SIG2 - Quantum Crystallography
Reported Period: **August 2022 – August 2023**
Report Date: **July 5, 2022**
Reported by: **Alessandro Genoni (chair), Anna Krawczuk (co-chair), Maura Malinska (secretary)**
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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)

43 members according to the last e-mail update received from ECA

152 members according to our own mailing list (+6 compared to the 2022 report)

We are always trying to convince people in our mailing list to become ECA individual members registered with SIG2 to fix the discrepancy currently existing between the official SIG2/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 152 members; +6 compared to the 2022 report). 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 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 ward 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: Robert F. Stewart school on electron density and related properties (ECM-33 satellite meeting; August 20th-22nd, 2022; Nancy, France) (https://stewart-school.event.univ-lorraine.fr/)

Number of Participants: ~ 50 participants

Level of involvement of SIG in the activity:

- SIG2/ECA individual members were involved in the organizing committee, chaired by SIG2/ECA member Nicolas Claiser.
- SIG2/ECA individual members were involved in the scientific advisory board.
- SIG2/ECA individual members were involved as lecturers/teachers.

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

Sponsored by ECA? No

Other Sponsors/Organizers: CNRS, Université de Lorraine, IJB (Institut Jean Barriol), Laboratory CRM2, ACF (Association Française de Cristallographie), STOE, Cegitek Innovation, Bruker, Dectris, Cristal Laser.

Short Description: The aim of this school was to teach all participants the basic knowledge about paired and unpaired electron density distributions using neutron and X-ray diffraction methods and to practice existing refinement software. In particular, the school was dedicated to electron density and its analysis, with emphasis on the combination of complementary experimental methods to enrich the electron density models and to lead to a more complete description of the electronic behavior of crystalline solids.

Title: Quantum Crystallography Workshop and Sessions at the 73rd American Crystallographic Association Annual Meeting (July 7th-11th, 2023; Baltimore, Maryland, USA) (https://www.acameeting.com/final-program-23)

Number of Participants: ~ 200 participants

Level of involvement of SIG in the activity:

- The Quantum Crystallography Sessions and Workshops were organized and chaired by Krzysztof Wozniak and Florian Kleemiss (both SIG2/ECA individual members) in collaboration with Yu-Sheng Chen (University of Chicago);
- 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: Rigaku for the Workshop entitled "Structure refinement and disorder modelling with Olex2 and NoSpherA2".

Short Description: Members of the SIG2 on Quantum Crystallography organized and participated in the following workshop and sessions at the 2023 Meeting of the American Crystallographic Association:

- Workshop *"Structure refinement and disorder modelling with Olex2 and 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 and Florian Kleemiss (SIG2/ECA individual member);
- Quantum Crystallography Sessions I and II. These two sessions were dedicated to advances and results obtained in the field of Quantum Crystallography (QCr). Both main aspects of modern methods of quantum crystallography (i.e., the improvement of crystallographic analysis based on quantum mechanical models and the improvement of quantum mechanical methods based on crystallographic data) were covered by the given presentations. The sessions were organized by the SIG2/ECA individual members Krzysztof Wozniak and Florian Kleemiss in collaboration with Yu-Sheng Chen (University of Chicago). Many SIG2/ECA individual members were invited speakers in these two sessions.

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

Number of Participants: 122 average number of participants, with a maximum of 173 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.

Number of participants in the whole series ranged from 71 up to 173. The lectures are recorded and posted on the website (https://qcrwebinar.chem.uw.edu.pl) 21-356 views per lecture.

9. Future/Programmed Activities.

Title: Sagamore Conference 2024, September 2024 (exact dates to be announced), 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 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: Third CECAM Workshop on Quantum Crystallography, February 2025, 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.

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

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.

Title: 2nd International School on Quantum Crystallography, June 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 were involved as lecturers or tutors.

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: 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.

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 "Bob Stewart school on charge density and related properties" in Nancy in August 2022 and 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 were regularly organized and many other congresses and workshops are already planned for the next years. It is also worth noting that, after a first edition in Nancy in 2017, the CECAM also agreed on patronizing the second edition of a workshop discussion meeting on Quantum Crystallography in 2021. A third one is probably envisaged in 2025. 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 (as already done in 2023 and already planned for 2024).

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 (CNRS & University of Lorraine, FR), e-mail: Alessandro.Genoni@univ-lorraine.fr

Co-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.