

Abstract Submitted  
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**Magnetism in FeAl, Ni<sub>3</sub>Al and Ni<sub>3</sub>Ga within DFT: Importance of asymmetry in the Exact Exchange potential** SANGEETA SHARMA, KAY DEWHURST, CLAUDIA AMBROSCH-DRAXL, Univeristy Graz, CLAS PERS-SON, KTH Stockholm, EXCITING GRAZ TEAM, EXCITING UPPSALA TEAM — We have calculated the magnetic properties of FeAl, Ni<sub>3</sub>Al and Ni<sub>3</sub>Ga with exact exchange DFT within the all-electron full-potential linearized augmented-plane-wave method, including core-valence interactions. The correct ground state for these materials is obtained in all cases: non-magnetic for FeAl and Ni<sub>3</sub>Ga and ferromagnetic in Ni<sub>3</sub>Al with a magnetic moment of 0.20  $\mu_B$  per formula unit, which is in excellent agreement with experiments. Both LDA and GGA fail to produce the correct magnetic ground state of all three compounds. This failure has been the subject of several investigations in the past. *Ad hoc* corrections to the LDA have been used to obtain the correct ground state for these materials, but are either not parameter free (LDA+*U*) or include dynamical variables (spin fluctuations) which are closer in spirit to the quasi-particle picture. We attribute the success of exact exchange to the strong asymmetry in the exchange potential. This should be a desirable feature for next generation approximate functionals.

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