

SIG2 Charge Spin and Momentum Densities

Reported Period: 2015-2016

Report Date: 21 July 2016

Reported by: Birger Dittrich (chair), Piero Macchi (co-chair), Nils Trapp (secretary)

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1. Introduction: This SIG promotes activities aimed at enhancing and diffusing the interest towards information which chemists/physicists/biologists/mineralogists and materials science researchers derive from charge, spin and momentum density (CSMD) studies. We are very active in organizing international CSMD congresses and act as organizers of and teachers in schools aimed at disseminating CSMD competences

2. SIG web site:

SIG2 <http://sig2.ecanews.org/>

3. Number of ECA individual members registered with the SIG according to (<http://www.xray.cz/eca/im-payment.htm>)

SIG2 Charge, Spin & Momentum Density: 99

4. Existence of a SIG mailing list? Yes

A google group was created (62 members). Moreover larger mailing lists are available after ECDM-6 meeting, Sagamore 2012 meeting, GRC-2013 meeting, Charge Density School 2011 (satellite of the 2011 IUCr Congress) which are kept continuously updated.

Address of the mailing list: 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 in the 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 ECM-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

MS 28: Charge density studies

Chairs: Anders Madsen (DK), Simon Coles (UK)

7. Prizes sponsored/coordinated

No prizes sponsored or coordinated by SIG2

8. Past Activities other than Microsymposia at ECM

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: Sagamore Conference 2015 (June), Sardinia, Italy

Number of Participants: ~ 120

Level of involvement of SIG in the activity: ECA individual members were involved in the organizing committee, chaired by C. Gatti (ECA SIG member, former SIG2 secretary). ECA individual members were involved as lecturers or discussion leaders and in the scientific committee.

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

Sponsored by ECA? yes

Other Sponsors/Organizers: IUCr, AIC, CNR-ISTM, Università degli studi di Milano, Dectris, Bruker, Stoe, Excillum, imXPAD, Rigaku

Short Description: The traditional meeting covered all the subjects related to this SIG. The IUCr commission for charge, spin and momentum density directly planned the scientific program.

Title: ECM& Center for Material Crystallography (CMC), Aarhus University, Aarhus, Denmark, 2010-2014

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

Level of involvement of SIG in the activity:

ECA individual Members registered with the SIG involved with CMC include the head of the 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: CMC first annual review meeting took place in Aarhus (DK), 2 Nov 2010. The composition of the Center and planned activity are illustrated in the CMC/website

<http://cmc.chem.au.dk/>. Involvement of SIG#2 members and European researchers in this world international center is large and increasing. Head of CMC is the former SIG#2 chair Bo Iversen, latest meeting took place in Aarhus, June 2015.

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 eight out of the ten CSMD Commission members belong to ECA SIG#2. The new commission was appointed at the IUCr meeting in Montreal; P. Macchi is now Commission chair.

9. Future/Programmed Activities.

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 are 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 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.

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

Title: ECM-30, ECA Meeting 2016 (August), Basel, Switzerland

Number of Participants: ~870, ~50 from SIG

Level of involvement of SIG in the activity:

ECA individual members are involved in the organizing committee.

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

Several ECA individual members registered with the SIG were involved in the planning of 3 Micro Symposia related to CSMD area:

Beyond multipolar refinement

(Chairs: Genoni & Grabowsky)

Charge and spin density of materials at extreme conditions

(Chairs: Casati & Guionneau)

Inorganic and metal-organic magnetic structures

(Chairs: Eickerling & Schaniel)

Additionally, Dr. Birger Dittrich will give a keynote lecture.

ECA individual members will be involved as lecturers or session chairs.

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

Sponsored by ECA? yes

Other Sponsors/Organizers: Sponsorship from IUCr and from X-ray diffraction firms, for full list see <http://ecm30.ecanews.org/2016/industry-information/list-of-sponsors.html>.

Title: School on Quantum Crystallography, 2018, Erice, Italy

Organized by Piero Macchi (SIG2 co-chair) and Dylan Jayatilaka. The school is still in early planning stage, but involvement of a large part of the SIG2 community is expected.

Title: Center for Material Crystallography (CMC), Aarhus University, Aarhus DK, 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-doc, PhD students, technicians)

Level of involvement of SIG in the activity:

ECA individual Members registered with the SIG involved 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: ECDM-VIII, European Charge Density Meeting (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 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

Title: Charge Density Workshop (2019), ECDM-VIII satellite meeting, Bremen, 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 S. Grabowsky.

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

10. Other matters. None

11. Brief annual activity report

SIG#2 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), a new school will be held in France in connection with the forthcoming ECM-30.

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: Birger Dittrich (Heinrich-Heine-Universität Düsseldorf, D), e-mail: dittrich@hhu.de

Co-chair: Piero Macchi (Bern University, CH), e-mail: piero.macchi@dcb.unibe.ch

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

Supplementary Materials.

(List of all supplementary materials, if any, related to the SIG report)

- Addendum 1 to n (to be sent in separate files)

No supplementary material is included with this report.