

Potential Application of Carbon Nanotubes and Ag-doped Carbon Nanotubes for Ethylene (C₂H₄) Adsorbent in Postharvest Agriculture

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Abstract: Ethylene (C₂H₄) control technologies in postharvest agriculture are critical for minimizing wastage and maintaining the market value of climacteric fruits. The present study reports molecular interactions between C₂H₄ and single-walled carbon nanotubes (SWCNTs) and Ag-doped single-walled carbon nanotubes (Ag-doped SWCNTs) using density functional theory-based simulations. The ground-state calculations demonstrate that C₂H₄ is attached to the sidewall of the prototype single-walled carbon nanotube (SWCNT) via weak physisorption, with bonding mediated by minor charge redistribution. The interaction between C₂H₄ and the prototype nanotube can be enhanced by introducing an Ag dopant into the SWCNT sidewall, forming an Ag-C₂H₄ π -complex. The Ag dopant can trap multiple C₂H₄ molecules, implying superior adsorbent performance. The NVT molecular dynamics simulations at 300 K predicted that the presence of competing H₂O and CO₂ weakens C₂H₄ binding on the surface of pristine SWCNT, leading to its diffusion. In contrast, the π -complex structure of C₂H₄ with Ag-dopant remains stable despite the presence of competing volatile gases. The simulations predicted that Ag-SWCNT is an effective adsorbent for C₂H₄ in H₂O- and CO₂-rich environments, such as in postharvest storage. Overall, the findings presented herein will serve as a reference for the design of C₂H₄ control technologies in postharvest agriculture.

Keywords: ethylene (C₂H₄); ethylene adsorbent; ethylene control technology; carbon nanotube; Ag-doped carbon nanotube; adsorption; postharvest agriculture; density functional theory; nanomaterial.

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1. Introduction

The waste of fresh produce induced by ethylene (C₂H₄) during the supply chain accounts for a significant fraction of global food losses [1,2]. C₂H₄ is a gaseous plant hormone that plays a central role in regulating plant growth, development, and postharvest physiology.

It is widely recognized as a key signaling molecule involved in climacteric fruit ripening and senescence processes. During ripening, even at very low concentrations, C_2H_4 triggers a cascade of physiological and biochemical changes, including increased respiration rate, softening of cell walls, color development, aroma formation, and eventual tissue senescence, all of which contribute to reduced postharvest quality and shelf life of fresh produce [3,4]. Therefore, it is critical to precisely regulate C_2H_4 during postharvest handling and storage to maintain fruit quality and market value. To mitigate this problem, various C_2H_4 management practices and control technologies are applied in postharvest systems. Existing C_2H_4 control technologies include adsorbents, scavengers, sensors, and C_2H_4 inhibitors. However, researchers have explored only a limited set of materials for this purpose [5], and many currently available technologies have poor reusability and may cause uneven fruit ripening [1]. Advanced materials (e.g., nanocarbons, nanocellulose, MXenes, and metal–organic frameworks) with extremely high surface areas and tunable properties may offer an effective strategy to mitigate the climacteric effects induced by C_2H_4 [6-9].

Standard approaches to minimize the effects of C_2H_4 during postharvest storage include the use of oxidizing scavengers (e.g., $KMnO_4$ and TiO_2), porous adsorbents (e.g., zeolites), and chemical inhibitors [1,10]. $KMnO_4$ is commonly used to oxidize C_2H_4 into H_2O and CO_2 . Another strategy involves the use of photocatalytic materials such as titanium dioxide (TiO_2), which promote the degradation of C_2H_4 under light irradiation [11]. Upon illumination, photogenerated electrons and holes react with O_2 and H_2O on the catalyst surface to generate superoxide (O_2^-) and hydroxyl ($\bullet OH$) radicals. These highly reactive species degrade C_2H_4 and other organic molecules into H_2O and CO_2 [12].

