

SIG13

Reported Period: September 2024 – August 2025

Report Date: 21st August 2024

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

1. Introduction:

SIG-13 members have been involved in the organization of several events and meetings devoted to the dissemination of structural studies and chemical properties. Its members participated in the work of the Organising and Programme Committees of the 34th and 35th European Crystallographic Meetings (Padova - ECM34, Poznan – ECM35). Alajos Kálmán Prize will be awarded the 4th time at ECM35. SIG13 and CrystEngComm outstanding Poster Award, established in 2024 will be awarded for the second time during ECM35. Two events supported by SIG13 took place during this period. Three events requested the support of SIG13 as per 2025-2026. SIG13 participated in the call for short video contributions showcasing its member activities

2. SIG13 web site: <https://ecanews.org/sig-13/>

3. Number of SIG-13 members: 87 (as on 16 August 2025),

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: 89, 15 emails were assigned inactive this year.

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) 87 from ECA website from two years ago, maximum ~150 from previous years.

6.a ECM35: The proposed Microsymposia related to the topic of SIG13, and mostly in close collaboration with SIG7 were:

The impact of supramolecular interactions on the dynamics of molecular crystals

The complex world of multicomponent crystals

Insight into crystals: crystal forms, isostructurality, symmetry, chirality

Molecular structure and chemical bonding

Non-covalent interactions in structures

Polymorphism and phase transitions

Supramolecular interactions behind crystal engineering

Driving anion-anion and cation-cation self-assembly

Designing the void: structural mastery in advanced porous materials

Most of them have, however, changed the title and/or been merged with others. They will be corrected and added here.

6.b SIG-13 keynote lecture at ECM35:

The keynote will be given by Prof Elena Simone from Politecnico di Torino, Torino in Italy

7. Prizes sponsored/coordinated:

The *International Kálmán 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 selection of the awardee is conducted by a panel nominated by ECA SIG-13 in close collaboration with the Hungarian Chemical Society. The Kálmán Prize awarded at the ECMs was established by the Hungarian Chemical Society and was endorsed by European Crystallographic Association in 2019. 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 third International Kálmán Prize will be awarded to Dr. Felipe Gándara at the ECM35 in Poznan.

The SIG13 and CrystEngComm outstanding Poster Award is settled and will be awarded at ECM35 in Poznan. By the request of the RSC it is a rolling agreement from ECM to ECM. The prize is a Eur250 voucher. The chair of SIG13 contacted Mike Andrews RSC about the financial planning, and before the ECM to plan all the details (poster panel, certificate, and handling).

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

At the ECM in Padova, SIG-13 members were active in the micorsymposia with good numbers of abstracts submitted to a variety of themes. This is a good reflection on the activity so we need to harness this and find ways to convert the conference activity into continual involvement throughout the year:

MS13 Molecular structure and chemical bonding in the view of quantum crystallography	13
MS20 When can ED challenge XRD in small molecule crystallography?	17
MS21 Electron diffraction joining forces with quantum crystallography towards materials science 6 applications	6
MS30 Noncovalent interactions in structure design	24
MS31 Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function	27
MS32 Correlate molecular structure with materials properties	23
MS33 Applications of 3D-PDF	25
MS40 Approaches and tools for learning crystallography efficiently and avoiding misconceptions	29

Title: 6th International Symposium on Halogen Bonding (ISXB-6)

Chair: Marijana Djakovic

Website: <https://isxb6.hkd.hr/>

Date: 20-25 October 2024

The 6th International Symposium on Halogen Bond (ISXB6) took place from October 20 to 25, 2024, in Dubrovnik, Croatia. This conference gathered 75 participants from 18 countries, including Croatia, Slovenia, Italy, Germany, Switzerland, the United Kingdom, Sweden, Poland, France, Finland, Portugal, Austria, the United States, Canada, Japan, China, South Africa, and Korea. Attendees presented their research across various chemistry fields, focusing on halogen bonds and

related interactions, which encompassed both experimental and theoretical approaches spanning advanced materials to medicinal chemistry.

The conference showcased a total of 7 keynote lectures, 22 invited lectures, 2 review lectures, and 6 oral presentations by distinguished scientists, 11 oral presentations by emerging researchers, and 22 poster presentations. Several sponsors generously supported the event, including the International Union of Crystallography (IUCr), the European Crystallographic Community (ECA), the Cambridge Structural Data Centre (CCDC), the University of Pennsylvania, and two RSC journals: CrystEngComm and the New Journal of Chemistry (NJC). Together with the CCDC, the RSC journals presented three awards for the best oral presentation (RSC-NJC) and the best poster presentations (CCDC and RSC-CrystEngComm) by young researchers. Additionally, the conference organising committee recognised several special prizes for outstanding oral and poster presentations from young participants. The presence of young researchers at the event was further enhanced through 16 scholarships provided by the IUCr, ECA and CCDC.

9. Future/Programmed Activities.

SIG13 participated in the Call for short video contributions showcasing SIG-13 member activities in 2025, but we got no answers. SIG 23 intends to promote this event again in 2025-2026. SIG will support all the events in its focus area.

10. Other matters. (50 words max.)

SIG13 is continuing in the promotion of the structural chemistry at all levels, members who are organizing and participating in official European Crystallographic Schools. We have supported the 4th International School on Porous Materials: MOFschool 2025 (16-20 June), the 10th European Crystallography School (ECS10) "From Nano to Macro: Elucidating Structures at Different Length Scales," for June 22-27, 2025 in Ohrid, the 32nd Croatian-Slovenian Crystallographic Meeting (CSCM32), the 19th European Powder Diffraction Conference (EPDIC-19), (June 23–26, 2026) Switzerland, and Zurich School of Crystallography (ZSC), (29 June to 11 July 2026)

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 but also actively emailing its members; (ii) by participating effectively in the planning process for the upcoming ECM and other Meetings/Schools in Crystallography, as reported previously.

The next Alajos Kálmán Prize will be awarded in Poznan, as well as the SIG13 CrystEngComm poster prize. SIG13 supported two events last year and gave its support to three forthcoming events. As it happened at the last ECM year, SIG-13 meetings will be held in-person at the ECM35 in Poznan, Poland, and an on-line meeting is also planned.

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

* *Chair*: Prof. Teresa Duarte (responsible for coordination of the SIG activities and for implementing/distributing news of SIG interest)

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