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Beyond RPA correlation energies: Evaluation of model exchange-correlation kernels[1] DEYU LU, Center for Functional Nanomaterials, Brookhaven National Laboratory — The adiabatic-connection fluctuation-dissipation theorem (ACFDT) has drawn considerable attention in describing van der Waals (vdW) dispersion interactions. Under the random phase approximation (RPA), the EXX/RPA method yields the correct asymptotic behavior at large distances. However, for many advanced materials, e.g., organic/inorganic interfaces and molecular crystals, it is important to capture the short-range dispersion interaction within several angstrom. Because RPA pair distribution function is incorrect at short distances, the contribution of the exchange-correlation kernel has to be included properly. In this work, we implemented several model exchange-correlation kernels in the framework of ACFDT. Special attention was paid to develop non-local kernels suitable for inhomogeneous electronic systems. The performance of the exchange-correlation kernels were evaluated for both bulk and molecular systems.

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