Electronic and magnetic properties of As10-nMn (n= 0-10, M= Co, Fe and Cu clusters by density functional theory

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Abstract

The arsenic clusters have been the topic of many experimental and theoretical studies [1-3].The mean reasons of this interesting subject are that arsenic has found wide applications in many fields, such as semiconductors, bio-pharmaceutics and it is one of the most toxic and carcinogenic element raising very important environmental issues [4]. In this work, we report the structures, electronic and magnetic properties of As10-nMn (n= 0-10, M= Co, Fe and Cu) clusters. All of this properties have been investigated using the density functional theory (DFT) with generalized gradient approximation functional (GGA) and pseudo-potential implemented in the SIESTA program. We find that the binding energies increase for n = 0 to 6 then they decrease for n = 7 to 10. This means that the M atoms enhance the stability for $n \leq 6$ and the stability of each system depends on the number of atoms of the dominating speciesthe clusters. The HOMO-LUMO gaps gradually decrease with some local oscillations as the cluster size increases. This may indicate that the metallic characteristics of As10-nMn clusters are enhanced by the doping M (M= Co, Fe and Cu) atom. The magnetic properties depend on the number and positions of M atoms. Indeed, we find that the magnetic moment increase with the number of atoms in the system in the case of As10-nCon and As10-nFen. In the case of As10-nCun, the total spin magnetic moment is not very influenced by the As caging. We have also examined the vertical electron affinity (VEA) and vertical ionization potential (VIP) for all As10-nMn (n= 0-10, M= Co, Fe and Cu) clusters. We find that there VEA show a decreasing tendency with the increasing cluster size. It indicates that the larger the clusters of As10-nMn will need more energy to capture electrons. We have also observed that

the *VIP* decreases slowly with the increasing of cluster size. This indicates that the different As10-nMn clusters tend to show a high metallic character which implies that these clusters can more easily lose one electron comparatively to the clusters of smaller size.

Keywords: ab intio calculations, clusters, As, Co, Fe, Cu, DFT, electronic and magnetic properties.

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