineering of thin film crystallinity for wear resistant coatings"</i>
<hr/>	
15h35 – 15h55	Coffee Break / Posters
<hr/>	
15h55 – 16h20	Dr. Michael Göbel, Prof. Thomas Klapötke, LMU, Germany <i>"Towards elucidating the exotic chemical reactivity of matter under extreme conditions"</i>
16h20 – 16h45	Special Guest
16h45 – 17h00	Poster Prizes, Closing Remarks, followed by Crystal Exhibition
<hr/>	
17h15 – 18h00	Annual Meeting of the Swiss Society of Crystallography & END

Abstract Invited Talks

T1: New Aspects of Borate Chemistry under High-Pressure

H. Huppertz

Institute for General, Inorganic, and Theoretical Chemistry, Leopold-Franzens-University
Innsbruck, Innrain 52a, A-6020 Innsbruck, Austria

At the moment, over 1100 borate crystal structures are listed in the Inorganic Crystal Structure Database ICSD. High-pressure investigations in this field are rare and were mainly performed from a geological point of view. Starting in 1999, systematic high-pressure / high-temperature experiments up to maximum pressures of 16 GPa have been carried out, using the multianvil technique to explore the synthetic possibilities in the field of borates under extreme conditions. Our research interest aims mainly at the structural behaviour and the synthesis of new inorganic materials under extreme conditions of pressure and temperature with a special view on borates, which are unattainable *via* conventional solid state syntheses. In these compounds, boron coordinates to oxygen in form of planar or non planar BO_3 groups as well as BO_4 tetrahedra. Due to the fact that nearly no synthetic work had been done under high-pressure / high-temperature conditions, we entered a new fruitful research area in the last years. We obtained several new compounds, which are presented in the talk including an outlook into further areas of high-pressure syntheses in solid state chemistry.

T2: Hydrogen induced metal-insulator transitions in metal – hydrogen systems

Klaus Yvon

Laboratoire de Cristallographie-MANEP, Université de Genève, Switzerland

Metal – hydrogen systems are of practical interest because they provide a safe and efficient way of storing hydrogen. Their storage densities tend to exceed that of liquid hydrogen and compressed gas cylinders while their risk of accidental ignition or explosion is minimal. Some have been commercialized for use in rechargeable nickel-metal hydride (Ni-MH) batteries and developed for energy conversion devices such as polymer electrolyte membrane fuel cell systems, while others are of use as switchable optical mirrors. Systems at the interface between metallic and insulating states are particularly interesting because they provide a useful playground for modelling metal-hydrogen interactions and thus to better understand fundamental properties such as hydrogen capacity and thermal stability. Metal-insulator (M-I) transitions in transition metal (T) based systems have only been discovered recently. They occur as a function of hydrogen concentration, lead to the formation of T-H bonds and leave the metal matrix nearly unchanged. The hydrogen-free compounds (e.g. Mg_2Ni and Mg_3Ir) are metallic while the hydrides are non-metallic (e.g. brownish-red Mg_2NiH_4 and red $\text{Mg}_6\text{Ir}_2\text{H}_{11}$; for a recent review see [1]). Quaternary metal-hydride systems such as $\text{LaMg}_2\text{Ni-H}$ [2] and $\text{La}_2\text{MgNi}_2\text{-H}$ [3] are particularly attractive for studies because they have a relatively large number of compositional parameters that allow one to tailor better properties for applications such as hydrogen detectors and sensors. A common feature of all these systems is the formation of closed-shell 18-electron T-metal-hydrogen complexes ($[\text{NiH}_4]^{4-}$ in Mg_2NiH_4 , $[\text{CoH}_5]^{4-}$ in Mg_2CoH_5 , $[\text{Ni}_2\text{H}_7]^{7-}$ and $[\text{Ni}_4\text{H}_{12}]^{12-}$ in $\text{La}_2\text{MgNi}_2\text{H}_8$) that correlate with the onset of the M-I transitions. Recent work in Geneva in that area will be highlighted.

- [1] *Hydrides: Solid State Transition Metal Complexes*. *Encycl. Inorg. Chem.*, 2nd edition, p. 1814-1846 (2005), John Wiley & Sons Ltd., ISBN 0-470-86078-2. K. Yvon, G. Renaudin,
- [2] *Hydrogenation Induced Insulating State in the Intermetallic Compound LaMg_2Ni* . *Phys. Rev. Lett.* **94** (2005) 066403. K. Yvon, G. Renaudin, C. M. Wei, M. Y. Chou.
- [3] *Isolated $[\text{Ni}_2\text{H}_7]^{7-}$ and $[\text{Ni}_4\text{H}_{12}]^{12-}$ Ions in $\text{La}_2\text{MgNi}_2\text{H}_8$* , *Angew. Chem. Int. Ed.*, **45**, (2006) 7770-7773. J.-N. Chotard, Y. Filinchuk, B. Revaz, K. Yvon.

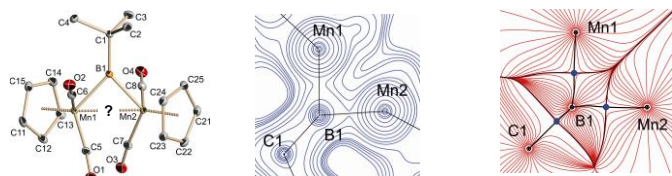
T3: Charge density based ligand design

Dietmar Stalke

Institut für Anorganische Chemie der Universität Göttingen, Germany

Recently we synthesised and experimentally determined the charge density in molecules to gain insight in their reactivity and coordination behaviour. Not to judge on the structure-reactivity relationship by mere bond lengths comparison [1] we rather rely on the topological analysis. Various topics are addressed in the talk:

- 1) S=N bonds in polyimidosulfite ylides are rather easy to cleave because they are electrostatically reinforced S⁺-N⁻ single bonds rather than hetero-olefin bonds and the formal S=C double bond is a polar S⁺-C⁻ single bond with no ylenic contribution [2].
- 2) The metallaphosphane [Me₂AlPy₂P] contains a divalent P(III) atom with two lone pairs at the central phosphorus atom. Following this finding the P-atom in the protonated phosphanide PPy₂(H) can be employed in bridging mimicking a 4-electron donor [3].
- 3) Multipole refinement of a lithiated benzyl silane provides insight in the electronic situation and thus the observed stereochemical course of transformations. Surprisingly the negative charge generated at the carbanion hardly couples into the phenyl ring [4].
- 4) The Laplacian distribution around the boron atom in [$\{\text{Cp}(\text{CO})_2\text{Mn}\}_2(\text{B}^t\text{Bu})$] clearly shows the difference between the borylene ligand and the carbonyl ligand [5].



5) The negative charge originating from lithiation of the methyl group in 2-picoline is distributed over the whole ring system with the largest increase at the methylene group. The bonding properties derived from the experimental and theoretical electron density distribution supports the interpretation as an enamide, but the preferred electrophilic attack at the anion generally occurs at the methylene group [6].

