

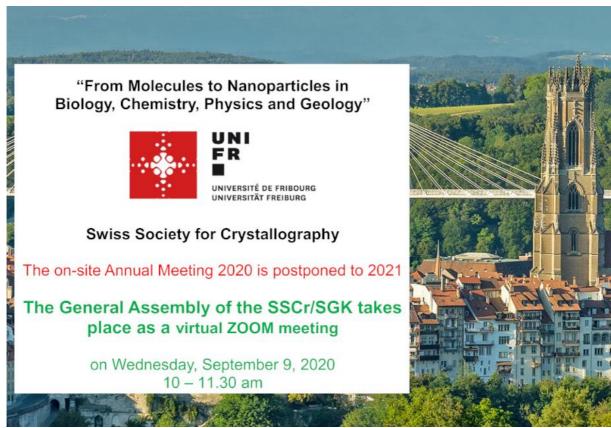
Schweizerische Gesellschaft für Kristallographie Société Suisse de Cristallographie Società Svizzera di Cristallografia Swiss Society for Crystallography

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



SGK / SSCr NEWSLETTER

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Postponed:Annual Meeting of the SGK/SSCr 2020 General Assembly 2020 as Virtual Meeting

On the cover: Regrettably we have had to postpone the 2020 Annual Meeting of the SGK/SSCr because of the uncertain situation with Covid-19 and the organisational constraints that this imposes. The University of Fribourg remains the location for next year's event. The General Assembly is held as an online meeting using ZOOM on Wednesday, September 9, 2020 from **10-11.30 am**

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The President's Page



Dear Members of the Swiss Society for Crystallography,

We all are experiencing a very special time and the COVID-19 pandemic has changed our lives considerably. We are still far from normality and the necessity of social distancing will also affect in the upcoming months our organization of meetings, teaching and, of course, the daily work in our labs and offices.

I believe that many of you have been looking forward to our Annual Meeting at the University of Fribourg which strengthens our exchange about advances in crystallography beyond your own research field. Our Annual Meeting is the platform not only for meeting colleagues, and

expanding and enforcing networks, but also for finding out about new instrumentation and related recent technology development. Our personal exchange between academia and industry is, however, difficult to replace via a digital solution. It is with great regret that this year's Annual Meeting at the University of Fribourg has been reduced to the general assembly of the SSCr. I would like to thank our colleagues from the Chemistry Department in Fribourg who prepared and announced an interesting program. However, only a pleasure deferred! Thank-you to our Fribourg colleagues for offering to host the next meeting in 2021!

I would like to invite you to the

Annual General Assembly of the SSCr / SGK

which will take place online (Zoom) on the 9th September 2020, 10:00-11:30.

I hope to see many of you at this Zoom meeting for an exchange on the activities of our society, details about the road mapping for large-scale facilities in Switzerland, upcoming actions, events and news from our members. You will find the agenda in this newsletter. Please contribute by signing on for the Zoom meeting and actively participating in the discussions in order to make the assembly as efficient as possible. I will send the Zoom connection details by e-mail to all members shortly.

I'm happy to see so many new crystallography related papers coming out in a growing number. Please use also the SSCr website for disseminating recent research achievements! Many conferences for 2020 have been postponed until 2021, including the IUCr-25, but be assured that we are prepared for an increase in requests for our travel support as soon as international on-site exchange ramps up. For the 'Howard Flack Crystallographic Lecture Series' we welcome your suggestions for the invited lecturer for 2021.

Even if digital communication occupies now an important space in our professional and private lives, it can't replace personal exchanges at meetings and conferences. I'm looking forward to these get-togethers which are sources of energy and contribute largely to progress in science.

I wish you a nice remainder of the summer and hope to see you 'virtually' at our General Assembly on the 9th September.

Antonia Neels
President of the SGK-SSCr

Swiss Society Annual Meeting 2020, Université Fribourg

Postponed to 2021

Regrettably, we have had to **cancel the 2020 annual meeting** of the SGK/SSCr because of the uncertain situation with Covid-19 and the organisational constraints that this imposes. The University of Fribourg remains the location for next year's event and we will keep you informed about the exact date.

Our decision has a two-fold impact on this year's activities and also organizational matters.

1) We will hold the:

General assembly (GA) of the society on the 9th September 2020, 10-11.30am, as an online meeting.

The president Antonia Neels will send a ZOOM invitation to all members and hopes that most of you will be able to join this part.



Figure 1: Continuing the work of the Society during the COVID-19 pandemic: the members of the SGK/SSCr

Board during their recent online meeting.

2) Scientific highlights from our community are nonetheless published in this issue of the newsletter.



Swiss Crystallographic Association SGK / SSCr

General Assembly 2020

Wednesday, September 9, 2020, 10:00-11:30 Virtual Meeting using ZOOM

Agenda of the General Assembly 2020

The minutes of our last General Assembly (PSI Villigen, Wednesday, September 4, 2019) are published on page 8-15 of the SGK/SSCr newsletter No. 104, Aug. 2020 (this issue), which is also available electronically at https://www.sgk-sscr.ch/news/newsletter

- 1) Determination of the quorum according to Art. 12/by-laws
- 2) Proposition for acceptance of the minutes of the General Assembly 2019, EPFL Sion
- 3) 2021/2022 Meeting and General Assembly: Decision on location/organizers (proposal 2022 in Bern, Simon Grabowsky)
- 4) Upcoming retirements from the Board and the election of new board members.
- 5)
- a) Annual report
- b) Annual financial statement
- c) Budget for the next year
- 6) Updates on SNBL arrangements
- 7) Road-mapping for large scale facilities and SSPh
- 8) Travel grants and PhD prize for 2020/2021
- 9) Other motions of members

Additional Information:

Year	Entries to SGK/SSCr	Exits from SGK/SSCr
2012	8	8 (since July 2012)
2013	7	15
2014	11	17
2015	23	18*
2016 (as of 06.06.)	3	4
2017 (as of 17.07.)	10	4
2018 (as of 18.08.)	8	19 [*]
2019 (as of 18.07.)	5	3
2020 (as of 17.08.)	10	13

^{*} in 2015 and 2018, a large number of SGK/SSCr members (18 and 19, resp.) have been excluded per decision of the Board because they were not paying the annual fees for more than 3 years, and could not be contacted.

