

MAR07-2006-000124

Abstract for an Invited Paper
for the MAR07 Meeting of
the American Physical Society

Using Constrained DFT to Define a Diabatic Configuration Space

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We show that several of the well-known shortcomings of approximate density functionals for treating electron transfer (ET) can be overcome by applying physically motivated constraints to the electron density. We summarize our implementation of this constrained density functional theory (CDFT) and present several illustrative applications that demonstrate the strengths of the new formalism: 1) CDFT allows charge transfer excitations to be treated accurately within a ground state formalism, including the long range $-1/r$ interaction between the electron and the hole 2) One directly obtains diabatic states, which can be unambiguously associated with Marcus theory parameters and 3) Long-standing ground state electronic structure problems – such as the prediction of exchange couplings and certain reaction barrier heights – can be treated accurately in a rigorous fashion.