- [1] a) J. Henn, D. Leusser, D. Stalke, *J. Comp. Chem.* **2007**, *28*, 2317;
b) H. Ott, D. Stalke, *Nachr. Chem.* **2008**, *56*, 131.
- [2] S. Deuerlein, D. Leusser, U. Flierler, H. Ott, D. Stalke, *Organometallics* **2008**, *27*, 2306.
- [3] a) T. Stey, J. Henn, D. Stalke, *Chem. Commun.* **2007**, 413; b) T. Stey, M. Pfeiffer, J. Henn, S. K. Pandey, D. Stalke, *Chem. Eur. J.* **2007**, *13*, 3636.
- [4] H. Ott, C. Däschlein, D. Leusser, D. Schildbach, T. Seibel, D. Stalke, C. Strohmann, *J. Am. Chem. Soc.* **2008**, *130*, 11901.
- [5] U. Flierler, M. Burzler, D. Leusser, J. Henn, H. Ott, H. Braunschweig, D. Stalke, *Angew. Chem. Int. Ed.* **2008**, *47*, 4321.
- [6] H. Ott, U. Pieper, D. Leusser, U. Flierler, J. Henn, D. Stalke, *Angew. Chem. Int. Ed.* **2009**, *48*, 2978

T4: Periodic and aperiodic crystals analysed by the maximum entropy method

Sander van Smaalen

Lehrstuhl für Kristallographie, Universität Bayreuth, 95440 Bayreuth, Germany

The Maximum Entropy Method (MEM) is a general method of data analysis with applications in image processing, NMR, crystallography and other sciences. We employ the MEM to determine the most probable electron density in the unit cell of a crystalline compound, given the set of measured intensities of Bragg reflections in the X-ray diffraction. For this purpose a computer program, BAYMEM, has been developed in Bayreuth, with which MEM-densities can be determined for electron densities in unit cells of periodic crystals as well as for superspace densities in four-dimensional space of aperiodic crystals [1]. Two disparate applications of the MEM are possible. With a reference density or PRIOR that is constant over the unit cell, local maxima in MEM-densities indicate positions of atoms, while the amount of electrons around each maximum is proportional to the occupancy of the site. In this way, disorder can be studied by the MEM, while the MEM in superspace can thus be used to determine the shapes of modulation functions of aperiodic crystals. The second approach employs a PRIOR equal to the density of the independent spherical atom model (ISAM). This results in highly accurate MEM-densities that exhibit the distribution of density in chemical bonds [2]. The latter application of the MEM is an alternative for the well-established method of multipole refinements. In this lecture I will introduce the MEM and I will provide several examples of its application to periodic and aperiodic crystals.

- [1] S. van Smaalen, L. Palatinus and M. Schneider, *Acta Crystallogr. A* **59**, 459-469 (2003). The Maximum Entropy Method in superspace.
- [2] A. Hofmann, J. Netzel and S. van Smaalen, *Acta Crystallogr. B* **63**, 285-295 (2007). Accurate charge density of Trialanine: a comparison of the multipole formalism and the maximum entropy method (MEM).

T5: Kinetics of chrysotile breakdown

Bernard Grobéty and Roy Trittshack

Department of Geosciences, University of Fribourg, Switzerland

Chrysotile is a phyllosilicate with a remarkable crystal structure. The layers, consisting of a tetrahedral and an octahedral sheet, are enrolled resulting in a tube morphology, with an outer diameter between 10 to 50 nm, and an inner diameter between 1 and 3 nm. The structure of chrysotile has no translational periodicity, but changes continuously with radius. Physical and chemical properties are, therefore, expected also to change with curvature. This is the case for the breakdown temperature. The dehydration temperature is inverse proportional to the curvature radius of the TO layers e.g. the reaction starts at the circumference of the tube. The primary reaction product is amorphous. For chrysotile tubes with diameters around 50nm dehydration starts at ca. 470°C and is terminated at ca. 570°C (Brindley and Zussman, 1957; Metraux and Grobéty, 2002). The kinetics of these reactions has been studied for temperatures between 600°C and 750°C (Brindley and Hayama, 1964a and b; Cattaneo et al., 2003). At these temperatures the entire tube dehydrates. In the present investigation, the kinetics of the chrysotile breakdown between 500°C and 650°C has been analyzed using in-situ high temperature X-ray diffraction. Both activation energy and reaction order change with temperature e.g. with the average curvature of the part of the chrysotile tube which dehydrates. The results will be discussed considering the asymmetry of the dehydration geometry.

T6: Engineering of thin film crystallinity for wear resistant coatings

Antonia Neels,¹ Leandro De Abreu Vieira,¹ Alex Dommann,¹ Jürgen Ramm²

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² OC Oerlikon Balzers AG, Iramali 18, LI-9496 Balzers, Liechtenstein

The XRD Application LAB of the CSEM participates in research and development projects and provides services which include structural analyses for coatings, thin films, micro- and nanocrystalline powders and single crystalline materials and especially quality control and reliability studies for the MEMS community (MEMS = Micro-Electro-Mechanical Systems).

The use of various XRD techniques and the evaluation of the microstructure in relation to macroscopic properties is discussed for α -alumina type structures used in coatings. Wear resistant coatings cover a wide range of industrial applications and are well accepted to increase tool life and productivity in cutting tool applications. α -alumina (corundum) has outstanding properties for hardness and chemical stability at high tool temperatures [1].

Corundum type $(Al_{1-x}Cr_x)_2O_3$ thin films present an effective oxygen diffusion barrier when they are annealed at 1000°C in ambient conditions (Figure 1).

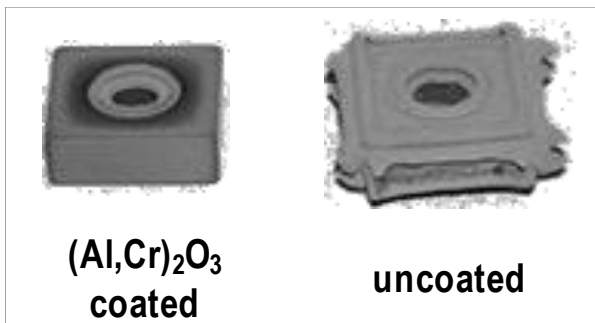


Figure 1: Appearance of the coatings / substrates after annealing at 1000°C.

One feature of the applied coating technology is the possibility to influence and adjust the stress in PVD oxide layers which is one major factor of influence in the wear behavior of the coating. For coatings on Si substrate, the strain can be determined by High Resolution X-ray Diffraction (HRXRD) by curvature measurements on the Si single crystal substrate (travelling peak technique, Figure 2a). The peak shift in dependence of the x position of the sample determines the curvature and layer stresses can be calculated. For these $(Al_{1-x}Cr_x)_2O_3$ coatings, moderate compressive and tensile stresses can be achieved.

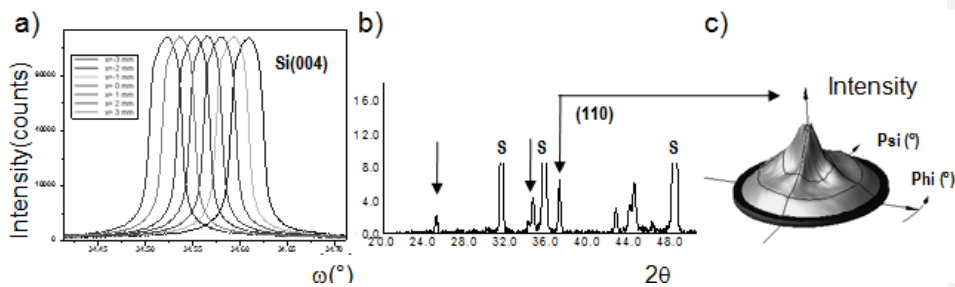


Figure 2: a) Curvature measurements on the Si substrate by means of Rocking Curves (RC's); b) $\omega/2\theta$ scan on the coating (S = substrate); c) texture determination, pole figure of $(Al_{1-x}Cr_x)_2O_3$ (110) reflection.

Phase analysis, composition (Al/Cr ratio), crystallite size and the preferred orientation of the grains in the coating are investigated. The preferred orientation is recognized performing ω/θ -scans (Figure 2b). The texture can be determined precisely by means of pole figures (Figure 2c). By understanding micro-structural features, XRD analysis supports actively the design and improvement of the coating properties such as hardness and resistance against oxidation at high temperature.

[1] J. Ramm, M. Ante, H. Brändle, A. Neels, A. Dommann and M. Döbeli, *Advanced Engineering Material*, 9 (2007) 604-608.

