

Abstract Submitted
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A comprehensive study of the structure and magnetic properties of Gd13 Cluster KUN TAO, PURU JENA, Department of physics, Virginia Commonwealth University, Richmond, VA — Several experimental and theoretical studies of Gd13 cluster have led to confusing results. While experimental studies using Stern-Gerlach technique yield different magnetic moments, theoretical studies provide different spin orientations and structures. We have carried out a comprehensive study of the structure-magnetic property relationship of Gd13 cluster by examining different isomers. Our calculations are based on density functional theory with GGA+U and takes into account spin-orbit interactions and spin canting. The cluster with icosahedra structure and collinear spins has the lowest energy irrespective of the level of theory used. However, the magnetic coupling between the central and surface atoms does depend upon the value of U. For U=0 the magnetic coupling in the ground state structure is antiferromagnetic between the central and surface atoms. The coupling changes to ferromagnetic when $U > 4$. The effect of temperature on the observed magnetic moment is also studied using Monte Carlo simulation.

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