



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

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## SGK/SSCr NEWSLETTER

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**No. 87**  
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**In this issue:** Minutes of the General Assembly of the SGK/SSCr 2012, June 21

### **On the Cover:**

The host town of the European Crystallographic Meeting ECM-30 will be Basel. The conference is scheduled for the end of August 2016 in the Kongress-Zentrum Basel.

Foto: Jean-Pierre Brog, Katharina Fromm, Claire-Lise Chanez and Jürg Schefer, presenting the bid at ECM-27 in Bergen.

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## The President's Page

### Dear members of the Swiss Crystallographic Society,

Introducing this column in our newsletter No. 70 in 2006, I never expected to write it once myself. But being elected as the new president at our last annual meeting, I am glad to take over also this obligation which is also an opportunity.

I first would like to congratulate our new members in the board of the society: Dr. Denis Sheptyakov, from *Paul Scherrer Institut*, Dr. Antonia Néels from the CSEM *Centre Suisse d'Electronique et de Microtechnique SA* in Neuchâtel and PD Dr. Tony Linden from the University of Zürich, but also the former president, Prof. Katharina Fromm. On its first meeting, the new board



in charge has appointed Prof. Macchi as vice president and Dr. Denis Sheptyakov in the double function as secretary and editor of the newsletter. I also take the opportunity to thank Prof. Walter Steurer for the huge effort he made during his long term activities in the board. He is now at the end of his term.

A first big event in front of us is the ECM-30 to be held in August 2016 in Basel. The Swiss Society for Crystallography is proud that the ECA council meeting in Bergen has approved our bid and we would like to thank all our supporters: The bid was not only backed by our society, but also by all the universities and research institutes of Switzerland. We will do everything to ensure that ECM-30 in Basel will be a successful scientific event.

Basel has been chosen as it has an excellent and very active teaching and research community, based at university institutes as well as at industrial sites and it also has a nice conference centre within the MUBA exhibition complex. The mathematician and physicist Leonhard Euler – known to all of you from the Eulerian angles - was born in this beautiful city on April 15, 1707, and you may want to visit his *Alma Mater*, just a few blocks from the conference centre.

We do not have to mention here that Basel is the centre of the Swiss pharmaceutical industry, as it hosts the world headquarters of many leading companies. Basel is also fantastically connected to Europe by a low-fare airport as well as by the railroad network of three countries. This will help the participants to partially compensate the costs caused by the (presently) strong Swiss Franc. We ask you all to spread this information at the conferences you are attending in the future.

But the main argument for Basel and Switzerland is the excellent science environment of our country and its great impact to the society. As you all daily contribute to this directly, the thanks go to everybody, and especially to our young scientists with their fantastic thesis work we always can enjoy.

With my best regards, Jörg Schefer

## International Year of Crystallography

The UN have approved year 2014 as the "International Year of Crystallography!"



*The United Nation General Assembly,*

*Recalling* Economic and Social Council resolution 1980/67 of 25 July 1980 on international years and anniversaries and General Assembly resolutions 53/199 of 15 December 1998 and 61/185 of 20 December 2006 on the proclamation of international years,

*Recognizing* that humankind's understanding of the material nature of our world is grounded, in particular, in our knowledge of crystallography,

*Stressing* that education about and application of crystallography is critical in addressing challenges such as diseases and environmental problems by providing protein and small molecule structures suited for drug design essential for medicine and public health as well as solutions for plant and soil contamination,

*Considering* that the impact of crystallography is present everywhere in our daily lives, in modern drug development, nanotechnology and biotechnology, and underpins the development of all new materials from toothpaste to aeroplane components,

*Considering also* the significance of the scientific achievements of crystallography, as illustrated by twenty-three Nobel Prizes awarded in the area, and that crystallography is still fertile ground for new and promising fundamental research,

*Considering further* that 2014 marks the centenary of the beginning of modern crystallography and its identification as the most powerful tool for structure determination of matter,

*Being aware* that 2014 provides an opportunity to promote international collaboration as part of the sixty-fifth anniversary of the founding of the International Union of Crystallography,

*Noting* the broader welcome by the crystallographic community worldwide of the idea of having 2014 designated as the International Year of Crystallography,

*Recognizing* the leading role of the International Union of Crystallography, an adhering body of the International Council for Science, in coordinating and promoting crystallographic activities at the international, regional and national levels around the world,

1. *Decides* to proclaim 2014 the International Year of Crystallography;
2. *Invites* the United Nations Educational Scientific and Cultural Organization, mindful of the provisions of the annex to Economic and Social Council resolution 1980/67, to facilitate the implementation of the International Year of Crystallography, in collaboration with Governments, the International Union of Crystallography and its associated organizations throughout the world, relevant organizations of the United Nations system, the International Council for Science, as well as other relevant non-governmental organizations, also invites the United Nations Educational Scientific and Cultural Organization to keep the General Assembly informed of progress made in this regard, and stresses that the costs of all activities that may arise from the implementation of the present resolution above and beyond activities currently within the mandate of the lead agency should be met from voluntary contributions, including from the private sector;
3. *Encourages* all Member States, the United Nations system and all other actors to take advantage of the Year to promote actions at all levels aimed at increasing awareness among the public of the importance of crystallography and promoting widespread access to new knowledge and to crystallography activities.

