



SIG-07 ANNUAL REPORT

Reported Period: mid August 2024 – mid August 2025
Report Date: August 14th, 2025
Report Authors: Simona Galli (SIG-07 Chair), Mark Elsegood (SIG-07 Co-chair)

1. Introduction

Established in 1999, the Special Interest Group #7 (SIG-07) encompasses the broad spectrum of theoretical, methodological and applicative fields of molecular interaction and recognition (MIR). SIG-07 activity includes (co-)proposing dedicated microsymposia and lectures at the European Crystallographic Meetings (ECMs) as well as specialist meetings, workshops and schools at the national and international level. Due to its interdisciplinary nature, SIG-07 has established a long-standing and fruitful collaboration with SIG-01 (Macromolecular Crystallography), SIG-02 (Charge, Spin and Momentum Densities), SIG-12 (Crystallography of Functional Materials), and SIG-13 (Molecular Structure and Chemical Properties) to define ECMs scientific programs, jointly proposing microsymposia topics and chairs, as well as plenary and keynote lecturers.

2. SIG website

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

The SIG-07 new website was initially populated by the previous officers (Catharine Esterhuysen, Chair; Simona Galli, Co-chair; Nikoletta Bathori, Secretary) in the period July-August 2024. Additional content was gradually introduced by the present officers (Simona Galli, Chair; Mark Elsegood, Co-chair) during the reported period and was brought to the SIG-07 membership's attention for comments and suggestions before launching it. The new website was officially launched in June 2025. The officers plan periodic updates, also based on the SIG membership's contributions. The SIG-07 officers acknowledge the ECA webmaster Andrea Ienco for his continuous support on this matter.

3. Number of crystallographers registered with the SIG

As *per* August 2025, based on the mailing list in the availability of its officers SIG-07 counts on 60 members from different European countries and South Africa.

4. Existence of a SIG mailing list

A mailing list provided by the former officers is in the availability of the present officers.



5. Approximate total number of researchers involved in the SIG activities (please indicate the basis for the estimate)

It is quite difficult to estimate the actual number of researchers involved in the SIG-07 activities. As anticipated above, the number of crystallographers registered with SIG-07 is limited to 60. Nonetheless, attendance at ECM microsymposia, plenary or keynote lectures (co-)proposed by the SIG is typically between 50 and 150 units.

To try to reduce this discrepancy, SIG-07 yearly produces an advert slide to be shown before the beginning of ECM (co-)proposed microsymposia. In addition, following an invitation by the ECA Executive Committee, in June and July 2025 the officers proposed to the SIG members to record short videos highlighting their research, teaching or outreach activities related to MIR as a catching form of publicizing SIG-07 and, to a broader extent, ECA activities. Finally, last June the officers recalled to the SIG membership the opportunity of contributing to the ECA lunchtime webinars, as the last contribution dates back to 2023. Both proposals will be renovated during the SIG meeting scheduled at ECM35 on August 29th, 2025, as well as by e-mail.

Sending periodical announcements regarding SIG-07 (research, teaching, outreach, organizational) activities to both the SIG members and potentially interested colleagues could be another action to increase the number of SIG-07 registered (advanced and early-career) crystallographers interested in MIR. Additional actions to address this aim will be solicited during the SIG-07 meeting scheduled at the ECM35.

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

At the ECM35 (to be held, August 25th – August 29th, 2025, Poznań, Poland, and Lviv, Ukraine), through its representative on the program committee Simona Galli, SIG-07 contributed to the definition of the scientific program co-proposing, jointly with SIG-13, 11 microsymposia and 3 keynote speakers. As already done in the recent past, while suggesting microsymposia potential chairs, the SIG representative posed attention to highlight both advanced and early-career researchers. Thanks to the work of the SIG representative, based on the SIG members' timely suggestions, the ECM35 final scientific program (<https://ecm35.ecanews.org/>) includes 8 microsymposia co-proposed by SIG-07, namely:

- *Supramolecular interactions behind crystal engineering*
jointly with SIG-13
- *The complex world of multicomponent crystals*
jointly with SIG-12 and SIG-13
- *Insight into the crystal: crystal forms, isostructurality, symmetry, chirality*
jointly with SIG-13
- *Molecular structure and chemical bonding*
jointly with SIG-02 and SIG-04
- *Impact of non-covalent interactions on dynamics in molecular crystals*
jointly with SIG-12 and SIG-13



- *Polymorphism and phase transitions*
jointly with SIG-05 and SIG-13
- *Crystallography in the world of mechanochemistry*
jointly with SIG-13
- *Designing the void: structural mastery in advanced porous materials*
jointly with SIG-12 and SIG-13

In addition, the SIG-07 members:

- Susan Bourne (University of Stellenbosh, South Africa) was invited as speaker for the MS *Supramolecular interactions behind crystal engineering*;
- Consiglia Tedesco (University of Salerno, Italy) was invited as speaker for the MS *Molecular structure and chemical bonding*;
- Petra Bombicz (Hungarian Academy of Sciences, Budapest, Hungary) was invited as speaker for the MS *Comparing crystal structures in massive dataset*;
- Simona Galli was invited as keynote speaker.

