

## **SIG 7 - MIRSIG**

**Reported Period: 2014-2015**

**Report Date: July 2015**

**Reported by: Paola Gilli (Secretary)**

### **1. Introduction.**

Established in 1999 as SIG #7, MIRSIG (Molecular Interaction & Recognition) covers the complete spectrum of theoretical, general and applicative fields of MIR. Activity includes organizing dedicated sessions at ECMs and specialist meetings, workshops and schools. Because of its interdisciplinary nature, MIRSIG has established collaboration with SIG #1 (Macromolecular Crystallography), SIG #2 (Charge, Spin and Momentum Densities), SIG #13 (Molecular Structure and Chemical Properties) and GIG #1 (Young Crystallographers) to organize ECM microsymbiosia.

### **2. SIG web site:**

SIG7 NO (still)

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

SIG7 Molecular Interaction and Recognition 197

### **4. Existence of a SIG mailing list : No**

**Address of the mailing list:**

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

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

The total number of researchers involved in the MIRSIG activities is difficult to estimate, but attendance at ECM microsymbiosia organized by SIG #7 tends to be between 70 and 200.

The number of ECA individual members registered with SIG #7 is 197, though we send announcements to a list of some 350 scientists working in the field. We are working to reduce this discrepancy by sending announcements to our members and trying to increase the number of young crystallographers. Awaiting for more precise measurements, we would suggest an estimated number of about 250 active members.

### **6. List of MS organized by the SIG at the last ECM**

At the **ECM28** (Warwick, 25-29 August 2013) MIRSIG has promoted:

one Keynote Lecture:

- PL1. Susan Bourne: "Building responsive metal-organic frameworks: modifying properties by structure"

and four Microsymbiosia, out of which one in collaboration with GIG #1 and three in collaboration with SIG #13.

- MS23 - Exploring crystal energy landscapes and crystal structure prediction (Chair: Graeme Day - Co-chair: Andrew Maloney) (with GIG1-YC)
- MS24 - Organic and inorganic multi-component crystals: structure and properties (Chair: Niki Bathori - Co-chair: Andrew Bond) (with SIG 13)
- MS25 - Molecular interactions: hydrogen bonding, halogen bonding, and beyond (Chair: Paola Gilli - Co-chair: Kari Rissanen) (with SIG 13)
- MS38 - Molecular recognition and complexation in small molecules (with SIG 13) (Chair: Alessia Bacchi - Co-chair: Janusz Lipkowski)

Both the plenary lecture and the four microsymbosia were attended by a wide audience, which testifies the interest of the European crystallographic community for MIR studies. We are indebted with the Chairpersons and all the members of SIG #13 and GIG #1 that have contributed to the success of the microsymbosia and take the occasion to thank the Chair and Co-chair of ECM28, Professors Sandy Blake and Elspeth Garman, for the excellent meeting in the beautiful campus of Warwick.

## 7. Prizes sponsored/coordinated

None

## 8. Past Activities other than Microsymbosia at ECM

As could be expected, during the year 2014, because of the concomitant 23<sup>rd</sup> Congress and General Assembly of the IUCr (Montreal, Canada, 5-12 August 2014), the activity of MIRSIG has been somehow reduced but not suspended. Though the SIG was not officially involved in the definition of the programme, many MIRSIG members have contributed to the success of this congress, which represents the main international event for the crystallographic community, as organizers, appointed chairs, co-chairs and invited speakers.

During the reported period, MIRSIG has supported the following activities:

Title: *Molecular materials: from fundamentals to applications*

9-13 February 2015, Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk (Russia)

Number of Participants: 45

Level of involvement of SIG in the activity:

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

Elena Boldyreva, Colin Pulham

ECA Individual Members registered with the SIG involved as lecturers:

Joel Bernstein, Elena Boldyreva, Bill Jones, Sarah Price, Colin Pulham

endorsed (SIG logo on the web page/leaflets) No

Sponsored by ECA? No

Other Sponsors/Organizers: British Council, Royal Society of Chemistry

Short Description:

Current challenges in the field of molecular materials require the unified efforts of chemists, crystallographers, physicists and engineers, with applications spanning many industries, including pharmacy, biology and medicine. This meeting offered an opportunity for 40 early career researchers to network with their peers and seek advice from five leading academics in solid state sciences. The workshop focused on various aspects of research into molecular materials ranging from fundamentals to applications, covering the topics of: (1) Polymorphism in Molecular Materials – control, prediction, and implications for applications; (2) Crystallisation of molecular materials under ambient and non-ambient conditions; (3) In situ studies of molecular crystals and molecular materials – diffraction, vibrational spectroscopy, lattice dynamics; (4) Solid-state chemical reactions of molecular materials - mechanochemistry

