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Boron nitride nanocone as an adsorbent and senor for Ampicillin: A Computational Study

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ABSTRACT

In this research, the performance of boron nitride nanocone for the detection and removal of ampicillin was investigated by infra-red (IR), natural bond orbital (NBO), frontier molecular orbital (FMO) computations. The calculated values of adsorption energy showed the interaction of ampicillin with BN nanocone is experimentally possible. The calculated values of Gibbs free energy and thermodynamic equilibrium constant showed the adsorption process is spontaneous and irreversible. The calculated values of enthalpy changes and specific heat capacity showed ampicillin adsorption is exothermic and BN nanocone can be used for the construction of a new thermal sensor for the detection of ampicillin. The effect of temperature on the thermodynamic parameters was also evaluated and the results indicated ampicillin adsorption is more favorable in room temperature. The NBO results demonstrated in both of the studied configurations a monovalent chemical bond is formed between the nanostructure and the adsorbate and the interaction process is chemisorption. The DOS spectrums showed the bandgap of BN nanocone increased from 1.888 (eV) to 7.030 (eV) which proved this nanomaterial is an appropriate electrochemical sensing material for detection of ampicillin. Some important structural parameters such as dipole moment, electrophilicity, maximum charge capacity, chemical hardness and chemical potential were also calculated and discussed in detail.

1. Introduction

Groundwater contamination by pharmaceutical ingredients is an environmental problem of widespread concern [1-2]. Residual pharmaceutical ingredients will be inevitably transported into biological wastewater treatment plants and have been recognized as part of the hazardous chemical substances able to alter the natural equilibrium system of the surrounding environment [3]. Recently, the presence of antibiotics in the environment has received much attention due to their impact on health and the environment because their presence in the waters provides the formation and development of antibiotic-resistant bacteria [4]. Therefore, it is of utmost importance to remove the antibiotic residues from the wastewater from sources such as households, hospitals and pharmaceutical factories before discharging them to the environment. Regular water and wastewater treatment may not be able to remove pharmaceutical compounds effectively. Accordingly, the development of new and effective wastewater treatment technologies, such as biodegradation, hydrolysis, chemical oxidation, volatilization and adsorption have been intensively studied in the past decade [5-8]. Among these techniques, adsorption is preferred due to simplicity in design, ease of fabrication, high efficiency, relatively lower cost and absence of high toxic by-product [9]. Many polymeric and inorganic materials such as activated carbon [10], zeolite [11] and carbon nanotube [12], etc. have been proven to be effective for the absorption of the pollutants. However, they frequently suffer from the disadvantage of limited adsorption capacity or slow adsorption rate [13]. Therefore, novel adsorbent materials with high adsorption capacity and easy cycling ability still keep a challenge.

Ampicillin (AM) (Figure 1) in its turn, is a β-lactam antibiotic of a large spectrum, able to interact with both