Electronic structure and magnetic properties of $L1_0$ binary compounds

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Materials exhibiting a large saturation magnetization (M_s), high Curie temperature (T_C), as well as a large magnetic anisotropy energy (MAE), are of great technological importance in a wide range of permanent magnet applications. Certain $L1_0$ ordered binary compounds reveal large MAE without containing scarce elements, such as platinum or rare-earths, making them potentially interesting from a technological perspective. In this work a combination of two different density functional theory (DFT) methods and Monte Carlo (MC) simulations is used for a thorough investigation into the electronic structure and magnetic properties of $L1_0$ structured binary compounds FeNi, CoNi, MnAl and MnGa. Large MAEs, in the order of 1 MJ/m^3 and higher, as well as high Curie temperatures, far above room temperature, are presented. Some investegation is also done into the effect of substitutional disorder and off stoichoimetric compositions. Disorder tends to decrease both MAE and T_C while going off stoichoimetry turns out to be important for the stability of a ferromagnetic phase in Mn-based compounds.