

密度泛函理论在分子磁学中的应用

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摘要 通过对桥联双核铁的磁耦合常数的计算,探讨了密度泛函理论计算条件对计算结果的影响。基于密度泛函理论下的破损态方法,着重讨论了双核 Fe(III)₂的 d_{xy}-d_{xy}电子通过氧桥的超交换作用。研究发现分子的反铁磁通道主要是Fe(III) d_{xy}和d_{xy}与μ-O的p轨道形成的,具有π*/π*和σ*/σ*特征的超交换通道。

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Application of Density Functional Theory in Molecular Magnetism

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Abstract Based on the density functional theory (DFT) combined with the broken symmetry (BS) approach, the magnetic coupling constant of the oxo-bridged iron (III) dimer [Cl₃FeOFeCl₃]²⁻ has been obtained under the various computational conditions in ADF code, including the numerical integration precision parameter, exchange-correlation energy functional and basis sets. The superexchange interactions between d_{xy}-d_{xy} unpaired electrons were also discussed, and the antiferromagnetic coupling of the title compound was attributed to the superexchange pathway characterized by π*/π* and σ*/σ* , coming from the d_{xy} and d_{xy} orbitals on Fe(III) ions and p orbital on μ-O atom.

Key words [IRON COMPOUNDS](#) [MAGNETISM](#) [density functional theory](#) [MOLECULAR ORBITAL THEORY](#)

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