

## **SIG13**

**Reported Period: September 2023 – August 2024**

**Report Date: 21<sup>st</sup> August 2024**

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

=====

### **1. Introduction:**

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 34<sup>th</sup> and 35<sup>th</sup> European Crystallographic Meetings (Padova - ECM34, Poznan – ECM35). Alajos Kálmán Prize is awarded the 3<sup>rd</sup> time at ECM34. SIG13 poster prize was established and will be first awarded during ECM34 sponsored by CrystEngComm. A Logo competition was performed. Three events were supported by SIG13 in the period. One event requested the support of SIG13 for the next year. A new website has been constructed.

**2. SIG13 web site:** old: [About SIG-13 – SIG-13 Molecular Structure and Chemical Properties – European Crystallographic Association \(ecanews.org\)](http://www.ecanews.org/about-sig-13), new: <https://ecanews.org/sig-13/>

**3. Number of SIG-13 members according to (<https://ecanews.org/groups/sig-13-molecular-structure-and-chemical-properties/>):** 82 (as on 16 August 2024), increase of 4 in the last year

### **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 from two years ago, maximum ~150 previous years, but additional contacts through French, British, Italian, Spanish, South African etc. Crystallographic Associations.

### **6.a ECM34: Microsymposia related to the topic of SIG13.**

M8 Nucleation and crystal growth/Chaperones and crystallization

M10 Structural-based drug discovery

M26 Chirality: Meeting point of crystallography, chemistry and topology

M27 High Pressure Crystallography: Exploring Structure and Method Development at Extreme Conditions

M28 Structural characterization of Energy Harvesting and Conversion Materials

M29 Structural characterization in Functional materials

M30 Porous functional materials

M31 Noncovalent interactions in structure design

M32 Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function

M33 Correlate molecular structure with materials properties

M40 Techniques to discover polymorphism: mechanochemistry, crystal growth and others

Also related:

M38 Things we no longer need to know – or do we?

M39 Common mistakes and problems in using black boxes

M41 Approaches and tools for learning crystallography efficiently and avoiding misconceptions

#### **6.b SIG-13 keynote lecture at ECM34:**

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* 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 ECA SIG-13, although the recognised field is wider, including all structural sciences. 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 Prof Piero Macchi at the ECM34 in Padova.

The *SIG13 poster prize*: CrystEngComm poster prize of ECA SIG13 is settled. It will be awarded the first time at the ECM34 in Padova. Pierangelo Metrangola as Editor-in-Chief of RSC CrystEngComm was very supportive of our plan (2023), 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 is a £125 voucher. The chair of SIG13 needs to contact Mike Andrews 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 activities other than Microsymposia at ECM which SIG-13 members have been involved with:**

**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:** 30<sup>th</sup> Croatian-Slovenian Crystallographic Meeting

Director: Ivica Đilović

Date: June 2024

Website: [CSCM 2024 – 30th Croatian-Slovenian Crystallographic Meeting \(hazu.hr\)](https://cscm2024.hazu.hr/)

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>

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.

## 9. Future/Programmed Activities.

**Title:** 6<sup>th</sup> International Symposium on Halogen Bonding (ISXB-6)

Directors: Marijana Đaković

Date: Dubrovnik, Croatia, 20-25 October 2024

Website: [ISXB6 – International Symposium on Halogen Bonding \(ISXB6\) \(hkd.hr\)](http://www.isxb6.hr)

The ISXB-6 brings together scientists from a variety of disciplines. The symposium will cover the fascinating phenomenon of halogen bonding and related interactions, from fundamental principles to applied technologies, both experimental and theoretical aspects. The knowledge of the properties of halogen bonding is relevant in many areas of research, such as chemical crystallography, medicinal chemistry, chemical biology, materials science as well as industrial applications.

## 10. Other matters. (50 words max.)

The logo expresses the scope and objectives of SIG13:

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 will be awarded the third time, as well as the SIG13 CrystEngComm poster prize the first time during ECM34 in

Padova. A logo competition took place resulting in a new logo of the SIG, a new website of SIG13 has been constructed. SIG13 supported three events last year and gave its support to one forthcoming event. As it happened at the last ECM year, SIG-13 meetings will be held in-person at the ECM34 in Padova, Italy, and an on-line meeting is also planned. The main order of business is to suggestion for microsymposia topics and keynote lecturers for the ECM35 Poznan programme committee meeting. 2024 is an election year, new officers will be voted.

## **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  
*Address:* Chemical Crystallography Research Laboratory, Research Centre for Structural Sciences, HUN-REN Research Centre for Natural Sciences, Magyar Tudósok körútja 2, H-1117 Budapest, Hungary  
Tel: +36 1 382 6513
  
- \* *Co-chair:* Prof. Teresa Duarte (responsible for coordination of the SIG activities and for implementing/distributing news of SIG interest)  
*E-mail:* teresa.duarte@tecnico.ulisboa.pt  
*Address:* Centro de Química Estrutural, Instituto Superior Técnico Universidade de Lisboa, Av Rovisco Pais, 1049-001 Lisbon, Portugal
  
- \* *Secretary:* Dr Katharina Edkins (responsible for the SIG web-page and for maintaining the SIG13 mailing list)  
*E-mail:* katharina.edkins@manchester.ac.uk  
*Address:* School of Health Sciences, The University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom  
Tel: +44 161 2758348