

SIG2 - Quantum Crystallography

Reported Period: September 2023 – August 2024

Report Date: July 16, 2024

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

1. Introduction:

SIG2 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:

SIG2 <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>)

56 members according to the SIG2 page in the ECA website

151 members according to our own mailing list.

We are continuously working to align the SIG2 mailing list with the official ECA membership list by encouraging non-registered members to formalize their affiliation with ECA, and, particularly with SIG2.

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: 151

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

Between 150-200 considering the different names of the participants in the last meetings related to SIG2 (90 was the number of participants in the CECAM workshop in September 2021, 119 was the number of participants in the Quantum Crystallography online meeting QCrOM2020 in August 2020; 75 was the number of participants in ICDM-9 in June 2022, 100 the number of participants in ICDM-1 in July 2019; 120 the number of participants in ECDM-7 in June 2016; 120 the number of participants in the Sagamore Conference in June 2015; 101 the number of participants in the Gordon Conference in June 2013).

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

- MS19 “Experimental and theoretical advances in quantum crystallography”, chaired by Paulina Dominiak (PL) and Simon Grabowsky (CH);
- MS20 “Electric, opto-electronic and magnetic properties from elastic and inelastic scattering”, chaired by Marlena Gryl (PL) and Jacob Overgaard (DK);

- MS26 “Quantum mechanical models for dynamics and diffuse scattering”, chaired by Anna Hoser (PL) and Anders Ø. Madsen (DK) [organized in collaboration with SIG-14];
- MS36 “Software development in quantum mechanics-based methods of crystallography, chaired by Regine Erbst-Irmer (DE) and Lukas Bucinsky (SK) [organized in collaboration with SIG-09]
- Keynote lecture given by Paulina Dominiak (PL): KN10 “Quantum crystallography of (macro)molecular crystals for everyone.”

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 SIG2. It is sponsored by Rigaku Oxford Diffraction. The recipient of the 2022 award was **Emilie Skytte Vosegaard** (Aarhus University, DK), who presented the poster *MS19-1-3* entitled “*Comparative study of in-house and synchrotron X-ray electron densities on molecular crystals*”

8. Past Activities other than Microsymposia at ECM

Title: Quantum Crystallography Workshop and Sessions at the 74th American Crystallographic Association Annual Meeting (July 7th-12th, 2024; Denver, Colorado, USA)
(<https://www.acameeting24.com/>)

Number of Participants: ~ 600 participants

Level of involvement of SIG in the activity:

- The Quantum Crystallography Sessions and Workshops were organized by Michael Bodensteiner and Florian Kleemiss (both SIG2/ECA individual members).
- SIG2/ECA individual members were involved as lecturers/teachers.

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

Sponsored by ECA? No

Other Sponsors/Organizers: OlexSys, Stoe, Dectris and Rigaku, for the Workshop entitled “Advanced Structure Refinement with Olex2 & NoSpherA2”.

Short Description: Members of the SIG2 on Quantum Crystallography organized and participated in the following workshop and sessions at the 2024 Meeting of the American Crystallographic Association:

- Workshop “*Advanced Structure Refinement with Olex2 & NoSpherA2*”, which was organized to further teach and spread the use of the *Olex2* software and particularly of its Hirshfeld atom refinement-based functionality *NoSpherA2* for structural refinements. Instructors: Michael Bodensteiner (SIG2/ECA individual member), Ilia Guzei, Oleg V. Dolomanov and Florian Kleemiss (SIG2/ECA individual member);

Session “*Latest Developments, Applications & Experiences Featuring Quantum Crystallography*” dedicated to advances and results obtained in the field of Quantum Crystallography (QCr). The session gathered both practitioners and method developers and included all theoretical and practical aspects of the application of quantum mechanics to the study of crystalline materials. The session was organized by Michael Bodensteiner (SIG2/ECA individual member) in collaboration with Brian Patrick from the University of British Columbia (Vancouver, Canada). Three SIG2/ECA individual members (Florian Keemiss, Anna Krawczuk and Sylwia Pawledzio) contributed to the session with oral presentation, two of them were invited speakers.

