



SIG 7 – MIRSIG ANNUAL REPORT

Reported Period: 2023-2024

Report Date: August 2024

Reported by: Catharine Esterhuysen (Chairman), Simona Galli (Co-chairman),
Nikoletta Báthori (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. Its activity includes organising dedicated sessions at European Crystallographic Meetings (ECMs) as well as specialist meetings, workshops and schools. Because of its interdisciplinary nature, MIRSIG has established long-standing 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 organise ECM microsymbosia.

2. SIG website

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

New: <https://ecanews.org/sig-07/>

3. Number of ECA individual members registered with the SIG according to <http://ecanews.org/mwp/groups/sig-07-molecular-interaction-and-recognition/members>

SIG-07	Molecular Interaction and Recognition	60
--------	---------------------------------------	----

4. Existence of a SIG mailing list: Yes

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 (co)organised by SIG #7 tends to be between 70 and 200.

The number of ECA individual members registered with SIG #7 is 60 (see point 3 above), though in the past we have sent announcements to a list of some 350 scientists working in the field inviting them to register in MIRSIG. We are working to reduce this discrepancy by sending periodical announcements to both our members and potentially interested colleagues, and trying to involve the young crystallographers. Awaiting more precise measurements, we would suggest an estimated number of about 250 active scientists interested in the MIRSIG topics.

6. List of MS organised by the SIG at the last ECM

At the *ECM34* (to be held, 26–30 August 2024, Padova, Italy, Organizing Committee: Gilberto Artioli and Giuseppe Zanotti - chair and cochair, respectively), MIRSIG, through its representatives on the program committee, Catharine Esterhuysen and Simona Galli, contributed to the definition of



the scientific programme with the suggestion of 13 microsymbiosia and 8 keynote speakers. The final programme includes 5 microsymbiosia jointly suggested with SIG #13 and/or with GIG #3, namely:

Porous functional materials

Noncovalent interactions in structure design

Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function

Correlate molecular structure with materials properties

Things we no longer need to know – or do we? Common mistakes and problems in using black boxes

Techniques to discover polymorphism: mechanochemistry, crystal growth and others

and 1 keynote lecture: Chiara Massera (University of Parma, Italy)

7. Prizes sponsored/coordinated

None

8. Past Activities other than Microsymbiosia at ECM

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

Title: *3rd International School on Advanced Porous Materials*

19-23 June 2023, Como, Italy

- Number of participants: 135 attendees, of which 15 lecturers and 2 sponsor delegates
- Level of involvement of SIG in the activity:
 - ECA Individual Members registered with the SIG involved in the organising committee: Simona Galli, School co-director
 - ECA Individual Members registered with the SIG involved as lecturers: N/A
 - endorsed (SIG logo on the web page/leaflets): No
- Sponsored by ECA? Yes
- Other Sponsors/Organisers: Italian Crystallographic Association, Alfatest, Anton Paar, Bruker, RSC Chemical Communications, Crystal Impact
- Short Description: Metal-organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs) are advanced porous materials deriving from the linking of (organic/inorganic and organic/organic) building units. In the past twenty years, the broad library of building units and synthetic conditions has allowed the preparation and consequent investigation of a huge number of MOFs and COFs showing intriguing functional properties – adsorption, separation, heterogeneous catalysis, sensing, drug delivery, to list a few – that outperform, in many aspects, those of classical porous materials. As this vast and interdisciplinary research field is advancing at a very fast pace, the third International School on Porous Materials gathered leading experts in the field to cover the current research advances in MOFs and COFs, focussing on synthesis, characterisation and applications.



