

SIG 7 – MIRSIG ANNUAL REPORT

Reported Period: 2022-2023

Report Date: September 2023

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 microsymbiosia.

2. SIG website

<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>

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| SIG7 Molecular Interaction and Recognition | 60 |
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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 microsymbiosia 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 4 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 members interested to the MIRSIG topics.

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

At the *ECM33* (23–27 August 2022, Versailles, France, Organizing Committee: Sylvain Ravy, Andrew Thompson and Jean-Paul Itié - chairs and cochair, respectively), MIRSIG, through its representatives on the program committee, Catharine Esterhuysen and Simona Galli, contributed to the definition of the scientific programme of ECM33 with the suggestion of 8 microsymbiosia in collaboration with SIG #13 (Molecular Structure and Chemical Properties) and 1 keynote lecture (Alessia Bacchi, University of Parma, Italy).

The keynote lecture and microsymbposia were attended by a wide audience, which testifies the interest of the European crystallographic community for the MIRSIG research topics. We are indebted to the Chairpersons and all the members of SIG #13 that contributed to the success of the microsymbposia and take the occasion to thank the Chairs of ECM33, Sylvain Ravy, Andrew Thompson and Jean-Paul Itie, for the excellent meeting in Versailles.

7. Prizes sponsored/coordinated

None

8. Past Activities other than Microsymbposia 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
 - 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: *PCCr3: 3rd Pan-African Conference on Crystallography*

17-22 January 2023, Nairobi, Kenya

- Number of participants: 80
- Level of involvement of SIG in the activity:
 - ECA Individual Members registered with the SIG involved in the organising committee: Susan Bourne, Delia Haynes
 - ECA Individual Members registered with the SIG involved as lecturers: Delia Haynes, Catharine Esterhuysen
 - endorsed (SIG logo on the web page/leaflets) No

- Sponsored by ECA? No
- Other Sponsors/Organisers: IUCr; Bruker, CCDC, ICDD, CrystEngComm
- Short Description: PCCr3 brought together crystallographers, mineralogists and solid-state scientists from Africa and beyond to contribute to the advancement of science on the African continent *via* crystallography in all its aspects, including topics concerning the structure and related properties of non-crystalline states, and to promote African cooperation in crystallography.

9. Future/Programmed Activities

Title: *ECM34*

26–30 August 2024, Padova, Italy

Organising Committee: Gilberto Artioli, Giuseppe Zanotti (Chair and Co-Chair, respectively MIRSIG, through its representatives on the program committee, Catharine Esterhuysen and Simona Galli, has contributed to the definition of the scientific programme of ECM34 with the suggestion of 13 microsymbiosia and 8 keynote lectures. The final programme includes 5 microsymbiosia jointly suggested with SIG 13, 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 2 keynote lectures:

Máté Erdélyi (Uppsala University, Sweden), Chiara Massera (University of Parma, Italy)

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

As evidenced by what has been reported above, during the period 2022-2023, 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 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>