*121st plenary meeting  
3 July 2012*

***UN-document***, *Sixty-sixth General Assembly, Plenary, 121<sup>st</sup> Meeting (AM)*:  
[http://www.un.org/ga/search/view\\_doc.asp?symbol=A/RES/66/284](http://www.un.org/ga/search/view_doc.asp?symbol=A/RES/66/284)

## **News for and from members**

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

#### **Personal members**

PD Dr. Heinz Josef Weyer  
(SwissFEL, Paul Scherrer Institut, 5232 Villigen PSI, Staff scientist)

Dr. Nicola Casati  
(Swiss Light Source, Paul Scherrer Institut, WLGA-229, Villigen PSI, Post-Doc)

Dr. Xavier Maeder  
(CSEM, 2002 Neuchâtel, Post-Doc)

Dr. Daniel Renciuik  
(Inorganic Chemistry, University of Zurich, 8057 Zürich, Post-Doc)

Jun Xu  
(Organisch-Chemisches Institut, Universität Zürich, 8057 Zürich, PhD).

Yolanda Sadikin  
(Laboratory for Crystallography, Université de Genève, 1211 Genève, PhD)

#### **Missing addresses** (with affiliation)

- Evans Shaun Russel, Chemistry and Biochemistry Departement, Bern
- Sebastian Basso, Laboratoire de Cristallographie, EPF Lausanne
- Dr. Donat Jozsef Adams, Gentilly, France

Please report new contact address to the secretary of the society,  
Denis.Sheptyakov@psi.ch  
Thanks.



## **Stellenausschreibung**

Wissenschaftler/in im Bereich Kristallographie (100%) wird momentan bei dem Departement für Chemie und Angewandte Biowissenschaften der ETH Zürich gesucht. Bei Interesse, wenden sie sich auf die Website:  
<http://internet1.refline.ch/845721/2222/++publications++/1/index.html>

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

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

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

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

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

Details for applications are given at:

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

## **ECA - New General Interest Group for Senior Crystallographers** (GIG of the European Crystallographic Association ECA)

Contributed by Svend Erik Rasmussen (Aarhus), ser@geo.au.dk

The European Crystallographic Association approved a new GIG, General Interest Group Senior Crystallographers.

Chair: Hans Beat Bürgi, University Bern (hans-beat.buergi@krist.unibe.ch)  
Co-Chair: Paul Beurskens, University Nijmegen (ptbeurskens@hetnet.nl)  
Secretary: open

This new GIG comes together to preserve the history of crystallography, the archive of materials, to play a part in teaching, consider special requirements of senior scientists and any other business connected and concerned to senior crystallographers. A scientist who is over 65 and retired is recognised as in this category.

The GIG for senior crystallographers would like to have a room at the ECM meetings where they can get together, and carry out all initiatives organized by this community. Senior crystallographers might, for instance, offer seminars on "who is who" in crystallography, the group could also arrange formal and informal sessions on the history of crystallography. It has been promoted by Svend Erik Rasmussen (Aarhus), Theo Hahn (Aachen) and Paul Beurskens (Nijmegen).

Old and still active crystallographers might also like to draw attention to the following matters:

- Readability of conference programmes and abstract books could be improved by the use of not too small font sizes and by avoiding the use of low contrasts such as using black print on grey or red backgrounds.
- Audibility of oral presentations would be facilitated by making sure that equipment for Tele coils and FM in auditoria is activated if available. Ideally, such facilities should be standard equipment.
- Conference buildings with as few stairs as possible should be chosen for future meetings.
- Some of the disabilities that inevitably follow with increasing age may also strike younger people and it might be of interest to know if young colleagues are actually prevented from attending meetings because of disabilities.

As in Europe the age average of crystallographers, and scientists in general, is increasing it may not be unreasonable to expect that the number of senior crystallographers may increase at future conferences.

# Report on the Annual Meeting of the Swiss Society for Crystallography held at the ETH Zürich, June 21, 2012

Contributed by Tony Linden, alinden@oci.uzh.ch

The annual meeting of the Swiss Society for Crystallography was held jointly with that of the Swiss Physical Society. 48 SSCr registrants along with some of the over 550 from the SPS enjoyed scientific sessions focussing on a historical review of some of the milestones in crystallography since the first diffraction patterns were observed 100 years ago in 1912. Dieter Schwarzenbach presented a plenary lecture where he described the initial experiments of Max von Laue and his team. The discovery of diffraction was revolutionary as it provided a method to study the geometry of matter at atomic resolution and opened up field of crystallography that is so essential today. Dieter further described some of the fundamental notions about structure determination that were worked out within the first 10 years. Some key events like methods for structure solution were critical, but also important was the development of instrumentation and computers to do the calculations which can today be accomplished in a few seconds, compared with the years of hand calculations done in the early days. Dieter closed with some remarks about some of the specialist areas of crystallography, such as the study of aperiodic and quasi crystals and charge densities.

