

Some of the recent history of quantum crystallography

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In my contribution, I plan to give a small overview of the history of the methods Hirshfeld Atom Refinement (HAR) and X-ray constrained wavefunction (XCW) fitting from the seminal work by Jayatilaka et al. at the end of the 1990s to today's modern software. I will underpin this journey with research examples from the work of our research group and from that of others.