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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Member of the
Swiss Academy of Sciences

SGK / SSCr NEWSLETTER

ISSN 1662-5358 (printed edition)
ISSN 1662-534X (electronic edition)

No. 97
March 2017

In this issue:

On the Cover:
Welcome to ECM30 in Basel by congress chair Katharina M. Fromm, introducing the organizing committee.

SGK / SSCr Newsletter No. 97

The President's Page

Well done!
Yes, the ECM30 was a great success, from many points of view. First, and most important, we had a very high level of science, represented by plenary and keynote lecturers, by speakers and chairs of the microsymposia, by the active audience and by the poster presenters.
Moreover, we had an incredibly high participation, exceeding 900 attendees, from almost 50 countries. This was quite unexpected for a meeting organized in a rather expensive country like Switzerland.
The meeting will be certainly remembered for the excellent organization of a very professional congress organizer, and for some novelties that were introduced for the first time, such as the science slams.
Last but not least, the location and the venue was perfect and the participants could not only find room for discussion and relax, but they also had occasion to sightsee. Basel is a very attractive city and was therefore ideal.

We will all preserve many memories of this meeting and this newsletter is dedicated to reporting the various aspects of the congress, scientific and social events, including some representative pictures. Moreover, we report on the satellites meetings that accompanied the main event and that contribute to the overall success.

I wish to thank all the organizers, the chair, the vice chair, the organizing committee and all the assistants that took care of all details of the organization. Of course, I also acknowledge the partners we had, in particular the commercial and institutional sponsors and exhibitors, the congress organizer, the local authorities who welcomed us in Basel.

What are our next objectives? We will archive ECM30, but we will preserve the enthusiasm for the next goals of our society. This year will be equally exciting as 2016: the IUCr general assembly will take place in Hyderabad (India) on 21-28 August 2017. Our society will continue supporting the traditional schools (the Zurich School of Crystallography, 11-22 June 2017) and workshops, the annual meeting of the society (Geneva, 12 September 2017) and the support of young scientists, including the PhD prize that will be issued in 2017, after the inaugural edition in 2015.
Very important is a renewal of interest for the *section of crystal growth* that in conjunction with the German society of crystal growth will organize a meeting in Freiburg (Germany), on March 8-10, 2017.
I am sure that the list of future activities will certainly grow.

I wish all our members a successful 2017.

Piero Macchi
(President of the SGK-SSCr)

Obituary Howard Flack (1943 – 2017)

Howard D Flack, 1943 - 2017

Howard has left us suddenly on Thursday, 2nd of February, 2017 at the age of 73 years. He was born in Surrey County in England. After having obtained his “honours degree” from the University of Nottingham he entered University College London where he was preparing his PhD project, Studies of Disorder in Anthrone and in Mixed Crystals of Anthrone-Anthraquinone, under the supervision of Kathleen Lonsdale. There can be no doubt that the direction of his life-long research interests were formed while working on this project. He realized that only a deep understanding of the diffraction process and its mathematical treatment brings him to the success of his work.

After gaining his PhD, Howard moved to Cambridge (England) to work as Research Assistant in Surface Physics in The Cavendish Laboratory. At this time, he met his future wife, Evelyne. By happy coincidence, Erwin Parthé offered Howard a position of Maître-assistant in the Laboratoire de Cristallographie at the University of Geneva, Switzerland. Howard’s arrival in Geneva coincided with a new start of crystallography in western Switzerland. Parthé’s interdisciplinary Crystallography Laboratory was a new central facility serving the Faculty of Science of the University. A year later, an Institute of Crystallography was newly created as part of Physics at the University of Lausanne, while the Universities of Neuchâtel and Basel gradually developed structure determination services. Howard generously collaborated with all these crystallography centres, and was involved in their success. He spent all his scientific life at the University of Geneva with short interruptions when he was invited to other institutions for teaching various mathematical methods of crystallography. He was employed in Geneva as part of the technical staff and as Chargé de cours. From 1984 to 1990, he was secretary of the Swiss Society for Crystallography, and initiated the creation of the SSCr. Newsletters.

Howard’s name is without any doubt connected with the Flack parameter. Since his thesis project, he had growing interest in the determination of absolute structure by X-ray diffraction. He realized that the problem could be posed by regarding the sample as a twin containing x and 1-x twin-fractions of the two enantiomers (with x a refinable parameter), in an analogous way to his treatment of disorder from 1970. This elegant solution of the problem of absolute structure determination proved to be enormously popular, with the twin-fraction x quickly being called The Flack Parameter.

His interest in mathematical crystallography was much broader than the chirality. He developed the way to treat merohedral twins, was involved in many projects dealing with statistical analysis of diffraction data, and suggested a method of absorption correction, implemented in his computer program CAMEL JOCKEY. He was a very good programmer, participating for many years in the development of the XRAY76 program system.

Howard saw, very early on, the contribution that modern computer-based communication systems could make to the dissemination of crystallography. His

contributions to the digital publication of IUCr material, to the structured archiving of data, and to the crystallographic community warrant their own description, and are detailed at http://www.iucr.org.

He particularly enjoyed being with students, and would take every opportunity to get them to talk about their own work. Many of Geneva students certainly remember his demonstration of 'la Coupe du Roi' - a method of dissecting an apple into two identical chiral halves. An experiment ending sometimes with teacher hurting himself when the knife was too sharp. Howard was giving the lecture Computational Methods in Crystallography and later on The Chirality of Crystals and Molecules in Geneva and at various other Swiss Universities. He certainly leaves a huge gap among the teachers of the Zurich Crystallography School.

My personal souvenir of Howard is his enthusiasm and never ending will of learning novel discoveries and finding the relations and laws governing the crystalline solids and beyond. He liked to share his knowledge. I believe not being the only one in Geneva who remembers that asking Howard a question was an adventure by itself. You left his office one hour later with the head full of novel and exciting information and had completely forgotten your original question.

With Howard, we have not only lost an influential scientist and teacher, we have also lost a widely interested and cultured person. He loved music, operas and concerts. He assembled an impressive collection of vintage toy trains and railway accessories produced by the British firm Hornby between 1920 and 1963. He liked down-hill skiing and horseback riding.

We will always remember his sense of humor, very “British”, his curiosity and willingness to share his knowledge.

Radovan Černý

Conference Pictures ECM30, Basel

A large collection of beautiful photographs can be found on the ECM-30 conference website:

http://ecm30.ecanews.org/2016/general-information/photo-gallery.html#prettyPhoto

Conference Report:
European Crystallographic Meeting in Basel

August 28 to Sept 1. 2016
Surrounded by eight satellites meetings

Katharina Fromm, University of Fribourg (chair)
Jürg Schefer, Paul Scherrer Institut (co-chair)
(Published in parallel in the Swiss Neutron News)

Alphorn Trio Solodurum, http://www.solodurum.ch/

Katharina Fromm (chair) and Jürg Schefer (co-chair) of ECM30 presenting chemical experiments.

In 2012, the general Assembly of the SGK/SSCr in Zurich decided to bid for an ECM meeting in Switzerland, which was approved in August of the same year by the ECA council in Bergen, Norway. After four years of preparation the European Crystallographic Meeting 2016 (ECM-30) finally saw the light on Sunday, August 28th, 2016 at 17h with some 500-600 people attending the opening ceremony in room San Francisco of the Basel Conference Center. The alphorn trio Solodurum entertained with its performance in a typical Swiss way. Chemical experiments after the welcoming talk by Katharina Fromm and the welcome address by Mauro Dell'Ambrogio, the Swiss State Secretary for Education, Research and Innovation were leading over to the scientific scope of the event. Hans-Peter Wessels from the Government of the Canton of Basel-City welcomed the participants on behalf of the hosting town, followed by Joël Mesot, Director of the Paul Scherrer Institute, Piero

Opening words of Joël Mesot, director of Paul Scherrer Institute, Villigen.

