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SIG: 2

Reported Period: 1 July 2007 - 30 May 2008

Report Date: 30 May 2008

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

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1. Introduction.

We continue 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 is the organization and the interest raised by the coming ECDM-V meeting

(50 words max.)

2. Past Activities.

For Each Activity

Title: Gordon Research Conference (GRC) on Electron Distribution and Chemical Bonding: Dynamics and Densities (1-6 July 2007), Mount Holyoke College, USA
Number of Participants: 99 (ever highest participation to this conference since 1978); 56% from Europe

Sponsors/Organizers: GRC organization, IUCr, NIH (National Institute of Health, General Medical Sciences, Bruker, Incoatec, Rigaku, Chemmetal/ GRC Chair : Carlo Gatti (ECA SIG-2)

Short Description: Large emphasis on time-dependent XRD, XFEL developments, biological aspects of CD research, and data quality for CD (temperature dependent) studies was given. Impressive progresses in deriving chemical concepts and computational tools from electron density and density matrices were reported. The conference has been judged favorably and approved for future scheduling

(50 words max.)

Title: ECM-24 (Marrakech, Maroc, 22-27 August 2007)

Number of Participants: about 40-50 from the CSMD community

Sponsors/Organizers: ECA

Short Description: Three MS were organized by SIG#2: on CD studies for coordination chemistry, on insights in materials science from combined CSMD studies and on new theoretical/experimental approaches for understanding atomic interactions. Pierre Becker gave a plenary lecture. Participation from SIG#2 members was not low considering time proximity of GRC-2007 and XD-workshop

(50 words max.)

Title: Workshop on XD2006 program package: Advanced Methods in X-ray Charge Density Analysis: Extracting Properties from a Multipole Refinement , September 3-6 2007, Martina Franca (Italy)

Sponsors/Organizers: ECA approval, IUCr, AIC (Associazione Italiana Cristallografia), BCA (British Crystallographic Association), XD-group, INSTM and several industries/ Piero Macchi, Chair, Scientific Committee (P. Coppens, C. Gatti, B.B. Iversen, W. Scherer, Y. Wang, i.e. 3 members of SIG#2 in the committee and one member as a chair)

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Short Description: The workshop, organized in morning lectures on cutting-edge developments in CD studies and in afternoon hands on sessions specifically dedicated to the use and main features of the new release of the XD program package, met a great success with about 80 participants from Europe, US, Asia.

(50 words max.)

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

DFG SPP-1178 program enters its fourth 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 is part of ECDM-V meeting

(50 words max.)

Title: Special interest group of DFG SPP-1178 (2005-2011),

Number of Participants: 10

Sponsors/Organizers: Max Planck Institute Dresden

Workshop (29.11. + 30.11.07 in Dresden) about possibilities to overcome problems of extinction problem and heavy atom scattering function in x-ray charge density analysis. Special guests (P.Becker and T. Koritzansky) presented state of the art of both topics followed by open discussion about possible experiments and numerical solutions.

(50 words max.)

3. Future/Programmed Activities.

For Each Activity

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

Sponsors/Organizers: ECA, IUCr, AIC (Associazione Italiana di Cristallografia), Fondazione Cariplo, CNR-ISTM, INSTM, University of Milano, several industries/Carlo Gatti, Piero Macchi, Riccardo Destro (Milano) and DFG

Short Description: The annual SPP-1178 DFG program meeting (see above) has been joined to ECDM-5 to strengthen the connection between the two scientific events and related communities.

(25 words max.)

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

Sponsors/Organizers: IUCr

Short Description : Members of SIG#2, as members also of IUCr CSMD commission, have been very active in making proposals for key-note lectures and MS titles and chairs

(25 words max.)

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

Sponsors/Organizers: ECA

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Short Description: SIG#2 has sent to the ECM-25 organizers proposals (title/chairs) for MS and KN lectures.

(25 words max.)

4. Other matters.

We decided to join SPP-1178 and ECDM-V meetings in the hope to set the grounds for establishing a European Charge Density Network, which could promote a further dissemination of the CD tools and facilitate participation of the SIG#2 community in important international projects.

(50 words max.)

5. Five year ‘overview’, brief activity report (2004-2008)

SIG#2 has promoted activities aimed at enhancing the interest towards (combined) CSMD studies among wider and 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-22 (2MS, 1PL), ECM-23 (2 MS, 1PL) and ECM-24 (2MS, 1PL)
 - b) ECDM-IV (2005), joint ECDM-V and SPP-1178 meetings (2008);
 - c) GRC-2004 and GRC-2007 on Electron Distribution and Chemical Bonding: Dynamic and Densities
 - d) IUCr-XX (2005), IUCr-XXI (2008)
 - e) SAGAMORE XV (2006) Conference on Electron CSMD
- Workshops : XD-2006 (in 2007), SIG SPP-1178 (in 2007)
Projects: DFG-1178 (2005-2011)

(100 words max.)

6. Estimated number of active members: 80 to 140 (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 wider and wider scientific communities)

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

Chair: Bo Brummersted 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.

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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