

Self-interaction correction for magnetic molecules

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The self-interaction error in density functional approximations is responsible for a number of errors in calculated properties such as smaller band gap, delocalization error, incorrect asymptotic decay etc. The self-interaction error can often lead to wrong spin states with density functional theory in systems with transition metal atoms. We present benchmark calculations on the self-interaction error in small transition metal oxide molecules and molecular magnet with Fermi Lowdin Orbital based self-interaction correction (FLOSIC) method. FLOSIC has been shown to provide improved description of a number of properties earlier such as atomization energies, magnetic coupling, dissociation energies, polarizabilities for organic and inorganic molecules etc. In this work, several systems with under-coordinated transition metal oxide molecules are chosen to assess its effectiveness for d-electron systems. Another application to be presented is on a Cu₂ molecular magnet. The properties of such molecules are highly dependent on the density functional approximations. The effect of self-interaction correction with local density approximation, generalized gradient approximation and with metaGGA functionals will be presented.