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Swiss Society for Crystallography

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The President's Page

Dear member of the Swiss Society for crystallography,

Here we are! In few weeks, the 30th European Crystallographic Meeting will take place in Basel. This project started in 2011, when we proposed Basel in a bid for the ECM29. The meeting was eventually assigned to Rovinji in Croatia, but one year later, we finally succeeded and we obtained the organization of ECM30.

In the past four years, a committee led by Katharina Fromm has intensively worked for organizing this meeting and we will see soon the outcome of this hectic activity.
It is certainly a great honor for our small community to be in charge of such an important event and to host so many scientists (more than 850, as of statistics on July 8th), who will certainly animate the meeting. At the same time, this event represents a unique opportunity to illustrate the enormous research activity in Crystallography, which is ongoing in Switzerland, as well as the laboratories and the large-scale facilities. For this reason, we decided to dedicate a large section of this newsletter to introducing all the crystallographic research groups currently active in Switzerland. In the following pages, you will see a brief description of the main ongoing research projects, the active group members and the most important publications. The newsletter will circulate also during the meeting and therefore all participants will have the occasion to learn more about the research carried out by their Swiss colleagues.

Before or after the main meeting, some satellite meetings will take place, including the traditional powder diffraction school organized at the PSI. The role of our members is also very important in the organization of all these satellites and I thank all those who contributed.

I wish also to remind you that on Wednesday August 31, within ECM30, we will have the annual assembly of the society. You will find in this newsletter more details about the agenda and the schedule. We hope you will be able to attend and discuss about the future initiative of our society and elect some new board members, replacing Katharina From, Jürg Schefer and Petr Leiman, who will leave the board. I warmly thank them for their activity in the past few years, in particular for the organization of ECM30 and the celebrations for the international year of crystallography in 2014.

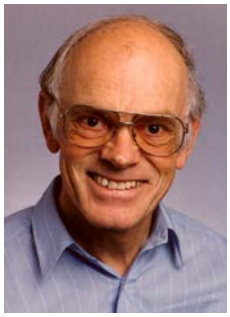
I hope to meet you in Basel and I wish you a very interesting and attractive meeting

Piero Macchi
(President of the SGK-SSCr)

Crystallography in Switzerland

The crystallographic community in Switzerland is a very active one. There is a large number of research groups and companies, either actively working in crystallography or are applying crystallographic methods to a large extent for their work*. The spectrum of the crystallographic topics is indeed amazing, too. For example, we have groups and companies working on routine single crystal structure analysis, powder diffraction, diffuse scattering, charge density determination, twinning, diffraction at non-ambient conditions (high-pressure, low temperature), modulated structures, protein crystallography, diffraction experiments with synchrotron radiation and neutrons, small-angle scattering and crystal growth, just to mention a few. In the following, we present an article on the history of crystallography (Hans Grimmer) and a survey on groups and companies in Switzerland, which have strong relations to crystallography.

History of Crystallography in Switzerland



Hans Grimmer, Paul Scherrer Institute. Reprinted (with updates) by courtesy of the communications of the Swiss Physical Society.

Introduction

Crystallography evolved from the study of the form of mineral crystals and of the anisotropy of their physical properties. After the discovery of X-ray diffraction by Laue (1912), the focus of crystallography shifted to structure analysis; chemists became the main users of crystallographic methods. Crystallographic institutes at universities were established first in Zürich, 1949 in Bern, in the 1970s in Geneva, Lausanne, Neuchâtel and Basel. In the beginning, the main focus in Switzerland was on methods and general principles. Due to the increasing demand of chemistry and biology institutes and the materials sciences, the focus shifted to the determination of ever more complicated structures, to disorder in crystals and to their dynamic properties. Crystallography laboratories were established also in institutes of chemistry and structural biology. The structure analysis of biological macromolecules and their application in drug design, although very successful and of great economic importance, will be mentioned only shortly in this article.

In addition to X-rays, neutrons became in the 1960s important probes to investigate crystals. Synchrotrons became a much more versatile and brilliant source of X-rays than X-ray tubes, especially when synchrotrons dedicated to the production of X-rays were built in the 1980s. Such sources are out of reach of university institutes, they were made available at Paul Scherrer Institute (PSI) in Switzerland and at national and international centres abroad. With the availability of the sources also the development of the corresponding beam-lines and of new applications gradually shifted from the universities to neutron and synchrotron radiation centres. As a consequence, full professors of crystallography who retired after 2000 were either not replaced or replaced at a lower level. On the other hand, joint appointments at PSI and Swiss universities, in particular ETH and EPFL have become common.

*If your research group is not listed here, please contact Michael Wörle woerle@inorg.chem.ethz.ch and your group page will be published in the next newsletter."

Crystallography overlaps with many sciences: mineralogy, solid state physics and chemistry, molecular biology, pharmacy and materials science. Crystallography is increasingly perceived as providing indispensable tools rather than as a science of its own at the crossroads of these disciplines [1].

The beginnings

Crystallography developed from mineralogy in the 17th century, when regularities in the forms of crystals and anisotropies of their physical properties were discovered. The term "Crystallographia" was actually introduced 290 years ago by the Swiss physician and scientist M. A. Kappeler [2]. In the 19th century the mathematical classification of 3-fold periodic structures was developed with the derivation of the 7 crystal systems, the 14 lattice types, the 32 crystal classes and the 230 types of space groups [3].

In 1855, the Polytechnic Institute (called ETH since 1911) was established in Zürich. Systematic crystallographic research started in Switzerland with Gustav Adolf Kenngott, who was Professor of Mineralogy at ETH from 1856 and at the University of Zürich (UZH) from 1857 until his retirement in 1893. The main activities of his successor Ulrich Grubenmann (1893-1920) were in petrography, where he made use of polarisation microscopy and chemical analytic methods. He was succeeded by Paul Niggli (1920-1953). All three were strong personalities and served the ETH as rectors, Niggli became rector also of UZH [4].

When Max von Laue was "Privatdozent" in Munich under Arnold Sommerfeld, he had in the beginning of 1912 the idea that X-rays might show interference effects with crystals. Paul Knipping and Walter Friedrich performed the experiments, showing interference spots compatible with the cubic symmetry of ZnS crystals. Laue's explanation of these spots proved the wave properties of X-rays and, simultaneously, the space group symmetry of crystals, i.e. that crystals are 3-fold periodic. Laue was not interested in determining the structure of crystals. This endeavour was started in England in 1913 by William Henry Bragg and his son William Laurence Bragg. Laue received the Nobel Prize for physics in 1914, the Braggs in 1915. British crystallographers remained the leaders in structure determination until the 1960s.

The cross-fertilization between crystallography and neighbouring disciplines is shown by the fact that Peter Debye became 1911 Professor of Theoretical Physics at UZH, succeeded by Max von Laue in October 1912.

In 1915 Debye developed in Göttingen together with his PhD-student Paul Scherrer a method to determine the distances between neighbouring lattice planes from the diffraction of X-rays by crystal powders, known as Debye-Scherrer method. In 1920, the ETH appointed Debye and Scherrer as professors of physics and the above-mentioned Paul Niggli as Professor of mineralogy and petrography [4].

The "Zürich school of crystallography" [3]

Niggli made important contributions to mineralogy and petrography, but his main interest was in showing how symmetry considerations can be used to determine the space group and the structure of crystals. In particular, his book "Geometrische Kristallographie des Diskontinuums", published in 1919, became the precursor of the volume "Space-group symmetry" of today's "International Tables for Crystallography" and already contained the concepts and tables that are most important for structure determination. Niggli collaborated with mathematicians as Georg Polya at ETH and Heinrich Heesch at UZH. Using symmetry and modern mathematical methods for the solution of general problems in crystallography is a distinctive feature of the research by Niggli and many of his successful students, often referred to as the "Zürich school of crystallography" [3].

In 1932 Conrad Burri was appointed professor for special mineralogy and petrography, whereas Niggli continued lecturing on crystal structure, crystal physics and crystal chemistry. These courses, named 'general mineralogy', were compulsory for chemists during their first three semesters [4].
In collaboration with the Swiss Federal Laboratories for Materials Science and Technology (EMPA), X-ray equipment was installed. Since 1930 this equipment was run by Ernst Brandenberger, who later became professor of materials science and testing, as well as a director of EMPA [4].
After the sudden death of Niggli at age 64, Fritz Laves, who had finished his thesis under Niggli, succeeded him from 1954 to 1976. He is best known for his work on the crystal structure of metals and alloys, where he was mainly interested in general structural principles from a crystal-chemical point of view, e.g. the 'Laves phases', intermetallic phases with composition AB2 [5].
The "Institute for Crystallography and Petrography" was strengthened by the appointment of two associate professors at UZH and ETH, Alfred Niggli (a pupil of Paul Niggli) in 1960 for crystal structure research and Walter Max Meier in 1966 for crystallography and mineral synthesis. Niggli, best known for his work in mathematical crystallography, was full professor from 1966 to his death in 1985. Meier was full professor 1973-1992; financially supported by Mobil Oil, he and his group determined the structure of many zeolites by powder diffraction.
The chemical institutes created their own chemical crystallography group, led with great success by Jack Dunitz from 1957 to 1990. Bernd Schweizer continued the activities until his retirement in 2013.

Bern
Zürich remained the unique center of crystallography until 1949, when Werner Nowacki [6], who had earned his doctorate under Paul Niggli with work on homogeneous space partitions into domains of influence, became professor in Bern. He founded the Section of Crystallography and Structural Studies. Feeling that the interests of crystallographers were not adequately represented by the "Swiss Society of Mineralogy and Petrology", he initiated the "Swiss Society for Crystallography" in 1968 and became its first president [7].
Nevertheless, Nowacki was very productive also in mineralogy by investigating the sulfosalt minerals found in the Lengenbach deposit in the valley of Binn. In order to determine the chemical composition of these often very small crystals he founded the Laboratory of Electron Microprobe Analysis in 1964.
When Hans-Beat Bürgi succeeded Nowacki in 1979, the Laboratory of Chemical and Mineralogical Crystallography was established. Bürgi's main interests are in static and dynamic structural chemistry, whereas research in mineralogical crystallography was continued by Thomas Armbruster and research in mathematical crystallography by Peter Engel. When Bürgi retired in 2007 (and became permanent academic guest at the organic chemistry institute of UZH) the Laboratory was split into the Laboratory for Mineralogical Crystallography led by Armbruster and the Laboratory for Chemical Crystallography led by Piero Macchi.

Crystallography in the French speaking part of Switzerland
Hans Schmid joined the Battelle Geneva Research Center in 1957, where he worked on the synthesis and potential applications of ferroelectrics, ferromagnetics and ferroelastics for display and data storage. In 1964 he synthesized a variety of boracites, in which he discovered for the first time, in collaboration with Edgar Ascher, the simultaneous occurrence and mutual coupling of ferroelectricity, ferromagnetism and

ferroelasticity in the same phase [8]. From 1977 to 1996 Schmid was Professor of Applied Chemistry at the University of Geneva.
In Geneva, a chair of crystallography was created in 1970, headed by Erwin Parthé until his retirement in 1993 [9]. His main interests were alloys and intermetallics. He developed a standard presentation of inorganic crystal-structure data, which helps to recognize similar structures. The results were published in a four volume series "TYPIX Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types". Klaus Yvon held a second chair 1982-2009. His main interests were new compounds for energy storage (metal hydrides) and energy conversion (superconductors, ferromagnets). At present, Radovan Cerný is in charge of teaching crystallography and Céline Besnard runs a service of structure determination.
Dieter Schwarzenbach taught crystallography at the University of Lausanne first as lecturer, then 1973-2001 as professor. He is an expert for the determination of electron densities in crystals. Gervais Chapuis joined him in 1975 and was full professor 1991-2009. He investigated incommensurate structures by diffraction and molecular dynamics. They initiated and led a project for the construction of a beam line at the European Synchrotron Radiation Facility (ESRF) in Grenoble. This effort resulted in the Swiss-Norwegian Beam Lines (SNBL), which started operation in 1995. In 2003 the Institute of Crystallography was transferred from the university to EPFL. Two former members of the institute, Phil Pattison and Kurt Schenk, are now attached to the X-ray diffraction service of the EPFL Institute of Chemical Sciences and Engineering (ISIC).
Helen Stoeckli-Evans taught chemical crystallography at the University of Neuchâtel 1972-2009, moving up from lecturer to professor. From 1997 to 2006 she was responsible for the small molecule crystallography service BENEFRI of the universities of Berne, Neuchâtel and Fribourg. The service was reorganized in 2006 and is now run jointly by the Institute of Microtechnology of the University of Neuchâtel and the Swiss Center for Electronics and Microtechnology (CSEM) under the responsibility of Antonia Neels (until 2014) and Olha Sereda (since), both former collaborators of Stoeckli.
At the University in Fribourg, the group of Katharina Fromm grows crystals and determines their structure for its research in the coordination chemistry of nano- and biomaterials.

Basel
Two years after the foundation of the "Biozentrum" of the University of Basel, Johan N. Jansonius started in 1973 as research group leader in the Department of Structure Biology. Prof. Jansonius retired in 1998. In 1997, Tilman Schirmer was promoted to Associate Professor in the above-mentioned department.
The Laboratory for Chemical Crystallography of the University of Basel started in 1980, led by Margareta Zehnder (Neuburger-Zehnder). It is now run by her husband Markus Neuburger, mainly as a service laboratory for structure determination.

Of course, important bio-crystallographic research was done in the pharmaceutical industry, e.g. by Markus Grütter, (a PhD student of Jansonius) at Ciba-Geigy (later Novartis) before he moved to UZH, or by Fritz Winkler at Hoffmann-LaRoche before he moved to ETH.

Newer developments in the Zürich area
When Walter Steurer was appointed Professor at UZH and ETH in 1993 after the retirement of Walter Max Meier, the institute was reorganized as "Laboratory of Crystallography"; it is now attached to the ETH department of materials. Steurer's main

research fields are quasicrystals, their structure analysis and description and the interpretation of both Bragg and diffuse scattering. Research on zeolites and powder diffraction continues with Lynne McCusker and Christian Bärlocher. After the retirement of Walter Steurer in 2016, the facilities were transformed into a crystallography platform headed by Thomas Weber.
With the appointment in 2010 of Nicola Spaldin as Professor of Materials Theory and in 2011 of Manfred Fiebig as Professor of Multifunctional Ferroic Materials, the department of materials has considerably strengthened its competence in developing new multifunctional materials.
Structure determination is done also in other departments of ETH. Michael Wörle is responsible for X-ray analysis in the Laboratory of Inorganic Chemistry led by Reinhard Nesper (retired in 2014). After the retirement of Bernd Schweizer (2013) the X-ray facilities of the Laboratories of Inorganic and Organic Chemistry were merged into the departmental technology platform Small Molecule Crystallography Center (SMoCC) headed by Michael Wörle.
Timothy Richmond is 1987-2014 full professor for the Crystallography of Biological Macromolecules, Nenad Ban since 2007 for Molecular Structural Biology. Fritz Winkler (1999-2009) and Gebhart Schertler since 2010 professors for Structural Biology headed simultaneously the Biology Department at Paul Scherrer Institute (PSI).
The leading position in crystallography-related research of ETH in the German speaking area [10] is due to all these contributions.
Also the activities at UZH deserve mentioning: Coming from Novartis, Markus Grütter was 1997-2013 full professor for macromolecular structural biology. Anthony Linden manages the X-ray crystallographic facility at the organic chemistry institute and organizes the biannual “Zurich school of crystallography” together with Hans-Beat Bürgi.
In the laboratory of Alex Müller at the IBM Research Center in Rüschlikon, Georg Bednorz synthesized in 1974 perovskites (SrTiO3) for his diploma work. He obtained his doctorate at ETH under the supervision of Heini Gränicher and Alex Müller. Back at IBM, he and Müller synthesized oxides that they considered to be candidates for superconductivity. In 1986 they found in La1.85Ba0.15CuO4 a superconducting transition temperature Tc = 35 K, higher than the highest known Tc in metals. For this discovery, they received the Nobel Prize for physics in 1987 [11].
Anke Weidenkaff was head of the Laboratory for Solid State Chemistry and Catalysis at EMPA Dübendorf and was teaching at the University of Bern, until she became professor at the University of Stuttgart in 2013. In 2014 the new Center for X-ray Analytics at EMPA was formed, headed by Antonia Neels. Alex Dommann, who applied X-ray diffraction to the characterization of coatings for industrial applications first at "Neutechnikum Buchs" and then at CSEM in Neuchâtel is now at EMPA St. Gallen.

The neutron sources at PSI [12]
Walter Hälg, since 1955 at ETH and full professor 1960-1984 started neutron scattering at the nuclear reactors SAPHIR and DIORIT of the Swiss Federal Institute for Reactor Research (EIR) in Würenlingen. The first instrument was a two-axis neutron diffractometer, used for single crystal studies of magnetic phase diagrams in external magnetic fields up to 6 Tesla. Albert Furrer was 1984-2004 head of the Laboratory for Neutron Scattering (LNS). In his period, EIR and the Swiss Institute for Nuclear Research (SIN) merged in 1988 to the Paul Scherrer Institute (PSI), and the Swiss Spallation Neutron Source SINQ was built and started operation in 1996. Successors of Furrer were Joël Mesot 2004-2008, who is now director of PSI and Professor at ETH and EPFL, Andrey Zheludev 2009-2010, now at ETH, and Christian

Rüegg since 2011. Crystallographic research at LNS is done mainly in the diffraction group. Using the strong features of neutrons, Peter Fischer, group head until 2002, made important contributions to hydrogen storage in metals, the structure of high temperature superconductors and to magnetism. At present, the diffraction group at LNS runs a single crystal neutron diffractometer and two powder diffractometers, one using thermal and the other cold neutrons. These instruments allow experiments in a wide range of conditions: temperatures between 50 mK and 1400 K, pressures up to 100 kbar for powders (2 GPa for single crystals) and magnetic fields up to 6 T for powders (15 T for single crystals). Dynamic properties of crystals are investigated in the spectroscopy group. This group operates five spectrometers. Some of its research topics are high temperature superconductors, critical phenomena in ferroelectrics, magnetism and colossal magnetoresistance.
Since 28 years, Switzerland is a member state of the Institut Laue-Langevin (ILL) in Grenoble; it also participates in the European Spallation Source (ESS) under construction in Lund, Sweden.

