Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electronic and Magnetic Structure of Fe Nanoparticle Embedded in FeAl[1] YANG WANG, Pittsburgh Supercomputing Center, G. MALCOLM STOCKS, AURELIAN RUSANU, DON M.C. NICHOLSON, MARKUS EISENBACH, Oak Ridge National Laboratory, J.S. FAULKNER, Florida Atlantic University — Magnetic nanostructures are of great scientific interest because of their potential applications in a wide range of technologies - data storage, magnetoelectronics, permanent magnets, smart drug delivery, etc. Unfortunately magnetic nanostructures present substantial theoretical challenges due to the need to treat the electronic interactions quantum mechanically whilst dealing with a, still, large number of atoms. In this presentation, we discuss our recent studies of magnetic nanoparticles using the Locally Self-consistent Multiple Scattering (LSMS) method, an order-N *ab initio* method capable of treating tens of thousands of atoms. In particular, we show results for a Fe nanoparticle embedded in a stoichiometric B2-FeAl binary alloy. The Fe nanoparticle, has the shape of a BCC Wigner-Seitz cell, contains 4,409 Fe atoms, and measures about 5 nm across the diagonal corners. Including the surrounding matrix the calculation involves 16,000 atoms. We show results for the moment and charge distribution within nanoparticle, on the facets, and in the FeAl matrix.

[1]The research of GMS, DMCN, ME, and AR is sponsored by DOE-OS, BES-DMEP under contract number DE-AC05-00OR22725 with UT-Battelle LLC. Calculations were performed at PSC, NERSC and ORNL-CCS.

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Date submitted: 28 Nov 2005 Electronic form version 1.4