MS21-01 | Possible Quantum Crystallography Solutions for N-Representable One-Electron Reduced Density Matrices Reconstruction

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One of the goals of Quantum Crystallography is to study to what extent experimental tools of crystallography such as X-ray, electron, neutron diffraction, in their polarized and non-polarized versions can be used to gain better access to fundamental quantum properties such as the N-electron wavefunction.

In recent years, our collaboration has developed methods to extend the range of scattering experiments to gain access to better one-electron reduced density matrices which fulfill N-representability conditions. Two such possible approaches will be described in the cases of spin-resolved and charge-only 1-RDM for model systems. The purpose is to assess the quality of a 1-RDM reconstruction using coherent-elastic and incoherent-inelastic pseudo-experimental data and critically compare the result to the original, periodic ab-initio derived, 1-RDM standard reference.