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Magnetic properties of small iron clusters: Nanoscale Dynamical Mean-Field Theory analysis[1] ALAMGIR KABIR, Department of Physics, University of Central Florida, Orlando, FL 32816, TALAT S. RAHMAN, VOLODYMYR TURKOWSKI, Department of Physics and NSTC, University of Central Florida, Orlando, FL 32816 — We analyze the role of correlation effects in determining magnetic properties of small iron clusters (Fe_2-Fe_5) by using the Nanoscale Dynamical Mean-Field Theory (NDMFT) approach. In particular, we study the dependence of the magnetization of the system on temperature, Coulomb repulsion and geometrical structure, including the Jahn-Teller distortion effect. We analyze the dynamical correlation effects in the magnetic behavior of the system by comparing our results with some static approaches, which take into account correlation effects, including the GGA+U approximation. It is shown that the NDMFT approach improves the results obtained by these approaches in the case of moderate Coulomb repulsion energy when the atomic coordination number is large. We discuss possible generalization of the approach to study the magnetic properties of nanoclusters on magnetic and non-magnetic substrates and embedded in matrices.

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