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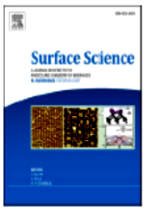

DFT insights into $B_3C_2N_3$ nanosheets: A promising biosensor for the earliest stage detection of exhaled breath biomarkers in lung cancer

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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.