Optimized Geometry of the Cluster Gd_2O_3 and Proposed Antiferromagnetic Alignment of f-electron Magnetic Moment

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Abstract

There is currently experimental interest in assemblies of Gd_2O_3 clusters. This has motivated the present study in which a single such cluster in free space is examined quantitatively by spin-density functional theory, with appropriate relativistic correction incorporated for Gd. First the nuclear geometry of the cluster is optimized and found to be such that the two Gd atoms lie in a symmetry axis perpendicular to the isosceles triangle formed by the O atoms. Then, a careful study is made of the magnetic arrangement of the localized f-electron moments on the two Gd atoms. The prediction of the present treatment is that the localized spins are aligned antiferromagnetically. An alternative picture using superexchange ideas leads to the same conclusion.

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