

**SIG2: Charge, Spin and Momentum Density**

**Reported Period: 2017-2018**

**Report Date: 17 July 2018**

**Reported by: Simon Grabowsky (chair), Krzysztof Woźniak (vice chair), Nils Trapp (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

**4. Existence of a SIG mailing list? Yes**

In 2016 we updated our e-mail directory and promoted our google group again, which consequently gained a lot of visibility (now 137 members). Most (active) participants from past events (e.g. ECDM-6, Sagamore 2012, GRC-2013 and more) have been merged into the google list.

**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\_CSMD

**Number of members in the SIG mailing list:** about 1000 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**

MS23 "Charge and Spin Density of Materials at Extreme Conditions", chairs Nicola Casati (CH) and Philippe Guionneau (FR)

MS22 "Beyond Multipolar Refinement", chairs Simon Grabowsky (DE) and Alessandro Genoni (FR)

KN Birger Dittrich (DE), chair Piero Macchi (CH)

**7. Prizes sponsored/coordinated**

No prizes sponsored or coordinated by SIG2

**8. Past Activities other than Microsymposia at ECM**

**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 for charge, spin and momentum density directly 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 chairman of SIG2 (Simon Grabowsky) together with SIG2 member Alessandro Genoni. 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.

See <http://qcrystcecam.weebly.com/>

**Title: International school on charge and spin densities (ECM-30 satellite meeting, August 2016), Nancy, France**

Number of Participants: 50

Level of involvement of SIG in the activity:

ECA individual members were involved in the scientific advisory board.

ECA individual Members registered with the SIG involved as lecturers/teachers.

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

Sponsored by ECA? no

Other Sponsors/Organizers: IUCr, CNRS, Bruker, CRM2, CristalLaser, Université de Lorraine, Dectris, IJB, GrandNancy

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 with existing refinement software.

See <http://crm2.univ-lorraine.fr/lab/en/education/congres/ecm30-congress-satellite-school/>

**Title: ECDM-VII, European Charge Density Meeting 2016 (June), Warsaw, Poland**

Number of Participants: 120

Level of involvement of SIG in the activity:

ECA individual members were involved in the organizing committee, chaired by K. Wozniak

ECA individual members were part of the Scientific Committee and International Advisory Committee (see <http://ecdm7.chem.uw.edu.pl/committees>)

ECA individual members were certainly involved as lecturers

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

Sponsored by ECA? yes

Other Sponsors/Organizers: IUCr, PAN, Rigaku Oxford Diffraction, Bruker, Oxford Cryosystems, Stoe, AXO Dresden GmbH, CeNT, University of Warsaw, Dectris

Short Description: (25 words max.): Presentation of latest results from experimental and theoretical charge density studies, accentuating methodological and statistical problems, resulting from recent advances in experimental hardware and software development.

**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 Charge Spin and Momentum Density (CSMD) Commission**

Number of Participants: 10 members

Sponsor/Organizers: IUCr

**Short description:** Membership was renovated at XXIII/IUCR/2014. Presently six out of the ten CSMD Commission members belong to ECA SIG2. The new commission was appointed at the J.-M. Gillet is now commission chair.

**9. Future/Programmed Activities.**

**Title: Tools For Chemical Bonding, July 15-19<sup>th</sup>, 2019 ICDM-VIII satellite meeting, Bremen, Germany**

Number of Participants: max. 80

Level of involvement of SIG in the activity:

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

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: (25 words max.): to be announced

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

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 SIG2 member D. Stalke.

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

ECA individual members will certainly 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: (25 words max.): to be announced. The name of the conference series was changed from “European” Charge Density Meeting to “International” Charge Density Meeting. This goes back to a discussion within the SIG2 members, started at the last ECM meeting in Basel.

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

Number of Participants: to be announced

Level of involvement of SIG in the activity:

SIG2 vice chair Krzysztof Woźniak is one of the chairmen of the organizing committee.

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

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

Sponsored by ECA? no

Other Sponsors/Organizers: to be announced

Short Description: (25 words max.): This satellite meeting will present an overview of a wide range of new laboratory instrumentation available from different companies, as well as new developments at several large scale facilities.

**10. Other matters.** None

**11. Brief annual activity report**

SIG2 keeps promoting activities aimed at enhancing the interest towards CSMD studies among ever wider scientific communities. The list of topics at the latest GRC meeting and preparation of books on Modern CD and on ED and Chemical Bonding clearly testify these efforts. Efforts to organize CSMD international schools/workshops have been made. After those in Marocco (2009) and Spain (2011), new schools were held in France (2016) in connection with ECM-30 and Erice (2018). This nontrivial and time-consuming activity is a *must* for promoting and spreading out the CSMD knowledge among new generations.

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

Chair: Simon Grabowsky (University of Bremen, DE), e-mail: [simon.grabowsky@uni-bremen.de](mailto:simon.grabowsky@uni-bremen.de)

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

Secretary/Webmaster: Nils Trapp (ETH Zürich, CH), e-mail: [nils.trapp@org.chem.ethz.ch](mailto:nils.trapp@org.chem.ethz.ch)

**Supplementary Materials.**

No supplementary material is included with this report.