

Abstract Submitted
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Magnetic properties of Fe nanoparticles: application of the DFT-Inhomogeneous-DMFT approach¹ ALAMGIR KABIR, Department of Physics, University of Central Florida, Orlando, Fl 32816, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NSTC, University of Central Florida, Orlando, Fl 32816 — Dynamical Mean-Field Theory (DMFT) in combination with Density Functional Theory (DFT) has been successfully applied to examine the properties of transition metal elements in which correlation plays an important role. It was recently shown that this approach can also be applied to study correlation effects in nanostructures [1]. Here we present results of a combined DFT-inhomogeneous-DMFT approach used to investigate the size dependent magnetic properties of small iron clusters containing 15 to 19 atoms. For the DMFT impurity solver we use the iterated-perturbation theory approximation. The numerical analysis with the code developed in our group allows one to study systems consisting up to several hundred atoms. The optimized structure of the Fe clusters is obtained from spin polarized DFT calculations. We find our approach to yield better agreement with experimental data [2] than that obtained using DFT and DFT+U, which generally overestimates the magnetization.

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

[2] M. B. Knickelbein, Chem. Phys. Lett. 353, 221(2002).

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