Structure, magnetic feature, open procedure interaction from density and self compatible hybrid methods

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Abstract

In the recent developments of density function methods; this array is allocated to the compression density function theory in the most important structural blocks of recognizing density theory and analyzing stages which include open consistent types. After discussion about theory, I want to report some selected studies to indicate potentials local limits and gradient modified density functions in contrast with structural, spectrometry, thermo chemical and kinetic energy. At the same time, I introduce you self compatible hybrid methods which gradient modified functions received by adding Hartree-Fock exchange.

Moreover, two basic group of EPR-II and EPR-III are introduced which optimized by density function methods to calculate permanent paired constants. EPR-II includes zeta paired basic groups as well as a single series of polar functions and an improved section of S. EPR-III include a series of triple zeta which contains influence function, double polar functions and single starting functions.

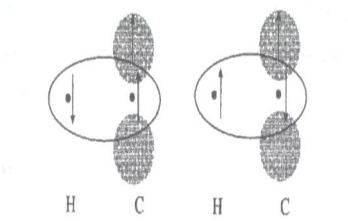

Fig. spin polarization mechanism

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