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**SIG:2 (Charge Spin and Momentum Densities)**

**Reported Period: 1 June 2008 - 30 May 2009**

**Report Date: 29 May 2009**

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

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## **1. Introduction.**

We keep promoting activities aimed at enhancing and diffusing the interest towards the information that chemists/physicists/biologists/mineralogists and materials-science researchers may derive from (combined) charge, spin and momentum density studies. Particularly important in this respect appears the interest raised by ECDM-V meeting and the schools/workshops currently being organized on this topic.

## **2. Past Activities.**

**Title: ECDM-V** (European Charge Density Meeting, 6-11 June 2008, Gravedona, Lake of Como, Italy)

**Number of Participants:** >170

**Sponsors:** ECA, IUCr, AIC (Associazione Italiana di Cristallografia), Fondazione Cariplo, CNR-ISTM, INSTM, University of Milano, several industries

**Organizers:** Carlo Gatti, Piero Macchi, Riccardo Destro (Milano) and Deutsche Forschungsgemeinschaft (DFG)

**Short Description:** ECDM conference was joined with the annual meeting of SPP-1178-DFG program on "New Information from Modern Charge Density Studies". The resulting meeting, composed of 3 DFG sessions, 8 ECDM microsymbosia and 11 common plenary lectures has enjoyed an extremely high participation (>170 attendants), about 70% more than previous ECDM meetings.

**Title : 2008 IUCr XXI General Congress, Osaka (Japan, 23-31 August)**

**Number of Participants:** >2000 (about 100-120 from ECA SIG#2 ?)

**Sponsors/Organizers:** IUCr

**Short Description :** SIG#2 members have heavily contributed to the success of the congress, covering 50% of the chair/co-chair roles and 56% of the delivered talks in the 5 MS organized by the IUCr Charge Spin and Momentum Density Commission. On top of this, the plenary lecture given by C. Lecomte (France).

**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

**Sponsors/Organizers:** DFG

**Short Description :** DFG SPP-1178 program enters its fifth year and it is aimed at diffusing and fostering cutting-edge CD research among chemists and physicists. SIG#2 members are taking active part in SPP-1178 either directly or through its supervision as external international referees. The 2008 DFG-1178 Annual Meeting was part of ECDM-V meeting

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

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**Number of Participants:** 10 members

Sponsor/Organizers : IUCr

**Short description :** Membership of the CSMD commission has been renovated at the Osaka 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.

### **3. Future/Programmed Activities.**

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

**Sponsors/Organizers:** IUCr, Los Alamos Neutron Scattering Center/Philip Coppens, Thomas Proffen

**Short Description:** 7 Sessions on cutting-edge topics in CSMD activities. SIG#2 members are largely involved as part of the Scientific Committee, as Session chairs and as speakers.

**Title :** ECM-25 (Instanbul, Turkey, 9-14 August 2009)

**Sponsors/Organizers:** ECA

**Short Description:** SIG#2 sent to the ECM-25 organizers timely proposals (title/chairs) for MS and KN lectures. Common MS with SIG#1, SIG#7 and SIG#6/12/13 have been proposed.

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

**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 is held by international teachers (Europe/USA).

**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

**Sponsors/Organizers:** University Cadi-Ayyad (UCA), Faculté des Sciences Marrakech (FSSM), Association Marocaine de Crystallographie (AMC), ECA, IUCr / N. Bouhaida , N.E. Ghermani

**Short Description:** A school devoted to disseminate knowledge on ED studies from high resolution X-ray diffraction data within the African/Magrebin communities. The school is held by international teachers.

**Tentative Title :** Workshop on XD-2010(?) program package July 2010, APS Argonne, USA?

Sponsors/Organizers: ?/XD-package developers and APS staff

**Short Description:** A workshop devoted to familiarize with XD multipole-refinement package and with CD analysis techniques (topology, electrostatics, energies). Format of the workshop is currently being elaborated.

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

<http://www.grc.org/programs.aspx?year=2010&program=elecdist>

**Sponsors/Organizers:** GRC, IUCr (?), ECA(?), DFG(?) / Dylan Jayatilaka (Perth, Australia), P. Macchi (Bern, Switzerland)

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**Short Description:** A list of preliminary session topics/speakers is currently being developed by the Conference Chair (available by 1/12/2009). Involvement of SIG#2 members expected to be large.

**Title :** Center for Material Crystallography, Aarhus University, Aarhus DK, 2010-2014

**Sponsors/Organizers:** Danish National Research Foundation / Bo B. Iversen (Chair)

**Short Description:** An international Center for Material Crystallography (CMC) has been approved by DNRF and will be established in 2010. Involvement of SIG#2 members is quite large.

**Title :** Preparing a new book devoted to "Modern Charge Density Analysis"

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

**Short Description:** A contributed book on modern aspects of charge density analysis is in preparation (publication date: 2010). Involvement of SIG#2 members as authors/editors is impressive.

**Title :** Preparing a Web-site of ECA SIG#2

**Sponsors/Organizers:** ECA / C. Gatti and S. Cenedese

**Short Description:** A SIG#2 website is under construction.

**Other matters.**

( 50 words max.)

Next ECDM meeting will probably take place in 2011. We are currently discussing whether to have it as a separate meeting or rather as a satellite of Madrid IUCr XXII congress. Both options have advantages and drawbacks. Suggestions on this matter from ECA President and Executive Committee are welcome.

**5. Five year 'overview', brief activity report (2005-2009)**

( 100 words max.)

(only compulsory for those who did not sent the 2004-2008 'overview')

We provided it last year. This is just an update for 2005-2009.

SIG#2 has promoted activities aimed at enhancing the interest towards (combined) CSMD studies among ever wider scientific communities. SIG active members seem increasing through the years as testified by increasing attendance to ECDM meetings. Conferences (in part or fully organized):

- a) ECM-23 (2 MS, 1PL) and ECM-24 (2MS, 1PL), ECM-25 (proposals: 4 shared MS, 1PL)
  - b) ECDM-IV (2005), joint ECDM-V and SPP-1178 meetings (2008);
  - c) GRC-2007 on Electron Distribution and Chemical Bonding: Dynamic and Densities
  - d) IUCr-XX (2005), IUCr-XXI (2008)
  - e) SAGAMORE XV (2006), SAGAMORE XVI(2009) Conference on Electron CSMD Workshops : XD-2006 (in 2007), SIG SPP-1178 (in 2007), Marrakech (October 2009)
- Projects: DFG-1178 (2005-2011)

**6. Estimated number of active members:**

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**80 to 200** (if we include the newcomers attracted by initiatives like SPP-1178 program and ECDM-5 meeting, both aimed at spreading the word of CD analysis among ever wider scientific communities)

**7. 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

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)

No Supplementary material. Available on request (book of abstracts, list of participants, etc.)

**NOTE: DO NOT FORGET TO SEND THE UPDATED LIST OF YOUR SIG OFFICERS**

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