Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie
Società Svizzera di Cristallografia
Swiss Society for Crystallography

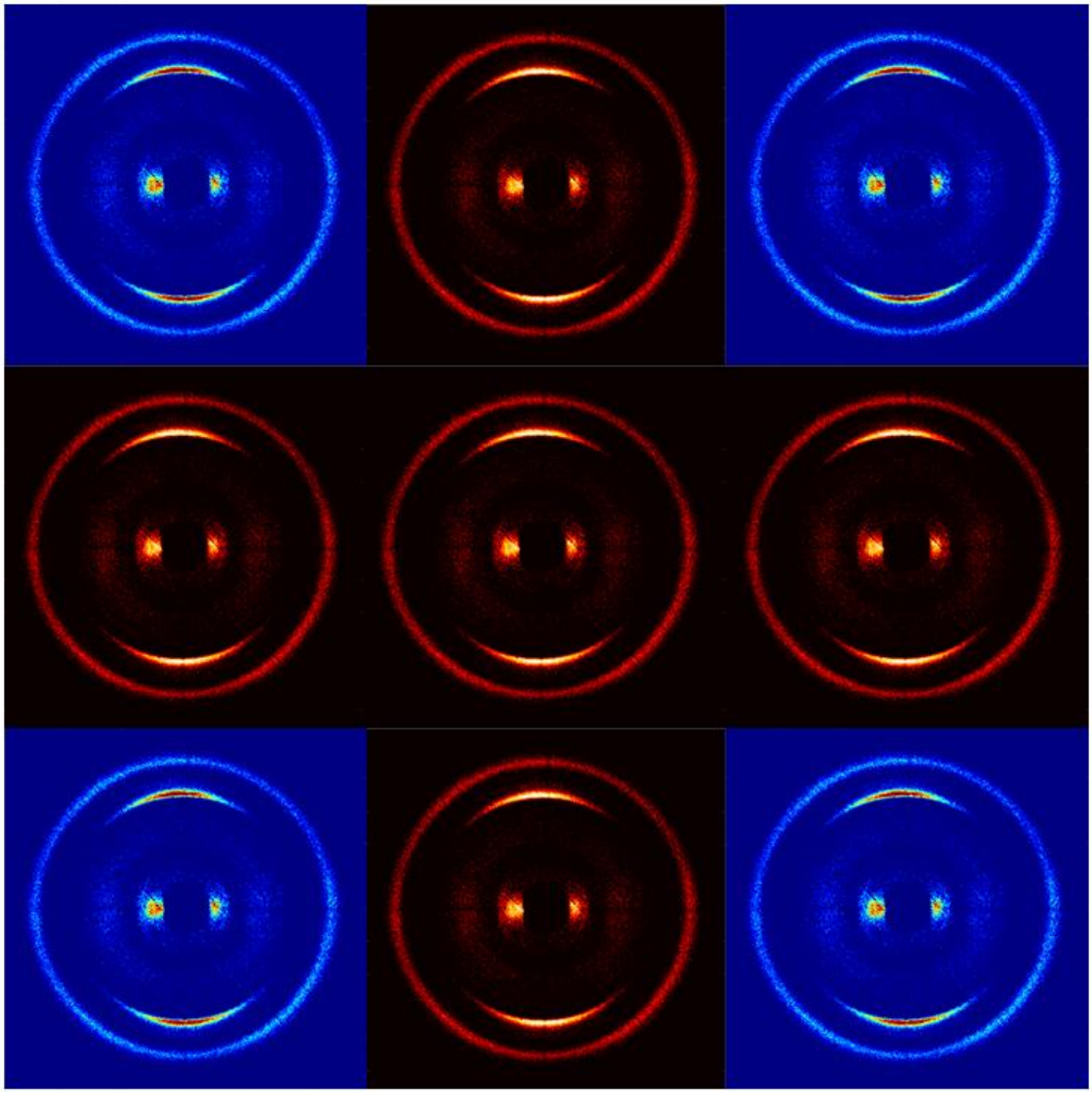
Sektion für Kristallwachstum und Kristalltechnologie
Section de Croissance et Technologie des Cristaux

member of the scnat swiss academy of sciences

SGK / SSCr NEWSLETTER

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

No. 103
April 2020



In this issue:

On the cover:
2D WAXD pattern from mineralized turkey leg tendon, A. Maurya, J. Schwiedrzik, A. Neels, Empa.

SGK / SSCr Newsletter No. 103

The President's Page

Dear Members of the Swiss Society for Crystallography,

It is my pleasure to address a few words to you during this period where science is called upon and challenged to answer the needs of our society.
Crystallography has its special role within the fight against the pandemic crisis we are currently facing. Today's crystallography ranges from X-ray, electron and neutron diffraction approaches to a variety of scattering technologies. Altogether, they provide a unique tool to look in 3D at biomolecules in the context of biological process understanding.
The Covid-19 virus has trimeric protein 'spikes' on its surface, which are able to attach to a receptor protein that is prevalent on cells of the human respiratory system. In addition, there are two long overlapping polyproteins being processed into smaller and functional polypeptides and being essential for replication. The current drug design approach concentrates on the two viral proteases, which are responsible for this process. Looking more deeply at the discoveries of the last few weeks, we realize that an enormous relevant outcome has been achieved with respect to the Covid-19 virus. Here, structural biology is the key and we find a number of new scientific breakthroughs in our crystallographic journals bringing us closer to the end of this pandemic! One of the basic elements is certainly the availability of databases, such as the Protein Data Base (PDB), where a constant international effort has been made by the crystallographic community over the last decades to share 3D structures of increasing complexity. I also welcome the initiatives of the SNSF and others to accelerate research in order to find vaccines and drugs for fighting COVID-19 diseases.
However, I look forward to a safe resumption of our activities!
In September 2019, we had an excellent annual meeting organized by Pascal Schouwink at the EPFL in Sion around the topic 'Energy Materials – From Bulk to Surface Crystallography' where also our PhD prize was awarded to Dr. Luzia German. For our precious Howard Flack lecture series, we had the chance to welcome Prof. Matt Rosseinsky. He traveled through five Swiss institutions and lectured about 'Design of Advanced Materials?' which attracted a broad audience from different fields of science that are connected to crystallography. Inside our newsletter you will find additional information about these respective highlights!
Please join us at our Annual Meeting 2020 at the Department of Chemistry, University of Fribourg on Wednesday 7th of September. The theme will be 'From molecules to nanoparticles in Biology, Chemistry, Physics and Geology'.
Especially for our young crystallographers, this is a great platform for presenting your research and to exchange ideas with and be inspired by the people you get to meet. Please submit your abstracts!
I wish you a safe time and take care.

