# Endohedral stannaspherenes: $Mn@Sn_{12}$ and its dimer. Ferromagnetic or antiferromagnetic?

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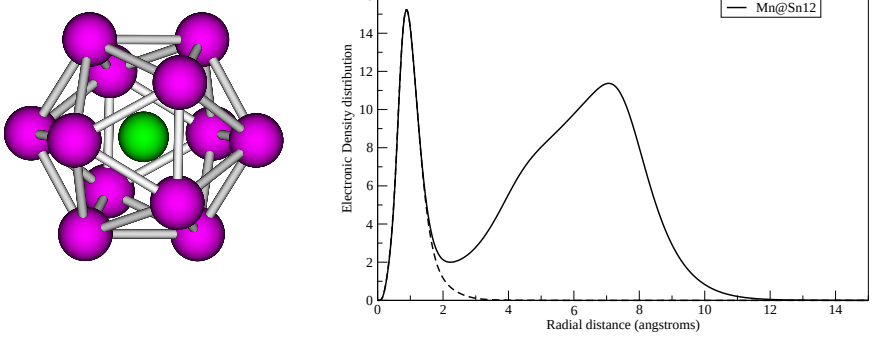
The endohedral $Mn@Sn_{12}$ has been characterized, where a $Mn^{2+}$ cation is trapped inside an icosahedral $Sn_{12}^{2-}$, also called stannasphere, as can be seen in Figure 1. This endohedral structure is a sextuplet, with the 3d orbitals of $Mn^{2+}$ singly occupied. Thermodynamically, this encapsulation process is highly permitted, being the encapsulation free energy of around 24 kcal/mol. These monomers yields to a ferromagnetic or antiferromagnetic coupling in the case of the dimer. Three different dimers have been tried. The difference between dimers is the orientation of the monomers, where one atom of one monomer faces one atom, or two atoms another two, or finally three atoms face other three atoms. The most stable dimer is the one where three atoms face another three. In all cases the ferromagnetic and the antiferromagnetic dimers are near degenerate.

Figure 1: Structure of the ground state of the endohedral $Mn@Sn_{12}$ (left) and its radial electronic density distribution (right)

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