Quantitative Convergent-Beam Electron Diffraction - The Nexus Between Electron and Quantum Crystallography

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Quantum crystallography as a field was originally defined as a "technique for extracting quantum mechanically valid properties from X-ray diffraction experiments" [1]. This definition was based on the premise that the confluence of quantum mechanics and crystallography is a direct consequence of the electron distribution around atoms being the origin of X-ray diffraction. This makes the electron distribution an observable that can be described by quantum mechanics [1].

Recently, this definition has been expanded to embrace electron diffraction, which is a direct consequence of electrons scattering from the crystal potential. As an observable, the crystal potential can of course also be described by quantum mechanics and is directly related to the electron distribution [2, 3]. This establishes the nexus between electron crystallography and quantum crystallography (and thereby X-ray crystallography).

In the last 30 years, quantitative convergent-beam electron diffraction (QCBED) has evolved into a technique that is now regarded as the most accurate and precise experimental method for measuring bonding-sensitive structure factors in crystals with small to moderately sized unit cells [2]. Some examples of key bonding studies exploiting QCBED's sensitivity are given in [4 - 9]. In this work, the most recent developments in the field are highlighted in their capacity to unlock new fundamental information about crystalline materials and new areas of research within the nexus between electron and quantum crystallography.

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