

SIG 7 - MIRSIG

Reported Period: 2013-2014

Report Date: July 2014

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 microsymposia.

2. SIG web site:

SIG7 NO (in preparation)

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 154

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 microsymposia organized by SIG #7 tends to be between 70 and 200.

The number of ECA individual members registered with SIG #7 is 154, though we send announcements to a list of some 250 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 more precise measurements, we would suggest an estimated number of about 200 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 Microsymposia, 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)

We are pleased to say that both the plenary lecture and the four microsymbiosia were attended by a wide audience, which testifies the interest of the European crystallographic community for MIR studies, and we 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. Thanks also to the Chairpersons and all the members of SIG #13 and GIG #1 that have contributed to the success of the microsymbiosia.

However, we would like to remark that four microsymbiosia in collaboration with another SIG correspond to a total of only two MIRSIG microsymbiosia, which is far from the numbers usually granted to our SIG during the last ten years as well as from our original proposal, which consisted of nine microsymbiosia, out of which six in collaboration (total of six). We are sure that this considerable reduction cannot be imputed to the scientific level or the too low attendance of our microsymbiosia, but rather to problems of time and space also due to the concurrent crystallographic centenary celebrations.

We confide that in future ECMs the number of MIRSIG microsymbiosia will come back to the average value of six registered so far. Moreover, as for the definition of the Scientific Programme, we would appreciate to come back to the old method of discussion, involving the Programme Committee, the Focus Area Representatives of the SIG Representatives.

7. Prizes sponsored/coordinated

8. Past Activities other than Microsymbiosia at ECM

During the **year 2014**, because of the concomitant *23rd Congress and General Assembly of the IUCr* (Montreal, Canada, 5-12 August 2014), the activity of MIRSIG has been reduced but not suspended. Though the SIG was not officially involved in the definition of the programme, many MIRSIG members (Enrique Gutierrez-Puebla, Dave Billing, Paul Raithby, Jim Wuest and our past-chair Susan Bourne) have contributed to the organization of this congress, which represents the main international event for the crystallographic community. A glance through the programme reveals one plenary and three keynote lecturers, at least ten microsymbiosia chaired by MIRSIG members, and many other names among the invited speakers.

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

Title: *Workshop "Hot Topics in Contemporary Crystallography", 2014*
10-15 May 2014, "Solaris" beach resort, Šibenik (Croatia)

Number of Participants: 40

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee: Aleksandar Višnjevac (Chair), Marijana Đaković, Biserka Kojić Prodić.

ECA Individual Members registered with the SIG involved as lecturers: Hans-Beat Büergi, Peter Wood, Andre Roodt.

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

Sponsored by ECA? Yes

Other Sponsors/Organizers: Ministry of Science, Education and Sports of the Republic of Croatia, Croatian Academy of Sciences and Arts, IUCr, Bruker, Dectris, Zagrebačka banka, PANalytical, Rigaku, Renacon, CCDC, Rofa, Agilent Technologies, Fidelta, AKD, Globtour, Solaris, Jamnica, Molecular Dimensions.

Short Description:

This summer school in crystallography, the first organized by the Croatian Association of Crystallographers (CAC) to mark the UN-proclaimed *iy-cr2014* in Croatia, was attended by 27 students coming from 14 countries. The programme of the four-days workshop, which addressed

six "hot topics" in contemporary crystallography, was particularly intense (12 90-min lectures, five 90-min hands-on sessions, one sponsored lecture, five short student oral presentations and a poster session). Many MIR themes were covered, particularly in the three lectures delivered by Prof. Hans-Beat Buergi and in the CSD seminars with hands-on demonstrations presented by Dr Peter Wood (CCDC).

Title: *1st European Young Crystallographers Satellite Meeting, 2013*

Sunday 25th August, Warwick Arts Centre, University of Warwick (UK)

Number of Participants: 120

Level of involvement of SIG in the activity:

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

Claire Murray and Andrew Maloney

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

Sponsored by ECA? Yes

Other Sponsors/Organizers: BCA, IUCr

Short Description:

A one day event for early stage researchers jointly organized by the Young Crystallographers Group of the British Crystallographic Association (YCG-BCA) and the European Crystallographic Association General Interest Group of Young Crystallographers (GIG-YC) as Satellite Meeting at the ECM28 in Warwick, to present their work in an informal and friendly environment. The event was attended by 120 participants. The 14 oral communications and 50 posters presented covered a wide range of crystallographic topics, a large part of them dealing with MIR studies.

Title: *5th European Master in Crystallography and Crystallization (E-MCC), 2013*

2012-2013 Edition, Europe – Mainly in Spain

Laboratorio de Estudios Cristalográficos (LEC), Universidad de Granada

Number of Participants: Limited to 25 by the organizers

Level of involvement of SIG in the activity:

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

Juan Manuel García-Ruiz (director), Fermin Otálora-Muñoz, Santiago García Granda.

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

Sponsored by ECA? Yes

Other Sponsors/Organizers: IUCr, CSIC, Factoria de Cristalizacion, GE3C, SEM.

