Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Magnetic nanodomains in small Mn_n clusters: a non collinearab initio study ALDO HUMBERTO ROMERO, Advanced Materials, IPICyT, San Luis Potosi, Mexico, JOSE MEJIA-LOPEZ, Physics Department, Pontificia Universidad Catolica de Chile, Chile, JOSE LUIS MORAN-LOPEZ, Advanced Materials, IPICyT, San Luis Potosi, Mexico, MARTIN GARCIA, Theoretische Physik, Fachbereich Naturwissenschaften,Universität Kassel, Germany — Small manganese clusters show an intriguing magnetic behavior[1-3]. with signatures of super paramagnetism and magnetic moments smaller than $1.5\mu_B$ per atom. This fact has called the attention of scientists due to the possibility of using Mn clusters as molecular magnets. Here we discuss the magnetic properties of small magnetic clusters by considering different topologies. Our calculation, a localized orbital pseudopotential, we include non collinear magnetism to describe the electronic properties. We find that only few clusters show noncolliner effects and the majority are collinear. We can assign a exchange constant that we find is antiferromagnetic to small distances and ferromagnetic to large distances, with this exchange we can use a Heisenberg Hamiltonian with dipolar interaction and we find very close results to the ab initio calculations, except that the noncollinear effect is much larger. Perspectives or our observations to larger clusters will be discussed. [1] M. B. Knickelbein, Phys. Rev. Lett **86** 5255 (2001). [2] K. M. Mertes *et al* Sol. Stat. Comm. **127** 131 (2003). [3] R. J. Van Zee *et al* J. Chem Phys. **76** 5636 (1982).

Aldo Humberto Romero
Advanced Materials, IPICyT, San Luis Potosi, Mexico

Date submitted: 26 Nov 2004 Electronic form version 1.4