Mauro Dell'Ambrogio, Swiss State Secretary for Education, Research and Innovation, addressing ECM30.

Macchi, President of the Swiss Society for Crystallography and Alessia Bacchi, President of the European Crystallographic Association.
During the second hour of the opening session, Udo Heinemann presented the Max Perutz Prize to Vaclav Petříček from Prague, who gave his prize lecture in the following. The welcome reception was sponsored by the City of Basel. The exhibitor area was the perfect place for this, allowing the participants and exhibitors to mix: ECM's are (and should be) also a yearly event for the crystallographic "family".

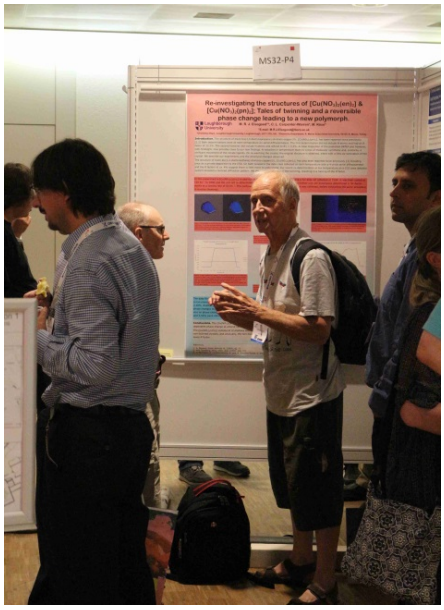
Ada Yonath, Nobel Prize Laureate in Chemistry (2009) during the opening plenary.

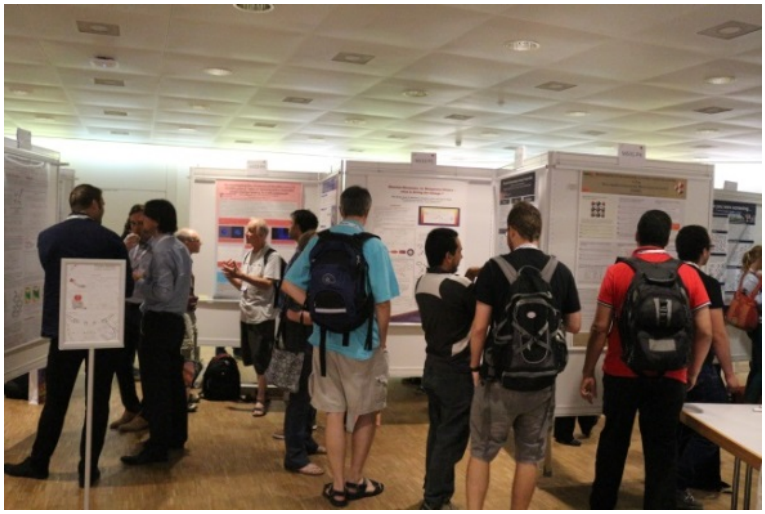
The second day started with the plenary lecture by Nobel Prize Laureate Ada Yonath from Israel. Her fascinating talk was appreciated by a very large and broad public, and her energy and enthusiasm were a model to many young scientists. The microsymposia kicked off at 10h with seven parallel sessions. Especially fascinating were the new approaches to overcome the problem of resistance to present antibiotics. Several special interest groups met over lunch time, a commercial user workshop and the software fayre also took place between 12h and 14h. From 14h-16h, again seven microsymposia took place. The next highlights were the keynote talks by Peter Schurtenberger and Francesca Fabbiani (in parallel from 16h30-17h30, while all participants had a chance to mix and meet around the first poster session which lasted until 19h30. A Young Crystallographers' Mixer took place later that evening 105m above Basel in the Bar Rouge, to which 100 out of the 200 registered young scientists turned up.
Tuesday morning started at 8h30 with two well-attended, excellent keynote lectures by François Diederich and Birger Dittrich, followed by six parallel microsymposia until 12h. The lunch break was again occupied by special and general interest group meetings, the software fayre and a commercial user workshop, as well as the first ECM-31 program committee meeting, where Katharina Fromm will be a member. Following the six parallel sessions from 14-16h, Sandra W. Jacob, and Marcus Neumann delivered their highly interesting keynote lectures. At 19h, a world premiere, the very first ECM-Science-Slam sponsored by STOE took place in room Sydney in front of ca. 300 listeners. Six young scientists from across Europe were selected from the poster abstracts and invited three months before the conference to participate. All six accepted the challenge, and the well-attended session was filled with six excellent three-minutes-presentations by these talented young candidates. It was Gregor Hofer from Zürich who convinced, in the end, the public with his presentation on the Zurich street parade to explain the pair-distribution-function. The Science Slam was immediately followed by the Bertaut Prize ceremony, during which Udo Heinemann presented the prize to Linda Reinhard.

Group picture of the participants of the first ECM science slam sponsored by STOE.

Wednesday morning saw two brilliant keynote presentations by Jan Pieter Abrahams and Simon Parsons before kicking off with six parallel sessions until 12h. The lunch break was again used for the ECA Council, several special and general interest groups, the software fayre and the general assembly of the Swiss Society for Crystallography. After six parallel microsymposia between 14h and 16h, Makoto Fujita and Olivier

Thomas as well as Robert von Dreele and Petra Fromme delivered their excellent keynote talks. Some 350 participants then joined the *apéro* and the conference dinner at the zoo of Basel. The excellent Basel transport system allowed a gapless transfer from the last session to this event.
Thursday started with two keynote lectures by Werner Paulus and Bob Cernik, followed again by six parallel sessions.





Lively discussion during the two poster sessions in the modern congress center, among them our long term members Hans Grimmer and Howard D. Flack (picture on the left).

The lunch breaks got filled with meetings of the European Crystallographic Association (ECA) and the special and general interest groups (SIG/GIG), the software fayre and some commercial presentations. The afternoon sessions were again well attended, as throughout the conference (the organizers were surprised to see the smaller lecture halls often more than full), before the last keynote lectures by Marek Grzelczak and Martin Schmitt took place. The room Sydney crowded up for the second plenary lecture by Nobel Prize winner Jean-Marie Lehn from Strasbourg, who gave a scientifically brilliant and fascinating talk. Immediately following this talk, the poster prize ceremony took place, and ECM-30 delivered a total of 21 prizes to promising young scientists. A list of the winners and the sponsors will be published on the ECA website. Short presentations invited the participant to future meetings, in particular, the crystallography school in Warsaw and ECM-31 in Oviedo. With short speeches from Piero Macchi, Alessia Bacchi, and Katharina Fromm, the conference was declared closed.

Apéro at the Basel Zoo next to the new modern elephant territory, just prrior to the conference dinner.

Some 60 participants had the opportunity to visit the SwissFEL just some weeks before its inauguration. As further social events, some 30-40 persons visited the Roche and Novartis Campus, and about the same number participated in the historical city tour, while others chose to participate in a guided tour through the zoo before the conference dinner.

In total, 931 participants from 47 countries were registered, showing that ECMs are not only visible in Europe but throughout the world. Indeed, participants from as far as Australia, Malaysia, Ecuador, Brazil, Mexico, Singapore, Canada, Taiwan, Hong Kong, Japan, the US or Korea were present. Close to 1/3 of all participants was female. 178 participants came from Switzerland, 166 from Germany, 116 from the UK. The fact that 47 different countries were present shows that the mobility of scientists across borders is very important for our community. Hence, the fact that governments hinder scientists from traveling is not acceptable as pointed out also in the opening ceremony by Swiss officials. A few registered members could not attend due to last minute visa issues.

