Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Magnetocrystalline anisotropy of L10 FePt nanoparticles[1] ALAMGIR KABIR, University of Central Florida, JUN HU, University of Calfornia Irvine, VOLODYMYR TURKOWSKI, University of Central Florida, RUQIAN WU, University of Calfornia Irvine, TALAT S. RAHMAN, University of Central Florida —
We perform theoretical investigation of Magneto Crystalline Anisotropy (MCA) of L10 FePt nanoparticles. Structural relaxation and magnetic moment of the clusters are evaluated using spin polarized *ab initio* density functional theory, and the MAE is calculated by using two approaches: (i) self-consistent inclusion of spin-orbit coupling and (ii) the torque method.[1] The clusters studied have 3(4) planes of Fe and 2(3) plane of Pt atoms and vice versa. We find an enhancement of MCA for the FePt clusters as compared to that of pure Fe nanoparticles and of bulk L10 FePt. We trace this enhancement to the increased spin and orbital moment of Pt atoms which raises the spin-orbit coupling. We also find that nanoparticles with Pt atoms in the central layer have larger MCA than the corresponding ones whose central layer is Fe. This is due to the fact that when Pt atom is the central layer it has more Fe atoms around so it more strongly hybridized resulting in higher orbital moments then Pt atoms on other layers. Detailed investigation of electronic structure of atoms on the clusters is also performed. Our finding can give useful insight to experimentalist for their studies of high density magnetic recording media. 1. X. D. Wang et al. Phys. Rev. B 54, 61(1996)

[1]Work Supported by DOE under Grant No. DOE-DE-FG02 -07ER46354

Alamgir Kabir
University of Central Florida

Date submitted: 15 Nov 2013 Electronic form version 1.4