

Understanding the Exchange Interaction between Paramagnetic Metal Ions and Radical Ligands: DFT and Ab Initio Study on Semiquinonato Cu(II) Complexes

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The exchange coupling, represented by the J parameter, is of tremendous importance in understanding the reactivity and magnetic behavior of open-shell molecular systems. In the past, it was the subject of theoretical investigations, but these studies are mostly limited to the interaction between metallic centers. The exchange coupling between paramagnetic metal ions and radical ligands has hitherto received scant attention in theoretical studies, and thus the understanding of the factors governing this interaction is lacking. In this paper, we use DFT, CASSCF, CASSCF/NEVPT2, and DDCI3 methods to provide insight into exchange interaction in semiquinonato copper(II) complexes. Our primary objective is to identify structural features that affect this magnetic interaction. We demonstrate that the magnetic character of Cu(II)-semiquinone complexes are mainly determined by the relative position of the semiquinone ligand to the Cu(II) ion. The results can support the experimental interpretation of magnetic data for similar systems and can be used for the in-silico design of magnetic complexes with radical ligands.

Słowa kluczowe

radicals, semiquinone, exchange coupling, DFT, ab initio, ferromagnetism, antiferromagnetism, broken symmetry

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