Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Density functional calculations of the magnetic structure of FePt nano-particles P.R.C. KENT, University of Tennessee, TN, D.M.C. NICHOLSON, Metals and Ceramics Division, Oak Ridge National Laboratory, M. EISENBACH, Metals and Ceramics Division, Oak Ridge National Laboratory, T.C. SCHULTHESS, Computer Science and Mathematics Division, Oak Ridge National Laboratory — The spin moment distribution in magnetic nano-particles is both scientifically interesting and technologically relevant. Here, we discuss the magnetic structure of FePt nano-particles, as determined by projector-augmented wave (PAW) and locally self-consistent multiple scattering (LSMS) local density calculations on nano-particles up to 3nm in size. The magnetic structure changes as a function of nano-particle size, composition, and chemical order, encompassing both ferromagnetic and anti-ferromagnetic tendencies. This behavior will be described and related to charge redistribution, structural relaxation, and local coordination. This work was enabled by computational resources of the Center for Computational Sciences at Oak Ridge National Laboratory and is supported by the Division of Scientific User Facilities and the Division of Materials Science and Engineering, U. S. Department of Energy.

P.R.C. Kent
University of Tennessee, TN

Date submitted: 30 Nov 2005 Electronic form version 1.4