ABSTRACT

THE INTERACTIONS BETWEEN MAGNETIC NANO CLUSTERS AND SURFACE MOLECULES BY USING DENSITY FUNCTIONAL THEORY ARE INVESTIGATED

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The electronic properties of platinum clusters are investigated at gamma point by using density functional theory (DFT) within generalized gradient approximation. The size dependence of binding energy**,** highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), magnetization, and bond length values are calculated for platinum clusters. It is observed that Pt_n clusters prefer to form 3D structures with increasing number of atoms., The electronic density of states is also calculated to explore the electronic properties of Pt_n clusters.

The NH_3 and H_2 molecules adsorbed Pt_n clusters are investigated by DFT calculations within generalized gradient approximation. The adsorption energy, highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), HOMO-LUMO gap (HLG), magnetization, and bond length values of H_2 ve NH_3 adsorbed platinum clusters are investigated as a function of atom number for the stable adsorption site . A strong interaction is found between Pt and N atoms. It is surprisingly observed that NH_3 dissociation occurs at Pt_{14} cluster. We found that H_2 molecule dissociates at different adsorption sites for all clusters except Pt_3 cluster. Each of H atom seems to prefer to bound different Pt atoms. We see that d orbital of Pt is dominant near the Fermi level in NH_3 and H_2 adsorbed Pt_n clusters. Metallic and conductivity properties of Pt_n clusters change with adsorption of NH_3 and H_2 molecules.

NH_3 adsorbed Pt_2 cluster can show half metallic properties. HOMO-LUMO gap (HLG) values for NH_3 and H_2 adsorbed Pt_n clusters are evaluated. The results also

imply charge transfer from Pt to H atoms in H_2 adsorbed Pt_n clusters and a polarization between Pt and N atoms in NH_3 adsorbed clusters. These results also comply with Lowdin analysis. The interactions between $MoSe_2$ monolayer and Fe, Mn atoms are investigated. Fe and Mn atoms prefer to bound to Mo atom in $MoSe_2$.

Keywords: Density functional theory, electronic structure, Pt_n cluster, Ammonia adsorption, Hydrogen adsorption, $MoSe_2$