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Abstract

The research work reported in this thesis deals with hydrogen storage in carbon and boron nitride nanostuctures using density functional theory. A new way to disperse metal atoms on surface of CNTs and fullerene is discussed. The porphyrin induction in CNTs and fullerene tune their electronic properties. It is found that dispersing metal atoms on surface of these functionalized system and subsequent optimization lead to strong bonding of such atoms on these systems. In case of Fe and Mg dispersion on PICNT, The binding energy of Fe and Mg is -7.84eV and -4.273eV, respectively. The binding energy of H_2 on the surface of Fe-PICNT and Mg-PICNT is found to be in terms of partial density of state (PDOS) and charge decomposition analysis (CDA) reveals that the mode of interaction of H_2 with former is Kubas type while for the later it is governed by physisorption. The optimized structure of Ca-PICNT shows binding energy of -5.23eV for dispersed Ca atom. The Ca-PICNT system hold maximum of 4-H_2 molecule with binding energy of -0.105eV/H_2. Transition metals (TMs) decoration on the the $C_{54}N_4$ reveals that the B.E value for Ti, V and Cr in this is -8.313, -8.37 and -8.76eV, respectively, which is much larger as compared to decoration of these TMs atom at the surface of fullerene. It is found that $3d_{xy}$ orbital from transition metal are in strong conjunction with valance $2p_x$ orbital of N-atoms and are responsible for formation of these proposed system. Single hydrogen molecule get adsorbed

on these system with binding energy values between 0.15 to 0.11eV and their interaction are consequence of electron transfer from H_2 sigma to d-orbital and back donation from d-orbitral to antibonding sigma(Kubas type).

To study the hydrogen storage in boron nitride system, borazine was selected as model system. The results of the Gibbs free energy corrected binding energy calculation for Ti-$B_3N_3H_6$ with 4-H_2 adsorbed show that the system continue to hold these hydrogen upto 400K. Presence of borazine results in the reduction of transition energy from triplet to quintet state of Ti and hence lead to easy accessibility to higher spin state. The binding energy for single hydrogen molecule in the quintet state of Ti-$B_3N_3H_6$ is found to be less as compared to triplet state of the same. In addition to these, the quantum chemical simulation have been carried out to study the structure and electronic properties of hybrid boron nitride nanotube obtained by substituion of carbon atom at half the periphery of boron nitride nanotube (namely CBNNT). The HOMO-LUMO gap of CBNNT is found to be intermediate of CNT and BNNT. Li atom decoration has been made at different sites of this proposed structure.