

SIG13

Reported Period: June 2022 – August 2023

Report Date: 11th September 2023

Reported by: Katharina Edkins (SIG secretary), Teresa Duarte (SIG co-chair) and Petra Bombicz (SIG Chair)

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1. Introduction:

During the last year the SIG-13 Committee has reinforced both the reorganisation and promotion of the SIG to the Structural Science Community. SIG-13 members have been actively involved in the organization of several events and meetings devoted to the dissemination of structural studies within the field of materials properties. Its members participate in the work of the Organising and Programme Committees of the 34rd European Crystallographic Meeting (ECM34). A Lunchtime Seminar was held by former SIG13 Secretary. SIG13 poster prize was established sponsored by CrystEngComm. A Logo competition was launched, still without a winner. Four events were supported by SIG13 in the period.

2. SIG web site: SIG13 [About SIG-13 – SIG-13 Molecular Structure and Chemical Properties – European Crystallographic Association \(ecanews.org\)](https://ecanews.org)

3. Number of SIG-13 members according to (<https://ecanews.org/groups/sig-13-molecular-structure-and-chemical-properties/>): 78 (as on 10 September 2023)

4. Existence of a SIG mailing list: Yes

Address of the mailing list: Mailing list through SIG secretary

Number of members in the SIG mailing list: 82

Through the ECA website above and the emailing list it is possible to advertise all events related to our activities.

5. The approximate total number of researchers involved in the SIG (please indicate the basis for the estimate) 103 from ECA website last year, maximum ~150 previous years, but additional contacts through French, British, Italian, Spanish, South African Crystallographic Associations, etc.

6.a SIG-13 microsymbiosia suggestions for ECM34: Number of suggested microsymbiosia was reduced to 8 after the request of the organisers of ECM34.

Microsymbiosia at ECM34 organised by the suggestion of SIG13	GIG / SIG
Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function	SIG-13, SIG-07
Non-covalent interactions in crystal growth and structure design	SIG-13, SIG-07, SIG-02, SIG-09

Microsymposia at ECM34 organised by the suggestion of SIG13	GIG / SIG
Correlate molecular structure with materials properties	SIG-13, SIG-07, SIG-14
Porous functional materials	SIG-13, SIG-07
Molecular structure and chemical bonding in the view of quantum crystallography	SIG-13, SIG-02
Chirality: Meeting point of crystallography, chemistry and topology	SIG-13, SIG-09
Things we no longer need to know – or do we? (Or Detecting and avoiding fraud and blunders in crystallography) Tricks in structure solution (or Common mistakes and problems in using black boxes)	SIG-13, SIG-07, GIG-02, GIG-01
Techniques to discover polymorphism: mechanochemistry, crystal growth and others	SIG-13, SIG-07

6.b SIG-13 keynote suggestions for ECM34: Number of suggested keynote lecturers was reduced to 2 by the request of the organisers of ECM34.

Máté Erdélyi is Professor of the Department of Chemistry-BMC, Organic Chemistry, Uppsala University, Sweden;

Chiara Massera is Associate Professor at the Department of Chemical, Life and Environmental Sustainability Sciences of the University of Parma, Italy.

7. Prizes sponsored/coordinated:

The *International Kálmán Prize* was established by the Hungarian Chemical Society and was endorsed by European Crystallographic Association in 2019. The ECA awards the Alajos Kálmán Prize twice in a three-year cycle at the ECMs. The Prize is awarded to an individual researcher in recognition for outstanding scientific contributions in the field of structural sciences within the last 5-10 years. The prize consists of a medal and a financial award, as well as the opportunity for the awardee to deliver a Prize Lecture at the ECM. The selection of the awardee is conducted by ECA SIG-13, although the recognised field is wider, including all structural sciences. The Executive Committee works on changes of By-law 8 of ECA about all the ECA Prizes in order to achieve a regulation integrated into the ECA Prizes' guidelines as much as possible. The amendment will be voted by the Council Meeting September 2023.

The first International Kálmán Prize was conferred to Professor Luigi Nassimbeni at ECM-32 in 2019. In its second iteration, the prize was given to Professor Eric Collet at the ECM-33 in 2022. The third International Kálmán Prize will be awarded at the ECM34 in Padova.

SIG13 poster prize: CrystEngComm poster prize of ECA SIG13 is settled. Pierangelo Metrangolo as Editor-in-Chief of CrystEngComm published by the RSC is very supportive of our plan, and Mike Andrews, Deputy Editor, has evaluated all the necessary details. By the request of the RSC it is a rolling agreement from ECM to ECM. The prize will be a £100 voucher for the RSC bookshop, a free subscription to the journal, and online promotion for the winner. The chair of SIG13 needs to contact Mike / RSC in November the year before the respective ECM for the financial planning, and 6 weeks before the ECM to plan all the details (poster panel, certificate, its handling etc).

8. Past/postponed activities other than Microsymposia at ECM which SIG-13 members have been involved with:

Title: Zürich School of Crystallography 2021 (postponed to June 2022 due to COVID-19)

Chairs: Tony Linden, Hans-Beat Bürgi

Website: <http://www.chem.uzh.ch/linden/zsc/Program.html>

The 'Zürich School of Crystallography' fills a niche by offering a course that allows young researchers in chemistry and physics to investigate crystals of immediate interest in their own research. The students profit from a combination of theoretical concepts and hands-on experience in all steps of small-molecule crystal structure analysis, from crystal growth to the interpretation and presentation of results.

