MAR12-2011-000218

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Weakly Interacting Subsystems in DFT

TROY VAN VOORHIS, MIT Department of Chemistry

In chemistry, one is frequently interested in systems that are composed of weakly interacting fragments: a solute dissolved in a solvent phase, the base pairs in DNA, molecules in a crystal. In all these cases, our physical picture is that electronic states of the assembly emerge from small perturbations of states localized on the fragments. In frustrating fashion, standard functionals completely fail to reproduce this qualitative picture: the excited states of molecular assemblies are dominated not by local, valence excitations, but by spurious charge transfer states; weak van der Waals forces that hold molecules together are typically absent; excess spin and charge tend to be strongly delocalized even when the physical coupling between centers is extremely weak. In this talk we will discuss how truly nonlocal density functionals can mollify these trends. In particular, we will highlight the recent derivation and implementation of nonlocal van der Waals density functionals that account for long-range correlation in terms of two-point density interactions.