Alternatively, porous materials such as zeolites can adsorb C_2H_4 through their well-defined pore structures and metal ions that facilitate gas capture [13–15]. These materials are typically incorporated into sachets, balls, rods, or tubes and deployed in industrial warehouses, supermarkets, and cold storage facilities to regulate ethylene levels in controlled-atmosphere environments [16]. Another widely used strategy employs an ethylene inhibitor, such as 1-methylcyclopropene (1-MCP), which binds to ethylene receptors and prevents ethylene-induced ripening. However, these approaches often suffer from limited efficiency, poor reusability, and the potential to induce uneven fruit ripening. These limitations highlight the need for new materials and alternative strategies for more effective C_2H_4 regulation.

The primary focus of this work is to evaluate the potential of carbon nanotubes (CNTs) as C_2H_4 -trapping materials in postharvest systems. CNTs exhibit a Young's modulus approaching 1 TPa and a high surface area of approximately $1315\text{ m}^2\text{ g}^{-1}$ [17,18]. In addition, their electronic properties vary with chirality, which may influence their interactions with gas molecules. Owing to these characteristics, CNTs have attracted considerable attention for gas adsorption and sensing applications [19–21]. For example, CNT-based materials have been explored for CO_2 capture with adsorption capacities as high as 253.99 mg g^{-1} [22], while surface functionalization with nitrogen-containing groups has been shown to enhance interactions with gases such as CO_2 and CH_4 [23]. These findings suggest that CNTs may also be promising materials for ethylene capture.

Various strategies have been proposed to enhance gas adsorption in porous materials, including modifying host frameworks (e.g., zeolites and metal–organic frameworks) by incorporating metal ions or clusters to strengthen interactions with target molecules [24–29]. These approaches suggest that metal modification may improve C_2H_4 adsorption in CNT-based systems. In this context, the present work employs density functional theory (DFT) calculations

to investigate the interaction of C₂H₄ with pristine and Ag-modified single-walled carbon nanotubes (SWCNTs). This work aims to elucidate the adsorption mechanisms and assess these systems' potential as C₂H₄-trapping materials for postharvest environments.

2. Simulation Details

All calculations were performed using the Quantum ESPRESSO package for first-principles materials simulations [30,31]. Exchange–correlation effects were treated within the generalized gradient approximation using the Perdew–Burke–Ernzerhof (PBE) functional [32,33], together with optimized norm-conserving pseudopotentials. The plane-wave kinetic energy cutoff and charge density cutoff were set to 60 Ry and 240 Ry, respectively. The self-consistent field (SCF) calculations were converged to an energy threshold of 10⁻⁸ Ry, and Gaussian smearing was employed to facilitate electronic convergence. Long-range dispersion interactions were included through the Grimme D3 correction scheme [34]. Brillouin-zone sampling was performed using a Monkhorst–Pack k-point grid of 1×1×9 for structural optimization, while a denser 1×1×30 mesh was used for electronic density-of-states calculations. The nanotube was modeled using a 1×1×5 supercell of the SWCNT(5,5). vacuum spacing of 13 Å was introduced in the directions perpendicular to the nanotube axis to avoid interactions between periodic images.

To quantify C₂H₄ adsorption on pristine and Ag-doped SWCNTs, the adsorption energy (E_{Ad}) was calculated according to the following expression:

$$E_{Ad} = E_{Complex} - E_{Adsorbent} - E_{Ethylene}. \quad (1)$$

Here, $E_{Complex}$, $E_{Adsorbent}$, and $E_{Ethylene}$ denote the total energies of the adsorption complex, the isolated nanotube adsorbent, and the isolated C₂H₄, respectively.

The recovery time (τ) was estimated using the Arrhenius-type expression:

$$\tau = \frac{1}{\nu_o} e^{\frac{E_{Ad}}{k_B T}}. \quad (2)$$

where ν_o is the attempt frequency, E_{Ad} is the adsorption energy, k_B is the Boltzmann constant, and T is the temperature. The ν_o is typically associated with the vibrational frequency of the adsorbed molecule on the surface. Following previous theoretical studies, a value of $\nu_o = 10^{12} \text{ s}^{-1}$ was adopted for direct comparison with the literature [35,36].

