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A DFT study of geometric, electronic, and magnetic properties of Fe_xAu_{113-X} (x=23, 56, 90) core-shell nanoparticles SAMPYO HONG, TALAT RAHMAN, University of Central Florida — We have performed density functional theory (DFT) calculations for Fe_xAu_{113-X} (x=23, 56, 90) nanoparticles to find that these nanoparticles prefer the formation of core-shell structure and the Fe core of the nanoparticles maintains almost constant magnetic moment of ~ 2.8 μ_B regardless of the Fe content, which is 27% enhancement from the bulk value, in agreement with previous studies. The local magnetic moment of Fe atoms are correlated with the local coordination of Fe atoms and the enhanced magnetic moment is a result of charge depletion from Fe atoms to Au atoms. We find that the more the depleted charge, the larger is the induced magnetic moment. This indicates that electron depletion is crucial for the enhancement of the induced magnetic moment for Fe atoms. The case of $Fe_{90}Au_{23}$ is interesting as only a partial Au shell can be formed owing to the lack of the sufficient number of Au atoms in the cluster. This core-shell structure is more stable than the segregated phase consisting of two Fe and Au nanoparticles. Segregation between Fe and Au phases may be driven by large surface energy mismatch and core stress, but another important factor for the formation of the core-shell structure could be low surface tension in the Fe-Au interface (i.e., strong Fe-Au interfacial interaction), which we attribute to the large charge transfer at the interface. Work supported in part by DOE grant DE-FG02-07ER46354.

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