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DFT insights into $B_3C_2N_3$ nanosheets: A promising biosensor for the earliest stage detection of exhaled breath biomarkers in lung cancer

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ABSTRACT

Density functional theory (DFT) was utilized to investigate the potential interactions between $B_3C_2N_3$ graphene-like nanosheets and three lung cancer biomarkers present in exhaled breath stage. This study focuses on sensing capability of three lung cancer biomarkers of volatile organic compounds (VOCs), namely, 2-propenal (C_3H_4O), acetone (C_3H_6O), and isoprene (C_5H_8). The selective capability of $B_3C_2N_3$ monolayer as an effective surface towards these biomarkers is demonstrated. The $B_3C_2N_3$ monolayer was theoretically confirmed to offer some sensing merits such as favorable adsorption energy, optical absorption, enhancing electrical conductivity, and preferable recovery time when conducted to the target VOCs biomarkers. To identify the adsorption mechanism between the target VOCs and the $B_3C_2N_3$ surface, charge transfer distribution was evaluated using Mulliken population analysis. The monolayer surface exhibited electronic and φ-type sensor characteristics in the detection process of all studied biomarkers. To identify the dynamic and thermal stability of the constructed systems: 2-propenal/$B_3C_2N_3$, acetone/$B_3C_2N_3$, and isoprene/$B_3C_2N_3$, molecular dynamics (MD) was performed after 5000 steps for 1 fs at ambient temperature. The results revealed that the $B_3C_2N_3$ monolayer surface may serve as a promising sensor for the earliest stage diagnosis of lung cancer depended on biomarkers detection of exhaled breath patients.

1. Introduction

Lung cancer is diagnosed and being ranked as the second most common cancers in the world [1]. Its morbidity and fatality rates have been announced as the highest cases among all cancer forms [2]. Malignant tumors are considered as a main cause of lung cancer that accompanies with common symptoms including coughing up blood, chest pain, shortness of breath, hoarseness, and wheezing [3,4]. Thus, the early diagnosis stage of lung cancer is highly needed for its potential remedies. Reportedly, the conventional procedures utilized to characterize lung cancer are imaging tests, sputum cytology, and biopsy process [5]. One approach with highly potential of early lung cancer detection is the screening of biomarkers found in the exhaled breath of patients. Particular substances are produced in the body of patients due to the presence of tumors and these substances act to release volatile organic compounds (VOCs) into the bloodstream [6,7]. The VOCs are ultimately exchanged in the lungs. As reported, the exhaled breath contains a high level of VOCs in lung cancer patients compared to those of healthy peoples. Consequently, the exhaled breath analysis is emerged as an expedient and workable technique for diagnosing lung cancer without the complications associated with invasive procedures. Therefore, the VOCs are found to be distinctive biomarkers for assessing the severity of lung cancer ones [8].

The VOCs including hydrocarbon compounds such as methyl cyclopentane (C_6H_{12}), isoprene (C_5H_8), 2-propenal (C_3H_4O), and acetone (C_3H_6O) in addition to some aromatic compounds like benzene (C_6H_6) and ethylbenzene (C_8H_{10}), have been recently investigated to show an effective detection towards liver and lung cancers [9–11]. A chemical resistance-type sensor offers significant promise in the VOCs detection due to its high sensitivity, rapid response, and inexpensive cost [12]. In the recent years, some two-dimensional (2D) materials possessing high reactivity and elevated electron mobility, have been improved to show favorable interactions with VOCs. These materials include III−IV compounds, transition metal dichalcogenides (TMDs), group V composite, and $B_xC_yN_z$ monolayers [13–15]. Bio-devices made from 2D nanomaterials can utilize for developing highly efficient sensing biomarkers

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