Title: 32nd Annual Meeting of the German Crystallographic Society (March 18th-21th, 2024; Bayreuth, Germany) (<https://dgk-conference.de/>)

Number of Participants: ~ 350 participants

Level of involvement of SIG in the activity:

- Sessions on “Theoretical methods II: Quantum crystallography and charge density studies” chaired by two SIG2/ECA individual members, Anna Krawczuk and Michael Bodensteiner.

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

Sponsored by ECA? No

Short Description: The session was dedicated to the popularization of quantum crystallography among German scientists, encompassing its field, applications, and method development. It was the first occasion on which a session entirely devoted to QCr was held during the meeting. One of the invited speakers was Florian Kleemiss, an individual member of SIG2/ECA.

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

Number of Participants from September 2023 to June 2024: 75 average number of participants, with a maximum of 121 participants

Level of involvement of SIG in the activity:

- Organized and chaired by Krzysztof Wozniak (former SIG2 chair and SIG2/ECA individual member) and Paulina Dominiak (current chair of the IUCr Commission on Quantum Crystallography and SIG2/ECA individual member);
- SIG2/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 2 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. Each appointment consists of two related lectures of approximately 35 minutes (+15 minutes for questions – with vivid discussions which usually lasted far longer), with one of the lectures about a traditional topic of Quantum Crystallography and the other one focused on a complementary field (for example, but not limited to, electron crystallography and quantum chemistry). These seminars are open to an as wide audience as possible and are supposed to continue on a regular basis in the next years.

Short Description: This series of seminars aims to disseminate recent research in Quantum Crystallography and broaden its horizons through related fields. Held monthly, each session consists of two 35-minute lectures followed by 15-minute Q&A sessions, promoting extensive discussions. Topics cover traditional Quantum Crystallography and complementary fields like electron crystallography and quantum chemistry. The series is open to a broad audience and is expected to continue regularly.

List of lectures:

Lecture 39: Peter Baum

Title: "Attosecond and femtosecond electron microscopy"

Date: April 18, 2024

Lecture 38: Martin Rahm

Title: "The Electron Density: a Fidelity Witness for Quantum Computation"

Date: April 18, 2024

Lecture 37: Eva Zurek

Title: "Theoretical Design of Light-Element Superconductors"

Date: February 29, 2024

Lecture 36: Julia Contreras-Garcia

Title: "Constructing New Models to Predict Superconductivity from the Electron Density and Localization"

Lecture 35: Marek Żukowski

Title: "Einstein-Podolsky-Rosen Paradox, Bell's Theorem, entanglement, GHZ paradox, 'nonlinear' crystals, quantum teleportation, and Nobel Prize 2022"

Date: January 25, 2024

Lecture 34: Krzysztof Szalewicz

Title: "Reliable predictions of crystal structures entirely from quantum mechanics"

Date: December 14, 2023

Lecture 33: Anna Krawczuk

Title: "Dipolar group polarizability as a multipurpose tool for predicting molecular and bulk properties"

Date: December 14, 2023

Lecture 32: Ulf Ryde, K. Lundgren, E. Oksanen

Title: "Recent development in quantum refinement of protein structures"

Date: November 16, 2023

Lecture 31: Cherif Matta

Title: "ATP Synthase: More than just a biocatalyst?"

Date: November 16, 2023

Lecture 30: F. Matthias Bickelhaupt

Title: "(Intermolecular) Covalent Interactions: A Quantitative Molecular Orbital Picture"

Date: October 26, 2023

Lecture 29: Simon Grabowsky

Title: "Quantum crystallography for chemical bonding analysis"

Date: October 26, 2023

Participation in the whole series:

- Range: 52 to 173 participants
- Lectures recorded and posted on the website <https://qcrwebinar.chem.uw.edu.pl> with 21-356 views per lecture.

The YouTube channel has 117 subscribers (<https://www.youtube.com/@quantumcrystallographywebi4529>); the most popular lecture by Piero Macchi has 481 views.

