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Geometry and electronic properties of platinum and palladium doped TiN (N = 1 – 15) nanoparticles

Nanoparticles with diameter 1.0 nm plays a significant role in catalysis because they constitute a new type of material possessing properties, which are distinct from individual atoms, molecules and bulk matter. Doped nanoparticles offers ways to explore fundamental properties of nanoparticles, in addition to a vastly greater range of parameters that can be tuned to obtain nanoparticles with desired properties. The synergistic effects of two metal nanoparticles show certain surprising new properties which increases their function and application in many different fields. These nano-systems shows better stability, selectivity and catalytic activity over monometallic nanoparticles. However, their indefinite composition and broad distribution hinder insightful understanding of the interaction between these invasive metals in bimetallic doped nanoalloys. In this study we report the density functional theory calculations with the PBEsol exchange-correlation functional. A 16 atoms TiN-1M (M = Pt, Pd) was considered. At N = 4, 6, 7, 9 and 10, the metal dopant preferred to occupy the position of the atom that on the face and surface of the nanoalloys. The substitution of Ti atom with Pt and Pd increases the relative stability of the nanoalloys and the maximum stability for lower bimetallic composition is reached for Ti5Pd Ti8Pt and Ti6Pt. However, the most stable nanoalloy is reached for Ti12Pd in comparison with Ti12Pt and pure Ti13 monoatomic nanocluster. Furthermore, N = 7 with Pt impurity displayed a non-magic nanoalloy, whereas, Pt impurity enhanced the stability of the nanoalloy. These observations were revealed by the binding energy, relative stability and dissociation energy. The HOMO-LUMO gaps also reveal the reduction of the quantum confinement as the cluster size increases.

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