The synchrotron radiation source SLS at PSI
Switzerland is a member state also of the European Synchrotron Radiation Facility (ESRF) in Grenoble, which started operation in 1994, and is engaged, in particular, in running the Swiss-Norwegian Beamlines (SNBL), as mentioned above.
In order to satisfy the increasing demand of synchrotron light, the Swiss Light Source (SLS) was constructed at PSI. Research at the SLS started in 2001 under J. Friso van der Veen, who was succeeded by Gabriel Aeppli in 2014. Van der Veen also was Professor of Experimental Physics at ETH 2000-2014, and Aeppli is Physics Professor at ETH and EPFL. The SLS provides photon beams of high brightness for research in materials science, biology and chemistry. At present, 16 beamlines are in operational mode, using synchrotron radiation at wavelengths ranging from the VUV to the hard X-ray regime.
Four laboratories operate these beamlines, provide user support and do research of their own: "Macromolecules and Bioimaging" runs among others 3 beamlines dedicated to macromolecular crystallography, "Femtochemistry" runs among others the PHOENIX beamline for X-ray microspectroscopic measurements (µ-XAS and µ-XRF), "Micro- and Nanotechnology" runs the X-ray Interference Lithography beamline. The various groups of "Condensed Matter and Materials Science", headed by Frithjof Nolting, operate 9 beamlines. At the MS beamline powder and surface diffraction techniques are used for research in condensed matter and materials science; at the two soft X-ray beamlines SIS and ADRESS the spectroscopy techniques ARPES and RIXS are used to investigate novel materials like high-temperature superconductors and low-dimensional magnets; the soft X-ray beamline SIM serves to study electronic and magnetic properties of thin films, multilayers, and bulk systems of metals and oxides; ultra-fast phenomena in solids are studied at beamline FEMTO using 100 fs X-ray pulses for diffraction or spectroscopy. Even shorter pulses will be available at the X-ray free-electron laser (SwissFEL) under construction at PSI.

The Swiss Society for Crystallography [7]
As mentioned above, the Swiss Society for Crystallography (SSCr) was founded in 1968 with Nowacki as its first president. The society included from its beginning members interested in crystal growth, which formed a section with activities of their own. Already in 1969, the SSCr was admitted as a member society of the 'Schweizerische Naturforschende Gesellschaft', the predecessor of the 'Swiss Academy of Sciences' (SAS). The SSCr is a member society of the International Union of Crystallography (IUCr) and of the European Crystallographic Association (ECA).

With financial support of the SAS, the SSCr produced a copiously illustrated brochure describing fascinating aspects of pure and applied crystallographic research in Switzerland. The German version 'Kristallographie in der Schweiz' appeared in 1999, the French version 'Cristallographie en Suisse' in 2001 [13].
In addition to many national meetings, the SSCr has organized several European meetings: A highlight for the society and its section was the organization of the 3rd European Crystallographic Meeting (ECM-3), immediately followed by the 1st European Conference on Crystal Growth, which both took place in Zürich in 1976. In 2006 the European Powder Diffraction Conference (EPDIC-10) was organized in Geneva and in 2016 ECM-30 will take place in Basel.
Table 1 shows the main officers of the SSCr. Until 2009 the chairman of the section for crystal growth acted as vicepresident of the society, until 1993 the secretary acted also as treasurer.
A majority of the SSCr officers were employed by a university, but also the Basel pharmaceutical industry is well represented with two presidents and with the treasurers from 1993 to 2010. The president Ascher worked at Battelle, the vicepresident Scheel was 1968-1982 at IBM Rüschlikon, 1989-2001 at EPFL, since 2001 self-employed. The growing importance of the neutron and synchrotron sources for crystallography is reflected by the fact that two of the SSCr presidents, the secretaries 2002-2015 and the editors of the 'SGK/SSCr Newsletter' 1998-2015, all work at PSI.
Table 1:

Period	President	Vicepresident	Secretary	Treasurer
1969-1972	W. Nowacki (Uni Bern)	E. Kaldis	P. Engel	P. Engel
1972-1975	E. Ascher (Battelle, Geneva)	E. Kaldis	P. Engel	P. Engel
1975-1978	A. Niggli (Uni / ETH Zürich)	H. J. Scheel	P. Engel	P. Engel
1978-1981	E. Parthé (Uni Geneva)	H. Arend	W. Petter	W. Petter
1981-1984	H.P. Weber (Sandoz, Basel)	H. Schmid	W. Petter	W. Petter
1984·1987	D. Schwarzenbach (Uni Lausanne)	S. Veprek	H. Flack	H. Flack
1987-1990	J. Daly (Hoffmann-LaRoche, Basel)	S. Veprek / E. Kaldis	H. Flack	H. Flack
1990•1993	M. Dobler (ETH Zürich)	E. Kaldis / J. Bilgram	H. Stoeckli-Evans	H. Stoeckli-Evans
1993-1996	H. Stoeckli-Evans (Uni Neuchâtel)	J. Bilgram	G. Chapuis	F. Winkler
1996-1999	G. Chapuis (Uni Lausanne)	J. Bilgram	V. Gramlich	F. Winkler
1999-2002	H. Grimmer (PSI, Villigen)	H.J. ScheeI	V. Gramlich / R. Cerny	J. Priestle
2002-2005	R. Cerny (Uni Geneva)	H.J. Scheel	H. Grimmer	J. Priestle / M. Hennig
2005-2009	W. Steurer (Uni/ ETH Zürich)	H.J. Scheel / K. Fromm	J. Schefer	M. Hennig
2009-2012	K. Fromm (Uni Fribourg)	M. Schiltz / J. Schefer	J. Schefer	M. Hennig / P. Macchi
2012-2015	J. Schefer (PSI, Villigen)	P. Macchi	D. Sheptyakov	P. Macchi
2015-	P. Macchi (Uni Bern)	A. Neels	M. Wörle	A. Neels

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Survey of the research groups/companies active in crystallography

The new campus in Sion where Energypolis is located

EPFL Valais Wallis
Rue de l'Industrie 17
Case Postale 440
1951 Sion
Switzerland
Website:
http://isic.epfl.ch/valais

LFIM
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XRD Platform
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Email: pascal.schouwink@epfl.ch

The research project "Energypolis", a joint venture between federal, cantonal and private institutions that has its home in the newly established EPFL satellite campus in Sion, was recently launched under the leadership of the Institute of Chemical Sciences and Engineering, ISIC, of EPFL in Lausanne. The numerous activities of Energypolis all have energy-related materials science as a common topic, in particular the storage and conversion of energy. The diversity of materials investigated gives rise to stimulating scientific problems calling for a range of crystallographic methods spanning from surface studies on thin-films via single crystal investigations to bulk *in-situ* and *in-operando* powder diffraction. Next to making frequent use of Swiss installations at the Paul Scherrer Institute and the Swiss-Norwegian Beamlines of ESRF (Grenoble), Energypolis is home to a young X-ray diffraction lab offering a number of *in-house* possibilities to its research teams as well as to external users. This lab serves as a flexible platform to users and to instrument development.

While 7 of the 9 research units hosted by Energypolis employ diffraction as part of their work, in particular the groups of Wendy Queen and Kyriakos Stylianou focus on crystallography to investigate novel nanoporous metal-organic frame-works (MOFs). These materials, construc-ted by metal-ions or metal-ion clusters that are interlinked by organic ligands, offer unprecedented internal surface areas allowing the adsorption of a wide range of guest species. The molecular nature of the organic ligands within the hybrid organic/inorganic newcomers, induces structural versatility, allows the introduction of multifunctional properties, and permits a modular approach to their design. Prof. Queen leads the Laboratory of Functional Inorganic Materials (LFIM) in Sion, The LFIM utilizes *in-situ* diffraction techniques to gain molecular level insight into what structural

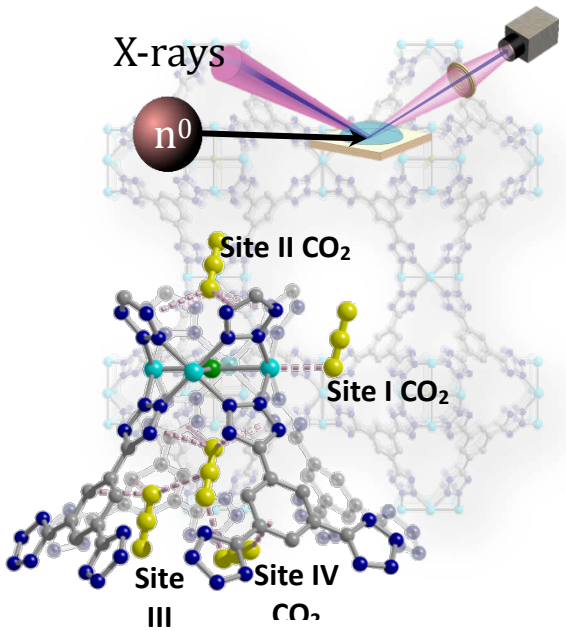

Figure 1: Ball and stick model revealing 4 CO_2 adsorption sites (yellow spheres) in a sodalite based MOF known as Cu-BTT as determined by neutron powder diffraction.

features give rise to enhanced or diminished properties, knowledge that is necessary to design new or chemically tune existing frameworks for specified functions. Diffraction is the most direct way to probe location and orientation of surface bound guest species, the relative difference in binding energy between neighbouring adsorption sites (Fig. 1), the structural response of materials under application relevant environments, and the existence of small-molecule activation. The initial focus of the LFIM is on assessing several aspects of these nanoporous materials including small molecule adsorption/separa-tion and their conversion into value-added chemicals and fuels. The ultimate goal is to contribute knowledge towards solving globally important problems related to the reduction of CO_2 emissions.

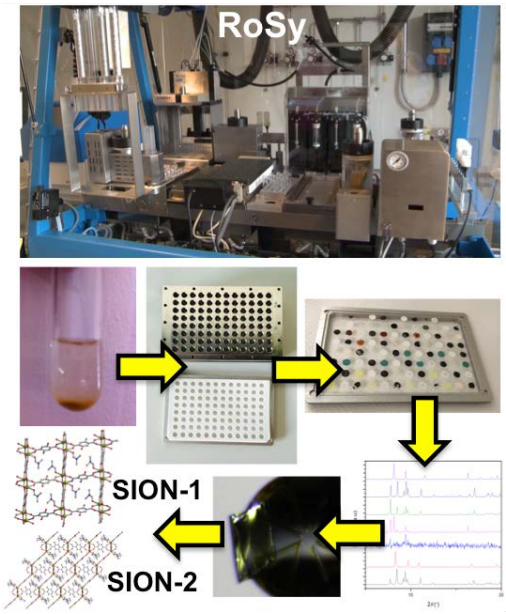

Figure 2: RoSy can be utilised to accelerate the discovery and characterisation of novel MOFs such as the SION-1 and SION-2.

To speed up the time-consuming and costly search for novel MOFs the Laboratory for Molecular Simulations (LSMO), directed by Prof. Berend Smit, initiates discovery at the computational level, where modelling gas adsorption requires a fraction of the cost when comparing with experimental isotherm measurements. Dr. Kyriakos Stylianou leads the synthetic activity within LSMO, aiming to accelerate the growth of large phase pure porous MOF materials using the robotic synthesizer (RoSy) available at EPFL Valais Wallis. The high-throughput automated microwave heating methodology used by RoSy (Fig. 2) is capable of improving synthesis times by a factor of 1000 compared to traditional synthesis pathways. This will enable the acceleration of MOFs discovery as a large number of reactions can be prepared in one batch by screening a wide variety of parameters; metal source, solvent mixtures, concentrations, pH of the reaction, heating time and temperature, and many more. Coupled with the rapid computational methods, high performing targets can be obtained through the use of cheap and abundant metal centres such as Mg(II), Al(III), Fe(III), Mn(II), Cu(II), Ti(IV), Zr(IV) and commercially available or easily prepared organic ligands. Dr. Stylianou's group uses single crystal diffraction to elucidate the structure of MOFs, after having optimized the synthesis conditions of the 100s of polycrystalline materials produced by RoSy, which are initially characterized by powder diffraction.

One of the diffraction lab's instruments will be largely dedicated to an optimized high-throughput setup that, assisted by a double-laser alignment system, allows fast screening of MOF powder samples but also the metal oxide photocatalysts, perovskite thin films, and 2-D porous membranes being investigated by Prof. Raffaela Buonsanti, Prof. Mohammad Khaja Nazeeruddin, and Prof. Kumar Varoon Agrawal, respectively.

Figure 1: Tilman, Dubravka, Andreas and Clemens cover single crystal and powder diffraction, and imaging techniques.

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DECTRIS Ltd is the technology leader in Hybrid Photon Counting X-ray detectors. It has its roots at Paul-Scherrer Institute, where PILATUS and MYTHEN were designed to open up new perspectives in protein crystallography and powder diffraction. Over the last decade, DECTRIS kept on "*detecting the future*" through strong collaborations with the scientific community, and today PILATUS, MYTHEN and EIGER dominate not only the synchrotron source, but also laboratory and industry diffractometer markets. The broad network of users and the variety of techniques, requirements and challenges kept DECTRIS' application scientists and support team at the cutting-edge of instrument development as well as the latest applications. On the frontier of protein crystallography stands Andreas Förster. Fascinated by the high-speed EIGER detectors, he is committed to advance structure determination methods and enable high data-rate protein crystallography. Tilman Donath, the imaging expert, gained his knowledge at several universities and synchrotron sources, and is now exploiting advances of the PILATUS3 X CdTe detectors for scientific and industrial applications. Dubravka Šišak Jung, the powder diffractionist with a background in pharma industry, combines her zeal for structure determination with the MYTHEN2 detectors, and takes further steps towards stress, texture and high-energy applications. While the support team keeps the things running smoothly, the driving force of the whole group, Clemens Schulze-Briese, crystallographer and beamline scientist, explores far horizons and patiently tunes new developments with future needs. In the autumn of 2016, X-DECTRIS year, this team of X-men joins forces and celebrates the company's 10th anniversary by opening up an application lab. Drop by for a chat at ECM-30 and check out what we're up to!

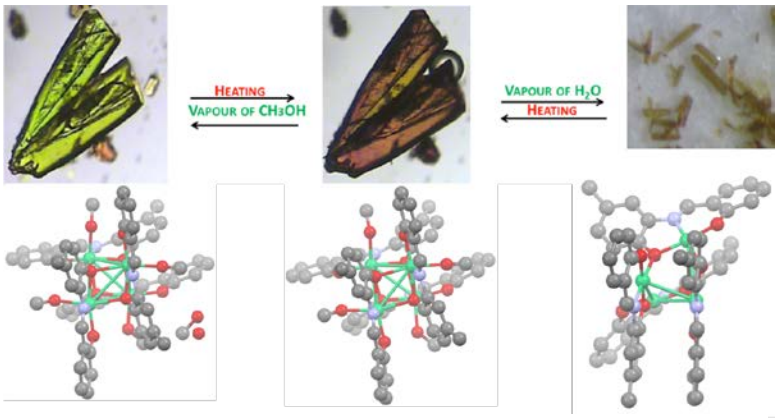

Figure 2: Robust Ni_4L_4 core of tetranuclear Ni(II) complexes allows for an exchange of coordinated and lattice solvent in the crystal, giving rise to similar structures with different magnetic properties [2].

Recent publications and highlights:
[1] Förster, A. *et al.*, https://www.dectris.com/white-papers.html
[2] Cindrić, M. *et al. J. New Chem*. (2016) Advance paper

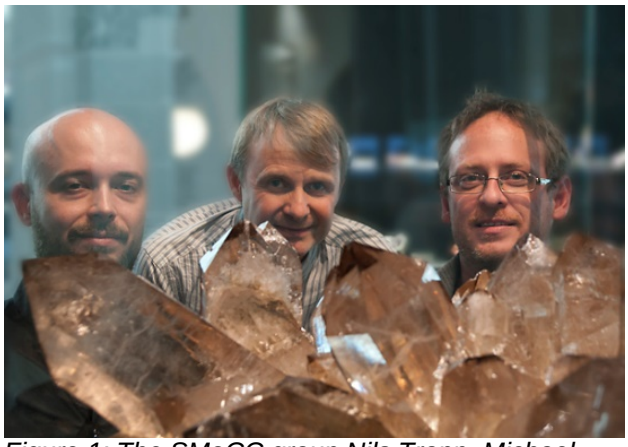

Figure 1: The SMoCC group Nils Trapp, Michael Wörle and Michael Solar (f.l.t.r)

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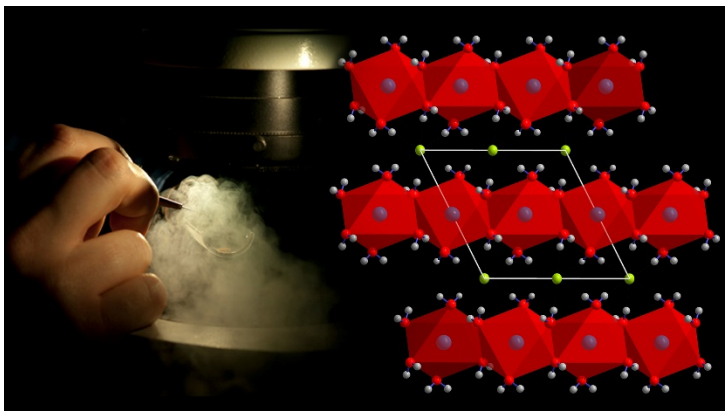
The Small Molecule Crystallography Center (SMoCC) is a technology platform of the Department for Chemistry and Applied Biosciences at the ETH Zurich. We support research activities by providing facilities for various characterizations by X-ray diffraction techniques. A large fraction of our work comprises high throughput routine single crystal structure analysis. Moreover, in order to ensure maximum flexibility and to be able to solve challenging crystallographic problems, we grant direct access to the instruments for interested (PhD) students and postdocs after adequate training. Support on crystallization techniques and problematic structures beyond simple routine structure analyses (charge density determinations, disorder and diffuse scattering, twin formation, incommensurate and modulated structures, phase transitions and *in situ* crystallizations) is given too. We develop devices for crystallization and sample handling at non-ambient conditions (low temperature, inert conditions). Our platform also hosts powder diffraction instruments and we perform routine phase identification (fingerprinting), as well as quantitative phase analysis and structure analysis on the basis of powder diffraction data (Rietveld refinements). As the National Affiliate Center of the Cambridge Crystallographic Data Centre the SMoCC hosts and distributes the Cambridge Structure Database (CSD) to all academic institutions in Switzerland and also provides acces to the Inorganic Crystal Structure Data Base (ICSD).



