MS27-O5 Pair Distribution Function calculated from electron diffraction data

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Structure description through Pair Distribution Function (PDF) analysis has attracted particular interest in the last years with the declination of the technology towards nanocrystalline and amorphous materials. The structure of these materials cannot be described by a set of lattice basis vectors and atomic coordinates, but by a continuous function representing the probability to find atoms at a particular distance - PDF. Experimentally, the PDF is calculated from continuous scattering data, as a rule X-ray, or neutron diffraction. The employment of electron diffraction data for the PDF analysis, although not being completely new, survives a renaissance within the last years. Electron diffraction data for the PDF calculation is collected in a Transmission Electron Microscope (TEM), which has to be operated in a special way in order to collect optimal data for PDF. 2D electron diffraction patterns should be integrated into the 1D intensity profile, which then after a proper normalization will be transformed into a PDF. Specifics of electron diffraction data handling as well as the limitation of the method will be discussed. PDFs calculated from electron diffraction data for different materials will be presented and type of structural information extracted from the PDFs will be discussed.

Keywords: Electron Diffraction, PDF, nanostructure

MS28. Charge density studies

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MS28-O1 Applications of hirshfeld surface analysis in crystal engineering and drug design

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The tool of Hirshfeld Surface (HS) analysis for exploring intermolecular interactions in molecular crystals developed by Spackman and co-workers has become very popular in recent years.[1] It applies Hirshfeld's idea of stockholder partitioning to the procrystal electron density in order to construct meaningful molecular surfaces inside the crystal. Only coordinates and tabulated spherically symmetric atomic electron densities are needed. Hence, it is not an electron-density-analysis technique, however, properties such as theoretically calculated electron density, electrostatic potential and others can be plotted onto the HS to investigate interactions mediated through the surface.

In the context of applications of HS analysis, the following assumptions have to be discussed: To which extend can gas-phase calculated properties for isolated molecules explain crystal packing, and to which extent can crystal structures of small biologically active molecules simulate the situation of the same molecule within a biological environment?

Presented applications towards crystal engineering will include correlations of purely geometric HS mediated properties to melting points of compounds, and the use of HS analysis for isomorphism and polymorphism considerations.

Presented applications towards drug design will include discussions of the electrostatic potential on HS's in a pseudoreceptor modeling experiment, and will show how HS analysis contributes to the understanding of enhanced physiological effects of well-known drugs.

References:

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