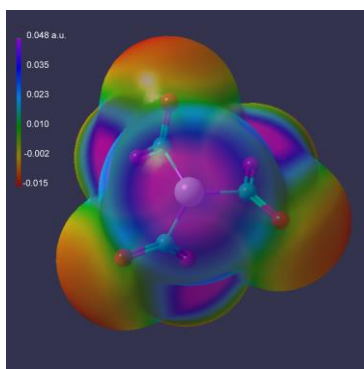
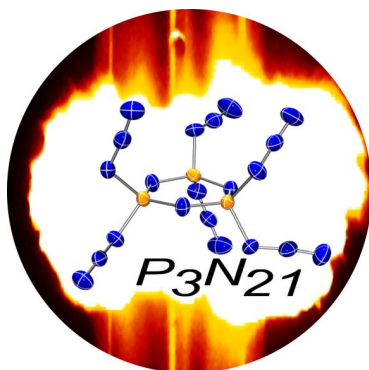
T7: Towards elucidating the exotic chemical reactivity of matter under extreme conditions

Michael Göbel and Thomas M. Klapötke

Department of Chemistry, Ludwig-Maximilians University (LMU), Munich, Germany

The development and testing of energetic materials is an exciting and challenging area of chemistry both as far as fundamental and applied aspects are concerned. Though the development of this kind of materials, which include high explosives, propellants, and pyrotechnics has a long standing tradition in the chemical sciences, research and efforts are undertaken world-wide as never before, foremost driven by the prospect of outstanding materials properties in general, and in order to discover new representatives having significant advantages over compounds currently used. Environmental considerations and safety requirements are important driving factors next to higher performance and tailored properties for special applications. Due to their unique properties, these materials are useful for manifold and highly diverse applications ranging from military to civilian areas in many industries including but not limited to construction, mining, oil exploration as well as space exploration. Obtaining such materials is complex owing to the fact that several different and mutually exclusive appearing material properties have to be met to find the molecule fulfilling all the qualification criteria in order to become widely accepted. The development of energetic materials is a whole world of trade-offs between energy content of a molecule and other desirable properties like higher performance, insensitivity against accidental initiation, thermal stability as well as a non-toxic and non-polluting behaviour when exposed to the environment next to other additional properties. The traditional procedure for formulating new materials has been largely guided by intuition, experience and testing, relying foremost on trial and error. In turn, a better understanding of the basic principles is highly desirable to yield a more rational design process. However, exploiting these possibilities requires an understanding of the properties of the individual molecules, their interaction amongst each other as well as to surrounding matter next to an understanding of kinetic energy release and dynamics of initiation and decomposition processes. This *bottom-up* approach to energetic materials would allow for a more fundamental understanding of the evolution of properties with the size of the system as well as an understanding of the effects of the interaction of matter at different molecular-length scales with external stimuli and finally a detailed understanding of the functionalities of matter at molecular-length scale. The information obtained could provide breakthroughs not only in the area of energetic materials but additionally also in all areas of material science and chemistry in general both as far as fundamental and applied aspects are concerned.

Energetic materials, due to their very nature, can offer a variety of unique insights into structure and matter. For example, detonations of high explosives produce thousands of Kelvin and a few hundred thousand atmospheres thus providing a unique means of elucidating the exotic chemical reactivity of matter under extreme conditions - similar to the conditions in the interiors of giant planets - as has recently been reported for the case of water.¹



At the same time, the extreme conditions inside a detonating explosive have made it extremely difficult to perform measurements and consequently the detailed chemical reactions that cause a detonation are largely not understood.² Empirical observations are important to gain a better understanding of the final chemical composition after detonation and the corresponding reaction mechanisms are still not known for many explosives rendering this science to be very young and advances to be likely with the advent of novel techniques allowing to acquire experimental information previously not available.³

Single crystal X-ray diffraction techniques will certainly become even more important in elucidating the nature of the chemistry of energetic materials with the advent of new bright light sources and the development of free electron lasers. Within the scope of this talk, a selection of structure determinations of rather elusive molecules will be shown. Examples include mercury fulminate⁴, a compound of historic interest that dates back to alchemists of the 17th century and finally allowed Alfred Nobel to successfully introduce Dynamite. Other examples include the highly energetic compound P_3N_{21} , representing the first example of a structure determination of the binary system phosphorus and nitrogen (top picture).⁵ The potential of single crystal X-ray diffraction in helping to design a more targeted development of novel highly energetic compounds with desirable properties will be demonstrated using the class of molecules carrying the trinitromethyl moiety.⁶ Finally, the intriguing structural properties of the chlorotrinitromethane molecule (bottom picture) will be briefly discussed.⁷

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- [4] Wolfgang Beck, Jürgen Evers, Michael Göbel, Gilbert Oehlinger and Thomas M. Klap *Z. Anorg. Allg. Chem.* **2007**, 633(9), 1417-1422.
- [5] Michael Göbel, Konstantin Karaghiosoff, Thomas M. Klapötke, *Angew. Chem.*, **2006**, 118(36), 6183-6186; *Angew. Chem. Int. Ed.* **2006**, 45, 6037-6040.
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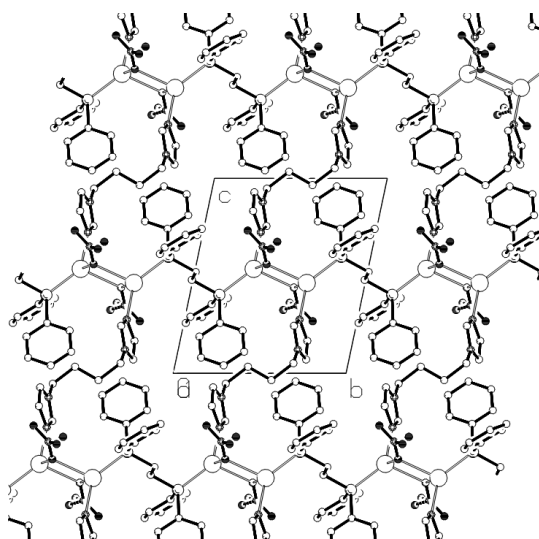
Abstract Posters

P1: Silver-Phosphine multi-dimensional coordination polymers: using exo-dentate ligands

Muhammad Altaf and Helen Stoeckli-Evans

Institute of Physics, University of Neuchâtel, Rue Emile-Argand 11, CH-2009 Neuchâtel

Interest in the preparation of extended networks using inorganic coordination polymers is based on the development of materials with tuneable properties similar to those observed in zeolites¹ and compounds with interesting biological,² and electrical properties.³⁻⁵ The rapidly growing area of coordination polymers based on metal cations with organic ligands and counter ions, has given rise to a wide variety of fascinating one-, two- and three-dimensional structures.⁶ The high degree of design arises from the coupling of the well understood coordination properties of the organic ligand, the individual metal ions, the anions and the solvent of crystallization. The selection of a highly developed ligand within the area of supramolecular chemistry and crystal engineering is most important.^{7,8}



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[5] R. Noguchi, A. Hara, A. Sugie, K. Nomiya, *Inorg. Chem. Commun.* **2006**, 9, 355.

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P2: α -NaLuF₄: a structure for all seasons.