This was followed by a very well attended joint microsposium on "100 Years of Diffraction". Michael Glazer enthralled us with details of lives of the Braggs, from their time in Australia, the insight leading to the deduction of Braggs Law and their later scientific activities. Jost Lemmerich described the life of Max von Laue, his later life and his interaction with many prominent colleagues of his time. Larry Falvello focussed on the origins and development of macromolecular crystallography, the key people involved in the early years, such as Astbury, Bernal, Hodgkin, Bragg, Pauling, Kendrew & Perutz, to name just a few, and the rapid rise in the number of macromolecular structure determinations being conducted today. Ton Spek rounded off a fascinating session by describing the life of Bijvoet and the development of the use of anomalous dispersion to determine absolute structure.

The final session of the afternoon focussed on current and new developments in crystallography. There was strong interest in the progress with the SwissFEL, the upgraded materials science beamline at the SLS, new methods for investigating disordered systems, high resolution X-ray diffraction applications and a status report on SINQ. These were supplemented by interesting talks on the use of charge flipping for structure solution from powder diffraction data, nanosized intercluster compounds and Brazil twinning in quartz.

The day finished with an evening poster session, where 12 interesting, well presented SSCr posters could be viewed – congratulations to Laure Guenée, Geneva, on winning the poster prize kindly sponsored by ScNAT. Those hardy souls who remained for the grill party afterwards were treated to a very spectacular thunderstorm!

*With thanks to the following sponsors for their generosity*



## Conference report: ECM 27 European Crystallographic Meeting, Bergen, Norway

Contributed by Dubravka Šišak,  
PhD student in the group of Lynne B. McCusker and Ch. Baerlocher,  
Laboratory of Crystallography, ETH Zurich

When Max von Laue conducted his first experiments with X-rays and crystals, their enormous impact on the field of crystallography and science in general could not be predicted. A century later, the anniversary of his work was celebrated in Bergen (6-11 August, 2012), at the 27<sup>th</sup> European Crystallographic Meeting. The size and the scope of the field that grew out of Laue's results was reflected in 47 microsymposia, distributed over 5 focus areas:

FA1 Biological and macromolecular crystallography

FA2 Materials and minerals

FA3 Physical and fundamental crystallography

FA4 Chemical crystallography

FA5 Experimental and computational techniques

Perhaps traditional and subjective view of the Meeting was that only small fraction of the topics dealt with the basic crystallographic problem, *ie* the phase problem. Admittedly, more than 70 years have passed since A. Patterson suggested the first systematic approach to the problem, and many more methods have been devised since, but nevertheless, difficulties still do occur. This is especially obvious in the cases of limited data resolution, incomplete data or reflection overlap, arising from the sample (*e.g.* macromolecules) or the technique (*e.g.* powder diffraction, XPD). However, many microsymposia did cover technical advances in overcoming these pitfalls (*e.g.* sample preparation, crystal growth, development of synchrotrons and detectors) or successful application of known approaches.

In comparison, improvements in algorithms for structure determination appeared to be quite limited. As seen through the eyes of a powder diffractionist, contributions dealing with structure determination from XPD data, in particular seemed to be more application work and overviews than method development. The subject was first addressed in the keynote lecture given by M. Tremayne. In the broad overview she covered the basic problems that occur with XPD data, and several classical approaches to overcome them. In particular, new developments in genetic algorithms and their application to molecular crystals were discussed. Although the achievements presented in this overview could have implied that structure determination from XPD data is almost a matter of routine, several subsequent lectures indicated the contrary.

Greater demands on XPD data imposed by complex structures (*e.g.* zeolites) has resulted in the development of non-routine approaches. Rather than improving a particular structure solution algorithm, the focus seemed to be shifted towards combining techniques. The fruitful combination of XPD and electron microscopy techniques (EM) was presented by L. B. McCusker, followed by lectures about the successful application of this approach to germanosilicates (K. Inge), porous silicates (X. Zou) and petrology (M. Gemmi). In addition to this "combinatory" technique, two lectures concerning structure determination from XPD data exclusively were given by D. Xie, who presented his 2D-XPD algorithm using charge flipping, and J. Rius, who introduced advances in TALP, a direct-space method program.

While some approaches (XPD+EM, 2D-XPD) are successful in the *ab initio* structure solution of inorganic compounds, the genetic algorithm and direct-space method approaches are particularly suitable for molecular crystals, if the molecular structure is known. However, in some cases, these structures need to be solved *ab initio*. The personal contribution of the author (D. Šišak) involved addressing such cases by applying and modifying the charge flipping algorithm incorporated in program *Superflip*. In the first step it was shown that the optimal values of input parameters can improve the solutions (inorganic compound, ZrPOF-q1), but cannot make an unsolvable structure solvable (organic compound, D-ribose). The following step addressed the problem of D-ribose by introducing "custom-made" starting phases. While the aforementioned XPD+EM strategy derives such phases from the EM experiment, this approach uses phase sets derived from an approximate structure. The construction of such a structure was done by optimizing a flexible molecule (chain) in direct space. The phases were then coupled with a re-optimized set of input parameter in *Superflip* and a number of fully interpretable solutions (*ca* 10 %) were thereby produced. However, identifying those maps in the 200 solutions generated turned out to be non-trivial.

