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Structural, electronic and magnetic properties of small bimetallic zirconium–palladium clusters: Ab initio study

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ABSTRACT

Structural, electronic and magnetic properties of small bimetallic zirconium–palladium clusters, Zr_nPd_m ($n+m\leqslant 5$), have been investigated using density functional theory with considering generalized gradient approximation and PBE functional. We have determined the ground state conformations of the bimetallic zirconium–palladium clusters by substitution of Zr and Pd atoms in the optimized lowest energy structures of pure zirconium and palladium clusters. Results reveal that binding energies of the pure Zr_n clusters are significantly higher than Pd_n clusters with the same number of atoms. Also it is found that binding energy of the Zr_n and Pd_n clusters increase with growth of the number of consisting atoms in the clusters. Results indicate that, for both Zr_n and Pd_n clusters the binding energy of planar forms is lower than three-dimensional structures. We have also found that the binding energy of the Pd_n clusters increase with substituting one or more Zr atoms in these clusters. We have also studied the HOMO–LUMO energy gap and magnetic moment of the pure and combined Zr and Pd clusters. The energy gap analysis of the pure and combined Pd and Zr clusters show that in generally the HOMO–LUMO gap of the bimetallic Zr_nPd_m clusters increase in comparison with their corresponding pure clusters with the same number of atoms. According to the spin polarization DFT calculations all of the Zr_nPd_m ($n+m\leqslant 5$) have net magnetic moments as instance the Zr_2, Pd_2 and ZrPd clusters show a total magnetic moment value of 2 μ_B. Some more discussions around charge population and density of states of considered clusters as well as their structural properties have been discussed in the context.

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1. Introduction

Bimetallic clusters constitute systems that are physically and chemically very attractive for science and technology. In addition to clusters size, the properties of the clusters are dependent on the chemical compositions and arrangement of atoms [1]. Unique and attractive structural [2–11], electronic [2,3,9–11] and magnetic [12–14] properties of the some bimetallic clusters have been reported so far. Also some studies have indicated that bimetallic systems have certain properties that make them better catalysts than pure metals [15–17]. The increase of the catalytic effects in bimetallic clusters is specified by several parameters such as overall composition, temperature, and preparation process of the catalyst [18–23]. As instance Sicolo and Pacchioni [24] have studied the properties of some bimetallic clusters such as PtAu adsorbed on MgO/Ag(100) ultrathin films. PdAg clusters also have been investigated by first principles studies [25]. Also clusters of Cu_nM (M = Ni, Pd, Pt; $n=1$–4) are discussed by Floreza et al. [26]. Transition-metal (TM) clusters are exclusively interesting because their magnetic properties are very sensitive to the local environment of the atoms and since magnetic materials derived from them have extensive potential applications in recording and storage devices. Recent studies have shown that the magnetic moments of some 3d-TM (Fe, Co, and Ni) clusters are significantly larger than the corresponding bulk magnetizations [27–33]. Also some experimental [34] and theoretical [35,36] studies have focused on the Pd, Zr clusters and bimetallic compounds [37,38] of these two elements. The Pd compounds can be used as catalysts as it is the subject of many articles [39]. Kwon et al. [40] have studied water oxidation in alkaline conditions using size-selected clusters of Pd to probe the relationship between cluster size and the water oxidation reaction. Also in recent work Yow et al. [41] have shown that the chemoselective C–O bond functionalization of benzofuran with an aluminum dihydride may be catalyzed by Zr compounds such as indenyl$_2$ZrCl$_2$.

Regarding to the mentioned properties of both Zr and Pd compounds the purpose of this paper is investigations on the structural and magnetic properties of Zr–Pd bimetallic clusters. We present a systematic study of the bimetallic $Zr_nPd_m(n+m\leqslant 5)$ clusters at

