

**SIG2: Quantum Crystallography**

**Reported Period: 2018-2019**

**Report Date: July 4, 2019**

**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: To integrate concepts from many experimental & theoretical methodologies into a coherent understanding of matter on the subatomic level beyond geometry; and to promote the application of this understanding in the physics, chemistry, materials and biology communities.

**2. SIG web site:**

SIG2 <http://ecanews.org/mwp/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>)**

SIG2 Charge, Spin and Momentum Density: 109 (according to ECA only 50 – we do not understand this discrepancy, maybe some of them have not paid the ECA fees. However, we can see that all our conferences are attended by at least ca. 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 135 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:** about 135 when including the event-based lists mentioned above.

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

About 200-250 (120 was the number of participants at the ECDM-7 in June 2016; 120 the number of participants at the Sagamore Conference in June 2015; 101 the number of participants at the Gordon Conference in June 2013).

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

MS21 “Intermolecular interactions from structural, energetic and charge density perspective(s)”, chairs Enrique Espinosa (FR), Ulli Englert (DE)

MS22 “Molecular structure and chemical properties: chemistry meets charge density”, chairs: Vladimir Stilinovic (HR), Jacob Overgaard (DK)

KN Piero Macchi (CH), chair Wolfgang Scherer (DE)

**7. Prizes sponsored/coordinated**

No prizes sponsored or coordinated by SIG2 in the past, however since the Vienna ECM meeting our SIG will have a poster prize award named after Prof. Philip Coppens and sponsored by Rigaku Oxford Diffraction and awarded at each ECM meeting.

## 8. Past Activities other than Microsymposia at ECM

### **Title: ICDM-1, International Charge Density Meeting, July 21-26<sup>th</sup>, 2019, Göttingen, Germany**

Number of Participants: yet unknown

Level of involvement of SIG in the activity:

ECA individual members were involved in the organizing committee, chaired by SIG2 member D. Stalke,

ECA individual members were part of the Scientific Committee and International Advisory Committee (<https://www.uni-goettingen.de/en/committees/590367.html>)

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 15-19<sup>th</sup>, 2019 ICDM-1 satellite meeting, Bremen, Germany**

Number of Participants: 83

Level of involvement of SIG in the activity:

ECA individual members were involved in the organizing committee, headed by SIG2 chair Simon Grabowsky.

ECA individual members were part of the Scientific Committee and International Advisory Committee.

ECA individual members were involved as lecturers

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

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.

### **Title: Progress in instrumentation for X-ray diffraction and CryoEM (ECM-31 satellite meeting, August 2018), Oviedo, Spain**

Number of Participants: 45

Level of involvement of SIG in the activity:

SIG2 chair Krzysztof Woźniak was the proposer of that meeting and the chairman of the organizing committee. The other cochairman were: Prof. Dr. Ullrich Pietsch (Siegen, Germany) and Dr. Michele Cianci (Ancona, Italy).

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

Sponsored by ECA? no

Other Sponsors/Organizers: Yes: Bruker, Jeol, Rigaku Oxford Diffraction, Excillum

Short Description: This satellite meeting presented an overview of a wide range of new laboratory instrumentation available from different companies, as well as new developments at several large-scale facilities. Very well attended and with very interesting presentations and discussions.

**Title: Sagamore Conference 2018 (July), Halifax, Canada**

Number of Participants: ~ 80

Level of involvement of SIG in the activity: ECA individual members were involved in the organizing committee, chaired by C. F. Matta. Many SIG2/ECA individual members were involved as lecturers or discussion leaders and in the scientific committees.

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

Sponsored by ECA? no

Other Sponsors/Organizers: IUCr, Mount Saint Vincent University, McMaster University, NSERC and others.

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

**Title: School on Quantum Crystallography, June 1-10<sup>th</sup>, 2018, Erice, Italy**

Number of Participants: ~ 90

Level of involvement of SIG in the activity: Organized by Piero Macchi (former SIG2 co-chair) and Dylan Jayatilaka. Many SIG2/ECA individual members were involved as lecturers or tutors.

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

Sponsored by ECA? yes

Other Sponsors/Organizers: AIC, Dectris, IUCr, MDPI, CCDC, Panalytical, Bruker, Stoe, University of Bern, OPCW, Crystal Solutions, MSD

Short Description: Topics included the beginnings of the Quantum Crystallography in the measurement of the electron charge or spin density; the Hohenberg-Kohn theorem and the importance of the X-ray diffraction experiment; multipole-based models for the charge density; polarizable-density models; momentum based experiments and orbital density expansions; joint refinement of charge, spin, and momentum density.

