On the structure and reactivity of Pt_nCu_n(n= 1-7) alloy clusters

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Abstract
The structure, electronic and reactivity properties of Pt_nCu_n(n= 1-7) clusters are investigated in the framework of density functional theory (DFT). The most stable forms of the clusters are obtained by a structure search procedure based in simulated annealing. The results show that the Pt_nCu_ncluster alloys adopt layered structure motifs with segregation of the Cu and Pt species. The total magnetic moments of the clusters adopt the low spin configuration. The bimetallic cluster reactivity is investigated by using the ionization potential, electron affinity, and the d-band center, respectively. The results show that the Pt_nCu_nclusters with (n= 5-7) have similar vIP and vEA parameters compared to the unary Pt clusters, but the d-band center is slightly higher suggesting an enhanced reactivity for the bimetallic clusters. On the other hand, the molecular electrostatic potential shows that the Cu species increase the available active sites on the cluster surface. The data on the infrared spectra of the clusters is also provided. These results are useful to understand the fundamental properties of Pt-M bimetallic alloys in the subnanometer region.

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