The role of ligands in controlling the electronic structure and magnetic properties of Mn_4 single-molecule magnets

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Abstract: We present our studies of electronic structure and magnetic properties of $Mn^{4+}Mn_3^{3+}$ single-molecule magnets (SMM), i.e, $[Mn^{4+}Mn_3^{3+}O_3Cl_4(OAc)_3(py)_3]$ (py = pyridine) and $[Mn^{4+}Mn_3^{3+}O_3Cl(OAc)_3(dbm)_3]$ (dbmH = dibenzoyl-methane) molecules by using a first-principles all-electron relativistic method within spin-polarized density functional theory. To investigate the possibility of ligands controlling the electronic structure and magnetic properties, we designed and calculated the geometric and electronic structures of twelve other $Mn^{4+}Mn_3^{n+}$ (n = 2, 3, 4) molecules with different peripheral-ligand configurations. The electronic structure of Mn^{n+} ions, and the interatomic distances, electronic structure and magnetic properties of $Mn^{4+}Mn_3^{n+}$ molecules display an interesting variation with n.

Author Keywords: First-principles calculation; Mn clusters; Molecular design; Nano-piezomagnets; Single-molecule magnets

Index Keywords: Density functional theory; Electronic properties; Electronic structure; Ligands; Magnetic materials; Magnetic properties; Magnets; Manganese; Manganese alloys; Methane; Molecules; Solid state physics; Structural properties; First-principles calculation; Mn clusters; Molecular design; Nano-piezomagnets; Single-molecule magnets; Manganese compounds

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