Title: *1<sup>st</sup> Meeting on POrous Molecular Solids and Satellite Meeting on Large scale facilities*

7-10 April 2015, Wallenberg Conference Center, STIAS - Stellenbosch Institute for Advanced Study, Stellenbosch (South Africa)

Number of Participants: 50

Level of involvement of SIG in the activity:

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

Leonard Barbour, Susan Bourne, Catharine Esterhuysen, Luigi Nassimbeni, Consiglia Tedesco

O ECA Individual Members registered with the SIG involved as lecturers:  
Leonard Barbour, Catharine Esterhuysen, Luigi Nassimbeni, Consiglia Tedesco, Clive Oliver,  
Dyanne Cruickshank

O endorsed (SIG logo on the web page/leaflets) No

Sponsored by ECA? No

Other Sponsors/Organizers: European Union, University of Stellenbosch, University of Salerno,  
ILL, ESRF

Short Description:

The meeting focused on the recent advances in the field of porous molecular materials with the aim to provide interesting and stimulating ideas for future research. The state of the art in the design and synthesis of new materials, their structural characterization, the chemical and physical analysis of their properties, the possible applications from materials science to nanomedicine were discussed in 10 keynote lectures, 32 oral contributions and 1 poster session. A satellite meeting was organized the last day to provide up-to-date information on how to access large facilities, as synchrotron and/or neutron sources at the ESRF and ILL beamlines.

Title: ***To.Sca.Lake: Total Scattering for Nanotechnology on the Como Lake***  
25-28 May 2015, Villa del Grumello, Como (Italy)

Number of Participants: 55

Level of involvement of SIG in the activity:

O ECA Individual Members registered with the SIG involved in the organizing committee:  
Norberto Masciocchi, Antonella Guagliardi

O ECA Individual Members registered with the SIG involved as lecturers:  
Norberto Masciocchi, Antonella Guagliardi, Hans-Beat Buergi

O endorsed (SIG logo on the web page/leaflets) No – Supported by SIG 7

Sponsored by ECA? No

Other Sponsors/Organizers: IUCr, AIC, IISS, Camera di Commercio Como, PANalytical, Assing,  
Rigaku, Dectris, Bruker

Short Description:

The complexity of state-of-art nano-objects needs the synergistic collaborations of scientists of different fields (chemists, physicists, material scientists, biologists, mineralogists) for the design of their structural aspects and multifunctional applications at a multiple scale, as well as the development of highly focused, advanced physico-chemical characterization tools. The To.Sca.Lake workshop, through theoretical lessons dedicated to fundamentals, experimental and computational aspects of the methods as well as demos and hands-on sessions, draws the attention of the Nanoscience and Nanotechnology community towards the potentiality of Scattering Methods, from Small and Wide Angle X-ray (SAXS and WAXS) to Low and Wide Angle Light Scattering (LALS and WALIS) Techniques, with emphasis on innovative Wide Angle X-ray Total Scattering (WAXTS) methods for the structural characterization of novel engineered nanomaterials.

Title: ***Engineering Crystallography: from Molecule to Crystal to Functional Form***  
5-14 June 2015, Ettore Majorana Centre, Erice (Italy)

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:  
Gerard Coquerel, Christer Aakeröy, Annalisa Guerri.

O ECA Individual Members registered with the SIG involved as lecturers:  
Christer Aakeröy, Gerard Coquerel, Aurora Cruz Cabeza, Ulrich Griesser, William Jones, Martin Schmidt

O endorsed (SIG logo on the web page/leaflets) No – Supported by SIG 7

Sponsored by ECA? Yes

Other Sponsors/Organizers: IUCr, CCDC, Dectris, PANalytical, Abbvie

Short Description:

The Course held in 2015 was 48<sup>th</sup> of the International School of Crystallography. About 120 scientists from some 30 countries attended the meeting. Participants were largely from universities, with some members of chemical and pharmaceutical companies. The programme contained about 50 lectures, including 6 chosen from poster abstracts submitted by participants. In addition, there were 2 software tutorials and 1 equipment demonstration. Purpose of the course was to equip the next generation of scientists with a deep understanding of the tools needed to prototype and engineer crystals to design materials with increasingly sophisticated properties.

## 9. Future/Programmed Activities.

Title: **ECM29**

23-28 August 2015, Rovinj (Croatia)

Organizing Committee: Aleksandar Višnjevac (Chair), Marijana Đaković (Co-chair)

During the last month of 2014 and the winter 2015 MIRSIG has contributed to the definition of the scientific programme of ECM29 with the organization of four microsymbiosia, out of which one in collaboration with SIG #13 (Molecular Structure and Chemical Properties), and one keynote lecture. Moreover, our Chairman has been proposed as keynote lecturer by SIG #13.

