



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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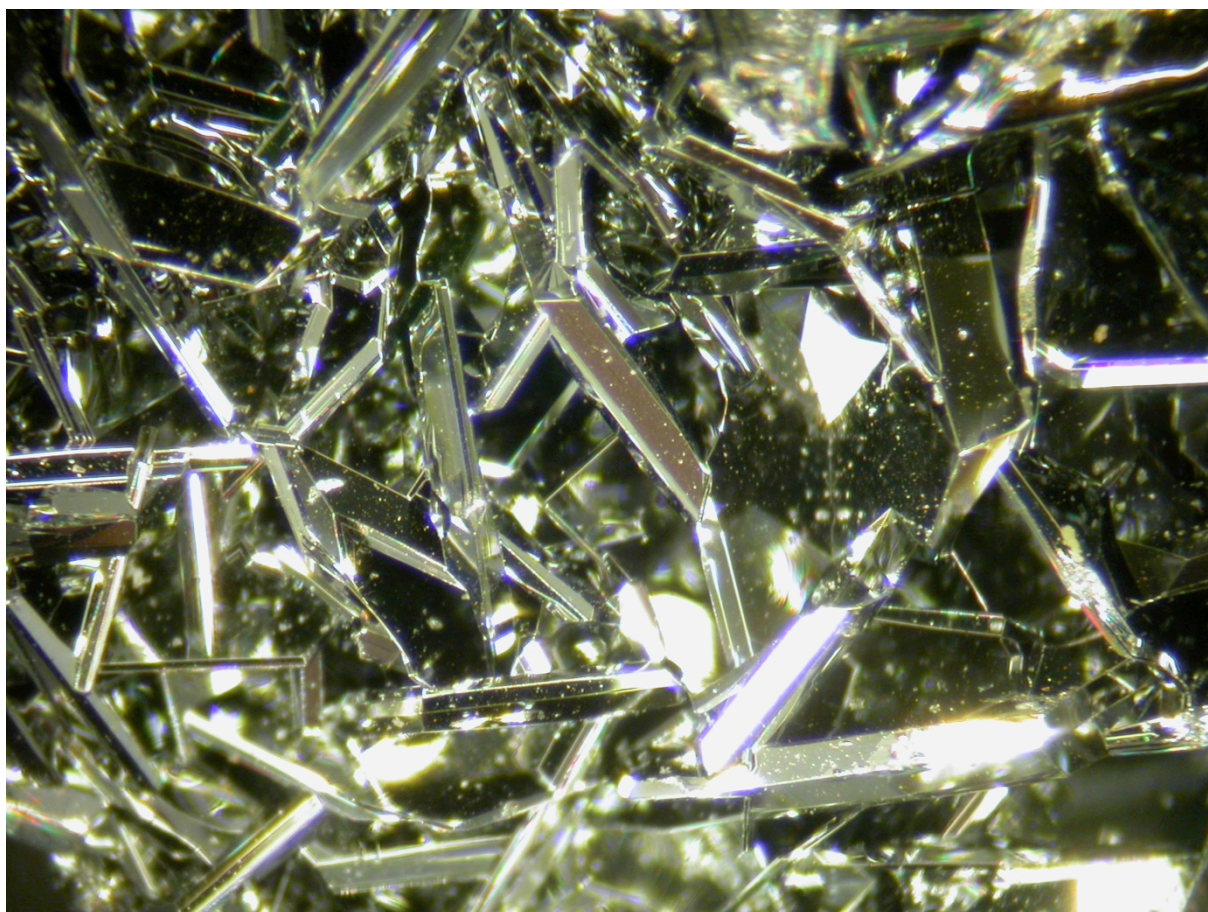
## SGK / SSCr NEWSLETTER

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**No. 93**

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In this issue:

First announcement of the 2015 SGK/SSCr Annual Meeting and  
General Assembly, Sept. 14, 2015, CSEM, Neuchâtel

On the Cover:

Crystals of the topological insulator  $\text{Bi}_2\text{Se}_3$  grown by the chemical vapor transport method (by using  $\text{I}_2$  as a transport agent). Crystals were grown by A. Ubaldini and E. Giannini, DQMP, University of Geneva. A dedicated topical meeting on crystal growth will be organized on June 11, 2015, in Geneva:  
[www.manep.ch/events/SwissCrystalGrowth](http://www.manep.ch/events/SwissCrystalGrowth)

## **SGK / SSCr Newsletter No. 93**

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## The President's Page

Crystallography makes important contributions to physics, chemistry, and biology. For example, solving magnetic structures depends on basic symmetry analysis and integration of these results into sophisticated computer codes is used by a wide community. In addition, crystal growth capabilities and the knowledge related thereto are essential. The Swiss Crystallographic Society appreciates therefore the effort by the University of Geneva and MaNEP (the Swiss Network on Novel Materials) to strengthen the collaboration within the crystal growth community – a workshop organized by Dr. Enrico Giannini in collaboration with crystal growers in Switzerland, and we hope this endeavor results in ongoing collaborations: [www.manep.ch/events/SwissCrystalGrowth](http://www.manep.ch/events/SwissCrystalGrowth)



International networks are also a key issue for enabling research into the problems that our society is facing, such as limitations in energy and resources, climate changes and pollution. A highlight in this regard has been the approval of Swiss participation to the European Spallation source ESS in Lund, Sweden. This involves a 3.5% share in the costs of construction and operation until 2026 and, as a benefit, the same share of instrument beam time, which will be offered to proposals from researchers in Switzerland evaluated on scientific merit, and as contracts to local industry providing equipment for ESS ([http://www.parlament.ch/d/sessionen/sda-sessionen/Seiten/20150309\\_bsd174\\_Forschung.aspx](http://www.parlament.ch/d/sessionen/sda-sessionen/Seiten/20150309_bsd174_Forschung.aspx)). The ESS facility will be complementary to the big investments in large scale facilities in Switzerland, such as the synchrotron SLS (upgrade program in preparation), the spallation neutron source SINQ and the free electron laser SwissFEL, and also to the excellent possibilities at the universities, for example at the Electron Microscope Center EMEZ at ETH Zürich, as well as all the laboratories with today's advanced X-ray laboratory equipment.

