

**SIG2 Charge Spin and Momentum Densities**

**Reported Period: 21 may 2010-1 June 2011**

**Report Date: 31 May 2011**

**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 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>)**

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**NOTE (Report 2010):** 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.

**Addendum to the note (Report 2011):** we notice that we were partly successful in what was said above, since the registered members, though being far less than the "real" ones, have increased in one year from 35 to 47, that is by about 35%

**4. Existence of a SIG mailing list  Yes /  No**

Not an official one yet (though planned within the SIG web site), but we have the ones used for ECDM-V meeting, Sagamore 2009 meeting, GRC-2010 meeting, Charge Density School 2011 (satellite of the 2011 IUCr Congress) which are kept continuously updated.

**Address of the mailing list:**

**Number of members in the SIG mailing list :** about 200 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) At least other 30-80 researchers can be added to this number, taking into account that not all researchers attended that event and that researchers in spin and momentum densities, usually present at Sagamore conference and IXS (Inelastic x-ray scattering) meetings were only poorly represented at ECDM-V. The number of attendees to Sagamore or IXS meetings is about 100 per meeting.

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

**MS 20: Charge, spin and momentum densities for the prediction of physical properties**

Chairs: Sebastian Pillet (Nancy/FR), Jozef Kozisek (Bratislava/SK)

## **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 (July 11-16, 2010, Mount Holyoke College, South Hadley, MA, USA)**

Number of Participants: 92

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)

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) : no

Sponsored by ECA? no

Other Sponsors/Organizers: GRC organization, IUCr, University of Western Australia, Rigaku, Bruker, Oxford Diffraction, Oxford Cryosystems , XD package

P. Macchi (SIG-2), co-chair.

Short Description: (50 words max.) : for a full list of sessions, talk titles, speakers and discussion leaders, see <http://www.grc.org/programs.aspx?year=2010&program=elecdist> . Involvement of SIG2 members was impressive. All sessions were well organized, with about 20 speakers or discussion leaders who have not spoken before at this GRC, and the discussions were all very intense.

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

Number of Participants: 162

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) : no

Sponsored by ECA?: no

Other Sponsors/Organizers: ESRF, Politecnico di Milano, IUCr / M. Krisch (ESRF) and C. Dallera (Politecnico di Milano)

Short Description: (50 words max.) : see <http://www.esrf.eu/events/conferences/ixs2010> for the list of sessions, talk titles and speakers. This triennial meeting attracted 162 participants (33 students) from 61 different institutions from Europe , America, and Asia. The conference included overview and plenary talks, conference sessions organized in ten themes, two poster sessions and a visit to ESRF

### **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 : this was the last year of activity of the project, aimed at fostering cutting-edge CD research among chemists/physicists. Such effort was achieved and new funding/organizing strategies are currently being explored to continue the program at European scale. SIG#2 members were involved in SPP-1178 as researchers or as external international referees

**Title : 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 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.

**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: (50 words max.): preparation of a contributed book on modern aspects of CD analysis is almost completed (publication date, 2011, hopefully in August before IUCr-2011). It is a 21 chapters didactic book covering the state-of-the-art methods and applications of electron, spin and momentum densities research. Involvement of SIG#2 members has been 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: (50 words max.): A contributed couple of books on modern aspects of the relationships between ED and chemical bonding has been almost completed. Already 7 contributed chapters are available on line : <http://springerlink.metapress.com/content/110355/>  
The final publication date of the series is planned for 2011. Involvement of SIG#2 members is impressive

## **9. Future/Programmed Activities.**

### **Title : XXII IUCr Congress, Madrid, 22-30 August 2011**

Number of Participants: >2000

Level of involvement of SIG in the activity:

Several ECA Individual members registered with the SIG have been involved in the planning of the 7 MicroSymposia related to CSMD area. One SIG-2 member (K. Hamalainen, Finland) has served in the International Program Committee.

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

1 ECA Individual members registered with the SIG, namely the present SIG-2 chair, Prof. B.B. Iversen will give a keynote lecture on Materials Crystallography and the chair for that talk will be C. Gatti (SIG-2 Secretary).

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.iucr2011madrid.es/index.php/home>

### **Title : 2011 *International School on Charge Density*, 30 August- 4 September, JACA (Spain), satellite of the Madrid XXII IUCr Congress.**

Number of Participants: limited to a maximum of 50 attendants

Level of involvement of SIG in the activity:

3 ECA Individual members registered with the SIG involved in the organizing committee (C. Lecomte, F. J. Lahoz, Pilar García Orduña )

10 ECA Individual members registered with the SIG involved as lecturers/tutors ;

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

Sponsored by ECA? No, as far as we know

Other Sponsors/Organizers: IUCr, CSIC, Université of Nancy, Agilent technologies, GESC, Oxford Cryosystems, Bruker, etc.

Short Description: (25 words max.) : see [http://iucr\\_csmd.istm.cnr.it/schools.html](http://iucr_csmd.istm.cnr.it/schools.html) for a full presentation of this 5-days school including lectures and practical tutorials with charge density software illustrated by the software authors themselves.

### **Title : ECDM-VI , European Charge Density Meeting, 15-20 September 2012, High Tatra , Slovakia**

Number of Participants: about 150

Level of involvement of SIG in the activity:

ECA Individual members are involved in the organizing committee, chaired by J. Kozisek

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-5 Conference hoping to attract many researchers from Europe, U.S.A, Japan, India, etc.

**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.): planned hiring of PhD students and exchange of PhD students within CMC consorted labs is running smoothly. The annual 2010 report has been published

<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 XXII/IUCR/2011; six/tenth of members belong to SIG#2, including C.Gatti as chair. We work to maintain such European *flavour* in the commission

**10. Other matters.** ( 50 words max.)

None

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

SIG#2 keeps promoting activities aimed at enhancing the interest towards CSMD studies among ever wider scientific communities. The list of topics at last GRC meeting and preparation of books on Modern CD and on ED and Chemical Bonding clearly testify these efforts. Organization of next ECDM-6 in Slovakia begun to continue the very successful ECDM-series. Efforts to organize CSMD international schools/workshops have been made. After that in Maroc (2009), we have organized a 5-days CD school in Spain (2011). 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: 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.