The electron localization function (ELF) was employed to characterize the interactions between subsystems. It provides a measure of the likelihood of finding an electron pair in a given region of space. The ELF was calculated using the following expression [37],

$$ELF = \frac{1}{1 + \chi(\mathbf{r})} \quad \text{where} \quad \chi(\mathbf{r}) = \frac{\frac{1}{2} \sum_{i=1}^N |\nabla \psi_i(\mathbf{r})|^2 - \frac{1}{8} \frac{|\nabla n(\mathbf{r})|^2}{n(\mathbf{r})}}{\frac{3}{10} (3\pi^2)^{\frac{2}{3}} n(\mathbf{r})^{\frac{5}{3}}}. \quad (3)$$

The electron density and wavefunctions are denoted by $n(\mathbf{r})$ and $\psi(\mathbf{r})$, respectively. The ELF ranges from 0 to 1, with values greater than 0.7 indicating strong electron localization, such as in core electrons, chemical bonds, and lone pairs. ELF values ranging from 0.2 to 0.7 indicate characteristics associated with metallic bonding. Non-covalent interactions were also examined by analyzing changes in the ELF contour. The optimized atomic configurations and the volumetric data are plotted using VESTA [38,39].

Finally, Born–Oppenheimer molecular dynamics simulations were performed for the nanotube–C₂H₄ systems in the presence of H₂O and CO₂ within the NVT ensemble. The

temperature was maintained at 300 K using a Nosé–Hoover thermostat. The simulations were run for 4 ps with a time step of 1.209 fs using the Verlet algorithm.

3. Results and Discussion

3.1. Structural properties of pristine SWCNT(5,5).

The equilibrium structure of the pristine SWCNT(5,5) was optimized and compared with previously reported theoretical and experimental data. The calculated unit-cell length was 2.455 Å, differing from the reported theoretical value of 2.460 Å by only 0.2%. Such a small difference can be attributed to the approximations inherent to the exchange–correlation functional employed in the calculations. The optimized C–C bond lengths along the axial and circumferential directions of the nanotube are found to be 1.423 Å and 1.428 Å, respectively. These values are consistent with previously reported DFT results for SWCNT systems [40]. The close agreement between the calculated structural parameters and the literature data confirms the reliability of the present computational approach for describing CNT-based systems.

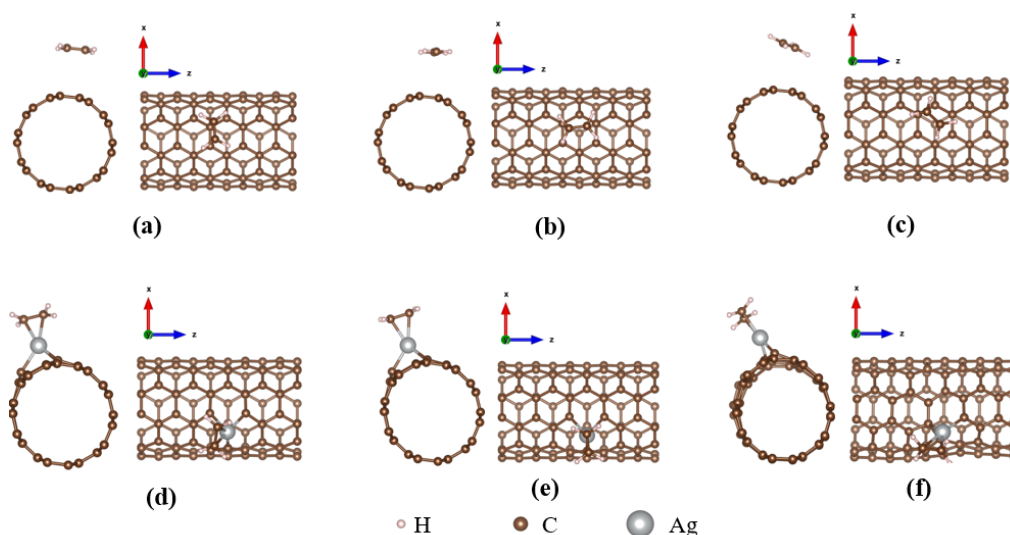


Figure 1. Optimized adsorption configurations of C_2H_4 on (a–c) pristine SWCNT(5,5) and (d–f) Ag-doped SWCNT(5,5), showing three distinct molecular orientations.

