

C2N2 Adsorption on the Surface of a BN Nanosheet: A DFT Study

Authors : Maziar Noei

Abstract : Calculation showed that when the nanosheet is doped by Si, the adsorption energy is about -85.62 to -87.43kcal/mol and also the amount of HOMO/LUMO energy gap (E_g) will reduce significantly. Boron nitride nanosheet is a suitable adsorbent for cyanogen and can be used in separation processes cyanogen. It seems that nanosheet (BNNS) is a suitable semiconductor after doping. The doped BNNS in the presence of cyanogens (C_2N_2) an electrical signal is generating directly and, therefore, can potentially be used for cyanogen sensors.

Keywords : nanosheet, DFT, cyanogen, sensors

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