van der Waals coefficients in DFT: a simple approximation for the polarizability STEFANO DE GIRONCOLI, SISSA and DEMOCRITOS, HUY VIET NGUYEN, SISSA, DEMOCRITOS and Hanoi University of Education — Long range van der Waals interaction plays a crucial role in many systems. Density functional Theory (DFT) within Local Density and Generalized Gradient Approximations for exchange-correlation energy is known to fail in describing properly this interaction, while direct calculations based on the exact Adiabatic Connection Formula are computationally impracticable, except for few simple systems. A simple and computationally fast scheme to calculate imaginary-frequency-dependent polarizability, hence asymptotic van der Waals interaction, within density functional theory is considered. The van der Waals coefficients for a large number of closed-shell ions and several molecules are calculated and compare well with available values obtained by more refined first-principle calculations. The success in these test cases shows the potential of the approximation in capturing the essence of long range correlations and may give useful information for constructing a functional which naturally includes van der Waals interaction in DFT.

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