

SIG 7 - MIRSIG

Reported Period: 2018-2019

Report Date: July 2019

Reported by: Catharine Esterhuysen (chairman) and Simona Galli (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://ecanews.org/mwp/groups/sig-07-molecular-interaction-and-recognition/members>)

SIG7 Molecular Interaction and Recognition 107

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 107, 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 *ECM31* (Oviedo, 22 – 27 August 2018, Oviedo, Spain):

MIRSIG contributed to the definition of the scientific programme of ECM31 with the organisation of seven microsymbosia, one in collaboration with SIG#1 (Macromolecular Crystallography) and six in collaboration with SIG #13 (Molecular Structure and Chemical Properties), and one keynote lecture together with SIG#13 (Aurora Cruz-Cabeza).

MS10- Hydrogen-bonding & weak interactions studied by neutrons and X-rays

Chairs: Marta Mosquera, Matthew Blakeley

MS30- Halogen and chalcogen bonding in the solid state

Chairs: Guillermo Minguez, Giuseppe Resnati

MS31- The role of supramolecular interactions in polymorphs and co-crystals

Chairs: Laszlo Fabian, Mino Caira

MS32- Molecular recognition and crystal engineering

Chairs: Berta Gómez-Lor, Delia Haynes

MS33- Prediction of molecular crystal structures

Chairs: Jacco van de Streek, Aurora Cruz-Cabeza

MS34- Exploring structural dynamics in crystals

Chairs: Panče Naumov, Leonard Barbour

MS35- From 0- to 3-dimensional porous systems

Chairs: Felipe Gandara, Wendy Queen

The keynote lectures and 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 Secretary of ECM31, Santiago García Granda and Enrique Pérez Carreño, for the excellent meeting in Oviedo.

7. Prizes sponsored/coordinated

None

8. Past Activities other than Microsymbosia at ECM

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

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

2-7 September 2018, Skukuza, Kruger National Park (South Africa)

Number of Participants: 80

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 assembled 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 discussed 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 were discussed.

9. Future/Programmed Activities.

Title: *ECM32*

18 – 23 August 2019, Vienna (Austria)

Organizing Committee: Kristina Djinovic-Carugo (Chair) and Klaudio Hradil (Chair and Treasurer)

MIRSIG, through its representatives on the program committee, Carl Henrik Gørbitz and Catharine Esterhuysen, has contributed to the definition of the scientific programme of ECM32 with the suggestion of eight microsymbosia, five alone, one in collaboration with SIG#2 (Charge, Spin &

Momentum Density) and two in collaboration with SIG #13 (Molecular Structure and Chemical Properties), and suggested four keynote lectures (Wais Hosseini, Angiolina Commotti, Alexander Buell and Colin Groom).

Title: *AIC International Crystallography School*

29 August – 3 September, Naples (Italy)

Number of Participants: ~50

Level of involvement of SIG in the activity:

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

Chiara Massera, Paolo Mazzeo, Simona Galli, Consiglia Tedesco

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

Chiara Massera,

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

Sponsored by ECA? No

Other Sponsors/Organizers: IUCr, Chiesi, Bruker, Crystal Impact, Anton Paar, crystals, Stoë, MiTeGen

Short Description:

The AIC International Crystallography School 2019 will offer an intensive course in Crystallographic Information, covering the extraction, dissemination and use of scientific knowledge from the structure determination experiment to database-driven discovery.

Title: *6th European Crystallographic School*

5-11 July 2020, Budapest (Hungary)

Number of Participants: 70-100 students, 30 lecturers

Level of involvement of SIG in the activity:

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

Petra Bombicz, Attila Benyei

ECA Individual Members registered with the SIG involved as lecturers:

Not yet known

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

Sponsored by ECA? Yes

Other Sponsors/Organizers: Hungarian Academy of Sciences

Short Description:

The 6th European Crystallography School will take place in Budapest between 5 and 11 July 2020. The previous Schools were on very high scientific level. The organisers of ECS6 would like to preserve the high standards to attract the students from different countries. The Research Centre for Natural Sciences, Hungarian Academy of Sciences (RCNS-HAS) will host the School. Based on the numbers of the previous schools we expect 70-100 participants: undergraduate, graduate and postgraduate students, postdocs, young scientists and professionals from the fields of chemistry, biology, solid state sciences who are seeking to participate on an intensive course in crystallography. Theoretical and practical lectures, hands-on tutorials, laboratory practices are planned. The lecturers will represent different areas of crystallography from different countries. The organisers make strong effort to invite eminent experts of crystallography. The school promotes crystallography among young researchers. It may be useful in further academic development of the participants offering a training for new generations of crystallographers.

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 2018-2019 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 ECM31 (Oviedo) in August 2018:

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

Co-Chairman: Simona Galli (Università degli Studi dell'Insubria) <simona.galli@uninsubria.it>