Quorum for final decisions (Art.12, by-laws):

As of 17.08.2020, we have 199 records in our database.

They are grouped as:

- 8 of these are companies (or corporate members),
- 29 are "libraries" (incl. some "quasi-personal" members, from whom we don't expect any fees, but to whom we are regularly sending our newsletters);
- 162 are personal members (full: 125, students: 33, honorary: 4)
- I.e. for the quorum to be able to make decisions, we should have **10%** out of **166** corporate and personal members, i.e. at least **17** people.

Board Members:

see last page of this newsletter

Delegates

ECA: A. Linden (Zurich)
IOCG: E. Giannini (Geneva)

ScNat: A. Neels (automatically assigned to the acting president)

Steering Comm. SNBL G. Chapuis (Lausanne), R. Cerny (Geneva)

Anthony Linden (Zurich)

Antonia Neels (Zurich)

Minutes of General Assembly 2019

Wednesday, September 4, 2019

EPFL Valais, 1950 Sion, Rue de l'Industrie 17, Zeuzier conference room, 12:50-13:40

Schweizerische Gesellschaft für Kristallographie

Agenda:

- 1) Determination of the quorum according to Art. 12/by-laws
- 2) Proposition for acceptance of the minutes of the General Assembly 2018, PSI Villigen
- 3) a) Annual report/Jahresbericht / le rapport annuel
 - b) Annual financial statement /Jahresrechnung / les comptes annuels
 - c) Budget for the next year / Aufstellung des Budgets für das kommende Jahr / le budget proposé pour l'année suivante
- 4) 2020 Meeting and General Assembly: Decision on location/organizer. Proposals are most welcome!
- 5) SNBL communication to the user community
- 6) Anträge von Mitgliedern other motions of members

Minutes:

Formalities:

The General Assembly was chaired by Antonia Neels, President, and started at 12:53 h The agenda has been published in the Newsletter 102 on 27. July 2019 (Art. 11) The secretary Michael Wörle, ETH, was appointed as keeper of the minutes.

Ad 1.

Additional Information:

Year	Entries to SGK/SSCr	Exits from SGK/SSCr
2012	8	8 (since July 2012)
2013	7	15
2014	11	17
2015	23	18*
2016 (as of 06.06.)	3	4
2017 (as of 17.07.)	10	4
2018 (as of 18.08.)	8	19 [*]
2019 (as of 18.07.)	5	3

^{*} in 2015 and 2018, a large number of SGK/SSCr members (18 and 19, resp.) have been excluded per decision of the Board because they were not paying the annual fees for more than 3 years, and could not be contacted.

With 33 members being present at this assembly, the necessary quorum of 10% (17) is reached to constitute a quorum (Art. 12).

As of 18.07.2019, we have 198 records in our database.

They are grouped as:

- 8 of these are companies (or corporate members),
- 29 are "libraries" (incl. some "quasi-personal" members, from whom we don't expect any fees, but to whom we are regularly sending our newsletters);
- 161 are personal members (full: 126, students: 31, honorary: 4) 10% out of 165 corporate and personal members, i.e. at least 17 people. Three corporate members present are Peter Kistler (Bruker Switzerland AG) and Marco Sommariva (Malvern-Panalytical) (named according to Art. 14 of the bylaws).

Ad 2.

The minutes of the General Assembly 2018 on 12/09/2018 at PSI in Villigen, reported in newsletter 102, have been approved unanimously, no abstentions.

Ad 3 a)

The President Antonia Neels gives the roadmap 2018-2021 and a report of the activities and cooperations:

- Three **SGK/SSCr PhD-prizes** were awarded in 2015, 2017 and 2019. Next one will be issued in 2021.
- **Travel support** for young scientists has increased from one in 2018 to 5 in 2019.
- The Howard Flack Lecture Series in 2018 was very successful. Prof. Omar Yaghi, who gave talks from 16th until 20th April at PSI Villigen, ETH Zurich, Uni Zurich, Uni Bern, EPFL Sion, Uni Geneve and Uni Fribourg. On 4th-8th November, 2019 Matt Rosseinsky (Uni Liverpool) will give talks at PSI Villigen, CSEM Neuchâtel, Uni Fribourg, EPFL Lausanne and Empa Dübendorf. Suggestions for 2020 are most welcome. Even two lecture series are possible, one in spring and one in autumn.
- The SGK/SSCr had several cooperations, as there are:
 2018 Powder Diffraction School at PSI Villigen

2018 Zurich School of Crystallography in Tianjin, China

2019 Zurich School of Crystallography in Zurich

2019 Chemical Landmark, Max Perutz event (together with SCS, SCNAT)

2019 Satellite Meeting for Neutron Scattering at ECM32 in Vienna.

- New special interest group (Sig-14, Dynamics, Disorder, Diffuse scattering (D3)) at European Crystallographic Association (ECA).
- Sine Larsen, who got eleventh Max Perutz Prize in 2018, has been at the Chemical Landmark
- Increase the participation in organisms
 ECA (new SIGs representatives), 2018 creation of SIG14
 IUCr (commission members and consultants)

Ad 3 b)

Budget report:

The treasurer Enrico Giannini gives the financial report for 2018.