Assembling in front of the PSI School building, ready for the SwissFEL tour at Paul Scherrer Institute.

The participation to the conference microsymposia proved to be very good and intense from the first to the last day including the closing ceremony. In particular, the exhibitors appreciated the conference center allowing an excellent mix of their exhibition and the participants. Also the professional tools of the professional Congress organizer (Congrex, Basel) such as the on-line program proved to be running perfectly. The atmosphere was thus overall excellent with a lot of smiles on people's faces. The opening with chemical experiments, the newly introduced Science Slam and the conference dinner at the zoo were perceived as "charming highlights" in addition to the top scientific talks of the conference. As an experience also from previous ECM's, it was hard to predict which sessions would be attended by how many delegates. It thus happened that some rooms got packed with people standing inside and outside of the room, despite the fact that we had taken into account the results/numbers from previous ECMs. Serving hot lunches and including this service into the conference fee allowed the participants to stay permanently in the conference venue, using the time for discussions with other participants and exhibitors.

8th Erwin Felix Lewy Bertaut Prize (ECA/ENSA) winner Linda Reinhard from the Department of Cell and Molecular Biology of the Karolinska Institute at DESY, Hamburg during the prize presentation. Right: Alessia Bacchi (president ECA), left: Udo Heinemann (Vice president ECA).

Concerning satellite meetings, there was a total of eight such workshops/meetings, organized mainly before ECM-30:

- PSI Powder Diffraction School PDS2016 – Modern Synchrotron Methods (PSI Villigen)
- Robert F. Stewart School on Electron Density and Related Properties (the University of Lorraine, Nancy, France)
- Young Crystallographers ECM-30 Satellite Meeting (Pharmacenter, University of Basel)
- Crystallography in the Pharmaceutical Industry Workshop (Biocenter, University of Basel)
- The CSD Python API: A Foundation for Innovation (Biocenter, Basel)
- High Data Rate MX Satellite Meeting (Biocenter, Basel)
- A Workshop on Methods in Crystallographic Computing (Lossburg-Wittendorf, Germany)
- SMARTER 5 Meeting – Structure elucidation by combining Magnetic Resonance, Computational Modelling and Diffraction (University of Bayreuth, Germany)

Young Crystallographers Mixer in the "Bar Rouge", displaying the ECM30 logo even before the conference start at the top of the Messetower, 105 meter above Basel.

The Young Crystallographers, for instance, had organized a satellite meeting on Sunday at which some 25 members participated. The Pharmaceutical Industry workshop counted 60 participants and was also held on Sunday. Most of the venues for these satellite meetings were at universities or research centers, bringing them closer to research but also benefitting from lower infrastructure costs.

For setting up the program, we counted on the help of all the SIGs and GIGs. However, we would suggest programming half a day by the local organizer to allow the ECM's to include local and global trends faster, attracting new communities and build up new SIGs.

ECM30 in Basel showed that crystallography is essential for today's science topics. Not only fields of physics, chemistry and biology are merging, but also the used technologies are widening, as reflected by talks involving microscopy or local probing techniques. We hope this will also be reflected in future teaching efforts in Switzerland, maybe by a common effort of universities.

Only thanks to the generous support from governments, science foundations and the support from volunteers all over the world, it was possible to organize this conference in the beautiful city of Basel. Overall, the conference was very successful from a scientific and organizational point of view. It was worth taking the risk to bring such a conference to Switzerland. We are glad having proposed it to the General Assembly of the Swiss Society for Crystallography in 2010 and thank all the participants, boards, and sponsors for making the meeting a success.

Appendix: Picture Galerie from the Plenary and the Keynote Lectures

Plenary Lecturers:

Ada E. Yonath
Nobel Prize Laureate in Chemistry, 2009

Jean-Marie Lehn
Nobel Prize Laureate in Chemistry, 1987

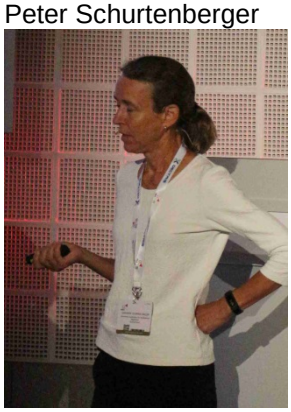
Keynote Lecturers:

Peter Schurtenberger

Francesca Fabbiani

François Diederich

Birger Dittrich



Sandra W. Jacob

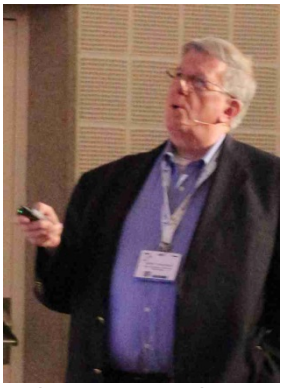
Marcus Neumann

Jan Pieter Abrahams

Simon Parsons

Makoto Fujita

Oliver Thomas



Robert von Dreele

Petra Fromme


Werner Paulus


Bob Cernik


Marek Grzelczak


Martin Schmidt

Picture Credits: Pictures have been contributed by numerous student and senior helpers. We gratefully acknowledge them here, but also the great effort of these “volunteers” before, during and after ECM30. A debriefing party in Bern, January 19, 2017, is especially dedicated to them.

Some Views and Statistics on ECM30

Key Facts:

931 registered delegates from **47** countries
30 international exhibitors
835 submitted abstracts
Almost **300** speakers presented in **75** sessions
296 women out of 931 delegates
467 poster submissions
250 oral submissions
36 retired scientists from 15 countries
179 students from 32 countries

Final Registration numbers:

ECA Individual Members:	152
Non-Members:	419
Students:	179
Retired:	36
Accompanying Persons:	26
Exhibitors:	94
Speakers:	25
Total:	931

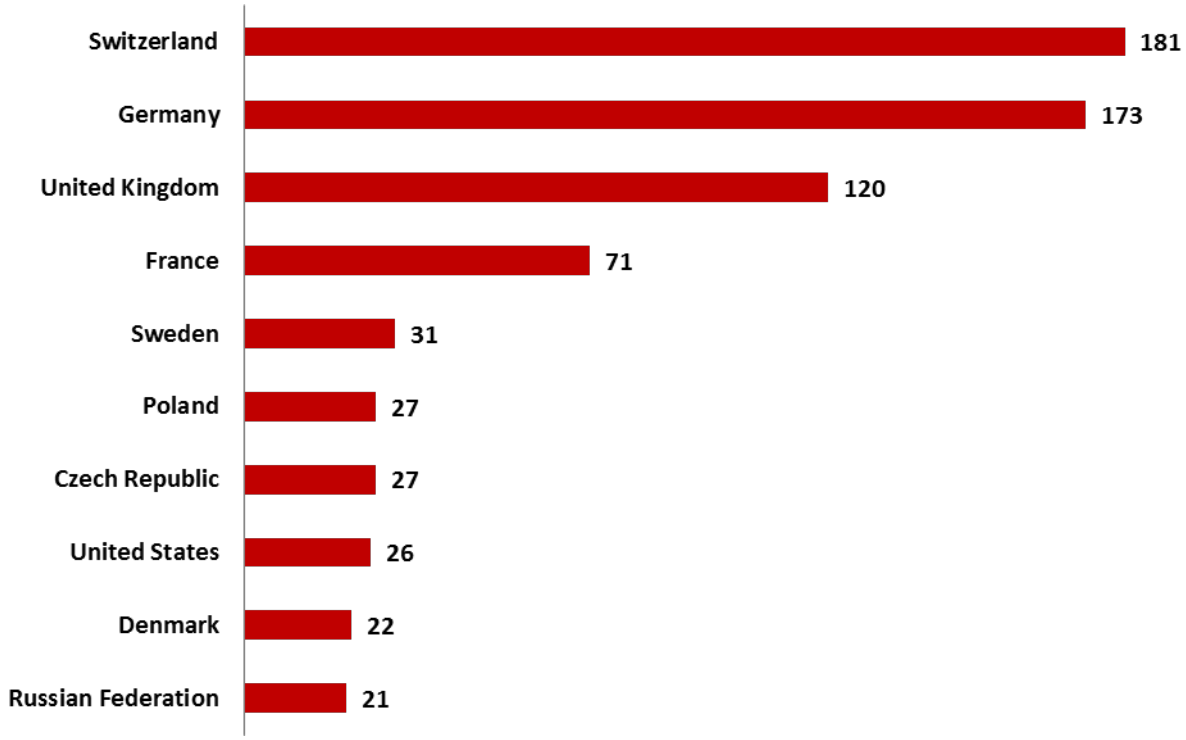
Submitted Abstracts:

