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Electronic and magnetic properties of endohedrally doped fullerene Mn@C_{60}: An all electron theoretical study[1] R.F. SABIRIANOV , G.P. LI, JING LU, W.N. MEI, Department of Physics, University of Nebraska at Omaha , X.C. ZENG, Department of Chemistry, University of Nebraska-Lincoln — In this work we calculated the total energy of a Mn atom encapsulated inside C_{60} cage by using GGA density functional theory at the PBE/PAW level. We found that the magnetic properties of free Mn are preserved when the atom is located at the central region and spin multiplicity M = 6 has the lowest energy among M = 6, 4 and 2. When we started to shift Mn away from the center, the energy and spin multiplicity initially remained the same, then gradually dropped when Mn reached about the half way between the center and edge of cage. The spin multiplicity M changed to 4 at a local minimum with energy lower than that at the center by about 0.2 eV. As we kept on moving Mn towards to the edge, the total energy increased monotonically and the spin multiplicity M reduced to 2. Hence the energy curve has two identical minima situated symmetrically with respect to the center of the cage.

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