At the **ECM29** (Rovinj, 23-28 August 2015) MIRSIG has promoted:

one Keynote Lecture:

- KL1. Jonathan Steed: "Crystallization and Gelation: Orthogonal Self-Assembly Far from Equilibrium"
- KL2. Carl Henrik Gørbitz: "Crystal structures of amino acids: investigations into CSD" (SIG 13)

and four Microsymbiosia, out of which one in collaboration with SIG 13.

MS-32. "**Halogen bonding in the solid state**" (with SIG 13)

Chairs: Christer Aakeröy, Lee Brammer

MS-34. "**Growth, structure and application of multi-component crystals**"

Chairs: Christopher Frampton, Tomislav Friščić

MS-36. "**Molecular crystals offering new insight into intermolecular interactions**"

Chairs: Paola Gilli, Carl Henrik Gørbitz

MS-37. "**Molecular crystalline processes at ambient and non-ambient conditions**"

Chairs: Elena Boldyreva, Gareth Lloyd

We take the occasion to thank the Chairpersons of ECM29, Aleksandar Višnjevac and Marijana Đaković, for the space granted to MIRSIG subjects within the meeting.

Title: **Indaba 8, 2015: "Serendipity vs. Prediction"**

16-21 August 2015, Skukuza, Kruger National Park (South Africa)

Number of Participants: anticipated to be limited to 120

Level of involvement of SIG in the activity:

O ECA Individual Members registered with the SIG involved in the organizing committee: Andreas Roodt (Chair), Demi Levendis, Dave Billing, Gideon Steyl, Len Barbour, Jan Boeyens, Susan Bourne, Catharine Esterhuysen

O ECA Individual Members registered with the SIG involved as lecturers: Len Barbour, Dave Billing, Jan Boeyens, Catharine Esterhuysen, Manuel Fernandez, Delia Haynes, Demi Levendis, Andreas Roodt, Wolf-Dieter Schubert

O endorsed (SIG logo on the web page/leaflets) No

Sponsored by ECA? Yes

Other Sponsors/Organizers: IUCr, South African Crystallographic Society, University of the Free State, International Council for Science Unions, Bruker

Short Description:

The last Indaba, dedicated to the theme “Serendipity vs. Prediction” considering the intriguing subject of prediction of phenomena versus discovering them 'by chance', will be the 8<sup>th</sup> in this successful series of interdisciplinary workshops open to various aspects of molecular structure (crystallography, spectroscopy, theory, etc.) and directed at all molecular scientists from chemistry, biology, physics, materials science and related fields. MIRSIG is well represented at the Indaba 8. Many of the organizers are members of MIRSIG, and the programme shows their influence. Moreover, we are glad to announce that during the Indaba 8, the Jan Boeyens Award will be assigned to our member Delia Haynes.

Title: **15<sup>th</sup> International Seminar on Inclusion Compounds (ISIC-15)**

17-21 August 2015, University of Warsaw, Old Library Building, Warsaw (Poland)

Number of Participants: 100-150

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee: Kinga Suwinska (Chair), Janusz Lipkowski, Jonathan Steed, Jerry Atwood, Mike Zaworotko, Luigi Nassimbeni, Len Barbour

ECA Individual Members registered with the SIG involved as lecturers: Israel Goldberg, Mike Zaworotko, Jerry Atwood, Kari Rissanen, Luigi Nassimbeni, Janusz Lipkowski, Consiglia Tedesco

endorsed (SIG logo on the web page/leaflets)  No

Sponsored by ECA?  No

Other Sponsors/Organizers: Bruker AXS, Rigaku Oxford Diffraction

Short Description:

The chemistry of inclusion compounds spans a wide area of MIR studies and ISIC represents an outstanding scientific event in this field. The main objective of this conference series, held every two years, is to present the frontiers of supramolecular chemistry as well as bring together young and experienced scientists from around the world to establish fruitful collaboration. The ISIC conference covers the following topics: Molecular inclusion and recognition, Self-organisation and self-assembly, New synthetic methods in supramolecular chemistry, Chemistry of supramolecular systems, Porous materials, Sorption/desorption properties, Nanomaterials, Applications.

