

SIG13: Molecular Structure and Chemical Properties

Reported Period: June 2012 – June 2013

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 ECM28 next coming meeting in Warwick (GB) and in the organization of the past ECM27 meeting in Bergen. The excellent result obtained in the involvement in the organization of the past ECM27 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 (already secretary in the previous officers) has been selected as new SIG13 Chair in a SIG13 meeting held during the ECM27 in Bergen. While Prof. Paul R. Raithby remains co-chair, a new and very active secretary has been decided in the name of Prof. Marijana Đaković.

SIG13 representatives have been active in the development of the programme for the ECM28 meeting and have made major contributions to the setting up, in strong collaboration with other SIGs, 9 Microsymposia. Then, in collaboration with all SIG13 members and with the help of the new mailing list, the microsymposia chairs and co-chairs have selected and suggested as well as the KN speakers.

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

6. List of MS organized by the SIG (also in collaboration with other SIGs) at the ECM28

The role of crystallography in chemical reactivity/kinetics/catalysis (MS37, SIG13) – due to the large number of high quality submitted abstracts as oral contributions the MS37 will take place in two sessions (with 10 speakers altogether)

General interests of single molecule crystallography, both large and small (MS10, SIG1 with SIG13 and SIG7)

Combined methods for soft matter crystallography (MS17, SIG4 with SIG13)

Organic and inorganic multi-component crystals: structure and properties (MS24, SIG7 with SIG13)
Molecular interactions: hydrogen bonding, halogen bonding, and beyond (MS25, SIG7 with SIG13)
Structural studies at extreme conditions by single crystal X-ray diffraction (MS32, SIG11 with SIG13)
Molecular compounds under high pressure (MS33, SIG11 with SIG13)
Crystallisation and crystal treatment (MS39, GIG1 with SIG1/SIG13 and SIG7)
Crystallographic Software Fayre introduction (MS44, General with SIG13)

Prizes sponsored/coordinated

none

8. Past Activities other than Microsymposia at ECM

For Each Activity

Title: Workshop: Past, Present, and Future of Crystallography@Politecnico di Milano:
From Small Molecules to Macromolecules and Supramolecular Structures, 6-7 June, 2013

Number of Participants: around 100

Level of involvement of SIG in the activity:

○ ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? no

Other Sponsors/Organizers: IUCr/AIC/ Usual Commercial Sponsors

Short Description: This workshop had the intention to bring together leading scientists with interests in crystallography and crystal engineering and will provide an excellent opportunity to disseminate the latest results in the field. In this framework, some SIG13 members had the opportunity to lecture, presenting their recent results on their crystallographic studies applied in the development of structure and properties relationships.

Title: 14th BCA/CCG **Intensive** Teaching School in X-Ray Structure Analysis

6-14 April, 2013, Durham UK

Number of participants: 75

Level of involvement of SIG in the activity:

Several ECA members registered for the meeting and gave aspects of the course. Some SIG input into the organization and delivery of the course.

Sponsored by ECA? No

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

Short Description: This is a comprehensive course that teaches all aspects of chemical crystallography to research students and post doctoral researchers from Europe and beyond. It has been running for almost 30 years and is recognized as the premier crystallography course in Europe. Some SIG13 members assisted in planning, organizing and delivering the course.

Title: 22nd Croatian-Slovenian Crystallographic Meeting

12-16 June, 2013, Biograd, Croatia

Number of participants: 70

Level of involvement of SIG in the activity:

Several ECA Individual Members registered, several SIG members involved as lecturers.

Sponsored by ECA? No

Other Sponsors/Organizers: commercial sponsors

Short Description: This is the annual joint meeting of the Croatian Crystallographic Association and the Slovenian Crystallographic Society with international participation that alternatively takes place in Slovenia and in Croatia. It has been running for 22 years and there is no registration fee for this Meeting. This year there were 70 participants from 13 countries. Some SIG13 members assisted in planning, organizing and delivering lectures.

9. Future/Programmed Activities.

For Each Activity

Title: MISSCA 2013

Number of Participants: 120

Level of involvement of SIG in the activity:

O ECA Individual members registered with the SIG involved in the organizing committee

Sponsored by ECA no

Other Sponsors/Organizers: IUCr/AIC/GE3C/ Usual Commercial Sponsors

Short Description:

Three years after their second successful Meeting (MISCA 2010, Oviedo, Spain), and six years after they organized their first joint Conference in Italy (MISCA 2007, Copanello di Staletti, Italy), the Italian and Spanish Crystallography Associations deemed it necessary to renew this traditional event. Stimulated also by the interest shown by the Swiss Crystallography Society, the three National Associations have merged their efforts to organize the first Meeting of the Italian, Spanish and Swiss Crystallography Associations - MISSCA 2013. The Conference will contribute to broaden the scientific contacts among the Members of the three communities. Moreover, thanks to the choice of an easily accessible location near Central Europe, it may attract scientists from neighboring Countries and fields.

Title: Workshop: Hot Topics in Contemporary Crystallography (HTCC)

10-15 May, 2014, Šibenik, Croatia

Number of participants: 30

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: waiting for ECA sponsor (requested)

Other Sponsors/Organizers: waiting for IUCr sponsor (requested)/commercial sponsors (diffractometer manufacturers)

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

Croatian Association of Crystallographers (CAC) is organizing the workshop

"Hot Topics in Contemporary Crystallography" (HTCC) that will take place

in Šibenik, Croatia, May 10-15, 2014. This will be 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.

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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