Magnetic Properties of Transition Metal Nanoparticles: A DFT-Inhomogeneous-DMFT Analysis

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To include electron-electron correlation effects in the nanosystem we are proposing a combined density-functional-theorydynamical-mean-field-theory (DFT + DMFT) approach, which we have recently shown to be suitable for including correlation effects in small (2-5 atoms) Fe and FePt clusters [1]. This method has several advantages as compared to the widely used DFT + U approach, the most important of which is that it takes into account dynamical correlation effects automatically. We find that the inclusion of dynamical effects leads to a reduction in the cluster magnetization (as compared to results from DFT + U) and that, the magnetization values agree well with experimental estimations. We will present results of application of this formalism to examine the size dependent magnetic properties of Fe_{15}, Fe_{17} and Fe_{19} clusters. For the above we have developed a computational code that should be capable of calculating the magnetic properties of systems containing hundreds of atom.

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

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