ABSTRACT

Density functional theory (DFT) calculations have been performed by B3LYP/6-31G (d,p) to calculate Hydrogen molecule interaction with Lithium, Sodium, Potassium, Beryllium, Calcium, and Magnesium doped Nanocage of $Al_{12}N_{12}$. After full optimization of the most stable structures are used to calculate, ionization energy, electron potential, Chemical hardness, softness potential, HOMO and LUMO energies, HOMO LUMO gaps, Adsorption energy, Fermi level, Dipole moment and Molecular electrostatic potential parameters were investigated. Results reveals that of Hydrogen molecule. Magnesium doped nanocage has the highest ionization energy, electron affinity, chemical softness chemical potential, HOMO LUMO energies, HOMO LUMO energy gap while in chemical softness Lithium, Sodium and Potassium doped nanocages have highest values. In Fermi level energies, Dipole moment and Adsorption energies are highest for Beryllium doped Nano cluster. In the case of Molecular Electrostatic Potential, the negative and positive charge is rotated in all Nanocluster on Aluminum and Nitrogen atoms. Although the result of Magnesium doped Nanocluster is different. All these nanostructures are promising possibility for detecting of the Hydrogen molecule, while Beryllium and Magnesium doped $Al_{12}N_{12}$ Nanoclusters can be chosen as the most delicate sensor for Hydrogen molecule adsorptions.