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B and C doped Cuboctohedral Mn_{13} Clusters with Giant Magnetic Moments PURU JENA, MENGHAO WU, Physics Department, Virginia Commonwealth University, Richmond, VA 23284, PROF.JENA TEAM — Using first-principles calculations based on gradient corrected density functional theory we show that an otherwise distorted icosahedric Mn_{13} ferrimagnetic cluster, when doped with six B or C atoms, transforms into a ferromagnetic cuboctahedral cluster with a magnetic moment that is an order of magnitude larger than that of the pure Mn_{13} cluster. The origin of this magnetic transition is attributed to the change in the Mn-Mn interatomic distance resulting from the structural transformation. These doped clusters remain ferromagnetic with giant moments even after removing a B or C atom. However, similar doping with N atom does not lead to ferromagnetic ordering and $Mn_{13}N_6$ remains ferrimagnetic with a magnetic moment of only 3 μ_B, just as in its parent Mn_{13} cluster.

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