

## **SIG13**

**Reported Period: July 2010 – June 2011**

**Report Date: 10<sup>th</sup> July 2011**

**Reported by: Fernando J. LAHOZ (SIG Chair)**

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### **1. Introduction.** (50 words max.)

During the last year the SIG13 committee has continued to reorganise and promote the SIG to the structural science community; the number of registered SIG members has increased from previous years. The SIG has been actively involved in the planning for the Madrid IUCr Meeting, and especially in the organization of a satellite workshop.

### **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            145

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

**Address of the mailing list:** <http://www.facebook.com/pages/ECA-SIG13/137466489407>

**Number of members in the SIG mailing list:** 79

We have maintained the dissemination of information of interest for SIG13 members both through the use of the conventional mailing list system and also using the facebook social network. All events related to our activities are promptly published and every member can be easily informed and eventually join the event. Obviously, we need to advertise more the existence of this facility and encourage people that a judicious use of facebook could help a scientific community to share in real time information and opinions.

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

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

### **6. List of MS organized by the SIG at the last ECM (some in close collaboration with SIG7)**

FA4 MS 26 - Molecular interactions in crystal packing and molecular assemblies

FA4 MS 27 - Molecular interactions in nanocrystalline, disordered and amorphous compounds

FA4 MS 29 - Inclusion compounds and porous materials

FA4 MS 30 - From hydrogen to halogen bonding: proton- against charge-transfer interactions

FA4 MS 31 - Supramolecular assemblies and crystal engineering

FA4 MS 33 - Structure-properties relationship in molecular crystals

FA4 MS 34 - Structural studies on coordination chemistry

FA4 MS 35 - Transformation in crystals: from polymorphism to solid-state reactivity

FA4 MS 36 - Interactions and reactivity in small and large molecules

*In collaboration with other SIGs:*

FA4 MS 24 - Quantitative electron crystallography

FA4 MS 25 - Modern electron diffraction – exploring structures and properties

FA2 MS 19 - Structure and properties of functional materials at extreme conditions

FA4 MS 28 - Applications of molecular crystals simulations

FA4 MS 32 - Crystallization in gels – a practical workshop

FA4 MS 37 - Charge density for understanding of chemical properties

FA5 MS 42 - Time-resolved X-ray diffraction and spectroscopy in biology and chemistry  
FA5 MS 43 - Charge Flipping  
FA5 MS 44 - Software development, automation and validation  
FA5 MS 45 - Recent developments in software for chemical crystallography

## **7. Prizes sponsored/coordinated**

**None**

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

Title: *MISCA 2010, 2<sup>nd</sup> Meeting of the Italian and Spanish Crystallographic Associations, Oviedo, Spain (July 2010)*

Number of Participants: around 195

Level of involvement of SIG in the activity:

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

16 ECA Individual members registered with the SIG involved as lecturers

Yes, endorsed (SIG logo on the web page/leaflets)

Sponsored by ECA? Yes

Other Sponsors/Organizers: ECA/National Associations/ Usual Commercial Sponsors

Short Description: (25 words max.) SIG13 was specifically involved in the organization of the microsymposium 'Structural Chemistry' and suggesting some plenary speakers. SIG13 members contributed to the Meeting speaking at several microsymposia.

Title: *13<sup>th</sup> BCA/CCG Intensive Teaching School, Durham, UK (March-April 2011)*

Number of Participants: 49

Level of involvement of SIG in the activity:

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

5 ECA Individual members registered with the SIG involved as lecturers

Sponsored by ECA?

No

Other Sponsors/Organizers: BCA/EPSRC/Industrial Sponsors

Short Description: (25 words max.) This was the 13<sup>th</sup> running of the world famous Intensive Crystallography School, held at Durham. SIG13 members are on the organising committee and contributed to the school by giving some of the lectures and running tutorial sessions.

Title: *Workshop on Weak Interactions in Crystals, Alcalá de Henares, Spain (20-22<sup>nd</sup> June 2011)*

Number of Participants: 18

Level of involvement of SIG in the activity:

2 ECA Individual Members registered with the SIG involved in the organizing committee

5 ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: University of Alcalá/Spanish Crystallographic Association/La Factoria Project

Short Description: (50 words max.) The workshop was addressed to the Spanish crystallographic community to make them familiar with the recognition of weak interactions in the crystallographic studies, and to help them in the interpretation of properties from the structural parameters. The workshop was structured on three days including lectures and practical sessions.