The surplus of about 15'000.- is due to the ECM30 in 2016. The Credit Suisse bank Account has been closed and the amount has been transferred to the UBS account.

Summary SGK Finances 2018

Total 31.12.2017	CHF 49'681.17
UBS account CS account Cash on hand	46'789.99 (account cancelled, money transferred to UBS account) 542.10
Total 31.12.2018	47'332.09
Balance	-2'349.08

SGK Financial Report 2018

UBS Balance 31.12.2017 30'798.60 CS Balance 31.12.2017 18'340.47

Income:

Membership dues:

Full members (various amounts due to debts)

5x30 + 66x40 + 1x40.02 + 1x45.48 + 1x50 + 1x60 + 1x70 + 1x75.53 + 1x80 + 1x120

 + 1x160 + 1x340.52
 3'831.55

 Students 8x10
 80.00

 Companies 5x130
 650.00

Subsidy SCNaT 6'237.30

Interest

5.65

Bank transfer: merger of the SKT and SGK bank accounts

3'540.44

Total Income

14'344.94

SGK Financial Report 2018

Expenses:

Membership dues to SANW (206 members)	1 ' 141.00
Travel costs for ECM delegates	2'000.00
Annual Meeting (PSI, Villigen)	3'000.00
Travel Grants	750.00
Howard Flack Lecture Series (Prof. Omar Yaghi)	7'030.26
Support to the PSI School on Powder Diffraction	2'000.00
Association to ECA	201.49
Printing and publishing costs (newsletter)	414.20
Website	8.87
Bank expenses	148.20

Total

Expenses 16'694.02

Income – Expenses - 2'349.08

SGK Financial Report 2018

Cash on Hand - 2018:

Status 31.12.2017	542.10
Total Income	0.00
Total Expenses	0.00
Balance (Income – Expenses)	0.00
Starting Balance + Income – Expenses	542.10
Cash on Hand 31.12.2018	542.10

Revisorenbericht für die Jahresrechnung 2018 der Schweizerischen Gesellschaft für Kristallographie (SGK)

Konten:

UBS UBS 279-C0291110.0

Die Unterzeichneten haben Kenntnis genommen von der Jahresrechnung der Schweizerischen Gesellschaft für Kristallographie. Die Rechnungsprüfung betrifft die Periode vom 1. Jan. 2018 bis 31. Dez. 2018. Die Unterzeichneten stellen fest, dass die Abrechnung mit den vorgelegten Belegen übereinstimmt.

Am 31. Dez. 2018 ist der Stand der Konten und der Kasse:

UBS	SFr.	46'789.99
Kasse	SFr.	542.10
Summe SGK	SFr.	47'332.09

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

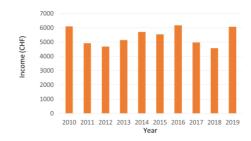
Ort / Datum Neuchâtel, 18.1.2019

Unterschriften

B. Spingler (Universität Zürich)

K. Schenk (EPF Lausanne)

- The budget 2018 has been approved by the auditors Kurt Schenk and Bernhard Spingler (Neuchâtel, 18.01.2019).
- Enrico Giannini presents an overview on the fluctuation of the membership dues:



- Enrico Giannini reports that the Credit-Suisse account has been suspended and the money was transferred to the UBS account. Hans Grimmer asked, if there will be every year costs of 7000.- for the Howard Flack Lecture Series. Antonia Neels answered no, cost depends mainly on the travel expenses, which are significantly lower if European speakers are invited.
- The Financial Report 2018 was unanimously approved by the members.

Ad 3 c)

Credits:

SGK Budget 2020 To be proposed at the SGK assembly 4.09.2019

- Deficit is desirable to reduce treasure (remark by Enrico Giannini). Antonia Neels comments, that SANW will give most likely only CHF 10'000.-, while CHF 12'500.- are budgeted.

The budget 2020 was approved unanimously by the members (no abstentions).

Ad 4)

- The Annual Meeting in 2020 is proposed to take place in Fribourg on Wednesday, Sept. 9th 2020, organized by Katharina Fromm and Aurelien Crochet.
- As a preliminary proposal is is discussed that the 2021 meeting might take place in Bern, organized by Simon Grabowsky.
- AN states, that no elections necessary since there are no vacant positions in the board. However, for the elections in 2020, members are invited to volunteer as a board member, since in two years some members of the board are leaving.
- At the moment there is only one delegate for ECA (Anthony Linden)
- At ECM32, there has been the highest number of participants ever, also many Swiss participants

Ad 5)

Radovan Cerny gave a short overview on the present situation and future concerning the Swiss-Norvegian Beamline (SNBL):

The PSI, the actual contractual partner in the SNX, has decided not to renew the SNX agreement with the Norway beyond 2020. The SNX board is currently looking for an institution, which will replace the PSI as contractual partner in the SNX agreement. The discussions are running on the ETHZ, EPFL and UNIGE. In parallel, the Swiss Steering Committee (SSC) has created a consortium of Swiss universities, according to the Norwegian model, which will be headed by the institution signing the SNX Agreement. The SERI will consider seriously any solution which will assure the continuation of the SNBL, including the financial contribution to the SNBL budget. The PSI fully supports these actions.

Antonia Neels asks for statistics of SGK-members in the IUCR-commission. Michael Wörle will deliver the data.

