

Abstract Submitted
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Local spin analyses using density functional theory BAYILEYEGN ABATE, JUAN PERALTA, Central Michigan University — Local spin analysis is a valuable technique in computational investigations magnetic interactions on mono- and polynuclear transition metal complexes, which play vital roles in catalysis, molecular magnetism, artificial photosynthesis, and several other commercially important materials. The relative size and complex electronic structure of transition metal complexes often prohibits the use of multi-determinant approaches, and hence, practical calculations are often limited to single-determinant methods. Density functional theory (DFT) has become one of the most successful and widely used computational tools for the electronic structure study of complex chemical systems; transition metal complexes in particular. Within the DFT formalism, a more flexible and complete theoretical modeling of transition metal complexes can be achieved by considering noncollinear spins, in which the spin density is 'allowed to' adopt noncollinear structures in stead of being constrained to align parallel/antiparallel to a universal axis of magnetization. In this meeting, I will present local spin analyses results obtained using different DFT functionals. Local projection operators are used to decompose the expectation value $\langle S^2 \rangle$ of the total spin operator; first introduced by Clark and Davidson.

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