

SIG13

Reported Period: February 2021 –June 2022

Report Date: 9th August 2022

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, its members participating on the organising and programme committees for the 33rd 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 dissemination 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/>): 103 (as on 09 August 2022)

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: 103

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 but additional contacts through French, British, Italian, Spanish, South African Crystallographic Associations, etc.

6. SIG-13 microsymbposia suggestions for ECM33: SIG-13 has suggested 15 microsymbposia 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.

| Microsymbposia at ECM33 organised bythe suggestion of SIG13 | GIG / SIG |
|--|-------------------|
| Structural Characterization of Functional Materials | SIG7-SIG13-GIG3/1 |
| Properties prediction and data mining Data Mining for Properties Prediction | SIG7-SIG13/2 |
| Supramolecular recognition | SIG7-SIG13 |

| Microsymposia at ECM33 organised by the suggestion of SIG13 | GIG / SIG |
|--|-------------------|
| Function optimization via unconventional interactions The Periodic Table of Chemical Interactions | SIG7-SIG13/5 |
| Crystal Engineering: structural flexibility, phase transitions and non-standard manipulation of synthons | SIG7-SIG13/6 |
| Crystallization Techniques and chemical reactions driven by solid state interactions | SIG13/7 |
| Navigating crystal forms in molecular and pharmaceutical materials | SIG13 |
| Advanced techniques to disclose structure-property relationships | SIG4-SIG7/9-SIG13 |

Prizes sponsored/coordinated:

The International Kálmán Prize has been established by the Hungarian Chemical Society and was endorsed by the 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 consists 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.

The first International Kálmán Prize was conferred to Professor Luigi Nassimbeni at ECM-32 in Vienna, Austria during August 2019. Now in its second iteration, the prize will be given to Professor Eric Collet from the University of Rennes, France, at the ECM-33 in Versailles, France, during August 2022. Prof Eric Collet is being recognized for his inspirational interdisciplinary research at the interface of material science, chemistry and physics with crystallography at the very heart of his work. Prof Collet is one of the pioneers who paved the way for the subsequent studies in the greatly innovative field of X-ray free electron lasers science. He with his collaborators made high impact studies of ultra-fast femtosecond experiments, ultra-fast photo excitations like photo induced structural dynamics, phase transitions and molecular switching. His outstanding achievement is based on the structural study of molecular complexes and new transition mechanisms, especially from the molecular to the crystal scale.

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

Title: The 6th 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 was a virtual school

The school welcomed a 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 wish to participate in an intensive crystallography course. Theoretical and practical lectures, hands-on tutorials, laboratory practices were delivered. Poster sessions were organised to allow students to present their results. 90 students participated from 4 continents, 35 scientists formed the international group of teachers.

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: 55th Course of International School of Crystallography 'Molecular Crystal Engineering'

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

Website: <http://www.crystalerice.org>

Postponed from 28 May – 5 June 2020 to 31 May – 4 June 2021, held online.

The Erice School provided theoretical and practical aspects of crystal engineering in form of lectures, workshops and hands-on trainings. The school was aimed at 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: 2nd International School on Advanced Porous Materials (MOFschool2021)

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

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

MOFschool took place from 21-25 June 2021 in remote mode with 130 participants, 108 of them were students. The School started with an introduction to metal-organic frameworks and related porous materials given by Prof. Omar Yaghi. The program continued 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 were discussed by Prof. Jeffrey R. Long and Prof. Mircea Dincă. Moreover, the young participants have been given the opportunity to present their research during one flash-presentation session and two poster-presentation sessions.

Title: Pan-African Conference on Crystallography virtual meeting (ePCCR),

Directors: Ahmadou Wague, Delia Haynes, Marielle Agbahoungbata and Thierry d'Almeida

Website: <https://events.saip.org.za/event/170/overview>

The Pan-African Conference on Crystallography (ePCCR) took place between 15th-19th November 2021 and brought together crystallographers, mineralogists and solid state scientists from Africa and beyond, towards the African Crystallographic Association. The meeting was part of the joint

event of the AfLS3-2021: African Light Source, ePCCr: Pan-African Conference on Crystallography Online and AfPS-2021: African Physical Society.

The topics of ePCCr covered Crystallographic Databases; Diffraction Physics; Phase Transitions; Inorganic Materials; Crystallography and Life Sciences; Crystal Engineering and Structural Chemistry; Large Facilities for Developing Countries.

The meeting was open to all, but the focus was to attract delegates particularly in Africa, and particularly among younger scientists. There is no registration fee for the virtual conference and bursaries of US\$75 were available to cover mobile phone data to further improve accessibility.

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 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 afternoons 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: 5th ECA lunchtime webinar

Talk by Katharina Edkins, SIG13

The 5th ECA lunchtime seminar was suggested by the members of the SIG13 to be presented by Katharina Edkins from the University of Manchester. She gave an introduction to hydrated crystal structures and their importance to pharmaceutical materials science. She then connected the crystal structures to the solution phase from which they crystallise indicating new ways to investigate and control hydrate formation.

9. Future/Programmed Activities.

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

Title: Cambridge Structural Database workshop at the ECM-33

Chair: Arie van der Lee

Website: <https://www.ecm33.fr/copie-de-ccp4-and-ccpem-workshops>

Date: 23 August 2022

This workshop is the initiative and organised by the French Professional Crystallographers' Network (RECIPROCS) with the chair of the Organizing Committee being Professor Arie van der Lee, Institut Européen des Membranes, CNRS, Université de Montpellier. The workshop will take place at the campus of the University of Versailles one day before the main meeting of the ECM-33. The teachers of the workshop will include representatives of the Cambridge Crystallography Data Center. This workshop is aimed at both chemical and biological crystallographers.

Title: ECM33 satellite meeting on high pressure crystallography

This satellite meeting would have focused on the structure-property relationships extracted from the study of functional materials under pressure, from inorganic to molecular materials or active pharmaceutical ingredients. Synthesis of new materials under pressure would have been also addressed. Unfortunately, this satellite meeting has been cancelled due to the low number of registrations.

Title: ECM33 satellite meeting on chirality in crystals

This satellite would have been covered the various aspects of chirality in the solid state and the contributions of crystallography to investigate properties of chiral crystals. Unfortunately, this satellite meeting has been cancelled due to the low number of registrations.

Title : Hot Topics in Contemporary Crystallography 5 workshop (HTCC5)

Chair: Aleksandar Višnjevac

Website: <https://htcc5.org/>

Date: 16-21 April 2023

The workshop of Hot Topics in Contemporary Crystallography is a successful series since 2014. This edition is dedicated to structural biology with the focus on the techniques which go beyond classical crystallography providing lectures and hands-on classes. Motivated young scientists in crystallography are expected to learn from leading experts of the field to present the most advanced methods in structural science. The workshop lasts 4 days and focuses on 4 topics: crystallization, processing, databases and visualization. These topics are highly important in molecular modelling, rational drug design, protein – ligand interactions, pharmaceutical development. The workshop is organised by the Croatian Association of Crystallographers and is anticipated to attract around 60 participants.

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 on 20 August 2019 during ECM32 in Vienna, Austria. 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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* *Co-chair:* Prof. Teresa Duarte (responsible for coordination of the SIG activities and for implementing/distributing news of SIG interest)

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