Title: *British Crystallographic Association Spring Meeting, Keele, UK (April 2011)*

Number of Participants: 284

Level of involvement of SIG in the activity:

5 ECA Individual Members registered with the SIG involved in the organizing committee  
23 ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA?

No

Other Sponsors/Organizers: BCA/Oxford Diffraction/Rigaku/Bruker

Short Description: (50 words max.) This was the annual British Crystallographic Association Meeting, about one third of which was devoted to “small molecule” crystallography, and symposia covered a range of topics involving molecular crystallography including high pressure and dynamic crystallography. The Meeting included plenary lectures from international speakers but also lectures from students and extensive poster sessions.

Title: ***Master on Crystallography and Crystal Growth (October 2010 – June 2011)***

Number of Participants: 19

Level of involvement of SIG in the activity:

3 ECA Individual Members registered with the SIG involved in the organizing committee

9 ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: Spanish National Research Council/La Factorial Project/UIMP University

Short Description: (50 words max.) This is an international official Master run by the CSIC and the International University Menendez-Pelayo. It is organized with a 60 ECTS dedication, and more than 40 lectures from all over the world. It is structured in three modules: a compulsory module with the basics of crystallography and crystal growth, a practical module of 20 ECTS to be done in different labs all along Europe and a third module of specialized courses. The SIG13 members are involved in the organization and as lectures.

## **9. Future/Programmed Activities.**

For Each Activity

Title: ***Current Research on Molecular Structures and Chemical Properties – A Young Perspective, Madrid, Spain (August 2011)***

Number of Participants: 60+

Level of involvement of SIG in the activity:

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

0 ECA Individual members registered with the SIG involved as lecturers

YES, endorsed (SIG logo on the web page/leaflets)

Sponsored by ECA?

No

Other Sponsors/Organizers: IUCr/Local Organising Committee/

Short Description: (25 words max.) This workshop, organized in collaboration with GIG-YC, is aimed to encourage the exchange of current experiences between different groups working in this area. Young researchers (under 35 years of age) will give short talks to explain the main objectives of the research carried out in their groups and on the specific research they are personally involved in. The main goal is to learn through these short talks the current work that is carried out on the binomial ‘Molecular Structures/Chemical Properties’ in different groups. We would like to stimulate the establishment of future collaboration.

Title: ***Categorizing Halogen Bonding and Other Noncovalent Interactions Involving Halogen Atoms, Sigüenza, Spain (August 2011)***

Number of Participants: 50

Level of involvement of SIG in the activity:

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

4 ECA Individual members registered with the SIG involved as lecturers

Sponsored by ECA?

No

Other Sponsors/Organizers: IUCr/IUPAQ project/Industrial Sponsors

Short Description: (25 words max.) The objective of this workshop is to gather several international leaders in the field around the task of giving a modern definition of halogen bonding that takes into account all current experimental and theoretical pieces of information on both gaseous and condensed halogen-bonded systems in chemical and biological systems

Title: ***IUCr XXII Congress and General Assembly, Madrid (August 2011)***

Number of Participants: 2500+

Level of involvement of SIG in the activity:

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

12 ECA Individual members registered with the SIG involved as lecturers

Sponsored by ECA?

Yes

Other Sponsors/Organizers: IUCr/ECA/National Associations/Industrial Sponsors

Short Description: (25 words max.) SIG13 members have been involved in the planning of the IUCr Meeting at all levels, there being representatives on the Organising Committee and on the International Programme Committee.

Title: ***2011 International School on Charge Density, Jaca, Spain (September 2011)***

Number of Participants: 54

Level of involvement of SIG in the activity:

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

5 ECA Individual members registered with the SIG involved as lecturers

Sponsored by ECA?

NO

Other Sponsors/Organizers: IUCr/GE3C/Comercial Sponsors

Short Description: (25 words max.) SIG13 members have been involved in the organization of this international school of lateral interest of the SIG members, as charge density is a powerful method to get a detailed description of chemical and physical properties.