Current delegates in the various bodies are:

ECA: A. Linden (Zürich)
IOCG: E. Giannini (Geneva)

ScNat: A. Neels (automatically assigned to the acting president)

Steering Comm. SNBL: G.Chapuis (Lausanne), R. Cerny (Geneva)

IUCR: A. Linden (Zürich)

A. Neels (Zürich)

Ad 6). Varia

- News from ECM32 in Vienna: Elspeth Garmann got the Max Perutz Prize.
 Sig-14, Dynamics, Disorder, Diffuse scattering (D3) organized a
 Microsymposium (Dimitri Chernichov).
- **ECM33** will take place 24-28- Aug. 2021 in Versailles, France.
- **ECM34** will take place 2022 in Padova, Italy
- **IUCR XXV** congress will take place 22-30. Aug. 2020 in Prague, Czech Republic. Radovan Cerny is a member of the organizing committee.
- **EPDIC17** will take place 26-30th may 2020 in Sibenic, Croatia.

AN presents the new regulations concerning 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

- Hans-Beat Bürgi, asks if the board has already discussed the introduction of an "Early Career Prize", as announced in the last annual meeting. The board will do so in its upcoming meeting. Master students would be a suitable target group for the "Early Career Prize".
- Antonia Neels thanks the reviewers evaluating the 2019 PhD-Prize applications.
- Antonia thanks the board members and especially Pascal Schouwink for the organizing of the Annual Meeting 2019. Next meeting will be in Fribourg Sept. 9th 2020 organized by Aurelien Crochet.
- Enrico Giannini explains that the International Organisation on Crystal Growth (IOCG) requires that the Section for Crystal Growth of the SGK/SSCr establishes its own board. The Board of the SGK/SSCr will decide how to proceed in its upcoming board meeting.

Meeting ends at 13:33

Minutes written by the Secretary Michael Wörle, 23.11.2019

Approved by the President Antonia Neels

Financial Report for 2019

Summary SGK Finances

 CHF

 Total 31.12.2018
 47'332.09

 UBS account
 46'718.63

 Cash on hand
 533.25

 Total 31.12.2019
 47'251.88

 Balance
 - 80.21

Revisorenbericht für die Jahresrechnung 2019 der Schweizerischen Gesellschaft für Kristallographie (SGK)

Konten:

UBS

UBS

279-C0291110.0

Die Unterzeichneten haben Kenntnis genommen von der Jahresrechnung der Schweizerischen Gesellschaft für Kristallographie. Die Rechnungsprüfung betrifft die Periode vom 1. Jan. 2019 bis 31. Dez. 2019. Die Unterzeichneten stellen fest, dass die Abrechnung mit den vorgelegten Belegen übereinstimmt.

Am 31. Dez. 2019 ist der Stand der Konten und der Kasse:

UBS SFr. 46'718.63 Kasse SFr. 533.25 Summe SGK SFr. 47'251.88

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

Ort / Datum

Neuchatel,

5. 2. 2020

Unterschriften

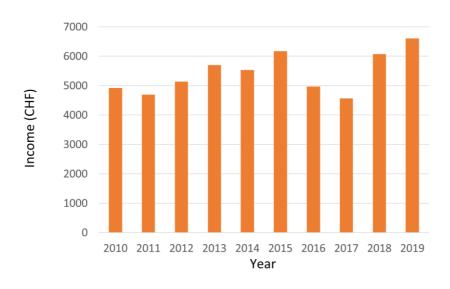
B. Spingler (Universität Zürich)

(EPF Lausanne)

Income:

Membership dues: Full members (various amounts due to debts) 2x30 + 1x38 + 62x40 + 1x43.91 + 1x45.48 + 3x50 + 1x70 + 1 + 1x100 + 3x120 + 1x150 + 1x220 Students 7x10 + 3x20 + 1x30 Companies 5x130 + 1x520 Total membership	9x80 + 1x84.50	5'276.41 160.00 <u>1170.00</u> 6606.41
Subsidy SCNaT Interest	1.90	12'300.00
	Total Income	18'908.31
Expenses:		
Membership dues to SCNat (163 members at 31.12.2019) Travel costs for ECM delegates Annual Meeting (PSI, Villigen) Travel Grants Howard Flack Lecture Series (Prof. Matthew Rosseinsky) Support to the Zurich School of Crystallography Satellite on neutron scattering at ECM32 Perutz symposium (collaboration with the SCS) Association to ECA Printing and publishing costs (newsletter) Website Bank expenses	Total Expenses Income – Expenses	1'141.00 1'000.00 3'000.00 5'077.00 2'070.51 2'000.00 1'500.00 2'000.00 200.51 830.15 8.85 160.50
	income – Expenses	- 80.21
<u>Cash on Hand - 2019</u> :		
Status 31.12.2018 Total Income Total Expenses Balance (Income – Expenses) Starting Balance + Income – Expenses Cash on Hand 31.12.2019		542.10 0.00 8.85 0.00 533.25 533.25

Fluctuation of the membership dues



SGK Budget proposal 2021

Membership dues	5'000.00
SCNat reimbursement for IUCr delegates	
(IUCr25 in Prague, Czech)	2'000.00
SCNat contribution for SGK annual meeting	
(including poster prize)	3'000.00
SCNat contribution for Zürich School	2'000.00
SCNat PhD / master students travel grants	4'000.00
SCNat Crystallographic Lectures:	01000
Howard Flack Series	3'000.00
SCNat ECA membership	250.00
Publication costs	500.00
Total Income	19'750.00
Delive	
Debits:	41450.00
Membership dues to SCNat	1'150.00
Annual meeting + poster prize	3'000.00
Travel Grants for Young Scientists	6'000.00
PhD thesis prize	
·	2'000.00
SGK support for Zürich School	2'000.00
SGK support for Zürich School Crystallographic Lectures:	2'000.00
SGK support for Zürich School Crystallographic Lectures: Howard Flack Series	2'000.00 4'000.00
SGK support for Zürich School Crystallographic Lectures: Howard Flack Series IUCr delegates (IUCr25, Prague, Czech)	2'000.00
SGK support for Zürich School Crystallographic Lectures: Howard Flack Series IUCr delegates (IUCr25, Prague, Czech) Sponsoring and event advertisement	2'000.00 4'000.00 2'000.00
SGK support for Zürich School Crystallographic Lectures: Howard Flack Series IUCr delegates (IUCr25, Prague, Czech) Sponsoring and event advertisement (posters, flyers, webpage)	2'000.00 4'000.00 2'000.00
SGK support for Zürich School Crystallographic Lectures: Howard Flack Series IUCr delegates (IUCr25, Prague, Czech) Sponsoring and event advertisement	2'000.00 4'000.00 2'000.00

