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.