Consequently, we are on a good track to contribute to the future demand for research projects and excellent personnel. Most important is the upcoming next generation of scientists: the Master's and PhD students. We have to make every effort to encourage our young researchers and provide them with good perspectives for their careers in research.

Last but not least I urge you to contribute to our next annual meeting to be held at CSEM in Neuchâtel, which is being organized by Dr. Olha Sereda. Details and the call for abstracts are printed within this issue.

Jürg Schefer

## **News for and from members**

### **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 at any time. You should have been a member for at least one year before applying for a grant.

Travel grants are a good opportunity for young scientists to profit from our society during a period when they have low income. By subsequently becoming 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/travel-grants/>

### **The PANalytical Award**

With the yearly PANalytical Award the company seeks to encourage and provide support for excellent young scientists who are at the beginning of their careers. The award recognizes and praises groundbreaking research that required the use of a laboratory X-ray diffraction, X-ray fluorescence or X-ray scattering instrument as the primary analytical technique. As such, recipients will not be limited to any brand of instrument, but rather to research that utilised an X-ray source to reach their conclusions. The annual award consists of a € 5 000 cash (or equivalent amount in the local currency) prize, a trophy and a certificate. The award is presented yearly at an event that is still to be confirmed.

Further information can be found at the following link:  
<http://www.panalytical.com/Events-overview/The-PANalytical-Award.htm>



## International Year of Crystallography postage stamps from Poland

I have received four International Year of Crystallography postage stamps from Poland as a gift for having provided some Swiss IYCr postage stamps to a friend/colleague in Poland. As I do not collect postage stamps myself, is there any member of the SGK who would be interested in receiving these Polish IYCr postage stamps as a gift? If there is more than one person interested, I shall have to decide who is the lucky person.



I do not collect postage stamps. If you want to know what I do collect, please have a look at:

<http://hornby.flack.ch/>

Howard Flack

Email: [crystal@flack.ch](mailto:crystal@flack.ch)

# LET'S GROW NICE – BIG – PURE !

## MINUTES OF A HAIR-RAISING CRYSTAL-GROWTH CONTEST FOR PUPILS

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d. Section de physique, University of Geneva

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### 2014 INTERNATIONAL YEAR OF CRYSTALLOGRAPHY: MAKE IT PUBLIC AND FUN!

Starting October 2013, it became obvious to a group of scientists from the *Chimiscope*, the *PhysiScope* and the Laboratory of Crystallography, University of Geneva, that “something had to be organised” for the general audience to commemorate 2014 International Year of Crystallography (IYCr-2014), which had been announced in 2012 by the UNESCO as a tribute to the centennial of X-ray diffraction.

Both at the international level (<http://www.iycr2014.org/>) and at the Swiss scale (<http://www.sgk-sscr.ch/iycr2014/>, website operated by the Swiss Society for Crystallography SSCR), a bunch of high-quality events were planned over the whole year 2014, with a focus on disseminating the front-edge knowledge on crystallography and its challenges among the general audience of non-specialists. In Switzerland, IYCr-2014 has been characterised in January by a special issue of *Chimia*, the international journal for chemistry published by the Swiss Chemical Society (<http://chimia.ch>), dedicated to the past, present and future of crystallography with 13 generous papers on the subject. By the end of February, Prof. Katharina Fromm, then President of SCNAT – Platform Chemistry and member of the SSCR, launched a public exhibition on crystals and crystallography in the University of Fribourg within the frame of its 125<sup>th</sup> anniversary; this exhibition opened its doors until mid-November. Then in March two wonderful stamps were issued by the Swiss Post in close collaboration with the President of the SSCR, representing spectacular crystals of natural epidote and amethyst. March was also the opportunity for the newspaper *Neue Zürcher Zeitung* to publish a long apology on crystals and crystallography in Switzerland, and for “Le Journal de l’UNIGE” to present an interview of Radovan Černý, head of the Laboratory of Crystallography, on the how’s

and why's of the science of crystals. Finally, the commemorative year ended up with a long radio coverage of crystallography on RTS – La 1ère. And this is of course not to forget the monthly calendar of wonderful pictures listing all Swiss events, published during the whole year 2014 by the SSCr and available to everybody on the society's website.

Something however seemed to miss to the authors of this report: while the great majority of events were focused toward adults, apparently no action was to be organised specifically for children, although crystals and crystal growing are among the fascinating subjects driven by natural or artificial processes that are fairly easy to bring to the curiosity of youngsters. We thus ultimately decided to organise a contest for school classes in Geneva, as a contribution to the spreading of knowledge and passion on crystallography among the younger audiences.

This contest, “Clair comme de l'Eau de Roche – Grand Concours de Croissance du Cristal le plus Superlatif” (Crystal-Clear – The Most Superlative Crystal Growth Contest; see the flyer in Fig.1), has been designed for all public and private schools of the Primary, Secondary I and Secondary II levels in Geneva.

To our knowledge, this contest has been the only one of its kind in Switzerland, while several other crystal growing competitions have been organised in other countries (a paper on such a contest organised in the USA has been published in the November 2014 issue of J. Chem. Educ.).

One year later, it is time to make an assessment of the contest and its outcomes.



