

Density and system dependent exchange-correlation potentials in density functional theory.

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Using the electron densities and the exchange-correlation potentials obtained from *ab initio* wave function theory (WFT) (HF, MP2, CCSD) [1], and optimized effective potential OEP-DFT [2] calculations, we received a new density- and system-dependent exchange (xHF) and correlation (TMP) potentials. By using this new density-dependent potentials, KS-DFT calculations have been performed for few atoms systems (He, Be, Ne, Ar), where results were compared with those obtained from standard density-dependent exchange-correlation DFT methods (SVWN5), several (WFT) methods such as MP2, CC and correlated OEP methods.

The results were compared in the terms of total ground state energies, correlation energies, exchange and correlation potentials. In addition to assess the impact of the new exchange and correlation KS-DFT potentials on the electron density, the analysis of the electron radial density has been performed [3].

Analysis of the energies, potentials and the electron radial density clearly showed, that the results obtained using new density-dependent exchange and correlation potentials are quantitatively and qualitatively comparable with results obtained from *ab initio* WFT and the correlated OEP-DFT methods also giving significantly better results than those obtained from standard density-dependent exchange-correlation functionals.

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