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Investigation of Nickle nanoclusters properties by density functional theory

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ABSTRACT

Clusters play important role for understanding and transferring microscopic to macroscopic properties.Geometric and electron properties of Small nickel clusters up to the tetramer has been investigated by Density Functional Theory (DFT). Raising the number of nickel clusters atoms were indicated decreasing the average equilibrium (Ni-Ni) distance of atoms and also the binding energy of per atom were showed increasing trend. Ni-Ni binding energy diagram shows a linear behavior in terms of ($n^{-1/3}$). It is correspond with the previous findings. During the process HOMO-LUMO gap energies reduce. The lowest HOMO-LUMO gap energy was related to Ni_8 cluster, so it proves that the cluster is more reactive and less kinetic stability. The linear relationship between size of clusters ($n^{-1/3}$) with some properties of clusters indicate that it can get these properties ($X\infty$) and extrapolated to the mass of the material.

Keywords: Ni nanocluster; DFT; Electronic properties; HOMO-LUMO gap; Binding energy