**Figure 1.** Flyer distributed to all Geneva schools to announce the launch of the contest.



### THREE AGE CATEGORIES – ONE KIT

The objective of the contest was self-contained in its title: Growing the most superlative crystal... but not whichever crystal. The organising committee had to identify a salt which met three criteria to be eligible as the starting material for all categories of ages (Primary level, Harmos 1-8; Secondary I level, Harmos 9-11; Secondary II level, Harmos 12-15): First, the salt, in its solid or solution or crystalline forms didn't have to be toxic or harmful or dangerous for the environment; second, it didn't have to be easily identifiable to avoid teachers purchasing extra stock in order to enhance their chance to grow larger quantities of crystal; third, the crystal had to be uncomplicated to grow with simple material that can be found in every school. Options such as copper sulfate pentahydrate ( $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ ; toxic and straightforward to identify) or potassium alum ( $\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ ; containing  $\text{Al}^{3+}$  suspected to be implied in breast cancer) were thus excluded, and the retained candidate was potassium dihydrogen phosphate ( $\text{KH}_2\text{PO}_4$  KDP, CAS Nr. 7778-77-0; white salt with no prominent characteristic and no toxicity); this salt shows a high difference in its water solubility at room temperature (ca. 230g/L) and at 90°C (ca. 835g/L), and it forms nice transparent tetragonal monocrystals which can grow humongous under highly controlled conditions.

All participating classes received the same kit, containing 100g of the unknown salt, a plastic container to prepare the solution and sending back unused substances for proper waste elimination, a plastic box for returning the grown crystal, and a set of simple instructions and hints to produce the most superlative crystal. Of course, the word superlative had a different meaning for each category of age: For Primary level classes (category "Kids"), the crystal had to be the funniest or most original, thus leaving a large creativity in the hands of the participants; for Secondary I level classes (category "Juniors"), the crystal had to be the heaviest and most bulky, thus bringing students to the concepts of scientific and quantitative approaches; for Secondary II level classes (category "Seniors"), the crystal had to be the largest and most crystallographically pure, thus requiring advanced skill and patience during all steps of the process.

Kits were distributed to participants between mid-January and mid-April, to allow for the Awards ceremony to be organised mid-May, i.e. before the end of the school term.

### CREATIVITY, SKILL, CHALLENGE, AND THEN PATIENCE

Approximately 200 teachers from Geneva were informed about the contest, and 90 kits were distributed to classes, thus reaching ca. 1800 students in Geneva. At the deadline, 54 samples had been returned to the organising committee, i.e. a very encouraging ratio of 60% of crystals returned. Actually, several teachers informed us that their growing process had been spoiled at a step or another by some disturbing parameters (mostly temperature or volume changes and sudden bulk crystallisation, but also because of improper reading of the instructions and hints); the authors

estimate that ca. 75% of all kits sent would have been returned as crystals if no team would have experienced troubles during the process.

The Table below summarises the main characteristics of the 54 crystal samples.

Category	Number of crystals received	Coloured crystals	Monocrystalline samples	Bulky samples
“Kids” (Primary)	25 (46%)	13 (52%)	10, partly (40%)	4 (16%)
“Juniors” (Secondary I)	14 (26%)	6 (43%)	10, partly (71%)	9 (64%)
“Seniors” (Secondary II)	15 (28%)	1 (7%)	14 (93%)	10 (67%)

The number of coloured samples (37% of all sets) was of a great surprise to the organising committee. Globally, the criteria required for becoming a winning crystal were followed in each category.

Evaluation of all samples and election of the Prize-winning crystals has been entrusted to the Jury, composed of Radovan Černý, crystallographer, Alan Francis Williams, chemist, Christoph Renner, physicist and Jacques Deferne, honorary curator of the *Musée d'Histoire Naturelle de Genève*. The ranking parameters used to evaluate the samples were as follows:

“Kids”: Score =  $0.54 \times [\text{Originality}] + 0.36 \times [\text{Beauty}] + 0.1 \times [\text{First Sight Impression}]$

“Juniors”: Score =  $0.70 \times [\text{Mass}] + 0.015 \times [\text{Originality}] + 0.015 \times [\text{Beauty}] + 0.27 \times [\text{First Sight Impression}]$

