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Layered antiferromagnetism with high Neel temperature in the intermetallic compound Mn_2Au SERGII KHMELEVSKYI, PETER MOHN, Center for Computational Materials Science, Vienna University of Technology, CMS TEAM — On the basis of earlier experimental studies the intermetallic compound Mn_2Au has been characterized as a non-magnetically ordered material. Here we report the results of first-principles calculations based on Local Spin-Density Approximation which describe Mn_2Au to have a narrow band antiferromagnetic ground state with rigid local moments on the Mn sites. Calculations of the inter-atomic exchange constants based on the magnetic force theorem and a Monte-Carlo modeling of the resulting Heisenberg-like Hamiltonian predict a very high Neel-temperature of $\sim$1580K. This temperature is considerably higher than for the other known high-temperature antiferromagnetic $L1_0$-type Mn based binary alloys, which are widely used in magnetic storage applications. The source of the difficulties in determining magnetic order from the earlier experiments is discussed. The observed metamagnetic like behavior and a susceptibility anomaly at low temperatures are linked to the frustrated magnetism on Mn anti-site impurities. We believe that the high temperature antiferromagnetism of Mn_2Au may have quite an impact in technology. In particular, it can be considered as a candidate for the application as a "pinning" layer in GMR devices.

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