KN10
Quantum crystallography of (macro)molecular crystals for everyone

P. Dominiak
Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw - Warsaw (Poland)

At the heart of X-ray crystallography is the scattering of the X-ray photon beam at the electron density of the crystal. Similarly, the electron beam is scattered at the electrostatic potential of the crystal or single particle. When analyzing the experimental diffraction(scattering) data, it is necessary to use the appropriate atomic scattering factors. To obtain them, the widely used model of independent atoms (IAM) with spherical symmetry was proposed about 100 years ago. However, the electron densities and electrostatic potentials of atoms in a molecule or crystal are not perfectly spherical, and the associated point charges are rarely close to formal ones. Currently, thanks to better measuring equipment, the shortcomings of the IAM are clearly visible in X-ray crystallography. To take advantage of more accurate, routinely collected data, more accurate electron density models should be used. The same soon happen with electron crystallography and modelling of electrostatic potential.

Quantum crystallography is usually associated with highly complex modelling using quantum chemistry methods and collecting experimental diffraction data of exceptional quality and resolution. Indeed, this is the heart of quantum crystallography. However, there is a branch of quantum crystallography which focuses on delivering new scattering models, data interpretation methods, and fast and reliable software tools to be applicable to standard measurements. The goal is to extract more information from routinely collected data. On the one hand, these new methods allow to achieve better fitting of the model to the data and improve the quality of the geometric data typically obtained from such measurements. On the other hand, they provide access to new types of information, i.e. electron density, electrostatic potential, interaction energy, and many more. Thus, quantum crystallography can be useful to all crystallographers, chemists, and structural biologists in their daily practice.

During the lecture, I will give general overview to the recent developments on the Hirshfeld Atom Refinement (HAR) and the Transferable Aspherical Atom Model (TAAM) refinement. I will focus on the Multipolar Atom Types from Theory and Statistical clustering (MATTS, formerly UBDB) data bank used to parametrize TAAM. I will present the results of TAAM refinements of organic crystal structures on the data from X-ray and 3D electron diffraction (3D ED). Prove that the time and effort needed to do TAAM refinement for organic crystals is almost the same as for IAM, including crystals with disorder and twinning. I will discuss how TAAM may help in the refinement of protein crystal structures against 3D ED (microED) data.

Acknowledgements: This work is supported by the National Centre of Science (Poland) through grant OPUS No.UMO-2017/27/B/ST4/02721.