3.2 Adsorption of C_2H_4 on pristine SWCNT(5,5).

To investigate the interaction between C_2H_4 and pristine SWCNT, three initial molecular orientations were considered, and the structures were optimized until the energy and force convergence criteria were met. The optimized configurations of the SWCNT– C_2H_4 complexes are shown in Figures 1a–c. According to Table 1, the equilibrium adsorption distances range from 3.33 Å to 3.53 Å. Different adsorption trends are observed depending on the molecular orientation. When the C–C bond of C_2H_4 is positioned above the hexagonal ring of the SWCNT, as illustrated in Figures 1b and 1c, an adsorption energy of approximately –0.15 eV is obtained. A slightly weaker adsorption energy of –0.14 eV is observed when the C_2H_4 molecule is oriented parallel to a C–C bond of the nanotube wall (Figure 1a). The relatively low adsorption energies lead to short recovery times, as predicted by the Arrhenius-type desorption relation. Under UV irradiation conditions, the increased attempt frequency further facilitates rapid desorption, resulting in recovery times on the order of 10^{-10} s. Such

values are characteristic of weakly bound systems dominated by van der Waals interactions. Furthermore, the adsorption of C₂H₄ on the nanotube sidewall does not induce noticeable deformation in the C–C bonds of the SWCNT, further confirming the physisorption nature of the interaction.

Table 1. Adsorption energy (E_{Ad}), recovery time (τ), and minimum adsorption distance (d_{min}) for C₂H₄ on pristine and Ag-doped SWCNT systems. The reported τ values represent the order of magnitude of the estimated recovery times.

Systems	E_{Ad} (eV)	τ (s)	d_{min} (Å)
SWCNT-C ₂ H ₄ Orientation 1 (Fig. 1a)	-0.14	10 ⁻¹⁰	3.53
SWCNT-C ₂ H ₄ Orientation 2 (Fig. 1b)	-0.15	10 ⁻¹⁰	3.45
SWCNT-C ₂ H ₄ Orientation 3 (Fig. 1c)	-0.15	10 ⁻¹⁰	3.33
Ag-doped SWCNT - C ₂ H ₄ Orientation 1 (Fig. 1d)	-1.09	10 ⁶	2.23
Ag-doped SWCNT - C ₂ H ₄ Orientation 2 (Fig. 1e)	-1.11	10 ⁶	2.22
Ag-doped SWCNT - C ₂ H ₄ Orientation 3 (Fig. 1f)	-1.82	10 ¹⁸	2.25
Ag-doped SWCNT with two C ₂ H ₄ (Fig. 2a)	-0.70	10 ⁻¹	2.23
Ag-doped SWCNT with three C ₂ H ₄ (Fig. 2b)	-0.54	10 ⁻³	2.43
Ag-doped SWCNT with four C ₂ H ₄ (Fig. 2c)	-0.43	10 ⁻⁵	2.24

3.3. Enhanced C₂H₄ adsorption on Ag-doped SWCNT(5,5).

The adsorption of volatile organic gases such as C₂H₄ can be enhanced by incorporating transition metals into the host material [10,41,42]. Following this strategy, we examined C₂H₄ adsorption on Ag-doped SWCNT. Unlike the weak interaction on pristine SWCNT, the Ag-doped system shows strong adsorption, with E_{Ad} values of -1.09 eV (Figure 1d), -1.11 eV (Figure 1e), and -1.82 eV (Figure 1f), comparable to those of the Ag-RHO zeolite-C₂H₄ complex (-0.97 to -1.18 eV) [37]. The corresponding minimum adsorption distances, d_{min} (2.23–3.43 Å), are much shorter than those in the pristine SWCNT-C₂H₄ system. This stronger interaction markedly increases the estimated recovery times τ to 10⁶–10¹⁸ s (Table 1). To assess the adsorption capacity of the Ag site, we optimized configurations with multiple C₂H₄ molecules (Figures 2a–c). The average adsorption energy per C₂H₄ decreases with coverage, from -0.70 eV (2 molecules) to -0.54 eV (3) and -0.43 eV (4), yet remains much stronger than on pristine SWCNT. These results indicate that the Ag site most strongly stabilizes a single C₂H₄ molecule, while additional molecules bind more weakly and are more prone to desorption.

