

SIG14 activity report September 2023-September 2024

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)

Organization of ECM

SIG14 representative in the organizing committee of **ECM34** in Paodva 2024 – Ella M. Schmidt.

List of MSs @ECM34 organized by SIG:

- **MS 12: Correlation between quantum crystallography and crystal dynamics**
Chairs: Maura Malińska (University of Warsaw, PL), Anders Østergaard Madsen (University of Copenhagen, DK)
Speakers: Silvia Capelli (ISIS, UK), Michał Chodkiewicz (University of Warsaw, PL)
- **MS 34: Applications of 3D-PDF**
Chairs: Thomas Weber (ETH Zürich, CH), Ella M. Schmidt (University of Bremen, DE)
Speakers: Nikolaj Roth (Aarhus University, DK), Matthew Krogstad (Argonne National Laboratory, USA)
- **MS 35: Methods for diffuse scattering analysis from powder to single crystals**
Chairs: Arkadiy Simonov (ETH Zürich, CH), Wojciech A. Slawinski (University of Warsaw, PL)
Speakers: Tatiana Gorelik (Helmholtz Centre for Infection Research, DE) Thomas Nicholas (Oxford University, UK)

KeyNote Speaker: **Anders Østergaard Madsen** (Copenhagen University, DK)

SIG14 representative in the organizing committee of **ECM35** in Pozań/Lviv 2025 – Anna Hoser.

SIG14 mailing list and webpage

The former mailing list had 32 members. We started using the newly provided tools via Wordpress and are currently launching a new mailing list.

We started filling the new webpage with content: <https://ecanews.org/sig-14/>

Organization of dedicated conferences

- **11th Conference on Aperiodic Crystals** Aperiodic 2024 is the latest in a series of conferences supported by the Commission on Aperiodic Crystals (CAC) of the International Union of Crystallography (IUCr), June 24-28, 2024
 - **SIG members of the programme committee:** Marc de Boissieu, Ella M. Schmidt.
 - **SIG members as invited speakers:** Marc de Boissieu, Andrew Goodwin

Organization of dedicated schools and workshops

- **UDM3. The complementary use of diffuse and inelastic X-ray scattering** User-Dedicated Microsymposia at the ESRF User Meeting, February 7th, 2024
 - **SIG Organizers:** Alexei Bosak, ESRF and Daniel Chaney, ESRF
 - **Purpose:** This user dedicated microsymposium (UDM) aims to highlight the complementary nature of diffuse and inelastic (IXS) X-ray scattering capabilities available at the ESRF and provide a space for scientific discussion amongst the user base in these areas. The IXS capabilities at the ESRF have been well developed over the last 20+ years and with the EBS upgrade remain one of the best in the world. However the addition of diffuse scattering capabilities in more recent years has provided many new opportunities. There is now an active and engaged user base utilising the synergy between the two techniques and this UDM aims to bring the community together to present their recent work as well as discuss both new scientific ideas and provide suggestions for additional desired capabilities at the ESRF. A non-exhaustive selection of areas that will be covered, includes thermal diffuse scattering, phase transitions and critical diffuse scattering, state-of-the-art modelling approaches, disorder-phonon coupling, diffuse "roadmapping" for IXS studies and the progress/challenges of sample environment development for diffuse and inelastic scattering studies.
 - **Webpage:** <https://www.esrf.fr/home/events/conferences/2024/user-meeting-2024/user-dedicated-microsymposia/udm3-complementary-use-of-inelastic-and-diffuse-scattering.html>
- **3D- Δ PDF and Diffuse Scattering Analysis** Satellite workshop to ECM 34, August 31-September 1, 2024:
 - **SIG Organizers:** Arkadiy Simonov, ETH Zurich, Ella M. Schmidt, University of Bremen, Thomas Weber, ETH Zurich, Reinhard B. Neder, FAU Erlangen
 - The Workshop administration was supported by ELECTRA e.V. and several members of **SIG 4**.
 - **Purpose:** Interest in diffuse scattering analysis and three-dimensional difference pair distribution function (3D- Δ PDF) 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- Δ PDF 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 [Discuss](#) on their own laptops.
 - **Webpage:** <https://www.geo.uni-bremen.de/kristall/Webseiten2022/ECMSatellite/DiffuseSatelliteWebpage.html>

Science communication and outreach activities

SIG officer Stefano Canossa is putting together a list of teaching resources that cover Fourier transforms for teaching purposes. Furthermore as a science communication project he posts Fourier transforms of aperiodic patterns, fractals and mathematical tilings on Instagram (@<https://www.instagram.com/specialdefects/>) and freely available on (<https://www.behance.net/specialdefects>). His teaching sets are now included in the Cambridge Crystallographic Data Centre teaching resources (DECOR, <https://www.ccdc.cam.ac.uk/community/education-and-outreach/education/decor/>).

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

Plenary and Keynote lectures:

- Ella M. Schmidt: “Supercell lattice dynamical calculations to predict thermal diffuse scattering in materials with correlated disorder.” User-Dedicated Microsymposia, ESRF User Meeting, Grenoble, France, February 2024.
- Arkadiy Simonov: “Insights into the local structure of materials from single crystal diffuse scattering.” User-Dedicated Microsymposia, ESRF User Meeting, Grenoble, France, February 2024.
- Marc de Boissieu: “Aperiodic crystals: atomic structure and phason modes”, German Crystallographic Meeting, Bayreuth, Germany, March 2024.
- Reinhard Neder: “General Introduction of diffuse scattering” Diffuse Scattering Workshop, Oak Ridge National Laboratory, USA. September 2023.
- Nikolaj Roth: “3D-magnetic PDF, model free approach for magnetic diffuse scattering”, Diffuse Scattering Workshop, Oak Ridge National Laboratory, USA. September 2023.
- Andrew Goodwin: “Truchet-tile architectures”, Structural Novelty Workshop, Liverpool, UK. January 2024.
- Andrew Goodwin: “Truchet-tile architectures in materials chemistry”, Correlated Disorder Workshop, Herzberg, Switzerland. February 2024.
- Stefano Canossa: “3D total scattering and the shifting paradigm of MOFs structural complexity”, 9th international MOF conference, Singapore, July 2024. **Awarded best oral presentation.**

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