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Linear scaling *ab initio* approach to the electronic structure calculation for L1₀-FePt nanoparticles embedded in FePt random alloy YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, G. MALCOLM STOCKS, AURELIAN RUSANU, DON NICHOLSON, MARKUS EISENBACH, Oak Ridge National Laboratory, QIMING ZHANG, J.P. LIU, University of Texas at Arlington — Magnetic nanostructures present substantial theoretical challenges due to the need to treat the electronic interactions quantum-mechanically whilst dealing with a large number of atoms. In this presentation, we show a direct quantum mechanical simulation of magnetic nano-structures made of spherical L1₀-FePt nanoparticles, with diameter within 2.5 nm \sim 5 nm, embedded in an fct-FePt random alloy. The calculation is performed using the locally self-consistent multiple scattering method, a linear scaling *ab-initio* all-electron method capable of treating tens of thousands of atoms. We found that there exists a screening region below the surface of each nanoparticle which essentially screens out the effect of the external random alloy to keep the physical properties of the interior region unchanged from the bulk of L1₀-FePt. Interestingly, the depth of this screening region is independent of the size of the nanoparticles we have investigated. We will show a non-collinear electronic structure calculation for the nano-structure and discuss the exchange coupling between the nanoparticle and the surrounding random alloy.

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