Antonia Neels
President of the SGK-SSCr

Science in Times of the Covid-19 Pandemic

Tony Linden –The X-ray Crystallography Facility in the Department of Chemistry, University of Zurich houses three single crystal diffractometers and one powder diffraction instrument. The facility supports the research within the department and beyond. Some instruments are accessible to authorized users in self-service mode, while the X-ray team provides full-service single-crystal structure determinations when desired. We are usually kept fully occupied with a constant stream of samples. Now, with Covid-19, the facility has been completely closed for the last several weeks. Users can still access existing data remotely, but no new data collections have been performed. Home Office has actually been quite productive for me. With less interruptions and no children at home, I have managed to complete and submit five papers. Giving lectures via Zoom has proven to be straightforward, although student interaction and feedback is reduced. With research at UZH slowly starting up again from 27th April, everyone is excited to be able to resume their lab work and the X-ray facility will open up again, although access will initially be restricted to members of the X-ray team. Will we be flooded with new samples, or will there be a lag while new compounds are synthesized and crystals grown? Time will tell. Ultimately, we look forward to the return of more normal days.

Antonia Neels – The Center for X-ray Analytics of Empa combines X-ray Diffraction, Small Angle X-ray Scattering and X-ray Imaging expertise for life and materials science with laboratories being located in Dübendorf, ZH and St. Gallen (www.empa.ch/x-ray). For the last few weeks we have been running in minimal operation because of the Covid-19 restrictions, while maintaining important relationships with our project partners and industry. However, most of our colleagues are in Home Office and I'm very happy to see how well this works and that communication is direct and focused. Certain experiments can be managed remotely, even if we concentrate on writing papers and projects. We switched with ease to online video conferences. That also works for teaching, even if jumping between the different tools is challenging! However,

the modality of the examinations is not yet totally clear. I experience a very intense and also direct exchange with colleagues and within the family. We care even more about our colleagues, neighbors and friends. We will ramp up to normal operation from the 27th of April – I am happy to be able to see you soon in person!

Dubravka Šišak Jung – Even in a lockdown, synchrotrons and laboratories are providing services for COVID19 research and preparing for the future. DECTRIS, a company developing and producing X-ray and electron detectors, continues to support current and planned applications.

As an application scientist, my main concern is to consult partners, collaborators and users in their technical and scientific questions. I can say two things about that: I am used to working with different time zones and I am not shy of using virtual meeting platforms. Except for teaching. Since I started my teaching activities (twenty years ago), I thought that good teaching requires physical presence. This year's online version of the HERCULES school has changed that. I based my lecture on interactive digital tools, which resulted in a very engaging atmosphere! This has inspired me to take a course on online teaching. Of course, this meant less time for writing, but after the last submission I needed a break from research articles. But I enjoy writing DECTRIS news. Pieces on the COVID19 research are particularly inspirational, as they demonstrate the power of crystallography and collaborative work (*I even donated my computer power to support folding protein structures (Fold@home)*).

Under the circumstances, things are working well. Still, I can't help to wish to meet all these people again, in person. Don't we all?

Antonio Cervellino – The Paul Scherrer Institute (https://www.psi.ch/) is the Swiss concentration of large scale facilities for X-rays (synchrotron and FEL flavours), neutrons, muons and many labs, notably bio-life, materials, energy, environment, fundamental physics. Between the hills of Villigen AG, straddling the Aare, we make and facilitate science for us, the Confederation, Europe and the world, and we are symbiotic with industry through InnovAARE AG (https://www.parkinnovaare.ch/). For the last few weeks we have been in "limited operation" of the lowest level (only experiments run completely in-house, max. 15% personnel on site) because of the Covid-19 pandemics. Even so we could fulfill a lot of our scientific activity, even with synchrotron experiments in remote control, and we plan now a careful but effective operation ramp-up, so that by the year's end the lost ground may be negligible, depending mostly just on the timely lifting of travel restrictions. Online video meetings have become the norm and will be very important also in the virus-free future. But if you want to come see us in person, we'll be happy to welcome you again soon!

Michael Wörle – Like most of the research facilities in Switzerland, also the Small Molecule Crystallography Center (SMoCC) at ETH Zürich had to close its doors during the lockdown and shift the activities to home-office. We really miss the hands-on work at the instruments and the interaction with the PhD-students, who keep us busy with samples and questions all day. On the other hand, now is the perfect time to take care of the things, which are usually pushed down in the To-Do list by the daily routine work. It was indeed worthwhile to read some crystallographic and also non-crystallographic literature and develop new ideas. We have also experienced that online meetings, emails and phone calls cannot completely substitute the personal contact at the workplace in the long run and we are happy that we are allowed to slowly ramp up our activities at ETH in the coming weeks.

