Equilibrium Geometries, Stabilities, and Electronic Properties of the Bimetallic Ag_2-doped Si_n ($n = 1-11$) Clusters: A Density-Functional Investigation

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An ab initio method based on the density functional theory has been employed to investigate the behaviours of the bimetallic Ag_2-doped silicon clusters at a size of $n = 1-11$. The possible geometrical configurations, growth-pattern behaviours, stabilities, energy gaps, and electronic properties are presented and discussed. The optimized geometries reveal that the silicon atom surface-capped and silver atom substituted 3D structures are dominant growth patterns. The calculated averaged binding energy, fragmentation energy, and the second-order difference of energy manifest that the most stable structures of Ag_2Si_n ($n = 1-11$) clusters are Ag_2Si_2 and Ag_2Si_5 isomers, which is in qualitative agreement with the $AgSi_n$ clusters. In addition, the gap between highest occupied and lowest unoccupied molecular orbital (HOMO-LUMO) exhibits that the Ag_2Si_3 and Ag_2Si_5 isomers have dramatically enhanced chemical stability. Natural population analysis shows that the charge-transfer phenomena are coincidence with the $AgSi_n$ clusters but different from Mo_2Si_n systems. Furthermore, the dipole moments of stable Ag_2Si_n ($n = 1-11$) display a pronounced odd-even oscillation with the number of silicon atoms.

Key words: Ag-Si Cluster; Geometric Configuration; Density Function Method.