

## **SIG 7 - MIRSIG**

**Reported Period: 2021-2022**

**Report Date: August 2022**

**Reported by: Catharine Esterhuysen (chairman), Simona Galli (Co-chairman), Nikoletta Báthori (Secretary)**

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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 organising 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 organise ECM microsymposia.

### **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>)**

SIG7 Molecular Interaction and Recognition 75

### **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 microsymposia organised by SIG #7 tends to be between 70 and 200.

The number of ECA individual members registered with SIG #7 is 75, 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 more precise measurements, we would suggest an estimated number of about 250 active members.

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

No ECM has been held in the reporting period.

### **7. Prizes sponsored/coordinated**

None

### **8. Past Activities other than Microsymposia at ECM**

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

Title: **6<sup>th</sup> European Crystallographic School**

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

Number of Participants: 90 students, 35 lecturers

Level of involvement of SIG in the activity:

- ECA Individual Members registered with the SIG involved in the organising committee:  
Petra Bombicz, Attila Benyei

- ECA Individual Members registered with the SIG involved as lecturers:  
Niki Báthori, Chiara Massera, Petra Bombicz, Attila Benyei, László Fábrián, Teresa Duarte
- endorsed (SIG logo on the web page/leaflets) No

Sponsored by ECA? Yes

Other Sponsors/Organisers: Hungarian Academy of Sciences

Short Description:

The 6<sup>th</sup> European Crystallography School took place online between 4 and 10 July 2021. The organisers of ECS6 preserved the high standards of the previous meetings and attracted students from four continents. The Research Centre for Natural Sciences, Hungarian Academy of Sciences (RCNS-HAS) hosted the School, which was attended by 90 participants: undergraduate, graduate and postgraduate students, postdocs, young scientists and professionals from the fields of chemistry, biology, solid state sciences seeking to participate on an intensive course in crystallography. The school consisted of theoretical and practical lectures, hands-on tutorials and laboratory practices from different areas of crystallography, with lecturers being eminent experts from different countries. The school thus promoted crystallography among young researchers and was important for the further academic development of the participants by offering a training for new generations of crystallographers.

Title: ***55<sup>th</sup> International School of Crystallography – Molecular Crystal Engineering***

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

Number of Participants: 61 students, 23 lecturers

Level of involvement of SIG in the activity:

- ECA Individual Members registered with the SIG involved in the organising committee:  
Ulrich Griesser, Annalisa 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/Organisers: IUCr; Italian Ministry of Education, University and Scientific Research; Sicilian Regional Government

Short Description:

Crystallisation 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 focused on molecular crystal engineering. The program highlighted the relevance of this discipline from both academic and industrial perspectives. Prominent scientists in the field illustrated 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 was discussed, with particular emphasis on synthetic strategies and the design of desired material properties.

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

21-25 June, originally planned for Como, Italy, finally held online

Number of Participants: 130 students and 14 lecturers

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: IUCr; Italian Association of Crystallographers, Eldico Scientific

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 second 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: *ePCCr (virtual meeting): Pan-African Conference on Crystallography*

15-19 November 2021, held online owing to COVID travel restrictions

Number of participants: 208

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, Andreas Roodt, Catharine Esterhuysen

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

Sponsored by ECA? Yes

Other Sponsors/Organisers: IUCr; Bruker, Dectris, CCDC, ICDD, CrystEngComm, Crystal Growth and Design, Rigaku, Brookhaven National Laboratory

Short Description: The ePCCr brought together crystallographers, mineralogists and solid-state scientists from Africa and beyond, with an important aim being to establish the African Crystallographic Association (AfCA). AfCA's mission is to contribute to the advancement of science on the African continent via crystallography in all its aspects, including related topics concerning the structure and related properties of non-crystalline states, and to promote African cooperation in crystallography.

## 9. Future/Programmed Activities.

Title: *ECM33*

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

Organising 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. The final programme includes eight microsymbiosia jointly suggested with SIG 13:

**MS27** Minerals and Materials Under Extreme Conditions

**MS28** Navigating crystal forms in molecular and pharmaceutical materials

**MS29** Crystal engineering: structural flexibility, phase transitions and non-standard manipulation of synthons

**MS30** Advanced porous materials : MOFs, COFs, SOFs....and what else?

**MS31** Unconventional interactions or symmetries for optimised and new properties, including chirality

**MS32** Advanced techniques to disclose Structure-Property Relationships

**MS33** Supramolecular recognition

**MS34** Crystallisation Techniques and chemical reactions driven by solid state interactions and one keynote lecture:

Alessia BACCHI (Parma University, 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:

ChemPlusChem and Chemical Record special collection: *4th International Symposium on Halogen Bonding (ISXB4)*, guest edited by Máté Erdélyi, Catharine Esterhuysen and Weiliang Zhu

#### **11. Brief annual activity report**

During the period 2021-2022, 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>