Research Article

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Adsorption behavior of mephentermine on the pristine and Si, Al, Ga- doped boron nitride nanosheets: DFT studies

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ABSTRACT

In this research, the adsorption behavior of pristine, Si- and Al- and Ga-doped boron nitride nano sheet are investigated toward mephentermine using density functional theory (DFT) calculations. Total energies, geometry optimizations were obtained and density of state (DOS) analysis was performed at B3LYP level of theory with the 6-31g (d) basis set. The adsorption energy (E_{ad}) between mephentermine and the pristine, Si- and Al- and Ga doped BNN is changed in the following order: Ga-Complex-N> Al-Complex-N>Si-Complex-N> complex -N. The E_{ad} of the BNN-mephentermine complex is -2.09 kcal/mol, which shows that the adsorption is weak physicaly. The E_{ad} of the Al-doped BNN-mephentermine complex is -34.06 kcal/mol, ΔE_g = -1.37%, indicating a low sensitivity of the Al-doped boron nitride nanosheet to the adsorption of mephentermine and is not suitable for sensing. As mentioned, due to the adsorption energy of −34.06 kcal/mol and the rather long recovery time, a strong interaction is not suitable for a sensor. The E_{ad} of the Ga-doped BNN-mephentermine complex is -46.46 kcal/mol, ΔE_g = -6.39%. the adsorption energy of -46.46 kcal/mol is not suitable for a sensor and indicates a long recovery time, As a result, it helps to decompose this compound and remove this compound.

1. Introduction

Mephentermine is a drug cardiovascular that It strengthens the heart and stimulates respiration. mephentermine helps release a chemical messenger that compresses blood vessels and also increases the heart's contractile power in pumping. The presence of medicinal compounds in the environment is considered a serious threat to humans and the entry of these substances into water and soil resources causes the pollution. Therefore A sensor is needed to detect the accumulation of drug waste. With the advent of nanotechnology, it was found that their surface /volume ratio is much higher than conventional micro-detectors [1, 2]. Nanostructures have received a great deal of attention as chemical sensors [3-10]. BN nanosheet is a two-dimensional structure of hexagonal boron nitride (h-BN) with a thickness of one to several atomic layers. It is geometrically similar to graphene, but has very different chemical and electronic properties [11]. BN nanosheets consist of sp^2-conjugated boron and nitrogen atoms that form a hexagonal structure [12, 13]. The BN nanostructures have a wide range of attractive properties such as stability high temperature strength, low dielectric constant, high thermal conductivity and oxidation resistance, which leads to a number of potential applications as electronic materials [14]. The BN nanosheet indicate a size controllable energy band Gap wich enable them a promising Materials for different thchnological application.

-In a study conducted in 2017 by Khaleghian and Azarbakhshi [15], the nonbonding interaction of single walled boron nitride nanotube with theophylline was studied theoretically, the effects of electron instability and bipolar interaction and spatial repulsion on structural and electronic properties and the amount Reactivity was investigated using quantum mechanics of density functional theory at the B3lyp theoretical level. Orbital analysis of natural bonding was performed and

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