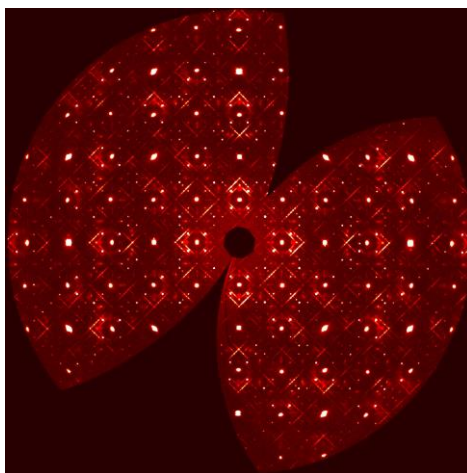
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NaLnF₄ (Ln=Y,La-Lu) crystallizes in two predominant phases. The low-temperature, stable hexagonal β -form, doped with various Ln³⁺ ions exhibits efficient light upconversion properties. Understanding these properties requires a knowledge of the local structure; the average structure of β -NaLaF₄ has occupational disorder within columns of mixed Na⁺/La³⁺ sites and Na⁺/vacancies; an examination of strong diffuse scattering allowed the relative alignments of the columns to be deduced [1]. At high temperatures, the unstable "cubic" α -phase forms. We are studying the structure of α -NaLuF₄ with likely composition Na₅Lu₉F₃₂, and have recorded



the full scattering using synchrotron radiation. Reconstructed reciprocal lattice (r.l.) layers reveal a rich, apparently cubic, diffraction pattern with very strong Bragg reflections, weaker satellites, strong diffuse scattering and mixed phases (the $hk0$ layer is shown). Bragg reflections in r.l. rows are not collinear. Therefore, the highest possible symmetry is tetragonal and 6-fold twinning accounts for the apparent cubic symmetry. Re-indexing as a tetragonal C -lattice places the satellites on r.l. rows; this allows definition of an orthorhombic supercell with one axis five times the tetragonal a -axis. Solving the structure in the C -superlattice with *SUPERFLIP* reveals two distinct commensurately modulated parallel columns of cations: one with varying Na⁺/La³⁺ occupancy and one with positional displacements of the ions from the average structure positions.

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We thank ESRF for time on the SNBL beamline, Dr. Karl Krämer (University of Bern, Switzerland) and the Swiss National Science Foundation for support.

P3: Interpretation of Opechowski-Guccione symbols of magnetic space groups independent of tabulated (0,0,0)+ sets

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The interpretation of Opechowski-Guccione (OG) symbols introduced in [1] depends in the case of centred conventional cells on the (0,0,0)+ set of general positions selected in [2]. Bertaut [3] claimed that the table of correspondences between OG and BNS (Belov-Neronova-Smirnova) symbols given in [1] contained a number of errors in the case of magnetic groups of class *mmm*. The disagreement was due in part to different interpretations of OG symbols. A new interpretation along the ideas of Bertaut is proposed, which leads to differences also for certain groups in class 222 and for some tetragonal and cubic groups. This interpretation requires using for two of the OG superfamilies names different from the standard Hermann-Mauguin symbol (HMS) of the corresponding space group [*Acm* → *Acc*, *A/mcm* → *A/mcc*] and ignoring the recent changes of 5 standard HMS, where double glide planes became denoted by *e*. The decisive advantages of the proposed interpretation are its independence of tabulated (0,0,0)+ sets and the possibility of reading a set of group generators off the OG symbol, similarly as in the case of BNS symbols.

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P4: Long and short range order in Laves phase deuterides

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The deuterides of cubic (C15) Laves phases have been widely studied for the influence of deuterium absorption on their magnetic properties. The systems YFe_2D_x and YMn_2D_x are particularly interesting due to the large variety of crystal structures depending on the D content [1,2]. When absorbing deuterium the metallic matrix retains the cubic cell ($Fd\bar{3}m$) above the deuterium ordering temperature. Below this temperature the symmetry is lowered and a fully ordered coordination of metals by deuterium atoms

is obtained in the deuterium rich phases. Complex structures with up to 12 metal atoms and 18 deuteriums in the asymmetric unit as for monoclinic $\text{YFe}_2\text{D}_{4.2}$ [3] are formed. Little is known about the local

deuterium configuration around the transition metal atoms in the disordered phase even if a considerable amount of diffuse intensity was reported in the neutron powder patterns.

Analysis of YFe_2D_x and YMn_2D_x by Rietveld and Pair Distribution Function (PDF) methods will be presented. Neutron Time-of-Flight (ToF) data were collected at IPNS, Argonne, and Lujan Center, Los Alamos on series of samples with different deuterium content. Each sample was measured below and above the temperature of deuterium ordering. The PDF in ordered and disordered states look very similar up to the radial distance of $\sim 8 \text{ \AA}$, which is comparable with the lattice parameter of a cubic Laves phase deuteride. The observed PDF was modeled in the disordered state using the same local model as in the ordered phase (Figure 1).

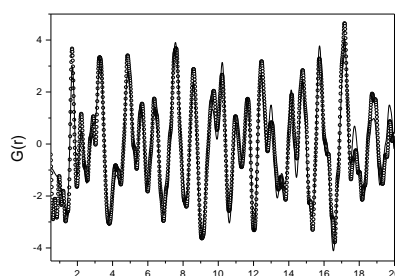


Fig. 1: Observed PDF (points) of $\text{YFe}_2\text{D}_{4.2}$ in disordered state: Modelling (solid line) by same local order of deuterium atoms around iron as in the ordered phase

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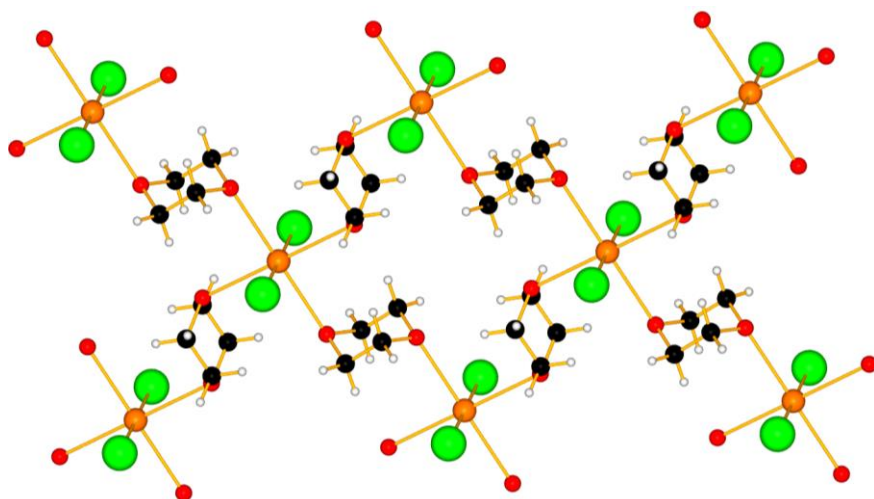
The collaboration with Thomas Proffen from Lujan Neutron Scattering Center, Los Alamos, USA, is highly appreciated. This work is supported by the Swiss National Science Foundation.

P5: Utility of absorption correction on transition metal complexes

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It is well known that a good absorption correction is necessary to obtain meaningful anisotropic thermal parameters for a crystal structure, especially when the absorption coefficient is high. Numerical absorption correction using a 3-dimensional integration over all X-ray beam paths in the crystal gives the most accurate results but it requires a crystal description in terms of face indices and distances. Measuring crystals of transition metal complexes of heavy metal ions like mercury(II), is this correction necessary or is it just an aid for solving structure more easily?



In the four examples, numerical absorption corrections are made with X-shape with the X-area[®] software [1], the starting regular form are icosahedrons with optimization of distances and hkl. Shelx 97 [2] is used for resolution, no restraints or any constraints are used, the resolution is stopped when all Q peaks are assigned, atoms are refined anisotropically and H-atoms are simulated.

