SIG14 activity report September 2024-August 2025

Editorial activity of SIG members

- **Marc De Boissieu:** section editor of Acta Cryst B (IUCr)
- **Tatiana Gorelik**: co-editor of Acta Cryst A (IUCr)
- **Reinhard B. Neder**: co-editor of Acta Cryst B (IUCr)
- **Anna Hoser**: special issue guest co-editor in Structural Dynamics (https://pubs.aip.org/sdy/collection/592020/Neutron-Scattering-and-Quantum-Crystallography)

Organization of ECM

SIG14 representative in the organizing committee of **ECM35** in Poznan 2025 – Anna Hoser.

List of MSs @ECM35 organized by SIG14:

- **M19 - Quantum mechanical models for disorder, dynamics, and diffuse scattering**
  Chairs: Johnathan Bulled (ESRF, Grenoble, FR), Anders Østergaard Madsen (U Copenhagen, DK)
  Speakers: Ella Schmidt (U Bremen, DE), Matthias Gutmann (ISIS Facility, Didcot, UK
  Abstract:
  Disorder and dynamics in the solid state materials are phenomena that may be difficult or impossible to unravel based on Bragg scattering data alone. The advent of very sensitive area detectors and state-of-the-art instrumentation have increased the possibilities to study diffuse scattering of such disordered structural components, from magnetic spins to entire protein molecules. At the same time, advanced models of dynamics and disorder can be obtained from quantum-mechanical calculations, e.g. ab-initio molecular dynamics simulations, lattice-dynamical models, and (quantum) Monte Carlo simulations. welcome broadly any contribution that applies quantum mechanical calculations – or related methods, e.g. tailor-made or machine-learned force fields – to learn more about thermal motion, magnetic correlations, and disorder in the solid state.
- **M22 - Short-range order as seen by different techniques**
  Chairs: Giovanni Orazio Lepore (U Florence, IT), Wojciech Sławiński (U Warsaw, PL)
  Speakers: Marta Morana (U Florence, IT), Przemyslaw Rzepka (J Heyrovsky Institute Physical Chemistry, CAS, Prague, CZ)
  Abstract:
  Short-range order becomes more and more important in materials studies, since it influences the properties. Unfortunately, it is commonly neglected because of experimental difficulties. Here, we invite scientists with experimental and/or theoretical expertise to move forward our understanding of materials with important local atom arrangements.
- **M23** - **Dynamics and disorder in complex systems and/or under extreme conditions**
  Chairs: Daniel Chaney (ESRF, Grenoble, FR), Ella Schmidt (U Bremen, DE)
  Speakers: Bryce Mullens (Stoney Brook U, New York, US), Björn Wehinger (ESRF, Grenoble, FR)
  Abstract:

This microsymposium will focus on recent advances in the study of dynamic behaviour, atomic disorder and the coupling that exists between them in complex systems formed under, or subjected to, extreme or unconventional conditions. "Extreme or unconventional conditions" are broadly defined to cover a wide range of non-ambient environments such as He-cryogenic or 'extreme' elevated temperatures (<80K or >500K), high pressure, applied electromagnetic fields, uniaxial strain and various in-situ gas or electrochemical environments as well as any other non-standard settings or combinations of them. Aside from experimental studies, any contributions that cover novel computational or theoretical approaches aiming to further our understanding of dynamics and disorder in complex systems under extreme conditions are also welcomed.

- **M24 Disordered and defective molecular systems, effect on chemical properties**
  Chairs: Hanna Boström (Stockholm U, SE), Stefano Canossa (ETH Zurich, CH)
  Speakers: Emily Meekel (Kyoto U, JP), Martin Schmidt (Frankfurt U, DE)
  Abstract:
  Disorder and defects are increasingly recognized for their key role in defining the real properties of materials, and for the potential of achieving novel functions by their synthetic control. This microsymposium showcases contributions covering these research topics at fundamental and applied levels, with a focus on materials assembled from molecular building blocks

Keynote Speakers supported:

- **Berthold Stöger** (Technical U Vienna, AT), together with SIG-05
- **Yasar Krysiak** (U Hannover, DE), together with SIG-04
- **Marc de Boissieu** (SIMaP-CNRS, Grenoble, FR), together with SIG-03

Poster Prize:
Dectris kindly sponsors a poster prize for the posters submitted to one of the SIG14 microsymposia listed above. The jury will consist of all SIG14 officers.

A SIG14 representative in the organizing committee of **ECM36** in Prague 2027 will be elected by the SIG at ECM25.