Orals:	250 (2 not registered)
Posters:	467 (82 not registered)
Invited Speakers:	102 (1 not registered)
Keynote Speakers:	16
Total:	**835**

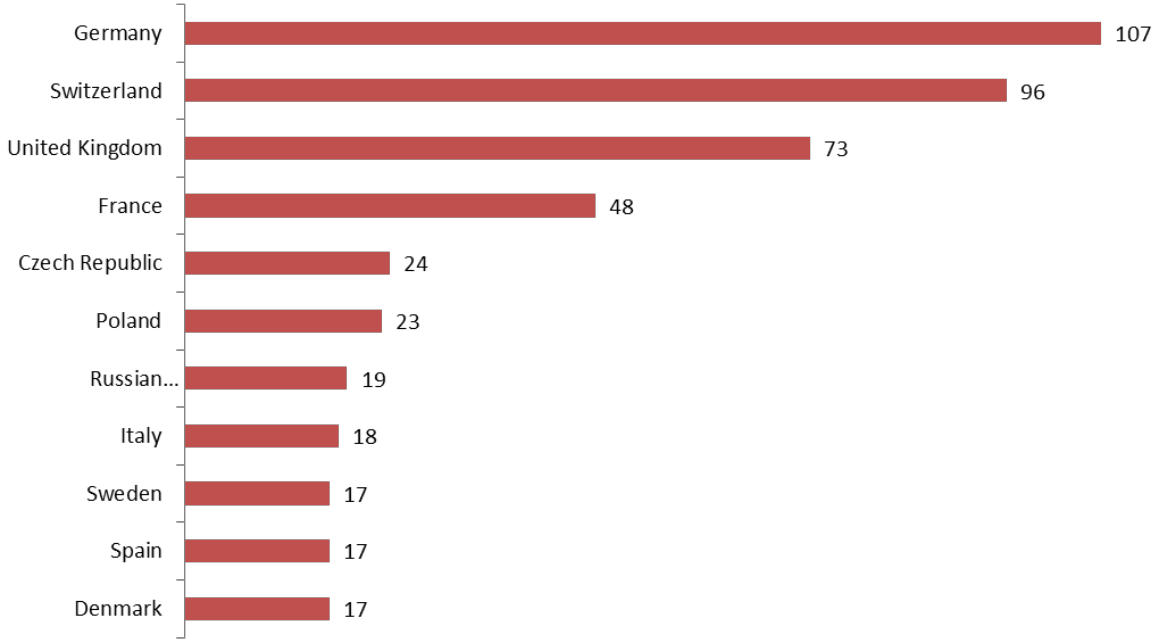
Top 14 Abstract Topics:

Topic name	No. subm. abstracts
Minerals and materials	24
Polymorphs, cocrystals, solvates, salts: a jungle for scientists and industries	21
Molecular interactions in crystal packing and molecular assemblies	19
Molecular recognition, supramolecular chemistry and crystal engineering	18
Biophysical characterization and crystallization	17
Solid state oxygen fuel cell, hydrogen storage & battery materials	17
Data collection and processing software (XFELS & synchrotrons)	16
Combining x-ray diffraction and other techniques for in situ and operando studies	16
Structural information in drug design	14
Hot structures in biology	14
Structural disorder and materials' properties at ambient and non-ambient conditions	14
Protein & glycobiology structure determination	13
Molecular compounds and MOFs at ambient conditions and under high pressure	13
New developments in phasing and refinement	12

Top 10 Countries (number of participants):



Top 10 countries (number of abstracts):



Exhibitors:

Name of Exhibitor	Name of Exhibitor
Anton Paar GmbH	Molecular Dimensions
Bruker	Nanotemper
CCDC - Cambridge Crystallographic Data Centre	NatX-ray
CSEM SA	Oxford Cryosystems
Dectris	Oxford University Press
Douglas Instruments	PANalytical
ECA	PDBe
ECM-31	Rigaku
ECM-32	Rigaku
Excillum	SCANZ
Formulatrix	STOE
Huber Diffraktionstechnik	Taylor & Francis
imXPAD	TTP Labtech
IUCr	Walter De Gruyter GmbH
marXperts	Xtal
	Total 30 companies

Sponsors:

Some external reports:

http://dgk-home.de/science-slam-ecm-30-basel/

http://dgk-home.de/ecm-30-basel-2016/

Final Budget of the 30th European Crystallographic meeting

The budget is provided by the professional congress organizer *Congrex Switzerland*. Noteworthy, due the agreement with the European Crystallographic Association (ECA), the positive balance will be shared between SGK and ECA

	Income	*Expenses*
Travel Bursaries		-13'660.30
Scientific program committee		-10'494.75
Promotion		-5'872.60
Coordination		-700.00
Administration of the participants		-8'134.80
Local Staff		-13'119.90
Printed matter		-24'721.71
Internet		-18'868.48
Equipment		-209'642.95
Social Program		-30'069.00
Young Crystallographer Mixer		-4'588.00
Conference Dinner	+32'400.00	-40'104.70
Catering		-94'897.70
Bank charges		-687.92
Organization Costs		-150'533.20
Registrations	+445'714.79	
Registration costs		-15'418.53
Exhibition	+150'000.00	-40'507.15
Sponsorship banners	+3'100.00	
Sponsored microsymposia	+18'200.00	
General Sponsorship	+49'215.90	
TOTAL	+698'630.69	-682'021.47
BALANCE	+16'609.22	

Reports of Satellite Meetings of the ECM-30

The international school on charge density and related properties
Nancy, August 23-26, 2016

Piero Macchi, University of Bern

The Robert F. Stewart School on Charge Density and related properties, a satellite of the 30th European Crystallographic Meeting, took place in Nancy at the Laboratory of Crystallography, Magnetic Resonance and Modelling (CRM^2) of the University of Lorraine, organized by Nicolas Claiser, Mohamed Souhassou and Piero Macchi, with the active contribution of the entire CRM^2 laboratory, directed by Dominik Schaniel.
The school was named after Robert Stewart, who unfortunately passed away on September 2015. Bob Stewart was one of the fathers of the modern charge density analysis. His contributions in the decades 1960s-1980s were enormous and this school was an occasion to teach the younger researchers about the historical developments in this field.
The aim of this School was to teach all participants the basic knowledge about paired and unpaired electron density distributions using experimental data. 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 precise spin resolved electron distributions in magnetic materials.
This school was dedicated to determination of the 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.
Theoretical lectures and tutorial sessions were offered to the participants (35 students and 17 lecturers and tutors), with hands-on sessions using software developed by the organizers, like XD2016, MoPro and MollyXN. Some new methodologies were presented and discussed, such as refinement of core polarizations, simultaneous charge and spin density refinements and the X-ray constrained wave function method.
The school ended with a round table about application of topological analysis and electrostatic properties of a charge distribution in chemistry, biochemistry and physics. The discussion focused also on the role of the spin density in material science and how to combine experimental and theoretical methods for a better electron density modeling.

