Extended Abstract

Study of the Adsorption Effects of Butanone, Propanal, and Pyridine Biomarkers on the Electronic Properties of Graphene Armchair Nanoribbons for the Early Detection of Gastric Cancer

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Received: 12.02.2026 Final revised: 02.06.2026 Accepted: 01.07.2026 Published On-Line: 05.09.2026

Doi: 10.22055/jrmbs.2026.20898

Abstract

In this study, the adsorption properties and electronic response of armchair graphene nanoribbons, as a sensing substrate for detecting three volatile organic compounds 2-butanone (C_4H_8O), pyridine (C_5H_5N), and propanal (C_3H_6O) as key biomarkers of gastric cancer, were investigated using density functional theory while taking van der Waals interactions into account. The results showed that armchair graphene nanoribbons adsorb these volatile organic compounds weakly, with adsorption energies in the range of −0.3 to −0.5 eV, indicating a physisorption process without the formation of direct chemical bonds. In addition, the density-of-states analysis showed that the adsorption of each molecule leads to the appearance of distinct peaks in the density-of-states plot of the armchair graphene nanoribbon. Therefore, the armchair graphene nanoribbon can be considered a potential substrate for gas sensing of gastric-cancer-related biomarkers in non-invasive diagnostic methods.

Keywords: Graphene, Volatile Organic Compounds, Gastric Cancer, Density Functional Theory, Gas Sensor

1. Introduction

Gastric cancer is one of the most lethal malignancies worldwide, largely due to late-stage diagnosis, which results in a five-year survival rate below 30%[1]. In contrast, early detection

can increase survival rates to over 90%. However, conventional diagnostic methods such as endoscopy and biopsy are invasive, costly, and unsuitable for large-scale screening[2].

Given these limitations, breath analysis has emerged as a non-invasive and cost-effective approach for early cancer detection through the identification of disease-related volatile organic compounds (VOCs)[3, 4]. Clinical studies have shown that several VOCs are elevated in the breath of gastric cancer patients, among which butanone, propanal, and pyridine have been identified as key biomarkers. Nevertheless, their low concentrations require gas sensors with high sensitivity and selectivity[5, 6].

Against this background, armchair graphene nanoribbons have attracted significant attention as sensing materials due to their tunable band gaps, high surface-to-volume ratios, and strong electronic response to molecular adsorption[7], making them promising candidates for selective detection of gastric cancer–related VOCs[8].

2. Computational Methodology

Density functional theory (DFT) calculations were performed using the Quantum ESPRESSO package[9] to investigate the adsorption behavior and electronic response of armchair graphene nanoribbons toward three gastric cancer–related VOC biomarkers: butanone, propanal, and pyridine. The generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional was employed, and van der Waals interactions were included via the Grimme-D3 dispersion correction[10]. Projector augmented-wave (PAW)[11] pseudopotentials were used to describe electron–ion interactions, with a plane-wave energy cutoff of 40 Ry and a 8 × 1 × 1 Monkhorst–Pack k-point grid for Brillouin zone sampling.

The model consisted of a hydrogen-passivated armchair graphene nanoribbon, with a vacuum spacing of approximately 15 Å to avoid interactions between periodic images. All structures were fully geometry-optimized until energy and force convergence criteria were satisfied. Adsorption energies were calculated using:

$$E_{ads} = E_{G+M} - E_G - E_M$$

where E_{G+M}, E_G, and E_M represent the total energies of the adsorbed system, pristine graphene nanoribbon, and isolated molecule, respectively. Negative adsorption energies indicate stable adsorption.