SIG14 mailing list and webpage

We keep the ECA SIG webpage updated with new activities from the SIG:
https://ecanews.org/sig-14/
The mailing list is hosted by the "Deutsches Forschungsnetz" and has been (re-)established after discussions of the SIG at ECM in Padova. Currently the list has 42 subscribers.

Organization of dedicated schools and workshops

- **3D-ΔPDF and Diffuse Scattering Analysis** Satellite workshop to ECM 35, August 24-25, 2024:
  - **SIG Organizers**: Arkadiy Simonov (ETH Zurich), Ella M. Schmidt (University of Bremen), Reinhard B. Neder (FAU Erlangen), Anna Hoser (University of Warsaw)

- **Purpose**: Interest in diffuse scattering analysis and three-dimensional difference pair distribution function (3D-ΔPDF) analysis has significantly increased in recent years, owing to the ability to utilize data from in-house laboratory instruments for analysis. However, data treatment and the initial stages of model building remain challenging. Therefore, the organizers are offering this workshop to assist participants in initiating data treatment and diffuse scattering analysis. The workshop will feature lectures by prominent figures in 3D-ΔPDF analysis from Europe and experienced users. Participants will benefit from a combination of lectures and practical sessions, where they will become familiar with a complete data processing workflow—from raw diffraction data to diffuse scattering refinement—using the programs Yell and Discus on their own laptops.
- **Webpage**: https://ecm35.org/3dds

List of plenary / invited / teaching lectures of individual SIG members

Plenary, Keynote and invited lectures (sorted by date):

- Anna Hoser: Sagamore XX Conference on Quantum Crystallography, India, Shiv Nadar Institute, 11.2024.
- Stefano Canossa: Bruker-MIT Symposium, Massachusetts Institute of Technology, USA, February 2025.
- Andrew Goodwin (Oxford University, German Crystallographic Meeting, Hannover, Germany, March 2025.
- Daniel A. Chaney: Seminar of the Institute of Solid State Physics, Graz, Austria, April 2025.
- Stefano Canossa: 2nd Swiss Symposium on Materials Chemistry, Fribourg, Switzerland, June 2025.
- Arianna Minelli (Oak Ridge National Laobratory, North American Solid State Chemistry Conference (NASSCC), Ames, Iowa (USA), July 2025.
- Anna Hoser: ICDM10 (International Charge Density Meeting 10), Durham, July 2025
- Stefano Canossa: 2nd Mediterranean conference on Porous Materials, Marrakech, May 2025.
- Invited Microsymposia at ECM 35 in Poznan August 2025:
  - Marta Mora MS 22
  - Anna Hoser MS 18
  - Stefano Canossa MS 48
  - Ella Schmidt MS 19
  - Björn Wehinger MS 23
  - Emily Meekel MS 24
  - Martin Schmidt MS 24
- Stefano Canossa: Early Career Researchers in MOFs and Related Materials, Cambridge, September 2025.

Teaching lectures (sorted by date):

- Reinhard Neder: MATRAC 2 school Herrsching, Germany, September 2024.
- Stefano Canossa: Workshop on interpretation of single crystal total scattering and data collection practices at the University of Valencia, February 2025.

- Reinhard Neder: MATRAC 1 school Seevetal, Germany, March 2025.
- Daniel A. Chaney: 15th School on the Physics and Chemistry of the Actinides - Grenoble, France, March 2025.
- Ella Schmidt: HERCULES school Grenoble, April 2025.
- Daniel A. Chaney: School on Finite Temperature and Anharmonic Response Properties of Solids in Theory and Practice - Liege, Belgium, April 2025.
- Stefano Canossa: 'Lake Como school on MOFs and porous materials', on theory and practice of single-crystal total scattering analysis, June 2025.
- Stefano Canossa: 'European Crystallography School in North Macedonia' on pretty much the same topic, but with more contents and interactive exercise on diffuse scattering interpretation, June 2025.

List SIG officers

Chair: Ella M. Schmidt – University of Bremen – ella.schmidt@uni-bremen.de
Vice Chair: Anders Ø. Madsen – University of Copenhagen - a.madsen@sund.ku.dk
Secretary: Anna Hoser - University of Warsaw - a.hoser@uw.edu.pl
Officers: Stefano Canossa, Dmitry Chernychov, Arkadiy Simonov, Wojciech Sławiński, Björn Wehinger

Elections will be held at ECM35 in Poznań..