

## ***SIG2 - Quantum Crystallography***

***Reported Period: January 2021 – July 2022***

***Report Date: July 5, 2022***

***Reported by: Krzysztof Woźniak (chair), Simon Grabowsky (vice chair), Alessandro Genoni (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. Goal: integrating concepts from many experimental & theoretical methodologies into a coherent understanding of matter on 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 e-mail updates that we regularly receive from ECA

146 members according to our own mailing list

We are currently 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 146 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](https://groups.google.com/forum/#forum/sig2_csmd)

*Name of the Google group:* SIG2\_QCr

*Number of members in the SIG mailing list:* 146

### **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**

- MS21 “Modern Quantum Crystallography”, chaired by Piero Macchi (IT) and Sajesh P. Thomas (DK);
- MS22 “Structure-Property Relationships via Charge Density Methods”, chaired by Anna Krawczuk (PL) & Lilianna Checinska (PL);

- MS29 “Accurate Treatment of Hydrogen Atoms”, chaired by Horst Puschmann (UK) & Matteo Lusi (IE);

## 7. Prizes sponsored/coordinated

Since the Vienna ECM meeting our SIG has had a poster prize award named after Prof. Philip Coppens and sponsored by Rigaku Oxford Diffraction. It will be awarded at each ECM conference. The first recipient of this prize was Vedran Vuković, Ph.D. student at the University of Lorraine (MS22-P07 | *QUINOID DIANION FORMING A LONE-PAIR PI-HOLE CONTACT* by Vuković, Vedran (CRM2, Université de Lorraine, Vandoeuvre-lès-Nancy, FRA); Jelsch, Christian (CRM2, Université de Lorraine, Vandoeuvre-lès-Nancy, FRA); Wenger, Emmanuel (CRM2, Université de Lorraine, Vandoeuvre-lès-Nancy, FRA); Molcanov, Krešimir (Institut Ruder Boškovic, Zagreb, HRV))



Vedran Vuković (in the middle) receiving the Prof. Philip Coppens ECA SIG2 Quantum Crystallography Poster Award at ECM32 in Vienna from Bo Brummerstedt Iversen (left) and SIG2 chair Krzysztof Woźniak (right).

The next one will be awarded at the ECM33 at Versailles.

## 8. Past Activities other than Microsymposia at ECM

**Title: CECAM Workshop “Second Discussion Meeting on Quantum Crystallography: Expectations and Reality”, September 9<sup>th</sup>-12<sup>th</sup>, 2021, online meeting (<https://www.cecarn.org/workshop-details/1051>)**

*Number of Participants:* 90 participants

*Level of involvement of SIG in the activity:*

- Organized by Piero Macchi (former SIG2 chair and vice-chair) and Alessandro Genoni (current SIG2 secretary);
- Many SIG2/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:* CECAM (Centre Européen de Calcul Atomique et Moléculaire)

*Short Description:* The workshop was 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, with invited speakers from other close fields (in particular, Quantum Chemistry, Electron Crystallography, X-ray Free Electron Laser communities). In addition to traditional talks and poster sessions, round table discussions on the state of the art and the future of the community were also organized (*New Experimental and theoretical methods for Quantum Crystallography; Wavefunction and charge density models for dynamical Quantum Crystallography*).

**Title: ICDM-9, International Charge Density Meeting, June 12<sup>st</sup>-16<sup>th</sup>, 2022, Aarhus, Denmark**  
(<https://chargedensitymeeting2022.wordpress.com/>)

*Number of Participants:* 75 participants

*Level of involvement of SIG in the activity:*

- Organized by SIG2/ECA members Jacob Overgaard and Anders Ø. Madsen;
- SIG2/ECA individual members were part of the International Advisory Board (<https://chargedensitymeeting2022.wordpress.com/committees/>)
- SIG2/ECA individual members were involved as lecturers.

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

*Sponsored by ECA?* No

*Other Sponsors/Organizers:* Rigaku, Dectris, Bruker, Oxford Cryosystems, STOE, iMAT (Aarhus University Centre for Integrated Materials Research);

*Short Description:* Presentation of the latest results from experimental and theoretical charge density studies. Covered topics: quantum crystallography in magnetism, photochemistry, theoretical quantum crystallography, large-scale facilities and data treatment, combined experiments in quantum crystallography, quantum crystallography for biological systems, quantum crystallography at non-ambient conditions. Round table discussion on past, present and future of “charge density” and related fields. Hands-on sessions on software for quantum crystallography (NoSpherA2, NoMoRe, MoPro).

**Title: Distinguished Lectures on Quantum Crystallography (December 2<sup>nd</sup>, 2021 – 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 (current SIG2 chair) 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.

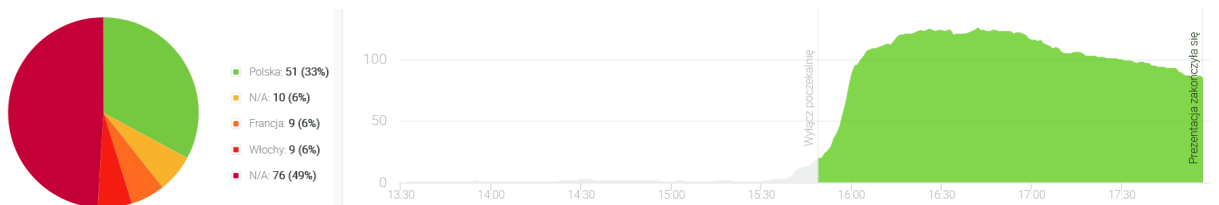
Number of participants in the whole series ranged from 75 up to 173. Below we report examples of statistical data for selected lectures:

### 17/02/2022

37% participants from Poland, 16% from Germany, 10% from France, and the rest from many other countries all over the world. Here is also an illustration of how the participation fluctuated during the lecture and the discussion time.



### Similar data for the first lecture on 2/12/2021



We want to stress the fact that we had interesting discussions after the lectures.

As mentioned above, we will regularly continue these lectures after the summer break.

## 9. Future/Programmed Activities.

**Title: Robert F. Stewart school on electron density and related properties (ECM-33 satellite meeting), August 20<sup>th</sup>-22<sup>nd</sup>, 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 are involved in the organizing committee, chaired by SIG2/ECA member Nicolas Claiser.
- SIG2/ECA individual members are involved in the scientific advisory board.
- SIG2/ECA individual members are 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 is 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 is dedicated to electron density and its analysis, with emphasis on the combination of complementary experimental methods to enrich the electron density models leading to a more complete description of the electronic behavior of crystalline solids.

**Title: Sagamore Conference 2024, India, August 2024, site to be announced**

*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, 2024, Lausanne, Switzerland**

*Number of Participants:* ~100 participants

*Level of involvement of SIG in the activity:*

- Organized by Simon Grabowsky (current SIG2 vice-chair)
- 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, 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: 2<sup>nd</sup> 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” will be created 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. Workshops every 6 months are already planned to facilitate the best integration of all software and components.
- Our members have been also invited to the conferences in the field of mineralogy, geology and high pressure including IUCR High Pressure Workshops.

## **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 2<sup>nd</sup> 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 2024. 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.

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: Krzysztof Woźniak (University of Warsaw, PL), e-mail: [kwozniak@chem.uw.edu.pl](mailto:kwozniak@chem.uw.edu.pl)

Co-chair: Simon Grabowsky (University of Bern, CH), e-mail: [simon.grabowsky@dcf.unibe.ch](mailto:simon.grabowsky@dcf.unibe.ch)

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

## **Supplementary Materials.**

No supplementary material is included with this report.