

Correlation Potentials and Electron Densities from Correlated DFT, WFT and OEP Methods - what we can learn from them?

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Direct comparison of the Kohn-Sham correlation potentials, electron densities and correlation energies, generated from few variants of correlated Optimized Effective Potential Method (OEP), standard Density Functional Theory (DFT) and from *ab initio* Wave Function Theory Methods (WFT), has been employed for analyzing the impact of the correlation effects on those quantities. These methods have been applied to a few atomic and molecular systems.

The correlation potentials, energies and densities generated from correlated OEP - OEP2-sc [1] and from WFT methods - Coupled Cluster and Second-Order Many Body Perturbation Theory show very similar and systematic behaviour, reconfirming the correctness of the *ab initio* DFT (OEP2) methods [2,3,4].

In a contrast it has been demonstrated that the standard VWN5 and LYP correlation functionals do not represent any substantial correlation effects on the KS-correlation potentials [3,4,5] and electron density [5], whereas these effects are well represented by the orbital dependent OEP correlation functionals. In the same time for the local, generalized-gradient, and hybrid functionals it has been found that the dynamic correlation effects are to a large extent accounted for by densities resulting from exchange-only calculations. Additional calculations with self-interaction corrected exchange potentials indicate that this finding cannot be explained as an artifact caused by the self-interaction error or non dynamic correlation effect.

The usefulness of such kind of analysis in a context of development new exchange correlation functionals in DFT will be also discussed. [6,7]

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