Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Towards an exact treatment of exchange and correlation in materials: Application to CO adsorption at transition-metal surfaces
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— We present an efficient scheme to correct the errors of density-functional theory (DFT) exchange-correlation (xc) functionals. The method locally corrects the xc interaction by analyzing clusters of the same local geometry as that of the calculations for the extended system. **The correction** is found to rapidly approach a universal dependence with cluster size, exhibiting a simple analytical behavior. As a consequence it is shown how high-quality cluster studies (e.g. using B3LYP, HF+MP2, or QMC) can be used to determine the DFT-LDA/GGA error for extended systems. The method is particularly efficient for defects in the bulk and at surfaces. — The approach is applied to CO adsorption at transition metals, where present xc functionals dramatically fail to predict the correct adsorption site.[1] The correct (experimentally confirmed) geometry is obtained by the correction scheme, and the origin of the LDA/GGA failure is discussed.

[1] P.J. Feibelman, B. Hammer, J.K. Norskov, F. Wagner, M. Scheffler, R. Stumpf, R. Watwe, and J. Dumesic, The CO/Pt(111) puzzle. J. Phys. Chem. B **1**05, 4018 (2001).

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Date submitted: 05 Jan 2006 Electronic form version 1.4