Credits:

Bank charges

Total Expenses

Income - Expenses

200.00 **23'600.00**

- 3'850.00

Candidature as New Board Member

Simon Grabowsky studied chemistry at Free University of Berlin and received his doctoral degree from the same institution in 2011 before he went to the University of Western Australia (UWA) in Perth for a postdoctoral stay with Professors Mark Spackman and Dylan Jayatilaka. Simon became Assistant Professor at UWA in early 2014, but left later in the



same year in order to take on an Emmy Noether fellowship of the German Research Foundation (DFG) which allowed him to be head of a research group at the University of Bremen, Germany. In 2015 he received the title "Professor" from the University of Bremen, and in 2019 he habilitated in physical chemistry. Since August 2019, Simon is a private docent and permanent research group leader in chemistry at the University of Bern as successor of Professor Piero Macchi.

His group's major interests lie in the principles of chemical bonding in inorganic molecular chemistry, exploring fundamental questions such as hypercoordination vs. hypervalency, covalency vs. ionicity etc. The group applies spectroscopic, crystallographic and theoretical methods of structure determination and advances them, especially quantum crystallography (QCr). QCr is based on the measurement of the sub-atomic distribution of electrons in solid matter via single-crystal diffraction experiments to investigate quantum phenomena experimentally. Technically, this requires high-resolution and high-quality/accuracy X-ray diffraction experiments at synchrotrons.

Scientific Contributions

Electron Diffraction and Nanocrystallography: a Device Dedicated to the Crystallographic Community

Gustavo Santiso-Quinones¹, Gunther Steinfeld¹, Eric Hovestreydt¹

¹ELDICO Scientific AG, Park Innovaare: deliveryLab, 5234, Villigen, Switzerland. <u>www.elidico-scientific.com</u>, <u>santiso@eldico.ch</u>

In the past two years, various achievements using Electron Diffraction (ED) techniques, have been made in the fields of inorganic or organic molecules, material sciences, geological sciences, archeological sciences, energetic materials, biological sciences and many others [1]. Such experiments are done in a (modified)-Electron Microscope. Though the realization of such experiments still requires plenty of expertise and efforts and it cannot be applied on daily basis. Pioneers in the field of Electron Diffraction [2], all agree that a dedicated device for the realization of such experiments, would be of great advantage to the crystallographic community. Though such a device doesn't exist (up to now) at all. Therefore, it is a necessity that such a device could be made available for the realization of this exciting field of nanocrystallography. ELDICO Scientific AG is developing a new device which is dedicated exclusively for such purposes. The device, an Electron Difftactometer, is built and optimized for diffraction experiments. Furthermore, it uses exclusively the crystallographic approach (continuous rotation method) and crystallographic software. The sample holder (goniometer) has been optimized to guarantee that the nanoparticles remain under the e- beam the whole time. The e- beam is optimized in such a way that the particles survive longer period of exposure time (in contrast to EM devices where the particles suffer from radiation damage very fast). This facilitates measuring beam sensitive organic samples. A single trained user (crystallographer) can performed the experiments, in contrast to (modified)-EM devices where an EM specialist and an experienced crystallographer are required. No add-ons are necessary (in contrary to an EM) to perform 3D-ED experiments.



Key facts of the ELDICO electron diffractometer

- Sample size from 10 to 1000 nm
- Improved beam intensity for ED experiments
- Improved goniometer for continuous rot. experiments
- Dedicated device for nano-crystallographic experiments
- R1 values comparable to X-ray diff. data

Goniometer

Type: single axis
Rotation: $-70^{\circ} - +70^{\circ}$ Speed: $1^{\circ}/s - 6^{\circ}/s$ Accuracy: $(0.01^{\circ} \text{ at } 1^{\circ}/s)$

Sphere of Confusion: $\sim 0.2 \,\mu\text{m}$

Possible: Semi-Auto. centering of particle

Figure 1: ELDICO Scientific Electron Diffractometer. A unique device dedicated for nanocrystallographic experiments.

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Magnetic network on demand: pressure tunes square lattice coordination polymers based on $\{[Cu(pyrazine)_2]^{2+}\}_n$

Rebecca Scatena^{1,2}, Fabio Montisci², Arianna Lanza³, Nicola P. M. Casati⁴ and Piero Macchi⁵

Coordination polymers, where metals ions are connected via organic ligands and stabilized by extraframework inorganic anions, are ideal platforms for the investigation of low-dimensional quantum magnetism [1],[2]. A special interest for this class of materials concerns the emerging field of spintronics [3]. Progresses in this field require a deep understanding of fundamental chemical and magnetic interactions in solid-state materials. Moreover, the relatively soft nature of coordination polymers provides the opportunity to tweak the spin behavior using external stimuli, potentially leading to multifunctional spintronic devices [4],[5].

