

Abstract Submitted
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Magnetic properties of Fe and Fe-Pt nanoparticles: application of nano-DFT+DMFT¹ ALAMGIR KABIR, Department of Physics, University of Central Florida, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NanoScience Technology Center, University of Central Florida, Orlando, FL — We apply a combined density-functional theory and dynamical mean-field theory (DFT + DMFT) approach [1] to handle reliably nanosized systems which display strong electron correlations. The code that we have recently developed allows one to examine systems containing several hundred atoms with feasible computational time. In particular, we calculate the magnetization of iron and iron-platinum nanoparticles by changing the system size (from 27 to 147 atoms), shape and composition. We demonstrate that the experimentally observed non-monotonous dependence of the magnetization as function of nanoparticle size can be rather accurately reproduced within DFT+DMFT, contrary to DFT and DFT+U approaches.

[1] V. Turkowski, A. Kabir, N. Nayyar and T.S. Rahman *J. Phys.: Condens. Matter* 22, 462202 (2010); *J. Chem. Phys.* 136, 114108 (2012).

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