

SIG2 Charge Spin and Momentum Densities
Reported Period: : 1 June 2009 - 20 May 2010

Report Date: 20 May 2010

Reported by: Bo Iversen(chair), Ulrich Pietsch(co-chair), Birger Dittrich (co-chair) and Carlo Gatti (secretary)

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1. Introduction. (50 words max.) We keep promoting activities aimed at enhancing and diffusing the interest towards the information which chemists/physicists/biologists/mineralogists and materials-science researchers derive from (combined) charge, spin and momentum density (CSMD) studies. We are in contact with IUCr to organize a CSMD school and possibly ECDM-VI meeting as satellites of 2011 IUCr Congress

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 35

NOTE!!!!!! : we checked this list and found that it does not include many members that should be surely included among the researchers in the CSMD area. In this report all figures given under the statement “Individual Members registered with the SIG” refers to the “ideal” list including these extra, presently non-official members. It will be our task in the next years to convince as many as possible researchers in the CSMD area to become ECA individual members and express their explicit interest for the SIG2 activities.

4. Existence of a SIG mailing list Not an official one yet (also planned within the SIG web site), but we have the ones used for ECDM-V meeting, Sagamore 2009 meeting and GRC-2010 meeting, which are kept updated.

Address of the mailing list:

Number of members in the SIG mailing list :

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

About 200 (>170 was the number of participants to last ECDM-V meeting in Gravedona, June 2008; at least other 30 researchers can be added to this number, taking into account that not all researchers attended this event and that the spin and momentum densities communities were only poorly represented at such meeting)

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

1) *Accuracy in experimental charge density determination* (chaired by AA Pinkerton and S van Smaalen)

2) *Very high-resolution protein structures* (chaired by C Jelsch and B Dittrich).

7. Prizes sponsored/coordinated

No prizes sponsored or coordinated by SIG2

8. Past Activities other than Microsymposia at ECM

Title : Sagamore XVI meeting (Santa Fe, New Mexico, USA, 2-7 August 2009)

Number of Participants: > 105

Level of involvement of SIG in the activity:

9 ECA Individual Members registered with the SIG involved in the program and Advisory committees

17 ECA Individual Members registered with the SIG involved as lecturers (11) and session chairs (6)

Sponsored by ECA? NO

Other Sponsors/Organizers: IUCr, NSF, Office of Basic Energy Sciences of the US Dept of Energy; Conference chair: Prof. Philips Coppens

Short Description: (50 words max.): Sagamore meeting is by tradition one of the most important activities of the CSMD community. 105 scientific participants from 16 countries. Opening keynote lecture: J. Schneider, DESY on the *Science at XUV and Hard X-ray Free Electron Lasers*. Eight oral sessions, three poster sessions and one session of poster talks

Title : International Workshop on the refinement and analysis of the electron density obtained from high resolution X-ray diffraction, Marrakech, Maroc, 28-30 October 2009

Number of Participants: about 35

Level of involvement of SIG in the activity:

6 ECA Individual Members registered with the SIG involved in the organizing or scientific committee

11 ECA Individual Members registered with the SIG involved as lecturers/teachers/tutors

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

Sponsored by ECA? Yes

Other Sponsors/Organizers: IUCr, University Cadi-Ayyad (UCA), Nonius Bruker, GASUP (Maroc) /Organizers: N. Bouhaida , N.E. Ghermani

Short Description: (50 words max.) Organized by N.Bouhaida and NE.Ghermani along with an international Scientific Committee, C.Lecomte, C.Gatti and C.Jelsch the workshop had the main aim to disseminate knowledge on ED studies from high resolution X-ray diffraction data within the African/Magrebin communities. A workshop booklet >100 pages-long with extended written lectures from teachers was distributed

Title : Charge Density School, Zaragoza, Spain, 31 May-6 June 2009

Note : we have no precise information about the various numbers related to this school

Number of Participants: about 30

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing or scientific committee

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: University of Zaragoza / Prof. Fernando Lahoz

Short Description: A five days school, within an international master on crystallography, on charge density research basics and applications. The school was held by international teachers (Europe/USA).

Title : DFG SPP-1178 (2005-2011), Deutsche Forschungsgemeinschaft Special Priority Program "Experimental charge densities for better understanding of chemical interactions"

Number of Participants: about 30 groups, involving about 150 individuals (permanent researchers, post-doc, PhD students, technicians)

Level of involvement of SIG in the activity:

About 10-15 ECA Individual Members registered with the SIG involved in the research within the various groups or as referees of such program

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

Sponsored by ECA? No

Other Sponsors/Organizers: DFG/ Prof. Dietmar Stalke, Prof. Wolfgang Scherer

Short Description : DFG SPP-1178 program enters its sixth and last year of activity. It was aimed at diffusing and fostering cutting-edge CD research among chemists and physicists, an effort which it surely achieved. SIG#2 members are taking active part in SPP-1178 either directly or through its supervision as external international referees

Title : Center for Material Crystallography (CMC), Aarhus University, Aarhus DK, 2010-2014

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 : CMC kick-off meeting took place in Aarhus (DK) in date 14-15 April 2010.

The composition of the Center and its 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 very large. Head of CMC is the present SIG#2 chair.