***F**igure 2: Mounting of an air/temperature sensitive crystal of a transition metal halogenide hydrate using a cold nitrogen gas stream and it's crystal structure.*

Recent publications and highlights:

[1] F. Diederich, N. Trapp, M. Wörle, T. Weber, Israel Journal of Chemistry 56 (2016), *in print*.
[2] M. Yarema, M. Wörle, M.D. Rossell, R. Erni, R. Caputo, L. Protesescu, K.V. Kravchyk, D.N. Dirin, K. Lienau, F. von Rohr, A. Schilling, M. Nachtegaal, M.V. Kovalenko, Journal of the American Chemical Society 136 (2014) 12422-12430.

Members of LPMC-EPFL at the MaNEP Swiss Workshop on Quantum Materials and Electronic Devices (SWM 2016), Les Diablerets.

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The activity of the Laboratory of Physics of Complex Matter (LPMC) covers a broad range of topics. Whether it concerns superconductivity, the movement of dislocations or living cells, the common denominator is complexity and materials' discovery. The laboratory provides a single crystal growth facility with nanosize to macroscopic samples, synthesizing more than 100 different compounds. Our material science centred research is complemented by the strong crystallography activities of Dr. Alla Arakcheeva and Dr. Bálint Náfrádi using X-ray and neutron diffraction techniques.

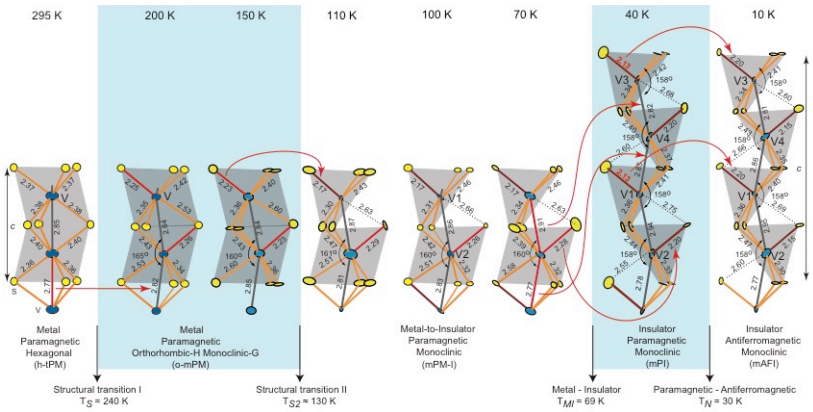

Fig. 1: Temperature dependent phase transformations in $BaVS_3$. Structural parameters relaxing at each phase transformation are indicated by red arrows. Specific V-S contacts are indicated: Typical (orange color) and polarized (brown color and dashed lines) V-S contacts are indicated. VS_6 octahedra and VS_5 pyramids are shown in gray. Atoms are shown using ellipsoids of 50% probability atomic displacements.

Dr. Arakcheeva obtained a PhD in Chemistry, DSc. in Physics, and is an expert in classical and aperiodic crystallography using X-ray diffraction with more than 35 years of experience in applications concerning crystallographic methods applied to the fields of physics, chemistry, electrochemistry, metallurgy, mineralogy and materials science.

Currently, Dr. Arakcheeva focuses on the study of correlated 5d-electron transition metal oxides [1]. The structural study of the superconducting $SmFeAsOH_x$ allowed us to localize H atoms [2]. For the organic-inorganic hybrid perovskite $CH_3NH_3PbI_3$ precise structural consequences of water absorption was investigated [3]. The structural aspect of 1D $BaVS_3$ correlated electronic series and the metal-insulator phase transitions was also investigated [4] (Fig. 1). Dr. Arakcheeva also heads the research services of Phase Solutions.

Bálint Náfrádi obtained a PhD in Physics from EPFL. He uses polarized neutron diffraction techniques to precisely determine magnetic structures with special emphasis on fine structural distortions and domain structures. Recently, he showed that minute lattice distortion in the rage of 10^{-6} rlu are responsible for magnetoresisitve anisotropy and domain formation in a high-T_C parent compound $YBa_2Cu_3O_6$ [5]. In Co-based multiferroic melilites the precise refinement of both magnetic and nuclear structures set the basis for a theoretical model describing the multiferroic coupling mechanism [6-9].

Recent publications and highlights:

[1] L. Yang, A. Pisoni, A. Magrez, S. Katrych, A. Arakcheeva, B. D. Piazza, K. Prsă, J. Jacímovic, A. Akrap, J. Teyssier, L. Forró, H. M. Rønnow. Crystal Structure, Transport, and Magnetic Properties of an Ir^{6+} Compound $Ba_8Al_2IrO_{14}$. Inorg. Chem. (2015) 54, 4371−4376.

[2] A. Pisoni, S. Katrych, A. Arakcheeva, T. Verebélyi, M. Bokor, P. Huang, R. Gaál, P. Matus, J. Karpinski & L. Forró. Single Crystals of Superconducting $SmFeAsOH_x$:
Structure and Properties. Phys. Rev. B (2016) Accepted.

[3] A. Arakcheeva, D. Chernyshov, M. Spina, L. Forró & E. Horvát. $CH_3NH_3PbI_3$: Precise Structural Consequences of Water Absorption at Ambient Conditions. Acta Cryst. B72 (2016). Accepted.

[4] A. Arakcheeva, P. Pattison, G. Chapuis, H. Berger, L. Forró. International School and Workshop on Electronic Crystals ECRYS-2014 August 11-23 2014 Cargèse, France.

[5] B. Náfrádi, T. Keller, F. Hardy, C. Meingast, A. Erb, B. Keimer. Magnetostriction and magneto-structural domains in antiferromagnetic $YBa_2Cu_3O_6$. Phys. Rev. Lett., (2016) 116, 047001.

[6] A. Sazonov, V. Hutanu, M. Meven, G. Roth, I. Kézsmárki, H. Murakawa, Y. Tokura, B. Náfrádi. The low-temperature crystal structure of the multi-ferroic melilite $Ca_2CoSi_2O_7$, Acta Cryst. B (2016) 72, 126-132.

[7] V. Hutanu, A. P. Sazonov, M. Meven, G. Roth, A. Gukasov, H. Murakawa Y. Tokura, D. Szaler, S. Bordacs, I. Kézsmárki, V. K. Gudurd, L. C. J. M. Peters, U. Zeitler, J. Romhányi, B. Náfrádi. Evolution of two-dimensional antiferromagnetism with temperature and magnetic field in multiferroic $Ba_2CuGe_2O_7$. Phys. Rev. B (2014) 89, 064403.

[8] V. Hutanu, A. Sazonov, M. Meven, H. Murakawa, Y. Tokura, S. Bordács, I. Kézsmárki, B. Náfrádi. Determination of the magnetic order and the crystal symmetry in the multiferroic ground state of $Ba_2CoGe_2O_7$. Phys. Rev. B (2012) 86, 104401.

[9] V. Hutanu, A. Sazonov, H. Murakawa, Y. Tokura, B. Náfrádi, D. Chernyshov.
Symmetry and structure of multiferroic $Ba_2CoGe_2O_7$. Phys. Rev. B (2011) 84, 212101.

Figure 1: The Team: On the picture: Tanja Kramer, Rolf Kaufmann, Antonia Neels, Michele Griffa, Kai Zweiacker, Yu Liu, Zoltan Balogh, Stefan Hartmann, Alex Flisch, Carina Stritt, Gelu Rotaru, Mario Beltran, Olga Kuzior, Alex Dommann, Thomas Lüthi, Mathieu Plamondon, Felix Reifler. Not on the picture: Selina Kolokytha, Ramon Schmid, Jürgen Hofmann.

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Empa
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The Center for X-ray Analytics was created in 2014 at Empa Dübendorf for the advancement and application of X-ray-based analytics and imaging to life and materials sciences and technology, which is done in partnerships with academic institutions and industry. Our studies are dedicated to exploiting and continuously improving X-ray methodologies to support materials research, also under different environmental conditions. Application areas are new materials and materials systems in biology, chemistry, metallurgy and semiconductor research. Our core activities relate with the evaluation of the structure-property relationship. We also focus on studies under different non-ambient environmental conditions, which give access to structure dynamics.

X-ray structural and imaging methods are developed (Fig. 2) using:

- X-ray Diffraction Techniques: HRXRD, 2D-XRD, WAXS, GI-XRD for single crystals, powders and thin films.
- X-ray Small Angle Scattering: SAXS combined with WAXS, 2D-SAXS for nano-materials and partially ordered systems.
- X-ray Computed Tomography (CT), combined with 3D image processing/analysis approaches, for a broad range of materials, e.g. biological materials, food, bones, concrete, wood, microsystems.

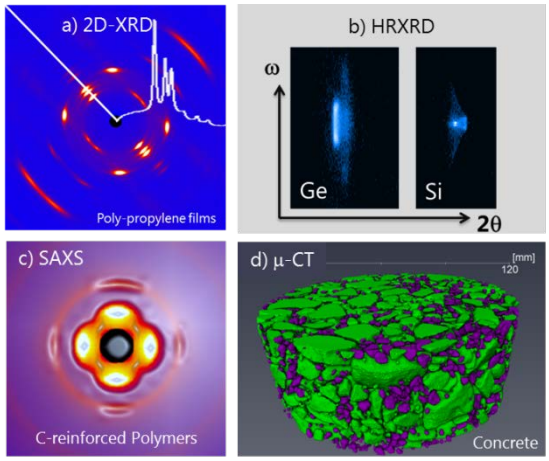

Figure 2: Applied X-ray methodology: a) 2D-XRD, b) HRXRD, c) SAXS and d) CT.

Recent publications and highlights:

[1] A. Schifferle, T. Bandi, A. Neels, A.Dommann, Phys. Status Solidi A, 2016, 102–107.

[2] D. Scopece, M. Döbeli, D. Passerone, X. Maeder, A. Neels, B. Widrig, A. Dommann, U. Müller, J. Ramm, Sci. Technol. Adv. Mater., 2016, 17, 20-28.

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Figure 1: Markus Neuburger (left hand side) and Alessandro Prescimone (right hand side)

Alessandro and me, Markus Neuburger, are running the crystallography lab in the Chemistry Department of University of Basel. We are providing a service for the research groups of the Chemistry Department and are working mostly with organic and metallo-organic samples. As crystals are getting smaller and smaller we are very happy that we can use for the difficult samples our new STADIVARI diffractometer, as depicted in figure 2.

With this new instrument it is possible to measure extremely small samples, as long as they are of sufficient quality. Sure, it still needs crystals, but size matters less when the primary beam is intense enough. Moreover the Pilatus R3 detector with its great dynamic range makes it easy to "see" even the tiniest little spots and produces data of outstanding quality.

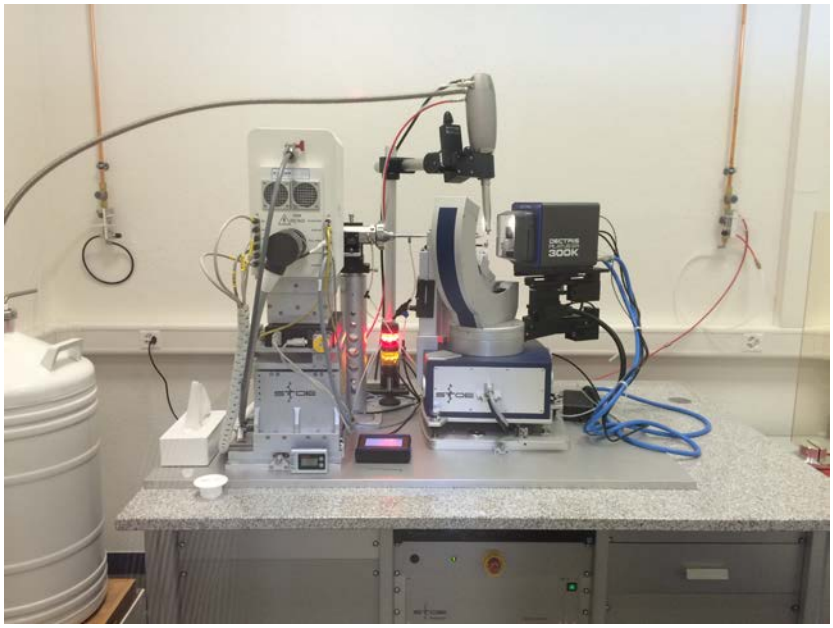

Figure 2: Our new STADIVARI with Metaljet generator and Pilatus detector

Some colleagues were asking me why we needed the Metaljet generator. After some month of use, and after repeating some measurements where we had got structures before, but no publishable data, it is clear that some extra power is always useful and we are happy to welcome everyone that wants to come and try, ☺.

Dr. Markus Neuburger

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Figure1: Thomas Weber

The X-ray platform of the Department of Materials at ETH Zurich was established as a departmental institution after the retirement of Prof. Walter Steurer early 2016. The platform offers a broad range of experimental possibilities, including standard single crystal data collection with a kappa four-cycle diffractometer, Laue diffraction, powder diffraction in Debye-Scherrer and Bragg-Brentano geometry, as well as typical material science specific X-ray characterization methods such as texture, particle size or crystallinity determination. A diffractometer dedicated to high resolution thin film analysis will be installed in September 2016. Most experimental possibilities are also available for external users within or outside ETH. The platform provides access to crystallographic data bases and offers assistance in the preparation of in-house and synchrotron experiments, data evaluation and manuscript writing. Beside the teaching of under- and postgraduate students, joint PhD or post-doc projects are accepted, if the scientific topic falls into the field of the platform manager's experience. Specialties are local structure determination from diffuse scattering and energy dispersive Laue diffraction with PILATUS detectors.

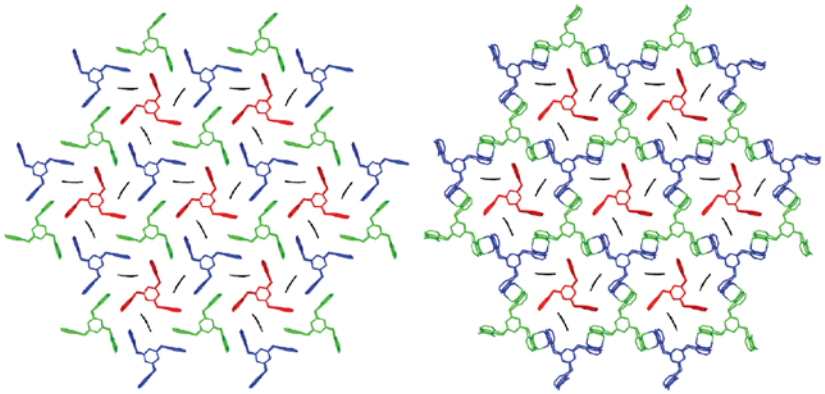
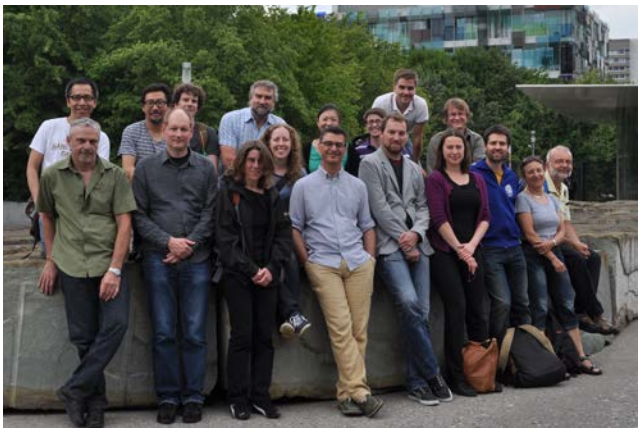


Figure 2: Formation of a two-dimensional polymer (right) from a monomer crystal (left) by light stimulated polymerization [1]. The determination of the reaction pathway via diffuse scattering analysis of the local order of intermediate structures is subject of a joint PhD project with the Schlüter group from the Department of Materials.

[1] Kory, M. J., Wörle, M., Weber, Th., Payamyar, P., van de Poll, S. W., Dshemuchadse, J., Trapp, N. & Schlüter, A.D.: Gram-scale synthesis of two-dimensional polymer crystals and their structure analysis by X-ray diffraction. *Nature Chem.* (2014) **6**, 779–784.