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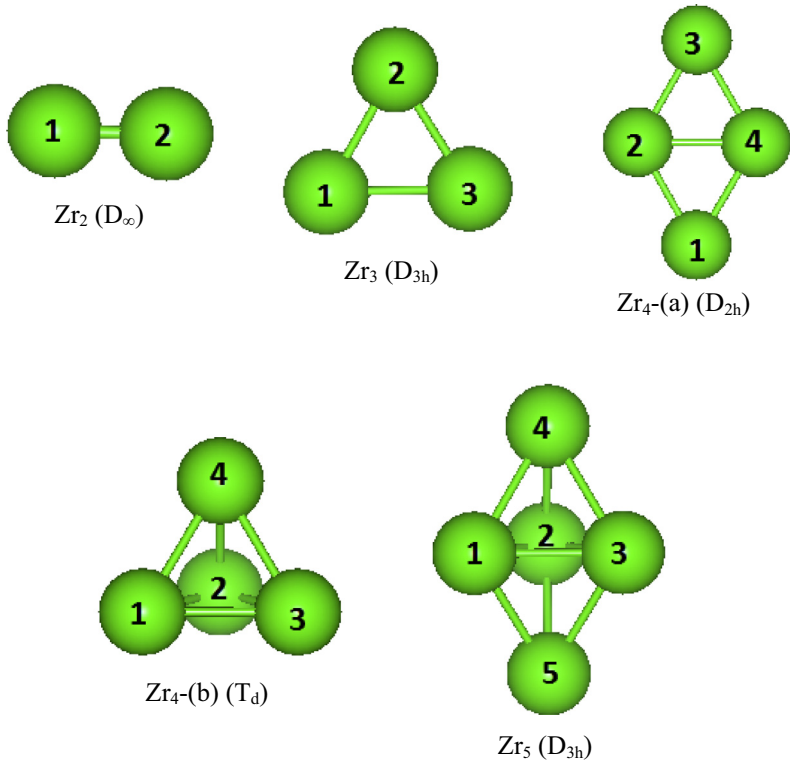

Fig. 1. Some lowest energy structures of the Zr_n ($n \leqslant 5$) clusters.

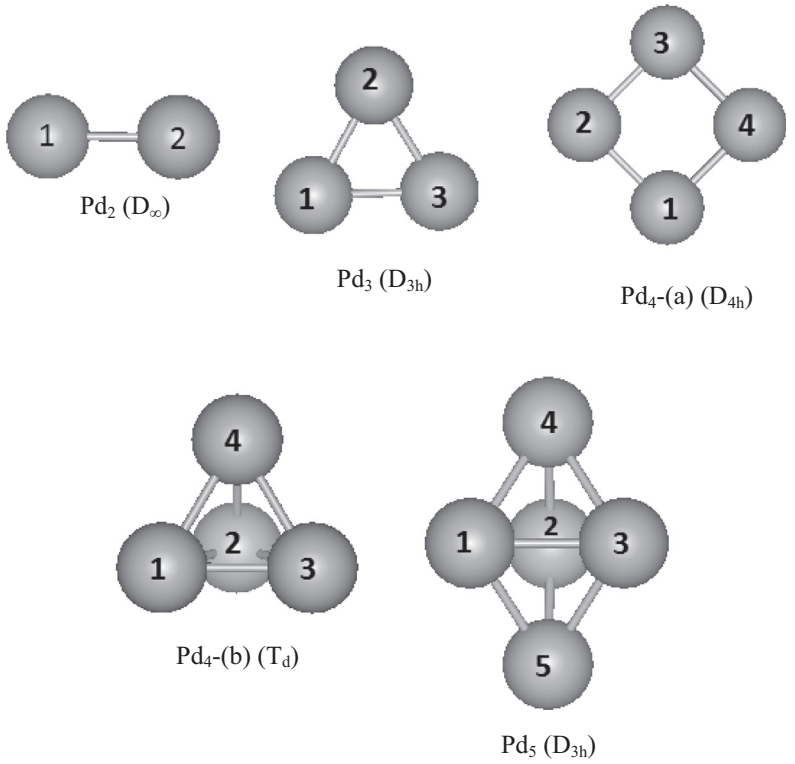

Fig. 2. Some lowest energy structures of the Pd_n($n \leqslant 5$) clusters.

their neutral states. Compared with pure Zr_n and Pd_n clusters, the Zr_nPd_m binary clusters exhibit some interesting structural evolutions. First-principles calculations based on a generalized gradient approximation to density-functional theory (DFT) have been

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