

SIG-02 - Quantum Crystallography

Reported Period: August 2024 – August 2025

Report Date: August 5, 2025

Reported by: Anna Krawczuk (chair), Alessandro Genoni (vice-chair), Maura Malinska (secretary)

1. Introduction:

SIG-02 brings together experimentalists and theoreticians in the field of quantum crystallography to study all aspects of quantum phenomena, e.g. charge and spin distributions in atoms, molecules and condensed matter. Goals: integrating concepts from many experimental & theoretical methodologies into a coherent understanding of matter at the subatomic level beyond geometry; promoting the application of this understanding in the physics, chemistry, materials, geology, mineralogy, high pressure and biology communities.

2. SIG web site:

SIG-02 <https://ecanews.org/groups/sig-02-charge-spin-and-momentum-density/>

3. Number of ECA individual members registered with the SIG according to (<http://www.xray.cz/eca/im-payment.htm>)

61 members according to the SIG-02 page in the ECA website

152 members according to our own mailing list

We are always trying to convince people in our mailing list to become ECA individual members registered with SIG-02 to fix the discrepancy currently existing between the official SIG-02/ECA list and our mailing list.

4. Existence of a SIG mailing list? Yes

In 2016 we updated our mailing list and promoted our Google group again, which consequently gained a lot of visibility (now 151 members). Most of the (active) participants from past events related to our SIG have been invited to our Google group.

Address of the mailing list: https://groups.google.com/forum/#forum/sig2_csmd

Name of the Google group: SIG2_QCr

Number of members in the SIG mailing list: 152

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

Between 100-150 considering the different names of the participants in the last meetings related to SIG-02 (~100 participants of Sagamore conference in India in November 2024, ~60 participants during the International Charge Density Meeting in June 2025).

6. List of MS organized by the SIG at the last ECM

- MS-11: New trends in quantum crystallography chaired by Simon Coles (UK) and Michael Bodensteiner (DE)
- MS-12: Correlation between quantum crystallography and crystal dynamics chaired by Maura Malinska (PL) and Anders Østergaard Madsen (DK) [organized together with SIG-14]
- MS-13: Molecular structure and chemical bonding in the view of quantum crystallography chaired by Catharine Esterhuysen (ZA) and Dietmar Stalke (DE) [organized together with SIG-13]

- MS-21: Electron diffraction joining forces with quantum crystallography towards materials science applications chaired by Paulina Dominiak (PL) and Richard Beanland (UK) [organized together with SIG-04]
- Keynote lecture given by Jean-Michel Gillet (FR)
- Keynote lecture given by Anders Østergaard Madsen (suggested together with SIG-14)

7. Prizes sponsored/coordinated

Poster prize award named after Prof. Philip Coppens in the field of broadly understood quantum crystallography in line with the scope of the ECA SIG-02. It is sponsored by Rigaku Oxford Diffraction. The recipient of the 2024 award was **Paulina Maria Rybicka** (University of Warsaw, PL), who presented the poster entitled “*The effect of (not) applying symmetry constraints during refinement and using different local coordinate systems on local symmetry of atoms and atom types in the MATTS data bank*”

8. Past Activities other than Microsymposia at ECM

Title: Quantum Crystallography Session at the 75th American Crystallographic Association Annual Meeting (18-23.07.2025; Lombard, Chicago, USA) (<https://www.acameeting2025.com/>)

Number of Participants: ~ 200 participants

Level of involvement of SIG in the activity:

- The Quantum Crystallography related session was organized and chaired by Anna Krawczuk and Sylwia Pawledzio (both SIG-02/ECA individual members);
- SIG-02/ECA individual members were involved as lecturers

Endorsed (SIG logo on the web page/leaflets): No

Sponsored by ECA? No

Other Sponsors/Organizers: Quantum Crystallography session was sponsored by Rigaku, Bruker, Stoe, Dectris, Mitegen and OlexSys

Short Description: Members of the SIG-02 on Quantum Crystallography organized and participated in the following session at the 2025 Meeting of the American Crystallographic Association:

- *Quantum Crystallography: Latest Developments, Applications, and Experiences:* The session was dedicated to advances and results obtained in the field of Quantum Crystallography (QCr). Both main aspects of modern methods of quantum crystallography were covered by the given presentations. SIG-02/ECA individual members were speakers during the session: Maura Malinska, Jean-Michel Gillet, Florian Meurer.

