

SIG12

Reported Period: 2022-2023

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Reported by: Jerome Rouquette, Claire Colin, Gabriella Cavallo

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1. Introduction. (50 words max.)

The main activities of the SIG team have been to prepare the Versailles and Padova ECMs. In Padova, the SIG12 representative to the program committee is Jérôme Rouquette.

2. SIG web site:

SIG12: <https://ecanews.org/groups/sig-12-crystallography-of-functional-materials/>

Future site should be: <https://ecanews.org/sig-12/>

3. Number of ECA individual members registered with the SIG

SIG12 Materials Science

88 (as of 06/09/2023)

4. Existence of a SIG mailing list: yes

SIG12 communicates with its members via the ECA webpages <https://ecanews.org/groups/sig-12-crystallography-of-functional-materials/>

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

66 members registered on <https://ecanews.org/groups/sig-12-crystallography-of-functional-materials/>

6. Plenary and Keynote speakers suggested by SIG12 for the ECM34 in Padova

1. Keynote (or plenary) speaker: *Beatriz Noheda, from Groningen University, <https://www.rug.nl/staff/b.noheda/>*

Noheda's research focuses on understanding the relationship between structure and functionality of thin films of ferroelectric, piezoelectric and multiferroic materials, the control of nano-domains that self-assemble by strain engineering, as well as the characterization of the distinct properties of domain walls. Her main scientific contributions have been the discovery of low symmetry (monoclinic) phases in high piezoelectric materials (PZT and MPB piezoelectrics) and the observation of domain walls as "vertical interfaces" with distinct structure and functionalities. Although her research is fundamental in nature, it is inspired by two main application areas that she believes will enable the next technological revolution: piezoelectric energy harvesting for low power electronics and the development of novel materials for neuromorphic computing.

2. Additional propositions (without any preference):

Len Barbour, from Stellenbosch University (South Africa) who is mainly focused on the discovery, design, assembly and characterisation of new functional materials with interesting properties. In particular, he is interested in exploring and understanding structure-property relationships relating to (i) porous materials and (ii) materials that undergo unusual thermal behaviour (e.g. anomalous thermal expansion, thermosalience, phase transitions, etc.)

Pance Naumov, from NYU Abu Dhabi, who is interested in Mechanical, dynamic and adaptive properties and peculiarities in molecular crystals.

Claudia Weidenthal (Max Planck Institute for Kohlenforschung), who is specialized in structural characterization of Catalysis based on Zeolite and porous Materials

Maksim Kovalenko from ETH Zurich, whose main interests are (i) the precision synthesis of highly luminescent semiconductor nanocrystals; (ii) nanocrystal surface chemistry; (iii) exploration of novel semiconductor materials by solution- and solid-state synthesis; (iv) novel semiconductors for hard radiation detection; (iv) novel materials and concepts for Li-ion and post-Li-ion rechargeable batteries.

Julien Haines from university of Montpellier. His research work focuses on multi-functional nanocomposites, sub-nanometric "host-guest" materials formed under pressure which make it possible to envisage enhanced one-dimensional properties, i.e. such as the electrical transport properties in graphene, photonics to thermoelectricity or even the photocatalytic production of hydrogen.

Paula Abdala from ETH Zurich; <https://ipe.ethz.ch/people/person-detail.MjEyMDcw.TGlzdC8zOTgzLDczMDQ4OTI0MA==.html>. The focus of her research is to understand the interplay between structure and function in materials for sustainable chemical and energy applications, such as heterogeneous catalysts, CO₂ sorbents and fuel cells. She uses synchrotron X-rays techniques to reveal the structure of the materials at working conditions and at different lengths and time scales. Among other projects, she works on the development of operando methods in collaboration with other researchers at LESE and at the synchrotron facilities. Combined X-ray absorption spectroscopy with X-ray powder diffraction, Raman spectroscopy and Pair Distribution Function analysis are key components of their operando toolbox to interrogate the structure of a material at work. The aim is to provide the basis for the design of new efficient materials.

7. List of MS organized by the SIG at the ECM34 in Padova

SIG12 proposed the following microsymbosia with support from other SIGs:

- Structural characterization in Functional materials
- Structural characterization of Energy Harvesting and Conversion Materials

- In situ and Operando diffraction with SIG6 and SIG8- (i.e. diffraction studies of working materials with simultaneous activity measurements. Not limited to powders). Time-resolved diffraction and scattering techniques

SIG12 supported the following microsymbosia proposed by other SIGs:

- High Pressure Crystallography: Exploring Structure and Method Development at Extreme Conditions
- New trends in quantum crystallography
- Aperiodic order and complex superstructures
- Electron diffraction joining forces with quantum crystallography towards materials science applications
- "Powder Diffraction at Synchrotron Source (Alternative titles: Advances in powder diffraction instrumentation at large facilities or Advances in powder diffraction instrumentation, or Progress in instrumentation)"

8. Prizes sponsored/coordinated

STOE regularly sponsors a poster prize in the field of the crystallography of functional materials at the ECMs.

9. Past Activities other than Microsymbosia at ECM

SIG12 supports he 18th European Powder Diffraction Conference (EPDIC18).

9. Future/Programmed Activities.

Currently, the SIG12 representative, Jérôme Rouquette, participates in the organization of the ECM34 in Padova as a member of the program committee.

SIG12 supports he 18th European Powder Diffraction Conference (EPDIC18).

10. Other matters. (50 words max.)

Members of SIG 12 are also involved in the design and use of experimental stations and new sample environments at large scale facilities (synchrotron-neutrons) to open new possibilities for the structural investigation of functional materials under *in situ* and *in operando* conditions.

11. Brief annual activity report (100 words max.)

SIG officers are involved in the organization of conferences related to materials crystallography, materials science and diffraction-related meetings, AFC 2024 (French Association of Crystallography), Montpellier, France; crystallography at high pressure, European High Pressure Research Group 2026, Montpellier, France. They participate in review and advisory committees in various European large-scale facilities.

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

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