Title: **2<sup>nd</sup> ICSU/IUPAC Workshop on Crystal Engineering**

30 August -1 September 2015, Politecnico di Milano, Como (Italy)

Number of Participants: Limited to 150 by the organizers

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee: Pierangelo Metrangolo (Chair), Giuseppe Resnati (Chair), Tullio Pilati, Giancarlo Terraneo

ECA Individual Members registered with the SIG involved as lecturers: Christer Aakeröy, Alessia Bacchi, Len Barbour, Andrew Bond, Susan Bourne, Dario Braga, Lee Brammer, Graeme Day, Gautam Desiraju, Janusz Lipkowski, Kari Rissanen, Jonathan Steed, Michael Zaworotko

endorsed (SIG logo on the web page/leaflets)  No

Sponsored by ECA?  No

Other Sponsors/Organizers: Fluorit, IUCr, SCI, AIC, IUPAC, ICSU, CrystEngComm, Crystal Growth & Design, IUCr Journals

Short Description:

The objective of the 2<sup>nd</sup> ICSU/IUPAC Workshop is to bring together a large number of scientists working in any areas related to crystal engineering: Computational Crystallography, 2D Crystal

Engineering, Pharmaceutical Co-crystals, Functional Crystals, Supramolecular Crystallography, Biomacromolecules, Metal-Organic Frameworks (MOFs), Organic Crystals, Inorganic Crystals, Functional Crystals, Industrial Crystallization, Porous Crystals, Liquid Crystals. The number of MIRSIG members in the programme reflects the role of crystal engineering in MIR studies.

Title: *ECM30*

28 August – 30 September 2016, Basel (Switzerland)

Organizing Committee: Katharina Fromm (Chair) and Jürg Schefer (Co-Chair)

The scientific programme of ECM30 is presently in phase of definition.

## 10. Other matters.

Thanks to the efforts of MIRSIG members several special issues covering topics of general interest for our scientific community were published in the most popular crystallographic journals during the reported period:

*Acta Crystallographica Section B*

Special Issue on “Non-ambient Crystallography”

Guest Editors: David G. Billing and Andrzej Katrusiak

<http://journals.iucr.org/b/issues/2014/03/00/issconts.html> (June 2014, 25 Articles)

*CrystEngComm*

Themed Issue on “Polymorphism”

Guest edited by: T.N. Guru Row and Ashwini Nangia

<http://pubs.rsc.org/en/journals/articlecollectionlanding?sercode=ce&themeid=9ee71c3d-fb4f-4539-aa0d-f3910ffac49f> (2015, 21 Articles)

*CrystEngComm*

Themed Issue on “Metal-Organic Frameworks and Hybrid Materials”

Guest edited by: Jin-Chong Tan and Bartolomeo Civalleri

<http://pubs.rsc.org/en/journals/articlecollectionlanding?sercode=ce&themeid=4aea0a02-e9b9-4707-8afc-03f96477a5bc> (2015, 33 Articles)

*CrystEngComm*

Themed Issue on “International Year of Crystallography Celebration: North America”

Guest edited by: Christer Aakeröy and Tomislav Friščić

<http://pubs.rsc.org/en/journals/articlecollectionlanding?sercode=ce&themeid=8273823f-8c2c-42c4-991b-5de65ee8e625> (2014, 25 Articles)

*CrystEngComm*

Themed Issue on “International Year of Crystallography Celebration: Europe and South Africa”

Guest edited by: Dario Braga and Michaele Hardie

<http://pubs.rsc.org/en/journals/articlecollectionlanding?sercode=ce&themeid=63416959-a562-4e3f-bdfe-d7b18c91509e> (2014, 24 Articles)

*Crystal Growth & Design*

Virtual Issue “Mikhail Antipin Memorial Issue”

Edited by: Tatiana V. Timofeeva and Ilia A. Guzei

<http://pubs.acs.org/page/cgdefu/vi/14.html> (2015, 30 Articles)

*Crystal Growth & Design*

Virtual Issue “10<sup>th</sup> International Workshop on the Crystal Growth of Organic Materials (CGOM10)”

Edited by: Gerard Coquerel and Kevin J. Roberts

<http://pubs.acs.org/page/cgdefu/vi/11.html> (2014, 14 Articles)

### **11. Brief annual activity report**

During the period 2014-2015 SIG 7 has been actively involved in its prime purpose – to organize discussions, sessions and microsymbiosia relating to molecular interactions and recognition processes at a variety of conferences around the world and within the ECA annual meetings. The committee of officers is working to update the SIG 7 mailing list and establishing a website which could act as a permanent point of contact among MIRSIG.

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

Elected during ECM27 (Bergen) in August 2012:

Chairman: Carl Henrik Görbitz (University of Oslo) <c.h.gorbitz@kjemi.uio.no>

Co-Chairman: Graeme Day (University of Southampton) <G.M.Day@soton.ac.uk>

Secretary: Paola Gilli (University of Ferrara) <paola.gilli@unife.it>