SIG12
Reported Period: 2024-2025
Report Date: 11/07/2025
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 Poznan ECM. In Poznan, the SIG12 representative to the program committee is Gabriella Cavallo.

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 83 (as of 30/07/2024)

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)

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

6. Plenary and Keynote speakers suggested by SIG12 for the ECM35 in Poznan

Mohamed Eddaoudi - King Abdullah University of Science and Technology, Saudi Arabia
https://www.kaust.edu.sa/en/study/faculty/mohamed-eddaoudi
His research activities are mainly aimed at developing new strategies for the design and synthesis of functional solid-state materials from molecular building blocks and advancing the understanding of the structure-property relationship of materials. His group at KAUST works towards developing of made-to-order MOFs that address some of our most challenging and enduring societal needs, such as: Clean energy alternatives: Advance the field of MOFs toward the construction of made-to-order MOFs that can store an adequate amount of H2 at room temperature and moderate pressures. Reduce greenhouse gas emissions: Advance the field of MOFs toward the construction of made-to-order and cost-effective MOFs that can sequester large amounts of CO2.Remediate chemical and biological threats: Construct superior MOFs that can rapidly detect and remediate life-threatening toxic reagents (i.e. chemical and biological warfare agents).

John Anthony - University of Kentucky, USA

https://chem.as.uky.edu/users/anthony
Aromatic molecules are a robust and versatile platform for the development of functional materials for electronic and optical applications. Using a tandem organic synthesis / device analysis approach, we seek to determine structure-property relationships that lead to materials with exceptional performance in organic thin-film transistors (for flexible flat-panel displays), organic solar cells (for low-cost generation of electricity), organic light-emitting diodes (for high-efficiency lighting) and other applications. Needless to say, students in my group learn a wide range of skills, from organic synthesis to materials characterization and device fabrication.

Andy Cooper - University of Liverpool, United Kingdom
https://www.liverpool.ac.uk/cooper-group/
Research Overview
Research activity focuses on the area of functional organic materials chemistry covering length scales from the atomic up to the macroscopic. Our core goal is to synthesize materials with structures and functions that are not found in other systems. We also focus on developing fundamental methods to achieve control over organic materials structure at the atomic level as a platform to enable a broad range of applications in areas such as energy. Our programme is a unique combination of computation, experiments, and robotics. Examples of materials with unique function developed in our group include the first nanoporous polymers with extended conjugation ('CMPs', Angew. Chem., Int. Ed., 2007), the first permanently porous organic cages (Nature Mater., 2009), the first 'porous liquids' (Nature, 2015; a collaboration with Prof. Stuart James), and organic polymers and covalent organic frameworks for photochemical hydrogen production from water (J. Am. Chem. Soc., 2015; Nature Chem., 2018).

Michaele Hardie - University of Leeds, United Kingdom
https://eps.leeds.ac.uk/chemistry/staff/4189/professor-michaele-hardie
Research interests :
- supramolecular chemistry;
- metallo-supramolecular assemblies;
- crystal engineering;
- synthesis of molecular hosts;
- X-Ray crystallography

Aurora Cruz-Cabeza (Durham University- United Kingdom)
https://www.durham.ac.uk/staff/aurora-j-cruz-cabeza/#publications
Research interests:
- Solid State Chemistry,
- Polymorphism,
- Crystallisation,
- Molecular Simulations,
- Nucleation,
- Crystal Growth

Len Barbour - Stellenbosch University, South Africa

https://academic.sun.ac.za/barbour/Home.html
Research Interests:
POROUS MATERIALS: The primary focus of the Barbour group is to develop the tools to understand counterintuitive behaviour (particularly the dynamics of structural flexibility) of porous materials. In addition to detailed crystal structure analyses, we carry out physico-chemical measurements of the kinetics and thermodynamics of sorption processes. We also actively develop new devices and protocols that we apply routinely to our own research: these include an environmental gas cell for in-situ structural analysis of gas-loaded crystals (by means of single-crystal and powder X-ray diffraction), and pressure-gradient differential scanning calorimetry.
ANOMALOUS THERMAL EXPANSION: For some solids thermal expansion occurs anisotropically, that is, with highly disparate linear expansion coefficients along the three directions. In rare cases, structural mechanisms exist that cause negative thermal expansion along one or more directions. This area of structural chemistry is still relatively unexplored and we are actively involved in establishing the structure-property relationships that influence anomalous thermal expansion.