Title: 10th International Charge Density Meeting (14-17.07.2025, Durham, United Kingdom)

Number of Participants: ~ 60 participants

Level of involvement of SIG in the activity:

- Conference organized by SIG2/ECA members: Horst Puschmann, Simon Coles and Paul Niklas Ruth
- SIG-02/ECA individual members were involved as lecturers and discussion leaders

Endorsed (SIG logo on the web page/leaflets): No

Sponsored by ECA? No

Other Sponsors/Organizers: OlexSys, Rigaku, IUCr, Dectris

Short Description: The meeting brought together leading researchers in quantum crystallography and related disciplines. While the conference has traditionally focused on charge, spin, and momentum densities, recent editions placed growing emphasis on quantum crystallography, which integrates quantum mechanics and crystallography to enable accurate modeling of crystal structures. Many of the SIG-02/ECA members were speakers during the conference.

Title: International School of Crystallography – Quantum Crystallography (30.05-07.06.2025, Erice, Italy) (<https://crystalalice.org/2025/welcome.php>):

Number of Participants: ~ 50 participants

Level of involvement of SIG in the activity:

- Organized by Paulina Dominiak (current chair of the IUCr Commission on Quantum Crystallography and SIG2/ECA individual member) and Julia Contreras-García.
- SIG-02/ECA individual members were involved as lecturers and tutors.

Endorsed (SIG logo on the web page/leaflets): Yes

Sponsored by ECA? Yes

Other Sponsors/Organizers: Bruker, Rigaku, CCDC, Dectris, OPCW, CNRS, University of Warsaw, Springer Nature, AFC, IUCr

Short Description: The Quantum Crystallography School provided an in-depth introduction to modern approaches that combine theoretical and experimental methods to study atomic and molecular structure, also and especially at subatomic level. Lectures covered quantum mechanical and semi-empirical methods, as well as data analysis techniques used in quantum crystallography. Hands-on workshops offered training in relevant software and case studies. The school ran in parallel with the Electron Crystallography School, with several joint lectures that encouraged interdisciplinary exchange between the two communities. Many of the SIG-02/ECA individual members were lecturers and tutors during the school.

Title: Quantum Crystallography Session at the 33rd Annual Meeting of the German Crystallographic Society (10-13.03.2025, Hannover, Germany):

Number of Participants: ~ 300 participants

Level of involvement of SIG in the activity:

- The session was organized and chaired by Florian Kleemiss (SIG-02/ECA individual member) and Marvin Treger;
- SIG-02/ECA individual members were involved as presenters.

Endorsed (SIG logo on the web page/leaflets): No

Sponsored by ECA? No

Other Sponsors/Organizers: none

Short Description: Members of the SIG-02 on Quantum Crystallography organized and participated in the following session at the 33rd DGK Meeting in Hannover:

- *New trends in quantum crystallography:* The session aimed to showcase the latest advancements in the field of quantum crystallography, highlighting both experimental and theoretical developments. SIG-02/ECA individual members were speakers during the session: Simon Grabowsky (CH), Anna Krawczuk (DE), Florian Meurer (DE) and Regine Herbst-Irmer (DE).

Title: Sagamore XX-2024 Conference on Quantum Crystallography (10-15.11.2024, Shiv Nadar Institute, New Delhi, India)

Number of Participants: ~ 100 participants

Level of involvement of SIG in the activity:

- Individual members of SIG-02 were involved in the scientific committee of the conference
- SIG-02/ECA individual members were presenting their research

Endorsed (SIG logo on the web page/leaflets): No

Sponsored by ECA? No

Other Sponsors/Organizers: Bruker, Crystal23, RSC, Rigaku, J. Mol. Struct. (Elsevier)

Short Description: The meeting brought together leading researchers in quantum crystallography and related disciplines. While the conference has traditionally focused on charge, spin, and momentum densities, recent editions placed growing emphasis on quantum crystallography, which integrates quantum mechanics and crystallography to enable accurate modeling of crystal structures. Many of the SIG-02/ECA members were speakers during the conference.

Title: Distinguished Lectures on Quantum Crystallography (September 2022 – present), webinars (<https://qcrwebinar.chem.uw.edu.pl/Home>)

Number of Participants: 65 average number of participants, with a maximum of 120 participants

Level of involvement of SIG in the activity:

- Organized and chaired by Krzysztof Wozniak (former SIG-02 chair and SIG2/ECA individual member) and Paulina Dominiak (current chair of the IUCr Commission on Quantum Crystallography and SIG2/ECA individual member);
- SIG-02/ECA individual members were involved as lecturers and, of course, as participants
- These lectures are organized under the auspices of the Quantum Crystallography Commission of IUCr and the European Crystallographic Association SIG-02 on Quantum Crystallography

Endorsed (SIG logo on the web page/leaflets): Yes

Sponsored by ECA? No

Other Sponsors/Organizers: IUCr, University of Warsaw, Crystallography Committee of the Polish Academy of Sciences