Macromolecular Crystallography group
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The Macromolecular Crystallography (MX) group (Figure 1) at the Swiss Light Source operates two high performance undulator beam lines, as well as a state-of-the-art bending magnet beam line complemented with an integrated Crystallization Facility. The group, which functions in a partnership with Swiss and international pharmaceutical companies, supports structural biologists from both academia and industry on experiments ranging from routine, automated data collection to advanced methods such as structure-based drug design, experimental phasing, and serial crystallography. Research in the MX group is primarily involved in advanced beamline instrumentation and crystallographic methods. In addition, we work closely with many structural biology groups on various projects.

We recently demonstrated how multi-axis goniometry can facilitate the solution of the most demanding Sulfur Single-wavelength Anomalous Diffraction (S-SAD) phasing experiments [1]. This phasing method, which has traditionally seen little utility due to the difficulty in collecting sufficiently accurate anomalous differences in native proteins, is now becoming the method of choice for *de novo* macromolecular structure determination. A multi-axis goniometer is equipped on our bending magnet beam line for S-SAD experiments.

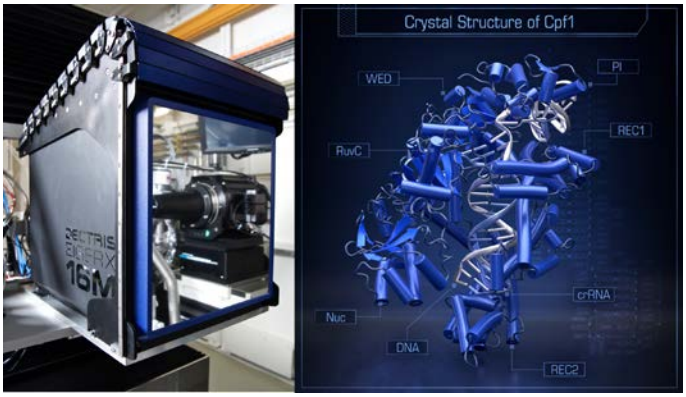

Figure 1: The EIGER 16M at PXI beamline and the first structure solved using this detector (Yamano et al. 2016 Cell)

Other developments include the possibility to collect *in situ* on micro-sized crystals (5-20 µm), typically obtained with membrane proteins [2]. Here, both micro-beam capabilities and fast grid scanning functionalities, together with fast readout detectors, such as the new Dectris EIGER detector (Figure 1), are essential to enable crystallography in a 'serial' fashion. This so-called serial crystallography method is of prime importance for the pharmaceutical industry since over 50% of drugs on the market target membrane proteins.

Recent publications and highlights:

1. Weinert T, Olieric V, Waltersperger S, et al (2015) Fast native-SAD phasing for routine macromolecular structure determination. Nat Methods 12:131–133.

2. Huang CY, Olieric V, Ma P, et al (2016) In meso in situ serial X-ray crystallography of soluble and membrane proteins at cryogenic temperatures. Acta Crystallogr D Struct Biol 72:93–112.

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The Caflisch group (Figure 1) at Department of Biochemistry, University of Zurich, is interested in broad and multidisciplinary aspects of computational structural biology. To this end, we are developing new computational protocols for studying protein dynamics, in particular protein folding and disease-relevant protein aggregation, as well as new methodologies to investigate protein-ligand interactions in the context of structure-based drug discovery.
The success of structure-based ligand discovery approaches predicates on the availability of the structural information on protein-ligand recognition to serve as a starting point of further optimization. In our studies we screen in silico library of fragments, small and mainly rigid molecules that represent a large chemical space. We prioritize fragments by using proprietary *in silico* docking approaches (the SEED program [1]), validate their binding by using biophysical and biochemical methods, and confirm the predicted pose(s) by the means of protein X-ray crystallography (Figure 2). Fragments are then collaboratively developed to potent inhibitors by the means of structure- and *in silico*-guided medicinal chemistry. The group has identified a number of tyrosine kinase inhibitors with cellular potency, and a lead compound has shown excellent anti-tumor activity in a mouse model of breast cancer. More recently, we have targeted epigenetic proteins, and have been working on the development of compounds blocking protein-protein interactions of human bromodomains [2].

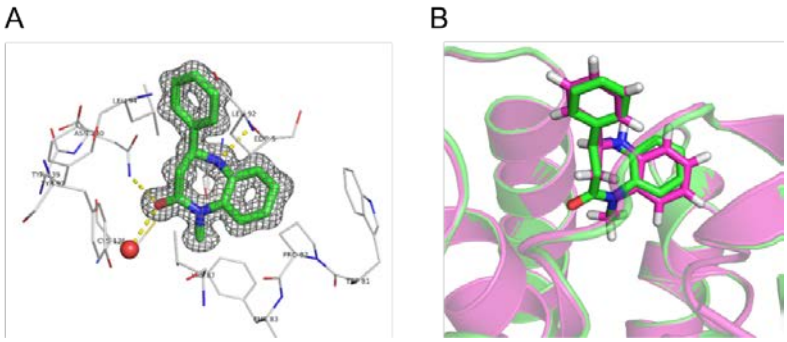

Figure 2: A) Crystal structure and experimental electron density of a fragment bound to the N-terminal bromodomain of the BRD4 protein (PDB code 4PCI). B) Comparison of docked (magenta) and crystal structure-derived (green) binding mode highlights accuracy of our computational docking methods.

The Caflisch group currently consists of nearly 20 people. Besides having the cutting edge position in development of computational methods and full in-house gene-to-structure capacity, the groups includes also experts in cell biology, protein chemistry and biophysics.

[1] Maieux N. et al., *Proteins*, **1999**, 37(1): 88-105.
[2] Zhu, J. and Caflisch, A., *J. Med. Chem*, **2016**, 59(11): 5555-5561.

Figure1: Crystallise! AG founders. Left: Dr. G. Steinfeld; right: Dr. G. Santiso-Quiñones

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Website:
http://www.crystallise.ch

Crystallise! AG (Schlieren/ZH, Switzerland) was founded in September 2014. The company provides crystallographic services for the identification of small molecule compounds and runs an independent laboratory for crystallographic analyses. The company focuses on the structural characterization of unknown or not fully characterized substances using single crystal X-ray analysis. Crystallise! main goal is to provide all kinds of crystallographic services to the chemical, pharmaceutical and agro industries.

Crystallise! services' include: Crystallization of samples, X-ray measurement, data analysis, interpretation of the data, and results. Our team even can handle sensitive (air, moisture, temperature) substances without any problem. Crystals that tend to loose solvent can be easily handle at our lab too.

The company's portfolio offers plenty of experience and know how in crystallization techniques, including a unique technique for the **Crystallization of Liquid Compounds**! [1]. Yes, we can crystallize liquid compounds and provide you a structural characterization of it (see Fig. 2)

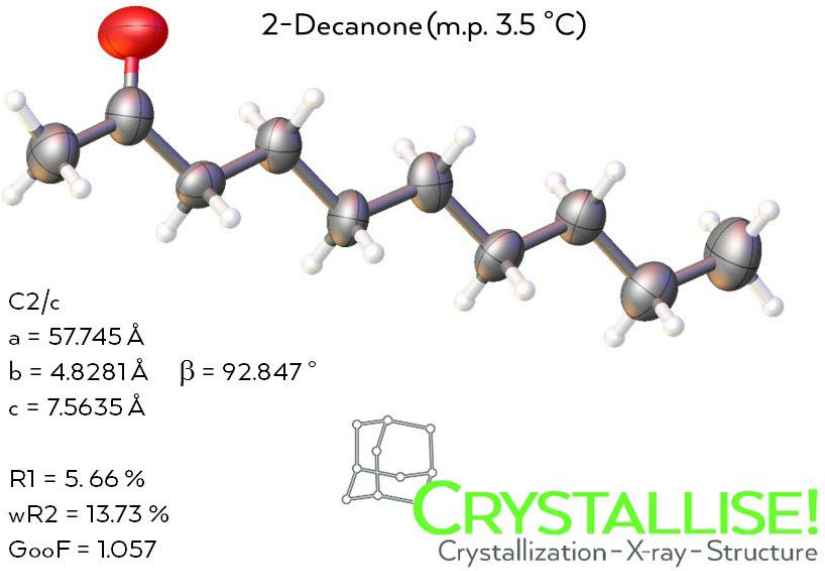

Figure 2: One example of a liquid compound crystallized at Crystallise! AG.[2]

At the present time, most of our customers are interested in the crystallization service. Where others have failed, Crystallise! AG has proven to be successful. Very often our costumers request the confirmation of the absolute configuration or they are interested in the composition of a specific polymorph form.

[1] G. Santiso-Quinones, I. Krossing. *Z. Anorg. Allg. Chem*. **2008**, 634, 704-707.
[2] As part of a collaboration with Prof. Dr. B Spingler (UZH).

Figure 1: The CSEM's Characterization crystallography group: S. Biselli, I.Marozau, J.Tillier, O.Sereda, J.Gobet, V.Courbat, M.Dadras (clockwise).

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Website:
http://www.csem.ch

The X-ray Application Laboratory was established in 2008 at CSEM thanks to the efforts of Prof. H. Stoeckli-Evans and Dr. A. Dommann. The laboratory was managed by Dr. A. Neels till 2013, focusing mainly on the BENEFRI (collaboration of three Swiss universities: Berne, Neuchâtel and Fribourg) service for 3-Dimentional structure determination of new chemical compounds, but not only. After five years, this team became more active in the investigation of the microstructure of a large pallet of materials. In 2013 the group was reorganized and successfully integrated into the CSEM's Characterization Center and it has been part of the Micro & Nano Systems Division since then. The center provides advanced crystallographic expertise in the development of the new materials for technology and product improvement. Currently, the Characterization Center brings several analytical techniques: X-ray, microscopic, spectroscopic, mechanical and tribology techniques, in which X-ray diffraction has a special place. This combination provides valuable information on a material's formation, defects, structural disorder and the output in physical properties of the investigated material. One of the strengths of the center is *in-situ* X-ray diffraction investigations (time-resolved studies), which shed light on a material's behavior under temperature, humidity and stress conditions. The research group consists of 8 highly qualified scientists (Fig. 1) and has ongoing research projects in several areas (PV, energy, metallurgy, solid -state chemistry, food, pharma, life science and micro-technology) [1-3]. The example below illustrates the benefits of using the *in-situ* Small Angle X-ray Scattering (SAXS) tech-nique in the field of electro-catalysis, *viz.* the investigation of polymer electrolyte fuel cell (PEFC) Pt cathode catalyst degradation. In PEFCs the electrochemical reactions, *viz*. the hydrogen oxidation reaction (HOR) and the oxygen reduction reaction (ORR), take place on the surface of typically Pt-based catalysts at the so-called three-phase boundary. Today, improving the performance of the cathode of PEFCs, where the ORR takes place, is probably one of the most urgent requirements because both the catalyst kinetics and its corrosion stability are clearly insufficient to make PEFCs cost competitive devices for automotive and stationary applications. In fact, Pt or Pt-alloy nanoparticles supported on high-surface area carbon supports display good performance as cathode catalysts under laboratory conditions despite the thermodynamic carbon instability at potentials above 0.206V_{NHE}. However, under real-life operating conditions, especially the cathode can reach potentials as high as 1.5V (e.g., during start-stop cycling) where the used

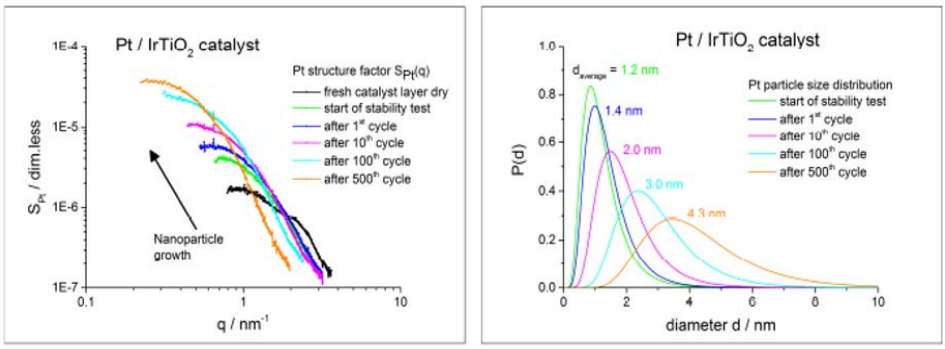

Figure 2: Pure Pt structure factor $S_{Pt}(q)$ extracted from the total scattering signal by using SAXS (on the left) and evolution of the Pt nanoparticles size distribution during electrochemical start/stop cycling (on the right).

carbon supported catalysts are lacking corrosion stability and become fuel cell lifetime determining. Thus, a special focus was made to establish structure-property relationships by means of SAXS, carried out *in-situ* during electrochemical measurements. Especially, we have successfully developed the *in-situ* X-ray electrochemical flow-cell which helped the understanding of (surface)-structural changes during potential cycling and created the important link between structural stability and reaction kinetics (Fig. 2). The *in-situ* SAXS provided the structural information at the nanoscale and has given direct hints to the electronic state of catalyst materials under electrochemical potential control [3]. This project was a collaboration together with PSI and ETHZ. We thank Umicore Ag & Co. KG and the Competence Center for Energy and Mobility (CCEM) of Switzerland for their support and for funding the project.

Recent publications and highlights:

[1]. E. Oakton, J. Tillier, G. Siddiqi, Z. Mickovic, O. Sereda, A. Fedorov, C. Copéret. Structural differences between Sb- and Nb-doped tin oxides and consequences for electrical conductivity. New Journal of Chemistry, 01/2016; 40(3).

[2]. E. Oakton, D. Lebedev, A. Fedorov, F. Krumeich, J. Tillier, O. Sereda, T.J. Schmidt, C. Copéret A simple one-pot Adams method route to conductive high surface area IrO2 –TiO2 materials. New Journal of Chemistry, 02/2016; 40(2).

[3]. T. Binninger, M. Garganourakis, J. Han, A. Patru, E. Fabbri, O. Sereda, R. Kötz, A. Menzel, and T. J. Schmidt, Particle-Support Interferences in Small-Angle X-Ray Scattering from Supported-Catalyst Materials. Physical Review Applied 02/2015; 3(2):024012.

The group of Prof. Dr. Spingler: from left to right: Ngọc An Lê, Ali Tuna, Bernhard Spingler, Philipp Nievergelt, Michele Larocca.

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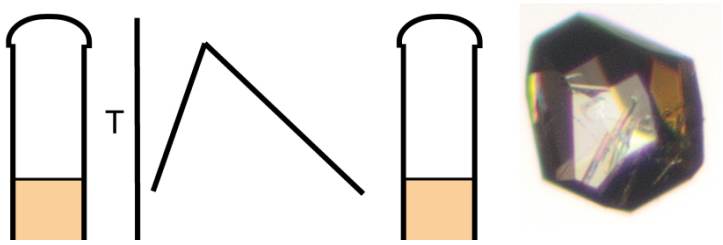
Research in the Spingler group focuses on crystallography and bioinorganic chemistry. Dr. Spingler has been involved in crystallographic studies for over 20 years. He has contributed more than 350 structures to the CSD and 19 structures to the PDB. The experiences made with many users of the crystallographic facilities resulted in the writing of a tutorial for the growth of single crystals of small molecules.[1] Current crystallographic activities are the suitability of thermal recrystallization for the generation of single crystals[2] and the crystallization of charged compounds. In the bioinorganic field, the Spingler group has studied the induction of the rare left-handed Z-DNA by mono- and dinuclear metal complexes (for recent examples see [3-5]). Currently, most of the group works on photodynamic therapy (PDT).[6, 7]



F*igure 1: Thermal recrystallization (left) used to grow excellent single crystals (right) within 6 hours.*

Recent publications and highlights:

[1] B. Spingler, S. Schnidrig, T. Todorova, F. Wild, CrystEngComm 2012, 14, 751.
[2] P. Nievergelt, B. Spingler, 2016, submitted.
[3] A. Medina-Molner, B. Spingler, Chem. Commun. 2012, 48, 1961.
[4] A. Medina-Molner, M. Rohner, D. Pandiarajan, B. Spingler, Dalton Trans. 2015, 44, 3664.
[5] M. Rohner, A. Medina-Molner, B. Spingler, Inorg. Chem. 2016, 55, 6130.
[6] A. Naik, R. Rubbiani, G. Gasser, B. Spingler, Angew. Chem. Int. Ed. 2014, 53, 6938.
[7] P. M. Antoni, A. Naik, I. Albert, R. Rubbiani, S. Gupta, P. Ruiz-Sanchez, P. Munikorn, J. M. Mateos, V. Luginbuehl, P. Thamyongkit, U. Ziegler, G. Gasser, G. Jeschke, B. Spingler, Chem. Eur. J. 2015, 21, 1179.

Figure 1: The PCC Team Beat Blattmann & Céline Stutz

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High Throughput Protein Crystallization @ University of Zurich

The Protein Crystallization Center high-throughput screening lab at the University of Zurich – PCC@UZH – assists professionally the academic and industrial research community for over 14 years in advancing their research in structural biology. Just over the past year, more than twenty academic and industrial research groups took advantage of PCC's expertise in a wide range of crystallization techniques for soluble and membrane proteins.

An experienced operator at PCC sets up the vapor diffusion and LCP crystallization experiments at 4° or 20°C according to the researcher's specifications at the nano-liter scale using automated liquid-handling robots. The crystallization plates are incubated in one of the two state-of-the-art Rock Imager 1000 (4°C or 20°C) and imaged using the visible (w/ & w/o cross polarizer) and a UV/Fluorescent imaging system from Formulatrix, Inc.

