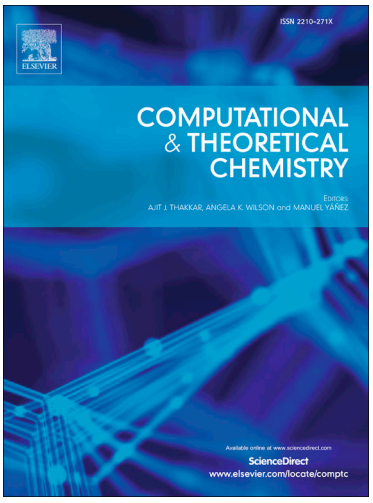

A Density functional theory study of Structural, electronic and magnetic properties of small Pd_nAg (n=1-8) clusters

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A Density functional theory study of Structural, electronic and magnetic properties of small Pd_nAg (n=1-8) clusters

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Abstract

The geometries, stabilities, electronic and magnetic properties of small Pd_nAg (n = 1-8) clusters have been estimated within the frame work of density functional theory (DFT) at B3P86/LANL2DZ level of theory. Various possible geometries have been examined in order to identify the lowest energy structures of the Pd_nAg clusters. It has been found that the lowest energy geometries of the binary clusters are in three-dimensional (3D) configurations. The stability analysis of the most stable structures has indicated that PdAg, Pd_2Ag and Pd_3Ag clusters are more stable and less reactive than their neighbouring clusters. A universal charge transfer from Ag atom to Pd atoms within the ground-state Pd_nAg clusters has been found. It has also been revealed that the electrons transfer internally from 5s and 4d states to 5p state in Ag atom, and from 4d state to 5s and 5p states in Pd atoms. Additionally, the Ag atom tends to lose some of its electrons to Pd atoms in the