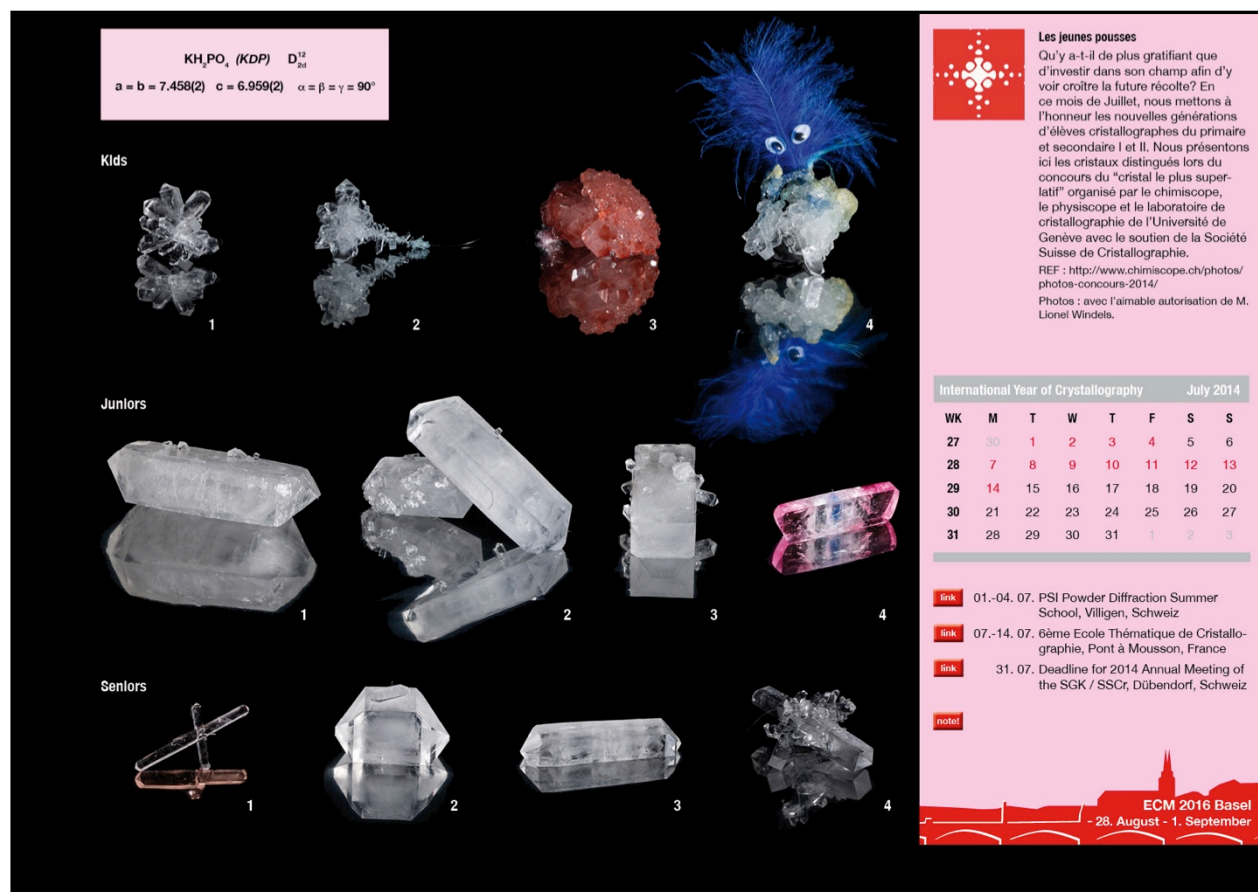
“Seniors”: Score =  $0.75 \times [\text{Crystallographic Quality}] + 0.25 \times [\text{Aesthetic Quality}]$   
 $= 0.75 \times \{ (0.5 \times [\text{Laue}] + 0.25 \times [\text{Visual Observation}] + 0.25 \times [\text{Polarised Light Observation}] ) \times \log_{10}(\text{Mass} + 10) \}$   
 $+ 0.25 \times \{ 0.9 \times [\text{First Sight Impression}] + 0.05 \times [\text{Originality}] + 0.05 \times [\text{Beauty}] \}$   
The Laue parameter was determined by recording the X-ray diffraction pattern produced by the monocrystal.

The apparently tortuous equation used for the evaluation of the samples provided by “Senior” classes allowed the Jury to take into account the crystallographic purity and the mass of the provided samples (both integrated under the parameter Crystallographic Quality).

Because of the large number of breath-taking samples received, the Jury ultimately decide to attribute a Special Prize to the crystal ranked fourth in each category. The table below summarises the statistics on all samples received.

Category	Maximum score	Average score	Median score	Minimum score
"Kids"	<b>5.4/6.0</b>	4.2 ± 0.7	4.3	2.8
"Juniors"	<b>5.7/6.0</b>	3.9 ± 1.2	4.2	2.1
"Seniors"	<b>6.0/6.0</b>	3.4 ± 1.5	2.8	1.7

Figure 2, extracted from the monthly calendar published by the Swiss Society for Crystallography during the year 2014, shows the four Prize-winning crystals in each of the three age categories.



**Figure 2.** French version of the Crystallographic Calendar (July) published by the SSCr during IYCr-2014, showing the magnificence of all Prize-winning crystals. Pictures were taken by Lionel Windels on a mirror surface. Reproduced with kind permission of the Swiss Society for Crystallography.

Complementing Figure 2, Figure 3 below shows some of the non-awarded crystals submitted during the contest. These crystals are definitely an arbitrary selection aimed at revealing to the reader the ingenuity of some participating classes, whichever their category. Thanks to the generous contribution of the Swiss Society for Crystallography and an anonymous Foundation active in science, the organising committee has been able to produce a luxurious catalogue exhibiting all crystals submitted, which has been offered to all participating schoolchildren after the award ceremony.



**Figure 3.**  
Selection of some  
of the crystals  
submitted to the  
contest.

By mid-May, the 12 Prize-winning classes were invited to participate in the final ceremony, which took place in the Faculty of Science, UNIGE, in the presence of the organising committee and the members of the Jury. The latter offered three presentations that intermingled history, science of crystallography and famous scientists (Wilhelm C. Röntgen and Max von Laue), order and disorder in Nature and in the research or industrial laboratory, and humour. Then Prizes were distributed to the award-winning classes. These Prizes are shown on Figure 4 below.



**Figure 4.** First, second and third Prizes, and Special Prize, distributed to all award-winning classes during the ceremony.



The first and second prizes for each category were large cubes of glass with a laser engraving showing the 3D structure of potassium dihydrogen phosphate monocrystals. The third prize was a 3D ball & stick model of this structure. And the fourth prize was a set of two scientific books related to chemical elements and atoms. All schoolchildren in the award-winning classes also received a nice quartz crystal. The ceremony was complemented by a nice tea party where students, teachers and researchers enjoyed sharing their enthusiasm for crystals.

But the nice story of this contest didn't end at the ceremony. In July 2014, all crystals were on exhibit during the 10<sup>th</sup> edition of the *Nuit de la Science*, organised around the *Musée d'Histoire des Sciences de Genève* (see Figure 5) where ca. 35'000 visitors gather every other year.