PCC and the Swiss Light Source (SLS) are offering a service for high-throughput crystallization screening combined with In-situ X-ray diffraction at the SLS without the need for a beamline proposal.

For more information, please contact Beat Blattmann or Céline Stutz by email or go to our web site at http://www.bioc.uzh.ch/research/core-facilities/protein-crystallization-center/

Figure 2: High Throughput Protein Crystallization combined with In-situ X-ray Diffraction Screening

Phase Solutions

Beyond your laboratory results

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Phase Solutions was created in 2010 to pursue independently the activities of the Laboratory of Crystallography at EPFL (École Polytechnique Fédérale de Lausanne), Switzerland. It was founded by Prof. Gervais Chapuis with Dr Alla Arakcheeva as CEO and Dr Philip Pattison as Adviser. The company is closely collaborating with EPFL.

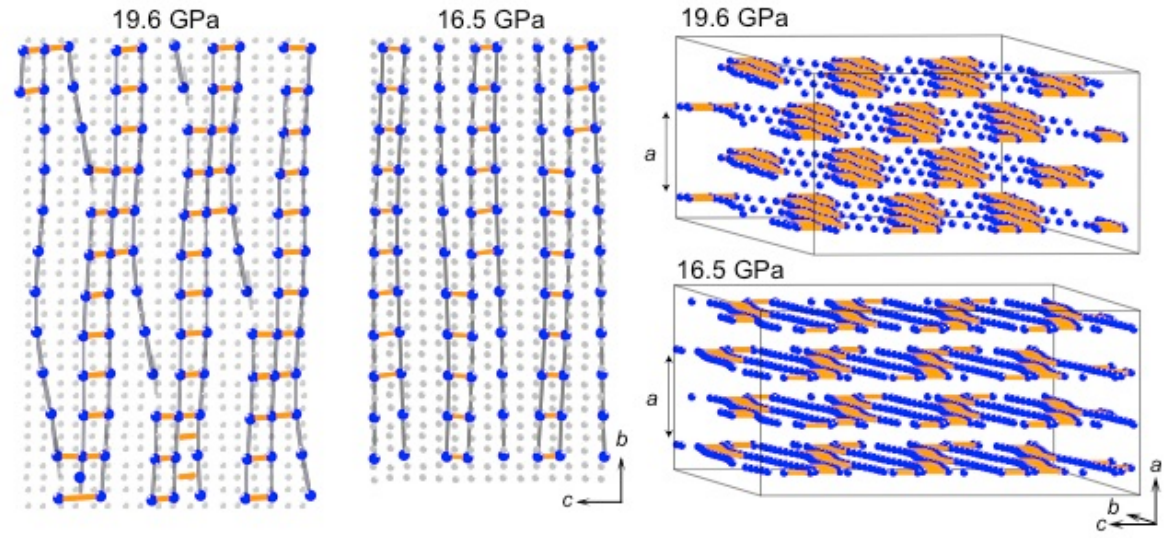

Fig. 1. Incommensurate density waves in BaIV-b

Phase Solutions (PS) provides crystallography research services including nano-particle size estimations, impurity tests of amount smaller than 1%, structural defects, incommensurately and commensurately modulated structures among others. PS also work with minimal amount of powder samples.

PS enables you to have access to top specialists in crystallography, the most advanced diffraction equipments and extended experience in the interpretation of X-ray results. Phase Solutions find solutions when others fail.

The following examples of studies have been performed with PS assistance:

- Study of the reaction products formed by the alkali–silica reaction in concrete [1]
- KEu(MoO4)2: Polymorphism, Structures, and Luminescent Properties [2]
- Novel nonlinear optical material with an incommensurate structure [3]
- Review on the aperiodic nature of incommensurately modulated structures [4]
- Crystal structure and modelling of polytypes using the superspace approach [5]
- $Na_{2/7}Gd_{4/7}MoO_4$: a modulated scheelite-type structure and conductivity [6]
- The luminescence of $Na_xEu^{3+}_{(2-x)/3}MoO_4$ scheelites [7]
- Incommensurate density waves (Fig. 1) in the high-pressure Ba-IVb phase [8]

Recent publications and highlights:

[1] R. Dähn, A. Arakcheeva *et al*., (2016) *Cement and Concrete Research*. **79**, 49.

[2] V. A. Morozov, A. Arakcheeva *et al*., (2015) *Chem. Mater*. **27**, 5519.

[3] A. Subashini, S. Leela *et al*., (2013) *CrystEngComm*. **15**, 2474.

[4] G. Chapuis & A. Arakcheeva. (2013) *Rend. Fis. Acc. Lincei*. **24**, 77.

[5] A. Arakcheeva, P. Pattison *et al*., (2013) *J. Appl. Cryst*. **46**, 99.

[6] V. Morozov, A. Arakcheeva *et al*., (2012) *Inorg. Chem*. **51**, 5313.

[7] A. Arakcheeva, D. Logvinovich, G. Chapuis *et al*., (2012) Chem. Sci. **3**, 384.

[8] A. Arakcheeva, M. Bykov *et al*., (2016) Submitted for publication.

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Figure 1: The crystallography equipment.

The Neuchâtel Platform of Analytical Chemistry (NPAC) is a state-of-the-art service and research facility affiliated to the Institute of Chemistry at the University of Neuchâtel. It is currently organized in three units, the Mass Spectrometry and Metabolomics unit, the Nuclear Magnetic Resonance unit, and the Crystallography unit. The primary mission of the NPAC is to serve as a support for research projects for the local and external academic community on a collaborative basis. The scientists running the platform develop and optimize methods for specific applications, and provide advice and assistance for sample preparation, as well as interpretation of the obtained data. In addition, the NPAC offers services to academia and the industry for routine protocols. The Crystallography unit houses a Stoe Mark II-Image Plate Diffraction System, using Mo-Ka graphite monochromated radiation, which is also connected to a low temperature device.
The crystallography equipment (Figure 1) is used by two groups, both dealing with single-crystals of small molecules. Professor Bruno Therrien interests lie in bioinorganic [1] and supramolecular chemistry [2], while Professor Helen Stoeckli-Evans is involved in projects concerning structural transformations induced by solvent loss on heating [3,4].

Recent publications:
[1] A. Grozav, O. Balacescu, L. Balacescu, T. Cheminel, I. Berindan-Neagoe, B. Therrien, Synthesis, anticancer activity and genome profiling of thiazolo arene ruthenium complexes, *J. Med. Chem.* 58, **2015**, 8475–8490.
[2] A. Pitto-Barry, N.P.E. Barry, V. Russo, B. Heinrich, B. Donnio, R. Deschenaux, B. Therrien, Designing supramolecular liquid-crystalline hybrids from pyrenyl-containing dendrimers and arene-ruthenium metalla-cycles, *J. Am. Chem. Soc.* 136, **2014**, 17616–17625.
[3] L. Schmitt, G. Labat, H. Stoeckli-Evans, Crystal-to-crystal transformation upon dehydration of a copper(II) 2,2′:6′,2″-terpyridine complex, *Acta Cryst.* C66, **2010**, m343–m347.
[4] H. Stoeckli-Evans, O. Sereda, A. Neels, S. Oguey, C. Ionescu, Y. Jacquier, *In situ* single-crystal to single-crystal (SCSC) transformation of the one-dimensional polymer *catena*-poly[[diaqua(sulfato)copper(II)]-μ_2-glycine] into the two-dimensional polymer poly[μ_2-glycine-μ_4-sulfato-copper(II)], *Acta Cryst.* C70, **2014**, 1057–1063.

Picture of the neutron diffraction group at PSI in 2/2015, from left: O. Zaharko, S. Gao, S. Butkute (now Vilnius), C. Canévet, M. Kubus, M. Frontzek (now SNS), T. Panzner, J. Schefer, V. Pomjakushin, L. Keller, D. Sheptyakov. Not on the picture: S. Toth, S.R. Maity (since 9/2015), R. Sibille (since 4/2016), F. Xiao, N. Van Well, P.G.R. Garbus (since 7/2016).

Neutron Diffraction Group

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The neutron diffraction group is responsible for the user service of the diffraction instruments at the Swiss Spallation Neutron Source SINQ (https:// www.psi.ch/sinq/instrumentation): The two powder diffractometers (HRPT and DMC), the single crystal diffractometer ZEBRA, the strain scanner POLDI and the test diffractometer ORION. Within our division at PSI (NUM), we are in close collaboration with the LDM laboratory, which is operating crystal growth facilities (e.g. a mirror furnaces), high-pressure and general analysis equipment (laboratory X-ray machines, SQUID, PPMS, e.g.). With HEIMDAL, we are also participating in novel NPD instrumentation for the ESS spallation source in Lund, Sweden.
Our research topics are focused in materials science, especially novel magnetic materials such as molecular magnets or novel permanent magnets. A strong focus is the investigation of materials for energy storage, new battery materials and oxygen diffusion at moderate temperatures. The industrial research goes towards spatially resolved measurements of residual stresses in engineering components, the study of stress/temperature induced phase transformations and in-situ deformation studies of metallic systems.
Further highlights are listed on the homepage of the NUM division (https:// www.psi.ch/num/scientific-highlights) and on the instruments web sites. A selcection of recent publications is listed below:

[1] R. Sibille, E. Lhotel, V. Pomjakushin, Ch. Baines, M. Kenzelmann: Candidate quantum spin liquid in the Ce3+ pyrochlore stannate Ce2Sn2O7, PRL 115, 097202 (2015).
[2] L. Keller, J.S. White, M. Frontzek, M. Babkevich, M.A. Susner, Z.S. Sims, A.Sa. Sefat, H.M. Ronnow, Ch. Rüegg: Pressure dependence of the magnetic order in CrAs: A neutron diffraction investigation, PRB B 91, 020409 (2015).
[3] O. Zaharko, M. Pregelj, A. Zorko, R. Podgajny, A. Gukasov, J. van Tol, S.I. Klokishner, S. Ostrovsky, B. Delley: Source of magnetic anisotropy in quasi-two-dimensional XY {Cu4(tetrenH5)[W(CN)8]4 7.2H2O)}n bilayer molecular magnet, PRB 87, 024406 (2013). [4] S. Song, D. Sheptyakov A.M. Korsunsk, H.M. Duong, L. Lu: High Li ion conductivity in a garnet-type solid electrolyte via unusual site occupation of the doping Ca ions, Mat.&Design 93, 232 (2016).

Figure 1: The Optics and Crystal Growth Group
From left to right: Dr. C. Barreteau (crystal growth, CG), Dr. E. Giannini (CG), Dr. S. Karlsson (CG), M. Brandt, Dr.M Tran, Dr. N. Bachar, Dr. J.-M. Poumirol, Prof. D. van der Marel (group leader), M. Philippi, Dr. J. Levallois, Dr. J. Teyssier (CG), Dr. M. Chhikara, Dr. A. Kuzmenko, Dr. A. Akrap, A. Stucky (CG), D. Valentinis, Dr. D. Stricker.

Optics and Crystal Growth
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DQMP of the University of Geneva belongs to the “Optics and Crystal Growth” Group lead by Prof. Dirk van der Marel. The main activity of the Optics and Crystal Growth Group is the study of fundamental excitations in strongly correlated solid matter, by various experimental techniques, mainly by optical spectroscopy.
The Laboratory for Crystal Growth (1 staff member, Enrico Giannini, 1 technician, 2 post-docs, 1 phD student) provides the research activity of the group with crystalline and polycrystalline materials, has external (both national and international) collaborations on various materials, and searches for novel materials with strong electron correlations. The interest is both on fundamental solid state physics and possible future applications (of superconductivity, spintronics, electronic devices…). This team has a long-standing experience in crystal growth, and has been working on a broad variety of compounds, with special focus on superconducting cuprates, magnetic transition metal silicides, Fe-based superconductors and, more recently, topological insulators and semiconducting transition metal chalcogenides.
The laboratory is equipped for a large versatility for the production of crystals of various and very different materials: two mirror furnaces for the Floating Zone growth, HF induction furnaces for Czochralski growth, even in oxidizing atmosphere and from levitating melt, arc furnaces, high-T high-P cubic anvil press (up to 10GPa 1500°C), high-p(O2) furnaces (100bar), resistive furnaces for the Bridgman method and the Vertical Gradient Freezing growth, many furnaces for solid state reactions under various conditions.
For crystallographics studies, the group takes advantages of the close collaboration with the Laboratory of Crystallography, lead by Prof. Radovan Cerny, in the same department.

Recent publications and highlights:
[1] J. Teyssier, E. Giannini, A. Stucky, R. Černý, M. V. Eremin,, D. van der Marel: ”Jahn-Teller induced nematic orbital order in tetragonal Sr2VO4”, Phys. Rev. B 93 (2016) 125138
[2] C. Barreteau, B. Michon, C. Besnard, E. Giannini: “High-pressure melt growth and transport properties of SiP,SiAs,GeP,and GeAs 2D layered semiconductors”, J. Cryst. Growth 443 (2016) 75–80

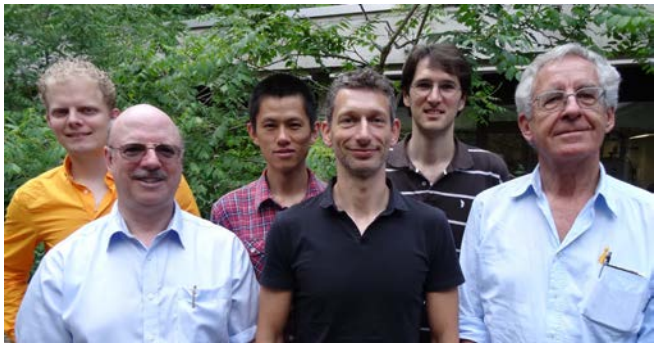

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Figure 1: The Linden group at UZH: Eric Stronks, Anthony Linden, Jun Xu, Olivier Blacque, Ruggero Frison, Hans-Beat Bürgi

The X-ray Crystallography Facility of the Department of Chemistry at the University of Zurich, currently lead by Prof. Anthony Linden, had its beginnings in 1969 and provides a small-molecule single-crystal structure determination service for all members of the department. Equipment includes Oxford Diffraction SuperNova and Xcalibur, Nonius KappaCCD, Stoe IPDS and Bruker D8 Advance single crystal and powder diffractometers. The Facility also conducts occasional analyses for researchers in other departments of the university and for some pharmaceutical companies, and has ongoing collaborations with academic colleagues at several external institutions.

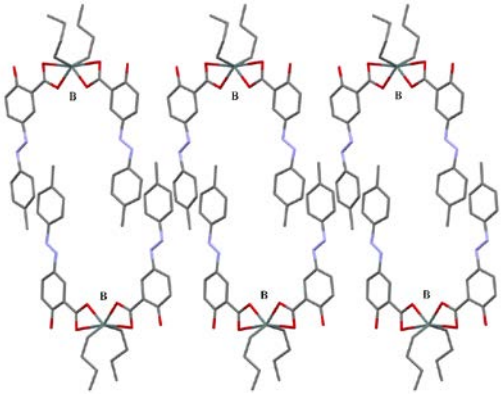

Figure 2: π-π stacking motifs in alkylcarboxylatotin(IV) **complexes**

The Facility organizes and hosts the popular biennial Zurich School of Crystallography, which trains budding young crystallographers from around the world. Prof. Linden is a Main Editor of Acta Crystallographica, Section C.

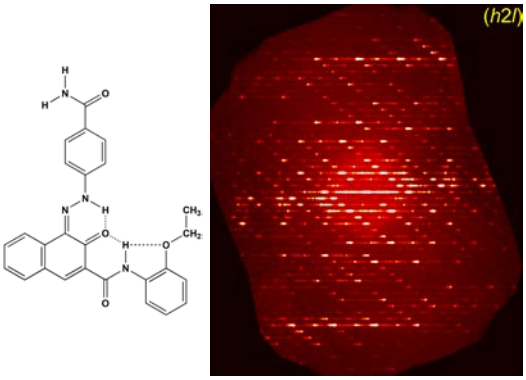

Figure 3: Diffuse scattering from layer stacking faults in Pigment

For research, the group has a general interest in solid-state intermolecular interactions and their relationship to the supramolecular and structural properties of crystalline materials (Fig. 2). The group is also interested in modelling the solid state local structures of disordered molecular materials through evaluation of the diffuse scattering (Fig. 3), because materials with interesting and useful physical properties are often disordered and knowledge of the local structure is necessary in order to fully understand the properties of the material. One aim is to further develop methods for analyzing diffuse scattering, which, unlike studies of ordered materials, are far from routine.

[1] A. Linden, T.S. Basu Baul, Acta Crystallogr. **2016**, *C72*, 313.
[2] R. Warshamanage, A. Linden, M.U. Schmidt, H.-B. Bürgi, Acta Cryst. **2014**, *B70*, 283.

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The group "New techniques for Ancient Materials" led by Prof. Claire Gervais is based at the Bern University of the Arts (HKB). The main core of our research activities lies in the study of physico-chemical processes in natural and cultural materials, with a focus on materials degradation and the development of innovative methods for investigation of disordered and sensitive materials [1]. We are developing various synchrotron and simulation techniques, from X (X-ray absorption spectroscopy, X-ray diffraction, X-ray tomography) ... to A (Algorithms for image processing and MC simulations).

We employed anomalous X-ray diffraction to estimate the ratio and location of Fe(II) and Fe(III) cations in the pigment Prussian blue (iron(III)hexacyanoferrate(II)). Prussian blue is found in various cultural heritage objects, from paintings to photographs, and shows extensive light-induced fading due to the photoreduction of iron(II) centers. Anomalous X-ray diffraction of faded and unfaded Prussian blue powders was performed around the Fe K-edge (Figure). It showed that a reduction indeed takes place upon fading and is likely associated to an increasing disorder between the two iron(II) and iron(III) sites in the faded structure [2]. Together with X-ray absorption spectroscopy, these findings allowed us to shed more light on the chemical and structural variations in faded Prussian blue cultural heritage artefacts.

