

Correlation energy from ACFD framework including the exact-exchange kernel

Nicola Colonna

*Theory and Simulation of Condensed Matter Physics
International School for Advanced Studies (SISSA), Trieste*

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Abstract: The accurate prediction of the electronic properties of weakly bound systems, such as molecules about to break during a chemical reaction or van der Waals bonded compounds, is one of the most challenging tasks for density-functional theory. The failure of conventional exchange-correlation functionals in describing these situations is due to their intrinsic local nature and calls for the development of more effective approximations to exchange and correlation energies. The Adiabatic-Connection Fluctuation-Dissipation (ACFD) formalism tackles this kind of problems at a very fundamental level, providing a perfect starting point for the development of truly non-local functionals; RPA is a successful example of such ACFD-derived functionals. Beside its good performance in predicting Van der Waals interactions and molecular dissociations, RPA is known to overestimate correlation energies and to poorly describe the total energy, pointing to the need for inclusion of exchange-correlation contributions to the kernel. In this respect we have developed and implemented an efficient scheme for the calculation of the correlation energy via the ACFD theorem going beyond RPA by including the exact-exchange contribution to the kernel (RPA_x). We will analyse how the new approximation performs in a few test systems.

[1] D.C. Langreth and J.P. Perdew, Solid State Commun. 17, 1425 (1975)

[2] D.C. Langreth and J.P. Perdew, Phys. Rev. B 15, 2884 (1977)

[3] M. Hellgren and U. von Barth, Phys Rev B 78, 115107 (2008)