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**Density functional study of structures, stabilities and electronic properties of AgAunλ (λ= 0, ±1; n = 1-12) clusters: comparison with pure gold clusters**

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**Abstract**

Geometrical structures, relative stabilities and electronic properties of neutral, cationic and anionic pure gold Auλn+1andAg-doped bimetallic AgAuλn(λ=0,±1; n=1−12)clusters have been systematically investigated by using density functionaltheory methodology. The optimized structures show that planar to three-dimensional structural transition occurs at n=5for cationic clusters. Due to strong relativistic effect of Au clusters, the ground state configurations of neutral and anionicbimetallic clusters favor planar geometry till n=12. Silver atoms tend to occupy the most highly coordinated position andform the maximum number of bonds with Au atoms. The computed HOMO-LUMO energy gaps, fragmentation energies andsecond-order difference of energies show interesting odd-even oscillation behavior. The result indicates that AgAu5, AgAu+2and AgAu−2are the most stable clusters in this molecular system. The DFT based descriptors of bimetallic clusters are alsodiscussed and compared with pure gold clusters. The high value of correlation coefficient between HOMO-LUMO energygaps and DFT based descriptors supports our analysis. A good agreement between experimental and theoretical data has beenobtained in this study

**Keywords:**

Density functional theory; bimetallic cluster; AgAu; structures; properties

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