Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Charge-transfer reactions, energy gaps, and electron-transfer diabatic surfaces NICOLA MARZARI, P. H.-L. SIT, Department of Materials Science and Engineering, MIT — Density-functional theory in the LDA or GGA approximation has become the widely-used standard model of condensed matter theory. I will discuss shortcomings and solutions to some of the problems that arise when addressing complex chemical reactions. These challenges include the correct description of electron-transfer processes, where electrons become delocalized and shared between ions that should be in different oxidation states. An effective solution can be obtained by introducing a penalty functional that imposes the correct charge state on the ions involved in the reaction [1]. This approach is validated in a model system, showing that the ground state and the charge-transfer excited state can be calculated with negligible errors, and then applied to the determination of the diabatic free-energy surfaces for ferrous and ferric ions in solution. [1] P. H.-L. Sit, Matteo Cococcioni and Nicola Marzari, Phys. Rev. Lett. 97, 028303 (2006).

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Date submitted: 20 Nov 2006 Electronic form version 1.4