Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Dynamical Mean-Field Theory approach to study the magnetic properties of nanostructures[1] NEHA NAYYAR, Department of Physics, University of Central Florida , VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NSTC, University of Central Florida — We extend the Nanoscale Dynamical Mean-Field Theory (NDMFT) approach [1] to study the magnetic properties of nanosystems. It is shown that the NDMFT solution becomes more accurate when the number of atoms in the cluster and their coordination number increase. We applied this method to study the magnetic properties of small cobalt clusters. The dependence of the cluster magnetization on the geometry, temperature and Coulomb repulsion energy was analyzed. We estimate the value of the Coulomb repulsion energy parameter, which is necessary to reproduce the experimental results in the case of different clusters. We compare our results with other approximations including GGA and GGA+U. In particular, we show that the last approximation in general overestimates the role of correlation effects. [1] S. Florens, Phys. Rev. Lett. 99, 046402 (2007)

[1]Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354

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Date submitted: 20 Nov 2009 Electronic form version 1.4