Structural, electronic and catalytic properties of bimetallic PtnAgn (n=1?7) clusters

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The geometrical, electronic and catalytic properties of PtnAgn (n = 1?7) clusters are investigated by means of density functional theory (DFT) computations. The ground state structures are obtained by a structure search procedure based in the simulated annealing method. In general, the PtnAgn clusters adopt structures with Pt cluster motifs at the central position surrounded by silver islands. We found that the Pt4Ag4 and Pt6Ag6 clusters have a closed shell geometric structure and are the most stable clusters in this series. The bimetallic cluster reactivity is investigated by using the ionization potential, electron affinity, the d-band center, and the adsorption energy descriptors, respectively. However, it turns out that the reactivity of these systems is more sensitive to the chemical element on the cluster surface exhibiting a local reactivity. The different reactive sites on the cluster surface can be explained by the molecular electrostatic potential surface. In the PtnAgn alloys, the Pt species perform similar interactions with a CO molecule in comparison to the unary Pt clusters, whereas the Ag species issue weaker interactions, increasing the catalyst resistance. In this context, the bimetallic clusters may serve as potential candidates for hydrogenation reactions. Furthermore, the distinct charge reorganization on the PtnAgn alloys is useful for incorporating a lower number of noble metals in order to achieve an increased catalytic and selectivity capabilities. Theoretical data on the infrared spectra of the clusters is also provided.

Alloys

Bimetallic

Clusters

DFT

Platinum

Silver

Binary alloys

Density functional theory

Electron affinity

Ground state

Hydrogenation

Platinum

Silver alloys

Simulated annealing

Adsorption energies

Bimetallic clusters

Catalytic properties

Geometric structure

Ground-state structures

Hydrogenation reactions

Molecular electrostatic potentials

Simulated annealing method

Ionization potential