School website: http://stewart-school.event.univ-lorraine.fr/
Invited Speakers/Instructors:
Dr. Nicolas. Claiser (Université de Lorraine, France)
Dr. Maxime Deutsch (Université de Lorraine, France)
Dr. Georg Eickerling (University of Augsburg, Germany)
Prof. Enrique Espinosa (Université de Lorraine, France)
Dr. Louis Farrugia (University of Glasgow Scotland UK)
Dr. Alessandro Genoni (CNRS/Université de Lorraine, France)
Prof. NourEddine Ghermani (ECP Paris, France)
Dr. Béatrice Gillon (LLB, Saclay, France)
Prof. Benoit Guillot (Université de Lorraine, France)
Dr. Arsene Gukasov (LLB-CEA Saclay, France)
Dr. Christian Jelsch (Université de Lorraine, France)

Prof. Maciej Kubicki (University of Poznan Poland)
Prof. Claude Lecomte (Université de Lorraine, France)
PD Dr. Piero Macchi (University of Berne, Switzerland)
Dr. Jacob Overgaard (Aarhus University Denmark)
Prof. Paul Popelier (University of Manchester, UK)
Prof. Dietmar Stalke (University of Göttingen, Germany)

Figure: Group Photo at the University of Lorraine.

Report Powder Diffraction School

Report on the PSI Powder Diffraction School 2016

Antonio Cervellino, Paul Scherrer Institute

This latest edition of the biennial PSI Powder Diffraction School, dedicated to the Modern Synchrotron Methods, has taken place on five full days, from 22 to 26 August 2016, at the Swiss Light Source synchrotron, part of the Paul Scherrer Institute. The students, limited to 40 in number, were guided through five days of lectures, practicals, and tutorials, aimed at giving them an operational knowledge of the techniques and methods of synchrotron x-ray powder diffraction, starting from general theory through experimental wisdom to target-oriented data analysis.
The IUCr support enabled us to offer 4 students the IUCr Young Scientist Award, including travel and subsistence support for frequenting the school. The award ceremony was held on the last day, in the afternoon of August 26, 2016, just prior to the Conclusions and Final Remarks session.
The school began on Monday, August 22, 2016 with a morning session including general introductory lectures about powder diffraction. The following afternoon session comprised lectures on crystal structure solution, instruments and experimental techniques, quantitative phase analysis and a short panoramic overview of data analysis programs. The day closed with the Bruker Welcome Reception, an apero and get-together.

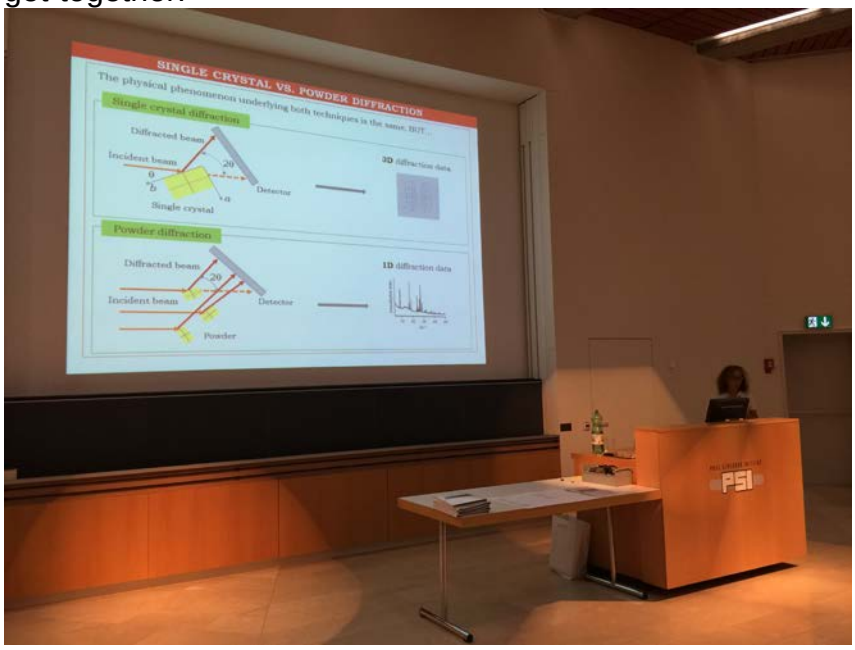


Photo 1: Taken during one of the general introductory lectures about powder diffraction, the “Introduction to Powder Diffraction” given by Dr. Simona Galli, University of Insubria, Como, Italy

Tuesday morning (August 23) was dedicated to lectures on two most important methods – total scattering and peak profile analysis – to extract structural and microstructural information. The afternoon menu offered two more exotic lectures - about complementarity of neutron powder diffraction and about perspectives in structure analysis – followed by the first of five practical sessions. For the practical sessions the students were divided in five groups, yielding a manageable number of 8 students per group. The groups were then in turn attending five different practical sessions, of about 2 hours each, that were repeated five times – the first on Tuesday afternoon, the following four taking the whole of Wednesday – so that each group could attend all five practical sessions. Those sessions were

a) Experimental practice at the Powder diffraction station of the X04SA-MS beamline at the Swiss Light Source synchrotron at the Paul Scherrer Institute;

b) Sample preparation methods, held at the Crystallization facility of the Swiss Light Source;
c) Guided visit to the SINQ neutron spallation source, sited as well at the Paul Scherrer Institute;
d) Guide to post-processing of the data, explaining the passage from channel-counts raw data to equally spaced, corrected and merged angle-intensity-error data;
e) Software installation session, propedeutic to the data analysis sessions held in the following days.

Among these, of course, practicals a) and b) are the most important in the spirit of this School, aiming to give the students a practical understanding of synchrotron x-ray powder diffraction experiments. Therefore all the various procedures related to sample handling and preparation and to beam optimization, energy and detector settings choice, and data acquisition were covered – with all relevant pitfalls and things to know.

Photo 2: Friday morning: Debussy2.0 tutorial session

Thursday morning, after the conclusion of the practical sessions, started with the first pair of parallel tutorials on data analysis. As powder diffraction is a rich multipurpose technique, many different software programs have been developed in time to obtain a certain type of information from the data, be it structural or microstructural. The school included therefore six tutorials, each one lasting about four hours, each dedicated to a different program - and a different analysis target. Due to time restrictions, the six tutorial sessions were organized in parallel running pairs. Therefore, on Thursday morning, the students could choose to attend a tutorial on TOPAS, given by Dr. Michael Evans, Bruker, or one on PdfGetX3 given by Dr. Mauro Coduri, ESRF. Thurdsay afternoon, again two parallel tutorials; this time the choice was between FullProf, explained by Dr. Tom Fennell, SINQ/PSI, and WPPM, introduced by Dr. Matteo Leoni, University of Trento. Friday morning again two parallel sessions. The choice was between FOX, introduced by Prof. Radovan Cerny from the University of Geneva; and Debussy 2.0, with Dr. Antonella Guagliardi and Dr. Federica Bertolotti from the Insubria University and CNR-IC, and Dr. Ruggero Frison from the University of Zurich. In all these tutorial sessions the students were guided in all the steps involved in analyzing one or more datasets (previously collected at the X04SA-MS beamline of SLS, the same of the practical sessions) up to obtaining the desired information (e.g. the atomic structure of a small molecular crystal, microstructural parameters, size and shape distributions of nanocrystals, interatomic distances distributions…). Thursday evening, at the conclusion of the first day of tutorials sessions, the social dinner was held at the Trotte Villigen, an historical rural building in the nearby village of Villigen restructured to hold large events. A catering service provided all participants with a selection of the finest Swiss barbecue.