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 Osaka IUCR 2008 meeting. Presently six out of the ten CSMD Commission members belong to ECA SIG#2 and one of them (C. Gatti) is also the present Commission chair.

9. Future/Programmed Activities.

Title : Gordon Research Conference on Electron Distribution and Chemical Bonding, July 11-16, 2010, Mount Holyoke College, South Hadley, MA, USA

Number of Participants: about 100?

Level of involvement of SIG in the activity:

1 ECA Individual members registered with the SIG involved in the organizing committee (P. Macchi co-chair of this 2010 GRC)

7 ECA Individual members registered with the SIG involved as lecturers; 4 ECA Individual members registered with the SIG involved as discussion leaders

Endorsed (SIG logo on the web page/leaflets) : we are not informed about that thus far

Sponsored by ECA? We are not informed about that thus far

Other Sponsors/Organizers: GRC organization, IUCr, AIC (Associazione Italiana di Cristallografia)

Short Description: (25 words max.) : see

<http://www.grc.org/programs.aspx?year=2010&program=elecdist> for a full list of sessions, talk titles, speakers and discussion leaders. Involvement of SIG2 members is impressive.

Title : IXS-2010 7th International Conference on Inelastic X-ray Scattering, 11-14 October 2010, World Trade Center, Grenoble

Number of Participants: about 100?

Level of involvement of SIG in the activity:

About 3 ECA Individual members registered with the SIG involved in the organizing/scientific committees

Several ECA Individual members registered with the SIG involved as lecturers

Endorsed (SIG logo on the web page/leaflets) : we are not informed about that thus far

Sponsored by ECA? We are not informed about that thus far

Other Sponsors/Organizers: ESRF, Politecnico di Milano, IUCr?

Short Description: (25 words max.) : see <http://www.esrf.eu/events/conferences/ixs2010> for a full list of sessions, talk titles and speakers.

Title : DFG SPP-1178 (2005-2011), Deutsche Forschungsgemeinschaft Special Priority Program "Experimental charge densities for better understanding of chemical interactions"

Number of Participants: about 30 groups, involving about 150 individuals (permanent researchers, post-doc, PhD students, technicians)

Level of involvement of SIG in the activity:

About 10-15 ECA Individual Members registered with the SIG involved in the research within the various groups or as referees of such program

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

Sponsored by ECA? No

Other Sponsors/Organizers: DFG/ Prof. Dietmar Stalke, Prof. Wolfgang Scherer

Short Description: (25 words max.): This program will end within a year. New funding/organizing strategies are currently being explored to continue and expand the program at a European scale.

Title : Center for Material Crystallography (CMC), Aarhus University, Aarhus DK, 2010-2014

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: (25 words max.): the planned exchange of PhD students within CMC consorted labs did already start. CMC research programs <http://cmc.chem.au.dk> did also start

Title : Preparing a new book devoted to "Modern Charge Density Analysis" (Springer)

Level of involvement of SIG in the activity:

2 ECA Individual Members registered with the SIG involved as Editors (C. Gatti and P. Macchi)

>15 ECA Individual Members registered with the SIG involved as authors/co-authors of book chapters.

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

Sponsored by ECA? No

Other Sponsors/Organizers: Springer / C. Gatti and P. Macchi (Eds)

Short Description: (25 words max.): A contributed book on modern aspects of charge density analysis is in preparation (publication date: end of 2010). Involvement of SIG#2 members is impressive.

Title : Preparing a series of two books for the *Structure and Bonding* series (Springer) on "Electron Density and Chemical Bonding I (experiment) and II (theory)"

Level of involvement of SIG in the activity:

2 ECA Individual Members registered with the SIG involved as Editors (D. Stalke and U. Flierler)
>15 ECA Individual Members registered with the SIG involved as authors/co-authors of book chapters.

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

Sponsored by ECA? No

Other Sponsors/Organizers: Springer / D. Stalke and U. Flierler (Eds)

Short Description: (25 words max.): A contributed couple of books on modern aspects of the relationships between ED and chemical bonding. Publication date: 2010/2011. Involvement of SIG#2 members is impressive

10. Other matters. (50 words max.)

Next ECDM meeting will probably take place in 2011 in Spain as a satellite of the 2011 Madrid IUCR-XXII Congress. First part of the satellite will be devoted to a CSMD school, while the second will constitute ECDM-VI. We are still waiting details from IUCR-XXII organizers about these planned activities.

11. Brief annual activity report (100 words max.)

SIG#2 keeps promoting activities aimed at enhancing the interest towards (combined) CSMD studies among ever wider scientific communities (the list of topics handled at last Sagamore meeting and next GRC testifies this). Sagamore meeting has been very successful and the contribution from SIG2 members impressive, despite it was held in US. With respect to the past, we have started an important effort for organizing CSMD international schools/workshops. This not easy and time consuming activity is a necessity for promoting and spreading out the CSMD knowledge among new generations and within new geographic areas.

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

Chair: Bo Brummerstedt Iversen (Aarhus University, DK), e-mail:bo@chem.au.dk

Co-chair: Ulrich Pietsch (Siegen University, Siegen, Germany) e-mail : pietsch@physik.uni-siegen.de

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

Secretary: Carlo Gatti (CNR-ISTM, Milano, Italy), e-mail: c.gatti@istm.cnr.it

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.