ADVANCED ELECTRON DENSITY REFINEMENT & TRANSFERABILITY. APPLICATION TO BIO-MACROMOLECULES AND MOLECULAR RECOGNITION.

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Latest tools for the multipolar refinement and analysis of charge density with MoPro[1] software at ultra high resolution will be described. A new procedure enables to compute an estimation of uncertainty on charge density properties. A series of charge density molecular models which are "at standard deviation" from the refined final model are generated for this purpose[2].

The charge density of structures determined at usual resolution, notably proteins, can be modelled via the electron density database approach. Examples on biological macromolecules like protein/ligand complexes will be shown.

The impact of multipolar charge density on molecular interactions, notably hydrogen bonds and halogen bonds will be discussed.

Multipolar modelling of the atomic electron density enables accurate computation of electrostatic energy between interacting molecules. Unlike the atomic point charges approximation, the integration procedure takes into account the penetration energy, which is essential in short distance interactions. The driving forces in a crystal packing can be revealed by a combination of statistical analysis of contacts on the Hirshfeld surface and of electrostatic energy calculations[3].

References