

Van der Waals Coefficients in Density Functional Theory: a Simple Approximation for the Polarizability

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Abstract: Long range interactions appear and play crucial roles in many systems, including soft matter, van der Waals complexes, biomolecules, etc. Density Functional Theory(DFT) within Local Density and Generalized Gradient Approximations for exchange-correlation energy is known to fail in describing properly van der Waals interaction, while approach from the exact Adiabatic Connection Formula of this quantity is computationally impracticable, except for few simple systems. We show in this report that a simple, computationally fast procedure to calculate van der Waals coefficients in DFT framework with reliable result can be developed from a simple approximation for the kinetic energy functional. Results of calculations applied to atomic and molecular systems strongly support the validity of the method in capturing essential part of long range correlations. This result may give useful information for constructing an exchange-correlation functional which includes van der Waals energies.

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