Report: Annual Meeting of the SSCr/SGK 2019

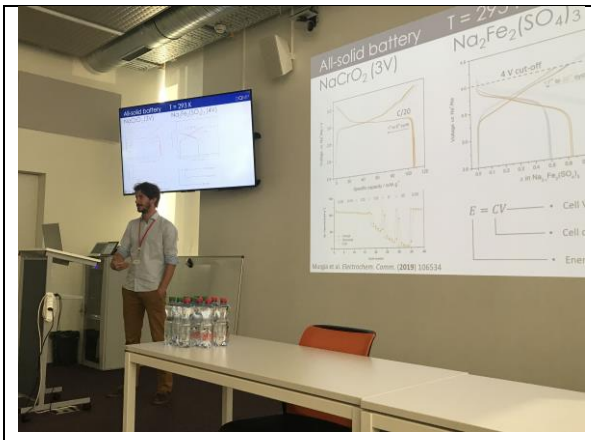
The annual meeting of the Swiss Society for Crystallography took place, for the first time, at the campus Energypolis of EPFL VS, the recently inaugurated satellite of the Ecole Polytechnique Fédérale de Lausanne (EPFL), which focusses on sustainable energy and is embedded in the beautiful Rhone valley and surrounded by the alpine mountains of the Wallis. In line with the venue, the general topic of the meeting was "*Energy Materials – From Bulk to Surface Crystallography*". The meeting aimed at bringing together contributions from different crystallographic disciplines that do not necessarily encounter each other on a daily basis, and attracted talks from electron microscopy to small-angle scattering. Three topical sessions provided a guideline to the general scientific program, centred on (1) *in-situ* and *in-operando* studies, (2) surface-sensitive X-ray scattering and nanoscopic order and (3) structural investigations using X-ray and electron diffraction.

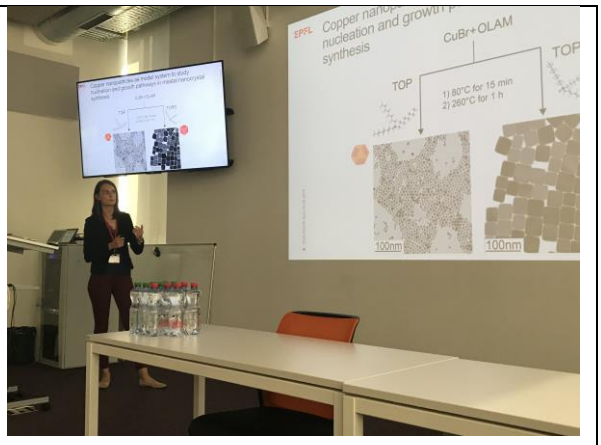
The meeting got off to a good start during the social dinner, for which 28 of the 65 registered participants of the meeting found their way to the vineyards above Sion, and enjoyed a sunny evening accompanied by wine-tasting and the local speciality raclette, as well as a beautiful view of the surrounding 4000 m high mountains.

The next day, the scientific program opened with an exciting lecture on how to improve our understanding of battery materials using powder diffraction, given by our first invited speaker Gwenaelle Rousse from Collège de France and Sorbonne University in Paris.

Battery materials indeed present a perfect playground for crystallography. Gwen was followed by Matteo Brighi (University of Geneva) and Valeria Mantella (EPFL) with topics on *in-situ* studies applied to sodium batteries and the synthesis of electro-

catalysts using nano-chemistry, respectively. Session two was opened by Ilja Gunkel, who was invited from the Adolphe Merkle Institute in Fribourg to speak about the application of grazing-incidence wide- and small-angle scattering (GIWAXS and GISAXS) to nanostructured polymer films. Ilja gave a beautiful and didactic talk on the basics of the methodology and the fabrication of polymer films.





This was followed by Anjani Maurya (EMPA), who also spoke about wide and small angle studies, this time not to decode structural insights of surfaces, but of nanofibers, using SAXS and WAXD. The session closed with Dmitry Chernyshov from ESRF in Grenoble, France, who presented the Swiss Norwegian Beamlines' plan and beamlines upgrades beyond 2020 at the ESRF.

From the discussion of nanoscopic order in the second session, the third dove into single crystal diffraction and atomic level order, starting with a very detailed case study on *operando* and *in-situ* electron diffraction tomography, presented by our third invited speaker Joke Hadermann from the University of Antwerp in Belgium, and highlighting not only the method itself, but also its maturity and pitfalls. This was followed by in-depth structural discussions on a pyrene-based metal-organic framework using X-ray crystallography, by Andrzej Gladysiak (EPFL) in the context of interchromophoric interaction and tuneable fluorescence. The last talk, concluding the scientific program,

brought us back to electron diffraction, now from the perspective of instrumental development, by Gustavo Santiso-Quinones from Eldico Scientifc AG in Villigen.

Embedded into the scientific program, just after the first session and before the General Assembly of the society, was a 10th talk, given by this year's PhD prize winner, Luzia Germann, from the Max Planck Institute in Stuttgart, Germany. Luzia gave us an interesting insight into her doctoral thesis, which dealt with the exploration of polymorphism in co-crystals using mechano-chemistry and *in-situ* powder diffraction during ball-milling. A poster prize was also awarded by votes lodged by all attendees, and went to Chethana Gadiyar for her very didactic poster on the nanocrystal-seeded synthesis of photocathodes. The poster session of 16 posters complimented the scientific program.

The Swiss Society for Crystallography warmly thanks all participants, as well as all our partners STOE, Dectris, Bruker, Rigaku and EPFL Valais who sponsored this meeting. At the time of this newsletter's publishing, most of us find ourselves having to adapt to unusual professional and private situations due to Covid-19. The current times are particular, but we very much look forward to seeing all of you again at our next meeting in Fribourg.

Pascal Schouwink

Scientific Organizer

Announcement of Annual Meeting of the SGK/SSCr 2020

Swiss Crystallographic Association
SGK / SSCr
Annual Meeting 2020

UNI FR
UNIVERSITÉ DE FRIBOURG
UNIVERSITÄT FREIBURG

Wednesday, September 9, 2020

Department of Chemistry
University of Fribourg
Chemin du musée, 9
1700 Fribourg

Call for Abstracts

The 2020 annual meeting of the SGK/SSCr and general assembly will take place at the Department of Chemistry, University of Fribourg on Wednesday 9th of September 2020. Three invited speakers from academia, 15 selected oral presentations and a poster session will show recent developments in the field.