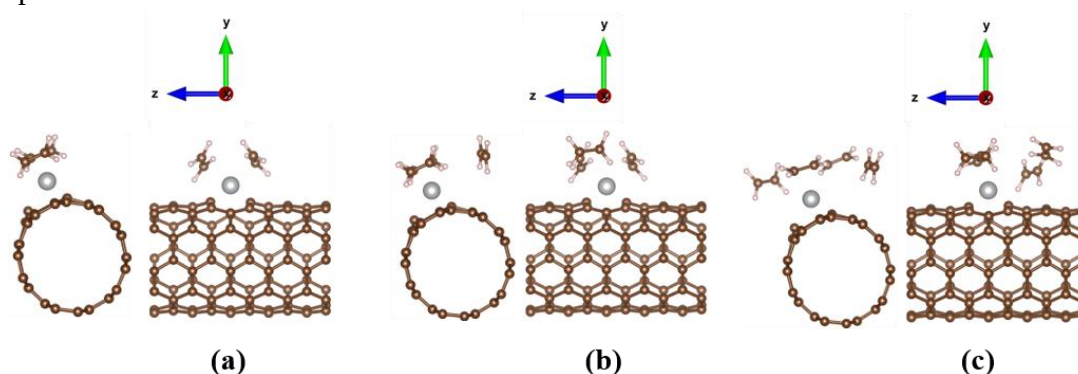


Figure 2. Optimized configurations of Ag-SWCNT with (a) two, (b) three, and (c) four adsorbed C₂H₄ molecules.

3.4. Charge transfer and electronic structure analysis.

To understand the interaction mechanism, we analyzed the charge density difference (CDD) and electron localization function (ELF), as shown in Figure 3. For the SWCNT-C₂H₄

complex (Figure 3a), the CDD isosurface ($10^{-4} \text{ e}/\text{\AA}^3$) indicates only minor charge redistribution at the interface. This observation is consistent with the Bader charge analysis, which shows negligible charge transfer between the nanotube and the adsorbed molecule. The corresponding 2D ELF contour also shows no significant electron localization between SWCNT and C_2H_4 , confirming the weak physisorption interaction. In contrast, the Ag-doped SWCNT– C_2H_4 system exhibits pronounced charge redistribution, as evidenced by the CDD isosurface ($10^{-3} \text{ e}/\text{\AA}^3$) and the 2D ELF contour shown in Figure 3b. The ELF map reveals a localization basin at the interface between the Ag dopant and the C_2H_4 molecule, indicating the formation of a covalent-type interaction. This behavior is further supported by the calculated charge accumulation of approximately 0.09 e on the C_2H_4 molecule, suggesting significant orbital hybridization with the Ag atom. These results explain the shorter adsorption d_{min} and the larger magnitude of E_{Ad} observed for C_2H_4 on the Ag-doped SWCNT compared with the pristine nanotube.

