TECHNISCHE UNIVERSITÄT DRESDEN

Institut für Festkörper- und Materialphysik

IFMP Institut für Festkörper- & Materialphysik

IFMP Seminar

Date Monday, June 17, 2024, at 14:50 (talk 1 of 2)

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Speaker **Krzysztof Wozniak**

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Title **Quantum Crystallography**

Abstract It is quite a paradox that more than a century after the introduction of the spherical Independent Atom Model (IAM, 1914 [1]) of atomic electron density (and in consequence spherical atomic scattering factors), 99.7% of all ~2M known crystal structures have still been refined using IAM which suffers from severe methodological deficiencies. Far better structural results can be obtained when new approaches of Quantum Crystallography (QCr) utilising aspherical atomic scattering factors are used in the refinement of X-ray data. In short, QCr is crystallography beyond IAM.

In this contribution, I will present details of several aspherical QCr approaches such as: Hansen-Coppens [2] pseudoatom refinement of experimental, quantitative electron density and the main ideas of Hirshfeld Atom Refinement (HAR) and some examples of its applications. My lecture will be complemented by several examples of our QCr [3-9] studies including: (1) multipole refinement of electron density in crystals of minerals including minerals under pressure, (2) Hirshfeld Atom Refinement (HAR) of ice structures against X-ray diffraction, electron diffraction and neutron diffraction data, (3) HAR refinement of H-atom positions in small-molecule organic compounds and hydrides, and, if I still have some time, I will present: (4) experimental HAR studies of relativistic effects and electron correlation in gold derivatives.

A century after the Braggs, it is possible to obtain H-atom positions from X-ray diffraction studies which are equally reliable as those from neutron diffraction. It is also possible to get reliable positions of H-atoms in the closest neighborhood of even some very heavy atoms, to study tiny redistributions of electron density in minerals under pressure, or to estimate the consequences of relativistic effects using X-ray diffraction data. So users of X-ray crystallography can do far better than just routinely refining a poor IAM model against precise, accurate and very often very dear diffractometer/synchrotron/XFEL X-ray data. QCr approaches can also improve the quality of macromolecular studies, powder X-ray diffraction results, PDF, XANES, EXAFS, CryoEM, electron diffraction, etc. In consequence, with Quantum Crystallography one can improve scientific results and stimulate progress in all fields of science/technology/medicine which utilize structural and electronic results.

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