Photo 3: Thursday evening: group photo before the school's social dinner

To conclude, after the end of the tutorial sessions, on Friday 26 afternoon, the usual session of concluding remarks was held. In this session, all students and teachers were invited in an open discussion about the school in all its aspects, especially to collect opinions and suggestions about what could or should be done differently or improved. After this fruitful discussion, the Young Scientists Award ceremony was held, where the organizers, Dr. Antonio Cervellino and Dr. Nicola Casati, were pleased to deliver the IUCr YSA diplomas to the award winners: Mrs Seham Abdel-Aal; Mr. Wei-Che Lin, PhD; Ms Ines Martins, PhD; Mr. Michal Andrzejewski, PhD.

Photo 4: The IUCr Young Scientist Award diploma ceremony

A final word of thanks to the teachers, who made freely available their knowledge to the benefit of the students:

Federica Bertolotti	Università dell'Insubria & To.Sca.Lab., Como, Italy
Nicola Casati	Paul Scherrer Institute, Switzerland
Radovan Cerny	University of Geneva, Switzerland
Antonio Cervellino	Paul Scherrer Institute, Switzerland
Mauro Coduri	ESRF, Grenoble, France
Michael Evans	Bruker AXS GmbH, Germany
Tom Fennell	Paul Scherrer Institute, Switzerland
Ruggero Frison	University of Zurich, Switzerland
Simona Galli	Università degli Studi dell'Insubria, Italy
Fabia Gozzo	Excelsus Structural Solutions S.P.R.L., Belgium
Antonietta Guagliardi	CNR-IC & To.Sca.Lab., Como, Italy
Matteo Leoni	University of Trento, Italy
Lynne McCusker	ETH Zurich, Switzerland
Steven Van Petegem	Paul Scherrer Institute, Switzerland
Philip Willmott	Paul Scherrer Institute & Uni Zurich, Switzerland
Dubravka Sisak-Jung	DECTRIS AG, Switzerland

As well thanks to the students, who attended numerous and did their best to learn the most; to Dr. Romain Sibille, Dr. Paolo Pio Mazzeo, Dr. Ban Voraksmy, Dr. Mathilde Léna Reinle-Schmitt, Dr. Tom Fenell, all of the Paul Scherrer Institute, for the assistance given during the practical sessions; and to

- the sponsors, including the IUCr, the SGK-SSCr Swiss Crystallographic Society, Bruker, DECTRIS, Excelsus Structural Solutions, and of course the Paul Scherrer Institut, which generously supported this edition;
- the secretariat, in the person of Ms. Martina Füglister, who made it at all possible;
- the technical staff of the X04SA-MS beamline, for the support during the practical sessions.

Swiss Society for Crystallography PhD prize

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

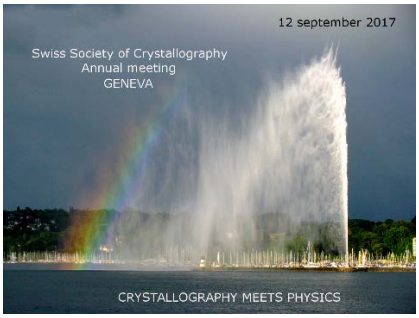
Requirements:
The prize is open to

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 **March 31st 2015 and March 31st 2017**.
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 **31st March 2017** 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)

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.
The award is endowed with CHF 2000.-



Swiss Society for Crystallography
SGK / SSCr
Annual meeting 2017

Tuesday, September 12, 2017
Faculty of Science - University of Geneva
30, quai Ernest-Ansermet – Geneva

Meeting Title:
"Crystallography meets Physics"

The 2017 annual meeting of the SGK/SSCr will take place at the Faculty of Science of the University of Geneva on Tuesday 12th of September 2017. The 2017 annual meeting will focus on various applications of crystallography in physics and will be structured in three main sessions: 1) Diffuse scattering, 2) Femto-crystallography, and 3) Low-dimensional materials and interfaces. Each session will be opened by an invited speaker and completed by two selected oral contributions. A poster session will complete the scientific program of the meeting.

Invited speakers:
Dr. Dmitry Chernyshov, ESRF, Grenoble, France
Dr. Jörg Standfuss, PSI, Villigen, Switzerland
Dr. Marco Gibertini, EPF, Lausanne, Switzerland

Contributions are welcome on any of the following topics:

- Novel experimental and analytical methods
- In-situ and in-operando crystallography
- Charge density and bonding analysis
- Molecular crystals
- Aperiodic crystals
- Low dimensional materials
- Disorder and diffuse scattering
- Design and synthesis of novel materials

Registration and abstract submission:
from May 1st on the website: http://SSCR-2017.unige.ch/
Deadline for abstract submission: July 1st, 2017

Program

Monday 11th of September:

19:30 – 22:30	Get together dinner (separate registration)

Tuesday 12th of September:

09:30 – 10:00	Welcome Coffee and Registration
10:00 – 10:10	Opening ceremony
10:10 – 10:50	**Session 1** - Invited Dr. Dmitry Chernyshov – ESRF, Grenoble
10:50 – 11:10	Session 1 - Contributed talk 1
11:10 – 11:30	Session 1 – Contributed talk 2
11:30 – 11:40	**SSCr PhD prize ceremony**
11:40 – 12:10	Prize-winner invited talk
12:10 – 13:50	**Lunch and Poster Session**
12:50 – 13:50	Assembly of the Swiss Society for Crystallography
13:50 – 14:30	**Session 2** – Invited Dr. Jörg Standfuss – PSI, Villigen
14:30 – 14:50	Session 2 – Contributed talk 1
14:50 – 15:10	Session 2 – Contributed talk 2
15:10 – 15:40	**Coffee Break**
15:40 – 16:20	**Session 3** – Invited Dr. Marco Gibertini, EPF Lausanne
16:20 – 16:40	Session 3 – Contributed talk 1
16:40 – 17:00	Session 3 – Contributed talk 2
17:00 – 17:10	**Poster award ceremony**
17:10 – 17:20	**Closing remarks**

ECM31 in Oviedo

ECM31
31st Meeting of the European Crystallographic Association
22/27 August

OVIEDO 2018 SPAIN

Lecture hall of the Palacio de Exposiciones Congresos of Oviedo by Santiago Calatrava

http://ecm31.ecanews.org/en/

4th European Crystallographic School (ECS4)

"High throughput structure analysis - from routine chemical problems to advanced applications"

http://ecs4.ecanews.org/index.html

5th German-Swiss Conference on Crystal Growth

March 8 – 10, 2017

Freiburg, Germany

http://dkt2017.de/

Photonics Spring Workshop 2017

The Paul Scherrer Institute is very happy to invite you to our:

Photonics Spring Workshop 2017

Date: 10 – 12 April 2017

Venue: Fachhochschule Nordwestschweiz, Brugg/ Windisch, Switzerland

Workshop Chairs: Dr. Luc Patthey, Prof. Dr. Philip Willmott, Paul Scherrer Institut

