Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Adiabatic-connection fluctuation-dissipation DFT for the structural properties of solids - the renormalized ALDA and other electron gas kernels[1] CHRISTOPHER PATRICK, KRISTIAN THYGESEN, Department of Physics, Technical University of Denmark — The adiabatic-connection fluctuation-dissipation formulation of density-functional theory (ACFD-DFT) provides a natural pathway for the calculation of electron correlation energies going beyond the random-phase approximation (RPA). The key ingredient of ACFD-DFT is the exchange-correlation kernel f_{xc} of time-dependent DFT. The last few decades have seen the development of a number of model kernels, often based on studies of the homogeneous electron gas (HEG). Here, we introduce a selection of these HEG kernels and use them to calculate the structural properties of a test set of solids within ACFD-DFT. Amongst our kernels we include the recently-introduced renormalized adiabatic local-density approximation (rALDA) [T. Olsen and K. S. Thygesen, Phys. Rev. B 88, 115131 (2013)], and also consider kernels which (a) satisfy known limits of the HEG, (b) carry a frequency dependence or (c) include a long-range component. By comparing the kernels to each other, to the RPA and to experiment we shall identify the essential properties of a kernel for ACFD-DFT applications. We shall also discuss the technical challenges of applying HEG kernels to inhomogenous systems, and identify key areas for future progress.

[1]Research supported by the Danish Council for Independent Research's Sapere Aude Program, Grant No. 11-1051390

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Date submitted: 07 Nov 2014 Electronic form version 1.4