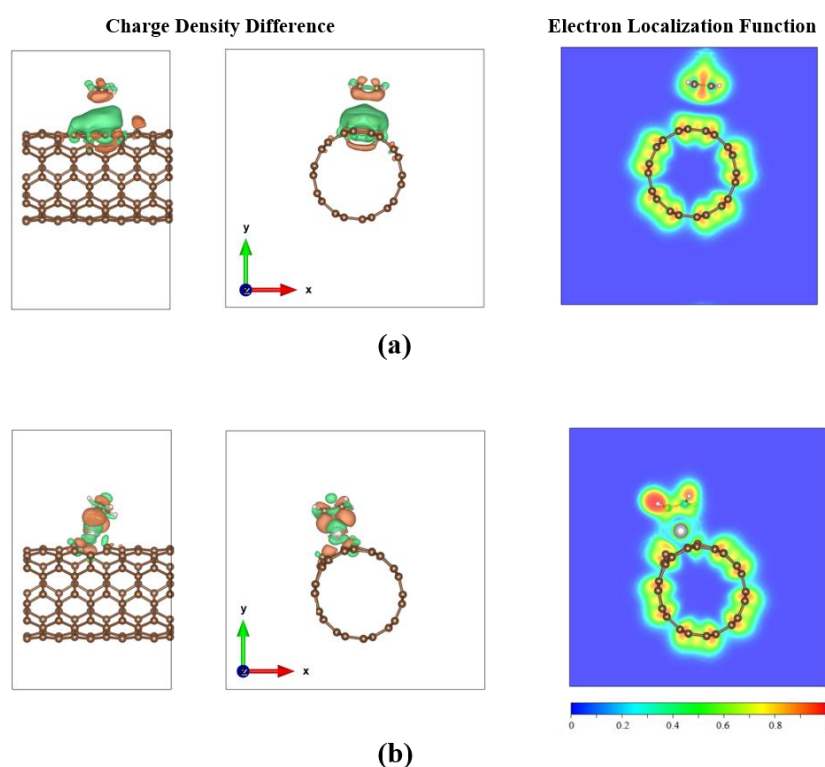


Figure 3. Charge density difference (CDD) and electron localization function (ELF) for C_2H_4 adsorption on **(a)** pristine SWCNT and **(b)** Ag-doped SWCNT. The left and middle panels present the three-dimensional CDD isosurfaces and corresponding side views of the adsorption geometries, while the right panels show the two-dimensional ELF contours. Green and brown regions denote charge accumulation and depletion, respectively, highlighting the weak interaction in the pristine system and the stronger bonding in the Ag-doped structure.

3.5. Electronic structure and orbital hybridization.

To examine the adsorption mechanism at the electronic level, the total and partial density of states (DOS and PDOS) were analyzed as shown in Figure 4. The calculated DOS for the pristine SWCNT(5,5) (Figure 4a) exhibits semimetallic behavior, consistent with previously reported theoretical studies of SWCNT's electronic structure [44–47]. Upon Ag doping, additional electronic states emerge near the Fermi level (Figure 4b), arising from the hybridization between Ag(4d) orbitals and neighboring C(2p) orbitals of the nanotube. Pronounced orbital overlap is also observed in the energy range -6 eV to -3 eV . For the SWCNT– C_2H_4 complex (Figure 4c), the main features of the pristine nanotube DOS remain

largely unchanged, indicating negligible orbital hybridization between the SWCNT and the adsorbed C_2H_4 molecule. Such behavior is characteristic of weak physisorption interactions [47,48]. On the one hand, the PDOS of the Ag-doped SWCNT- C_2H_4 system (Figure 4d) reveals clear orbital hybridization between Ag(4d) and C(2p) states of the nanotube with the C(2p) orbitals of C_2H_4 in the energy region between -6 eV and -4 eV. This hybridization accounts for the enhanced adsorption of C_2H_4 on the Ag-doped SWCNT compared with the pristine nanotube.