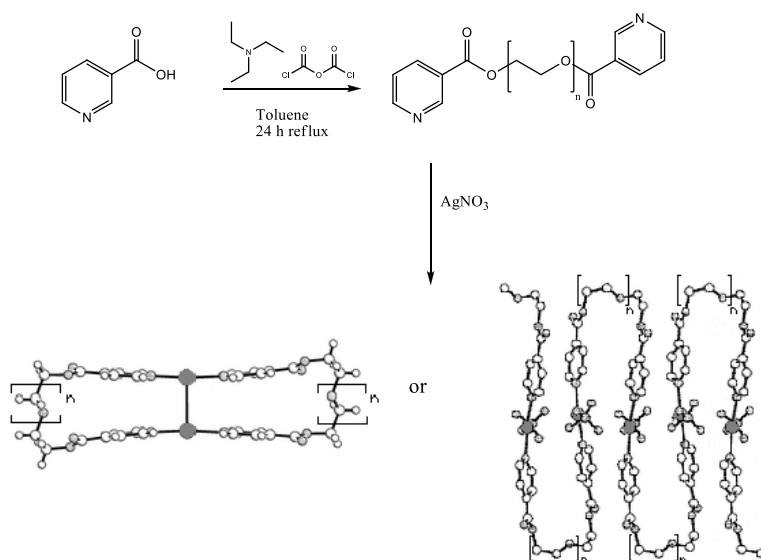
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P6: Synthesis of New Silver Compounds with derivatives of nicotinate

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Silver ions have antibacterial properties, and complexes with this ion have a great potential of applications in medical uses. Complexes of silver with several ligands derived from nicotinic acid and with up to three ethylene oxide groups as spacer are already known. In our group, we obtain metallacycles, and under special conditions, chain structures. We propose the development of complexes with longer spacers and to study the possible formation of solids, liquid crystals or polymers.



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P7: Fracture behaviour of single crystal Silicon structures

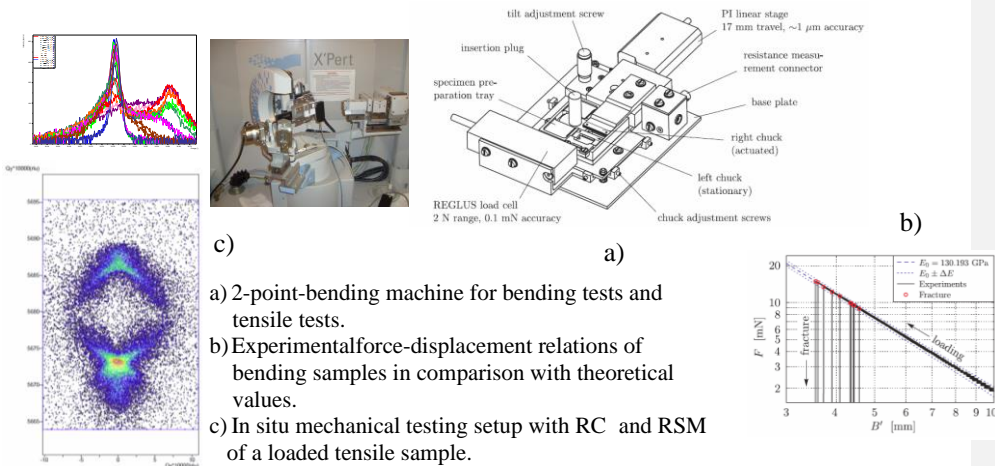
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Single Crystal Silicon (SCSi) is the preferentially used material in microsystem engineering. Imperfections—like surface roughness and defects—of the perfect lattice introduced by the manufacturing processes are recognized to favor failure. An experimental setup for mechanical tests as 2-point-bending test and tensile test was developed and is used to realize large deformations (>3% strain) on particular DRIE etched SCSi devices to assess the resistance of SCSi structures to loading [1]. The experiments are analyzed for Young's modulus and fracture strength. The results are in good agreement with literature values (relative error less than 0.5%) [2]. Understanding of failure requires further information about material conditions on the atomic scale which may be determined by HRXRD. In situ measurements of local deformations and the analysis of the strain field and defects in the critical regions of the structure by HRXRD allow the comparison and correlation with the simulation of deformations by Finite Element Method (FEM), which includes the characteristic surface roughness.



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P8: Structural transformations of cyano-bridged coordination polymers

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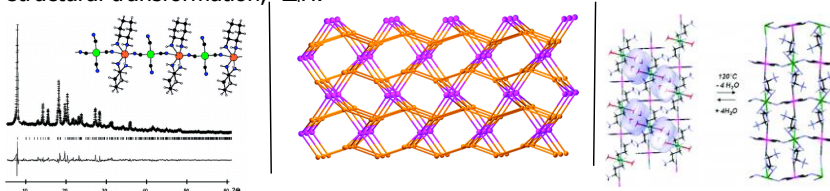
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Dynamic structural transformations, based on flexible porous frameworks are a major challenge in material sciences, both from a fundamental and a practical point of view. We have focused our efforts on the synthesis of crystalline materials, since the attainment of well-defined structures is intimately linked to an understanding of the design, synthesis and properties of such materials.^[1] We have constructed a number of metal-organic coordination polymers based on metallocyanides, some of which show structural transformations on dehydration/rehydration. Their “sponge-like” behaviour, often accompanied by a colour change, has been shown by in-situ powder X-ray diffraction and immersion calorimetry to be reversible.^[2-7] In one case, using a combination of DSC, powder XRD and immersion calorimetry, it was possible to obtain the net heat of the structural transformation, $-\Delta H$.^[8]



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P9: New borohydrides – crystal structures and vibrational spectra

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The first 3d-metal borohydride - Mn(BH₄)₂

Solvent-free manganese borohydride Mn(BH₄)₂ was prepared at ambient conditions in ball milled mixtures of alkali metal borohydrides and MnCl₂ [1]. The milling conditions were optimized, and especially a cooling break was found to be important for the successful synthesis by ball milling. Mn(BH₄)₂ crystallizes with the space group symmetry P3₁12 and is stable up to 450 K. Mn(BH₄)₂ shows interesting relation with α-Mg(BH₄)₂ [2,3]: both structures are made of similar layers. Like α-Mg(BH₄)₂ the structure of Mn(BH₄)₂ is not densely packed and contains isolated voids with the estimated volume of 21 Å³ each, which occupy in total 6% of the space.

New Sc-based double cation borohydride – NaSc(BH₄)₄

Double cation alkaline- and transition-metal borohydride – NaSc(BH₄)₄ was prepared by two different research groups in ball-milled mixtures of NaBH₄ and ScCl₃ at ambient conditions. A competing reaction producing a new ternary chloride Na₃ScCl₆ has prevented from higher borohydride yield than 22 wt. %. Optimization of the starting ratio between NaBH₄ and ScCl₃ to 2:1 allowed to solve this challenging problem from synchrotron powder diffraction data. NaSc(BH₄)₄ crystallizes with the space group symmetry Cmc and is stable up to 523 K. Compared to LiSc(BH₄)₄ [4] the isolated [Sc(BH₄)₄]⁴⁻ anions in NaSc(BH₄)₄ are more deformed and differently oriented inside the deformed alkaline-metal cubes.

The deformed tetrahedral coordination of transition-metal cation by four [BH₄]⁻ anions as observed in Mn(BH₄)₂ and NaSc(BH₄)₄ is common also for cations in many other borohydrides. On the other side, in most of these borohydrides each [BH₄]⁻ is approximately linearly coordinated by two cations. An idealized structure based on such local configurations is that of inversed Cu₂O, as already discussed for α-Mg(BH₄)₂ [2]. The similarity of the structures on the local level is in favor of alloying the stable alkaline-metal with unstable transition-metal borohydrides in the view of tuning the desorption properties of borohydrides.

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The collaboration with University of Hawaii at Manoa, Department of Chemistry, USA, and with Interdisciplinary Nanoscience Center (iNANO) and Department of Chemistry, University of Aarhus, Denmark is highly appreciated. This work is supported by the Swiss National Science Foundation.

