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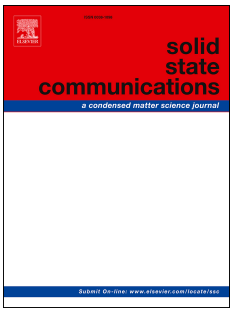

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Theoretical Investigation of Existence of Meta-stability in Iron and Cobalt Clusters

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Abstract

Nowadays considerable attention has been given for researches on magnetic properties of transition metal clusters (specifically Fe_N and Co_N). This is because these clusters offer big hopes for the possibility of presenting significant magnetic anisotropy energy which is critical for technological applications. This study intends to find out the causes for the existence of the two states (ground and meta-stable) in Iron and Cobalt clusters. The study also explains the role of valence electrons for the existence of magnetism in the two states by using the concept of ionization potential, electron dipole polarizabilities, chemical hardness and softness of the clusters. Assuming that, when all itinerant electrons are at s-level and also at the d-level ($n_s = n \; and \; n_s \to 0$) the ground state and meta-stable state energies with distinct energy minima are ($E_{gs} = l/2n + \varepsilon_c n - 2\mu_B hn \;\; and \; E_{ms} = \varepsilon_d n - g\,\mu_B hn$) respectively. The findings also showed that polarizability of small cluster of the specified elements are increased compared with the bulk value, which means that there is an effective increase in the cluster radius due to the spilling out of the electronic charge. Furthermore, it is obvious that 4s electrons are more delocalized than the 3d electrons so that they spill out more than the 3d electrons. This leads to the conclusion that 4s electrons are primarily responsible for the enhanced polarizabilities and for shell structure effects. This indicates that polarizability at the meta-stable state is less than that of the ground state i.e. the meta-stable state loses its s electron. Therefore the two minima represent a ground state of configuration $3d\uparrow^5 3d\downarrow^{2+\delta} 4s^{2-\delta}$ with energy $E_{gs}$and meta-stable state of configuration $3d\uparrow^5 3d\downarrow^{3+\delta} 4s^{1-\delta}$ with energy E_{ms} for Co clusters and a ground state configuration $3d\uparrow^5 3d\downarrow^{1+\delta} 4s^{2-\delta}$ with energy E_{gs} an meta-stable state of configuration