Title: 1st Stellenbosch Introductory Crystallography School

9-15 July 2023, Stellenbosch, South Africa

- Number of participants: 55 attendees, of which 10 lecturers
- Level of involvement of SIG in the activity:
 - ECA Individual Members registered with the SIG involved in the organising committee: Delia Haynes (School director), Catharine Esterhuysen (School co-director)
 - ECA Individual Members registered with the SIG involved as lecturers: Delia Haynes (School director), Catharine Esterhuysen
 - endorsed (SIG logo on the web page/leaflets): No
- Sponsored by ECA? No
- Other Sponsors/Organisers: Stellenbosch University
- Short Description: The school focused on single crystal X-ray diffraction covering the topics of symmetry, point groups and space groups, diffraction physics, data collections, structure solution and refinement and reporting results, including utilisation of the Cambridge Structural Database. The aim of the school was to give participants an understanding of the principles and practice of crystallography through a combination of lectures and hands-on tutorials.

9. Future/Programmed Activities

Title: 17th International Seminar on Inclusion Compounds and Porous Materials (ISIC17)

2-6 September 2024, Poznań, Poland

- Number of participants: ~100 attendees
- Level of involvement of SIG in the activity:
 - ECA Individual Members registered with the SIG involved in the organising committee: N/A
 - ECA Individual Members registered with the SIG involved as lecturers: Consiglia Tedesco
 - endorsed (SIG logo on the web page/leaflets): No
- Sponsored by ECA? No
- Other Sponsors/Organisers: Adam Mickiewicz University, Polish Crystallographic Association, Bruker, Hidden Isochema, TestChem, 3P Instruments, ChemAT, Chemistry Europe, ACS Crystal Growth and Design, RSC CrystEngComm and Dalton Transactions
- Short Description: ISOC17 is not only dedicated to pure inclusion phenomena, recognition and supramolecular chemistry, but also to the porous, nano- and advanced 'smart' materials and the methods of their research, including the exploration of MOF, COF, and ZIF type porous materials, along with their potential applications. The main goal of this meeting is to bring together both young and 'experienced' scientists from across the world for healthy discussion at all levels as well as an exchange of ideas within this society.



Title: *6th International Symposium on Halogen Bonding (ISXB-6)*

20–25 October, 2024, Dubrovnik, Croatia

Number of Participants: ~100

Level of involvement of SIG in the activity:

- ECA Individual Members registered with the SIG involved in the organizing committee:
Marijana Đakovic, Mario Cetina, Mateja Pisačić
- ECA Individual Members registered with the SIG involved as lecturers:
Susan Bourne, Catharine Esterhuysen
- endorsed (SIG logo on the web page/leaflets): No

Sponsored by ECA? Yes

Other Sponsors: Cambridge Structural Database, Croatian Chemical Society, University of Zagreb

Short Description: The ISXB-4 aims to bring together researchers from all over the world who are interested in the fascinating phenomenon of halogen bonding and related interactions, from fundamental principles to applied technologies, covering both experimental and theoretical approaches in various areas of research ranging from advanced materials to medicinal chemistry and chemical biology. The **ISXB6** will feature keynote addresses and invited lectures by internationally renowned experts, contributed presentations, posters, and flash communications by young and promising researchers. The Symposium will also provide ample opportunities for networking and socializing in a friendly and stimulating atmosphere.

Title: *ECM35*

August 2025, Poznan/Lviv, Poland/Ukraine

MIRSIG, through its representative on the program committee, Simona Galli, is contributing to the definition of the scientific programme of ECM35.

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. In particular, Susan Bourne and Delia Haynes co-edited a *CrystEngComm* themed collection on "**Crystal Engineering in Africa**", and Delia Haynes co-edited a Virtual Special Issue of *Crystal Growth & Design* on the "**Legacy and Future Impact of the Cambridge Structural Database: A Tribute to Dr. Olga Kennard**".

11. Brief annual activity report

As evidenced by what has been reported above, during the period 2023-2024, SIG #7 has been actively involved in its prime purpose – to organise discussions, sessions and microsymbiosia relating to molecular interactions and recognition processes at a variety of conferences and schools 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 IUCr25 (Prague) in August 2021:

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

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

Secretary: Nikoletta Báthori (Cape Peninsula University of Technology)
<BathoriN@cput.ac.za>