To this end, we report the pressure induced structural and magnetic changes in $[CuCl(pyz)_2](BF_4)$ (pyz = pyrazine) and $[CuBr(pyz)_2](BF_4)$, two members of a family of 3D coordination polymers based on square mesh $\{[Cu(pyz)_2]^{2+}\}_n$ layers. High pressure x-ray diffraction and DFT calculations have been used to investigate the structure/magnetic property relationship. Although structurally robust and almost undeformed within a large pressure range, the $\{[Cu(pyz)_2]^{2+}\}_n$ network can be electronically modified by adjusting the interaction of the apical X linkers interconnecting the layers, with strong implication on the magnetic properties. Our analysis shows that the degree of covalent character of the apical Cu–X interaction explains the difference in magnetic exchange between the two species. We have also investigated the mechanical deformation of the network induced by non-hydrostatic compression that affects the structure depending on the crystal orientation (Figure 1). The obtained results suggest the existence of a "Jahn-Teller frustration" triggered at highest hydrostatic pressure [6].

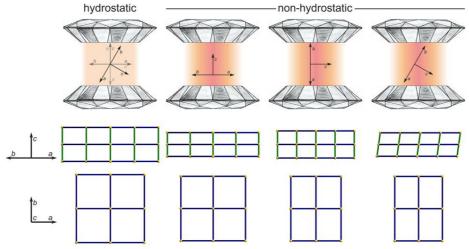


Figure 1: Pressure-induced structural deformations of the tetragonal framework of [CuX(pyz)₂](BF₄) (X=Cl,Br) coordination polymers in different pressure regimens and as a function of the single crystal orientation inside the diamond anvil cell. Reprinted with permission from Scatena *et al.* (2020) *Inorg. Chem.* 59, 10091–10098. Copyright 2020 American Chemical Society.

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Time-resolved and dynamic investigations on nanoparticles agglomeration using Small Angle X-ray Scattering

Neda Iranpour Anaraki^{1,2,3}, Amin Sadeghpour^{1,4}, Claudio Toncelli⁴, Alex Dommann^{1,7}, Peter Wick², Antonia Neels1,3

Nanoparticles (NPs) agglomeration in biological environments is one of the main issues in their applications in biology and medicine [1]. The colloidal stability of NPs depends on the physiochemical properties of media like pH, ionic strength (IS), temperature, and the presence of competing molecules like proteins [2]. Understanding the role of each parameter in the NPs agglomeration process and colloidal stability in biological media is crucial since it steers NPs uptake, accumulation and fate in living systems. There is a lack of information about the dynamic NPs behavior when changing the media from the NP stock dispersion to a biological flow environment [3]. An approach combining small-angle X-ray scattering (SAXS) and a microfluidic system has been used (Fig1.a) for in-situ and dynamic observations related to the early stage of NP agglomeration and primary NPs interactions when surrounding media is changing [4]. It is shown, that the presence of proteins in the NP surrounding triggers the NP agglomeration differently than changing the IS and pH of the environment. Agglomeration in the presence of protein is an extremely fast process, and in less than 1 min, the NP radius increases by around 15 nm. It contrast, with a much slower influence of IS and pH on NP agglomeration, in 2M salt solution the NP radius changed around 7 nm after 150 min. The time scales in Fig. 1 show that this method is sensitive and precise in depicting the dynamics of fast and slow NP interactions in colloidal conditions. Together with classical biochemical analysis, as well as modeling and simulation, our concept fills the knowledge gap in understanding NP agglomeration processes and provides the rationale for novel NP designs in particular for biomedical applications.

The applied dynamical microfluidic-SAXS method monitors early stage of NP agglomeration directly and shows advantages with respect to Cryo-TEM and DLS [4].

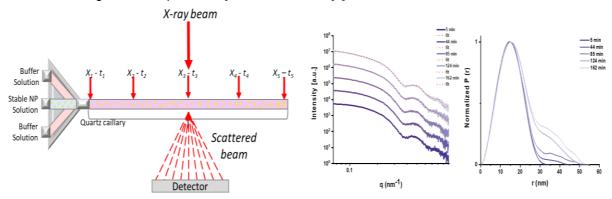


Figure 1: (a) Microfluidic-SAXS combination (b) Experimental data and fitted curves for stable silica NP colloidal solution and KCl salt solution in five different positions along the quartz capillary from the beginning to the end (1-5). The slope of the scattering curves in the smaller q range increases with time, showing the continuous agglomeration process along the quartz capillary. (c) The pair-distance distribution function (PDDF) for each scattering curve in positions 1 to 5

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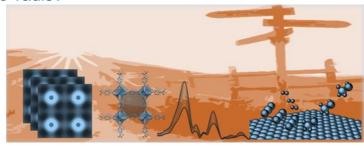
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News

Important meeting: Synchrotron tools for the chemistry/materials science community beyond 2024: quo vadis?

16 September 2020



This meeting will gather existing and future users of synchrotron radiation in Switzerland to discuss perspectives of synchrotron tools for research in chemistry and materials science. The aim is to provide a forum to set an agenda for future planning and development of beamline facilities, with special focus on X-ray absorption and emission, diffraction and scattering techniques. The meeting was originally scheduled for May 8th, 2020, in Bern, but due to Covid constraints, it is planned for September 16th probably as a virtual meeting. The Zoom link will be sent soon to all synchrotron users and will be announced on the SSCr. web page (https://www.sgk-sscr.ch/swiss-society-crystallography).

The availability of cutting-edge X-ray based methods to probe a material's structure, at different length and time scales combined with infrastructure for in situ/operando studies, is essential to obtain fundamental insight in research relevant in chemistry and material science. SNBL and SLS beamlines provide reliable access to the state of the art tools. There is, however a need to increase the user's participation to tailor the development of these facilities to meet the requirements that will allow addressing key scientific challenges in the next decade.

Invited speakers will present an overview and future challenges of the use of synchrotron techniques in representative scientific areas. The current and upcoming experimental infrastructure at the SNBL (at ESRF) and SLS2.0 will be presented by experts at these synchrotron facilities.

