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**A Comparative Study of Structure, Stabilities And Electronic Properties Of Neutral And Cationic [AuSin]Λ And [Sin+1]Λ (Λ = 0, +1; N = 1–12) Nanoalloy Clusters**

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**Abstract**

Structure, stabilities and electronic properties of [AuSin]λ and [Sin+1]λ (λ = 0, +1; n=1-12) nanoalloy clusters are studied invoking Density Functional Theory methodology. To understand the chemical stability of the lowest energy structure of cluster, chemical parameters like, Binding Energy, Fragmentation Energy, Second Order Difference in Energy and HOMO-LUMO energy gap are studied with the variation of cluster size. The binding energy of neutral and cationic Sin+1 and AuSin clusters is gradually increasing along with the cluster size n. The second order difference in energy for pure Sin+1 and doped cluster AuSin shows an interesting odd-even alternation behavior. It is found that Si7, AuSi5, [Si5]+ and [AuSi7]+ are the most stable clusters. The HOMO-LUMO energy gap of neutral and cationic AuSin cluster is high as compare to their corresponding neutral and cationic Sin+1 cluster. It indicates that doping of Au atom enhances the energy gap of silicon clusters. The computed HOMO-LUMO gap of neutral and cationic AuSin clusters are in the range of 1.35–2.94 eV, which is suitable for microelectronics, optoelectronic devices and photovoltaics applications. Density Functional Theory based descriptors viz. Electronegativity, Hardness, Softness and Electrophilicity Index are also reported. The HOMO-LUMO energy gap of pure Si and doped cluster AuSin displays odd-even oscillation behavior as a function of cluster size, n. The close agreement between theoretical and experimental results supports and validates our computational analysis.

**Keywords:**

Density functional theory, Cluster Silicon Au-Si, HOMO-LUMO energy gap

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