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Role of disorder and structural inhomogeneity on the magnetic structure of FePt nanoparticles PAUL KENT, DON NICHOLSON, MARKUS EISENBACH, THOMAS SCHULTHESS, Oak Ridge National Laboratory, Oak Ridge, TN — Recent experiments (e.g. [1]) have demonstrated a substantial increase in Fe magnetic moment on annealing of FePt nanoparticles, underscoring the likely importance of local composition variations at the nanoscale. To test these ideas, we have calculated the magnetic structure of FePt nanoparticles up to 3nm in size using density functional theory. We investigate the role of disorder and the influence of explicitly constructed Fe and Pt rich regions, both at the center and at the surface of the particles. The size and disorder dependent spin-moment distributions are related back to changes in the electronic structure of the materials relative to the bulk. Even for 3nm nanoparticles, the magnetic structure deviates significantly from the bulk due to the large fraction of near-surface atoms. Structural relaxation is shown to significantly influence the magnetic structure, particularly reducing the magnetic moments of surface atoms. This work used resources of the National Center for Computational Sciences at Oak Ridge National Laboratory (ORNL) and is supported in part by the Division of Scientific User Facilities, U. S. Department of Energy as well as the Laboratory Directed Research and Development program at Oak Ridge National Laboratory. [1] C. Antoniak *et al.* Phys. Rev. Lett **97** 117201 (2006).

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