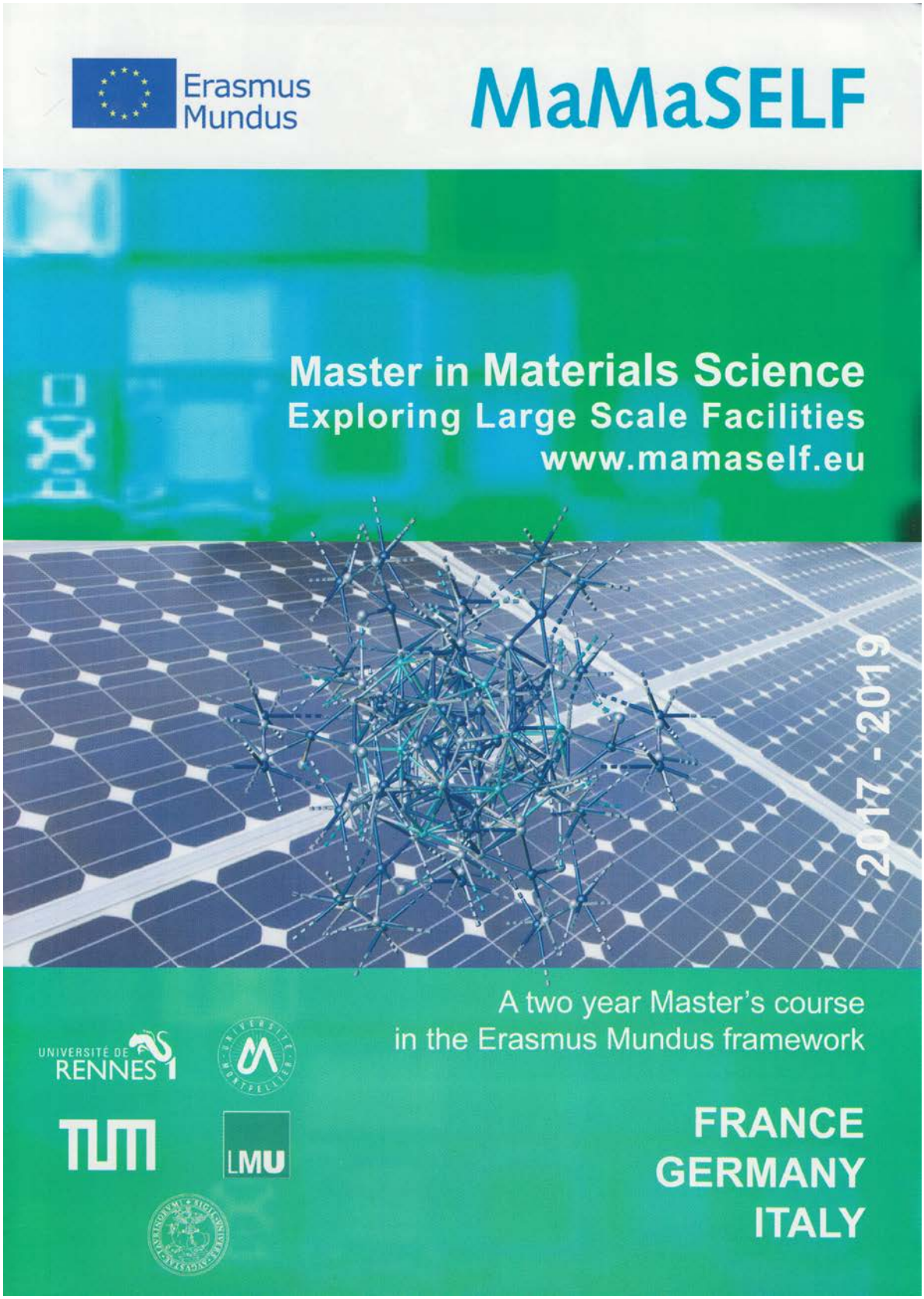
The workshop will focus on the SwissFEL Athos soft X-ray instruments and the SLS-2 upgrade project.

We invite you to participate in this workshop that will be guided by science rather than machine design, focusing on the identification of grand challenges in condensed-matter research, magnetism, chemistry, catalysis, imaging, and structural biology.

The workshop will include Keynote Lectures from the following speakers:

Magnetism – Prof. Dr. Stefan Eisebitt, Max-Born-Institut Berlin
Surface Chemistry – Prof. Dr. Anders Nilsson, Stockholm University
Imaging – Prof. Dr. Chris Jacobsen, Argonne National Laboratory
Structural Biology – Prof. Dr. David Stuart, University of Oxford
Heterogeneous Catalysis – Prof. Dr. Bert Weckhuysen, Utrecht University
SCES/CM – Prof. Dr. Dragan Mihailovic, Jozef Stefan Institute
Condenced Matter - Prof. Dr. Jerry Hastings, SLAC National Accelerator Laboratory

Master in Materials Science



https://www.mamaself.eu/

To.Sca.Lake 2.0

Dear Colleagues,

Following the successful edition of spring 2015, we are pleased to announce that the 2nd To.Sca.Lake Summer School will take place in Como, Italy, from May 29th to June 2nd 2017.
Information on the Program, Venue, Registration and availability of Grants for young attendees can be found on the tsnl.lakecomoschool.org webpage.
Extended Tutorials on Debussy and PDFGui are scheduled within the Program. In order to optimize their organization, the maximum number of participants is fixed at 50, on a first-come first-served criterion. Registration is already opened!
The Summer School “To.Sca.Lake 2.0: Total Scattering for Nanotechnology on the Como Lake” offers an extended overview on Total Scattering Techniques (from X-rays to visible light) for Nanotechnology, complemented by lectures on synthesis and applications of advanced nanomaterials. Theoretical, experimental and modeling aspects of Wide and Small Angle scattering methods will be integrated by hands-on tutorials on well renowned programs for DSE and PDF Analysis (Debussy and PDFGui) and Demo sessions on SAXS and Light Scattering. The Workshop is open to all aspiring scholars and scientists in any area related to Nanoscience and Nanotechnology, and it is especially addressed to PhD students and young postdocs. The aim of the school is to deepen into both theoretical and applied frontier developments in these fields.

The School Directors
Antonella Guagliardi (Institute of Crystallography, CNR)
Norberto Masciocchi (University of Insubria)

Job Opportunities

Researcher/Senior Researcher for Instrument (HEIMDAL) Design and Construction at the European Spallation Source (ESS) 891313

Aarhus University (AU) is contributing to the European Spallation Source ESS in Lund, Sweden, by leading the construction of the proposed combined neutron powder and small angle scattering instrument HEIMDAL. In this connection the Department of Chemistry at Aarhus University offers a fixed-term position as researcher or senior researcher (Instrument Lead Scientist at ESS) for a total of 4 years. The intended starting date is 1st of October 2017 or as soon as possible thereafter.

Description of work:
The mission is to supervise the design, and define the scientific scope of the neutron instrument HEIMDAL at ESS. The long term goal is to become Instrument Responsible, once the instrument has moved into the operations phase. The Instrument Lead Scientist will work closely together with the Instrument Lead Engineer forming an instrument team. The Instrument Lead Scientist and Instrument Lead Engineer, together with a core team of specialists from the instrument consortium at ESS in Lund will define the scientific specifications of the instrument. The Instrument Lead Scientist provides scientific project leadership, including defining scope scientific and initial hot commissioning experiments. He/she must also be active in a scientific program on the leading edge in the field of materials science.

Your role:
- Provide the scientific and technical leadership of the HEIMDAL instrument project.
- Deliver scientific plans for the proposed scientific scope of HEIMDAL.
- Prepare the detailed design together with the core instrument team. The project is dependent on passing the Tollgate 2 review.
- As part of the Core Instrument Team, deliver a neutron scattering instrument according to the scope, budget and schedule determined at Tollgate 2 review as defined by ESS rules

Your tasks:
- Provide scientific guidance and support to HEIMDAL work package team.
- Lead the planning of the HEIMDAL work package and contribute to its implementation.
- Assemble and coordinate the HEIMDAL work package team.
- Delegate work packages to Technical Groups and In-Kind partners.
- Provide final approval of technical designs.
- Manage scientific and technical project changes in accordance with project goals.
- Represent the project during Scientific and Technical Advisory Panel (STAP) and Scientific Advisory Committee reviews.
- Assist in tracking and ensuring timely project deliverable using ESS processes and appropriate tools.
- Monitor, communicate, and report on progress according to the ESS Construction Project requirements.
- Participate in risk reviews and help manage risks.
- Providing requirements to ensure the integration of the scientific capabilities of the instrument software, sample environment and support labs.
- Conduct your own research using neutron/X-ray powder and small angle scattering.
- To a leaser extend participate in teaching activities.

