

SIG13

Reported Period: June 2013 –June 2014

Report Date:

Reported by: Alessandra Crispini (SIG Chair)

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1. Introduction. (50 words max.)

During the last year the SIG13 committee has reinforced both the reorganisation and promotion of the SIG to the structural science community, participating actively in the scientific organization of the ECM29 next coming meeting to be held in Rovinj, Croatia, between 23-28th August, 2015 and in the organization of the past ECM28 meeting in Warwick (GB). The excellent result obtained in the involvement in the organization of the past ECM28 meeting has implied the obtainment of a successful number of MS, all of them fully participated by high quality number of experts in the field. In continuity with the previous officers, Prof. Alessandra Crispini has remained SIG13 Chair, Prof. Paul R. Raithby co-chair and Dr. Marijana Đaković the secretary.

SIG13 representatives have been active in the development of the programme for the ECM29 meeting and have made major contributions to the setting up, in strong collaboration with other SIGs. In particular, Prof. Paola Paoli has strongly contributed to the development of the ECM29 scientific program within the SIG13 community. Then, in collaboration with all SIG13 members and with the help of the new mailing list, the microsymbiosia chairs and co-chairs have been selected and suggested as well as the KN speakers.

All SIG13 members are involved actively in the celebration of IYCR2014 with various activities. In particular Prof. Attila Benyei is co-author of a university textbook for MSc students of Chemistry in Structure determination by X-ray diffraction published in 2013. The book is in Hungarian and will be published electronically, hopefully soon. The topic is small molecule and protein crystallography and the book is dedicated to IYCR2014 (the logo is also used).

2. SIG web site:

SIG13 <http://sig13.ecanews.org/>

3. Number of ECA individual members registered with the SIG according to (<http://www.xray.cz/eca/im-payment.htm>)

SIG13 Molecular Structure and Chemical Properties 205

4. Existence of a SIG mailing list: Yes

Address of the mailing list: ECA-SIG13@chem.pmf.hr

<http://www.facebook.com/pages/ECA-SIG13/137466489407#!>

Number of members in the SIG mailing list: 183

Through the ECA-SIG13 Facebook home page is possible to advertise all events related to our activities: <http://www.facebook.com/pages/ECA-SIG13/137466489407#!>

5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate):

120 from ECA registration, but additional contacts through French, British, Italian and Spanish Crystallographic Associations.

6. List of MS organized and proposed by the SIG (also in collaboration with other SIGs) at the ECM29

Molecular crystals with tailored physical properties; Chair: Pilar Gomez-Sal (Spain); Co-chairs: Sebastian Pillet (France), Alessandra Crispini (Italy). SIG13

Structure and function in coordination compounds; Chair: Attila Benyei (Hungary); Co-chairs: Marijana Dakovic (Croatia), Wolfgang Scherer (Germany). SIG13

Mechanical effects and properties of ordered matter; Chair Pance Naumov (Japan); Co-Chairs: Anthony K. Cheetham (United Kingdom), Elena V. Boldyreva ((Russian Federation). SIG13

Molecular dynamics on molecular compounds; Chair: Jacco van der Streek (Denmark), Co-chairs: Graeme Day (UK), Matthew Habgood (UK). **SIG13**

Halogen Bonding in Polymorph and Co-crystal Screening; Chair: Mike Zaworotko, (Ireland); Co-chairs: Christer Aakeroy (USA); Tayur N. Guru Row (Republic of India).

Dynamics in Nanoporous Molecular Crystals; Chairs: Angiolina Comotti (Italy), Gareth Lloyd (UK), Len Barbour (South Africa) SIG13

Topology of crystal structures; Chair: Davide M. Proserpio (Italy); Co-chairs: Igor Baburin (Germany), Sven Lidin (Sweden); SIG13 **in collaboration with SIG12.**

We have agreed to support the following MS suggested from SIGs 11 and 12:

- High Pressure Solid State Chemistry and Materials Synthesis (from SIG-11)
- Advances in high-pressure methods (from SIG-11)
- In situ and in operando crystallography (from SIG-12)

Prizes sponsored/coordinated

none

8. Past Activities other than Microsymposia at ECM

Title: Hot Topics in Contemporary Crystallography (HTCC)

10-15 May, 2014, Šibenik, Croatia

Number of participants: 35

Level of involvement of SIG in the activity:

Several ECA Individual members involved into the delivery of the course, some SIG input into the Organizing Committee

Sponsored by ECA: yes

Other Sponsors/Organizers: IUCr and 15 commercial sponsors (diffractometer manufacturers)

Short Description: To celebrate the International Year of Crystallography (IYCr 2014)

Croatian Association of Crystallographers (CAC) organized the workshop "Hot Topics in Contemporary Crystallography" (HTCC) that took place in Šibenik, Croatia, May 10-15, 2014. This was a course that teaches selected topics of crystallography to research students and post-doctoral researchers from Europe. Some SIG13 members assisted in planning and organizing the course.

