Electronic and magnetic properties of $As_{10-n}M_n$ (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 $As_{10-n}M_n$ (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 $As_{10-n}M_n$ 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 $As_{10-n}Co_n$ and $As_{10-n}Fe_n$. In the case of $As_{10-n}Cu_n$, 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 $As_{10-n}M_n$ (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 $As_{10-n}M_n$ 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 $As_{10-n}M_n$ 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.

References

[1] S. Safer, S. Mahtout, K. Rezouali, M.A. Belkhir and F. Rabilloud, Comp. Theo. Chem. 1090 (2016) 23–33
[2]. X. bai, Q. C. Zhang, J. C. Yang. H. M. Ning, J. Phy. Chem. A 116 (2012) 9382 - 9390.
[3]. K. S. Bhatia, W. E. Jones, Can. J. phy. 49 (1971) 1773 - 1782.
[4]. M.Z. Shen, H.F. Schaefer, J. Chem. Phys. 101 (1994) 2261–2266.