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MS49 Charge Spin and Momentum Densities in Material Science

Chairpersons: John Charles Spence, Brummerstedt Iversen

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High-Energy Synchrotron Radiation for Charge Density and Materials Science Experiments

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Recently it has been shown that high-energy synchrotron radiation is an excellent tool for the measurement of charge densities, because there is no significant affection of the data by absorption and extinction in most practical cases [1,2]. Thus, the enhancement of the data quality compared to 'low-energy' data sets now allows detailed comparisons between experimental and theoretical charge densities, even in the case of 'new materials' like high-Tc superconductors [3].

On the other hand high-energy synchrotron radiation is also very useful for 'classical' materials science experiments, e.g. texture or stress and strain analyses, because of the large intrusion depth, i.e. the possibility of studying not only academic but also 'realistic' samples (size). GKSS is currently building up two high-energy materials science beamlines at DESY, Hamburg, Germany. The concepts of the beamlines will be presented here. Both will be equipped with materials science diffractometers, which can also be used for charge density studies.

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Keywords: synchrotron radiation experimental, charge density, materials science

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Charge Density Studies of Ultra High Resolution Protein Structures

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The recent advances in synchrotron radiation and crystallogenesis methods have bought bio-crystallography in a context favorable to subatomic resolution protein structures. At this resolution, electron density reveals fine details related to the deformation of the valence electron density due to chemical bonding and intermolecular interactions. A spherical atom model of electron density does not allow to take into account these features in the refinement. However, in small molecules charge density studies, the Hansen & Coppens [1] multipolar model is commonly used, and allows the asphericity of the atomic electron density to be parameterized and quantified against experimental data.

Here we will show how charge density studies principles can be applied with the software MoPro [2] on protein structures obtained at subatomic and atomic resolution, using specific methods like the multipolar parameter transferability from our experimental database [3]. We will also present derived electrostatic properties based on the multipolar formalism and computed on high resolution Human Aldose Reductase – inhibitors complexes [4] of pharmacological interest.

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Keywords: charge density, protein structure, very high resolution

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Hypervalency – Experimental Charge Density Uncovers a False Concept

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Recently we synthesised and experimentally determined the charge density in molecular species containing so-called hypervalent central atoms. In those compounds formally the amount of valence electrons at the central atom exceeds the number of eight. Typical text book examples are SiF_6^{2-}, PF_6 or SO_3. Historically 3d orbitals are employed to explain the valence expansion and the generate sp^3d or sp^3d^2-hybrid-orbitals. However, the promotion of a phosphorus 3p electron to the d-orbital 16 eV are required but only 1 to 5 eV received by each covalent bond. Theoretical chemistry uncovered hypervalency as a false concept long time ago.[1] We investigated the phenomenon in terms of experimental charge density and topological analysis[2] of the hexacoordinated silicon complex $[F_2Si\{O(Me_2NN)\ CPh\}_2]$, the lithiumiminophosphoranate $[(Et_2O)Li\{Ph_2P(CHPy)(NSiMe_3)\}]$, and the sulfur triimide $S(N^tBu)_3$.[3]

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Measurements of Electron Densities in Solids

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This talk reports the recent progress in the measurement of electron densities in inorganic crystals and its significance for our understanding of bonding and electronic structure [1]. The talk is organized in two parts. The first part first emphasizes the importance of accuracy in experimental structure factors for electron density mapping and the challenge of studying inorganic crystals, which is then followed by an introduction of the convergent beam electron diffraction technique for accurate structure factor measurement. The second part of the talk reports the study of electron density in several inorganic crystals of materials interest with focus on transition metals and ions. Comparison between experiment and theory will be made to highlight the significance of experimental electron density and the need for further study. The talk will be concluded by looking into future challenges and opportunities in materials science for crystallography.

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Orbital-wise Decomposition of Magnetic Compton Profiles and Spin Moments in UGe_2

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The uranium ferromagnet UGe_2 has drawn much attention because of possible coexistence of superconductivity and ferromagnetism [1].