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The roots of Quantum Crystallography

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The term *Quantum Crystallography* has recently entered the scientific language, following a definition by Massa, Huang & Karle (1995). Their vision was quite narrow-focused, identifying quantum crystallography with the possibility of improving an electronic wave function by means of X-ray scattering intensities, or otherwise using wavefunction-based methods to improve the traditional crystal structure models.

Instead, if quantum crystallography refers to the extraction of quantum-based information from crystallographic measurements or the use of theoretical quantum chemistry to improve the quality of the crystallographic models, then it is clear that this field finds its roots directly at the beginning of modern crystallography, after the discovery of X-rays. In facts, it was only in the 1960s that this kind of studies became technically available, especially under the impulse of R. Weiss (1966), who showed how electron charge density, in position or in momentum space, could be determined from X-ray diffraction.

A terrific development occurred in the 1970s, fostered by P. Coppens (1984) and R. F. Stewart (1976) and many coworkers who paved the way to extract a huge array of quantum mechanical quantities from crystallographic experiments. The progresses have involved also the determination of magnetization densities and spine distributions (Becker, 1980), the refinement of reduced density matrices (Gillet, 2007) and the calculation of X-ray restrained wavefunctions (Jayatilaka, 1998).

Many methods to analyze those quantities have been developed and adopted, mostly based on electron density partitions and quantum topology (Bader, 1990).

These roots enable nowadays a modern and broader science, which is under development and takes advantage of improved modelling techniques, for example combining different kinds of experiments, and from the new types of source that are currently available at large scale facilities.

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KN-6

Application of advanced transmission electron microscopy techniques to structure solution and refinement of complex inorganic materials

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The crystal structure solution of complex inorganic compounds, including commensurately or incommensurately modulated compounds, is often very challenging, even using the well-established methodology of single-crystal X ray crystallography. This task becomes even more difficult for materials that cannot be prepared in a single-crystal form, so that only polycrystalline powders are available. Transmission electron microscopy (TEM) has a strong advantage in such cases, as it can study separate nm sized crystallites, turning a "powder sample" into a sample with a multitude of "single crystals". A TEM furthermore allows using many different techniques, from diffraction to imaging to spectroscopy. Huge advances were made in both high resolution imaging and spectroscopy as well as electron diffraction methods over the last decade. In this lecture, an overview will be given which and how advanced transmission electron microscopy techniques can be specifically well used to aid the structure solution and refinement of complex inorganic materials, as well as the potential of some recent analysis tools and instrumentation towards this target.

Keywords: TEM, modulated, structure