

Quantum Crystallography: What is it about?

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Quantum Crystallography is a multidisciplinary field where (mostly, but not exclusively) diffraction experiments involving X-rays, electrons, and neutrons are used to try to understand and model atomic and subatomic structure and behaviour.

The “quantum” in Quantum Crystallography emphasizes that the focus is on trying to determine *model wavefunctions from the experiments* — a hybrid of quantum chemistry and crystallography — not only to make better predictions, but also to allow the wealth of physical and chemical information obtainable from this approach more easily available to chemists and physicists.

In this talk I will focus on explaining the basic idea of trying to reconstruct an experimental wavefunction (an idea which goes back to Pauli). I’ll also describe the improvements that have been made over time, including briefly describing some recent work adjusting periodic wavefunctions to reproduce experimental electron densities in some boronitrogen molecules. I’ll also describe briefly our aims to try and introduce these techniques into molecular biology, with the Chari group at the MPI.