

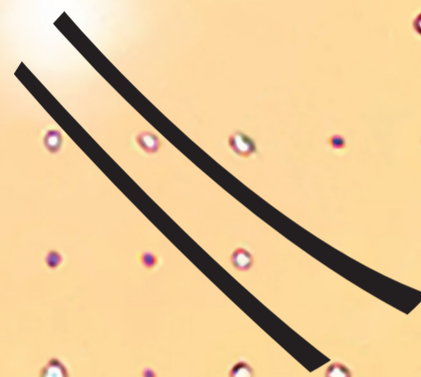
Seminar

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Online

The connubium between crystallography and quantum mechanics



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Seminar abstract

The link between the Quantum Mechanics and Crystallography is much tighter than what most scientists think. The entanglement started quite soon after the first X-ray diffraction experiments in the early 1900's because the emerging technique was suitable to solve some fundamental questions of quantum physicists. On the other hand, crystallography needed models to exhaust the increasing flow of information possible thanks to X-ray diffraction. To see the atomic content of a crystal, one must adopt a quantum mechanical perspective. This synergy continues nowadays. The technique in use is not only X-ray diffraction, but also neutron diffraction or electron diffraction (together with many spectroscopic techniques). The models are ever more sophisticated and enable reconstruction of the charge and spin electron density and even a calculation of wavefunctions restrained to the experimental data.