HIGH CURIE TEMPERATURES IN (GA,MN)N FROM MN CLUSTERING.

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The effect of microscopic Mn cluster distribution on the Curie temperature (T_C) is studied using the spin-polarized total energy density functional calculations with the projector augmented wave method. We find that the calculated T_C depends crucially on the microscopic cluster distribution. The partially dimerized Mn_2-Mn_1 distribution is found to give the highest T_C. In general, the presence of the Mn_2 dimer has a tendency to enhance T_C. The lowest T_C values are obtained for the Mn_4 -Mn_1 and Mn_4-Mn_3 distributions. In general, the presence of the symmetric Mn_4 tetramer has a tendency to suppress T_C to very low temperatures.

References:

T. Hynninen, H. Raebiger, A. Ayuela, and J. von Boehm, Appl. Phys. Lett. (accepted).