

SIG 7 - MIRSIG

Reported Period: 2016-2017

Report Date: July 2017

Reported by: Carl Henrik Görbitz (chairman) and Catharine Esterhuysen (Co-chairman)

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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 microsymbosia.

2. SIG web site:

<http://ecanews.org/mwp/groups/sig-07-molecular-interaction-and-recognition/>

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

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 microsymbosia 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 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 *ECM30* (Basel, 28-30 August 2016) MIRSIG has promoted:

MIRSIG contributed to the definition of the scientific programme of ECM30 with the organization of six microsymbosia, three alone (MS 29, 30, 31) and three (MS 32, 34, 37) in collaboration with SIG #13 (Molecular Structure and Chemical Properties), and suggested four keynote lectures together with SIG#13 (Martin Schmidt, Simon Parsons, Francesca Fabbiani, Marcus Neumann).

- KL1. Martin Schmidt: "New methods for structural investigations of nanocrystalline and amorphous organic compounds"
- KL2. Simon Parsons: "Understanding the driving forces of phase transitions in molecules"
- KL3. Francesca Fabbiani: "Exploring crystalline molecular materials at high pressure"
- KL4. Marcus Neumann: "Organic crystal structure prediction – from fundamental research to industrial application"

- MS 29 – "Molecular interactions in crystal packing and molecular assemblies"
Chairs: Doris Braun, Kari Rissanen
- MS 30 – "Hydrogen bonding from theory to applications"

- Chairs: Nikoletta Bathori, Laszlo Fabian
- MS 31 – “Crystal energy landscapes: computation and uses”
Chairs: Marcus Neumann, Anthony Reilly
 - MS 32 – “Polymorphs, cocrystals, solvates, salts: a jungle for scientists and industries”
Chairs: Martin Schmidt, Catharine Esterhuysen (with SIG 13)
 - MS 34 – “Molecular recognition, supramolecular chemistry and crystal engineering”
Chairs: Carl Henrik Gorbitz, Chiara Massera (with SIG 13)
 - MS 37 – “Molecular compounds and MOFs at ambient conditions and under high pressure”
Chairs: Francesca Fabbiani, Wendy Queen (with SIG 13)

The keynote lectures 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 to the Chairpersons and all the members of SIG #13 (Molecular Structure and Chemical Properties) that have contributed to the success of the microsymbosia and take the occasion to thank the Chair and Co-chair of ECM30, Katharina Fromm and Jürg Schefer, for the excellent meeting in Basel.

7. Prizes sponsored/coordinated

None

8. Past Activities other than Microsymbosia at ECM

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

Title: *International Conference on the Chemistry of the Organic Solid State*

3-7 April 2017, Wallenberg Conference Center, STIAS - Stellenbosch Institute for Advanced Study, Stellenbosch (South Africa)

Number of Participants: 135

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee:
Leonard Barbour, Nikoletta Báthori, Susan Bourne, Catharine Esterhuysen, Delia Haynes, Luigi Nassimbeni, Clive Oliver

ECA Individual Members registered with the SIG involved as lecturers:
Graeme Day, Kari Rissanen, Jonathan Steed

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

Sponsored by ECA? No

Other Sponsors/Organizers: University of Stellenbosch

Short Description:

The meeting was the latest in the ICCOSS conference series, with the main objective being to showcase frontier research relating to various aspects of organic solid state chemistry, as well as to bring together young and experienced scientists from around the world to establish fruitful discourse. This was an excellent meeting that was thoroughly enjoyed by all attendees.

9. Future/Programmed Activities.

Title: *ECM31*

22 – 27 August 2018, Oviedo (Spain)

Organizing Committee: Santiago García Granda (Chair) and Enrique Pérez Carreño (Secretary)

MIRSIG, through its representative on the program committee Susan Bourne, has contributed to the definition of the scientific programme of ECM31 with the suggestion of eight microsymbosia, two alone, one in collaboration with SIG#2 (Charge, Spin & Momentum Density) and five in

collaboration with SIG #13 (Molecular Structure and Chemical Properties), and suggested three keynote lectures together with SIG#13 (Aurora Cruz-Cabeza, Giuseppe Resnati and Mark Spackmann).

Title: *IUCr 2017*

21-28 August 2017, Hyderabad (India)

The SIG is not officially involved in the definition of the programme, however Petra Bombicz, Andrej Katrusiak and Piero Macchi, who are members of the SIG, are contributing through their involvement on the programme committee.

Title: *Horizons in Hydrogen Bonding, 2017 (HBOND2017)*

2-7 September 2017, Skukuza, Kruger National Park (South Africa)

Number of Participants: ~120

Level of involvement of SIG in the activity:

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

Kari Rissanen

- ECA Individual Members registered with the SIG involved as lecturers:

Giuseppe Resnati, Kari Rissanen

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

Sponsored by ECA? No

Other Sponsors/Organizers: University of Jyväskylä, Federation of Finnish Learned Societies, CCL.net

Short Description:

Hydrogen bonded systems play very important role in many disciplines like chemistry, biology, astrophysics, supramolecular chemistry and nanoscience, chemical engineering, and material sciences. The International Conference on "Horizons in Hydrogen Bond Research" is a biennial conference series with a long tradition, which gather scientists working in the field of hydrogen bonding research, from weak to strong interactions, studied virtually all states of matter by a multitude of experimental and theoretical methods. Also, studies of similar interactions like halogen bonds, chalcogen bonds and pnictogen bonds are in the focus area of HBOND2017. HBOND2017 is the twenty second in the series of conferences on hydrogen bonding which was originally initiated by Prof. Lucjan Sobczyk in Poland in 1977.

Title: *Indaba9, 2018: "Modeling of Structures and Properties"*

2-7 September 2017, Skukuza, Kruger National Park (South Africa)

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:

Demi Levendis (Chair), Dave Billing, Manuel Fernandes

- ECA Individual Members registered with the SIG involved as lecturers:

Catharine Esterhuysen, Delia Haynes, Demi Levendis, Andreas Roodt, Wolf-Dieter Schubert

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

Sponsored by ECA? No

Other Sponsors/Organizers: IUCr, South African Crystallographic Society, Bruker

Short Description:

The 9th Indaba in the successful series of interdisciplinary workshops will assemble scientists from around the world, from chemistry, physics, life and materials sciences, crystallographers, theoreticians and spectroscopists, scientists interested in the correlation of structure and function, in dynamics, activity and selectivity. The meeting aims at discussing the recent progress of

experimental structural methods, structural modeling, the correlation of structures with properties and the prediction of properties and function. In particular, fundamental and new theories and methods, and their application to small molecule activation, energy conversion and storage, and the life sciences will be discussed.

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:

11. Brief annual activity report

During the period 2016-2017 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 ECM29 (Rovinj) in August 2015:

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

Co-Chairman: Catharine Esterhuysen (University of Stellenbosch) <ce@sun.ac.za>

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