As the tools provided in *Superflip* (convergence *R* value, consistency of symmetry, peakiness) proved to be unreliable as evaluation criteria in this case, two other approaches were investigated. Reasoning that the good solutions would be similar, two cluster analyses, one based on the comparison of electron density maps and the other on the comparison of phase sets were put to the test, but did not yield useful results. Then, the ranking of the solutions based on their entropies was tried and resulted in comparably good correlation. In the cases where the solution selected on the basis of its entropy was not fully interpretable, it was shown that adding and averaging several maps with low entropy resulted in either a fully interpretable map, or a phase set that could be used for further recycling in *Superflip*. Such a recycling procedure generated over 50 % correct solutions. As both approximate structure approach and the entropy-based evaluation seemed to be promising, they were applied to several known and unknown structures and yielded successful results.

More than 70 years of the phase problem has left a rich legacy of algorithms, approaches and equations, so the importance of keynote lectures and historical overviews should not be underestimated (S. Parsons, D. Swarzenbach). The modification, combination and application of these "old" ideas can be inspiring and successful.

Although this report is based on rather traditional views (and expectations) of X-ray crystallography, perhaps one of the most exciting aspects in this field is at the extreme, where the "phase problem" is solved without a crystal or diffraction data. One of the mycosymposia, dedicated exclusively to the developments in structure prediction of crystalline and amorphous materials attracted not only the personal curiosity of the author, but also indicated one of the exciting directions that is being pursued after 100 years of conventional X-ray crystallography.

The author thanks the SGK for the financial support for the trip to Bergen.

**Minutes of the General Assembly 2012**  
**ETH Höggerberg, Chemistry Building HCI J6**  
**June 21, 2012**

**Agenda**

Published in the SGK/SSCr Newsletter No. 86, page 46

The minutes of our last General Assembly (2010) available at  
<http://www.sgk-sscr.ch/Newsletters/SGK-News-81.pdf>.  
Correction: Year is 2011, issue is 85

- 1) Welcome by the vice president, J. Schefer
- 2) Election of a keeper of the minutes (Protokollführer)  
A. Linden
- 3) Opening of the General Assembly 2012  
Meeting opened 11.55, ETH HCI J6, Chair J. Schefer,  
Apologies K.Fromm (business travel, US)
- 4) Feststellung der Beschlussfähigkeit gemäss Art. 12/by-laws:  
Members June 1, 2012: 139 regular, 18 students, 6 companies  
157 personal members = 10% equals to 16 persons for quorum  
31 members are present – the quorum is reached.
- 5) Antrag auf Genehmigung der Minutes General Assembly 2011, Bern  
The minutes are published on page 12-16 of the SGK/SSCr newsletter  
No. 85, Dec. 2011  
Approved unanimously.

Only remark: made to item 8 that the poll of members concerning the ECM bid (different option to Basel) had not been carried out. The president apologizes for this. The board apologizes for not to carry out this poll. The reason was the lack of manpower to present a full bid for different locations.

- 6) Approval of the agenda for the Assembly 2012  
Approved unanimously
  - a) Jahresbericht  
le rapport annuel
  - b) Jahresrechnung  
les comptes annuels
  - c) Aufstellung des Budgets für das kommende Jahr/  
le budget proposé pour l'année suivante
  - d) Festsetzung des jährlichen Mitgliederbeitrages/  
le montant de la cotisation annuelle  
*Antrag des Vorstandes : wie bisher (CHF 30/regular und CHF 10/students)*

**e) Wahlen/Elections:**

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

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

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

**A. Jahresbericht 2011 - Activities in 2011 - Résumé**

The annual meeting in Bern in September, organized by Piero Macchi and Thomas Armbruster.

It was again a big success, especially in terms of young participants and the cross-over to mineralogy. Three poster prizes were given to young scientists. The 2013 Meeting to be planned in Como, together with the Italian Crystallographic Society.

In a cross-over to chemistry and its International Year of Chemistry 2011, we participated in the organization of the Fribourg Chaim Weizmann Lectureship, given to Nobel Prize Winner Ada Yonath. The Israeli crystallographer received this lectureship for her contributions on the crystal structure and functioning of the Ribosome. Some 300 participants, mostly students, came to her lecture in Fribourg on March 21st.

SGK/SSCr has also put together an application, trying to bring the European Crystallography Meeting to Switzerland in the medium future. An application will be submitted in 2012 (first refused in 2011, went to Rovinj, Croatia)

The Society has published three newsletters and supported young scientists in terms of travel grants, poster prizes and financial support for the school of crystallography.

## Conferences and Courses

The SSCr supported the Crystallography School in Zurich, "Bring your own crystals", organized and hosted biannually by our member Tony Linden at the University of Zürich. 21 students participated with financial and scientific support from SGK/SSCr.

The annual meeting took place in Bern in September 2011. Nine international and national speakers presented their research in front of ca. 80 participants, out of which many young scientists. More than 22 posters were presented by young scientists. Three poster prizes for the best contributions were given to young scientists.

Three travel grants were given to three young scientists in order to present their research at international conferences Yvens Cheremond (Fribourg), Abita Chimpri (Bern), Volodymyr Svitlyk (Grenoble)

Piero Macchi was our representant at the IUCr meeting in Madrid in August 2011 where he participated also in the ECA-annual meeting.

## ECA

The ECA regularly provides financial support to schools within the ECA region, including Europe, as well as Africa and the Middle-East (typically in recent years 7000 Euros per annum overall as student bursaries).