Finally while the minutes of the event were published in the December issue of the journal *Chimia*, all details on the contest, including pictures of all crystals and the luxurious catalogue, have been made available on the website of the *Chimiscope* (<http://chimiscope.ch>).



**Figure 5.** Crystals on display during the *Nuit de la Science*, July 2014, in the *Perle-du-Lac* gardens, Geneva.

## AND SO WHAT?

After the lights of the contest were switched off, the organising committee noticed that the significantly increased number of visits at the *Chimiscope* and the *PhysiScope* had been booked by many of the teachers who initially participated in the contest with their classes. This observation has convinced the organisers that a unifying event focused on science and youngsters can have unexpected and positive consequences in terms of incentive interactions between researchers and schoolchildren.

## ACKNOWLEDGEMENTS

The authors warmly acknowledge the financial support provided by the Swiss Society for Crystallography and an anonymous Foundation active in science, which helped the organising committee to publish the catalogue that has been distributed to all participating schoolchildren.





**Swiss Crystallographic Association  
SGK / SSCr  
Annual Meeting and General Assembly 2015**

**Monday, September 14, 2015**

CSEM SA  
Rue Jaquet-Droz 1  
2000 Neuchâtel

Meeting Title:

**“The role of X-ray Diffraction in Materials for a Sustainable Future”**

**Call for Abstracts**

The 2015 annual meeting and general assembly of the SGK/SSCR will take place at CSEM SA (Swiss Center of Electronics and Microelectronics) on Monday 14<sup>th</sup> of September 2015. Three invited speakers from academia, seven selected oral presentations and a poster session will show recent developments in the field.

More details and a template for an abstract on the website:  
[indico.psi.ch/event/SGK-SSCR-Annual-Meeting-2015](http://indico.psi.ch/event/SGK-SSCR-Annual-Meeting-2015)

**Deadline for Abstract submission:** July 1, 2015

Abstract should be sent by email to: [secretariesdivt@csem.ch](mailto:secretariesdivt@csem.ch)  
Any crystallographic topic is welcome. Meeting Organizer: Dr. Olha Sereda.

**Registration:** Please register on our webpage  
[indico.psi.ch/event/SGK-SSCR-Annual-Meeting-2015](http://indico.psi.ch/event/SGK-SSCR-Annual-Meeting-2015)

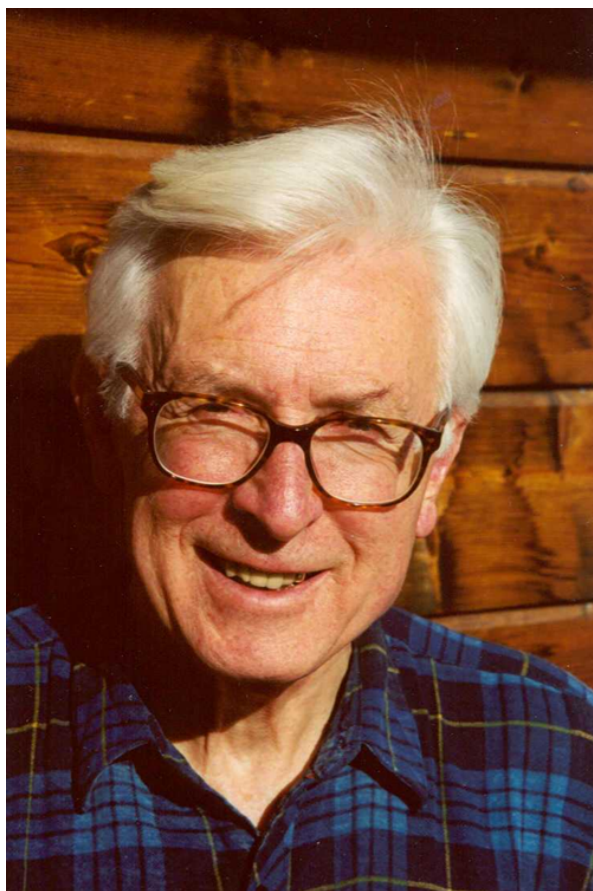
In order to register, you will have to create an account for you.

The meeting is free of charge (except for accommodation and conference dinner in the evening). Means of payment for the dinner will be provided on the conference webpage.

## Program

<b>9.00-09.45</b>	<b>Registration and Poster session</b>
09.45-10.00	Welcome message
<b>10.00-10.45</b>	<b>Prof. Dr. Helena Van Swygenhoven</b> (NXMM, Paul Scherrer Institute and École Polytechnique Fédérale de Lausanne) <i>"In-situ X-ray techniques applied to metallurgy"</i>
10.45-11.00	<i>Posters + Coffee break</i>
<b>11.00</b>	<b>Session 1</b>
11.00-11.20	Talk 1 selected from the abstracts
11.20-11.40	Talk 2 selected from the abstracts
<b>11.40-12.30</b>	<b>Lunch and Posters</b>
12.30-13.55	General Assembly of the SGK
<b>14.00-14.45</b>	<b>Dr. Colin Groom</b> (Cambridge Crystallographic Data Centre, Cambridge, UK) <i>"Fifty years of sharing crystal structures"</i>
<b>14.45</b>	<b>Session 2</b>
14.45-15.05	Talk 4 selected from the abstracts
15.05-15.25	Talk 5 selected from the abstracts
15.25-15.45	<i>Coffee Break and Posters</i>
15.45-16.30	<b>Dr. Taras Slobodskyy</b> (Institut für Nanotstruktur und Festkörperphysik, Universität Hamburg) <i>"X-ray diffraction studies of thin film solar cells"</i>
<b>16.30</b>	<b>Session 3</b>
16.30-16.50	Talk 6 selected from the abstracts
16.50-17.10	Talk 7 selected from the abstracts
<b>17.10-17.30</b>	<b>Poster Prize Winners &amp; Final remarks</b>
<b>17.30-18.30</b>	<b>Aperitif</b>
<b>19.00-23.00</b>	<b>Dinner</b>

## In Memoriam Hans Schmid (1931 - 2015)



Hans Schmid, Professor Emeritus at the Faculty of Science of the University of Geneva passed away on Thursday, April 2. He was a member of the Swiss Society for Crystallography from its beginnings and served as chairman of its section for crystal growth from 1981 to 1984.

