About the connections and possible contaminations between quantum chemistry and quantum crystallography

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Although an ultimate definition has not been provided yet, nowadays quantum crystallography can be considered as a field of science having the goals of studying and interpreting properties and phenomena occurring in the crystalline state by exploiting the laws of quantum mechanics [1, 2].

To accomplish the above-mentioned tasks, several techniques have been devised. Prominent examples are the multipole models to determine experimental charge densities from high-resolution X-ray diffraction data or the quantum chemical topology strategies (e.g., the quantum theory of atoms in molecules) to analyze experimental or theoretical electron densities.

However, in this context, new methods strongly based on quantum chemistry also recently emerged. They can be subdivided into two great families [3]. On the one hand, we have the techniques where the experimental X-ray diffraction data are used to enhance and possibly improve the information content of wavefunctions and electron densities resulting from traditional quantum chemistry calculations, as in the case of the so-called X-ray restrained/constrained wavefunction (XRW/XCW) fitting approach [4]. On the other hand, we also have strategies where, on the contrary, the usual quantum chemical computations are exploited to significantly improve the refinements of crystal structures, as through the quite popular Hirshfeld atom refinement (HAR) approach [5].

In this pedagogical lecture, a general overview on the XRW/XCW and HAR methods will be given. In particular, while describing the bases and the recent developments of these two techniques [3], the focus will also be on the possibilities of mutual fertilization/contamination between the already very close fields of quantum chemistry and quantum crystallography.

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