

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First principle calculations of long range correlation effects within the random phase approximation¹ DEYU LU, YAN LI, HUGH WILSON, GIULIA GALLI — The local and semi-local approximations to Density Functional Theory fail to describe correctly certain types of weak interactions (e.g. van der Waals forces) due an incorrect account of long range correlation effects. Such effects may be described by computing correlation energies within the random phase approximation (RPA), using the fluctuation-dissipation theorem and the adiabatic connection. We present an approach to compute RPA correlation energies based on an eigenmode expansion of the dielectric matrix [1,2]. By solving the frequency dependent Sternheimer equation within linear response theory [3], we eliminate the need to compute single particle unoccupied states, which makes our approach more efficient than methods using the direct-summation technique. Furthermore, the use of a dielectric eigenmode representation allows for a physical interpretation of several, different contributions to correlation energies. Results for graphite and the benzene crystal will be discussed. [1] H. Wilson, F. Gygi and G. Galli, Phys. Rev. B, 78:113303, (2008). [2] D. Lu, F. Gygi and G. Galli, Phys. Rev. Lett., 100:147601(2008). [3] S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Giannozzi, Rev. Mod. Phys. 73:515, (2001).

¹Work supported by DOE SciDAC grant DE-FC02-06ER25794.

Deyu Lu
UC Davis

Date submitted: 10 Dec 2008

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