The sixth Max Perutz Prize of the European Crystallographic Association goes to Professor Hartmut Fuess from the Department of Materials Science at the University of Technology in Darmstadt (Germany).

## Support from ScNat 2011

<b>Mittel für</b>	<b>ScNat-Rubrik</b>	<b>Beitrag</b>
Jahrestagung	Organisation von Anlässen	<b>2'500</b>
Publikationen	Printprodukte zur Wissensverbreitung	<b>0</b>
Nachwuchsförderung	Organisation von Anlässen	<b>500</b>
	Reisekostenbeiträge an Dritte	<b>1'500</b>
Reise-und Werbungskosten (inkl. 2'500 für ECM Bid in Bergen)	Organisation von Anlässen	<b>5'000</b>
Mitglied ECA	Mitgliedschaften	<b>120</b>

## B. Jahresrechnung 2011

### Jahresrechnung 2011

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



Approved:	31
Not-approved:	0
Abstention:	0

Der Vorstand wird entlastet.

### C. Budget 2012

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

In favour: 31, Not-approved: 0, Abstention 0 votes.  
The budget 2012 is approved.

### D. Annual Membership Fees

No change (30CHF regular, 10 students).  
Approved by the general assembly.

### E. Elections and Votings

After 10 years, Prof. Walter Steurer comes to the end of his long-time membership in the board of our society, where he was a member from 2002 to 2012. We would like to thank him for his work within this time. From 2006 to 2009, he was leading the board. A great thank from all our members!

A second member leaving us is Prof. M. Schiltz. He is now heading the National Science Foundation of Luxemburg. We also would like to thank him for his work and wish him the best in this new position in his home country.

The assembly agrees to make block-votings.

**1) Elections, present members:**

K. Fromm, J. Schefer, P. Macchi , C. Besnard, M. Hennig  
In favour: 31, Not-approved: 0, Abstention 0 votes.

**2) New members:**

Anthony Linden, Zürich  
Antonia Neels, Neuchâtel  
Denis Sheptiakov, PSI  
In favour: 31, Not-approved: 0, Abstention 0 votes.

We welcome our three new members in the board.

**3) President**

Jürg Schefer, PSI Villigen  
In favour: 31, Not-approved: 0, Abstention 0 votes.

**4) Auditors**

Ch. Bärlocher, K. Schenk  
By acclamation.

**F. New Art. 6 of our by-laws**

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

After some discussion on legal aspects, especially the reliability with losses/gains by organizing such a big conference like ECM-30, the voting was as following:

In favour: 29, Not-approved: 0, Abstention 2 votes.

New Art 6 is approved

**G. Bid for ECM-30, 2016 Basel**

ECM-30, Kongresszentrum Basel (bei der Mustermesse Basel)

SGK/SSCr will bid at the ECM Meeting in Bergen

Window for start of conference:

Present time window for the conference should be within the last weeks of August 2016, with no known overlaps to other major conferences in our science field.

Some discussion of budget/costs.

Some discussions came up on the budget and costs of the conference. As a positive point it was noted that the location is easy and relatively inexpensive to get to from major ECA countries, due to good train/flight connections. This

balances the additional cost of registration and accommodation for a meeting in Switzerland.

Discussion on whether or not an e-mail vote from all SSCr/SGK members was required to approve such a substantial undertaking / financial risk (as noted in the minutes of the 2011 Assembly)

**Vote 1:**

on if we want to make a bid and do an e-mail ballot of whether Basel should be the site: 1 for, 30 against.

**Vote 2:** on if we want to have Basel as the location: majority approved

**Vote 3:** on if we should bid in Bergen for Basel as the host of ECM-30:

For: 26, against: 5, abstention 5 votes.

We will bid for ECM-30 to be held 2016 in Basel.

Any other business? None

Meeting closed 12.45

The new president thanks for attending the meeting.

## 6<sup>th</sup> Max Perutz Prize

(<http://ecm27.ecanews.org/home/34-max-perutz-prize-to-prof-hartmut-fuess.html>)



The sixth Max Perutz Prize of the European Crystallographic Association goes to **Professor Hartmut Fuess** from the Department of Materials Science at the University of Technology in Darmstadt (Germany).

Hartmut Fuess is recognized for his outstanding contributions to structure research of functional materials such as zeolites, fuel cells, and magnetic materials, the construction of scientific instruments at large-scale synchrotron and neutron facilities and the skilled and enthusiastic service to crystallography in Europe and the broader international community.

## 5<sup>th</sup> Erwin Felix Lewy Bertaut Prize

(<http://ecm27.ecanews.org/home/36-bertaut-prize-goes-to-dr-pavel-afonine.html>)



The Fifth Erwin Felix Lewy Bertaut Prize of the European Crystallographic Association (ECA) and European Neutron Scattering Association (ENSA) is awarded to **Dr. Pavel V. Afonine** from the Lawrence Berkeley National Laboratory, Berkley, USA.

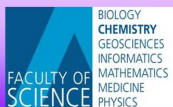
Dr Pavel Afonine is recognised for his notable work on the theoretical and methodological aspects of X-ray and neutron macromolecular crystallography. In particular he has developed software to use neutron diffraction data in combination with or separately from X-ray diffraction data.