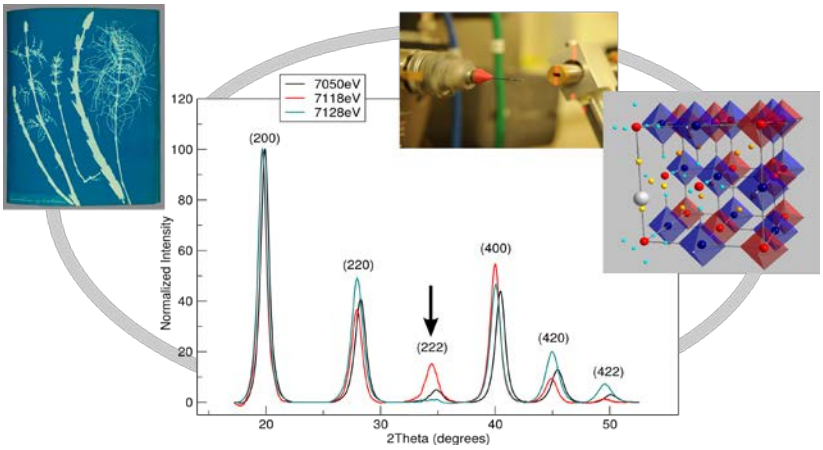

Figure 1: X-ray diffraction of Prussian blue obtained around the iron K-edge at CRISTAL beamline, synchrotron SOLEIL. After Rietveld refinement, the average oxidation states on both iron sites could be estimated.

[1] C. Gervais, M.A. Languille, G. Moretti, S. Reguer, "X-ray Photochemistry of Prussian Blue Cellulosic Materials: Evidence for a Substrate-Mediated Redox Process", *Langmuir*, 31:8168, 2015.
[2] C. Gervais, M.A. Languille, S. Reguer, S. Pelletier, E. Elkaim, E. Vicenzi, L. Bertrand. “Estimation or iron valencies of Prussian blue pigment by anomalous X-ray diffraction” *Acta Cryst. A67*, C111, 2011.

Figure 1: The crystallography group with names of the group members. Note that P. Schouwink is since June 2016 at the crystallography laboratory of EPFL Valais Wallis, Sion.

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The Laboratory of Crystallography at the University of Geneva is a part of the Dpt. of Quantum Matter Physics. The laboratory awards a Ph.D. degree in crystallography, teach the crystallography for students in physics, (bio-)chemistry and mineralogy, and in collaboration with the Section of Chemistry provides the crystallographic service. The laboratory was created in 1970 as the first Chair of Crystallography in the French-speaking Switzerland. The actual research directions are in the field of crystallography based design of light metal hydrides [1] as materials for solid state hydrogen storage, solid electrolytes in Li- and Na-batteries [2], luminescence [3] and magnetocaloric applications (group of R. Černý), in collaboration with the Section of Chemistry on spin crossover materials and rare earths based coordination polymers (C. Besnard, P. Schouwink, L. Guénée) and in the development of Pearson's Crystal Database (K. Cenzual). It is also the place where the computer program Fox [4] has been created, and the improvement of the methods for crystal structure solution from powder diffraction data stays one of the important activities. The laboratory worked also in the field of crystallography and crystal chemistry of inorganic compounds (E. Parthé), and of intermetallics and their properties such as hydrogen storage, magnetism and supraconductivity (K. Yvon, R. Černý). The methods of structure solution from single crystal data, especially the absolute structure determination are another important contribution of the laboratory (H. Flack, G. Bernardinelli).

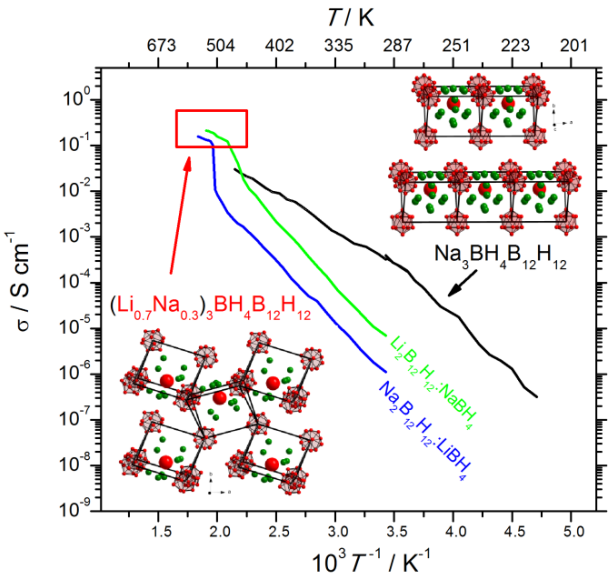

Figure 2: Crystal structure of $Na_3BH_4B_{12}H_{12}$ and $(Li_{0.7}Na_{0.3})_3BH_4B_{12}H_{12}$; mobile species ($Li^+$,$Na^+$) in green, boron as red spheres, $[B_{12}H_{12}]^{2-}$ as molecule. Ionic conductivities obtained from impedance spectroscopy [2].

Recent publications and highlights:

[1] Borohydride-oxide analogy: *Acta Cryst. B* (2015), 71, 619-640
[2] Superionic hydroborates: *Adv. Energy Mater*. (2015), 1501016
[3] Borohydrides-perovskites: *Nature Comm*. (2014) 5:5706
[4] Program Fox: http://fox.vincefn.net/

Figure 1: Some members of the group spanning several generations: Simon Brenner, Fabian Gramm, Javier de Oñate, Lynne McCusker, Christian Baerlocher, Stef Smeets, Catherine Dejoie, Dubravka Sisak Jung, Ana Belen Pinar, Ken Inge.

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Website:http://www.crystal.mat.ethz.ch/research/ZeolitesPowderDiffraction.html

When Walter Meier retired from the ETH in 1992, Christian Baerlocher and Lynne McCusker continued to pursue the theme of zeolite structure analysis that he had started, and eventually built up their own group with a slight change in emphasis. Because zeolites, especially the newly synthesized ones, tended to be polycrystalline and their structures complex, getting an initial structural model of the framework structure was a challenge and this was the focus of the new group. By taking advantage of the new synchrotron radiation opportunities and the ever increasing computing power, a number of methods/tools for solving structures from powder diffraction data were developed over the years: FOCUS [1], structure envelopes [2], the texture method [3], and powder charge flipping [4]. By combining X-ray powder diffraction with electron microscopy data in various ways, the power of these tools could be exploited even further [5]. Several methods also proved to be applicable beyond the realm of zeolites.

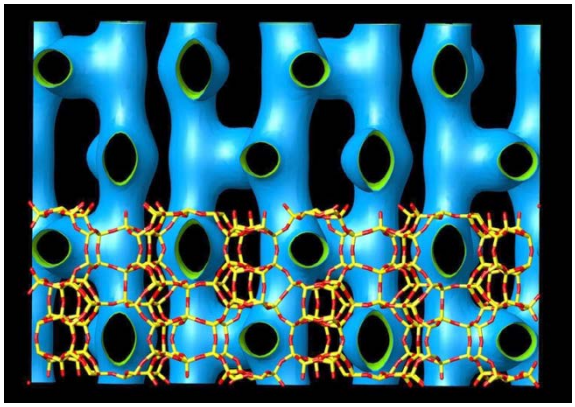

Figure 2: The framework structure of IM-5 with its unusual channel system, solved by combining HRTEM and XPD data in the powder charge flipping algorithm.

More recently, the possibility of obtaining single-crystal data from micron-sized crystals using white beam (Laue) micro-diffraction was explored [6], and this in turn led to experiments for the SwissFEL facility that should come online next year (with a unique 4% energy bandpass mode). These experiments showed that the superimposed diffraction patterns of up to 10, stationary, randomly oriented, micron sized crystallites exposed to a single (*ca.* 20 femtosecond) pulse can be indexed and reliable intensities extracted [7]. The group disbanded at the end of 2015 when the Laboratory of Crystallography at ETH closed, but the work continues with the next generation in several places around the world.

[1] RW Grosse-Kunstleve, LB McCusker, Ch Baerlocher (1997) *J Appl Cryst* **30** 985-995; S Smeets, LB McCusker, Ch Baerlocher, E Mugnaioli, U Kolb (2013) *J Appl Cryst* **46** 1017-1023
[2] S Brenner, LB McCusker, Ch Baerlocher (1997) *J Appl Cryst* **30**, 1167-1172
[3] T Wessels, Ch Baerlocher, LB McCusker (1999) *Science* **284** 477-479; J Grässlin, LB McCusker, Ch Baerlocher, F Gozzo, B Schmitt, L Lutterotti (2013) *J Appl Cryst* **46** 173-180
[4] Ch Baerlocher, LB McCusker, L Palatinus (2007) *Z. Krist* **222** 47-53; Ch Baerlocher, F Gramm, L Massüger, LB McCusker, Z He, S Hovmöller, X Zou, (2007) *Science* **315** 1113-1116

[5] F Gramm, Ch Baerlocher, LB McCusker, SJ Warrender, PA Wright, B Han, SB Hong, Z Liu, T Ohsuna, O Terasaki (2006) *Nature* **444** 79-81; LB McCusker, Ch Baerlocher (2013) *Z Krist* **228** 1-10
[6] C Dejoie, LB McCusker, Ch Baerlocher, R Abela, BD Patterson, M Kunz, N Tamura (2013) *J Appl Cryst* 791-794
[7] C Dejoie, S Smeets, Ch Baerlocher, N Tamura, P Pattison, R Abela, LB McCusker (2015) *IUCrJ* **2** 361-370

Rosario Scopelliti

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The X-ray diffraction group at EPFL is a joint service offered by ICMP, IPSB and ISIC of FSB to EPFL and industry. It is directed by Professors Paul Dyson, Pëtr Leiman and Henrik Rønnow.

The service carries out, using the diffraction of X-rays, data collection on single crystals and powders. CIF-files for deposition in data-bases and for publications are completed. The service is always open to discuss less common applications of X-ray diffraction and to provide synchrotron facilities when needed.

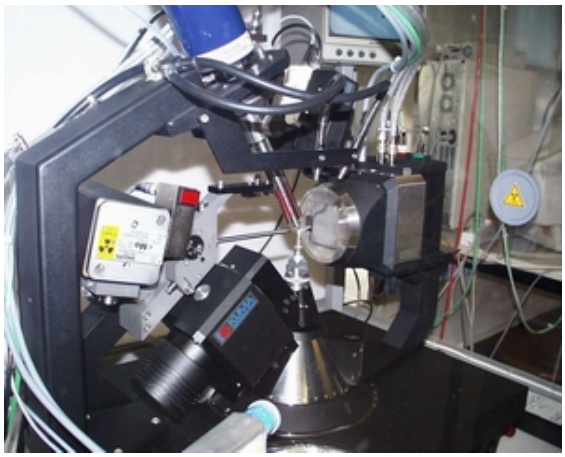

Figure 2: A picture of one of our diffractometers equipped with a CCD-detector and crystal cooling.

Recent publications and highlights:

[1] M. Marmier, M. Wise, J.J. Holstein, P. Pattison, K. Schenk, E. Solari, R. Scopelliti, K. Severin, *Inorganic Chemistry*, **2016**, 55(8), 4006-4015.
[2] T.Xu, C.–J.M. Yin, M. D. Wodrich, S. Mazza, K. M. Schultz, R. Scopelliti, and X. Hu, *J. Am. Chem. Soc.*, **2016**, *138* (10), 3270–3273.

Prof. Hans-Beat Bürgi

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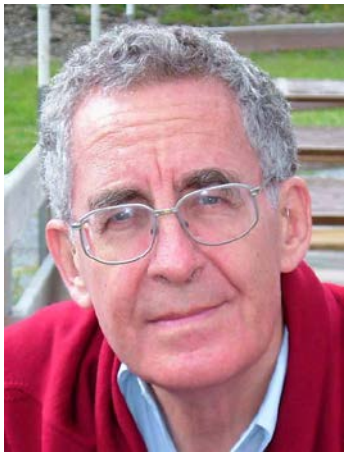
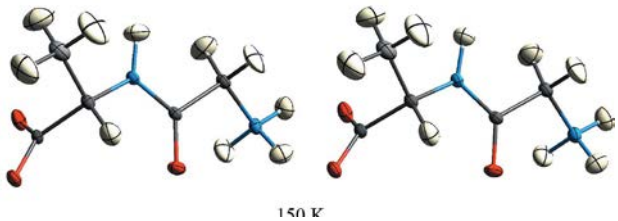


Hans-Beat Bürgi is a permanent academic guest at the Chemistry Department of the University of Zürich, Professor Emeritus at the University of Bern, Switzerland and a co-director with Prof. Anthony Linden of the *Zurich School of Crystallography*, a two-week intense course for international students, which was inaugurated in 2007. His research interests include:

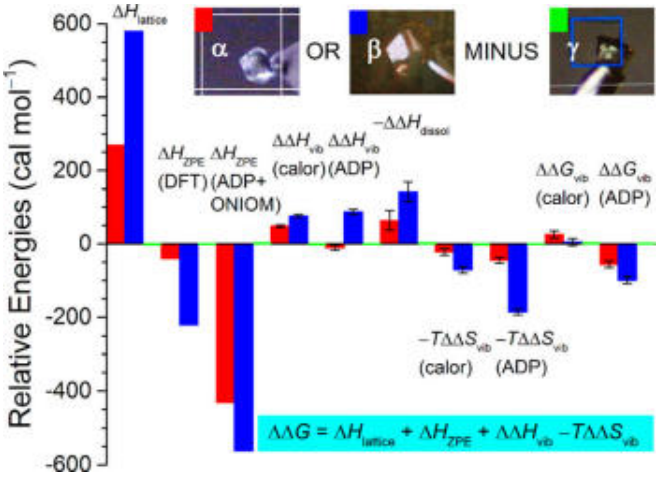
- *Quantum Crystallography*: by combining diffraction and quantum chemical calculations the scope of X-ray crystal structure determination is extended. Hirshfeld atom refinement (HAR) provides accurate anharmonic ADPs, hydrogen atom positions and their ADPs [1].



Gly–l-Ala molecule from X-ray data after HAR at the BLYP/cc-pVTZ level (left) and from neutron data (right)

- *Dynamics and Thermodynamics of Crystalline Polymorphs*. 3. γ - Glycine, Analysis of Variable-Temperature Atomic Displacement Parameters, and Comparison of Polymorph Stabilities [2].

- *Analyzing diffuse scattering with supercomputers* [3]: the interesting properties of many crystalline materials result from packing faults. The resulting diffuse scattering is interpreted in terms of atomistic models with Monte Carlo calculations and genetic algorithms (with Prof. Anthony Linden).



Differences in crystal enthalpies, entropies and free energies between α-, β- and γ-glycine from combining diffraction data with DFT and ONIOM calculations

[1] S. C. Capelli, H.-B. Bürgi, B. Dittrich, S. Grabowsky, D. Jayatilaka, *IUCrJ* **2014**. *1*, 361–379.
[2] T. Aree, H.-B. Bürgi, D. Chernyshov, K. W. Törnroos, *J. Phys. Chem. A* **2014**, *118*, 9951−9959.
[3] T. M. Michels-Clark, V. E. Lynch, C. M. Hoffmann, J. Hauser, T. Weber, R. Harrison, H. B. Bürgi, *J. Appl. Cryst.* **2013**, *46*, 1616–1625; **2016**, *49*, 713–714.

Figure 1: The current members of the group. Some former group members who contributed to the recent publications: Leonardo dos Santos, Luzia Germann, Martin Fisch, Elena Marelli

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The main research activities of the group concern the determination and analysis of the accurate electron density distribution in metal-organic materials and the investigation of molecular crystals and metal organic frameworks at high pressure.
The goal of the research is finding precise correlation between atomic or electronic structure and electric, magnetic and mechanical properties of materials.

For this research, the group uses experimental as well as theoretical methods: solvothermal synthesis and crystallization, single crystal X-ray diffraction at ambient and non-ambient conditions, optical and dielectric measurements, calculation of electronic structures in molecules and solids, modelling and analysis of the electron density distribution.
A strong cooperation exists with the material science beamline (Dr. Nicola Casati) at the Paul Scherrer Institute.