More details on the website: http://frommgroup.ch/sgk-sscr-2020/

Deadlines for Abstract submission:

Oral Presentation: June 30, 2020
Poster Presentation: July 31, 2020

Please use the template .doc available on the meeting website.
Abstract should be sent by e-mail to sgk-sscr-meeting2020@unifr.ch

Registration: The meeting is free of charge, however please register by email to sgk-sscr-meeting2020@unifr.ch before the 01.09.2020.

“From molecules to nanoparticles in Biology, Chemistry, Physics and Geology”

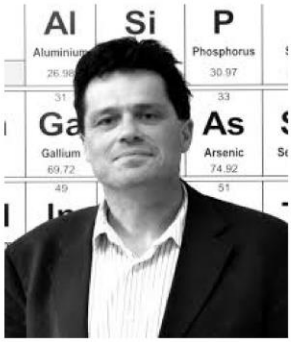
Tentative program:

9.00-9.30	Registration and Poster session
9.30 - 9.45	Welcome message
9.45 - 10.30	**Keynote 1: Robin Teufel, Freiburg**
10.30 - 10.45	Coffee break and Posters
10.45-12.15	Session 1 (15 min talks); 5 talks selected from the abstracts
12.15 - 13.00	Lunch and Posters
13.00 – 14.00	General Assembly of the SGK
14.00 – 14.45	**Keynote 2: Catherine Housecroft, Basel**
14.45 – 15.30	Session 2 (15 min talks); 5 talks selected from the abstracts
15.30-15.45	Coffee Break and Posters
15.45 - 17.15	Session 3 (15 min talks); 5 talks selected from the abstracts
17.15 - 18.00	**Keynote 3: Nicola Hüsing, Salzburg**
18.00	Poster Prize Winners announcement and closing ceremony

Swiss Society for Crystallography

Howard Flack Crystallographic Lectures Series

Prof. Dr. Matthew J. Rosseinsky
Department of Chemistry, University of Liverpool, Liverpool L69 7ZD, UK



Lecture Series:

Design of Advanced Materials?

Monday, **4 November 2019, 14:15**
Paul Scherer Institute
PSI East, room OSGA/EG06 (in front of the OASE mensa), 5232 Villigen

Tuesday, **5 November 2019, 10:00**
CSEM Neuchâtel
Rue Jaquet-Droz 1, CH-2002 Neuchâtel

Wednesday, **6 of November 2019, 17:00**
University of Fribourg
Main auditorium, Chemistry Department, Chemin du Musée 9, 1700 Fribourg

Thursday, **7 November 2019, 17:15**
EPFL Lausanne
Auditorium BCH 2201, ISIC, Station 6, 1015 Lausanne

Friday, **8 November 2019, 11:00**
Empa in Dübendorf
Empa Academy II, Empa, 8600 Dübendorf, Überlandstrasse 129

Abstract of the lecture series

'Design of Advanced Materials?'

M.J. Rosseinsky

Department of Chemistry, University of Liverpool, Liverpool L69 7ZD, UK

The knowledge we have developed through the synthesis and experimental study of extended solids allows us to efficiently identify new materials, in many cases with scientifically interesting or technically important changes in properties. An example is the chemical control of the transparent conducting behaviour of correlated metals (1), evaluated as epitaxial films through optical and transport data. The selection of d^0 cations to stabilise oxygen-oxygen bond formation upon deep oxidation of lithium ion cathodes is a further example (2). Here computation provides underpinning guidance in the selection of experimental targets.

However, the large potential range of accessible compositions and structures challenges our present capabilities. As part of the current interest in exploring computationally-enabled routes to new materials, we are developing computational tools for the identification of stable new compositions. We have recently (3) been able to predict *ab initio* the regions of composition space that afford new materials, and then subsequently isolate those materials experimentally, using the computation of the energies of probe structures identified by new crystal structure prediction methods (4) to explore the space. The presentation will discuss the potential offered by informatics approaches often referred to as machine learning in such work.

(1) J.L. Stoner *et al.*, *Advanced Functional Materials* **29**, 1808609, 2019

(2) Z. Taylor et al., *J. Am. Chem. Soc.* **141**, 7333, 2019

(3) C. Collins *et al., Nature* **546**, 280-284, 2017

(4) C. Collins *et al.*, *Faraday Discussions* **211**, 117, 2018

CV

M.J. Rosseinsky

Matthew Rosseinsky obtained his undergraduate degree and D. Phil in chemistry from the University of Oxford. He was a postdoctoral member of the technical staff at AT&T Bell Laboratories before returning to the University of Oxford as a lecturer in chemistry. In 1999, he moved to the University of Liverpool as professor of inorganic chemistry. In 2009, Matthew received the inaugural De Gennes Prize from the Royal Society of Chemistry (RSC) — a lifetime achievement award in materials chemistry that is open internationally and is one of the RSC's three premier awards. He was elected a Fellow of the Royal Society in 2008, and was awarded the Hughes Medal of the Royal Society in 2011 for his highly influential discoveries in the synthetic chemistry of solid state electronic materials and novel microporous structures. In 2013, he became a Royal Society Research Professor, and was awarded its Davy Medal in 2017.

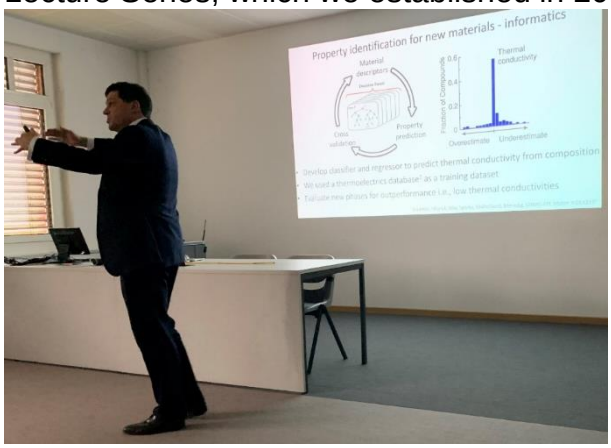
Matt's work addresses the synthesis of new functional materials in bulk and thin-film form for energy and information storage applications, and has been characterized by extensive collaboration with many academic and industrial colleagues. The Rosseinsky group's current areas of interest include materials for batteries and solid oxide fuel cells, multiferroics, thermoelectrics, superconductivity, materials for separation and catalysis, high-throughput materials discovery, and materials for solar energy conversion.

