Abstract Submitted
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Effect of Hydrogen Absorption on the Magnetic Moment and Anisotropy of Fen and Con Clusters[1] M.R. BELTRAN, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, A.P. 070-360, C.P. 04510 Mex.D.F., N.O. JONES, S.N. KHANNA, Physics Department, Virginia Commonwealth University, Richmond, VA 23284-2000, T. BARUAH, M.R. PEDERSON, Complex Systems Theory, Naval Research Laboratory, Washington, D. C. 20375 — Theoretical investigations have been carried out to examine the effect of H absorption on the magnetic moment and anisotropy of small Fe_n and Co_n clusters. Our studies use a gradient corrected density functional approach and cover clusters containing up to 4 transition metal and 2 H atoms. We show that the successive addition of H atoms can lead to monotonic or oscillatory change from the free cluster magnetic moment. An analysis of the density of electronic states shows that the variations in the magnetic moment can be related to the location of the lowest unoccupied molecular orbital in the parent cluster. It is shown that the addition of hydrogen can substantially change the magnetic anisotropy, yielding a particularly high magnetic anisotropy for Co_3H_2 that is higher than the known molecular nano-magnets.

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