Quasi-local approximation of non-local exchange-correlation kernels in the adiabatic-connection fluctuation-dissipation theorem[1] DEYU LU, Brookhaven National Laboratory — The adiabatic-connection fluctuation-dissipation theorem (ACFDT) is a formal theoretical framework to treat van der Waals (vdW) dispersion interactions. Under the random phase approximation (RPA), it yields the correct asymptotic behavior at large distances, but the short-range correlation is overestimated. It has been demonstrated that non-local exchange-correlation kernels can systematically correct the errors of RPA for homogenous electron gas. However, direct extension of non-local kernels derived from the electron gas model to inhomogeneous systems raises several issues. In addition to the high computational expense, the non-local kernels worsen the rare gas dimer binding curve as compared to RPA. In this study, we propose a quasi-local approximation of the non-local kernel in order to address these issues.

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