Results and Discussion

The results indicate that the adsorption of butanone, propanal, and pyridine does not induce significant structural deformation in the armchair graphene nanoribbon, and the lattice symmetry remains well preserved, confirming the non-destructive nature of the interaction and its suitability for sensing

applications. The optimized adsorption geometries of these molecules on the graphene nanoribbon surface are illustrated in Figure1:

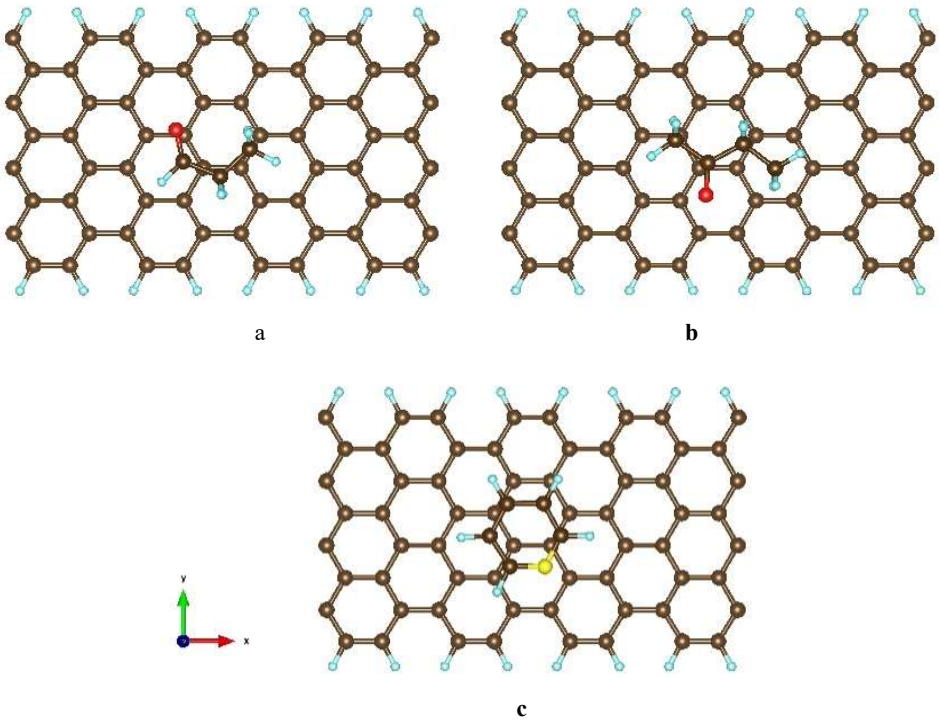


Figure 1. Optimized adsorption configurations of (a) butanone, (b) propanal, and (c) pyridine on the graphene nanoribbon surface.

All molecules exhibit stable adsorption with negative adsorption energies, with butanone showing the strongest interaction (−0.465 eV), followed by propanal (−0.355 eV) and pyridine (−0.437 eV). The stronger adsorption of butanone is attributed to its larger size and higher polarizability, while the weaker adsorption of propanal and pyridine results from their smaller size and, in the case of pyridine, the presence of a nitrogen atom that induces local electrostatic repulsion. The equilibrium adsorption distances are consistent with this trend, being approximately 2.87 Å for butanone, 2.77 Å for propanal, and 3.36 Å for pyridine

Based on the calculated adsorption energies, the interaction between the VOC molecules and the graphene nanoribbon is non-destructive in nature, indicating stable physisorption and confirming the suitability of this system for sensing applications. To gain deeper insight into the electronic effects induced by molecular adsorption, the density of states (DOS) of the pristine and molecule-adsorbed graphene nanoribbons was analyzed. The total density of states of the systems adsorbed with butanone, propanal, and pyridine as well as the pristine armchair graphene nanoribbon are shown in Figure 2:

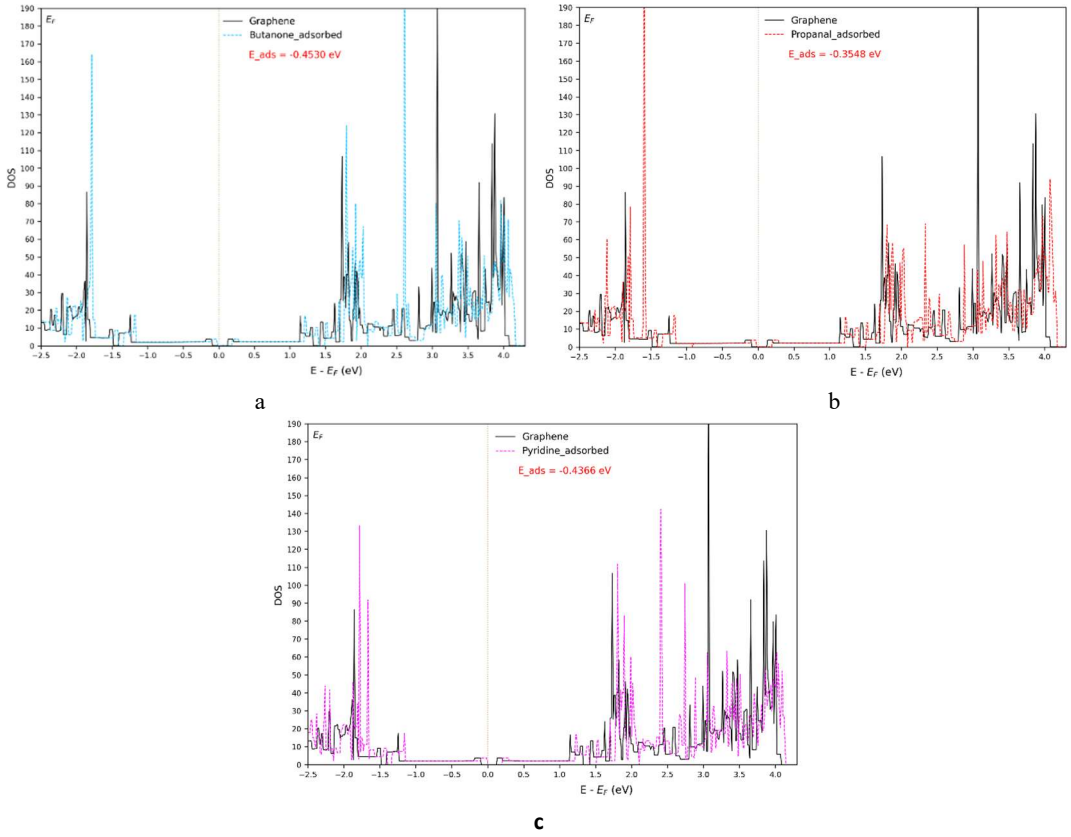


Figure 2. Total density of states (DOS) of the pristine armchair graphene nanoribbon and the molecule-adsorbed systems: (a) butanone, (b) propanal, and (c) pyridine

The pristine nanoribbon is represented by a solid blue line, while the adsorbed systems are shown by dashed orange lines, with the Fermi level aligned at zero energy. Comparison of the DOS profiles indicates that the adsorption of each molecule induces distinct changes in the density of states, particularly in the vicinity of the Fermi level. These changes, manifested as the appearance or shifting of DOS peaks, reflect the different electronic interactions between each VOC and the graphene nanoribbon. Such molecule-dependent behavior demonstrates the presence of unique electronic signatures and highlights the strong potential of graphene nanoribbons for the selective detection of gastric cancer–related biomarkers.

Conclusion

This theoretical investigation demonstrated that armchair graphene nanoribbons exhibit strong potential as sensing materials for the detection of gastric cancer–related volatile organic compounds. The adsorption of butanone, propanal, and pyridine on graphene nanoribbons is stable and primarily

physical in nature, yet sufficiently strong to induce measurable changes in the electronic structure. The distinct DOS signatures associated with each molecule highlight the possibility of selective detection, which is crucial for practical breath-based diagnostic applications. These findings provide valuable theoretical insights and a solid foundation for the future design and optimization of graphene nanoribbon–based gas sensors aimed at non-invasive, early diagnosis of gastric cancer.

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