P10: Novel Silver Coordination Complexes with Fluorescent Ligands

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Metal-organic complexes have attracted extensive attention due to their potential application in electronics, magnetism, optical, and catalytic materials as well as their fantastic structures.^[1-4] Our idea is to design and synthesize some new ligands having fluorescent properties and coordinating with silver ions, the latter of which is regarded as a powerful antibacterial material used for many years, to obtain the corresponding fluorescent silver complexes. Furthermore, we want to coat them on a gold surface by molecular self-assembly, to study the structures and the morphologies of the surfaces, and investigate the optical and antibacterial properties. Herein, the structures and fluorescence spectra of some compounds will be presented.

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P11: Hydrogen bond evolution in molecular crystals

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X-ray diffraction crystal structures of oxalic acid dihydrate at high pressure, up to 5.3 GPa, show impressive changes in the molecular geometries of the chemical species, which suggest a proton transfer from $\text{H}_2\text{C}_2\text{O}_4$ to H_2O and therefore the creation of ionic species [1]. This is confirmed by theoretical prediction (using periodic DFT calculations) and by powder neutron diffraction on deuterated species [2]. The nature of the proton transfer (continuous or discontinuous) is presently under investigation.

The behavior of oxalic acid in similar crystalline environments is currently under study, in order to obtain more information on hydrogen bonding changes in these systems.

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P12: Synthesis of silver nanoparticles in polyelectrolyte matrix

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Nowadays, a wide variety of composite materials consisting of polymers containing metal nanoparticles have been extensively investigated to realize their potential applications ranging from optoelectronics to biomaterials. Nanostructured materials consisting of silver nanoparticles (Ag-NPs) embedded in polymeric matrices show physico-chemical, optical and antibacterial properties [1, 2]. A simple method to prepare a AgNP/polyelectrolyte composite was successfully used. Thus, Ag-NPs were obtained through spontaneous formation of nanostructured silver from an Ag_2O /polystyrene sulfonate (PSS) solution. The kinetics of AgNP-formation was investigated by dynamic light scattering and UV/vis spectroscopy, and related morphology was investigated by X-ray diffraction techniques. The synthesis of the Ag-NP/polystyrene sulfonate composite was performed by mixing a PSS solution in water with a Ag_2O solution in diluted ammonia during 48 hours. The nanoparticle size was determined by TEM and SEM.

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P13: Multitopic Ligand Approach for the Synthesis of Oxidic Materials

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Mixed metal materials can be used in different applications, for instance in opto-electronic devices or as metal oxides in high-Tc superconductors (BSSCO, YBCO) [1, 2, 3]

A synthetic strategy to obtain mixed metal oxides is to use decomposition techniques like (metal-organic) chemical vapor deposition (MO-CVD) to combust metal-containing volatile complexes. Complexes of alkaline earth and group 11 metal ions may for example provide such precursors.

We developed a multitopic ligand system, where different metal ions can be successively coordinated. This way, it is possible to tailor the properties (e.g magnetic, opto-electronic) of the multimetallic compounds.

To obtain mixed metal oxides ($\text{Ca}_x\text{Cu}_y\text{O}_z$ or $\text{Ba}_x\text{Cu}_y\text{O}_z$), we use different methods like combustion/sintering of the compounds or also evaporation techniques like MO-CVD. The so obtained oxides are characterized by XRD, SEM and EDS.

We will show that this concept works by presenting the synthesis pathways and also by showing first results obtained for mixed metal oxides, which could be used for the synthesis of BSSCO or YBCO. [4]

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P14: Magnetic and Structural Properties of $\text{Pb}_3\text{Mn}_7\text{O}_{15}$

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² Laboratory for Neutron Scattering, ETH Zürich & Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

³ Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

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The wide variety of physical properties in perovskite manganites stimulates the study of other Mn oxide families without perovskite structure, but a mixed valence state of the Mn ions ($\text{Mn}^{3+}/\text{Mn}^{4+}$). The material under investigation is the quasi 2D compound $\text{Pb}_3\text{Mn}_7\text{O}_{15}$ (Fig.1). Both existing models describing its crystal structure [1,2] were disproved by high-resolution X-ray powder diffraction investigations at the Swiss Light Source Materials Science (SLS-MS) beamline. A new model based on the orthorhombic space group *Pnma* could be identified [3]. Magnetization measurements give evidence of strong antiferromagnetic correlations. A huge step at $T = 70$ K indicates a 3D long range ordered state and a second smaller step at $T=20$ K is interpreted as reorientation of some moments due to a variation of the magnetic anisotropy with temperature. Neutron single crystal and powder diffraction measurements revealed the coexistence of two magnetic phases in $\text{PbO-MnO}_2\text{-Mn}_2\text{O}_3$ indicating the presence of different oxidation states. The disappearance of magnetic peaks at $T=20$ K and $T=70$ K is consistent with the magnetization measurement.

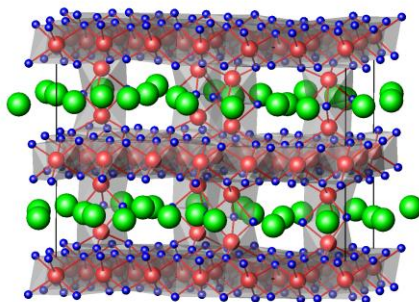


Fig. 1: Layered structure of $\text{Pb}_3\text{Mn}_7\text{O}_{15}$. Pairs of Mn atoms are bridging the layers separated by Pb atoms.

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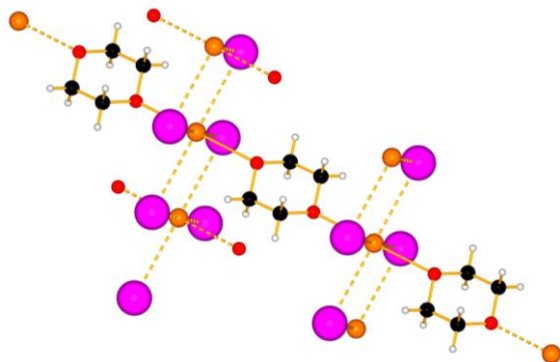
This work has been performed with the support of ILL Grenoble and the PSI FoKO, as well as INTAS Grant 06-100013-9002.

P15: Polyether adducts of d-block metal compounds as starting materials for new cluster compounds.

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We are interested in molecular compounds, especially oxygen donor adducts of metal halides, because they are used as starting materials in the synthesis of low-dimensional polymeric compounds, i. e. clusters, and polymers or metal organic frameworks.^[1-5] Indeed, since more than two decades, metal aggregates are used in the low-cost synthesis of superconductors and other oxide materials by the sol-gel technique, or as volatile precursors in the MOCVD (Metal Organic Chemical Vapor Deposition) process if they present the required properties, namely solubility and volatility. One of the major problems of the synthesis of organo-alkaline earth metals compounds is their tendency to form insoluble due on one hand to their low metal oxidation state (II) which only allows two anionic ligands, and on the other hand, their large ionic radii which demand a high coordination number. However, the chemistry of such metal halide or pseudo-halide adducts with neutral Lewis-coordinating ligands (usually non-polar aprotic solvents) is still not systematically studied. In this context, we have synthesized and characterized some new molecular compounds using polydentate neutral Lewis-coordinating ligands such as DME, dioxane, diglyme and triglyme in order to, in a fundamental way, know and understand better the chemistry of d-block metal halides in aprotic solvents. Secondly, we were interested in the study of the influence of the size of the ligand on the coordination sphere of the metal cation using monodentate, bidentate, tridentate and finally tetradentate O-donor ligands.



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- [5] A. Crochet, K. M. Fromm, *in preparation*

P16: Dehydration-induced phase transition in D-xylose isomerase

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D-xylose isomerase, which causes the isomerization of glucose to fructose, has a large market in the food industry because of its application in the production of high-fructose corn syrup. In order to fully understand and control the activity of the protein a good knowledge of the structural response of the protein to changes in the environmental conditions is necessary. Since proteins function in aqueous media and nearly half of the volume of protein crystals is occupied by water, protein-water interactions are of great interest.