A central topic of Matt's research is the development of new methods of identifying functional materials, emphasising the integration of experiment with computational methods for materials discovery, which includes new tools for crystal structure prediction.

https://www.liverpool.ac.uk/chemistry/research/rosseinsky-group/

Report on the 2019 Howard Flack Crystallographic Lecture Series

From 4th to 8th November 2019 it was our great pleasure to welcome Prof. Matthew Rosseinsky from the Department of Chemistry of the University of Liverpool, UK. He gave five lectures in the frame of our distinguished Howard Flack Crystallographic Lecture Series, which we established in 2018.



1 Matthew Rosseinsky lecturing at PSI

After arriving on Monday morning at Zurich airport, he started his Switzerland tour at the PSI in Villigen. Before his lecture in the afternoon, we had time for discussions with colleagues.

After Matt travelled by train to Neuchâtel, we enjoyed dinner at the Hotel 'Alpes et Lac' where he stayed for two nights and also profitted from a visit to downtown Neuchâtel. On Tuesday morning, Matt visited the research and technology organization CSEM, where a large audience of materials scientists, researchers in micro and nano systems and from the energy and life science departments welcomed him. Mattt was impressed by such a huge interest in his research topic and made an excellent presentation. Colleagues form the UniNE, UniGe and UniBe also came to CSEM to attend Matt's lecture. Prof. Rosseinsky had several discussions on the importance of computational investigations of interfaces (especially at the nanoscale), for the control of functional interfaces for medical diagnostics, single molecule electronics and for energy applications. By the end of the day, Matt underlined that he had had an outstanding scientific exchange at CSEM.

2 Exchange with students at the University of Fribourg

On Wednesday morning, he travelled by train through the 'Seeland' to Fribourg where the students of the Fromm group started discussions during the afternoon before his lecture in the late afternoon at the Department of Chemistry of the University of Fribourg.

In the evening, lively discussions continued with Katharina Fromm during dinner. The next morning, Matt's journey brought him to EPFL in Lausanne, where he arrived still very much in shape after the last three intense days and just in time for lunch, which was shared with colleagues while enjoying the view of the Lake of Geneva. Although the weather was lousy, spirits where high and the discussion with known and new colleagues was lively. A busy four-hour afternoon schedule had been prepared for Matt to meet colleagues one-on-one, until shortly before he presented his Flack Lecture. A brief slot of 15 minutes to relax and prepare was enough for Matt to deliver an energetic and didactic lecture that was thoroughly enjoyed by students from EPFL and colleagues from the University of Geneva, who had made the trip for this occasion. The lecture was followed by an

apéro, after which Matt had to get back on the train, the next stop being Empa near Zurich, on the other side of Switzerland. It was a pleasure having Matt at EPFL.

After the long and intense day in Lausanne, Matt started early on Friday morning at Empa in Dübendorf. We initiated the day with lab visits at the Center for X-ray Analytics followed by discussions with Empa colleagues. At 11am he started his talk at the Empa Academy, where we were fascinated by his lecture about his current interest in exploring computationally-enabled routes to new materials and the application of ML (machine learning) tools for the identification of stable new material compositions.

3 *Matthew Rosseinsky' s lecture at the Empa Academy in Dübendorf*

The lecture was followed by a lunch accompanied by lively discussions between Matt and colleagues and friends from the ETHZ, the University of Zurich and, of course, Empa.

4 *Lunch at Empa Dübendorf with Matt Rosseinsky and colleagues from the SSCr after the lecture*

In the early afternoon, he returned to Zürich airport to catch his flight back to Liverpool. It has been a great experience and a real pleasure to welcome Prof. Matthew Rosseinsky here in Switzerland. We thank him very much for the fascinating lecture series and for accepting our dense travel and lecture schedule.

Pascal Schouwink, Olha Sereda and Antonia Neels

Report on Gordon Research Conference on Nanoporous Materials

Ilia Kochetygov
Laboratory for Functional Inorganic Materials, EPFL Valais, Sion, Switzerland

A Gordon Research Conference (GRC) on Nanoporous Materials and Their Applications was held in Andover, NH, U.S. during August 4-9, 2019. This conference brought together the influential researchers in the field, from students to professors, to share their scientific discoveries and ideas. The unique feature of GRCs, that is a choice of a remote, countryside venue, significantly helped with establishing informal contacts with peers and professors. A balanced program that interweaves plenary talks of professors, presentations of students, poster sessions, outdoor activities and an evening bar, kept the attendants active from 9AM to 9 PM. A careful choice of topics in the program highlighted the most notable areas in the field of porous materials. Thus, for instance, a researcher working in a field of metal-organic frameworks not only can get a state-of-the-art update on these materials, but also can learn well about the adjacent field of zeolites and other inorganic porous materials. As porous materials are connected to the large-scale industries and everyday applications, several talks from the industrial researchers were also included in the program. For a student working in the field, it is important to learn how the research and overall work direction in industry is different from academia, a knowledge necessary for an educated choice of further career directions.

During the conference, I established contacts with many peer students and postdoctoral researchers, as well as with professors on different career stages. Those include Prof. Casey Wade (Ohio State University), Prof. Erich Bloch (University of Delaware), Prof. Natalia Shustova (University of South Carolina), Prof. Omar Farha (Northwestern University). I had a great opportunity to present my research to them and we had numerous fruitful discussions on research results, management and further career planning. I was happy to meet fellow students and postdoctoral researchers from the U.S. to discuss my research with them and learn the features of their doctoral and postdoctoral studies and careers as well.

Overall, I am sure that the network established at this conference will be helpful for my research in various aspects: collaborations, choice of further career and workplaces, education, etc. I would therefore like to thank the SGK for supporting my trip to the U.S. so that I could participate in this GRC.

