Beyond RPA Correlation Energies: Evaluation of Model Exchange-Correlation Kernels

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The adiabatic-connection fluctuation-dissipation theorem (ACFDT) provides a formal frame work to treat the exchange-correlation energy. Under the random phase approximation (RPA), the effect of the exchange-correlation kernel is neglected, leading to the so-called EXX/RPA method. It has been shown that EXX/RPA yields overall a good description of structural properties of materials with different dimensionalities and different types of chemical bonds. In particular, the description of van der Waals systems is significantly improved over the density functional theory in the local or semi-local approximations. However, due to the lack of exchange-correlation kernel, EXX/RPA overestimates absolute correlation energy and slightly underestimates the cohesive energy. In this work, we applied the full ACFDT by including model exchange-correlation kernels. Two types of model kernels were studied: a local kernel proposed by Dobson and Wang [1] and a non-local kernel proposed by Corradini *et al.* [2]. We generalized the original Corradini kernel to inhomogeneous systems, and developed a new algorithm to allow an efficient numerical implementation. Results on benchmark systems were discussed.

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[1] J. F. Dobson and J. Wang, Phys. Rev. B **62**, 10038 (2000).

[2] M. Corradini, R. Del Sole, G. Onida, and M. Palummo, Phys. Rev. B **57**, 14569 (1998).

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