

MAR09-2008-005055

Abstract for an Invited Paper
for the MAR09 Meeting of
the American Physical Society

Insights and Progress in Density Functional Theory.

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Density functional theory of electronic structure is widely and successfully applied in simulations throughout engineering and sciences. However, there are spectacular failures for many predicted properties, which can be traced to the delocalization error and static correlation error of commonly used approximations. These errors include underestimation of the barriers of chemical reactions, the band gaps of materials, the energies of dissociating molecular ions and charge transfer excitation energies. Typical DFT calculations also fail to describe degenerate or near degenerate systems, as arise in the breaking of chemical bonds, and strongly correlated materials. These can all be characterized and understood through the perspective of fractional charges and fractional spins introduced recently. Understanding the errors of functionals in the simplest way possible — as violations of exact conditions for fractional charges and fractional spins — opens the path forward for reduction of the errors and for applications of density functional theory in new frontiers. [P. Mori-Sanchez, A. J. Cohen, and W. T. Yang, *Phys. Rev. Lett.* 100:146401(2008); *Phys. Rev. B*,77:115123(2008); *J. Chem. Phys.* 129:121104(2008); *Science*, 321:792(2008)]

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