Impressions from the GRS/GRC on Organellar Channels and Transporters in Mount Snow, West Dover, VT, USA

Pascal F. Meier, Stockholm

I was awarded an SGK Travel grant to attend the Gordon Research Seminar (GRS) and Gordon Research Conference (GRC) on Organellar Channels and Transporters. The conference started off with a 2-day GRS meeting. It was a great opportunity to connect with fellow early career scientists and network with our peers in the field. We presented and discussed our current research, ranging from newly developed optical techniques for imaging protein interactions and signaling cascades to atomic structures of membrane proteins.

The GRC had a great variety of talks dedicated to ion channels and transporters that are located on different intracellular organelles as well as the cell membrane. These ranged from exciting discoveries from current structural and mechanistic studies by cryo-EM and X-ray crystallography towards protein regulations and crosstalk between distinct organelles or systematic responses.

What I enjoyed the most during the conference was the crosstalk between investigators, working in fields from structural biology, plant biology to physiology and human diseases.

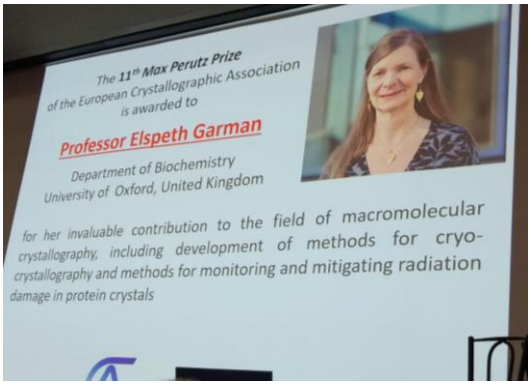
I received my Master of Biochemistry from the University of Zürich. I then moved to Stockholm where I am currently doing my PhD in the group of David Drew at the Department of Biochemistry and Biophysics at Stockholm University. We are a structural biology group that has been traditionally focused on using X-ray crystallography to gain functional and structural insight into ion and sugar transport proteins of the Solute Carrier (SLC) family. We are currently extending our techniques towards using single-particle cryo-EM, NMR and MD simulations.

My gratitude goes to the SSCr board for the travel grant that allowed me to present my work at this GRS and GRC.

32nd European Crystallographic meeting 2019 – Report from a participant

The ECM-32 2019 was one of the most memorable conferences in crystallography that I have visited and has largely exceeded my expectations in terms of high standards and quality of scientific presentations and talks. I was also very impressed by the venue that the organizers decided to use, namely the campus of the University of Vienna, which gave an additional inspiration with beautiful and unique historical reflections on the walls.

The uniqueness of the ECM-32 was in its really rich scientific programme which allowed one to choose preferred topics and gave me a great opportunity to learn about advances in new areas of crystallography, such as electron and neutron diffraction, structure solution and refinement of macromolecules. Many talks were also devoted to structure solution from powder diffraction data and twin refinements. I have extensively enriched my background with valuable tricks which were discussed and demonstrated in practical examples apart from theoretical knowledge in the microsymposium "Teaching new dogs old tricks". A crystallographic prize in the name of the 11th Max Perutz Award was given to Prof. Elspeth Garman for her valuable contribution to the field of crystallography. This award ceremony gave a large motivation to me and the people around for the importance of crystallography and its moving forces for the discovery of macromolecular crystallography which can be only described precisely by crystallographic methods.

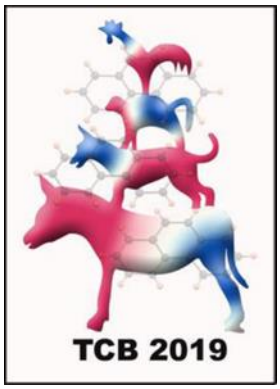


Needless to say, the 2019 ECM-32 enriched and brought new outstanding research to the area of crystallography, which inspired not only me, but also others who have come from all over Europe. The conference featured many breaks and scientific discussions that also allowed me to meet others and establish collaborations. The conference has demonstrated that crystallography is a very versatile field and continuously brings new advances and triggers new discoveries to come. I am very thankful for this generous and unique opportunity and support of the Swiss Crystallography Association to be a participant at the ECM-32 conference 2019 in Vienna and present my own research. I have definitely widened my horizons and have learnt many new things, which will certainly guide me in the future to stay in the field of crystallography and pursue my career in crystallography as a researcher.

Serhii Vasylevskyi, University of Fribourg, Switzerland

Tools for Chemical Bonding – Report from a Participant

General remarks



The workshop *Tools for Chemical Bonding* took place from the 14-19th July 2019 in Bremen (Germany). As the name proposes, this workshop focused on various, mainly theoretical, tools to analyze bonds. Although widely used in chemistry, the concept of a chemical bond is lacking a unique definition. Instead, a plethora of techniques and theories can be employed to define and analyze bonds as well as intermolecular interactions, depending on the context and personal preference. It is therefore important to get on overview of the existing techniques, their advantages and disadvantages, and their applications. This workshop gathered experts in the field of chemical bonding analysis; often the developers of specific software themselves were present. In addition, roughly 50 students from all over the world could attend the workshop. During five days, sessions on different topics were given by the experts. These usually started with a presentation and were followed by hands-on tutorials and exercises. Every student had his or her own laptop and was given access to a locally set-up computer cluster where the presented software was preinstalled. In addition to these sessions, several keynote presentations and a poster session were hold.

Personal experience

Since all night trains to Bremen were booked out weeks before the conference took place, the train trips from Bern to Bremen and back were done during the day and included touristic stops in Cologne and Hamburg. Arriving in Bremen, I found the hotel not really outstanding (e.g. wifi did not work) but the conference place, instead, was very convenient. Everybody could connect the personal laptop to the computer cluster and everybody had easily access to all lecture notes. Furthermore, the lectures as well as the coffee and lunch breaks took place in the same building, which allowed frequent exchanges with the other participants.