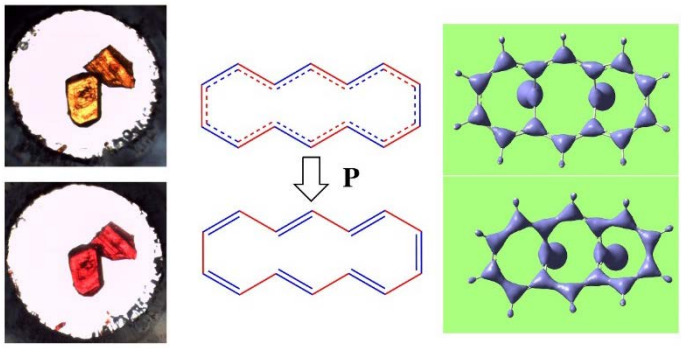
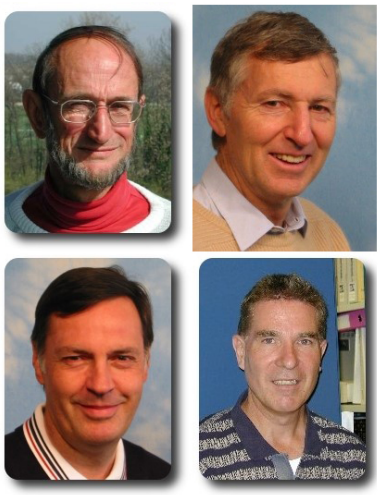


Figure 2: Breaking the aromaticity of Biscarbonyl[14]annulene at High pressure, recently published in Nature Comm. 2016, 7, 10901

Recent publications and highlights:
[1] Dos Santos, L.; Lanza, A.; Barton, A.; Brambleby, J.; Blackmore, W.; Goddard, P.; Xiao, F.; Williams, R.; Lancaster, T.; Pratt, F.; Blundell, S.; Singleton, J.; Manson, J.; Macchi, P. *J. Am. Chem. Soc.* **2016**, *138*, 2280–2291
[2] Casati, N.; Kleppe, A.; Jephcoat, A.; Macchi, P. *Nature Comm.* **2016**, *7*, 10901
[3] Lanza, A.; Germann, L. S.; Fisch, M.; Casati, N.; Macchi, P. *J. Am. Chem. Soc.*, **2015**, *137*, 13072–13078



Crystallography Competence Centre,
SB **IPSB** **LCR**
BSP - Cubotron

EPFL

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dieter.schwarzenbach@epfl.ch
web: http://ccc.epfl.ch

Dieter Schwarzenbach was offered a chair in crystallography and the creation of an Institute of Crystallography starting in the winter term of 1973. Gervais Chapuis was appointed maître assistant; he has since moved up through the levels of assistant professor (1979) and associate professor (1981) to ordinary professor (1991). In 1988 the position of a service crystallographer (chef de projet) was created and occupied by Kurt Schenk. Since 1990, we have initiated and lead a project for the construction of a beamline at the European Synchrotron Radiation Facility (ESRF) in Grenoble. This effort has developed into the Swiss-Norwegian Beamlines (SNBL) funded by the Swiss and Norwegian National Science Foundations, Swiss and Norwegian Universities, and more recently by the Swiss State Secretariat for Education, Research and Innovation. Philip Pattison has been responsible for the coordination between groups in Switzerland interested in making use of SNBL. In recent years, the Institute has been reformed as a Crystallography Competence Centre, providing a service to any groups at the EPFL and University of Lausanne interested in the characterization of materials based on X-ray diffraction. Research topics include quasicrystals, aperiodic and composite crystals and, in particular the structures of incommensurately modulated crystals. Dieter Schwarzenbach and Gervais Chapuis are now Professors Emeriti, while Kurt Schenk and Philip Pattison have recently retired.

SNBL – Planning for the next decade" Swiss-Norwegian Workshop May 28-29, 2015

The Swiss-Norwegian Beamlines (SNBL) @ ESRF

ESRF - The European Synchrotron
CS 40220
38043 Grenoble
Cedex 9
France

web:http://www.esrf.eu/UsersAndScience/Experiments/CRG/BM01/
email: dmitriev@esrf.fr

The mission of the **SNBL** is to provide scientists from both Norway and Switzerland, from both academia and industry, with increased access to synchrotron radiation. A user on SNBL has access to state-of-the-art, custom-designed instrumentation for diffraction and absorption experiments. Both partner countries have relatively large and exceptionally active scientific communities using X-ray diffraction and absorption as their main probes; for these groups the amount of public beamtime offered by ESRF was insufficient from day one, and this is the raison d'être of the Swiss-Norwegian Beam Lines at ESRF. Nowadays, it is fully understood by the scientific community that many of the most challenging problems in structural crystallography can be solved only with the use of synchrotron radiation, and even then, often enough, only by harnessing the combined power of two or more experimental techniques (such as, e.g., powder and single-crystal diffraction). The SNBL has four such different experimental techniques, which are distributed over two beamlines (BM01 and BM31). The experiments are supported by a team of seven scientists plus technical, computing and secretarial staff.

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http://www.psi.ch/les

Figure 1: Sergey Churakov

Prof. Sergey Churakov holds the Professorship of Mineralogy at the University of Bern and is the head of the Laboratory for Waste Management (LES) at the Paul Scherrer Institute. At the University of Bern the professorship carries responsibilities for leading the research group, for managing the Institute's mineralogy laboratories and for teaching mineralogy. The Competence Center for Secondary Raw Materials at the University of Bern (www.rohstoff.unibe.ch) is associated with the Mineralogy group. Current studies focus on characterization, process-optimization, and the use of secondary raw materials. The Center is known for its mineralogical and crystallographic expertise, it collaborates with geological consulting companies, industry and authorities and is responsible for powder X-ray diffraction. The Laboratory of Waste Management at the Paul Scherrer Institute is the Swiss competence center for geochemistry and multi scale radionuclide and mass transport in argillaceous rocks and cement and their applications to deep geological systems and Swiss radioactive waste repositories. The research projects at LES benefit from unique state-of-the-art research infrastructure (X-ray synchrotron, neutron source, hot laboratory, high performance computing, etc.). We study the extra-framework cation arrangement of natural zeolites (and in general of microporous materials) under different environmental conditions (temperature and humidity) by single crystal X-ray diffraction methods to understand the bonding between framework and cavity occupants and its influence on framework distortions. This basic research approach has strong bearing on application of zeolites in chemical technology and environmental remediation.

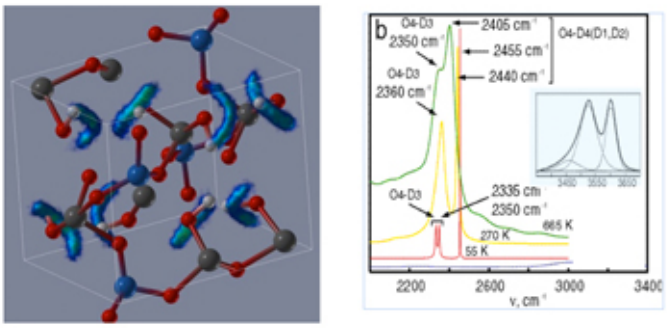

Figure 2: Thermodynamics and mobility of fluids in mineral systems, fundamental aspects of mineral surface reactivity (interaction with charged mineral surfaces, nucleation processes in confined environments)

Recent publications and highlights:

[1] Churakov S.V. (2016) Ab initio simulations of mineral surfaces: Recent advances in numerical methods and selected applications, In Highlights in Mineralogical Crystallography, Ed. Armbruster Th. and Danisi R., p. 75-108. De Gruyeter, 210 pp. ISBN 978-3-11-041704-3

[2] Churakov S.V., Labbez Ch., Pegado L., Sulpizi M. (2014) Intrinsic acidity of surface sites in calcium silicate hydrates and its implication to their electrokinetic properties J. Phys. Chem. C, 118, 11752–11762.

Schweizerische Gesellschaft für Kristallographie

Société Suisse de Cristallographie
Società Svizzera di Cristallografia
Swiss Society for Crystallography
Sektion für Kristallwachstum und Kristalltechnologie
Section de Croissance et Technologie des Cristaux

Basel 2016
ECM-30

Invitation

SGK-SSCr - Annual Assembly of the Swiss Society for Crystallography

August 31, 2016 12.00 – 14.00h

Congress Center Basel, Messeplatz 21, 4058 Basel
Room Rio (Level 2)

This invitation is valid as entrance ticket, please bring it with you to the assembly.

Swiss Crystallographic Association SGK / SSCr

General Assembly 2016

Wednesday, August 31, 2016
Congress Center Basel, Room Rio (Level 2), 12:00-14:00

Members who want to attend the General assembly and have not registered to the ECM-30, may use the invitation printed on the previous page as an entrance ticket,
VALID ONLY FOR THE SGK GENERAL ASSEMBLY

Agenda of the General Assembly 2016

The minutes of our last General Assembly (Neuchâtel, CSEM, Monday, September 14, 2015) are published on page 50-53 of the SGK/SSCr newsletter No. 96, July 2016 (this issue), which is also available electronically at http://www.sgk-sscr.ch/newsletter/

1) Determination of the quorum according to Art. 12/by-laws

2) Proposition for acceptance of the minutes of the General Assembly 2015, Neuchâtel

3) a) Annual report/Jahresbericht / le rapport annuel

   b) Annual financial statement /Jahresrechnung / les comptes annuels

   c) Budget for the next year / Aufstellung des Budgets für das kommende Jahr / le budget proposé pour l'année suivante

   Elections / Wahlen / Élections

4) a) definition of a chairperson for the elections

   b) confirmation of the present board members

   c) elections of 3 new board members
   (replacement for Petr Leiman, Jürg Schefer, Katharina Fromm).
   Already available candidates are: Dr. Antonio Cervellino (SLS, PSI) and Prof. Enrico Gannini (Solid State Physics, University of Geneva). Further nominations should be communicated to the president prior to the meeting.
   Candidates are asked for a short 1-2 minute oral presentation.

   e) election/confirmation of the auditors

5) 2017 Meeting and General Assembly: Decision on location/organizer. Proposals are most welcome!

6) PhD Prize 2017 (rules, amount)

7) Anträge von Mitgliedern
other motions of members

Additional Information:

Year	Entries to SGK/SSCr	Exits from SGK/SSCr
2012	8	8 (since July 2012)
2013	7	15
2014	11	17
2015	23	18*
2016 (as of 06.06)	2	2

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

Quorum for final decisions (Art.12, by-laws):
As per 06.07.2016, we have 201 records in our database.
They are grouped as:
- 9 of these are companies (or corporate members),
- 30 are “libraries” (incl. some “quasi-personal” members, from whom we don’t expect any fees, but to whom we are regularly sending our Newsletters);
- 162 are personal members (full: 128, students: 30, honorary: 4)
I.e. for the quorum to be able to make decisions, we should have 10% out of 171 corporate and personal members, i.e. at least 17 people.

Board Members:
see last page of this newsletter

Delegates
IUCr: P. Macchi (Bern), Radovan Cerny, Geneva
ECA: J. Schefer (PSI)
IOCG: K. Fromm (Fribourg)
ScNat: P. Macchi (automatically assigned to the acting president)

Summary SGK Finances

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

SGK Budget 2017
To be proposed at the SGK assembly 31.08.2016

Credits:	**Budgeted**
Membership dues	5'000.00
SANW reimbursement for IUCr delegate	1'500.00
SANW master students travel grants	2'000.00
SANW contribution for SGK annual meeting	3'000.00
SANW contribution for Zurich School	2'000.00
SANW contribution for PhD prize	1'000.00
Interest (est.)	100.00
Total Income	**14'600.00**
Debits:	
Membership dues to SANW	2'000.00
Annual meeting + poster prize	3'000.00
Travel Grants to Young Scientists	2'000.00
SGK support for Zurich School	2'000.00
PhD poster prize	1'500.00
IUCr delegates	2'000.00
ECA national membership dues 2017	250.00
Bank charges	250.00
Total Expenses	**13'000.00**
Income – Expenses	**1'600.00**

Revisorenbericht für die Jahresrechnung 2015 der Schweizerischen Gesellschaft für Kristallographie (SGK)

Konten:

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

Die Unterzeichneten haben Kenntnis genommen von der Jahres-rechnung der Schweizerischen Gesellschaft für Kristallographie. Die Rechnungsprüfung betrifft die Periode vom 1. Jan. 2015 bis 31. Dez. 2015. Die Unterzeichneten stellen fest, dass die Abrechnung mit den vorgelegten Belegen übereinstimmt.

Am 31. Dez. 2015 ist der Stand der Konten und der Kasse:

UBS account	15’892.54
CS account	18'278.82
Cash on hand	542.10
ScNat Credit	8’000.00
Total 31.12.2015	42’713.46

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

Ort / Datum
BERN, 11 März 2016

Unterschriften

B. Spingler
(Universität Zürich)

K. Schenk
(EPF Lausanne)

Minutes of General Assembly 2015

Neuchâtel CSEM, Monday, September 14, 2015
Schweizerische Gesellschaft für Kristallographie

Agenda:

1. Decision, if quorum is reached according to Art. 12 / by-laws
2. Acceptance of the Minutes of the General Assembly 2014 in Dübendorf
3. Reports
    a) Annual Report
    b) Auditor Report
    c) Budget 2016
    d) Regulation of the annual membership fees
4. Elections
    a) Chairperson for the elections (if required)
    b) Confirmation of the present board members
    c) Elections of 2 new board members
    d) Election of a new president out of the elected board members
    e) Election/confirmation of a new vice-president
    f) Election of a new secretary
    g) Election/confirmation of the auditors
    h) Election of the delegates to ECA, IUCR and IOCG
5. Information on the preparations for ECM-30 in 2016 (Basel)
6. Other motions of members

Minutes:

Formalities:

- The General Assembly was chaired by Jürg Schefer, President, and started at 12.30h.
- No objections against the period of notice for the invitation to this assembly, being part of Newsletter 94, despite having only 17 days instead of the required 21 days (Art. 11), which was due to problems with missing abstracts.
- The Agenda (published in the Newsletter 94) was approved unanimously by the participating 27 members.
- As keeper of the minutes Natalija van Well, PSI was elected unanimously.

Ad 1.
With 27 members being present at this assembly, the necessary quorum of 10% is reached to constitute a quorum. As per 28.08.2015 the SKG has 154 individual and 8 corporate members.

Ad 2.
The Minutes of the General Assembly 2014 in Dübendorf have been approved unanimously.

Ad 3 a)

- Three newsletters (No. 92, 93 and 94) were published. Big thanks to the secretary, Denis Sheptyakov for this.
- One board meeting with the local organizing committee ECA-30 (30.1.2015) and three program meetings for ECM-30 (5.12.2014, 30.01.2015, 08.05.2015) were performed in Bern.
- Attendance of the MAP Meeting (Natural science sub-organisation of the Swiss Academy of Science (ScNAT) by Jürg Schefer.
- Attendance at the assembly of delegates of the ScNAT:
    - 24.03.2015: Jürg Schefer (Marcel Tanner, Basel, has been elected as new president >2017)

- 05.06.2015: Antonia Neels (ScNat receives slightly increased support from the Swiss administration)
- ScNat will handle international memberships in future (i.e. ECA), but only formally It will not influence the election of the delegates.
- Next assembly of delegates will be on 23.09.2015. The new president of SGK/SSCr will attend.

- "200 Years of ScNat" started with an exhibition in Davos on 17.06.2015 (research live etc.); further 12 cities will follow.
- The following support was approved by the board:
  - Powder Diffraction School PDS 2014: CHF 1.000,00
  - Annual Meeting 2014 in Dübendorf:
    - CHF 3.000,00 (SGK/SSCr, ScNat)
    - CHF 500,00 Poster Prize for Nadja Opara
    - (Additional support received from STOE, BRUKER, Panalytical, Anton Paar)
  - Travel support
    - Two travel grants were given to three young scientists in order to present their research at international conferences:
      - A. Finelli ECM 2015 – Poster
      - Y. Sadikin, Gordon Conference – Poster
    - Jürg Schefer / Katharina Fromm: ECA annual meeting (reimbursed by ScNat)
    - Radovan Cerny / Piero Macchi: IUCr Montreal (reimbursed by ScNat)
- Commemoration of the deceased members:
  - Prof. Marc Vuagnat, member since 1969*, died on 23.03.2014
  - Prof. Hans Schmid, member since 1969*, died on 02.04.2014
  - Dr. Roland Prewo, member since 1985, died on 26.08.2014
  - PD Heinz Josef Weyer, member since 2012, died on 22.10.2014
  - Prof. Hans Wondratschek, member since 1969*, died on 26.10.2014
  - Prof. Wolfgang Hoffmann, member since 1986, died on 11.02.2015

  (* founder members of our society)
- Membership statistics
  As per 20.08.2015 SGK/SSCr has 154 individual members (thereof 21 students) and 8 corporate members. In 2014/2015 the society gained 12 new and lost 18 members. Presently, a gap in the representation of senior scientist to open.
- ECM-29 in Rovinj, Croatia, 23.08.2015 – 28.08.2015
  - 1052 participants (44 from Switzerland), 223 delegates, 761 abstracts (29 from Switzerland), 11 satellite meetings.
  - 13 student assistants for the auditorium, the registration etc.
  - Ca. 12 poster prizes given by the SIG's to ca. 30 students (for details see ECA homepage).
  - 55 bursaries to support students (given by a bursary committee).
  - John R. Helliwell has been awarded the MAX PERUTZ Prize (laudatio: http://ecanews.org/perutzprize.php).
  - Thanks to Katharina Fromm for the preparation of our booth at the ECM-29.
- The new SGK/SSCr- PhD-Prize
  This newly established prize was awarded for the first time to Dr. Dr. Arkadiy Simonov, one of the three candidates.
  - This award, given once a year (depending on the applications) comprises a certificate and CHF 1.000,00 cash.
  - Cuurently, the funding of the prize is out of the SGK/SSCr budget. Future sponsors have to be identified, i.e. support from senior members in future through increasing membership fees (CHF 50 to CHF 100) if SGK/SSCr could not provide this funding – see also 3.d.
  - The 2015 committee comprises:
    Hans-Beat Bürgi (Bern), T. Schirmer (Basel), D. Schaniel (Nancy).
  - Thanks to Hans-Beat Bürgi for his initiative at the last general assembly to establish this prize.

- Crystal growth activities
  - With the help of Hans Scheel, a letter has been sent to Prof. Sarah Springman, rector of ETH Zürich with the recommendation to improve these crystal growth activities also with the focus on the education of engineers in the technical/industrial direction. As a reaction the Materials Science Department of ETH was informed. The board has to keep track of the future actions taken by this department.
  - Based on the initiative of Enrico Giannini within the MANEP-consortium, a crystal growth workshop was held at the University of Geneva (11.06.2015) with ca. 20 participants. The intention is to better use and share the scientific knowledge and equipment at our universities. More details will be presented in the next newsletter.
- IUCr – International Union of Crystallography
  - Delegates: Piero Macchi and Radovan Cerny
    There were no new after the IUCr Meeting in Montreal to be repored.
    Piero Macchi only asks to take influence on the program of the next conference in Hydarabad/India/2017 by contacting the representatives and making suggestions.

