

## Density fitting approach to many-body calculations in molecules and solids

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Density fitting is well established in quantum chemistry as a method for accelerating SCF and post-SCF calculations, including GW and BSE methods [1,2]. Here an all-electron, Gaussian orbital, Coulomb-metric density fitting method with applications to molecules and solids is reported. Calculation of Hartree-Fock exchange in solids is well known to present difficulties to numerical simulations owing to its divergent behaviour at small wave-vector. Local orbital basis approaches also suffer from the problem that contributions to the Fock operator do not converge when summed entirely in real-space. A Coulomb-metric density fitting approach to calculation of Hartree-Fock exchange or to Coulomb matrix elements over Bloch functions which appear in many-body methods leads to an Ewald summation in real and reciprocal space which is absolutely convergent. This is a feature of the factorisation introduced by density fitting. Performance of the density fitting methods with respect to auxiliary fitting basis, etc is analysed. The method is illustrated by time-dependent Hartree-Fock and GW/Bethe-Salpeter equation calculations on Na clusters [3] with up to 20 atoms, molecular crystals and simple covalent solids using the Exciton code [4].

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[4] C. H. Patterson, *Mol. Phys.* 108, 3181 (2010)