

SIG2 Charge Spin and Momentum Densities

Reported Period: 2014-2015

Report Date: 17 July 2015

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: 88

4. Existence of a SIG mailing list? Yes

A google group was created (56 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 (122 was the number of participants at the ECM-6 in September 2012; 101 the number of participants at the Gordon Conference in June 2013; 120 the number of participants at the Sagamore Conference in June 2015).

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

MS 29: Getting more from your electron density

Chairs: Claude Lecomte (FR), Annamaria Mazzone (IT)

MS 13: Charge and spin density measurements of materials

Chairs: Beatrice Gillon (FR), Krzysztof Wozniak (PL)

MS30: Beyond harmonic treatment (Ensemble)

Chairs: Birger Dittrich (DE), Simon Grabowsky (AU)

7. Prizes sponsored/coordinated

No prizes sponsored or coordinated by SIG2

8. Past Activities other than Microsymposia at ECM

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

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.

Title: XXIII IUCr Congress, Montreal, August 2014

Number of Participants: >2000

Level of involvement of SIG in the activity:

Several ECA Individual members registered with the SIG were involved in the planning of the Micro Symposia related to CSMD area.

There were two plenary lecture KN29 by M. Spackman on Rationalising molecular crystal structures using Hirshfeld surfaces and KN03 by W. Scherer on Charge Density and Chemical Bonding in Inorganic Materials, and two sessions dedicated to charge density research: MS19 - Computational Methods for Charge Density Studies organized by C. Lecomte and P. Macchi with talks from B. Guillot, T. Sakakura, C. Gatti, R. Herbst-Irmer, N. Wahlberg, A. Genoni and N. Dadda and a session MS65 on Charge Density and Drug Design chaired by C. Matta and B. Dittrich, with talks by Christian Jelsch, F. Cortes-Guzman, M. Pitak, J. Graf, M. Malinska and L. Massa. Contributions to CD research were of course not limited to these sessions, as illustrated by the microsposium on Maximum Entropy in Crystallography chaired by M. Takata and S. Van Smaalen with talks by V. Juve, E. Nishibori, K. Sugimoto, C. Huebschle, D. Sisak Jung and S. Christensen. All these and other MS were accompanied by numerous interesting poster presentations.

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

Sponsored by ECA? no

Other Sponsors/Organizers: IUCr

Short Description: (25 words max.): see <http://www.iucr2014.org/>

Title: Sagamore Conference 2015 (August), 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 covering all the subjects related to this SIG. The IUCr commission for charge, spin and momentum density directly planned the scientific program.

9. Future/Programmed Activities.

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

Number of Participants: about 150

Level of involvement of SIG in the activity:

ECA Individual members are involved in the organizing committee, chaired by K. Wozniak

ECA Individual members will be part of the Scientific Committee and International Advisory Committee (composition being decided soon but not yet available)

ECA Individual members will certainly be involved as lecturers

Endorsed (SIG logo on the web page/leaflets): information not available at the moment

Sponsored by ECA? ECA sponsorship will be requested

Other Sponsors/Organizers: Sponsorship from IUCr and from X-ray diffraction firms will be requested.

Short Description: (25 words max.): it is planned to follow the successful format of the previous ECDM-6 Conference hoping to attract many researchers from Europe, U.S.A, Japan, India, etc.

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): information not available at the moment

Sponsored by ECA? ECA sponsorship will be requested

Other Sponsors/Organizers: Sponsorship from IUCr and from X-ray diffraction firms will be requested.

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: ~700, ~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 are involved in the planning of Micro Symposia related to CSMD area.

ECA Individual members will certainly be involved as lecturers.

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 will be requested.

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>

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. Organization of next ECDM-7 in Poland begun to continue the very successful ECDM series. Efforts to organize CSMD international schools/workshops have been made. After those in Maroc (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: Piero Macchi (Bern University, CH), e-mail: piero.macchi@dcb.unibe.ch

Co-chair: Birger Dittrich (Institut für Anorganische Chemie, Göttingen University, Göttingen, Germany) e-mail: bdittri@gwdg.de

Secretary: Nils Trapp (ETH, Zurich, 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.