Hans Schmid was born on January 11, 1931 in Reichenberg (Liberec) in the then German speaking part of the present Czech Republic. In 1945 he moved with his family to Innsbruck. He studied at the Technical University Graz, where he received his doctoral degree in inorganic physical chemistry in 1955. After two years as research assistant in the Austrian aluminum industry, he moved in 1957 to the Battelle Research Laboratories in Geneva, where he worked on the synthesis and physical properties of ferroelectric and ferroelastic materials, mainly with a view to application in the fields of heat detection, display and data storage. This research culminated in 1964 in the synthesis of single crystals of the boracite  $\text{Ni}_3\text{B}_7\text{O}_{13}\text{I}$ , the first material that was found to be simultaneously ferroelectric, (weakly) ferromagnetic and ferroelastic. Together with Dr. E. Ascher, he showed in [1] that in this boracite the spontaneous electric polarization can be switched by a magnetic field and the spontaneous magnetization by an electric field. Hans Schmid presents a very lively account of this discovery in [2], mentioning the collaborators that contributed to the success as well as the many obstacles he had to overcome for gaining financial support to continue his research. In 1973 he organized and chaired in Seattle (USA)

the first international conference on "Magnetoelectric Interaction Phenomena in Crystals". In 1974 he was appointed head of the "Crystal Physics Section" and in 1976 "Senior Scientist" at Battelle Geneva Research Center. In 1975 he became "Privat-docent" in Crystallography at the Faculty of Science of the University of Geneva.

From 1977 to 1996 he lectured in the Department of Inorganic, Analytical and Applied Chemistry of the University of Geneva, first as associate professor and from 1978 as full professor of Inorganic Applied Chemistry, Solid State Chemistry and Materials Science. With Dr. J.-P. Rivera, he set up one of the best equipped laboratories for the study of the magnetoelectric effect and the optical properties of crystals. Together with Rivera, several talented postdocs and PhD students he continued his research on magnetically ordered ferroelectrics and ferroelastics and their magnetoelectric interactions. He was director of the department 1989-1992 and organized in 1993 the second international conference on "Magnetoelectric Interaction Phenomena in Crystals" (MEIPIC-2), which took place in Ascona, Switzerland. In his over 500 times quoted contribution [3] to this conference he coined the term "multiferroic" to describe crystals that show at least two of the three properties ferroelectric, ferromagnetic and ferroelastic. This conference stimulated interest in multiferroic materials, which have become a very active field of research.

Hans Schmid successfully continued research also after his emeritation in 1996, especially on multiferroic properties in the perovskite  $\text{BiFeO}_3$  and in  $\text{LiMPO}_4$  ( $M = \text{Fe}, \text{Co}, \text{Ni}$ ). His last paper has been accepted for publication after his death.

The undersigned got to know Hans Schmid during their common time at Battelle. He is very grateful to him for many valuable research proposals and for being invited to help organizing MEIPIC-2. He likes to remember Hans Schmid as a most helpful, generous, fair and friendly colleague. Thanks are due also to Dr. Jean-Pierre Rivera for his unfailing help in preparing this obituary.

Hans Grimmer  
Paul Scherrer Institut, 5232 Villigen-PSI, Switzerland

[1] E. Ascher, H. Rieder, H. Schmid & H. Stössel, "Some properties of ferromagnetoelectric nickel-iodine boracite  $\text{Ni}_3\text{B}_7\text{O}_{13}\text{I}$ ", *J. Appl. Phys.* **37** (1966) 1404-1405.

[2] H. Schmid, "The Dice-Stone, der Würfelstein: Some personal souvenirs around the discovery of the first ferromagnetic ferroelectric", *Ferroelectrics* **427** (2012) 1-33.

[3] H. Schmid, "Multi-ferroic Magnetoelectrics", *Ferroelectrics* **162** (1994) 317-338.

## Advanced Training in X-Ray Crystallography

with Carmelo Giacovazzo

**Excelsus Structural Solutions** in collaboration with the University of Bologna organizes the 1<sup>st</sup> of a series of advanced trainings addressed to a scientific industrial audience with interest in X-Ray Powder Diffraction and its applications to small organic molecular compounds.

Topic of this 1<sup>st</sup> event is **X-Ray Crystallography** with lectures delivered by **Prof. Carmelo Giacovazzo**, Consiglio Nazionale Ricerche, Institute of Crystallography (CNR-IC)-Bari, Italy.

When: **September 9<sup>th</sup>-12<sup>th</sup>** (intensive, all day)

Where: **“G. Ciamician” Chemistry Department, University of Bologna - Italy**

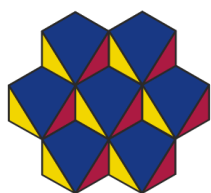
Interested people should contact:

Crystallography-Lectures@excels.us OR fabia.gozzo@excels.us  
(see also [www.excels.us](http://www.excels.us) OR [www.ciam.unibo.it/crystal\\_engineering](http://www.ciam.unibo.it/crystal_engineering))

- Limited number of participants, first-comes first served
- Registration fees: 800 Eur (before May 30<sup>th</sup>), 1200 Eur (after May 30<sup>th</sup>)
- **Mandatory:** study of the first **24 pages** of *Fundamentals of Crystallography* (2<sup>nd</sup> Edition) plus exercises assigned by Carmelo Giacovazzo prior to the lectures! Material (i.e. 24-pages + exercises) distributed by Excelsus to the confirmed participants 3 months before the training!
- Any question about the distributed material? Carmelo Giacovazzo is available to answer them BEFORE the lectures via email.

