Abstract Submitted
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Electron-electron correlations and magnetic properties of small FePt clusters[1] ALAMGIR KABIR, NEHA NAYYAR, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NSTC, University of Central Florida, Orlando, FL 32816 — We have applied the DFT+U and the Nanoscale Dynamical Mean-Field Theory (NDMFT) [1] approaches to study the magnetic properties of small FePt clusters. The role of correlation effects in determining the geometry and the magnetic properties of the clusters as a function of chemical composition and the effective local Coulomb repulsion energy U is examined. We find that the magnetization to decrease with increasing number of Pt atoms. Interestingly, contrary to the bulk case, Pt clusters have nonzero magnetization. The magnetic properties are found to be very sensitive to the value of U, as a result of the dependence of the single particle energy levels on this parameter. Dynamical correlation effects, which are taken into account in the DFT+DMFT approach and which lead to an increase of the average in time double occupancy of the d-orbitals, results in a significant decrease of magnetization as compared to the results from the DFT+U case.

[1] V. Turkowski et al, J. Phys.: Condens. Matt. 22, 462202 (2010)

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