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 H₂ adsorbed Ptₙ clusters and a polarization between Pt and N atoms in NH₃ adsorbed clusters. These results also comply with Lowdin analysis. The interactions between MoSe₂ monolayer and Fe, Mn atoms are investigated. Fe and Mn atoms prefer to bound to Mo atom in MoSe₂.

**Keywords**: Density functional theory, electronic structure, Ptₙ cluster, Ammonia adsorption, Hydrogen adsorption, MoSe₂