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Theoretical study of interaction between Mexiletine drug and pristine, Si-, Ga- and Al-doped boron nitride nanosheet.

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ABSTRACT

In this study, the adsorption behavior of pristine, -Si, -Ga and -Al doped boron nitride nanosheet (BNN) is investigated toward the mexiletine drug 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* basis set. The adsorption energy (E_{ad}) between mexiletine and the pristine, Si-, Ga- and Al-doped BN nanosheet was changed in the following order: Ga-Complex-N(NH_2) > Al-Complex-N(NH_2) > Si-Complex-O. The E_{ad} of the mexiletine/BNN complex is −4.73kcal/mol, which is very low interaction so that the adsorption is not suitable. The E_{ad} of the mexiletine/Si-doped BNN complex is −22.14kcal/mol, which is a suitable interaction so that the desorption may be occurred readily. Besides, the E_g significantly increased from 4.47 eV to 5.68 eV and the rate of the change is % ΔE_g = −27.20% which shows the suitable sensitivity of the Si-doped BN nanosheet to the adsorption of drug. Therefore, it can be concluded that the Si-doped BN nanosheet can be a promising candidate to being a sensing ability over the mexiletine drug from both E_{ad} and E_g parameters.

1. Introduction

Mexiletine is a medication used to treat abnormal heart rhythms, chronic pain, and some causes of muscle stiffness. Common side effects include abdominal pain, chest discomfort, drowsiness, headache, and nausea. It works as a non-selective voltage-gated sodium channel blocker and belongs to the Class IB group of anti-arrhythmic medications [1].

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 of plants, soil, humans and animals and creates problems through manufacturing processes, agriculture and waste disposal. The drug is often released into the environment. These toxic compounds eventually enter the body of organisms through nutrition and drinking water. When a drug is released in large quantities into the environment and nature, it is dangerous and requires sensing to determine where the drug accumulates, for example in water and soil and in the environment in general, and therefore sensors are used. These sensors can be nanoparticles. As a result, nano-scale methods have been developed to identify drug compounds to address environmental pollution and concerns about human health [2-6]. With the advent of nanotechnology, due to their surface/volume ratio, which is much higher than conventional micro detectors [7, 8]. Nanostructures have received a great deal of attention as chemical sensors [9-16].

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 [17]. A sheet is not essentially completely flat but it is considered by a plate-like form or structure. There are various kinds of nanosheets including boron nitride nanosheets (BNN) which show suitable character in the stability and electronic properties comparing with carbon nanosheet [18-20].