

Abstract for an Invited Paper  
for the MAR10 Meeting of  
The American Physical Society

**DFT and beyond: A discussion of exact exchange plus local- and nonlocal-density approximations to the correlation functional**

MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, Germany

Local- and semilocal-density approximations (LDA/GGA) to density-functional theory, although tremendously successful for describing the properties of many molecules and materials, suffer from, amongst others, self-interaction errors and the absence of long-range van der Waals interactions. One at present most systematic approach for handling the xc functional appears to be exact exchange combined with the random phase approximation for correlation. We show that significant insight can be obtained by this approach, e.g. for studying the interaction between two graphene sheets [1], cohesive and surface energies of transition metals [2], or the adsorption of CO on close-packed transition metal surfaces [3]. For some of these systems the LDA and GGA give an even qualitatively wrong description. — Despite the success for the mentioned systems we also identify shortcomings of the approach, in particular for molecules. — A second route discussed in this talk concerns the linkage of LDA+ $U$  and many-body perturbation theory:  $G_0W_0@LDA+U$ . We discuss results for the  $4f$  lanthanide-oxide series [4] as well as for  $3d$  transition metal oxides. — 1) A. Sanfilippo, X.G. Ren, P. Rinke, A. Tkatchenko, V. Blum, K. Reuter, and M. Scheffler, in preparation. 2) A. Soon and Matthias Scheffler, in preparation. 2) X. Ren, P. Rinke, and M. Scheffler, Phys. Rev. B **80**, 045402 (2009). 4) H. Jiang, R.I. Gómez-Abal, P. Rinke, and M. Scheffler, Phys. Rev. Lett. **102**, 126403 (2009).