Prospects for Self-Interaction Corrected Density-Functionals with Unitary Invariance: Applications to Molecules

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Gradient corrected density-functionals, such as PW91 and PBE GGA[1], have proved to be very successful for describing materials and molecular properties. In applications to spin-ordered molecular magnets, gradient corrected density functionals have allowed for the calculation of spin excitations and magnetic anisotropies with relatively good success[2]. However, improvements in these functionals are necessary if one is interested in obtaining quantitatively accurate spin excitations in molecules containing 3d transition metal ions, extending these methods to systems containing f electrons, or in understanding transport across such molecular magnets tethered to electrodes. In this talk, I review some of the general improvements that have been offered by the Perdew-Zunger self-interaction correction (SIC) and past approaches to solving these equations[3]. A new version of the self-interaction correction to density functional theory is briefly introduced[4-5] which seems to be simpler to use and which provides two formal improvements over the original version. Applications of this SIC, within the local spin-density approximation, give improvements to atomization energies of molecules, total energies and ionization energies in atoms, and the uniform electron gas is obtained. By example, it is shown that the method is fast enough to apply to systems with open metal centers such as porphyrins.