

IUCr COMMISSION NEWS

Contributions intended for this section should be submitted to The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

COMMISSION ON CHARGE, SPIN AND MOMENTUM DENSITIES

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Newsletter No. 1

Following a suggestion by M. Nardelli, President of the International Union of Crystallography, the Commission decided to publish an annual newsletter, in general after the Sagamore Meeting, the Gordon Research Conference on Chemical Bonding or the Congress of the IUCr. The newsletter is intended to inform those interested in the field of charge, spin and momentum density studies of the activities of the Commission, especially new scientific projects and related meetings.

The Commission on Charge, Spin and Momentum Densities supports new experimental and theoretical concepts in this interdisciplinary field of research. The interplay between experiment and theory is considered essential for progress in this field and the Commission organizes meetings where these two aspects are well represented and stimulates common projects. A major effort is made to bring researchers from various laboratories together, in order to cross-check the experimental techniques applied and to make developments available to a larger community.

In this newsletter details are given of the Sagamore IX Conference held in Luso, Portugal, 26 June-2 July 1988, of a two-day workshop on density matrices held in Coimbra, Portugal, 25-26 June 1988, and of new scientific projects. Finally, a complete list of the members of the Commission, together with their addresses, is given in order to facilitate communication. Please contact a Commission member whenever you have suggestions or questions related to charge, spin and momentum densities.

Sagamore IX in Luso

The meeting was organized by L. Alte da Veiga, M. M. R. Costa, M. J. M. de Almeida, L. R. Andrade, A. Matos Beja and J. A. Paixao from the Physics Department of Coimbra University and was considered as most successful by the

approximately 100 participants. The stimulating and agreeable social activities offered by the organizers were highly appreciated. The program included the following invited contributions:

- J. R. Schneider (Berlin, FRG): *New Frontiers in Charge Densities.*
- J. B. Forsyth (Rutherford Laboratory, UK): *New Frontiers in Spin Densities.*
- S. Manninen (Helsinki, Finland): *New Frontiers in Momentum Densities.*
- S. W. Lovesey (Rutherford Laboratory, UK): *The Companionship of Neutron and Photon Magnetic Scattering in Condensed Matter Research.*
- D. Feil (Enschede, Netherlands): *Charge Density Distribution and Chemical Bonding.*
- R. F. Stewart (Pittsburgh, USA): *Electrostatic Potentials and Energies from X-ray Diffraction Data.*
- K. Hermansson (Uppsala, Sweden): *Electronic Density Distribution, Intermolecular Potentials and Molecular Mechanics.*
- L. Leiserowitz (Rehovot, Israel): *Crystal Growth and Electron Density in Organic Molecules.*
- V. S. Urusov (Moscow, USSR): *Electron Density Distribution and Crystal Properties.*
- K. Schwarz (Vienna, Austria): *Electronic Structure Calculations of Transition Metals and Alloys.*
- D. E. Ellis (Evanston, USA): *Defect Structure Studies of Transition Metal Compounds.*
- M. M. R. Costa (Coimbra, Portugal): *Electron Densities in Transition Metals.*
- G. H. Lander (Karlsruhe, FRG): *X-ray Studies of Magnetic Properties in Actinides.*
- M. J. Cooper (Warwick, UK): *Magnetic X-ray Scattering.*
- W. Schülke (Dortmund, FRG): *Inelastic Scattering of Synchrotron Radiation.*
- M. Nielsen (Roskilde, Denmark): *Surface Structures and Phase Transitions Studied by X-ray Diffraction.*
- G. P. Felcher (Chicago, USA): *Grazing Incidence Studies: Neutrons.*
- S. Berko (Waltham, USA): *Positronium Velocity Spectroscopy of the Electronic Structure of Metal Surfaces.*

About 60 posters were presented in three sessions. The conference proceedings will be published in *Portugaliae Physica*.

Workshop on density matrices

Experimental charge and momentum density studies yield complementary information on the ground-state wavefunction of a system. One-particle density matrices are considered the most appropriate quantity for combining the two types of information; their diagonal elements are related to the charge, the off-diagonal elements to the momentum density. In order to acquaint the community with this approach, and in preparation for a possible Commission project, D. Feil, J. R. Schneider, W. Schülke, L. Alte da Veiga and M. J. M. de Almeida organized a workshop on *Density Matrices as Intermediates between Wavefunctions and Experiments* in Coimbra, preceding Sagamore IX. The following lectures were presented:

- V. Smith Jr (Kingston, Canada): *Basic Theory of Density Matrices*.
 G. E. W. Bauer (Eindhoven, Netherlands): *The Energy Electron Density Relationship*.
 D. Feil (Enschede, Netherlands): *Examples of Density Matrices of Simple Systems*.
 C. Pisani (Torino, Italy): *Density Matrices of Crystals*.
 J. R. Schneider (Berlin, FRG): *Experimental Methods to Obtain Charge and Momentum Densities*.
 W. Schülke (Dortmund, FRG): *Experimental Methods to Obtain the Off-Diagonal Terms*.
 S. R. Gadre (Pune, India): *From Positional Density to Momentum Density*.
 L. Massa (New York, USA): *From Experiment to Wavefunction*.
 W. Weyrich (Konstanz, FRG): *Experimental Results on Off-Diagonal Terms and Conversion to Wavefunctions*.

Proceedings of the workshop will be published in *Portugaliae Physica*.

Magnetic form factors

Following a suggestion by the IUCr Commission on Neutron Diffraction, J.-X. Boucherle prepared an updated compilation of magnetic form factors and magnetization densities. Anyone interested in obtaining a copy should contact J.-X. Boucherle (CENG, DRF/DN, 85 X, F-38041 Grenoble CEDEX, France).

New Commission projects

V. Smith (Department of Chemistry, Queen's University, Kingston, Ontario K7L 3N6, Canada) and W. Weyrich will devise a project on density matrices with emphasis on: (a) silicon, for which many experimental data and theoretical calculations are available; and (b) other suitable compounds, still to be determined.

E. D. Maslen (Crystallography Centre, University of Western Australia, Nedlands, Western Australia 6009, Australia) and D. Feil, assisted by K. Hermansson, will write a feasibility study on electron densities and atomic charges in ionic compounds such as perovskites and organic salts. This will indicate suitable compounds and appropriate questions, and will be presented at the next Gordon Research Conference on Chemical Bonding, in summer 1989.

J. R. Schneider, together with S. Berko, will initiate a workshop on the various experimental techniques probing the bulk electronic properties of solids.

With respect to Commission projects the following rule is adopted: A project is undertaken for two years. It requires the initiative of somebody – member of the Commission or not – to extend its duration.

Sagamore X

The next Sagamore Conference on Charge, Spin and Momentum Densities will be held in Konstanz, FRG, at the end of August 1991. W. Weyrich (Fakultät für Chemie, Universität Konstanz, Postfach 5560, D-7750 Konstanz 1, FRG) is the Chairman of the Organizing Committee.

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