I would group the talks and exercise sessions into three main categories: orbital localization methods, techniques to analyze intermolecular interactions, and combination of X-ray diffraction data with quantum chemical calculations. The latter gives rise to the evolving field of quantum crystallography. All of these three categories are key topics of my PhD project and therefore it was useful to hear more details about these research fields. For my personal research, the most interesting talks were the ones by Matthias Bickelhaupt about energy decomposition analyses and Jean Christophe Tremblay about different localizations of molecular orbitals. During the poster session, I presented a poster about the “Analysis of interactions in crystals using extremely localized molecular orbitals”, also recently published in the Journal of Molecular Structure.

The opportunity to attend this workshop, which really fitted my personal research interest, was highly appreciated. Therefore, I express my gratitude for the generous support of the Swiss Society for Crystallography, which provided me with such a successful experience during my PhD.

Bern, 30.03.2020, Michelle Ernst

Swiss Society for Crystallography PhD prize

The **winner 2019** is announced at the beginning of August on the following web-site:

https://www.sgk-sscr.ch/news/crystallographic-news/winner-phd-prize-2019

TRAVEL GRANTS for SGK/SSCr Scientists

Our Society is supporting members participating at international conferences, workshops and schools.

Conditions for travel grants for young SSCr members (under 35):

- Only current members of the SSCr can be supported financially
- Student members can get up to CHF 500 for a poster presentation and CHF 750 for an oral presentation. Attendance at a workshop or school outside Switzerland, if the programme does not permit participant presentations, can be supported with CHF 500.
- Postdocs can be supported only for oral presentations with a maximum of CHF 500

Per institute and year, a maximum of two persons can be supported.

Please submit applications to the President of the Society including the following:

- conference abstract if applicable, type of presentation/involvement and letter of motivation
- letter of support from your supervisor
- brief budget of expected costs of attending the meeting
- specify the date you first joined the SSCr

A 1-2 page scientific report for the SSCr newsletter is expected within 2 months of the meeting.

Financial support can also be granted to retired SSCr members:

- Active participation at an event is required: e.g. presentation, lecture, session chair, organizer
- Young researchers have priority if our budget is limited
- The grant amount will be decided by the board, depending on the available budget

The board of the SSCr wishes you an exciting year with lots of scientific exchanges around the world!

News

Updates from the SLS about the SLS 2.0 project
https://www.psi.ch/en/sls2-0

New Board Members

The SGK/SSCr is looking for two new board members starting Sept 2021. Interested members may apply, please include one support letter of a member.

Meetings, Conferences, Workshops, Schools, Courses

Due to the Covid-19 pandemic many events have been postponed. Please check the respective websites.

Scientist for beamline P02.1/PETRA III DESY

Deutsches Elektronen-Synchrotron DESY
A Research Centre of the Helmholtz Association

For our location in Hamburg we are seeking:

Scientist for beamline P02.1/PETRA III

DESY

DESY is one of the world's leading research centres for photon science, particle and astroparticle physics as well as accelerator physics. More than 2400 employees work at our two locations Hamburg and Zeuthen in science, technology and administration.

The position

- Work as part of a team to provide operational support for the beamline, with close collaboration with the international user community
- Develop and actively pursue own in-house research program in the field of powder diffraction or total scattering
- Contribute to the existing in-house research programs at the beamline
- Work with colleagues in promoting the beamline through conferences and training workshops

Requirements

- PhD in chemistry, physics or equivalent field or qualification
- Experience of collecting data at a synchrotron source and working with beamline instrumentation
- Experience of analysing data from either total scattering or powder diffraction data experiments
- Experience with a technique such as in-situ catalytic or gas sorption studies, battery materials etc.
- Knowledge of Rietveld refinement or PDF fitting would be considered a strong asset
- Practical problem solving abilities
- An interest in software development (esp. using python) or in instrumentation would be an asset

For further information please contact Martin Etter, +49 40 8998 5648, martin.etter@desy.de.

We are looking forward to your application via our application system: www.desy.de/onlineapplication

Deutsches Elektronen-Synchrotron DESY
Human Resources Department | Code: FSMA014/2020
Notkestraße 85 | 22607 Hamburg Germany
Phone: +49 40 8998-3392
http://www.desy.de/career

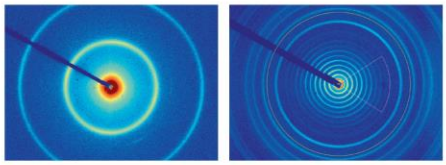
Deadline for applications: 2020/05/03

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

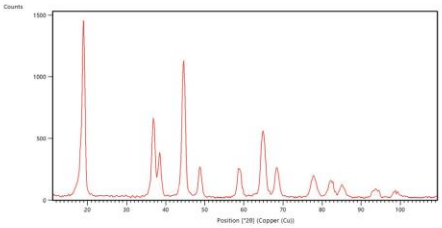
https://www.desy.de/career/job_offers/index_eng.html?joboffer=103152

The Empyrean X-ray diffraction platform, equipped with Mo/Ag radiation and the GaliPIX^{3D} detector, enables high-energy X-ray diffraction/scattering experiments in your laboratory.

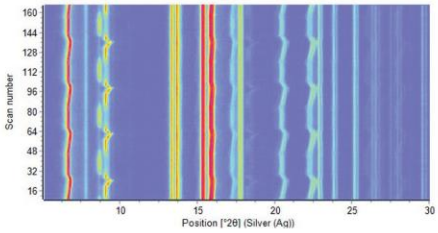
It is designed for advanced studies of materials; for applications requiring the use of hard radiation e.g. easy and quick setup of PDF experiments on nano-crystalline materials, *in operando* XRD measurements on battery cells, high-resolution crystallography over large q-range to refine thermal parameters, penetrating through a diamond anvil cell, ultrafast XRD measurements and more.



2D SAXS (left) and 2D WAXS (right) of Silver behenate using Cu radiation.



Hyper-speed full pattern snapshot (33° 2θ with Ag radiation, equivalent to ~100°2θ with Cu radiation) recorded in just 2 seconds.



