The realization of the considerable potential of the Compton spectroscopy has however been hampered in practice due primarily to the fact that the best momentum resolution possible via γ -ray sources and solid state detectors is about 0.4 au, which is too limited to explore delicate Fermiology related issues in materials. But the advent of synchrotron radiation sources capable of providing high energy, high flux and well-defined polarization offers revolutionary new opportunities since momentum resolution of 0.1 au has been demonstrated and better resolution should be possible.
Bearing these considerations in mind, the Commission on Charge, Spin and Momentum Density has recently started a new project, "Fermiology of High T_c Superconductors via High Resolution Synchrotron-based Compton Scattering Spectroscopy". This effort is particularly timely since the third generation synchrotron sources are at various stages of development around the world (ESRF in France, APS in USA and Spring-8 in Japan). The plan is to proceed in two steps, exploring simpler systems first, as a prelude to developing the Compton technique fully in order to investigate complex materials, the goal being the High-T_c's. This talk will discuss the objectives of this new Commission Project, giving an overview of the important theoretical questions to be addressed, and discuss the experimental challenges facing the Compton community towards this end. Some very recent relevant theoretical and experimental results will also be presented.

PS–14.02.06 STANDING WAVE INELASTIC SCATTERING FROM **Si**

By A. Kaprolat* and W.Schülke, Institute of Physics, University of Dortmund, Germany; K. Sturm, Forschungszentrum Jülich GmbH, Germany

Conventional inelastic scattering experiments using x-rays are known to yield information about electron correlations in space and time. For momentum transfers comparable to reciprocal characteristic length's of the system (inelastic x-ray scattering spectroscopy **IXSS**), the experiments yield the dynamical structure factor $S(\vec{q},\omega)$, a quantity connected to diagonal elements of the inverse dielectric matrix ε^{-1}, wherefrom electronic properties such as plasmon dispersion and excitation spectra can be calculated.

An extension to this experimental technique is to use a coherent superposition of two plane waves, forming a standing wave field, rather than one single plane wave as initial photon state of the scattering process. These experiments (coherent **IXSS**) yield the nondiagonal dynamical structure factor, connected to nondiagonal elements of ε^{-1}, so one has at least in principle experimental access to the full dielectric matrix.

We present an experimental setup for coherent **IXSS** using synchrotron radiation. Experimental results for coherent inelastic scattering from single-crystal **Si**-samples are shown and discussed within the framework of a two-plasmon-band model. The results show for the first time direct experimental evidence for the existence of a bulk plasmon band structure showing a band gap for scattering vectors close to the [111]-Brillouin zone boundary in **Si** (A. Kaprolat, W. Schülke, Phys. Rev. Lett., 1991, 67, 879). It is shown that using coherent **IXSS**, the line shape of the two plasmons at the Brillouin zone boundary can be reconstructed (K. Sturm, W. Schülke, Phys. Rev. **B**, 1992, 46, 7193).

OCM–14.02.05

UNIFIED DESCRIPTION OF ELECTRONIC STRUCTURE BY DENSITY MATRICES FROM THEORY AND EXPERIMENT. By Vedene H. Smith, Jr.* and Hartmut Schmider, Dept. of Chemistry, Queen's University, Kingston K7L 3N6, Ontario, Canada; Wolf Weyrich, Fak. für Chemie, Universität Konstanz, D-W-7750 Konstanz, Fed. Rep. of Germany; Winfried Schülke, Inst. für Physik, Universität Dortmund, D-W-4600 Dortmund, Fed. Rep. of Germany.

The one-particle reduced density matrix (ODM) is the carrier of all single-particle information about a chemical system, and plays therefore a central rôle in the theoretical description of the latter. Both charge and momentum densities are respectively a cut and a transformed projection of this function, and are directly or indirectly accessible by experiment. The attempt to reconstruct the ODM from these densities or directly from experimental data in the framework of a given basis set is the subject of this paper. To this end, a methodology employing a restrained least-squares technique that ensures so-called $N-$ *representability* conditions has been developed and tested. Applications to atomic and molecular systems, including isotropic and directional data from both spaces are presented. The impact of the combination of complementary information and the necessity of partial inclusion of correlation effects are discussed. The quality of the results is judged employing suitable representations of the ODM and its functionals. It is emphasized that a *direct* experimental access to projections of nondiagonal elements of the ODM in momentum space becomes feasible for highly perfect crystalline solids by means of coherent Compton scattering. Thus an additional experimental test for the quality of the ODM reconstruction is available.

PS–14.02.07 ELECTRON DENSITY DISTRIBUTIONS IN ATOMS, MOLECULES AND CRYSTALS. A NEW APPROACH OF ANALYZING INTRA- AND INTERMOLECULAR INTERACTIONS. By W.H.E. Schwarz*, J.E. Niu, and S. Irle. Theoretical Chemistry Group, The University, Siegen, Germany.

Electron density distributions $\rho(r)$ contain three types of features, which give rise to a new natural approach of analyzing ρ with respect to chemical bonding. These features are 1) the very large, nearly spherical atomic core densities, defining the geometric structure, 2) the smaller multipolar atomic valence densities, defining the orientation and population of partially filled p- and d-shells of the "independent atoms" in the molecule or crystal, and 3) the very small density deformations due to the interatomic interactions.
The valence shell parameters (orientation and shape of independent atoms in the promolecule or procrystal) and the Chemical Deformation Densities are determined theoretically and experimentally for molecules and crystals. The features are brought in relation to intramolecular and intermolecular interactions. The atomic shapes correlate well with the intermolecular bond type. Intramolecular interactions affect the atomic orientations. Positive chemical deformation densities are found on all covalent bonds including those to F and O atoms. Previous results have been published by Schwarz et al. in J. Mol. Struct. **225** (1992) 435 and Ber. Bunsenges. Phys. Chem. **96** (1992) 1545.