Ad 3 b)
- Financial report 2014 presented by Piero Macchi, Treasurer
  (details have been sent to the board and the auditors)
- Full details were already published in the Newsletter No. 94.
- Reduction of the credit balance of the society by CHF 2.594,06 to CHF 37.744,97 as per 31.12.2014.
- Different activities in future should increase the credit balance of the society again.
- Financial report was approved by the auditors.
- Approval of the financial report and discharge of the board with 26 votes in favour and one abstention.

Ad 3 c)
- Budget for 2016 with a proposed loss of CHF 4.000,00 (without the reimbursement by the ECM-30 budget – CHF 4.500,00) was presented by the President
- Full details in Newsletter No. 94.
- Unanimously approval of the budget 2016.
- Thanks to the Treasurer for his efforts.

Ad 3 d)
- Discussion about the financing of the appropriate cash prize for the PhD award; no final decision was taken.
- After a lively discussion, a proposal to change the membership fees for regular individual members in 2016 to CHF 40 p.a. in 2016 has been accepted; the other membership fees remain unchanged. The board has to make such a suggestion at the next general assembly for a change of the by-laws. The final improvement has to be made by our next general assembly in Basel, 2016.

Ad 4 a)
- The assembly does not ask for a special day president for the votings.

Ad 4 b)
- Beside Denis Sheptyakov (Secretary) and Michael Henning (member), whose terms are ending, all other member of the board were reconfirmed. The president thanks them for the work done.

Ad 4 c)
- As new members of the board Petr Leimann (Lausanne) and Michael Wörle (ETH Zürich) were proposed to the members and voted in unanimously. The general assembly welcome the two new board members.

Ad 4 d)

- Jürg Schefer's term as president is ending. As new president Piero Macchi, University of Bern, was proposed to the members and voted in with 26 votes in favour and 1 abstention (himself).

Ad 4 e)
- No election or confirmation.

Ad 4 f)
- To be elected by and out of the board members.

Ad 4 g)
- As auditors Bernhard Spingler (University of Zürich) and Kurt Schenk (EPF Lausanne) were proposed and voted in unanimously by the members. The delegates thank both for their work.

Ad 4 h)
- As delegates for the IUCr, Switzerland can nominate 2 persons. Currently, Piero Macchi (Bern) and Radovan Cerny (Genève) are the delegate. They were proposed again as delegates and voted in by 26 votes in favour and one abstention.
- As delegate for the IOC (International Organisation of Crystal Growth) Katharina Fromm was proposed again and approved unanimously.
- As delegate ECA (European Crystallographic Association) Jürg Schefer (also vice president of the ECM-30 local committee) was proposed again and voted in unanimously.

Ad 5
- Information in detail about the timing and preparation of the SGK/SSCr annual meeting in Basel will be circulated in due time by the board.

Ad 6
- No further points to be discussed.

The old president thanked everyone for attending the general assembly and closed the meeting at 13.55h.

N. van Well, 14.09.2015

Excursion to the SwissFEL – ECM30, Basel

http://ecm30.ecanews.org/2016.htm

ECM-30 offers an after conference excursion to the X-ray free-electron laser. SwissFEL. The Paul Scherrer Institute is presently completing this new scientific large-scale facility. It will provide new opportunities for cutting-edge research. The SwissFEL is scheduled to go into operation at the end of 2016.

Registration fee, CHF 50.-, few places left

Program of the excursion, Sept. 2, 2016:

09:00	Departure from Basel by bus
10:15 – 10:30	Arrival at PSI (Educational Center OSGA)
10:30 – 10:50	Welcome address (OSGA)
10:50 – 13:00	Excursions on the SwissFEL site
13:00 – 14:00	Lunch at the OASE restaurant (self-service, not included)
14:00 – 14:20	Possibility to attend the PSI visitors' center PSI-Forum
14:30	Departure of the bus back to Basel
~16:00	Arrival to Basel

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Satellite Meetings of the ECM-30

PSI Powder Diffraction School PDS2016 – Modern Synchrotron Methods

Where: Paul Scherrer Institute, Villigen, Switzerland

When: **22-26 August, 2016**

Accommodation: at the PSI guest house and nearby hotels and B&B

More information and registration: indico.psi.ch/conferenceDisplay.py

Powder-diffraction methods have demonstrated an ever increasing range of applications in materials science, chemistry, physics, life sciences and engineering.

Modern synchrotron-radiation methods not only provide data of exceptional quality, but have allowed previously inaccessible experiments to be performed. Along with determining the atomic structure and the relative abundance of crystalline phases in bulk samples, information on disordered materials, microstructural features, defects and their evolution in response to external stimuli over a wide range of timescales is now possible.

The school, with an updated in-depth programme, aims at giving a broad overview of all the modern possibilities using synchrotron radiation, starting with a general theoretical introduction to the various methods and applications. Hands-on practice with selected synchrotron XRPD experiments and exhaustive analysis of the collected data are the central part of the school and will provide the student with a solid fundamental understanding of these essential and versatile experimental techniques.

Organizers:
Antonio Cervellino, PSI, Switzerland, antonio.cervellino@psi.ch
Nicola Casati, PSI, Switzerland, nicola.casati@psi.ch

Robert F. Stewart School on Electron Density and Related Properties

Where: Faculté des Sciences, Université de Lorraine, Nancy, France

When: **23-26 August, 2016**

Accommodation: at the Université de Lorraine guest house

More information and registration:
crm2.univ-lorraine.fr/lab/fr/education/congres/ecm30-congress-satellite-school/

Focus: High resolution X-ray diffraction and polarized neutron diffraction are the most relevant methods for respectively modeling charge density and magnetic moment (spin) distributions. Combining both experimental methods in a joint refinement leads to a precise spin resolved electron distributions in magnetic materials.

The aim of this School is to teach all participants the basic knowledge about paired and unpaired electron density distributions using neutron and X-ray diffraction methods

and to practice existing refinement software. This school is dedicated to electron density and its analysis with the emphasis on the combination of complementary experimental methods to enrich the electron density models leading to more complete description of the electronic behavior of crystalline solids. The school will end with a round table about application of topological analysis and electrostatic properties of a charge distribution in chemistry, biochemistry and physics. Also we will discuss the role of the spin density in material science and how to combine experimental and theoretical methods for a better electron density modeling.

Target Audience: The audience will be typically early career scientists e.g. assistant professors, post-doctoral research fellows, and graduate students of crystallography, medicinal chemistry, solid state and materials science, biochemistry, theoretical, quantum and computational chemistry.

The number of participants is limited to 50.

Organizers:
Piero Macchi, University of Bern, Switzerland, piero.macchi@dcb.unibe.ch
Mohamed Souhassou, Université de Lorraine, France, mohamed.souhassou@crm2.uhp-nancy.fr

Crystallography in the Pharmaceutical Industry Workshop

Where: Biozentrum, University of Basel, Klingelbergstrasse 70, 4056 Basel, Switzerland

When: **Sunday, 28 August 2016, 2016, 9:00–15:30h**

Registration via the ECM-30 registration page

Registration Fee: CHF 50

Download the flyer with the preliminary programme here.

This satellite meeting will cover various aspects of modern day pharmaceutical crystallography and its contribution to drug design and drug development. We will provide have an informative mix of presentations and round table discussions.

Target Audience: The audience will be typically early career scientists e.g. assistant professors, post-doctoral research fellows, and graduate students of crystallography, biology, medicinal chemistry, biochemistry, theoretical, quantum and computational chemistry.
The number of participants is limited to 80.

Organizers:
Trixie Wagner, Novartis Institutes for BioMedical Research, Switzerland, trixie.wagner@novartis.com
Carien Dekker, Novartis Institutes for BioMedical Research, Switzerland, carien.dekker@novartis.com
Sascha Gutmann, Novartis Institutes for BioMedical Research, Switzerland, sascha.gutmann@novartis.com

The CSD Python API: A Foundation for Innovation

Where: Biozentrum, University of Basel, Klingelbergstrasse 70, 4056 Basel, Switzerland

When: **Sunday, 28 August 2016, 9:30–12:30h with lunch until 13:30h**

Registration via the ECM-30 registration page

Registration Fee: CHF 20.00

The Cambridge Structural Database (CSD) is the world's repository for small molecule organic and metal-organic crystal structures. As such, this chemically diverse database of more than 800,000 structures is a highly valuable resource for structural chemistry research and education. The Cambridge Crystallographic Data Centre (CCDC) not only distribute the CSD but also provide a comprehensive set of software tools that enable the valuable structural data to be searched, analysed, visualised and explored.

This workshop will introduce attendees to the CSD Python API – a new platform providing programmatic access to the complete range of CSD data and functionality. The CSD Python API enables scientists to perform crystallographic and chemical data analysis through tailored scripts from within the Mercury interface, on the command-line or even through 3rd party software. The CSD Python API can also provide an excellent educational platform to engage undergraduates with Chemistry and Computing.

The CSD Python API workshop is ideal for researchers that have some basic familiarity with the CSD-System, but are interested in learning about more flexible and sophisticated ways to interact with CSD data and functionality; however, anyone is invited to attend. Attendees will not need to be expert in programming or scripting languages, but simply be comfortable with computer systems. Our experienced staff will be available to assist with any questions you might have and at the end of the workshop there will be an opportunity to trouble-shoot with the instructors. The instructors will remain for the duration of the ECM conference to provide any additional help and feedback that attendees might appreciate after the workshop.

The workshop is free, but all participants must pre-register through the ECM website for an administration fee of CHF 20.00.

Almost all ECM attendees will already have access to the CSD Python API through their institution's CSD-System licence, but if attendees do not already have a licence, we can provide short-term workshop licences in advance. Participants will be expected to bring along their own laptops and to have already installed the CSD-System, Python and the CSD Python API on their laptop prior to the workshop.

Organizers:
Peter Wood
CSD-System Product Manager, CCDC
wood@ccdc.cam.ac.uk
Steve Maginn
Director of User Services, CCDC
maginn@ccdc.cam.ac.uk

A Workshop on Methods in Crystallographic Computing

Where: Hotel Sonnenrain, Lossburg-Wittendorf, Germany

When: **25-28 August, 2016**

Accommodation: on site

More information and registration:
www.mrc-lmb.cam.ac.uk/harry/ecacomsig/freudenstadt.html

Following our successful Computing Schools held before ECM-28 (Warwick) and ECM-29 (Rovinj), SIG9 will hold a Workshop prior to ECM-30. The Workshop aims to bring developers together from across the main Crystallographic disciplines (Powder, Small Molecule and Macromolecular) to learn from each other and to cross-pollinate their ideas. To this end, we will have very few formal lectures with the emphasis on tutorials and small group seminars, so that methods can quickly and efficiently be propagated.

The Workshop will cover two full days and two part days - it starts on the afternoon of Thursday 25th August and finishes on the morning of Sunday 28th August. Transport will be provided between the Workshop's location and the ECM-30 site in Basel.

Organizers:
Harry Powell, MRC Laboratory of Molecular Biology, UK, harry@mrc-lmb.cam.ac.uk
Martin Lutz, Utrecht University, The Netherlands, m.lutz@uu.nl

Young Crystallographers ECM-30 Satellite Meeting

Where: Pharmazentrum, University of Basel, Klingelbergstrasse 50, 4056 Basel, Switzerland

When: **Sunday, 28 August 2016, 9:00–15:30h**

More information and registration: ecanews.
org/mwp/groups/gig-01-young-crystallographers

We would like to invite young crystallographers and early career researchers to join us at our ECM-30 satellite meeting on Sunday 28th of August, 2016. At this event, you will have the opportunity to present your work, socialise and network with your peers in an informal and friendly environment. Oral and poster presentations from all aspects of crystallography will ensure that there is something for everyone’s interests. We are looking forward to meeting you all.

Organizer:
Andrew Maloney, Cambridge Crystallographic Data Centre, UK,
maloney@ccdc.cam.ac.uk

High Data Rate MX Satellite Meeting

Where: Biozentrum, University of Basel, Klingelbergstrasse 70, 4056 Basel, Switzerland

When: **Friday, 2 September 2016, 2016, 9:00–16:00h**

Registration via the ECM-30 registration page

Registration Fee: CHF 20.00

This one-day satellite meeting will discuss issues in doing very high-data-rate macromolecular crystallography (High-Data-Rate MX). Scientists and programmers working to create methods to handle diffraction images produced by the Dectris Eiger-16M detector have recently discovered challenges. These challenges relate to speed and parallelism of reading the images, a problem that all of the software systems for data analysis must address in adapting techniques to keep pace with the rate at which diffraction images are produced. Developers and users of MX data processing software all need to consider this challenging task and adjust both software and data collection strategies appropriately.

This satellite meeting will be a follow-on to a workshop held 26-28 May 2016 at NSLS-II at Brookhaven National Laboratory and an informal session at the American Crystallographic Association meeting in Denver, Colorado in July 2016. It will be an excellent opportunity for members of the community to understand what has been done thus far to support efficient processing and to comment on what additional issues need to be considered. In addition to talks on the data formats and how they are handled in the major packages, there will be time for open discussion and recommendations for the future.

The number of participants is limited to 70.

Organizers:
Herbert J. Bernstein, Rochester Institute of Technology, USA, yayahjb@gmail.com
Robert M. Sweet, Brookhaven National Laboratory, USA, rsweet@bnl.gov
Nicholas K. Sauter, Lawrence Berkeley National Laboratory, USA, nksauter@lbl.gov

SMARTER 5 Meeting – Structure elucidation by combining Magnetic Resonance, Computational Modelling and Diffraction

Where: University of Bayreuth, Bayreuth, Germany

When: **4 - 8 September 2016**

Accommodation: Hotels in Bayreuth (for further information visit the local homepage)

More information and registration: www.smarter5.uni-bayreuth.de

Materials Science and Engineering present increasingly challenging problems to scientists dealing with the elucidation of solid-state structures due to the raising complexity and hierarchical structuring of modern materials. In particular, without access to crystals suitable for single crystal X-ray diffraction, even today, unravelling the structure of such compounds is limited.

By combining different analytical techniques, each providing complementary information, we expect to be able to significantly improve the structure solution process in such cases. Therefore, the SMARTER meeting aims at bringing together scientists in the areas of solid-state magnetic resonance and other spectroscopic techniques, diffraction as well as modelling to resolve questions about how to optimally implement information from various techniques into a general strategy for ab initio structure determination of complex materials.

The conference in Bayreuth is the latest in a series of meetings designed to encourage cross-fertilisation across subject boundaries, with invited speakers chosen to reflect the diversity of approaches required to solve demanding structural problems, such as obtaining crystal structures from powdered samples or understanding disordered systems.

Organizers:
Brad Chmelka (Santa Barbara, USA)
Andrew Goodwin (Oxford, United Kingdom)
João Rocha (Aveiro, Portugal)
Jürgen Senker (Bayreuth, Germany), juergen.senker@uni-bayreuth.de
Renée Siegel (Bayreuth, Germany), renee.siegel@uni-bayreuth.de
Francis Taullele (Versailles, France)
Jonathan Yates (Oxford, United Kingdom)

Contact for the meeting
Email: smarter5@uni-bayreuth.de

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	15.03. and 15.09.	www.psi.ch/useroffice
Protein crystallography beamlines (PX)	15.04. and 15.10.	
SINQ: Swiss Spallation Neutron Source		
All instruments (regular calls)	15.05. and 15.11.	www.psi.ch/useroffice
SINQ/SLS		
Joint x+n proposals (MS/HRPT)	15.02.	www.psi.ch/useroffice
SμS: Swiss Muon Source		
All instruments	07.12. and 12.06	www.psi.ch/useroffice
ESRF: European Synchrotron		
long term proposals	15.01.2017	www.esrf.eu/
short term proposals	10.09.2016	UsersAndScience/
ILL: Institut Laue Langevin		
All instruments	Feb., Sept.	www.ill.eu
FRM II: Heinz Maier-Leibnitz		
All instruments	06.05.2016	www.mlz-garching.de/user-office
Rapid Access program	08.07.2016	www.mlz-garching.de/user-office
SNS Spallation Neutron Source Oak Ridge	various	neutrons.ornl.gov

Calendar of forthcoming meetings

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

			Application Deadline
2016			
June 26 – July 01	Les Diablerets	Intrinsically Disordered Proteins (GRS) http://www.grc.org/programs.aspx?id=14532	July 15
Aug. 22-26	Villigen	Powder Diffraction School. Modern Synchrotron Methods https://www.psi.ch/pds2016	July 31
Aug. 28-Sept. 01	Basel	30th Meeting of the European Crystallographic Association http://ecm30.ecanews.org/ecm2016/home.html	July 6
Sept. 7-11	Rimini, Italy	Italian Crystallographic Association, 2016 International School Polymorphism, stability and phase transitions in crystals: theory, experiments, applications. http://www.aicschool2016.org/	June 12
Sept 21 – Sept 23	Berlin	2nd Meeting of the "Young Crystallographers" / "Junge Kristallographen" http://dgk-home.de/aks/jkyc/berlin-2016/	July 15
2017			
Aug. 21-29	Hyderabad, India	The XXIV Congress & General Assembly of the International Union of Crystallography (IUCr-2017) http://www.iucr2017.org	to be announced

Become a member of SGK/SSCr

If you are working in the field of crystallography, you might be interested in becoming a member of our society. For more information as well as online registration, please go to our website (http://www.sgk-sscr.ch).
Presently, the yearly membership fee is CHF 40 (CHF 10 for students).

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

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