9. Future/Programmed Activities.

Title: Sagamore Conference 2024, November 10-15, 2024; Shiv Nadar Institute, New Delhi, India

Number of Participants: expected ~120 participants

Level of involvement of SIG in the activity:

- SIG2/ECA individual members will be involved in the international organizing committee, chaired by Parthapratim Munshi (Shiv Nadar University, India);
- SIG2/ECA individual members will be involved in the scientific committee;
- SIG2/ECA individual members will be involved as lecturers or discussion leaders.

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

Sponsored by ECA? No

Other Sponsors/Organizers: to be announced

Short Description: The traditional meeting will cover all the subjects related to this SIG. The IUCr commission of Quantum Crystallography will plan the scientific program.

Title: 2nd International School on Quantum Crystallography, May 30 – June 7, 2025; Erice, Italy

Number of Participants: ~ 100 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.
- Many SIG2/ECA individual members will be involved as lecturers or tutors.

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

Sponsored by ECA? to be announced

Other Sponsors/Organizers: to be announced

Short Description: The school will cover different topics related to the field of Quantum Crystallography, starting from fundamentals of crystallography (symmetry, diffraction, modelling) and quantum mechanics (Schrödinger equation, wavefunction, physical bases of the models). The lectures will also focus on the most adopted methodologies (experimental as well as computational) to determine charge and spin electron densities, wavefunctions, electric and magnetic properties of crystalline materials from experimental diffraction data. Application of quantum crystallographic studies in fields like materials science, chemistry and structural biology will be also presented and discussed.

Title: ICDM-10, International Charge Density Meeting, July 2025, Durham, UK

Number of Participants: expected ~120 participants

Level of involvement of SIG in the activity:

- SIG2/ECA individual members will be involved in the organizing committee, chaired by SIG2/ECA members Horst Puschmann and Simon Coles.
- SIG2/ECA individual members will be part of the Scientific Committee and International Advisory Committee
- SIG2/ECA individual members will be involved as lecturers and discussion leaders.

Endorsed (SIG logo on the web page/leaflets): to be announced

Sponsored by ECA? To be announced

Other Sponsors/Organizers: to be announced

Short Description: presentation of the latest results from experimental and theoretical charge density studies.

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

Number of Participants: ~100 participants

Level of involvement of SIG in the activity:

- Organized by Simon Grabowsky (former SIG2 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: CECAM, Rigaku, Quantum Espresso and other sponsors 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.

10. Other matters.

As a result of the Virtual Regensburg Meetings (online meetings that took place in August, November and December 2020 also to discuss possible funding schemes in the framework of Quantum Crystallography), Simon Coles (University of Southampton) and Horst Puschmann (Durham University) were able to get an important grant from the UK Research Agency. Thanks to this grant, a new “QCr integrated workbench” is currently under development to bring software and components for all aspects of Quantum Crystallography together “under one roof” for the whole community. This will also be beneficial to further spread the research activities and the methodologies of quantum crystallography.

11. Brief annual activity report

SIG2 keeps promoting activities aimed to enhance the interest towards Quantum Crystallography studies among ever wider scientific communities. The list of topics at the latest meetings and the preparation of books on Quantum Crystallography clearly testify these efforts. In this context, it is also very worth noting the organization of the *Distinguished Lectures on Quantum Crystallography* (see above in the report). Efforts to organize Quantum Crystallography international schools/workshops are also continuously made (see the already planned 2nd edition of the International School on Quantum Crystallography in Erice in June 2025 in the framework of the well-known Erice International School of Crystallography). Moreover, conferences within the community are regularly organized and already planned for the next months and years. It is also worth noting that, after a first edition in Nancy in 2017 and a second one held online in 2021, a third CECAM discussion meeting on Quantum Crystallography is probably envisaged in 2026 (proposal submitted to the CECAM). Since 2019 we also have had a Philip Coppens poster prize that will be awarded at each ECM meeting. This will increase our visibility at the ECM meetings. Finally, to further spread the research activities within the SIG2 on Quantum Crystallography, the SIG2 members will regularly organize and give lectures in dedicated workshops and sessions at the annual meetings of the American Crystallographic Association (already done in 2023 and 2024, already planned for 2025). In conclusion, the SIG2 community is very vivid, full of discussions and new ideas.

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

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

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

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

Supplementary Materials.

No supplementary material is included with this report.