Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Self-consistent calculations of correlation energies within the random phase approximation[1] STEFANO DE GIRONCOLI, NGOC LINH NGUYEN, SISSA and CNR-IOM DEMOCRITOS,Trieste, Italy, VIET HUY NGUYEN, GIULIA GALLI, University of California, Davis, USA — Calculations of correlation energies within the the formally exact Adiabatic Connection Fluctuation-Dissipation (ACFD) formalism, within the Random Phase Approximation (RPA) for the exchange-correlation kernel, have been recently carried out for a number of isolated and condensed systems. The efficiency of such calculations has been greatly improved by exploiting iterative algorithms to diagonalize RPA dielectric matrices [1]. Unfortunately, for several systems, it has been found that RPA correlation energies may significantly depend about the choice of input single particle wavefunctions [2]. In this work, we derive an expression of the RPA self-consistent potential based on Density Functional Perturbation theory and we present self-consistent RPA calculations for weakly bound molecular dimers, including the controversial case of the Beryllium dimer.

[1] H.-V. Nguyen and S. de Gironcoli, Phys. Rev. B 79, 205114 (2009); H. F. Wilson, F. Gygi, and G. Galli, Phys. Rev. B 78, 113303 (2008).
[2] Huy-Viet Nguyen and G.Galli, J. Chem.Phys. 132, 044109 (2010).

[1]Work partly supported by DOE-scidac-e DE-FC02-06ER25777.

Stefano de Gironcoli
SISSA and CNR-IOM DEMOCRITOS,Trieste, Italy

Date submitted: 24 Nov 2010 Electronic form version 1.4