

## **SIG13**

**Reported Period: June 2015 –June 2016**

**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 ECM30 next coming meeting to be held in Basel, Switzerland.

SIG13 representatives have been active in the development of the programme for the ECM30 meeting and have made major contributions to the setting up, in strong collaboration with other SIGs (SIG 7 and 11). In particular, Prof. Prof. Marijana Đaković has strongly contributed to the development of the ECM30 scientific program within the SIG13 community. During the ECM29, after a stimulating meeting between members of the SIG13, the new SIG Officers have been decided. In continuity with the previous team, Prof. Alessandra Crispini has been selected as new SIG13 Chair, and the new co-chair and secretary are Prof. Petra Bombicz and Dr. Clive Oliver, respectively. 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 ECA individual members registered with the SIG according to (<http://www.xray.cz/eca/im-payment.htm>)**

SIG13 Molecular Structure and Chemical Properties                      180

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

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

**Number of members in the SIG mailing list: 188**

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)** 180 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 ECM30**

<b>MS</b>	<b>Organized by</b>
Polymorphs, cocrystals, solvates, salts: a jungle for scientists and industries	SIG7 / SIG13
Molecular compounds and MOFs at ambient conditions and under high pressure	SIG7 / SIG13

Molecular recognition, supramolecular chemistry and crystal engineering	SIG7 / SIG13
Hot structures of small molecules	SIG13
Simulation of dynamics in molecular compounds	SIG13
Crystallography in solid state reactions and catalysis	SIG13
Nanomaterials & graphene	SIG13
Inorganic and metal-organic magnetic structures	SIG11/SIG13

### Prizes sponsored/coordinated

none

### 8. Past Activities other than Microsymposia at ECM

Title: IV Meeting of the Italian and Spanish Crystallographic Associations 21st -25th June 2016, Tenerife Spain

Number of participants: around 125

Level of involvement of SIG in the activity: Several SIG13 members have participated

Sponsored by ECA: no

Other Sponsors/Organizers: Spanish Group of Crystallography (GE3C), Italian Crystallography Association (AIC), Real Sociedad Española de Química (RSEQ)

Short Description: MISCA meeting continues to be the place to reinforce the strong bonds between the Italian and Spanish crystallographic communities, and it is also the opportunity to award the MISCA Medal, a tradition to honor our excellent crystallographers. This IV MISCA was organized around seven microsymposia covering the state-of-the-art in the many fields the crystallography plays a central role, but there was time for discussion, group meetings and collaborative work whilst enjoying the beautiful sunsets at Puerto de la Cruz. During the meeting, the MISCA Medal Award was conferred to Prof. Carlo Mealli, founding father and one of the most active members of the special interest group meeting SIG13.

The IV MISCA was organized around seven microsymposia covering the state-of-the-art in the many fields the crystallography plays a central rôle.

Title: A seminar tour dedicated to CSD-Enterprise for researchers who use molecular structural information in the life sciences and in the organic solid state chemistry

Level of involvement of SIG in the activity: organized by Consiglia Tedesco (University of Salerno) and by Chiara Massera, Claudia Graiff and Alessia Bacchi (University of Parma).

Number of participants: 150

Sponsored by ECA: no

Other Sponsors/Organizers: CCDC, AIC

Short Description: The tour consisted in two hands-on workshops aimed at researchers who use molecular structural information in the life sciences and in the organic solid state chemistry, with

the following program:  
June 14th 2016 - University of Salerno, Uses and Applications of Crystallographic Data in Structural Chemistry and Drug Discovery  
June 16th 2016 - University of Parma, Uses and Applications of Crystallographic Data in Studies of Solid State Properties and Behaviour  
The event has been developed with the support and sponsorship of the CCDC; Steve Maginn, Ilenia Giangreco and Ghazala Sadiq from CCDC lectured during the two days.

## 9. Future/Programmed Activities.

Title: 23<sup>rd</sup> International Conference on the Chemistry of the Organic Solid State

Number of Participants: 200

Level of involvement of SIG in the activity: Several ECA members are part of the organizing committee, which is chaired by Len Barbour.

Sponsored by ECA: to be applied for

Other Sponsors/Organizers: to be applied for

Short Description: This conference is part of an international series held around the world. All aspects of the chemistry and physics of organic materials are included in the scope of the conference. The website will be active soon: [icross2017.co.za](http://icross2017.co.za)

## 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 ECM29 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)

*E-mail:* [crispini@unical.it](mailto:crispini@unical.it)

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\* *Co-chair*: Prof. Petra Bombicz (responsible for coordination of the SIG activities and for implementing/distributing news of SIG interest)

*E-mail*: bombicz.petra@ttk.mta.hu

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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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