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# Recent publications of our members: IUCr Poster Prize at the ECM-27

We congratulate Claire-Lise Chanez for receiving the IUCr poster prize at ECA-27. The prize has been presented to her by the former ECA president, Prof. Santiago Garcia-Granda at the closing ceremony in Bergen. ([http://www.ecanews.org/figures/Poster\\_Prizes\\_ECM27.jpg](http://www.ecanews.org/figures/Poster_Prizes_ECM27.jpg)).

## Multi-topic precursors for mixed-metal oxides



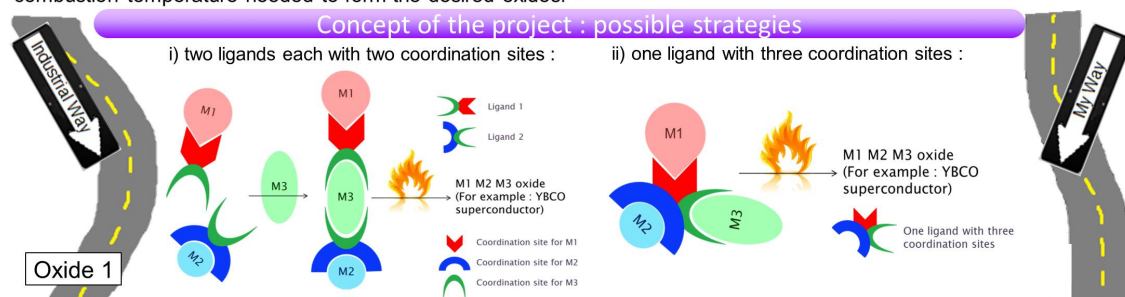
Claire-Lise Chanez, Katharina M. Fromm\*

[claire-lise.chanez@unifr.ch](mailto:claire-lise.chanez@unifr.ch), [katharina.fromm@unifr.ch](mailto:katharina.fromm@unifr.ch)

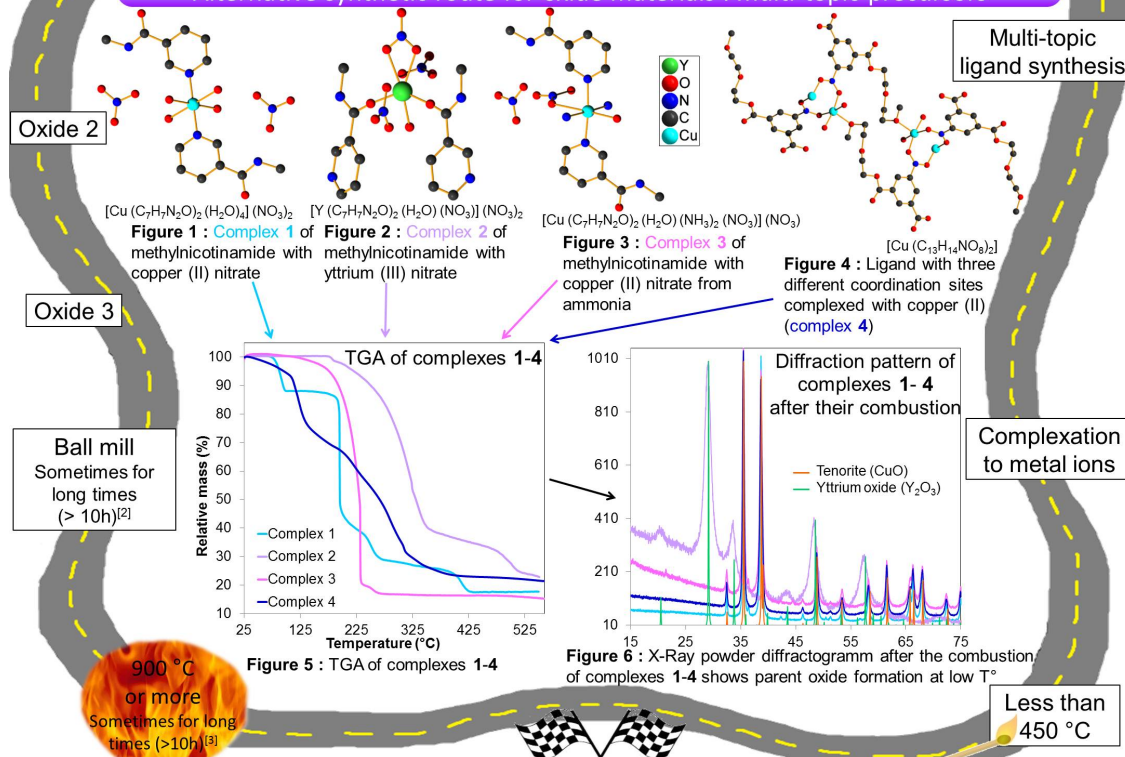
### Introduction

Oxides are increasingly used for example in ceramics, pigments, anodes, batteries or high- $T_c$  superconductors. The actual synthesis of mixed-metal oxides (left road) cost a lot of energy due to the high temperatures needed to form the oxides ( $> 900^\circ\text{C}$ ). Our goal is to obtain the same mixed-metal oxides at relatively low temperatures (less than  $450^\circ\text{C}$ ) by using precursors (right road) which organize the metal ions in the space. This preorganization should decrease the combustion temperature needed to form the desired oxides.<sup>[1]</sup>

### Concept of the project : possible strategies



### Alternative synthetic route for oxide materials : multi-topic precursors



### References :

- [1] F. Gschwind, O. Sereda, K. M. Fromm, Multitopic Ligand Design : A concept for Single-Source Precursors, *Inorg. Chem.*, **48**, 10535, 2009.
- [2] B. D. Fahlan, Superconductor Synthesis-An Improvement, *J. Chem. Educ.*, **78** (9), 1182, 2001.
- [3] L.B. Kong et al., Preparation of  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  ceramics via a high-energy ball milling process, *Mat. Lett.*, **50**, 108, 2001.