We have now identified a dehydration-induced phase transition in D-xylose isomerase from *Streptomyces rubiginosus*. The transition, characterized using both powder and single crystal diffraction, occurs at room temperature for relative humidity around eighty percent. After the transition, the crystal recovers its crystalline state and diffracting power. The symmetry is reduced from space-group I222 to its subgroup P2₁2₁2 but the effects of this symmetry break on the structure are subtle. The decrease of the unit-cell volume by more than 15 percent produces more pronounced and interesting structural rearrangements in the crystal.

[1] Gummow R.J., Liles D.C., *Mat. Res. Bull.*, 1993, **28**, 1293

[2] Grirrane, A.; Pastor, A.; Galindo, A.; Ienco, A.; Mealli, C. *Chem. Commun.* 2003, 512.

P17: Structure modulations of scheelite related compounds affect their luminescence properties

Alla Arakcheeva¹, Gervais Chapuis¹, Phil Pattison^{1,2}, Vladimir Morozov³, Semen Shmurak⁴

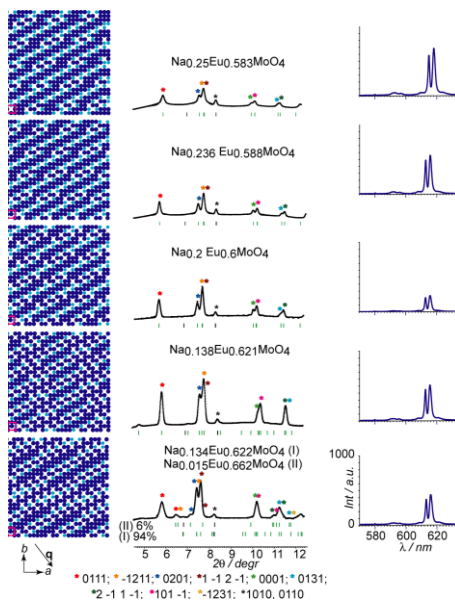
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Some scheelite related compounds (SRCs), such as $\text{KGd}(\text{WO}_4)_2$:Nd,Yb, $\text{NaBi}(\text{WO}_4)_2$, PbMoO_4 and MWO_4 ($\text{M} = \text{Cd}, \text{Pb}, \text{Ca}$), are well known in industry; many more of them are the subject of advanced research studies owing to their optical properties, stability and relatively simple preparation. Many SRCs form incommensurately modulated structures, which can only be characterized [1] using the superspace symmetry approach. The example of the $\text{Na}_x\text{Eu}^{3+}_{2/3-x/3}\text{MoO}_4$ ($0 < x < 0.5$) series of SRCs illustrates the potential of this approach for the investigation of crystal structure-property relations. Six new different compositions (with $x = 0.015, 0.134, 0.138, 0.2, 0.236, 0.25$) are characterized by different satellite reflections in their XRD patterns (green marks and colored stars in Figure, centre) described with the unique superspace group, $I2/b(a\beta 0)00$, and similar unit cell parameters, but with different modulation vector \mathbf{q} . Different luminescence intensity induced by the $^5\text{D}_0$ - $^7\text{F}_2$ transitions of Eu^{3+} ions (Figure, right) correlates with different orderings of cations (dark and light blue colors show Eu and Na respectively in Figure, left) defined by the vector \mathbf{q} and occupation modulation function of the cation position, which are specific for each member of the family. Hence, the superspace approach can guide the materials scientist toward the search for an optimum composition and structural ordering to obtain the desired physical properties of SRCs, which vast majority form incommensurately modulated structures.



[1] A. Arakcheeva, G. Chapuis, Acta Cryst. 2008, **B64**, 12-25.

Acknowledgements:

This work has been performed with the support of the Swiss National Science Foundation, (grants No 20-105325/1 and 200021-109470/1) which is gratefully acknowledged.

P18: Understanding the oxygen diffusion process in Ruddlesden-Popper phases at room temperature : the special case of $\text{La}_2\text{CoO}_{4+\delta}$.

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The understanding of chemical reactivity of solids at low temperatures in terms of structural modifications and disorder occurring during the reaction process is still a relatively unknown and poorly understood field. La_2CoO_4 plays - due to the relatively high stability of Co^{3+} - a key role in terms of chemical reactivity as it shows with $\delta = 0.25$ the highest oxygen intercalation rate compared to Cu or Ni with a δ_{max} of 0.07 and 0.18 respectively. For stoichiometric $\text{La}_2\text{CoO}_{4.00}$, the same octahedral LTO (Low Temperature Orthorhombic) tilting arrangement as the one present for the isostructural La_2CuO_4 compound is observed at 293 K (space group *Bmab*), but small quantities of intercalated oxygen are sufficient to induce local lattice distortions as the extra oxygen atoms are located on interstitial sites [2]. Applying electrochemical oxidation we were, however, able to intercalate relatively high extra oxygen contents up to $\delta = 0.25$, which for $\text{La}_2\text{CoO}_{4.19}$ results in a 2D incommensurately modulated structure due to the ordering of the extra oxygen atoms, which at a stoichiometry of $\text{La}_2\text{CoO}_{4.25}$ shows a lock-in transition to a 2D commensurately modulated structure ($4a \times 4a \times c$ unit cell) which is directly related to the ordered distribution of the extra oxygen atoms.

[1] W. Paulus *et al. Solid State Sciences* **4** (2001) 565

[2] R. Le Toquin, W. Paulus³, A. Cousson, G. Dhalenne, A. Revcolevschi,
Physica B **350** (2004) 269

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This work has been performed with the support of CNRS and ESM, Entwicklungsfond Seltene Erden (www.esmfoundation.org).

P19: Proof of liquid layering in nanometre confinement

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Manfred Heuberger³ and J. F. van der Veen^{1,2}

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³ EMPA, 9014 St. Gallen, Switzerland

The lubricating properties of a molecular liquid between two surfaces may change if the surfaces approach each other to within a few molecular diameters¹. The question arises whether the liquid remains 'liquid' in this case². We performed the first synchrotron X-ray reflectivity (XRR)³ study of a liquid under extreme confinement in order to determine the density profile of the liquid's layer structure. We show that squeezing a tetrakis-trimethylsiloxysilane (TTMSS) drop between two mica single crystals causes the liquid's molecules in the film region to order in discrete layers parallel to the surfaces. Electron density profiles determined across gaps of 8.6 and 11.2 nm reveal hydrated mica surfaces which confine 8 respectively 10 equidistant monolayers of TTMSS. The monolayer densities suggest closed-packed ordering, while the measured interlayer distance of 1.0 nm sterically enables sliding of single layers out of the film.

- [1] Persson, B. N. J. & Tosatti, E. Layering Transition In Confined Molecular Thin-Films - Nucleation And Growth. *Physical Review B* **50**, 5590-5599 (1994).
- [2] Jinesh, K. B. & Frenken, J. W. M. Capillary condensation in atomic scale friction: How water acts like a glue. *Physical Review Letters* **96** (2006).
- [3] Als-Nielsen, J. & McMorrow, D. *Elements of Modern X-ray Physics* (John Wiley and Sons, New York, 2001).

Agenda of the SGK/SSCr General Assembly 2009

September 8, 2009, 17¹⁵-18 h

Big Lecture Hall, Department of Chemistry, Chemin du Musée 9
University of Fribourg, 1700 Fribourg



According to our by-laws, Art. 11, we invite all our members for the annual meeting by publishing the meeting agenda 20 days in advance.

Our president, Prof. W. Steurer, is terminating his term after guiding our society for the past three years. According to our by-laws (Art. 13e), the assembly has to elect a new president. Corporate members may delegate their vote to a member of the society. Eligible is every member of the society. We refer to our by laws published on the internet (http://www.sgk-sscr.ch/Statuts_SSCR.html). All present board members declared to candidate for a further term in the board.

