

Abstract Submitted
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Accounting for spin fluctuations beyond LSDA in the density functional theory¹ LUCIANO ORTENZI, Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany, IGOR I. MAZIN, Naval Research Laboratory, 4555 Overlook Avenue SW, Washington, D.C. 20375, USA, PETER BLAHA, Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria, LILIA BOERI, Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — We present a method to correct the magnetic properties of itinerant systems in local spin density approximation (LSDA) and we apply it to the ferromagnetic-paramagnetic transition under pressure in a typical itinerant system, Ni₃Al. We obtain a scaling of the critical fluctuations as a function of pressure equivalent to the one obtained within Moriya's theory. Moreover we show that in this material the role of the bandstructure is crucial in driving the transition. Finally we calculate the magnetic moment as a function of pressure, and find that it gives a scaling of the Curie temperature that is in good agreement with the experiment. The method can be easily extended to the antiferromagnetic case and applied, for instance, to the Fe-pnictides in order to correct the LSDA magnetic moment.

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