### Acknowledgements :

The authors thank the Swiss National Science Foundation, the University of Fribourg and Frimat for generous funding.



## **Call for nominations for the ECA Perutz Prize 2013**

The European Crystallographic Association is pleased to announce the Seventh Max Perutz Prize, that will be awarded in recognition of meritorious achievements in any branch of crystallography to an individual scientist clearly affiliated with the ECA.

The nominator must indicate briefly why the candidate is nominated and may include matters such as publication record and impact of their research in the scientific community. However, the uniqueness of their pioneering contributions and the usefulness of the nominee's work will be of prime consideration to the selection committee.

The winner receives the award at the official opening of the following ECM and presents a lecture at this occasion.

More information can be found at <http://www.ecanews.org/ecaprize.php>

Nominations are now open and will close on March 8th 2013.

Nominations must be sent to the ECA Secretary at the address: [secretary@ecanews.org](mailto:secretary@ecanews.org)

## Walter Petter, 1926 - 2012



When Walter Petter passed away at his home in Zürich on 21 September 2012, his 86<sup>th</sup> birthday, the Swiss crystallographers lost a great teacher, an unselfish and dear friend always ready to serve the common good. He died suddenly in apparently good health.

Walter was born and raised in Mannheim (D). He was just old enough to be drafted into the German army at the end of World War 2, be captured by the victorious Russians and return home unscathed. In 1953, he earned a Diploma (masters degree) in Physics at the University of Karlsruhe. The award of a Humboldt fellowship enabled him then to enter the ETH in Zürich, where he joined the *Institut für Experimentalphysik* of Paul Scherrer. He served as teaching assistant supervising physics experiments for undergraduate students, where I first met him in 1957. He was clearly the most popular assistant, and the students were trying hard to be assigned to experiments supervised by him. He then transferred to the *Institut für Kristallographie und Petrographie* (IKPETH) directed by Fritz Laves, where I met him again in 1959. We were to remain lifelong friends. Still being himself a graduate student, he was the mentor, scientific authority, and also sort of older brother for many graduate students and collaborators of the IKPETH, helping them, discussing their scientific issues with them, kind, unassuming, honest, capable and rigorous. In modern parlance, it may be said that he sold himself below his true scientific value: he was keenly interested in science and published well-cited papers, but he did not care for the competition based on publication and citation records, spending his time and sharing his knowledge unreservedly with everyone. Human relations were as important to him. Thus, he not only organized the *Röntgenkurs* (in the 1960s a practical course on the use of diffraction cameras, later also on structure determination), he also organized the *Fondue* at the end of the week. In 1967, he evaluated the first 4-circle diffractometer of IKPETH and was thereafter responsible for its operation, producing superb intensity data sets. During the summer of 1974, he helped the fledgling *Institut de cristallographie* of the University of Lausanne to get off the ground. The success of the 3<sup>rd</sup> European Crystallographic Meeting in Zürich in 1976 owed much to Walter's efforts on finances, book of abstracts, excursion and banquet. Walter has also well served the Swiss Society for Crystallography as secretary (1983 - 1985). At the ETH-Z, he became *Oberassistent* in 1969, and was promoted *wissenschaftlicher Adjunkt* and titular professor in 1980.

Walter was a remarkably cultivated man. He loved classical music, concerts and operas. After his retirement from ETH-Z, he studied musicology and Japanese at the University of Zürich, seriously as ever. He was an expert in enology, and a fine connoisseur of the wines from his native *Rheinland-Pfalz*. He liked to walk long distances, *e.g.* the Jura mountains from Basel to Geneva. The students whom he taught over several decades and his many friends will remember him dearly and are grateful for the privilege to have known him.