7. List of MS organized by the SIG at the ECM35 in Poznan

MS: Structural characterization of Materials for Energy Storage and Conversion

Chairs/Speakers
Laure Monconduit from University of Montpellier. After many years dedicated to new materials, new crystallographic arrangements and their structure-properties relationship, LM progressively specialized to materials for electrochemical energy storage, as Li batteries.
Her current research directions include the synthesis and characterization of new electrodes materials, especially anodes for Li-ion, and for post-Li electrochemical systems: Na-, K-, Mg-, Ca-ion batteries. She is specialist of p-bloc element electrode material, with a great specific attention paid on silicon. LM participates to the renewal of metal batteries (electrode protection and the electrolyte's modification (polymers, gel, composite electrolytes). More recently she has embarked on the path of batteries recycling, especially by mechanochemistry. The understanding of the electrochemical mechanism through operando characterization technics (XRD, IR-ATR, Raman, Mössbauer spectroscopy) is the centre of all her research topics.

Will Chueh - Stanford University
https://chuehlab.stanford.edu/people/will-chueh
Will Chueh is an Associate Professor in the Department of Materials Science and Engineering and Energy Science & Engineering at Stanford University, Department of Photon Science at SLAC National Accelerator Laboratory, and a Senior Fellow of the Precourt Institute for Energy. He leads a group of more than thirty researchers pursuing the following missions: (1) understand reactions and transport involving ions and electrons, and (2) decarbonize various energy transformation pathways.

MS; Structure-Property Relationships in Functional Materials

Chairs/Speakers:
Claudia Weidenthale (Max Planck Institute for Kohlenforschung), who is specialized in structural characterization of Catalysis based on Zeolite and porous Materials.

Giancarlo Terraneo (Politecnico di Milan). He's research interests are in the field of crystal engineering, supramolecular chemistry and structural characterization of molecular functional materials through X-ray diffraction techniques.

Prof. C Malla Reddy - Department of Chemistry IIT Hyderabad, Telangana, India
https://people.iith.ac.in/cmreddy/

MS: Structure and dynamics in porous frameworks

Chairs/speakers:

Simon Krause - Max Planck Institute for Solid State Research
https://simonkrause-chem.de/#about
Research interests:

- Functional and Dynamic Framework Materials
- Molecular Machines and Switches
- Dynamic Phenomena and Catalysis
- Chemistry and Catalysis with Light

Wendy Lee Queen- EPFL Valais, Sion/CH
https://www.epfl.ch/labs/lfim/queen/
Synthesis and characterization of metal-organic frameworks (MOFs), that are of interest in a number of host-guest applications. The team offers a highly innovative approach to the design, synthesis, and characterization of hybrid organic/inorganic materials for applications in the fields of gas and liquid separations, small molecule storage, and catalysis. Of particular interest among her projects are the study of interactions between "host" hybrid materials and "guest" molecules using advanced characterization techniques and the development of post-synthetic modification strategies to enhance MOF performance.

Supramolecular interactions behind crystal engineering

Chairs/Speakers:

Len Barbour - Stellenbosch University, South Africa
https://academic.sun.ac.za/barbour/Home.html

Prof. C Malla Reddy - Department of Chemistry IIT Hyderabad, Telangana, India
https://people.iith.ac.in/cmreddy/

Pierangelo Metrangolo – Politecnico di Milano
https://www.cmic.polimi.it/en/persone/docenti-e-ricercatori/metrangolo-pierangelo/

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 Microsymposia at ECM

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

9. Future/Programmed Activities.

Gabriella Cavallo will be the SIG12 representative in Poznan for the ECM35.

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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