Short Description:

The 5th European Master in Crystallography and Crystallization (E-MCC), jointly organized by the Universidad Internacional Menendez Pelayo (UIMP) and the Consejo Superior de Investigaciones Científicas (CSIC) within the framework of the European Space for Higher Education provides to the young scientists a unified, in-depth vision of the crystalline state, their properties and applications. The master is based in Granada but involves teaching activities in several European laboratories, mainly in Spain (Oviedo, Madrid, Barcelona, Alcala, La Laguna, Zaragoza, Bologna, Grenoble). The E-MCC program, organized in three modules plus Master Thesis, covers a wide range of crystallographic topics, out of which many are of keen interest for SIG 7. Crystallization has been the subject of a number of microsymposia and workshops organized by SIG 7 over the years, and not by chance all the organizers and several professors of the international teaching team are SIG 7 members.

9. Future/Programmed Activities.

Title: *ECM29*

23-28 August 2015, Rovinj (Croatia)

Organizing Committee: Aleksandar Višnjevac (Chair)

Following the established procedure of ECMs organization, MIRSIG has submitted a number of suggestions for microsymposia and plenary lectures to be held at ECM29, taking into account the indications of our members. The scientific programme of ECM29 is presently in phase of definition. The Programme Committee will meet in Montreal during the IUCr Congress and the definitive programme is expected to be on web within November 2014.

Title: ***Indaba 8, 2015: “Serendipity vs. Prediction”***

Skukuza, Kruger National Park (South Africa)

August-September 2015 (dates to be confirmed, before or after ECM29)

Number of Participants: anticipated to be limited to 120

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee: Andre Roodt (Chair), Jan Boeyens, Len Barbour, Susan Bourne, Dave Billing, Melanie Rademeyer, Demi Levendis.

ECA Individual Members registered with the SIG involved as lecturers: unknown at this stage

endorsed (SIG logo on the web page/leaflets) Unknown

Sponsored by ECA? Possibly

Other Sponsors/Organizers: IUCr, South-African Universities and scientific organizations unknown at this stage

Short Description:

The next in this successful series of interdisciplinary workshops considering the intriguing subject of prediction of phenomena *versus* discovering them 'by chance' will take place in the traditional location of the Kruger Park. The exact date will be announced soon.

Title: ***Engineering Crystallography: from Molecule to Crystal to Functional Form***

5-14 June 2015, Ettore Majorana Centre, Erice (Italy)

Number of Participants: 120 (expected)

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee: Gerard Coquerel, Christer Aakeröy, Annalisa Guerri.

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

endorsed (SIG logo on the web page/leaflets) Unknown

Sponsored by ECA? Possibly

Other Sponsors/Organizers: Unknown at this stage

Short Description:

The Course held in 2015 will be 48th of the International School of Crystallography. About 120 scientists from around 30 countries are expected to attend the meeting. The purpose of the course is to equip the next generation of scientists with a deep understanding of the tools they need to prototype and engineer crystals to design materials with increasingly sophisticated properties.

10. Other matters.

- The MIRSIG founding member and IUCr President 2005-2008, Prof. Yuji Ohashi, has recently published a book entitled “Crystalline State Photoreactions” (Springer Japan 2014), which describes the fascinating results of his life work dedicated to the direct observation of reaction processes and metastable intermediates in crystals.

<http://link.springer.com/book/10.1007%2F978-4-431-54373-2>

- During the reported period, thanks to the efforts of several MIRSIG members, some exciting special issues covering topics of keen interest for all MIR scientists have been published in the most popular crystallographic journals:

Crystal Growth & Design

Virtual Issue “In Honor of Prof. Gautam R. Desiraju”

Edited by: Kumar Biradha and Michael J. Zaworotko

(October 2013, 42 Articles) <http://pubs.acs.org/page/cgdefu/vi/9>

Acta Crystallographica Section B

Special Issue on “Crystal Engineering”

Guest editor: Andrew D. Bond

(February 2014, 20 Articles) <http://journals.iucr.org/b/issues/2014/01/00/issconts.html>

CrystEngComm

Themed Issue on “Structural Macrocyclic Supramolecular Chemistry”

Guest edited by: Len Barbour, Len MacGillivray and Kari Rissanen

<http://pubs.rsc.org/en/journals/articlecollectionlanding?sercode=ce&themeid=864a589a-50ac-4c5b-8099-c0337422302f> (2014, 25 Articles)

CrystEngComm

Themed Issue on “Functional Co-crystals”

Guest edited by: Colin Pulham

<http://pubs.rsc.org/en/journals/articlecollectionlanding?sercode=ce&themeid=a7a254a9-f54f-4945-9f7b-2374f7991d87> (2014, 27 Articles)

11. Brief annual activity report

During the period 2013-2014 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 recognizes the need for a SIG 7 mailing list and website which could act as a permanent point of contact among MIRSIG members and is presently working on the matter.

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>

The 2014 MIRSIG–SIG7 Assembly will be held in occasion of the 23rd Congress and General Assembly of the IUCr and is scheduled for

**Wednesday 6 August 2014, 19.30–20.20,
Room 522a** of the Palais des Congrès de Montréal.

All the MIRSIG members, or potentially interested members, are cordially invited to the assembly to discuss the future activities of our SIG. Suggestions and communications are always welcome and can be sent to the Secretary by e-mail at the address: <paola.gilli@unife.it>
