Beyond RPA correlation energies: Evaluation of model exchange-correlation kernels

DEYU LU, Center for Functional Nanomaterials, Brookhaven National Laboratory, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — The description of van der Waals dispersion interactions using the so called EXX/RPA method has recently attracted a widespread interest. Overall, equilibrium distances and cohesive energies of weakly bound molecular systems exhibit a significant improvement over the results of semi-local Density Functional Theory calculations [1,2], due to the proper inclusion of long-range correlation effects. However, cohesive energies still result to be underestimated with respect to experiments in several cases. This is mainly due to the neglect of the exchange-correlation kernel in evaluating response functions entering the correlation energy expression. In this work, we study the effect of several model exchange-correlation kernels and evaluate their performance for molecular systems.