Short Description: A series of seminars having a dual goal: i) further disseminating the research activities and the most recent results in the field of Quantum Crystallography; ii) broadening the horizons of Quantum Crystallography through possible contamination from related and neighboring fields. The seminars generally take place monthly. Seminars are held monthly, each typically featuring two lectures of approximately 35 minutes plus extended discussion time. One talk focuses on a core topic in Quantum Crystallography, while the second explores a complementary or emerging area. The series is open to the widest possible audience and is expected to continue in future years. Distinguished speakers from recent sessions include: Christopher J. Bardeen, Deepak Chopra, Małgorzata Biczysko, Benoît Guillot, Sarah L. Price, Paul Popelier, Louis Massa, Sarah Guerin, Sajesh Thomas, Huibo Cao, and Nicola Claiser.

Number of participants in the whole series ranged from 52 up to 173. Lectures are recorded and posted on the website <https://qcrwebinar.chem.uw.edu.pl> with 21-356 views per lecture.

9. Future/Programmed Activities.

Title: Third CECAM Workshop on Quantum Crystallography, February 11-13, 2026, Lausanne, Switzerland

Number of Participants: ~100 participants

Level of involvement of SIG in the activity:

- Organized by Simon Grabowsky (former SIG-02 Chair and individual SIG2/ECA member), Julia Contreras-García and Jean-Michel Gillet (former chair of the IUCr Commission on Quantum Crystallography).
- Many SIG2/ECA individual members will be involved as lecturers and discussion leaders.
- Proposal submitted

Endorsed (SIG logo on the web page/leaflets): Yes

Sponsored by ECA? To be announced

Other Sponsors/Organizers: to be announced.

Short Description: The workshop is organized to discuss the state of the art of Quantum Crystallography in all its modern aspects and to also discuss possible new perspectives for this research field.

Title: Sagamore Conference, Nancy, France (2027)

Expected number of Participants: ~100 participants

Level of involvement of SIG in the activity:

- Organized by CRM2 including individual members of SIG-02/ECA
- SIG2/ECA individual members will be part of the scientific committee
- SIG2/ECA individual members will be included as lecturers.

Endorsed (SIG logo on the web page/leaflets): Yes

Sponsored by ECA? To be announced

Other Sponsors/Organizers: to be announced.

Short Description: Conference will be primarily dedicated to charge, spin, and momentum densities and latest development in the field

Title: 11th International Charge Density Meeting, Lecco, Italy (2028)

Expected number of Participants: ~120 participants

Level of involvement of SIG in the activity:

- Organized by Alessandro Genoni (Former Chair and current Vice-Chair of SIG-02 and individual member of SIG-02/ECA)
- SIG2/ECA individual members will be part of the scientific committee
- SIG2/ECA individual members will be included as lecturers.

Endorsed (SIG logo on the web page/leaflets): Yes

Sponsored by ECA? To be announced

Other Sponsors/Organizers: to be announced.

Short Description: Conference will be dedicated to advancements in experimental and theoretical charge density studies.

10. Other matters.

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11. Brief annual activity report

SIG-02 continues to promote activities aimed at increasing awareness and engagement with Quantum Crystallography across broader scientific communities. In particular, the past 12 months have been especially active, with numerous meetings, schools, and other events organized by members of the community. We particularly highlight the ongoing Distinguished Lectures on Quantum Crystallography, which remain a key outreach initiative, and the successful 2nd International School on Quantum Crystallography, held in Erice in June 2025 as part of the well-established Erice International School of Crystallography. Efforts to strengthen and expand our network. The upcoming third CECAM Discussion Meeting on Quantum Crystallography, following the earlier editions in Nancy (2017) and online (2021), has now been confirmed for 2026 and is expected to be highly impactful in terms of scientific exchange and visibility, building on the success of previous meetings. Our community is also preparing for strong participation in the IUCr Congress 2026 in Calgary, as well as other international events in the coming year. Since 2019, the Philip Coppens Poster Prize has been awarded at each ECM meeting, further increasing our presence and recognition within the crystallographic community. In addition, SIG-02 members regularly contribute with lectures and organize dedicated sessions at the annual meetings of the American Crystallographic Association – a tradition successfully upheld over the past several years.

In summary, SIG-02 remains a dynamic and engaged community, marked by ongoing dialogue, collaboration, and the continuous development of new ideas in quantum crystallography.

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

Chair: Anna Krawczuk (University of Göttingen, DE), e-mail: anna.krawczuk@uni-goettingen.de

Vice-chair: Alessandro Genoni (Politecnico di Milano, IT), e-mail: alessandro.genoni@polimi.it

Secretary: Maura Malinska (University of Warsaw, PL), e-mail: mmalinska@chem.uw.edu.pl

Supplementary Materials.

No supplementary material is included with this report.