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A first-principles study of Ni_nPd_n (n = 1 − 5) clusters

Aldo Cervantes-Flores[1] · Heriberto Cruz-Martínez[2] · Omar Solorza-Feria[1] ·
Patrizia Calaminici[1]

Abstract A first-principle investigation of structures and properties of Ni_nPd_n (n = 1−5) clusters is presented. For this study, the linear combination of Gaussian-type orbitals auxiliary density functional theory (LCGTO-ADFT) method has been employed. In order to determine the lowest energy structures, several isomers in different spin multiplicities were studied, for each cluster size. Initial structures, for which successive geometry optimization was computed without any constrain, were taken along Born–Oppenheimer molecular dynamics (BOMD) trajectories. To discriminate between minima and transition state structures, harmonic frequency analyses were performed at the optimized structures. Ground state structures, bond lengths, harmonic frequencies, dissociation energy, ionization potential, electron affinity and spin density plots are presented. This work demonstrates, that the Pd atoms prefer to allocate on the surface of the *cluster* structures whose core is formed by the 3d TM atoms type. Moreover, it has been observed that the ground-state structure spin multiplicity increases as the system size grows. The results of this study contribute to gain insight into how structures and energy properties

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✉ Patrizia Calaminici
pcalamin@cinvestav.mx

1 Departamento de Química, CINVESTAV, Av. Instituto Politécnico Nacional 2508, AP 14-740, México D.F. 07000, México

2 Programa de Doctorado en Nanociencias y Nanotecnología, CINVESTAV, Av. Instituto Politécnico Nacional 2508, AP 14-740, México D.F. 07000, México

change with cluster size in bimetallic Pd-based alloys.

Introduction

The investigation of transition metal (TM) clusters has developed as a very important research area due to the fact that their properties are strongly related to their shape and size (see for examples the Refs. [1–10] and references therein.) Bimetallic TM clusters are particularly interesting systems because their structures and properties are quite distinct with respect to the ones of homo-nuclear TM clusters [11]. Moreover, these TM compounds are also attractive since they are considered as the seeds of nanoclusters with potential catalytic behavior. In particular, different alloys formed with palladium, such as PdFe, PdCo, PdNi, and PdCu have been shown to possess a catalytic performance comparable to the one of most expansive Pt supported on carbon catalysts for oxygen reduction reaction in fuel cells [12–16]. For this reason, the study of these systems is of great experimental and theoretical interest. What is theoretically challenging is to gain understanding into the arrangement of the individual atoms in these alloys, as it is difficult to obtain this information experimentally.

A few bimetallic TM compounds of different sizes formed by nickel and palladium atoms with various compositions have been theoretically investigated [17–25]. Density functional theory (DFT) was employed to study the binding energy of $Pd_{13-x}Ni_x (x = 1−13)$ clusters. The obtained results indicate that the thermodynamic stability of Ni substituted Pd_{13} clusters is higher than the one of the naked

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