Your qualifications:

- PhD in Physics, Chemistry or Materials Science.
- Experience in scattering techniques, preferably powder diffraction.
- Experience in building and maintaining experimental infrastructure.
- Experience of working in an international environment.
- Excellent oral and written English skills are a prerequisite.

Further expectations for the two levels of appointment are:

Researcher: Candidates must demonstrate potential for excellent research and industrial or public sector collaboration. Extensive postdoctoral training or similar is expected (see below for tenure-track program)

Senior researcher: Candidates must have an excellent record of independent research accomplishments including experience in construction and operation of experimental facilities for X-ray or neutron science, in the preparation of technical reports, collaborations with industry or public organisations, scholarly achievement, an established record of external funding, as well as concomitant strong evidence of emerging leadership in their field.

Applicants are expected to meet the criteria listed for senior researcher in: http://scitech.medarbejdere.au.dk/fileadmin/site_files/scitech.medarbejdere.au.dk/files/Evaluation_Criteria.pdf

We offer an international and dynamic working environment, where time will be spent both at Aarhus University, Denmark and at the ESS, in Lund, Sweden. The time spent in Aarhus and Lund is expected to vary during the project, initially most of the work can be carried out in Aarhus, but as installations starts more time will be spent in Lund. After the commissioning of the instrument, ESS is expected to offer you a position as a local contact for the instrument in Lund, Sweden, while an affiliation to Aarhus University is maintained.

Place of work and area of employment:
The place of work is Langelandsgade 140, 8000 Aarhus, and the area of employment is Aarhus University with related departments.

For further information on the position please contact Associate Prof. Mogens Christensen (mch@chem.au.dk, tel +45 87 15 53 39) or Head of Department, Prof. Birgit Schiøtt (birgit@chem.au.dk, tel +45 87 15 59 75). Application procedure

Application Deadline: 30.04.2017

More Information:
http://chem.au.dk/profil/ledige-stillinger/videnskabelige-stillinger/?tx_peoplexs_pi1%5Bid%5D=891313&tx_peoplexs_pi1%5BportalId%5D=5285&tx_peoplexs_pi1%5Baction%5D=show&tx_peoplexs_pi1%5Bcontroller%5D=Vacancy&cHash=64badaed0231862ece657d5c0ef674b5

Expert in X-ray techniques and crystallography

The Institute of Physics at EPFL is seeking to hire an expert in X-ray techniques and crystallography in charge of the Institute's X-ray facilities.
Operating within the Institute's Crystal Growth Facility, the successful candidate will work with laboratories across the EPFL campus to maximize their scientific output.

Responsibilities include:

- Assist EPFL laboratories with planning and execution of measurement, including single crystal and powder diffraction, texture and thin-film analysis etc.
- Partake in analysis of data, including structural refinements, and interpret results in relation to other techniques
- Train researchers in diffraction techniques and structure refinement
- Author concise reports and relevant paragraphs in scientific publications.
- Maintain and expand a state of the art suite of in-house instrumentation including diffractometers, sample changers, LT devices, HP accessories etc.
- Maintain relevant crystallographic software and train collaborators in their use.

Desired qualifications:

- Solid experience with X-ray methods such as diffraction of single crystals (including Laue method), powders (including diffuse and total scattering), thin films, textures
- Technical expertise in X-ray instrumentation, including ability to specify equipment to be procured, maintain, service and upgrade existing instrumentation.
- Experience with synchrotron and other large scale facility methods are an advantage
- Experience with experiments under non-ambient conditions (P,T)
- Capability and desire to train diffraction techniques and crystallography
- Experience with complementary scattering techniques such as electrons, neutrons etc.
- A broad understanding of complementary scientific disciplines such as Raman, NMR, magnetic structures, phase transitions, electron microscopy, crystal optics and X-ray fluorescence or spectroscopy would be favorable.

What we offer:

EPFL is a leading university with strong emphasis on basic sciences, engineering and life sciences. Multiple laboratories in physics, chemistry and materials science rely on high level diffraction and crystallographic analysis. As responsible for Physics' X-ray facilities of the Crystal Growth Facility, the successful candidate will have the opportunity to interact and collaborate with scientists from multiple disciplines and contribute to a broad span of activities and exciting science.
We offer internationally competitive salaries, excellent working conditions and a state-of-the-art infrastructure in a highly dynamic and international environment.
Start date: as soon as possible; **Deadline for application:** until the position is filled
Contract: Initial appointment is 2 years with possibility for extension, including possibility of promotion to permanent staff.
Motivated and qualified candidates should submit their application including: detailed CV including list of technical skills (techniques and software mastered), teaching/training and publication record as well as names of at least 3 references to arnaud.magrez@epfl.ch and henrik.ronnow@epfl.ch.

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)	20.02.2018 (no beam in 2019 due to guide upgrade)	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	approx.. Jan. 2018	www.esrf.eu/ UsersAndScience/
short term proposals	01.03.2017	
ILL: Institut Laue Langevin		
All instruments	Feb., Sept.	www.ill.eu
FRM II: Heinz Maier-Leibnitz		
All instruments	21.07.2017	www.mlz-garching.de/user-office
Rapid access program	21.04.2017 28.06.2017	www.mlz-garching.de/user-office
SNS Spallation Neutron Source Oak Ridge	12.04.2017	neutrons.ornl.gov

Calendar of forthcoming meetings

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

			Application Deadline
2017			
March 8-10	Freiburg, Germay	German-Swiss Conference on Crystal Growth http://dkt2017.de/	31.01. (early bird)
June 11 -22	Zurich	Zurich School of Crystallography http://www.chem.uzh.ch/linden/zsc/	16.01.
July 02 - 07	Warsaw, Poland	4th European Crystallographic School (ECS4) http://ecs4.ecanews.org/index.html	01.04. (early bird)
Aug. 21-28	Hyderabad, India	The XXIV Congress & General Assembly of the International Union of Crystallography (IUCr-2017) http://www.iucr2017.org	31.05. (early bird)
Sept 12	Geneva	Annual SGK/SSCr-Meeting http://www.sgk-sscr.ch/en/geneva2017/	
2018			
Aug. 21-29	Oviedo, Spain	31th Meeting of the European Crystallographic Association http://ecm31.ecanews.org/en/index.php	to be announced
June 1-10	Erice, Italy	Erice International School on Quantum Crystallography	To be announced
2019			
Aug.	Vienna, Austria	32th Meeting of the European Crystallographic Association http://ecm32.ecanews.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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(If you would like to see your logo here, please contact our treasurer, Dr. Antonia Neels)

Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie
Società Svizzera di Cristallografia
Societad Svizera per Cristallografia

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SGK/SSCr Newsletter (ISSN 1662-5358, online version: ISSN 1662-534X)

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Bank Account: UBS Zürich
IBAN: CH39 0027 9279 C029 1110 0
BIC: UBSWCHZH80A
BLZ: 279

Printing and Mailing: PAUL SCHERRER INSTITUT PSI

The newsletter of SGK/SSCr is published 2-4 times a year in a circulation of 250. Contributions are welcome at any time, as well as illustrations for the cover. Articles in English, German or French may be submitted. Please send all interesting material directly to the editor.
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