- 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
- e) Wahlen: (Art. 13e)
 - e1) Wahl/Bestätigung des Vorstandes 2009-2012
 - e2) Wahl des neuen Präsidenten 2009-2012
- f) Anträge von Mitgliedern

News for and from members

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

Personal members

Jing CHEN, Departement de Chimie, Université de Fribourg
(Ph.D. student)

Francesco GRAMICCIA, Laboratoire de Cristallographie, EPF Lausanne (Ph.D. student)

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

If you wish to apply for a travel grant, please send the above mentioned documents to the president of the SGK/SSCr anytime.

Details for applications are given at:

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

Pending Membership Fees 2009

We would like to thank (most of you) for the prompt payment of the 2009 membership fee.

—However, several of the fees for 2008 and even a few back to 2007 are still missing. The cover letter indicates the **total amount due** (a negative balance means that you paid in advance and no action is needed).

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Please pay the full amount due immediately **by bank transfer** to the UBS account:

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Please avoid cash payments at a post office (PC 80-2-2, UBS Zürich, Account No. 230-C0291110.0) as Postfinance is charging significant handling fees to the society.

Thank you for your cooperation.

Your treasurer,
Michael Hennig

Calls for proposals

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

Facility	Deadline(s)	Link
SLS: Swiss Light Source All except PX lines Protein beam lines (PX)	March 15, Sept. 15 Feb. 15, June 15, Oct. 15	user.web.psi.ch user.web.psi.ch
SINQ: Swiss Spallation Neutron Source All instruments (regular calls)	May 15, Nov. 15	user.web.psi.ch
SμS: Swiss Muon Source All instruments	Dec. 5	user.web.psi.ch
ESRF: European Synchrotron All instruments, long term proposals All instruments, short term proposals	Jan. 15 March 1, Sept. 1	www.esrf.fr www.esrf.fr
SNBL: Swiss Norwegian Beam Line	March 1, Sept. 1	www.esrf.fr/ exp_facilities/BM1A
ILL: Institut Laue Langevin All instruments	Sept. 15, 2009	www.ill.fr
FRM II: Heinz Maier-Leibnitz All instruments	Jan. 29 & Aug. 27, 2010	user.frm2.tum.de

Calendar of forthcoming meetings

(please mail missing information on meetings of interest to Jurg.Schefer@psi.ch)

Call for Abstracts

2009

Aug. 2-Aug. 8	Zuoz CH	8 th PSI Summer School on Condensed Matter Research Functional Materials, http://sls.web.psi.ch	closed
August 14-15	Istanbul Turkey	Symmetry and Crystallography in Turkish Art and Culture, Satellite Conference of the ECM-25 www.lcm3b.uhp-nancy.fr/mathcryst/istanbul2009.htm	closed
August 16-21	Istanbul Turkey	ECM-25: European Crystallographic Meeting http://www.ecm25.org	closed
Aug. 30 - Sept. 12	Zurich CH	The Zurich School of Crystallography: Bring Your Own Crystal, http://www.oci.uzh.ch/diversa/xtal_school/	closed
Sept. 2-4	Innsbruck Austria	Swiss Physical Society, Joint Annual Meeting of ÖPG/SPS/ÖGAA, http://oepg2009.uibk.ac.at/	closed
Sept. 7, 19h	Fribourg, CH	Welcome Dinner of the SGK/SSCr Annual Meeting	page 7
Sept. 8	Fribourg CH	Annual Meeting of the SGK/SSCr University Fribourg, http://www.sgg-sscr.ch/	closed
Sept. 16-19	Aachen Germany	43. Metallurgie-Tagung http://www.dgm.de/dgm/metallographie	closed
Sept. 21-25	Moscow Russia	Clays, Clay Minerals and Layered Materials – 2009 http://www.cmlm2009.ru/	
Oct. 12-13	Villigen CH	JUM@P'09, 1 st PSI User Meeting (SLS,SINQ, SMS) http://user.web.psi.ch/jump09/html/index.shtml	Sept. 15, 2009
Nov. 5-11	Pfanzelt Germany	Zeit- und temperaturaufgelöste Röntgen-Pulver-Diffraktometrie (XI) In-situ Untersuchungen paul-bernd.kempa@ict.fraunhofer.de	

2010

January 20-21	Gif-Sur- Yvette France	5 th SOLEIL Users Meeting http://www.synchrotron-soleil.fr/Soleil/ToutesActualites/Workshops/2010/SUM10	Dec. 7, 2009
March 8-12	Grindelwald CH	ICANS-XIX: The 19 th Meeting of the International Collaboration on Advanced Neutron Sources	Sept. 1, 2009
March 25-26	Grenoble France	HERCULES XX: HERCULES Symposium	
June 3-13	Erice Italy	International School of Crystallography www.ccsem.infn.it	Nov. 30, 2009
June 21 – July 2	Nancy France	Summer Schools on Mathematical Crystallography Nancy, France, 21 June - 2 July 2010 http://www.crystallography.fr/mathcryst/nancy2010.php	to be announced
July 4-9	Sorrento Italy	16 th International Zeolite Conference http://www.iza-online.org/ConfSched.htm	to be announced
Sept. 7-9	Geneva CH	SGK/SSCr Annual Meeting 1 day ,meeting, will be decided later To be approved by the general assembly in Fribourg, 2009	to be announced
Aug. 27-30	Darmstadt Germany	EPDIC-12 http://www.epdic12.org/	to be announced
Aug. 29 – Sept. 3	Darmstadt Germany	ECM-26 http://ecm26.ecanews.org/	to be announced
to be decided	Villigen CH	PSI Powder Diffraction School	to be announced

2011

July 17-21	Prague Czech Rep	5 th European Conference on Neutron Scattering http://www.ecns2011.org	to be announced
Aug. 22-29	Madrid	IUCr-2011, 22 nd General Assembly and Congress of IUCr http://www.iucr.org/iucr/cong/iucr-xxii	to be announced
to be decided	Zurich CH	The Zurich School of Crystallography: Bring Your Own Crystal, http://www.oci.uzh.ch/diversa/xtal_school/	to be announced

2012

Aug/Sept.	Bergen Norway	ECM-27	to be announced
April 29- May 4	Vancouver Canada	ARRS 2012 – Meeting of the American Roentgen Ray Society	to be announced
to be decided	Villigen CH	PSI Powder Diffraction School	to be announced

2013

April 14-19	Moscow Russia	17 th International Zeolithe Coneference	to be announced
to be decided	Washington DC, USA	ARRS 2013 – Meeting of the American Roentgen Ray Society	to be announced
to be decided	Zurich CH	The Zurich School of Crystallography: Bring Your Own Crystal, http://www.oci.uzh.ch/diversa/xtal_school/	to be announced

2014

August	Montreal Canada	IUCr-2011, 23 rd General Assembly and Congress of IUCr http://www.iucr.org/iucr/cong/iucr-xxiii	to be announced
to be decided	Villigen CH	PSI Powder Diffraction School	to be announced

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). For new members, the membership is free until the end of 2007. Please note: SGK/SSCr members can also apply to be a member of the subsection crystal growth (no additional charge) or for individual membership of the European Crystallographic Association, ECA (additional charge: 10 Euro).

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

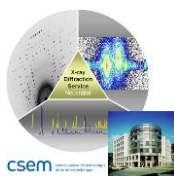
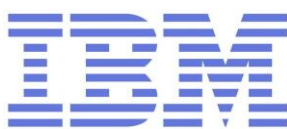
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Interest			
Membership subsection crystal growth	Yes ()	No ()	
Birth date	Day:	Month:	Year:
Language(s)			
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Highest degree received			
from university			
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