A Comparative Study of Different DFT Based Methodologies of Bi-Metallic Ag-$Au_{n\ (n=1-7)}$ Nano Alloy Clusters

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There are a number of reports available in favour of bi-metallic nano alloy for a wide range of applications. As the bi-metallic nano alloy clusters have diverse physicochemical properties, among such nano clusters, the compounds formed between Ag-Au have gained a considerable interest because they possess unique optical, electronic and magnetic and mechanical properties, which have extensive applications in the field of radiation medicine, biophysics and nanoscience. Density Functional Theory (DFT) is one of the most popular techniques of quantum mechanics to study the electronic properties of materials. Recently, conceptual DFT based descriptors have been turned to be indispensable tools for studying the experimental properties of compounds. In this report, we have analysed Ag-$Au_{n\ (n=1-7)}$ system invoking two different DFT based methodologies *viz.* B3LYP and Local Density Approximation (LDA). The electronic properties of Ag-Au_n are successfully investigated and compared in terms of DFT based global descriptors. This report reveals that $AgAu_6$ has the maximum reactivity and the least stability, whereas $AgAu_2$ system exhibits the highest stability. This study is probably the first attempt to establish such type of comparison for Ag-Au nano alloy clusters.