Lectures program and downloadable pdf announcement at:  
[http://www.excels.us/index/pages/id\\_page-192/lang-en/](http://www.excels.us/index/pages/id_page-192/lang-en/)





# CAC 2015



## XXIII Conference on Applied Crystallography

**20 - 24 September 2015**

**Krynica Zdrój, Poland**

### Invited Speakers

- Dan Shechtman  
2011 Nobel Prize Laureate
- Vincent Favre-Nicolin
- Andrew Fitch
- Maria Gdaniec
- Wolfgang Hofmeister
- Ute Kolb
- Bogdan Kotur
- János Lábár
- Ron Lifshitz
- Jean Paul Morniroli
- Reinhard Neder
- Václav Petříček
- Janusz Wolny

The conference will be held in Krynica Zdrój, Poland in the Czarny Potok\*\*\*\* SPA & Resort hotel, offering beyond the largest conference center, variety of attractions like Health SPA and Baths, Swimming Pool, Cardio Studio and Fitness.



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33-380 Krynica Zdrój,  
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tel. +48 18 530 30 00  
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**[www.cac.us.edu.pl](http://www.cac.us.edu.pl)**

## Crystallography at an X-ray Free Electron Laser

There are presently two operating X-ray Free Electron Lasers (XFEL): LCLS (Stanford) and SACLA (Japan). These will be joined during the next two years by additional additional facilities: European XFEL (Hamburg), PAL FEL (Korea) and SwissFEL (PSI). The SwissFEL building is now complete in the Würenlingen forest near the Paul Scherrer Institut, and the first Swiss X-ray pulses are expected early in 2017.

A major part of the research at these ultrabright, ultra-short-pulse machines is and will continue to be based on X-ray crystallography – albeit with some major modifications to present synchrotron-based techniques. In a recent article (*Crystallography Reviews* 20, 242-294 (2014)), the status of XFEL-based crystallography experiments, on both organic and inorganic samples, is summarized and an outlook is presented on how the field may develop in the near future. The emphasis of the article is on novel aspects and opportunities particular to the XFEL. The abstract and contents of the article are reproduced below.

*An X-ray Free Electron Laser (XFEL) produces short pulses (10-50 fs) of intense ( $\text{mJ}/\text{mm}^2$  at 120 Hz) X-rays, with high transverse coherence. Such pulses open novel spectroscopic and scattering methods for static and time-resolved studies of matter, and many are based on X-ray crystallography. With serial femtosecond crystallography, the XFEL allows high-resolution structural determination on sub-micron protein crystals. Although the XFEL pulse is destructive, its short duration insures that effectively undamaged material is probed. Coherent scattering features provide information on the physical crystal form and may assist in determining the crystallographic phase. By introducing synchronized optical laser pulses, one can perform “pump-probe” measurements of dynamic properties, on the sub-picosecond time-scale. These include photo-initiated structural modifications in biomolecules, photo-excited lattice vibrations and photo-driven structural phase transitions. As with synchrotron radiation, the XFEL wavelength can be tuned to atomic resonances, allowing time-resolved resonant-diffraction measurements, which are particularly sensitive to selected order parameters (lattice, charge, spin, orbital) in magnetic or correlated-electron materials. Finally, it is anticipated that the special properties of XFEL pulses will allow entirely new types of X-ray scattering measurements, such as ptychographic crystallography on 2D bio-crystals, correlation-function determination of nanoparticle geometry and non-linear crystallographic mixing of optical and X-ray pulses.*

- 1. Introduction**
- 2. Generation and properties of XFEL pulses**
  - 2.1 The XFEL principle
  - 2.2 SASE pulses
  - 2.3 A self-seeding filter for the XFEL based on dynamic diffraction
- 3. Serial femtosecond crystallography of proteins**
  - 3.1 Serial crystallography at an XFEL
  - 3.2 Monte Carlo determination of scattering factors
  - 3.3 Sample damage issues
  - 3.4 New opportunities for phase determination
  - 3.5 Outlook for SFX
- 4. Femtosecond diffraction in inorganic crystals**
  - 4.1 Time-resolved XRD studies of photo-excited coherent phonons
  - 4.2 Photo-induced phase transitions
  - 4.3 Time-resolved resonant diffraction in correlated-electron systems
- 5. Special and prospective issues in XFEL crystallography**
  - 5.1 2D ptychographic crystallography
  - 5.2 Correlation-function analysis of scattering data
  - 5.3 Non-linear X-ray optics and diffraction
- 6. Summary and outlook**

Bruce D Patterson, Paul Scherrer Institut, February, 2015

## **Swiss Society for Crystallography PhD prize**

The Swiss Society for Crystallography establishes a prize for the best PhD thesis in crystallography.

### **Requirements:**

The prize is open to

- a) Students, of any nationality, who earned a PhD title from a Swiss University
- b) Students, of any nationality, who earned a PhD title from a University abroad, but carried out significant amount of work for the PhD title at a Swiss Research Institution, like EMPA, PSI or SNBL.
- c) Students of Swiss nationality who earned a PhD title from any University worldwide.

The student must have earned the title between **July 1<sup>st</sup> 2013 and June 30<sup>th</sup> 2015**.

The subject of the thesis can be in any area of crystallography (structural biology, chemical crystallography, solid-state physics, crystallography of materials, etc.). The implications of the obtained results for crystallography should be evident.