Four complete charge-discharge cycles of a commercial prismatic battery cell, measured with Ag radiation (5 minutes per scan, 14 hours total measuring time).

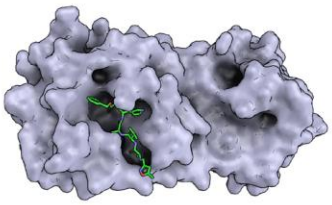
www.malvernpanalytical.com

Malvern Panalytical
a spectris company

DECTRIS
detecting the future

Every structure counts

Even during lockdown, many synchrotron beamlines and research laboratories are tirelessly providing services for COVID19-related research.



We are privileged and honored to support their current and future applications, because every structure counts.

Our support engineers and application scientists are available for a consultation on a variety of technology and application topics.

Don‘t hesitate to reach out to us at info@dectris.com

Calls for proposals

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

Facility	Deadline(s)	Link
Priority access call for work on combating COVID-19, see		www.psi.ch/useroffice/
No external users until 31.05.2020 for SLS, SwissFEL, see		www.psi.ch/useroffice/
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)	June/July 2020	www.psi.ch/useroffice/
SINQ/SLS		
Joint x+n proposals (MS/HRPT)	28.02.	www.psi.ch/useroffice/
SμS: Swiss Muon Source		
DOLLY, GPD, GPS, HAL-9500, LEM , LTF	28.02., second call	www.psi.ch/useroffice/
GPD, GPS, LTF, HAL-9500, LEM	to be announced	
SwissFEL		
ARAMIS-Alvra, ARAMIS-Bernina	15.03, 15.09	
ESRF: European Synchrotron		
long term proposals	02.03.2020	www.esrf.eu/
short term proposals (standard)	02.03.2020	UsersAndScience/
ILL: Institut Laue Langevin		
All instruments	17. 09. 2020	www.ill.eu/
FRM II: Heinz Maier-Leibnitz		
All instruments	To be announced	www.mlz-garching.de/user-office/
Rapid access program	31.07.2020	www.mlz-garching.de/user-office/
SNS Spallation Neutron Source	16.09.2020	neutrons.ornl.gov
Oak Ridge		

Calendar of forthcoming meetings

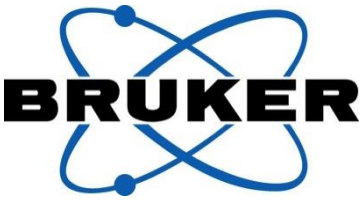
(Please mail the missing information on meetings of interest to woerle@inorg.chem.ethz.ch)

News from the IUCR about the **Melbourne Congress and General Assembly of the IUCr**
https://www.iucr.org/news/notices/announcements/26th-iucr-congress#.XqYdlcJJGvU.twitter

			Application Deadline
2020			
Aug. 22-29	Prague, CZ	25th Congress & General Assembly of the IUCR, Congress postponed to August 2021 https://www.xray.cz/iucr/	To be announced
2021			
June 6-17	University of Zurich	Zurich School of Crystallography http://www.chem.uzh.ch/linden/zsc	15.01.2021
Aug. 14-22	Prague, CZ	25th Congress & General Assembly of the IUCR, Congress postponed to August 2021 https://www.xray.cz/iucr/	Abstracts for Lectures: 21.03.2021
2023			
Aug. 22-29	Melbourne, Au	26th Congress & General Assembly of the IUCR, https://scanz.iucr.org/	To be announced

Institutional members and supporting institutions

Corporate members



Supporting institutions

(If you would like to see your logo here, please contact our treasurer, Dr. Enrico Giannini)

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).

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

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

Members of the Board of the Society for the period 2018 – 2021

President	**Prof. Dr. Antonia Neels** Center for X-ray Analytics Empa Überlandstrasse 129, CH-8600 Dübendorf +41 58 765 4507, antonia.neels@empa.ch
Vice-President	**Prof. Dr. Anthony Linden** Department of Chemistry A University of Zürich Winterthurerstrasse 190, CH-8057 Zurich +41 44 635 4228, anthony.linden@chem.uzh.ch
Secretary	**Dr. Michael Wörle** Small Molecule Crystallography Center ETH Zürich Vladimir-Prelog-Weg 1, CH-8093 Zürich +41 44 632 5684, woerle@inorg.chem.ethz.ch
Webmanager	**Dr. Pascal Schouwink** EPFL Valais Wallis Rue de l'Industrie 17 Case postale 440, CH-1951 Sion +41 21 695 82 80, pascal.schouwink@epfl.ch
Treasurer	**Dr. Enrico Giannini** Department of Quantum Matter Physics Université de Genève 24, Quai Ernest Ansermet, CH-1211 Genève 4 +41 22 379 6076, enrico.giannini@unige.ch
Other members	**Dr. Dubravka Sisak-Jung** DECTRIS LTD Taefernweg 1, CH-5405 Baden-Daettwil +41 56 500 21 00, dubravka.sisak@dectris.com. **Dr. Olha Serada** XRD Application LAB CSEM Jaquet Droz 1 / CP 526, CH-2002 Neuchâtel +41 32 720 5437/5551 olha.sereda@csem.ch **Dr. Antonio Cervellino** Material Science Group Paul Scherrer Institute WLGA/229, CH-5232 Villigen PSI +41 56 310 4611 antonio.cervellino@psi.ch
Auditors:	**Prof. Dr. B. Spingler** (University of Zürich), **Dr. K. Schenk** (EPF Lausanne)

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

Editor:
Dr. Michael Wörle
ETH Zürich
HCI H103
Vladimir-Prelog-Weg 1
CH-8093 Zürich, Switzerland

e-mail: woerle@inorg.chem.ethz.ch

www.sgk-sscr.ch

SGK/SSCr, CH-1700 Fribourg

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

Printing and

Mailing:

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

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.
Commercial advertisements of material of interest to members of the SGK/SSCr are welcome. Please contact the treasurer for details of the advertising rates.