The presentations will be followed by discussions of the participants to identify key challenges, evaluate and propose strategies for the current and future X-ray based facilities and supporting infrastructure.

The conclusions of the meeting will be included in a Scientific Roadmap 2025 for synchrotron facilities for the chemistry/materials science community beyond 2024.

Organization Committee:

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Radovan Cerny (UNIGE)
Christophe Copéret (ETHZ, SCNat)
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Antonia Neels (Empa, SSCr)
Wendy Queen (EPFL)

Chairs:

Radovan Cerny (UNIGE) Wendy Queen (EPFL)

Obituary Max Dobler

The life and the work of Max have already been described in detail: see https://trauer.nzz.ch/traueranzeige/max-dobler

and therefore, some reminiscences at a more personal level are appropriate to reveal other aspects of his life.

In our case, it all began in Oxford, where Max and his family, as well the late professor Mario Wiesendanger (later Professor of Neurophysiology, University of Fribourg), myself and Fritz had converged from different horizons in the Fall of 1969. Max came on a sabbatical leave from ETH Zürich to work for Professor David Phillips in the Department of Molecular Biophysics, and I started my first post-doctoral year with Professor Dorothy Hodgkin in the Inorganic chemistry laboratory. The Swiss connection was rapidly established, and it took only a few days for Max, Mario, and Fritz to meet at *Halifax House*, where they quickly founded a mini-Swiss society speaking the dialect of Zürich at lunch time. I was also invited to join them, and this became the basis of a long-lasting friendship.

In the Autumn of 1971, I moved to the University of Neuchâtel. My task was to set up the local X-ray laboratory, which became an important tool for the local chemists. Max was of great help to me advising what equipment to buy with our modest budget and lending us a *Charles Super* precession camera which together with the *Stoe Weissenberg* camera enabled me to begin a career of over 38 years in chemical crystallography. During the academic year 1971-1972 Max gave the introductory lecture in X-ray crystallography to the advanced students here in Neuchâtel. His knowledge of French was excellent, and it gave me a chance to get acquainted with this new language (as my second language, Welsh, was of little use). Thanks to Max I was able to collect valuable data on the 4-circle *Hilger & Watts* diffractometer in Zurich and I regularly attended the lunchtime seminars of the group of Professor Jack Dunitz.

In 1976 Max was involved in the organisation of the highly successful 3rd European Crystallography Meeting that was held in Zürich. From 1984 to 1993 he was a member of the Committee of the Swiss Society for Crystallography and president for the period 1990-1993. I joined the committee in 1987 and acted as secretary/treasurer while Max was president. The organisation of the annual meetings was always a pleasure as we visited the various locations searching out restaurants for diner after the meeting.

Retirement proved to be an extremely productive period for Max. He was a founding member of the Biographics Laboratory 3R in Basel and together with the late Angelo Vedani and his collaborators established the OpenVirtualToxLab – A platform for generating and exchanging in silico toxicity data.

Max Dobler was a dear colleague and friend and he was much esteemed by his Swiss colleagues and the many students who enjoyed learning crystallography under his guidance.



Figure 2 Max Dobler (left) and Angelo Vedani (right)

Helen Stoeckli-Evans & Fritz Stoeckli University of Neuchâtel, July 2020.

Prize André Guinier 2020 of the Association Française de Cristallographie

Chers tous,

Il m'incombe le grand honneur de vous annoncer que le CA de l'AFC a décerné le <u>premier</u> **prix André Guinier de l'AFC** conjointement à :

Gérard Bricogne et Vincent Favre-Nicolin

Félicitations à eux!

Vous trouverez les détails de la **genèse** de ce prix, les **parcours** des lauréats et leurs **réactions** sur le site de l'AFC, rubrique "*Les prix de l'AFC*". https://www.afc.asso.fr/prix-de-these/le-prix-andre-guinier/millesime-2020

Ce prix leur sera remis à l'occasion de notre congrès général, AFC2021 à Grenoble.

N'hésitez pas à faire la publicité de ce prix 2020 dans vos entourages professionnels. Pour information, ce résultat et son contexte seront relayés par l'IUCr dans la prochaine IUCrnewsletter.

Bon travail et bonne continuation à tous,

Philippe Guionneau Président de l'AFC

Howard Flack Lecture Series

Unfortunately, due to the coronavirus-related travel restrictions, we had to cancel this year's Howard Flack Lecture Series, scheduled for November 2020. For the Lecture Series in 2021 we are open to suggestions for potential lecturers. Please email your suggestions to the President Antonia Neels (antonia.neels@empa.ch).

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

Due to the limited meeting and travel possibilities this year, the remaining funds from 2020 will be available additionally for 2021. Nonetheless, if you are attending a meeting later this year, or have recently attended a 2020 meeting, you are welcome still to apply for 2020 support.

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

IUCR XXV



More info at: https://www.xray.cz/iucr/

The Zürich School of Crystallography

The Zürich School of Crystallography 2021 Bring Your Own Crystals University of Zürich June 6 – 17, 2021 Organized and directed by

Anthony Linden and Hans-Beat Bürgi

More info at: https://www.chem.uzh.ch/linden/zsc/

IUCr XXVI



26th Congress & General Assembly of the International Union of Crystallography 2023 22 Aug 2023–29 Aug 2023 in Melbourne, Australia

More info at: https://scanz.iucr.org/

7th European Conference on Crystal Growth, ECCG7

Date: July 26-28, 2021

Venue: Marriott Rive Gauche Conference Center, Paris, France

(no website available yet)

3rd European School on Crystal Growth, ESCG-3

Date: July 21-24, 2021

Venue: Chimie-Paris (IRCP) and Physico-Chemical Biology Institute (IBPC), Paris,

France

(no website available yet)



https://www.epdic17.org/

Positions

W2 Position at LMU München



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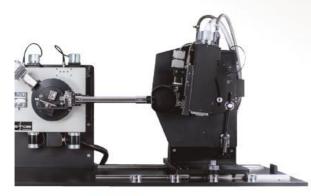






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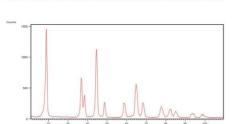
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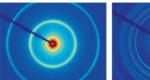


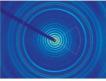
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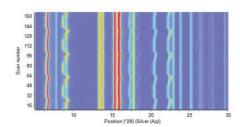


Hyper-speed full pattern snapshot (33° 2 θ with Ag radiation, equivalent to ~100°2 θ with Cu radiation) recorded in just 2 seconds.





