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Mn clusters: a nanoscale magnetic transition SUDHA SRINIVAS, KOBLAR A. JACKSON, PETIA BOBADOVA-PARVANOVA, MIHAI HOROI, Department of Physics, Central Michigan University, Mt. Pleasant, MI 48859 — Small Mn clusters exhibit remarkable magnetic behavior. Early ESR experiments[1] found the smallest clusters (n=2-5) to be ferromagnetic (FM), while later Stern-Gerlach measurements[2] found larger clusters (n>12) to have very small net moments. Our calculations show that these data reflect a transition in magnetic *ordering* as a function of cluster size, occurring at n=7 atoms. Specifically, the FM arrangements of the atomic spins favored in smaller clusters give way to antiferromagnetic (AF) arrangements in larger clusters. We find that the FM $\rightarrow$ AF transition occurs at n=7, in agreement with experimental data, and is driven by a large change in the relative energies of the FM and AF structures. We present results for the structures and magnetic properties of Mn_n (n = 2-13), focusing on correlations between the structural, electronic and magnetic properties of the clusters and discuss the effect of substitutional impurities on the magnetic properties of the clusters.

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2. M. B. Knickelbein, Phys. Rev. Lett. **86**, 5255 (2001).

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