Effect of Ni and Pd on the geometry, electronic properties, and active sites of copper clusters

Florez, Elizabeth

Mondragón, Fanor

Fuentealba, Patricio

The geometry, electronic properties, and active sites of copper clusters doped with Ni or Pd atoms, Cun-1M (n = 2-6; M = Ni, Pd) have been investigated using first-principles methods. Planar structures are energetically favorable in Cun-1Ni (n = 2-6). However, for Pd-doped clusters, three-dimensional structures are competitive in energy, and for n = 6, the most stable structure is not planar. Several properties of doped copper clusters present odd-even oscillations as the number of copper atoms grow. The different atomic ground-state configuration of Ni and Pd determines the bonding and electronic properties of doped copper clusters. The interaction between impurities and copper atoms can modify the chemical hardness and active sites of doped copper clusters markedly inducing directionality in the reactivity. This effect is relevant to the behavior of catalysts as well as in the growth of metallic films.