Abstract

The adsorption of NO molecule on neutral, cationic and anionic Pd_n (n=1-5) clusters were studied using density functional theory. Adsorption takes place at the top, bridge and hollow sites of the clusters. In all the cases NO adsorbed in a bent geometry. The adsorption mostly takes place at the low coordination sites rather than the three coordinated hollow sites. Charge transfer between Pd clusters and NO molecule and the corresponding weakening of N-O bond is an essential factor of the adsorption. The N-O stretching frequency follow the order of cationic > neutral > anionic. Binding energy of NO on anionic clusters is found to be greater than those of neutral and cationic clusters.

Keywords: Nitrogen oxide adsorption; neutral, cationic and anionic Pd-clusters; Pd_n (n=1-5); DFT.