Magnetic Properties of $[Mn_n]Ce_m$ Clusters

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Abstract

Manganese oxide single-molecule magnets $[Mn_n]$ (with *n* up to 84) have attracted much attention in the last few decades. More recently, $[Mn_n]Ce_m$ compounds have been synthesized. Using first-principles quantum calculation, we studied several $[Mn_n]Ce_m$ clusters including Mn_3Ce_2 and Mn_5Ce_3 with three different ligands. Magnetization in these clusters is mainly from the Mn ions. The magnetic interaction between the Mn ions can be either ferromagnetic or antiferromagnetic. We investigated energies of all spin configurations for each molecule. We fitted the total energies from first-principles calculations to Heisenberg model and extracted the exchange parameters, *J*. The *J* values from first-principles calculations and *J*'s from the experimental susceptibility curve were compared. Pathways of magnetic interaction were analyzed using the Wannier function method.