Dieter Schwarzenbach

## Calls for proposals

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

<b>Facility</b>	<b>Deadline(s)</b>	<b>Link</b>
<b>SLS: Swiss Light Source</b> All except PX lines Protein crystallography beamlines (PX)	March 15, Sept. 15 Feb. 15, June 15, Oct. 15	<a href="http://www.psi.ch/useroffice">www.psi.ch/useroffice</a>
<b>SINQ: Swiss Spallation Neutron Source</b> All instruments (regular calls)	May 15, Nov. 15	<a href="http://www.psi.ch/useroffice">www.psi.ch/useroffice</a>
<b>SINQ/SLS</b> Joint powder instrument (MS/HRPT)	Feb. 15, 2013	<a href="http://www.psi.ch/useroffice">www.psi.ch/useroffice</a>
<b>S<math>\mu</math>S: Swiss Muon Source</b> All instruments	Dec. 5	<a href="http://www.psi.ch/useroffice">www.psi.ch/useroffice</a>
<b>ESRF: European Synchrotron</b> All instruments, long term proposals All instruments, short term proposals	Jan. 15 March 1, Sept. 1	<a href="http://www.esrf.eu">www.esrf.eu</a> <a href="http://www.esrf.eu">www.esrf.eu</a>
<b>SNBL: Swiss Norwegian Beam Line</b>	March 1, Sept. 1	<a href="http://www.esrf.eu/UsersAndScience/Experiments/CRG/BM01/">www.esrf.eu/ UsersAndScience/ Experiments/ CRG/BM01/</a>
<b>ILL: Institut Laue Langevin</b> All instruments	Feb. 15, Sept. 15	<a href="http://www.ill.eu">www.ill.eu</a>
<b>FRM II: Heinz Maier-Leibnitz</b> All instruments	Jan. 25, 2013	<a href="http://user.frm2.tum.de">user.frm2.tum.de</a>
<b>SNS Spallation Neutron Source</b> Oak Ridge	March 6, 2013	<a href="http://neutrons.ornl.gov">neutrons.ornl.gov</a>



## Calendar of forthcoming meetings

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

			<b>Abstract Deadline</b>
<b>2012</b>			
Nov. 18-23	Sydney Australia	SAS'2012: International Small Angle Scattering Conference <a href="http://www.sas2012.com/">http://www.sas2012.com/</a>	in the past
Nov. 19-22	Prague Czech Rep.	Polymorphism and Crystallization <a href="https://www.scientificupdate.co.uk/conferences/conferences-schedule/register/89-Polymorphism-and-Crystallization.html">https://www.scientificupdate.co.uk/conferences/conferences-schedule/register/89-Polymorphism-and-Crystallization.html</a>	in the past
Nov. 27-29	Villigen CH	PSI Powder Diffraction School <a href="http://www.psi.ch/pds2012">http://www.psi.ch/pds2012</a>	N / A
			<b>Abstract Deadline</b>
<b>2013</b>			
January 21-25	Stoos CH	7 <sup>th</sup> Int. Symposium – Hydrogen and Energy, <a href="http://www.empa.ch/h2e-symposium">www.empa.ch/h2e-symposium</a>	Oct. 10, 2012.
January 23-25	Grenoble France	International Workshop on Single-Crystal Diffraction with Polarised Neutrons (Flipper 2013) <a href="http://www.ill.eu/flipper2013">http://www.ill.eu/flipper2013</a>	Nov. 30, 2012.
March 10-15	Regens- burg, DE	DPG-Frühjahrestagung, Condensed Matter Research <a href="http://www.dpg-physik.de/veranstaltungen">http://www.dpg-physik.de/veranstaltungen</a>	
March 19-22	Freiberg DE	21. Jahrestagung der Deutschen Gesellsch. für Kristallographie, <a href="http://www.dgk-conference.de">http://www.dgk-conference.de</a>	to be announced
April 14-19	Washington DC, USA	ARRS 2013 – Meeting of the American Roentgen Ray Society	to be announced
June 9-22	Zurich CH	The Zurich School of Crystallography 2013 <a href="http://www.oci.uzh.ch/group.pages/linden/zsc">http://www.oci.uzh.ch/group.pages/linden/zsc</a>	Jan. 15, 2013
July 2-5	Lucerne CH	4 <sup>th</sup> European PEFC & H <sub>2</sub> Forum <a href="http://www.efcf.com/">http://www.efcf.com/</a>	to be announced
July 2-7	Diablerets CH	Gordon research conference on Electron Distribution and Chemical Bonding, <a href="http://www.grc.org/programs.aspx?year=2013&amp;program=elecdist">http://www.grc.org/programs.aspx?year=2013&amp;program=elecdist</a>	
July 7-12	Moscow Russia	17 <sup>th</sup> International Zeolite Conference <a href="http://www.izc17.com">http://www.izc17.com</a>	to be announced
July 7-12	Marseille France	18th European Symposium on Organic Chemistry (ESOC 2013) <a href="http://esoc2013.eu/">http://esoc2013.eu/</a>	to be announced
Aug. 25-29	Warwick UK	European Crystallographic Association, ECM-28 <a href="http://ecm28.org">http://ecm28.org</a>	
Sept. 9-13	Como Italy	Joint Annual Meeting of the Swiss and Italian Crystallographic Societies	to be announced

**2014**

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

**2015**

To be fixed	Rovinj	ECM-29 2015	to be announced
	Croatia	<a href="http://www.ecm29.org">http://www.ecm29.org</a>	

**2016**

21-25. Aug	Basel	European Crystallographic Association, ECM-30	to be announced
	CH	<a href="http://www.ecm30.org">http://www.ecm30.org</a>	

**2017**

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

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

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



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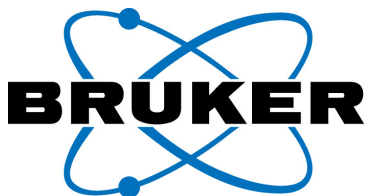
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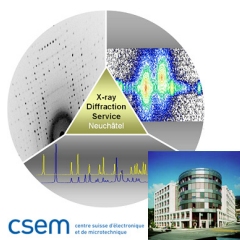
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