

SIG2: Quantum Crystallography

Reported Period: 2019-2020

Report Date: January 29, 2021

Reported by: Krzysztof Woźniak (chair), Simon Grabowsky (vice chair), Alessandro Genoni (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. 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>)

The link to the individual member lists via the webpage given above does not work, so we had to estimate the number of members using different sources. SIG2 Quantum Crystallography: 138 (according to our own mailing list), 50 (according to the webpage <https://ecanews.org/how-to-start-an-ig/>). We will investigate where this discrepancy comes from. Maybe some of them have not paid the ECA fees. However, we can see that all our conferences are attended by at least 100 people.

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 138 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: 138

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

About 200-250 (119 was the number of participants for the Quantum Crystallography online meeting QCrOM2020 in August 2020; 100 the number of participants for the first ICDM in July 2019; 120 the number of participants for the ECDM-7 in June 2016; 120 the number of participants for the Sagamore Conference in June 2015; 101 the number of participants for 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).

8. Past Activities other than Microsymposia at ECM

Title: QCrOM2020, Quantum Crystallography Online Meeting 2020, August 26th-29th, 2020, online meeting (<https://qcrom2020.cs-campus.fr/>)

Number of Participants: 119

Level of involvement of SIG in the activity:

- SIG2/ECA individual members were involved in the organizing committee, chaired by SIG2 member Jean-Michel Gillet (also current chair of the IUCr commission on Quantum Crystallography);
- SIG2/ECA individual members were part of the Scientific Committee and International Advisory Committee;
- 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: STOE, World Scientific.

Short Description: talks and poster presentations on traditional topics of quantum crystallography, such as experimental and theoretical charge/spin/momentum density studies in ambient and non-ambient conditions, investigations on non-covalent interactions and new technologies for charge density studies. Round table discussions on the state of the art and the future of the community were also organized (*How do scattering and spectroscopy methods combine in Quantum Crystallography?; Quantum Crystallography at the crossroad: the challenge of becoming popular; What is hot in Quantum Crystallography, what needs to be solved?*)

Title: Quantum Crystallography Virtual Regensburg Meeting(s), August 19th, 2020 – November 18th, 2020 – December 18th, 2020 online meeting(s)

Number of Participants: 16

Level of involvement of SIG in the activity:

- SIG2/ECA individual members were involved in the organizing committee, chaired by SIG2 member and vice-chair Simon Grabowsky;
- SIG2/ECA individual members were involved as participants and discussion leaders.

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

Sponsored by ECA? No

Other Sponsors/Organizers: No, although representatives of some companies were invited and participated in the discussions during the different meetings.

Short Description: The three meetings that took place so far mainly aimed at discussing the state of the art of the field of quantum crystallography, with a particular attention to finding/proposing possible funding opportunities to make our community more and more competitive and visible also towards other research fields. To this purpose, researchers that do not belong to our community were also invited and participated in the round table discussions. Other meetings are already scheduled in 2021.

Title: ICDM-1, International Charge Density Meeting, July 21st-26th, 2019, Göttingen, Germany

Number of Participants: 100

Level of involvement of SIG in the activity:

- SIG2/ECA individual members were involved in the organizing committee, chaired by SIG2 member Dietmar Stalke;
- SIG2/ECA individual members were part of the Scientific Committee and International Advisory Committee (<https://www.uni-goettingen.de/en/committees/590367.html>);
- SIG2/ECA individual members were involved as lecturers.

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

Sponsored by ECA? Yes. Nevertheless, there was a misunderstanding regarding the e-mail address to be used for the application. When this was sorted out, the ECA Commission in charge of this task (chaired by Prof. Gorbitz) reacted very quickly and competently.

Other Sponsors/Organizers: Deutsche Forschungsgemeinschaft (DFG), Excillum, Dectris, Incoatec, STOE, Roth.

Short Description: Presentation of the latest results from experimental and theoretical charge density studies. Covered topics: non-covalent interactions; data and model quality, charge, spin and momentum densities from computational methods; charge density in life science; materials profiles from charge and spin densities; non-ambient conditions; new technologies for experimental charge density.

Title: Tools for Chemical Bonding, July 15th-19th, 2019 ICDM-1 satellite meeting, Bremen, Germany

Number of Participants: 83

Level of involvement of SIG in the activity:

- SIG2/ECA individual members were involved in the organizing committee, headed by SIG2 vice-chair Simon Grabowsky;
- SIG2/ECA individual members were part of the Scientific Committee and International Advisory Committee;
- SIG2/ECA individual members were involved as lecturers.

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

Sponsored by ECA? Yes

Other Sponsors/Organizers: Deutsche Forschungsgemeinschaft (DFG), Physical Chemistry Chemical Physics (PCCP), Emmy Noether Program, Schüttinger

Short Description: Hands-on workshop to learn how to use different software packages in quantum chemistry and quantum crystallography for the analysis of chemical bonding. The software developers directly taught how to use the software. In addition, experts on chemical bonding gave six keynote lectures.

9. Future/Programmed Activities.

Title: CECAM Workshop “Second Discussion Meeting on Quantum Crystallography: Expectations and Reality”, September 9th-12th, 2020, Milan, Italy

Number of Participants: ~40 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 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. If the sanitary condition due to the current COVID-19 pandemic will not allow an on-site meeting, the workshop will be on-line.

Title: Quantum Crystallography (Virtual) Regensburg Meeting(s), 2021 online/onsite meeting(s)

Number of Participants: 15-20

Level of involvement of SIG in the activity:

- SIG2/ECA individual members will be involved in the organizing committee, chaired by SIG2 member and vice-chair Simon Grabowsky;
- SIG2/ECA individual members will be involved as participants and discussion leaders.

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

Sponsored by ECA? No

Other Sponsors/Organizers: No, although representatives of some companies will be always invited and participate in the discussions during the different meetings.

Short Description: The meetings will be a continuation of the online meetings that already took place in 2020 to discuss the state of the art of quantum crystallography, with a particular attention to finding/proposing possible funding opportunities to make our community more and more competitive and visible also towards other research fields. If the current COVID-19 pandemic will allow it, an on-site meeting will be organized in Regensburg (Germany) in August 2021.

Title: Sagamore Conference 2022, India, 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: ICDM-2, International Charge Density Meeting, 2022 or 2023, Denmark, 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 a SIG2 members Jacob Overgaard and Anders Ø. Madsen.
- 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.

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 at enhancing 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. Efforts to organize Quantum Crystallography international schools/workshops have been made. After those in Morocco (2009) and Spain (2011), new schools were held in France (Nancy, 2016) in connection with ECM-30, Italy (Erice, 2018) and in Germany (Bremen, 2019). An online conference was also efficiently organized in August 2020 to guarantee a continuous scientific exchange between the members of the community also in a year overturned by the COVID-19 pandemic. This nontrivial and time-consuming activity is a *must* for promoting and spreading out the Quantum Crystallography knowledge among new generations.

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, which will take place in Milan in September 2021 (COVID-19 permitting). Furthermore, the second edition of the school on Quantum Crystallography is already planned for 2026 in the framework of the well-known Erice International School of Crystallography.

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

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

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

Supplementary Materials.

No supplementary material is included with this report.