

# Proceedings of the Sagamore X Conference on Charge, Spin and Momentum Densities

Konstanz, September 1–7, 1991 · Z. Naturforsch. **48a**, 1–446 (1993)

## The IUCr Commission on Charge, Spin and Momentum Densities

WINFRIED SCHÜLKE	(Fed. Rep. of Germany) – Chairman
EDWARD D. STEVENS	(USA) – Secretary
JEAN-XAVIER BOUCHERLE	(France)
DIRK FEIL	(Netherlands)
J. BRUCE FORSYTH	(United Kingdom)
KERSTI HERMANSSON	(Sweden)
FUMITAKE ITOH	(Japan)
SEppo O. MANNINEN	(Finland) – Consultant
PETER MIJNARENDs	(Netherlands)
KARLHEINZ SCHWARZ	(Austria)
VADIM S. URUSOV	(Russia) – Consultant
SAX A. MASON	(France) – Chairman of the Neutron Diffraction Commission

## Organising Committee

WOLF WEYRICH	(Universität Konstanz) – Chairman
HELGARD V. POEPPINGHAUSEN	(Universität Konstanz) – Secretary
VEDENE H. SMITH, JR.	(Queen's University, Kingston, Ontario)
EBERHARD HEUSER-HOFMANN	(Universität Konstanz)
MICHAEL SPRINGBORG	(Universität Konstanz)

## Sponsors

We acknowledge the assistance and the financial support of the following institutions and organisations:

- International Union of Crystallography (IUCr)
- Deutscher Akademischer Austauschdienst (DAAD)
- Universität Konstanz
- Gesellschaft der Freunde und Förderer der Universität Konstanz
- Town of Konstanz
- Blumeninsel Mainau GmbH, Konstanz
- BASF AG, Ludwigshafen
- Bodenseewerk Perkin-Elmer GmbH, Überlingen
- Byk Gulden Lomberg Chemische Fabrik GmbH, Konstanz
- Convex Computer GmbH, Frankfurt a. M.
- Cray Research GmbH, München
- MBraun GmbH, München
- Rich. Seifert & Co., Ahrensburg
- Siemens AG, München



Dieses Werk wurde im Jahr 2013 vom Verlag Zeitschrift für Naturforschung in Zusammenarbeit mit der Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V. digitalisiert und unter folgender Lizenz veröffentlicht: Creative Commons Namensnennung-Keine Bearbeitung 3.0 Deutschland Lizenz.

Zum 01.01.2015 ist eine Anpassung der Lizenzbedingungen (Entfall der Creative Commons Lizenzbedingung „Keine Bearbeitung“) beabsichtigt, um eine Nachnutzung auch im Rahmen zukünftiger wissenschaftlicher Nutzungsformen zu ermöglichen.

This work has been digitalized and published in 2013 by Verlag Zeitschrift für Naturforschung in cooperation with the Max Planck Society for the Advancement of Science under a Creative Commons Attribution-NoDerivs 3.0 Germany License.

On 01.01.2015 it is planned to change the License Conditions (the removal of the Creative Commons License condition "no derivative works"). This is to allow reuse in the area of future scientific usage.

## Preface

Sagamore X, held at the Universität Konstanz from September 1 to 7, 1991, was the tenth in the series of the interdisciplinary Sagamore Conferences on Charge, Spin and Momentum Densities. The previous nine were held at Sagamore/New York (1964 and 1967), Aussois/France (1970), Minsk/U.S.S.R. (1973), Kiljava/Finland (1976), Mont Tremblant/Canada (1979), Nikko/Japan (1982), Sånga Säby/Sweden (1985) and Luso Buçaco/Portugal (1988).

The general subjects behind the title of the Sagamore Conferences are experimental and theoretical studies of the electronic structure of matter in all of its aspects by considering the wealth of information contained in multi-dimensional distribution functions (particle, charge, spin) in position and momentum space. The extension of the scope to nuclear coordinates in both spaces is natural. As a consequence of the interdisciplinary nature of the general themes, the Conferences have always been open to contributions from physics, chemistry, crystallography, mineralogy, etc., and have benefited from the resulting exchange of ideas.

Prior to the Conference, the Sagamore community lost two of its members. Moving memorial lectures were given in honour of Stephan Berko and Fred Hirshfeld by A. T. Stewart and P. Coppens, respectively. Since these lectures have been published elsewhere (Proc. 9th Int. Conf. Positron Annihilation, Materials Sci. Forum **105–110**, 3 (1992) and Trans. Amer. Crystallogr. Assoc. **26**, 91 (1990), resp.), they are not included here.

Twenty of the 45 invited talks and 50 of the 99 poster papers are now collected in the present volume. The papers cover almost all areas presented at the Conference in a well-balanced way and are arranged under the following headings:

	<i>Page</i>
I. Charge Densities	3
II. Spin Densities	109
III. Theoretical Charge and Momentum Densities	127
IV. Density Matrices in Theory and Experiment	203
V. Scattering Theory	233
VI. Inelastic Photon Scattering	266
VII. Inelastic Electron Scattering	358
VIII. Positron Annihilation	390
IX. Inelastic Neutron Scattering	406
X. Optical Properties	443

This structure of the Proceedings and the order of the papers within each of the ten sections reflect an attempt to find a continuous path through the multi-dimensional space of subjects and aspects. I hope that I have succeeded to the extent that the reader will feel the continuity and will be sufficiently curious to follow that path.

Organising the Sagamore X Conference as well as editing the Proceedings have been very interesting experiences for me. I thank all participants, all authors, and all those who have helped me in many ways. I am particularly grateful for the critical and very constructive support that I have received from the referees. Their efforts have contributed substantially to the quality of our Proceedings. The beautiful layout is the work of the Managing Editor, Mrs. T. Littmann, in cooperation with the very experienced printing-house K. Tritsch/Würzburg. Finally, I want to express my gratitude to Professor A. Klemm, who has been a very cooperative Editor and was very patient with an unsteady flow of manuscripts. It is his standards that I have tried to meet with the Proceedings.

Wolf Weyrich