Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

***Ab initio* study of the possibility of noncollinear magnetism in small Mn clusters**[1] R.C. LONGO, MANUEL ALEMANY, Universidad de Santiago de Compostela, Spain, J. FERRER, Universidad de Oviedo, Spain, A. VEGA, Universidad de Valladolid, Spain, L.J. GALLEGO, Universidad de Santiago de Compostela, Spain — We investigated the possibility of noncollinear magnetism in small Mn_n clusters (n = 2-6) using the density-functional method SIESTA with the generalized gradient approximation (GGA) to exchange and correlation. The lowest-energy states identified were ferromagnetic for Mn_2 and Mn_3, and magnetically noncollinear for Mn_4, Mn_5 and, most decidedly, Mn_6. These SIESTA/GGA results, which are compared with those of an earlier SIESTA study that used the local spin density approximation, are qualitatively in keeping with the result obtained by VASP/GGA calculations.

[1]Work supported by the Spanish Ministry of Education and Science (Projects FIS2005-04239, FIS2006-12117-C04-04, MAT2005-03415 and Program "Ramon y Cajal"), by the Junta de Castilla y Leon (Grant No.VA068A06), and by the Galician Supercomputing Center.

Manuel Alemany
Universidad de Santiago de Compostela, Spain

Date submitted: 26 Nov 2007 Electronic form version 1.4