Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Structural and magnetic properties of Ni_2MnGa from first-principles VAMSHI KATUKURI, BURAK HIMMETOGLU, MATTEO COCOCCIONI, CEMS University of Minnesota — Ni_2MnGa is the prototype magnetic shape-memory alloy. In this work we use ab-initio calculations to characterize structural and magnetic transitions and to identify possible strategies to tune them towards the same critical point. To this aim both the austenite and the martensite phases of the Ni_2MnGa alloy are studied with particular attention to the electronic factors controlling their stability and the onset of the structural transition. Our results indicate that, in spite of its metallic character, electronic correlations play an important role in determining the behavior of this compound and, in particular, the entity (and sign) of the deformation accompanying the transition from the austenite phase to the martensite one. The vibrational properties of the austenite phase are also studied and structural instabilities (soft modes) are investigated as possible signatures of intermediate "modulated" structures.

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Date submitted: 19 Nov 2010 Electronic form version 1.4