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Interatomic exchange in Mn-based alloys[1] PRIYANKA MANCHANDA, RALPH SKOMSKI, Univ of Nebraska - Lincoln, ARTI KASHYAP, IIT Mandi, DAVID SELLMYER, Univ of Nebraska - Lincoln — The ongoing quest for new rare-earth free permanent magnets includes the search for new magnetic phases with high magnetization and magnetic anisotropy. Manganese alloys could be used because Mn^{2+} ion has a moment of 5 μ_B per atom. However, manganese is in the middle of the $3d$ transition-metal series, and it is well-known and easily explained in terms of general electronic structure trends that such elements prefer to form antiferromagnetic (AFM) rather than ferromagnetic (FM) spin structures. Most of the Mn compounds are antiferromagnetic and the few existing ferromagnetic compounds, such as MnAl and MnBi, have low magnetization, of the order of 1 μ_B per atom. In this presentation, we used first-principle calculations to study interatomic exchange in Mn based alloys. As a model system, we use $L1_0$-ordered MnAl. Interestingly, we find a strong ferromagnetic interatomic exchange in the Mn planes of the alloy, in spite of the short Mn-Mn interatomic distances. Furthermore, we study modifications of the $L1_0$ structure, such as the effect of Fe substitution on the exchange interactions in MnAl derivatives.

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