

SIG2 Charge Spin and Momentum Densities

Reported Period: 2013-2014

Report Date: 20 June 2013

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

=====

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 72 (a considerable increase with respect to the past, ca. 40%)

4. Existence of a SIG mailing list? Yes

A google group was created (48 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: -

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 (170 was the number of participants to last ECDM-V meeting in Gravedona, June 2008; 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).

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 : Gordon Conference on electron Distribution and Chemical Bonding

Number of Participants: 101

Level of involvement of SIG in the activity:

SIG2 chair was chair of the meeting; the SIG2 co-chair was lecturer; many ECA individual members involved as lecturers or session chairs.

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

Sponsored by ECA? yes

Other Sponsors/Organizers: IUCr, Rigaku, Bruker, Agilent, Dectris, AIC, SGK,

Short Description: it was the most participated GRC meeting in this series but unfortunately the last. Very high level of presentations and discussions. For a full list of sessions, talk titles, speakers and discussion leaders, see <http://www.grc.org/programs.aspx?year=2013&program=elecldist>.

Title : ECM& Center for Material Crystallography (CMC), Aarhus University, Aarhus DK, 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 on 24.01.2014.

Title : IUCr Charge Spin and Momentum Density (CSMD) Commission

Number of Participants: 10 members

Sponsor/Organizers: IUCr

Short description: Membership of the CSMD commission has been renovated at the Madrid IUCR 2011 meeting. Presently six out of the ten CSMD Commission members belong to ECA SIG#2.

The new commission will be nominated at IUCr meeting in Montreal; P. Macchi is designated candidate for the Commission chair.

9. Future/Programmed Activities.

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 are involved in the planning of the MicroSymposia related to CSMD area.

Several ECA Individual members registered with the SIG will be involved as MS chair or co-chairs or will be involved as MS's lecturers.

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 : ECDM-VII , European Charge Density Meeting, (date not yet established), 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 : Sagamore Conference 2015 (August), Sardinia, Italy

Number of Participants: > 100

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

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 traditional meeting covering all the subjects related to this SIG. The IUCr commission for charge, spin and momentum density will directly plan the scientific program.

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 : IUCr Charge Spin and Momentum Density (CSMD) Commission

Number of Participants: 10 members

Sponsor/Organizers : IUCr

Short description : Membership will be renovated at XXIII/IUCR/2014. We work to maintain such European *flavour* in the commission

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 that in Maroc (2009) and Spain (2011), it is envisaged the need of a new school, perhaps in connection with one of the forthcoming meetings. This not easy 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: Simone Cenedese (CNR-ISTM, Milano, Italy), replaced by 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.