

# Influence of local atomic disorder on the electronic and magnetic properties of Ni<sub>2</sub>MnGa Heusler alloy

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The electronic and magnetic properties of Ni<sub>2</sub>MnGa Heusler alloy depend strongly on the atomic disorder in the fcc sublattices of L2<sub>1</sub> type structure and the tetragonal distortion. In this work we present the electronic structure of Ni<sub>2</sub>MnGa obtained by ab-initio methods, SIESTA [1-2] and LMTO [3]. We study the influence of the atomic disorder on the shape of the density of states near the Fermi level as well the effect of the tetragonal distortion. Using the SIESTA code we have shown that the shape of the density of states depends on the form of the pseudopotentials and the parametrization of the exchange-correlation potentials.

[1] SIESTA 1.3 <http://www.uam.es/siesta>

[2] J.M.Soler, E.Artacho, J.Gale, A.Garcia, J.Junquere, P.Ordejon, D.Sanchez-Portal, J.Phys.Cond. Matter **14**, 2745 (2002)

[3] O.K.Andersen, O.Jepsen, Phys. Rev. Lett. **53**, 2572 (1984)

13.4 cm

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9.7 cm