

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**Molecular dissociation within the adiabatic connection fluctuation dissipation framework** MARIA HELLGREN, NICOLA COLONNA, STEFANO DE GIRONCOLI, SISSA — The adiabatic connection fluctuation dissipation (ACFD) framework provides an exact expression for the correlation energy in terms of the dynamical density-density response function where the latter can be approximated using time-dependent density functional theory or many body perturbation theory. The first level of approximation is the so-called random phase approximation (RPA) which already incorporates many desirable features known to be difficult to capture with standard correlation functionals. For example, it contains the weak van der Waals forces, and the problem of large static correlation errors which appear in the dissociation limit of molecules are completely absent within the RPA. However, many properties are in quantitative error with experiment and certain features of strong electron correlation are missing. We will here show how the inclusion of exchange effects in the response function yields correlation energies, van der Waals coefficients and molecular dissociation energies in excellent agreement with experimental values. Some attention will be given to how an open-shell atom should be described in the dissociation limit. This further allows one to analyze a given approximate ACFD functional in terms of a so-called fractional charge analysis.

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Date submitted: 15 Nov 2013

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