

Abstract Submitted
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***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.

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