

SIG13

Reported Period: June 2017 –June 2018

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 31st European Crystallographic Meeting, ECM31, will take place in Oviedo, Asturias, Spain from 22-27 August 2018. SIG13 representatives have been active in the development of the programme for the ECM31 meeting and have made major contributions to the setting up, in strong collaboration with other SIGs (SIG 7 and 11). In particular, Dr. Clive Oliver has strongly contributed to the development of the ECM31 scientific program within the SIG13 community. All SIG13 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 <http://ecanews.org/mwp/groups/sig-13-molecular-structure-and-chemical-properties/>

3. Number of SIG-13 members according to (<http://ecanews.org/mwp/groups/sig-13-molecular-structure-and-chemical-properties/>)

SIG13 Molecular Structure and Chemical Properties 132

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: 132

Through the ECA website above as well as the ECA-SIG13 facebook home page it 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) 199 from ECA website but additional contacts through French, British, Italian, Spanish and South African Crystallographic Associations.

6. List of MS represented by SIG-13 (also in collaboration with other SIGs) at the ECM31

Microsymposium topic/title	SIG / SIG
1. MS 21 – Intermolecular interactions from structural, energetic and charge density perspectives	SIG 2 / SIG 7 / SIG 13
2. MS 22 – Molecular structure and chemical properties: Chemistry meets charge density	SIG 2 / SIG 13
3. MS 30 - Halogen and chalcogen bonding in the solid state	SIG 7 / SIG 13

Microsymposium topic/title	SIG / SIG
4. MS 31 – The role of supramolecular interactions in polymorphs and co-crystals	SIG 13
5. MS 32 – Molecular recognition and crystal engineering	SIG 7 / SIG 13
6. MS 33 – Prediction of molecular crystal structures	SIG 7 / SIG 13
7. MS 34 – Exploring structural dynamics in crystals	SIG 7 / SIG 13
8. MS 35 - From 0- to 3-dimensional porous systems	SIG 13
9. MS 36 - Structure and function in inorganic and coordination complexes	SIG 13
10. MS 37 - Mechanochemistry: structure and reaction	SIG 13

Prizes sponsored/coordinated

none

8. Past Activities other than Microsymposia at ECM

Title: 2nd POMOS - 2nd Meeting on Porous Molecular Solids - 6-8 June 2018 Vietri sul Mare (Italy)

Number of Participants: 100

Level of involvement of SIG in the activity: Several ECA members were part of the organizing committee, which was chaired by Consiglia Tedesco.

Sponsored by ECA: no

Other Sponsors/Organizers: none

Short Description: This is the 2nd conference after the 1st successful POMOS held in Stellenbosch, South Africa, in April 2015. "The meeting is an opportunity to focus on the recent advances in the field of porous molecular materials with the aim to provide interesting and stimulating ideas for future research." - <http://www.pomos.org/>

Title: BCA Spring Meeting, 26-29 March, 2018, Warwick University (United Kingdom)

Number of Participants: 150

Level of involvement of SIG in the activity: Several ECA members are part of the organizing committee.

Sponsored by ECA

Other Sponsors/Organizers: none

Short Description: The meeting was preceded by the Young Crystallographers meeting from Monday, 26 March to lunchtime on Tuesday, 27 March. The main part of the meeting started at 10.30 on Tuesday, 27 March and finished on at 13.30 on Thursday, 29 March. A varied programme was assembled, promising relevant topics for everyone. Of particular note was a first dedicated session to electron diffraction at a BCA meeting.

website: <http://www.bcaspringmeetings.org.uk/home> (no longer available)

Title: 11th Edition of Symposium with International Participation: New Trends and Strategies in the Chemistry of Advanced Materials with relevance in Biological Systems, Techniques and Environmental Protection, Institute of Chemistry, Timisoara (Romania), 28-99 June 2018.

Level of involvement of SIG in the activity: ECA members participants

Number of participants: 50

Sponsored by ECA: no

Other Sponsors/Organizers: none

Short Description: The main goal of the Symposium is to present the latest trends in the chemistry of materials, with reference to theory of structures and therefore new applications.

Title: The 5th European Crystallographic School, 8 - 14 July 2018 (South Africa)

Level of involvement of SIG in the activity: ECA members participants

Number of participants: 90

Sponsored by ECA: yes

Other Sponsors/Organizers: Several sponsors

Short Description: "The aim of the school is to give attendees a fundamental understanding of the principles underpinning crystallography through a combination of lectures and hands-on tutorials. We will begin by covering the basic principles of point groups, space groups, crystallisation, data collection, and structure refinement from a theoretical perspective." – Chaired by Catharine Esterhuysen

Website: <http://www0.sun.ac.za/ecs5/>

Title: 1th International Symposium on Metallocrowns and Metallacryptates, which will be held in Parma on the 27-28 of September 2017

Number of Participants: 100

Level of involvement of SIG in the activity: ECA members are part of the organizing committee.

Sponsored by ECA: to be applied for

Other Sponsors/Organizers: to be applied for

Short Description: The Symposium is held as the final meeting of the EUFP7 Marie Curie IRSES Project "Metallocrowns" and as the final meeting of the Bilateral Italy.USA Project "Development of porous magnetic Metallocrowns for sensing applications". Within the Marie Curie Project, Dr Matteo Tegoni and the involved team of the Department of Chemistry, Life Science, and Environmental Sustainability of the University of Parma, have been strongly involved in the work package of title "X Ray Structures of large MC Assemblies", designing, synthesizing and structural characterizing (X ray) large MC assemblies including MOF-like architectures.

SIG-13 also provided support letters to Consiglia Tedesco (2nd Meeting on Porous Molecular Solids: 6-8 June 2018), Tony Linden (Zurich School of Crystallography: 16-27 June 2018) and Simona Galli (International Schools on Advanced Porous Materials: June 2019 and in aid of ECA sponsorship applications.

9. Future/Programmed Activities.

Title: V Meeting of the Italian and Spanish Crystallographic Association (MISCA), [June](#), Napoli (Italy) 2019

Number of Participants: 100

Level of involvement of SIG in the activity: ECA members are part of the organizing committee.

Sponsored by ECA: to be applied for

Other Sponsors/Organizers: to be applied for

Short Description: The MISCA meeting represents an opportunity to reinforce the strong bonds between the Italian and Spanish Crystallographic communities. This MISCA will cover the state of the arts in many fields where the crystallography plays a central role. There will be time for discussion, group meetings and collaborative work.

Title: 9th Spanish School on X Ray Diffraction applied to single crystal, Saragoza (Spain), September, 2019

Number of Participants: 30

Level of involvement of SIG in the activity: ECA members are part of the organizing committee and tutors

Sponsored by ECA: no

Other Sponsors/Organizers: to be applied for

Short Description: This a crystallographic school addressed to PhD students and young researchers willing to introduce themselves in this discipline. The school will review the basic concept of X ray Diffraction and practical tutorial.

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.

A SIG-13 meeting was held during ECM30 in Basel on 31 August 2016. The SIG officers presented the 2016 report to the meeting. The members discussed cooperation between SIG-13 members and the possibility of a triennial scientific meeting around specific themes. An immediate outcome of the meeting was the nomination of Clive Oliver to the ECM-31 Programme Committee as the SIG-13 representative. Updating of the SIG-13 website in terms of adding content to the “Scope and Objectives” section, to include more activities and thus improving visibility and publicity of SIG-13 Clive Oliver mentioned that the new website is intended to be used for the dissemination of information to SIG-13 members (the meeting notice was also sent via the website), thus negating the need to have a continually updated e-mail list.

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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- * *Co-chair:* Prof. 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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