Spin-Flip DFT, Effective Hamiltonians, and Molecular Magnetism

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ABSTRACT

Spin-flip approach provides a simple solution for certain types of strongly correlated systems, which traditionally are described as "multi-reference". It can be used both within wave-function methods and within DFT. Originally developed for diradicals and triradicals, SF method can be applied to systems with more extensive degeneracies by using effective Hamiltonian approach. When augmented with calculations of properties (e.g., spin-orbit couplings), SF-DFT provides effective and reliable tool for computational studies of molecular magnetism.

References

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