

SIG 7 - MIRSIG

Reported Period: 2019-2020

Report Date: January 2021

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 112

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 112, though in the past we have sent 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 *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, 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).

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#2 (Charge, Spin & Momentum Density) and SIG #13 (Molecular Structure and Chemical Properties) that contributed to the success of the microsymbosia and take the occasion to thank the Chairs of ECM32, Kristina Djinovic-Carugo (Chair) and Klaudio Hradil (Chair and Treasurer), for the excellent meeting in Vienna.

7. Prizes sponsored/coordinated

None

8. Past Activities other than Microsymposia at ECM

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

Title: *AIC International Crystallography School*

29 August – 3 September, 2019 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
- ECA Individual Members registered with the SIG involved as lecturers:
Chiara Massera, John Helliwell
- endorsed (SIG logo on the web page/leaflets) No

Sponsored by ECA? Yes

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

Short Description:

The AIC International Crystallography School 2019 offered 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: *4th International Symposium on Halogen Bonding (ISXB-4)*

2–5 November, 2020, Online event owing to COVID travel restrictions (originally to be hosted in Stellenbosch, South Africa)

Number of Participants: 229

Level of involvement of SIG in the activity:

- ECA Individual Members registered with the SIG involved in the organizing committee:
Catharine Esterhuysen, Nikoletta Báthori, Delia Haynes
- ECA Individual Members registered with the SIG involved as lecturers:
Susan Bourne, Marijana Đakovic, Giuseppe Resnati, Filip Topic
- endorsed (SIG logo on the web page/leaflets) No

Sponsored by ECA? Yes

Other Sponsors/Organizers: IUCr, Bruker, GodoShigen, Crystal Growth & Design, Crystals Journal, CrystEngComm, Devos, Kimix, Rigaku, Springer

Short Description:

The ISXB-4 brought together scientists from a variety of disciplines, but with a common interest in the halogen bond and related interactions. The symposium covered both experimental and theoretical aspects of a broad range of fields such as medicinal chemistry, chemical biology, materials science and industrial applications through keynote addresses, contributed presentations and posters.

9. Future/Programmed Activities.

Title: *ECM33*

23 – 27 August 2022, Versailles (France) – delayed from 2021

Organizing Committee: Jean Paul Itié, Sylvain Ravy and Andrew Thompson

MIRSIG, through its representatives on the program committee, Catharine Esterhuysen and Simona Galli, has contributed to the definition of the scientific programme of ECM33 with the suggestion

of twelve microsymbiosia, and suggested five keynote lectures (Christine Beavers, Franziska Emmerling, Alessia Bacchi, Chilla Malla Reddy, K. Travis Holman).

Title: 6th European Crystallographic School

Originally 5-11 July 2020, Budapest (Hungary); postponed to 4-10 July 2021 to be held online owing to COVID travel restrictions

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.

Title: 55th International School of Crystallography – Molecular Crystal Engineering

31 May-4 June 2021, to be held online owing to COVID travel restrictions

Number of Participants: ~100 students, 22 lecturers

Level of involvement of SIG in the activity:

- ECA Individual Members registered with the SIG involved in the organizing committee:
Ulrich Griesser, Annalise Guerri

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

Ulrich Griesser, Martin Schmidt

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

Sponsored by ECA? Yes

Other Sponsors/Organizers: IUCr; Italian Ministry of Education, University and Scientific Research; Sicilian Regional Government

Short Description:

Crystallization experiments are still difficult to control and the development of crystal forms with superior properties remains a challenging task that requires specific synthetic, analytical and computational skills. Recent scientific advances highlight that a thorough understanding of intermolecular interactions is the key to modern crystal engineering and the conception of relations between structure and properties. Such insights are increasingly exploited to design and produce new materials with desired functions. Successful examples of this approach include pharmaceutical, agrochemical, separation and optoelectronic research, at a fundamental and applied level. The 2021 Course at the International School of Crystallography in Erice will focus on molecular crystal engineering. The program will highlight the relevance of this discipline from both, academic and

industrial perspectives. Prominent scientists in the field will illustrate theoretical and practical aspects of crystal engineering in lectures, workshops and hands-on trainings. Additionally, the significance of crystal forms in different areas of chemical industry will be discussed, with particular emphasis on synthetic strategies and the design of desired material properties.

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:

CrystEngComm Editor's collection: *Chromism in Frameworks*, guest edited by Susan Bourne

CrystEngComm Editor's Collection: *Mechanochemistry*, guest edited by Elena Boldyreva

11. Brief annual activity report

During the period 2019-2020 SIG 7 has been actively involved in its prime purpose – to organize discussions, sessions and microsymbosia relating to molecular interactions and recognition processes at a variety of conferences around the world and within the ECA annual meetings.

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>