9. Future/Programmed Activities.

Title: The Zürich School of Crystallography 2015

SIG13 is going to strongly support the sixth Zürich School of Crystallography that will take place in 2015. The Zürich School is now well established and has a deserved reputation for excellence in the teaching of chemical crystallography to practitioners throughout Europe.

The Zürich School is targeted specifically at providing state-of-the-art training in crystallography for early career researchers, and specifically allows young researchers in chemistry, materials science and physics to investigate crystals that are of immediate interest to their own research. This is a high level of training that is not available in individual institutions throughout Europe and is certainly well above the level of crystallography taught in undergraduate programs across Europe.

The School will be organized by two leading exponents of crystallography, Professors Tony Linden and Hans-Beat Bürgi, both of whom have outstanding international reputations. The course presented will be of the highest standard.

Title: The International Erice School of Crystallography 2015 on “Engineering Crystallography: from Molecule to Crystal to Functional Form“

SIG13 is going to strongly support the 48th Erice International School of Crystallography that will take place in 2015. The Erice schools have a long history of excellence providing a great way of spreading the crystallographic word to young scientists from any country, with special attention to developing countries. This course will help to equip the next generation of scientists with a deep understanding of the tools they need to prototype and engineer crystals to design materials with increasingly sophisticated properties. To do this goal, it is fundamental the development in the understanding of the molecular structures of these molecular materials, which is best achieved using diffraction methods, and at the heart of these studies lies single-crystal X-ray crystallography which provides a full three-dimensional representation of the structure.

Title: Contemporary Crystallography in Croatia, Croatian Academy of Science and Arts, Zagreb, Croatia, September 30, 2014

Number of Participants: 80

Level of involvement of SIG in the activity: ECA Individual members registered with the SIG involved in the organizing committee

Sponsored by ECA: no

Other Sponsors/Organizers: usual commercial sponsors

Short description: The meeting *Contemporary Crystallography in Croatia, Croatian Academy of Science and Arts, Zagreb, Croatia, September 30, 2014* is organized by Croatian Crystallographic Association (CCA) and Croatian Association of Crystallographers (CAC) to celebrate the International Year of Crystallography (IYCr 2014).

Title: 15th BCA/CCG Intensive Teaching School in X-Ray Structure Analysis

21st March - 29th March 2015, Trevelyan College, Durham, UK

Number of participants: 50-80

Level of SIG involvement: A number of the lecturers and tutors are SIG members.

Sponsored by the ECA: No

Other sponsors: usual commercial sponsors.

Short description: The school is intended primarily for younger scientists **with some experience of structure analysis** who wish to improve their understanding of the underlying principles and practice.

10. Other matters. (50 words max.)

SIG13 is continuing in the promotion of the structural chemistry at all levels, participating in “crystallographic schools” across the European Economic Community. Members will also participate in the Networks and Programmes set up by the European Research Council (and some of the national Research Councils) with the aim to provide a better understanding of structure/property relationships in solid state materials.

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

The SIG13 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 SIG Committee has met at the ECM and has corresponded regularly by e-mail, and has encouraged participation of SIG members at relevant national and international meetings. There has also been regular exchange of information between the SIG and officers of the IUCr Commission for Structural Chemistry to the benefit of both organisations.

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

- * *Chair:* Prof. Alessandra Crispini (responsible for the general coordination of the SIG, and specially for interacting with the steering committee)
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Address: Department of Chemistry and Chemical Technologies
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- * *Co-chair:* Prof. Paul R. Raithby (responsible for coordination of the SIG activities and for implementing/distributing news of SIG interest)
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- * *Secretary:* Prof. Marijana Đaković (responsible for the SIG web-page and for maintaining the SIG13 mailing list)
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