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Stability and Magnetic Coupling between Mn doped Stannaspherenes ANIL KANDALAM, GANG CHEN, PURU JENA, Virginia Commonwealth University — The discovery of carbon fullerenes has stimulated considerable interest in the search of cage clusters involving not only group IV elements but also metallic systems. The recent discovery of stannaspherene, a highly stable Sn_{12}^{2-} hollow cage cluster with a reported diameter of 6.1 Å has triggered a renewed interest in the search for stable endohedral cage complexes with $3d$ transition metal atoms as dopants. It is anticipated that these complexes may carry large magnetic moments and can be used as building blocks for novel magnetic materials. We report the first density functional theory based study of the interaction between two Mn doped stannaspherenes ($Mn@Sn_{12}$) and show that $Mn@Sn_{12}$ is not only highly stable and carry a magnetic moment of 5 μ_B, but the clusters retain their structural identity even when they interact with each other. Equally important, the magnetic coupling depends strongly on the orientation of the clusters. We believe that these new results would encourage the scientific community to explore the possibility of synthesizing novel magnetic materials with magnetic element doped Sn_{12} clusters as building blocks.

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