Abstract Submitted
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Effect of a Fe substitutional impurity on the geometric and electronic structure of Au_{13} cluster[1] GHAZAL SHAFAI, TALAT RAHMAN, University of Central Florida — We have carried out spin-polarized density functional theory calculations based on the pseudopotential method to determine the changes in the characteristics of the Au_{13} cluster when one Au atom is replaced by Fe. For a pure Au_{13} cluster, the 2D geometry is the lowest-energy isomer, followed closely by a flake structure, while the icosahedron is higher in energy by 2.98 eV and is not stable since it is found to undergo Mackay transition to form a cuboctahedron. When a surface or central Au atom is replaced by Fe, we find dramatic changes in the energy ordering of these nanoparticles, since Fe tries to move inwards so as to be highly coordinated. In fact the distorted icosahedron and a biplanar structure obtain the lowest energy. The structure of the Fe-centered icosahedron is slightly distorted (Jahn-Teller distortion), so that the degeneracy on two bands near Fermi level is removed. The lowest energy isomer in this study has the highest magnetic moment (3.98 μ_B) in comparison with that of the other isomers. The magnetic moment of the icosahedron with an Fe atom at the center is 3.1 μ_B, which is in in agreement with previous findings.

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