Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

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 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.

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[2] Y. Li, D. Lu, H-V Nguyen and G. Galli, J. Phys. Chem. A, 114, 1944-1952 (2010) and D. Lu, H-V Nguyen, and G. Galli, J. Chem. Phys. 133, 154110 (2010)

Deyu Lu
Center for Functional Nanomaterials, Brookhaven National Laboratory

Date submitted: 18 Nov 2010 Electronic form version 1.4