**Title: CECAM Discussion Meeting on Quantum Crystallography: Current Developments and Future Perspectives (June 19-20<sup>th</sup> 2017), Nancy, France**

Number of Participants: 27

Level of involvement of SIG in the activity: the conference was organized by the current secretary of SIG2 (Alessandro Genoni) and the current vice chair of SIG2 (Simon Grabowsky); 22 of the 27 participants were SIG2 members.

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

Sponsored by ECA? no

Other Sponsors/Organizers: CECAM, Bruker, Turbomole, Wien2k, Université de Lorraine, GrandNancy, Societe Chimique de France, Institut Jean Barriol

Short Description: The aim of this discussion meeting was to start an initiative for the redefinition of Quantum Crystallography (QCr), and to discuss strategies for a broader dissemination of the techniques behind QCr and new applications. A very interesting review paper has been published jointly coauthored by participants of this meeting: A. Genoni, L. Bucinsky, N. Claiser, J. Contreras-Garcia, B. Dittrich, P. M. Dominiak, E. Espinosa, C. Gatti, P. Giannozzi, J-M Gillet, D. Jayatilaka, P. Macchi, A. Ø. Madsen, L. Massa, Ch. F. Matta, K. M. Merz, P. N. H. Nakashima, H. Ott, U. Ryde, K. Schwarz, M. Sierka, S. Grabowsky, "Quantum Crystallography: Current Developments and Future Perspectives", Chem. Eur. J. 2018, 24,10881 – 10905. See also <http://qcrstcecam.weebly.com/>

**Title: Center for Material Crystallography (CMC-2), Aarhus University, Denmark, 2015-2019.**

The materials crystallography center was extended for five more years.

**Number of Participants:** 7 international groups, involving about 70 individuals (permanent researchers, post-docs, PhD students, technicians)

Level of involvement of SIG in the activity:

ECA individual Members registered with the SIG include the head of this center (Bo Iversen, Aarhus University) and two (D. Stalke and C. Gatti) of the six international partners constituting the center along with Aarhus University ECA individual Members registered with the SIG involved as lecturers/teachers

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

Sponsored by ECA? No

Other Sponsors/Organizers: Danish National Research Foundation (DNRF) / Bo B. Iversen (Chair)

Short Description: planned hiring of PhD students and exchange of PhD students

within CMC consorted labs is running smoothly. See <http://cmc.chem.au.dk>

**Title: IUCr Quantum Crystallography Commission**

Number of Participants: 10 members

Sponsor/Organizers: IUCr

**Short description:** Membership was renovated at the 24<sup>th</sup> ICUR Meeting in Hyderabad (August 2017). Presently six out of the ten Quantum Crystallography Commission members belong to ECA SIG2. J.-M. Gillet is now the new commission chair and the current Chair of SIG2 (Prof. Wozniak) has been asked to represent the IUCr QCr Commission in the International Program Committee (IPC) of the next IUCr Congress in Prague (2020). As a consequence of the IPC. meeting in Prague in May 2019, the numbers of keynote lectures and microsymbosia associated with Quantum Crystallography have significantly increased. There will be 3 keynote lectures and 6 microsymbosia related to our field compared to 1 keynote and 4 microsymbosia at the previous IUCr congresses. We hope that within next years we will also increase our visibility (by having more lectures and microsymbosia) within ECA.

**9. Future/Programmed Activities.**

**Title: CECAM Workshop on Quantum Crystallography, 2020, Milan, Italy**

Number of Participants: ~40 participants

Level of involvement of SIG in the activity: Organized by Piero Macchi (former SIG2 co-chair).

Many SIG2/ECA individual members will be involved as lecturers.

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 workshop will be 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 2021, Goa, India**

Number of Participants: to be announced

Level of involvement of SIG in the activity: ECA individual members will be involved in the organizing committee, chaired by Parthapratim Munshi (Shiv Nadar University, India). Many SIG2/ECA individual members will be involved as lecturers or discussion leaders and in the scientific committees.

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, July 2022, site to be announced**

Number of Participants: to be announced

Level of involvement of SIG in the activity:

ECA individual members will be involved in the organizing committee, certainly chaired by a SIG2 member.

ECA individual members will be part of the Scientific Committee and International Advisory Committee

ECA individual members will be involved as lecturers.

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.** None

**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 GRC meeting and preparation of books on Modern Charge Density and on Electron Density and Chemical Bonding clearly testify these efforts. Efforts to organize Quantum Crystallography international schools/workshops have been made. After those in Marocco (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). This nontrivial and time-consuming activity is a *must* for promoting and spreading out the Quantum Crystallography knowledge among new generations.

Since this year (2019) we will also have a Philip Coppens poster prize awarded at each ECM meeting, which will increase our visibility at the ECM meetings. 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 Bremen, DE), e-mail: [simon.grabowsky@uni-bremen.de](mailto:simon.grabowsky@uni-bremen.de)

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.