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



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



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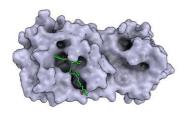




Every structure counts



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



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



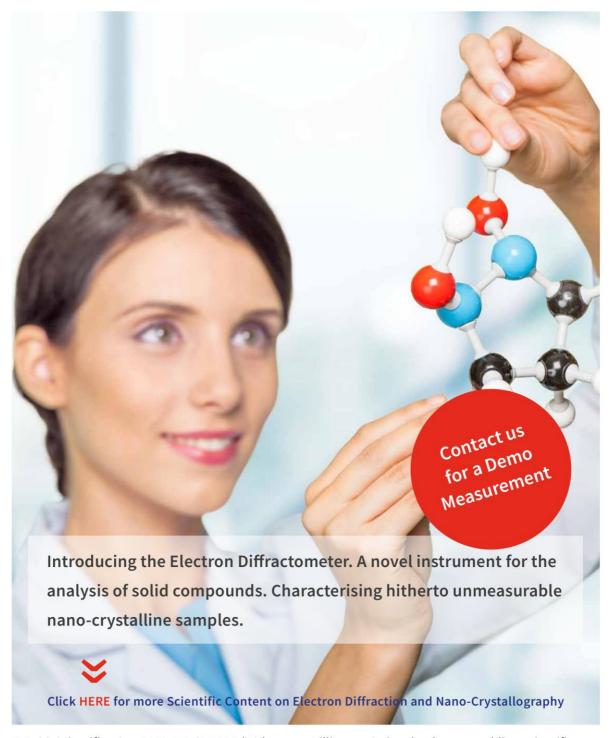
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Calls for proposals

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

Facility	-	Deadline(s)	Link
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For news about current s			www.psi.ch/useroffice/
SLS: Swiss Light Source All except PX lines Protein crystallography bea	mlines (PX)	15.03. and 15.09. 15.04. and 15.10.	ffice/proposal-deadlines
SINQ: Swiss Spallation N All instruments (regular calls)			psi.ch/de/useroffice/proposal-
SINQ/SLS Joint x+n proposals (MS/HRPT)	29.02.	https://www. deadlines	psi.ch/de/useroffice/proposal-
SµS: Swiss Muon Source DOLLY, GPD, GPS, HAL- 9500, LEM SwissFEL	Dec. 2020.,	https://www. deadlines	psi.ch/de/useroffice/proposal-
ARAMIS-Alvra, ARAMIS-Bernina	15.03, 15.09	1	
ESRF: European Synchrotron long term proposals short term proposals (standard)	15.01.2021 10.09.2020	www.esrf.eu/ UsersAndScie	
ILL: Institut Laue Langevin All instruments	17. 09. 2020	www.ill.eu/	
FRM II: Heinz Maier- Leibnitz All instruments Rapid access program	tba tba	www.mlz-gar	ching.de/user-office/
SNS Spallation Neutron Source Oak Ridge	16.09.2020	neutrons.orn	i.gov

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

Prague, CZ	25 th Congress & General Assembly of the IUCR, Congress postponed to August 2021 https://www.xray.cz/iucr/	To be announced
Prague, CZ	Congress postponed to August 2021	To be announced
Prague, CZ	Congress postponed to August 2021	To be announced
	https://www.xray.cz/iucr/	
University of	Zurich School of Crystallography	15.01.2021
Zurich		
Prague, CZ	25 th Congress & General Assembly of the IUCR,	Abstracts for
	Congress postponed to August 2021	Lectures:
	https://www.xray.cz/iucr/	21.03.2021
Paris, F	7th European Conference on Crystal Growth, ECCG7	tba
Paris, F	3rd European School on Crystal Growth, ESCG-3	tba
Šibenik, HR	EPDIC17, https://www.epdic17.org/	see website
Versailles, F	33rd European Crystallographic Meeting	To be announced
	https://ecanews.org/	
Melbourne, Au	26 th Congress & General Assembly of the IUCR, https://scanz.iucr.org/	To be announced
	Prague, CZ Paris, F Paris, F Šibenik, HR Versailles, F Melbourne,	Zurich http://www.chem.uzh.ch/linden/zsc Prague, CZ 25 th Congress & General Assembly of the IUCR, Congress postponed to August 2021 https://www.xray.cz/iucr/ Paris, F 7th European Conference on Crystal Growth, ECCG7 Paris, F 3rd European School on Crystal Growth, ESCG-3 Šibenik, HR EPDIC17, https://www.epdic17.org/ Versailles, F 33 rd European Crystallographic Meeting https://ecanews.org/

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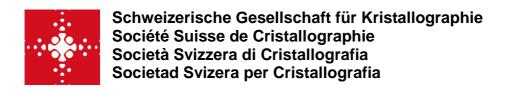
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If you are working in the field of crystallography, you might be interested in becoming a member of our society. For more information as well as online registration, please go to our website (http://www.sgk-sscr.ch).

Presently, the yearly membership fee is CHF 40 (CHF 10 for students).

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



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