### **Application:**

The application for the prize should be submitted before **30 June 2015** by the student himself or by the thesis supervisor. The applicant should submit: a) a pdf copy of the thesis; b) a letter of the supervisor approving his/her candidature; c) pdf copies of the articles published from the results obtained during the thesis; d) a pdf scan of the PhD diploma; e) a short CV of the candidate.

The application should be sent to the secretary of the Swiss Society of Crystallography ([info@sgk-sscr.ch](mailto:info@sgk-sscr.ch))

### **The award**

The winner will be selected by a commission, based on the quality of the research, the quality of the publications, and the effective contribution of the candidate to the scientific work. The commission may decide not to assign the prize if none of the candidates fit the minimal prerequisites concerning the topic, the quality of the thesis, the papers published from it and the approval of the supervisor.

The winner will be announced before the annual meeting and will be invited to give a short talk of the results of his/her thesis.

The Swiss Society of Crystallography will award the winner with a diploma and will reimburse the participation of the student to the annual meeting.

## Calls for proposals

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

Facility	Deadline(s)	Link
<b>SLS: Swiss Light Source</b> All except PX lines Protein crystallography beamlines (PX)	15.03. and 15.09. 15.04. and 15.10.	<a href="http://www.psi.ch/useroffice">www.psi.ch/useroffice</a>
<b>SINQ: Swiss Spallation Neutron Source</b> All instruments (regular calls)	15.05. and 15.11.	<a href="http://www.psi.ch/useroffice">www.psi.ch/useroffice</a>
<b>SINQ/SLS</b> Joint x+n proposals (MS/HRPT)	20.02.2016	<a href="http://www.psi.ch/useroffice">www.psi.ch/useroffice</a>
<b>SμS: Swiss Muon Source</b> All instruments	08.12. and 10.06	<a href="http://www.psi.ch/useroffice">www.psi.ch/useroffice</a>
<b>ESRF: European Synchrotron</b> long term proposals short term proposals	15.01.2016 10.09.2016	<a href="http://www.esrf.eu/UsersAndScience/">www.esrf.eu/ UsersAndScience/</a>
<b>ILL: Institut Laue Langevin</b> All instruments	Feb., Sept.	<a href="http://www.ill.eu">www.ill.eu</a>
<b>FRM II: Heinz Maier-Leibnitz</b> All instruments	11.09.2015	<a href="http://user.frm2.tum.de">user.frm2.tum.de</a>
<b>SNS Spallation Neutron Source</b> Oak Ridge	various	<a href="http://neutrons.ornl.gov">neutrons.ornl.gov</a>



## Calendar of forthcoming meetings

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

				Application Deadline
<b>2015</b>				
May 25-28	Como Italy	Total Scattering for Nanotechnology on the Como Lake <a href="http://www.toscalake.com">www.toscalake.com</a>		now open
Jun. 5-14	Erice Italy	The 48th crystallographic course, Erice, Italy <a href="http://www.crystalerice.org/Erice2015/2015.htm">www.crystalerice.org/Erice2015/2015.htm</a>		in the past
Jun. 7-12	Santa Margherita di Pula Italy	SAGAMORE XVIII Conference on Charge, Spin and Momentum Densities (CSMD) <a href="http://www.sagamorexviii.org">www.sagamorexviii.org</a>		in the past
Jun. 7-20	Zurich Switzerland	Zurich School of Crystallography – Bring Your Own Crystals <a href="http://www.chem.uzh.ch/linden/zsc/">www.chem.uzh.ch/linden/zsc/</a>		in the past
Jun. 11	Geneva, Switzerland	Topical meeting on Crystal Growth in Switzerland <a href="http://www.manep.ch/events/SwissCrystalGrowth">www.manep.ch/events/SwissCrystalGrowth</a>		24.05.2015
Jun. 14-18	Cavalese-Trentino, Italy	DSE 2015 – 100 Years of Debye Scattering Equation <a href="http://dse2015.org">dse2015.org</a>		As long as vacant places are available
Jun. 30 – Jul. 03	Lucerne Switzerland	5th European Pefc & H2 Forum <a href="http://www.efcf.com">www.efcf.com</a>		now open
Aug. 23-28	Rovinj Croatia	The 29th European crystallographic meeting (ECM-29) <a href="http://ecm29.ecanews.org">ecm29.ecanews.org</a>		23.03.2015
Aug. 30- Sep. 4	Zaragoza Spain	VI European Conference on Neutron Scattering (ECNS) <a href="http://www.ecns2015.eu">www.ecns2015.eu</a>		15.03.2015
Sep. 1-4	Wien Austria	Joint Annual Meeting of the Austrian and Swiss Physical Societies – 2015. <a href="http://www.sps.ch">www.sps.ch</a>		
Sep. 14	Neuchâtel Switzerland	Annual Meeting of the SGK / SSCr <a href="http://indico.psi.ch/event/SGK-SSCr-Annual-Meeting-2015">indico.psi.ch/event/SGK-SSCr-Annual-Meeting-2015</a>		01.07.2015
<b>2016</b>				
Aug. 28 – Sep. 01	Basel CH	The 30th European crystallographic meeting (ECM-30) <a href="http://ecm30.ecanews.org">ecm30.ecanews.org</a>		to be announced
<b>2017</b>				
Aug. 21-29	Hyderabad India	The XXIV Congress & General Assembly of the International Union of Crystallography (IUCr-2017) <a href="http://www.iucr2017.org">www.iucr2017.org</a>		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 30 (CHF 10 for students).



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Please FAX the completed form to: Denis Sheptyakov, +41 (0)56 310 2939  
or use our online application form at [www.sgk-sscr.ch](http://www.sgk-sscr.ch)

You may also use this form if you need to update your contact information.

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