Title: ***40 Congress of the Italian Crystallographic Association, Siena, Italy (September 2011)***

Number of Participants: over 150

Level of involvement of SIG in the activity:

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

10 ECA Individual members registered with the SIG involved as lecturers

Sponsored by ECA?

NO

Other Sponsors/Organizers: IUCr/GE3C/Comercial Sponsors

Short Description: (25 words max.) This is the usual annual national meeting of the Italian association where a significant number of SIG13 members are particularly active. At least one microsymposium has been organized focussed towards proper research interest of our SIG.

Title: ***British Crystallographic Association Spring Meeting (April, 2012)***

Number of Participants: 250-300

Level of involvement of SIG in the activity:

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

O ECA Individual members registered with the SIG involved as lecturers  
Sponsored by ECA?

No

Other Sponsors/Organizers: BCA/Industrial Sponsors

Short Description: (25 words max.) This is the British Crystallographic Association Annual Meeting where, as usual, there will be a strong contribution from SIG13 members, who are on the organising committee and will be planning and presenting some of the lectures.

Title: *ECM27, Bergen, Norway (August 2012)*

Number of Participants: over 700(?)

Level of involvement of SIG in the activity:

1-2 ECA Individual members registered with the SIG involved in the organizing committee

10-20 ECA Individual members registered with the SIG involved as lecturers

Yes, endorsed (SIG logo on some microsymposium)

Sponsored by ECA? Yes

Other Sponsors/Organizers: ECA/National Associations/Commercial Sponsors

Short Description: (25 words max.) SIG13 will be hardly involved in the planning of the ECM27 Meeting through its representative at the Programme Committee (Prof. Paul R. Raithby), submitting proposals collected from the steering committee and from individual SIG members.

Title: *Workshop on 'Single Crystal Diffraction at High Pressure' (August 2012)*

Number of Participants: 50(?)

Level of involvement of SIG in the activity:

1-2 ECA Individual members registered with the SIG involved in the organizing committee

5-6 ECA Individual members registered with the SIG involved as lecturers

No, endorsed (SIG logo)

Sponsored by ECA? Yes(?)

Other Sponsors/Organizers: ECA/National Associations/Commercial Sponsors

Short Description: (25 words max.) The chemical properties of molecular compounds can be strongly influenced by the application of hydrostatic pressure and many new polymorphs have been discovered in high pressure experiments. SIG13 members are quite interested in this workshop and we are supporting it.

#### **10. Other matters.** (50 words max.)

SIG13 will continue to promote 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) to develop structural methods and provide a better understanding of structure/property relationships in solid state materials.

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

The SIG13 Committee has concentrated on the two key areas within its remit: (i) the general promotion of "Molecular Structure and Chemical Properties" through greater publicity for the SIG, particular through its new website, and (ii) by participating effectively in the planning process for the upcoming IUCr Meetings in Crystallography. We are working to improve the representation of SIG13 steering committee to have representatives from all countries participating in ECA.

The SIG Committee 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. Fernando J. Lahoz (responsible for the general coordination of the SIG, and specially for interacting with the steering committee)  
*E-mail:* lahoz@unizar.es  
*Address:* Instituto de Síntesis Química y Catálisis Homogénea (ISQCH)  
Dpto. Química Inorgánica, Facultad de Ciencias  
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(Tel: +34 976 761147; Fax: +34 976 761187)
- \* *Co-chair:* Prof. Paul R. Raithby (responsible for coordination of the SIG activities and for implementing/distributing news of SIG interest)  
*E-mail:* p.r.raithby@bath.ac.uk  
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University of Bath  
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- \* *Secretary:* Prof. Alessandra Crispini (responsible for the SIG web-page and for maintaining the SIG member list)  
*E-mail:* crispini@unical.it  
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- \* SIG13 Steering Committee: (responsible for coordinate initiatives from/to SIG13 in their countries – some countries without representatives!)
- |              |                   |  |
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**Supplementary Materials.**

(List of all supplementary materials, if any, related to the SIG report)

- Addendum 1 to n (to be sent in separate files)