

Abstract Submitted  
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**First Principles Approach to the Magnetic Structure of Realistic Models of Nanoparticles**<sup>1</sup> G. MALCOLM STOCKS, AURELIAN RUSANU, DON NICHOLSON, MARKUS EISENBACH, Oak Ridge National Laboratory, YANG WANG, Pittsburgh Supercomputer Center, SAM FAULKNER, Florida Atlantic University — Magnetic nanostructures are of great interest because of their potential applications in a wide range of technologies - data storage, magneto-electronics, 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 – e.g., a 5nm cube of Fe contains  $\sim 12,000$  atoms, 4,000 of which are in the surface and subsurface layers. Here, we discuss a new implementation of the *ab initio* order-N Locally Self-consistent Multiple Scattering (LSMS) method that is capable of treating tens of thousands of atoms. We will present scaling data that show the performance of the code both in the real space mode of the original method and in the k-space mode based on screened structure constants and sparse matrix solvers. Illustrative results will be shown for a BCC Fe-nanoparticle embedded in a stoichiometric B2-FeAl binary alloy, a magnetic nanostructure model containing 16,000 atoms.

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