7. Prizes sponsored/coordinated

No prizes were coordinated or sponsored by SIG-07 in the reported period.

8. Past Activities other than Microsymposia at ECM

During the reported period, SIG-07 has supported the following event:

4th International School on Porous Materials, June 16th – 20th, 2025, Como, Italy

(<http://mofs.lakecomoschool.org/>)

- Number of participants: 155 attendees, namely: 48 in-presence scholars; 58 in-remote scholars; 19 lecturers (among whom the 3 school directors); 5 teachers' assistants; 16 local organizing committee members; 9 sponsor delegates.
- Level of involvement of SIG-07 in the activity:
 - Crystallographers registered with SIG-07 involved in the organising committee:
Simona Galli, School co-director.
 - Crystallographers registered with SIG-07 involved as lecturers:
Simona Galli.
 - Endorsed (SIG logo on the web page/leaflets): No.
- Sponsored by ECA: Yes.
- Other Sponsors: Non-commercial: University of Insubria (Italy), University of Milan (Italy), University of Granada (Spain), Lake Como Schools of Advanced Studies, Fondazione Alessandro Volta, Italian Crystallographic Association, Italian Consortium on Materials Science and Technology; commercial: Alfatest, Bruker, Frontiers in Chemistry, Hiden Isochema, Crystal Impact, Micromeritics, MDPI (Materials), Nordtest, RSC (Chemical Sciences, CrystEngComm, Materials Advances, Materials Horizons), Verder.

- Short Description: MOFschoo2025, the fourth edition of this event, was designed to introduce undergraduate, graduate and Ph.D. students and post-doctoral fellows into the broad and interdisciplinary field of metal-organic frameworks (MOFs) and related porous materials. Indeed, through a series of cutting-edge lectures and two parallel hands-on sessions, the event provided the scholars with the opportunity of deepening their knowledge on up-to-date synthetic protocols, characterization techniques, theoretical-calculation approaches, and some representative applicative contexts. An entire day was dedicated to crystallography-related topics, namely: fundamentals and ambient-conditions for single-crystal (F. Gándara) and powder (S. Galli) X-ray diffraction; non-ambient-conditions for powder X-ray diffraction (V. Colombo); single-crystal total scattering analysis (S. Canossa); topology with hands-on session on the software Topos Pro (D. Proserpio); hands-on session on the software Topas (Bruker) (R. Vismara, F. Carmona, M. Vandone). With reference to the scholars, the goals of geographical diversity – with representation from 26 countries across 5 continents – and gender balance – with 54% female students – were successfully achieved. The scholars had the opportunity to communicate the results of their research during 2 flash-presentation sessions and 2 poster sessions, one in-person, and one through the social medium Bluesky. ECA generous financial support was employed to cover the registration fee and accommodation of two deserving Ph.D. candidates from Brazil (male) and Australia (female).

9. Future/Programmed Activities

32nd Croatian-Slovenian Crystallographic Meeting (CSCM32), June 17th - 21st, 2026, Vodice, Croatia (<https://cscm32.hazu.hr/>, under construction)

- Number of participants: ca. 100.
- Level of involvement of SIG in the activity:
 - ECA Individual Members registered with the SIG involved in the organising committee: Marijana Đaković (University of Zagreb, Croatia), Chair of the Meeting.
 - ECA Individual Members registered with the SIG involved as lecturers: Not available at this stage.
 - Endorsed (SIG logo on the web page/leaflets): Not available at this stage
- Sponsored by ECA: Not available at this stage.
- Other Sponsors/Organisers: Not available at this stage.
- Short Description: The meeting will encompass the broad spectrum of crystallographic topics, e.g.: macromolecular and small-molecule systems, materials science, crystal engineering, mineralogy, metallurgy, solid solutions, powder diffraction, small-angle scattering, crystal structure prediction, as well as interdisciplinary approaches combining diffraction and microscopy with complementary techniques. The CSCMs have been traditionally held without conference fees for early career crystallographers. This model favours the attendance of the next generation of crystallographers - graduate students, Ph.D. candidates, and postdoctoral



fellows, who will have the opportunity to present their work orally, as no poster sessions will be organized.

ECM36, August 2027, Prague, Czechia

Through its representative on the program committee, Simona Galli, who will collect proposals from the SIG members and will coordinate with other SIGs, SIG-07 is committed to contribute to the definition of the scientific program of ECM36.

10. Other matters

No matters other than those exposed above characterized the activities of SIG-07 during the reported period.

11. Brief annual activity report

As evidenced by what has been reported above, during the period mid august 2024 – mid august 2025 SIG-07 has been actively involved in its prime purpose, namely: to organise microsymposia and lectures relating to molecular interaction and recognition processes within the ECA annual meetings and to endorse meetings, workshops and schools covering MIR-related topics.

12. List SIG officers, name and e-mail, and specify their main function in the SIG

The present SIG-07 officers, namely:

Chair: Simona Galli, Università degli Studi dell'Insubria, Italy
simona.galli@uninsubria.it

Co-chair: Mark Elsegood, Loughborough University, United Kingdom
m.r.j.elsegood@lboro.ac.uk

were elected through an in-remote election organized by the former officers in September 2025. The position of Secretary has been vacant since then.