MP2, RPA AND GW WITHIN THE GAUSSIAN AND PLANE WAVES METHOD

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New developments in the electronic structure code CP2K have been implemented for large scale simulations using wavefunction correlation methods [1]. The focus was on MP2, RPA and GW methods for periodic systems with gamma-point sampling. Resolution-of-the-identity (RI) with a Coulomb metric is used together with canonical orbitals and all necessary periodic two-electron Coulomb integrals with two and three orbital indices are calculated using the Gaussian and plane waves approach [1,5].
Forces and stress tensor have been derived for the MP2 method [3] and MP2 and RPA methods have been used in Monte Carlo and molecular dynamics simulations of water at ambient conditions[4]. These correlation methods can be combined with accelerated Hartree-Fock calculations using the auxiliary density matrix approach (ADMM)[2]. Additional improvements in efficiency were achieved by using semi-analytic Ewald integral calculations for Gaussian basis sets [6]. Reduced scaling approaches based on overlap metric RI and imaginary time integration was recently implemented for RPA and GW methods[6,7].
Together with their also reduced memory footprint, these new methods allow the calculation of systems with 1000's of atoms at the RPA and GW level.

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