

## **SIG13**

**Reported Period: September 2019 –January 2021**

**Report Date:**

**Reported by: Clive Oliver (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, its members participating on the organising and programme committees for the 33<sup>rd</sup> European Crystallographic Meeting, ECM33, which was postponed to 2022 due to COVID-19. All SIG-13 members have been involved actively in the organization of events and meeting devoted to the diffusion of structural studies within the field of materials properties.

**2. SIG web site:** SIG13 <https://ecanews.org/groups/sig-13-molecular-structure-and-chemical-properties/>

**3. Number of SIG-13 members according to (<https://ecanews.org/groups/sig-13-molecular-structure-and-chemical-properties/>):** 151 (as on 28 January 2021)

**4. Existence of a SIG mailing list: Yes**

**Address of the mailing list:** Mailing list through ECA website

**Number of members in the SIG mailing list:** 151

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)** 151 from ECA website but additional contacts through French, British, Italian, Spanish, South African Crystallographic Associations, etc.

**6. SIG-13 microsymposia suggestions for ECM33:** SIG-13 has suggested 15 microsymposia for ECM33 to be co-hosted with either GIG-1, GIG-3, SIG-2, SIG-3, SIG-4, SIG-5, SIG-7, SIG 8 or SIG-9. Two keynote and three plenary speakers have also been suggested.

<b>Suggested microsymposia</b>	<b>GIG / SIG</b>
Combining Techniques to Disclose Structure-property Relationships in Smart Materials  Structure and properties relationships at work, combined techniques for characterization	SIG7-SIG13-GIG3/1
Properties prediction and data mining  Data Mining for Properties Prediction	SIG7-SIG13/2

<b>Suggested microsymbosia</b>	<b>GIG / SIG</b>
Supramolecular recognition: matching molecular partners Supramolecular Recognition: Can We Trust Synthons?	SIG7-SIG13/4
Function optimization via unconventional interactions The Periodic Table of Chemical Interactions	SIG7-SIG13/5
Aspects in Crystal engineering: structural flexibility and phase transitions Disorder and Structural Flexibility inside Crystals	SIG7-SIG13/6
Solid State interactions driven chemical reactions and catalysis	SIG13/7
Navigating pharmaceuticals crystal forms	SIG13/8
Nanocrystallography of organic and metallo-organic crystals	SIG4-SIG7/9-SIG13

### **Prizes sponsored/coordinated:**

The first International Kálmán Prize was conferred to Professor Luigi Nassimbeni at ECM-32 in Vienna, Austria during August 2019. The prize is in memory of Alajos Kálmán, an eminent scientist in the field of chemical crystallography. The Prize is established by the Hungarian Chemical Society and is endorsed by European Crystallographic Association. The ECA awards the Alajos Kálmán Prize twice in a three-year cycle at the ECMs. The Prize will be 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 awardee delivers a Prize Lecture at the ECM.

The chair of the ECA SIG-13 is the chairperson of the Alajos Kálmán Prize Committee. The Chair sets up the Prize Committee. The Committee consist of five members, one of them is delegated by the Hungarian Chemical Society. The Alajos Kálmán Prize Committee is an independently convened group that works in confidence to discuss candidacies for the Kálmán Prize. The selection of the awardee is conducted by ECA SIG-13, although the recognised field is wider, including all structural sciences. Nominations must be sent to the ECA SIG-13 Chair.

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

**Title:** The 6<sup>th</sup> European Crystallographic School, Budapest,. Hungary, 4-10 July 2021 – Chair: Petra Bombicz

Website : <https://ecs6.ecanews.org>

This school was originally planned for 5-11 July 2020 but was postponed by one year due to COVID-19. Additionally, it has been moved to an online platform, i.e. it will be a virtual school.

The organization of the school is progressing well with the involvement of professional conference organizers. Registration is open with the early-bird registration being 01 March 2021. Opportunities exist for partial waiving of registration fees by applying for bursaries, made possible through the generosity of ECA and IUCR funding.

Short Description: The school welcomes wide range of participants, including undergraduate, graduate and postgraduate students, postdocs, young scientists and professionals from the fields of chemistry, biology, solid state sciences who wishes to participate in an intensive crystallography course. Theoretical and practical lectures, hands-on tutorials, laboratory practices are planned. Poster sessions will be organised to students to present their results. The school will be useful in further academic development of the participants offering a training for new generations of crystallographers.

**Title:** ISXB-4: 4<sup>th</sup> International Symposium on Halogen Bonding, 2-5 November 2020 – Chair: Catharine Esterhuysen

Website: [ISXB-4 Symposium 2020 | Halogen Bonding Symposium \(isxb42020.net\)](http://isxb42020.net)

This conference was originally planned for 23-27 March 2020, to take place in Stellenbosch, South Africa. Due to COVID-19 it was postponed to 2-5 November 2020 and took place in an online format. There were two hundred participants thanks also to bursary support provided by ECA and IUCr by the waiving of registration fees. This allowed more attendees than expected for an in-person meeting.

Short description: The aim of ISXB-4 was to bring together scientists from multiple disciplines, with halogen bonding and related interactions being the common interest. The symposium covered both experimental and theoretical aspects of fields as diverse as medicinal chemistry, chemical biology, materials science and those pertain to industrial applications. There was also a strong focus on young scientists, with special sessions for emerging investigators and for undergraduates and high-school learners.

## 9. Future/Programmed Activities.

SIG-13 also provided several support letters for schools/conferences:

**Title:** Zurich 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:** 55<sup>th</sup> Course of International School of Crystallography ‘Molecular Crystal Engineering’

Organiser: Annalisa Guerri, Directors: Matteo Lusi, Ulrich J. Griesser, Lucia Maini

Website: [www.crystalerice.org](http://www.crystalerice.org)

Postponed from 28 May – 5 June 2021 to 31 May – 4 June 2021 to be held online.

The Erice School provides theoretical and practical aspects of crystal engineering in form of lectures, workshops and hands-on trainings. The school aims the understanding of intermolecular interactions which is the fundament of modern crystal engineering and exploitation of the relations between structure and properties which is the interest of SIG13.

**Title:** 2<sup>nd</sup> International School on Advanced Porous Materials (MOFschool2021)

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

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

MOFschool2021 will take place between 21-25 June 2021 planned as an in-person meeting with max 55 participants. The School starts with an introduction to metal-organic frameworks and related porous materials given by Prof. Omar Yaghi. The program continues with lectures on cutting edge synthetic and post-synthetic methods, advanced characterization techniques (e.g. infrared spectroscopy with probe gas molecules; in situ and operando X-ray diffraction techniques with lab instruments or at large scale facilities; X-ray absorption spectroscopy; molecular modelling), pertinent software with tutorials and hands-on sessions. The applications of porous materials in energy- and environment-related fields will be discussed by Prof. Jeffrey R. Long and Prof. Mircea Dincă. Moreover, the young participants will be given the opportunity to present their research during one flash-presentation session and two poster-presentation sessions.

**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.

**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.

The last SIG-13 meeting was held during ECM32 in Vienna, Austria on 20 August, 2019. The chair, co-chair and secretary were present, as well as five other SIG-13 members. The main order of business was to suggest microsymposia topics for the ECM33 programme committee meeting that was to take place soon after. Teresa Duarte was chosen to be SIG-13’s representative on the ECM33 programme committee.

**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)

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\* *Secretary:* Dr Clive Oliver (responsible for the SIG web-page and for maintaining the SIG13 mailing list)

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