Title: The 7th European Crystallography School, Lisbon, Portugal

Chair: Teresa Duarte

Website: <https://ecs7.events.chemistry.pt/>

The 2022 European Crystallographic School was the first one to be attended IN PERSON after the COVID19 pandemic. The school was held in Lisbon, Portugal, at the Chemical Engineering Department of Instituto Superior Técnico, Lisbon University. The program of the 2022 School was focused on X-ray crystallography of powders, small molecules and proteins, covering topics from the fundamentals of diffraction to the latest developments in the fields. There were 47 students and 25 teachers/tutors. The overall program was organised so that each morning students had their theoretical classes and in the afternoon they had hands-on tutorials. The attendees were divided into small groups for tutorials and laboratory practical sessions, so that they could have hands-on experience.

Title: The 8th European Crystallography School, Berlin, Germany

Chair: Manfred Weiss

Website: https://www.helmholtz-berlin.de/events/ecs8/index_en.html

The organisers of the 6th and 7th European Crystallographic School contributed with their experience to the organisation of the 8th School that took place in June 2023. The school was held at the BESSY II electron storage ring, operated by the Helmholtz-Zentrum Berlin. The focus of the school was to cover the various applications of X-ray crystallography to powders, small molecules, and proteins, with topics ranging from the fundamentals of diffraction to the latest developments in the fields. The school was directed to undergraduate, graduate, postgraduate and young scientists from different fields (biology, biochemistry, chemistry, material science, physics, etc.) who are eager to learn more about the possibilities of crystallography. Following the standard format, the school had fundamental lectures taught during the mornings, while the afternoons were dedicated to lectures on applications and hands-on tutorials.

Title: 21st ECA lunchtime webinar

Talk by Clive Oliver, SIG13

The 21st ECA lunchtime seminar took place on 25 May 2023 was suggested by the members of the SIG13 to be presented by Clive Oliver from the University of Cape Town on "Small molecular and

crystal structure changes in MOFs leading to large differences in sorption and thermosensitive properties”.

SIG-13 provided support letters for schools/conferences:

Title: 3rd International School on Advanced Porous Materials (MOFsSchool2023)

Directors: Valentina Colombo, Simona Galli, Jorge A. R. Navarro

Date: 19-23 June 2023

Website: <https://mofs2023.lakecomoschool.org>

MOFsSchool took place from 19-23 June 2023 as a hybrid meeting.

9. Future/Programmed Activities.

Title: Hot Topics in Contemporary Crystallography 6 workshop (HTCC6)

Chair: Martina Vrankić

Website: <https://htcc6.org/>

Date: 7-12 April 2024

Since 2014, HTCC workshops have tackled the most fascinating achievements in both experimental methods and theoretical approaches, that have recently brought structural research to the forefront of natural sciences. We try to bring together leading experts in selected domains as lecturers, and motivated scientists in crystallography or related fields as “students”, who may come from both academia and industry, and who are interested in acquiring new knowledge on cutting-edge methods in structural science and exploring ways to apply them in their ongoing research. Since HTCC4 held in 2019, HTCCs are dedicated exclusively to macromolecular crystallography and are taking place in Dubrovnik.

Title: 30th Croatian-Slovenian Crystallographic Meeting

Director: Ivica Đilović

Date: June 2024

Website:

The conference covers all general fields of crystallography, from various small molecule systems to macromolecules, as well as materials, crystal engineering, mineralogy, metallurgy, solid solutions, powder diffraction, small angle scattering, crystal structure prediction, and many more. Contributions showing the synergy of diffraction, and microscopy with other methods, are also presented.

Title: Zürich School of Crystallography – Bring Your Own Crystals

Directors: Tony Linden and Hans-Beat Bürgi

Date: 16-28 June 2024

Website: <http://www.chem.uzh.ch/linden/zsc>

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10. Other matters. (50 words max.)

SIG13 has announced an invitation for a **logo competition**. The logo should express the scope and objectives of SIG13. There is no restriction in shape and colour, but originality, scalability, proportions, simplicity, timelessness are the aspects of evaluation. The winner is offered a small gift by the CCDC.

Scope and Objectives: SIG 13 is supporting advances in molecular and crystal structure, in chemical crystallography through both theoretical and experimental methods and their applications with the aim to discover the relationship between the molecular structure and the chemical properties. We provide a coherent forum for molecular crystallographers working in many of the cutting edge areas of materials design, crystal engineering, tailoring molecular materials for physical properties etc. The aim of the SIG is to promote activity where chemistry is seen through the eyes of the crystallographer, and to represent and connect researchers in this area.

SIG13 is continuing in the promotion of the structural chemistry at all levels, members who are organizing and participating in official European Crystallographic Schools.

11. Brief annual activity report (100 words max.)

The SIG-13 Committee has worked actively on the two main goals within its remit: (i) the promotion of “Molecular Structure and Chemical Properties” through greater publicity for the SIG, particular through its new website; (ii) by participating effectively in the planning process for the upcoming ECM and other Meetings in Crystallography. Alajos Kálmán Prize was awarded during ECM33. Support of SIG13 was given to four forthcoming events. The last two SIG-13 meetings were held in-person at the ECM33 in Versailles, France, and on-line on 18th November 2022. The main order of business was to suggestion for microsymbosia topics and keynote lecturers for the ECM34 programme committee meeting. During the last year a lunchtime seminar was held by a SIG13 member, SIG13 poster prize was established, a logo competition was announced.

12. List SIG officers, name and e-mail, and specify their main function in the SIG:

- * *Chair:* Dr Petra Bombicz (responsible for coordination of the SIG activities and for implementing/distributing news of SIG interest)
E-mail: bombicz.petra@ttk.hu
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- * *Co-chair:* Prof. Teresa Duarte (responsible for coordination of the SIG activities and for implementing/distributing news of SIG interest)
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- * *Secretary:* Dr Katharina Edkins (responsible for the SIG web-page and for maintaining the SIG13 mailing list)
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