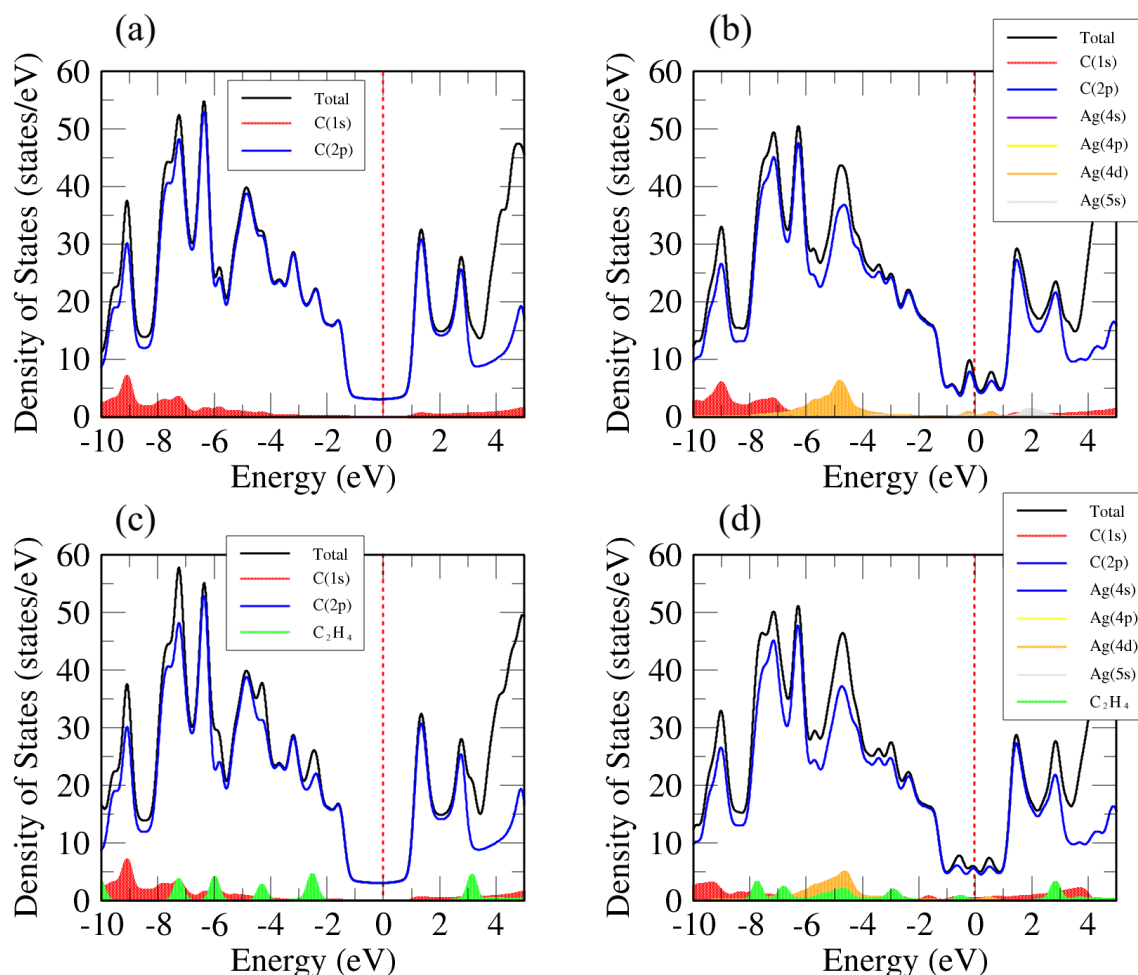


Figure 4. Electronic density of states (DOS) of (a) pristine SWCNT(5,5), (b) Ag-doped SWCNT(5,5), (c) SWCNT(5,5)- C_2H_4 , and (d) Ag-doped SWCNT(5,5)- C_2H_4 .

3.6. *Ab initio* molecular dynamics under a competitive gas environment.

Ab initio molecular dynamics (AIMD) simulations were performed to investigate the adsorption behavior of C_2H_4 on pristine and Ag-doped SWCNTs in the presence of competing volatile molecules, namely H_2O and CO_2 . Representative snapshots of the trajectories are shown in Figure 5. In the pristine SWCNT system, the C_2H_4 molecule remains adsorbed on the nanotube sidewall throughout the 4 ps simulation, despite the presence of competing H_2O and CO_2 molecules. However, all species exhibit comparable mobility and diffuse along the nanotube surface without being strongly confined. Meanwhile, in the Ag-doped SWCNT system, the C_2H_4 molecule remains localized around the Ag active site throughout the simulation. This restricted motion indicates that the Ag-doped region acts as an effective trapping center, suggesting that Ag-doped SWCNT can selectively capture C_2H_4 even in the presence of other volatile molecules under postharvest conditions.

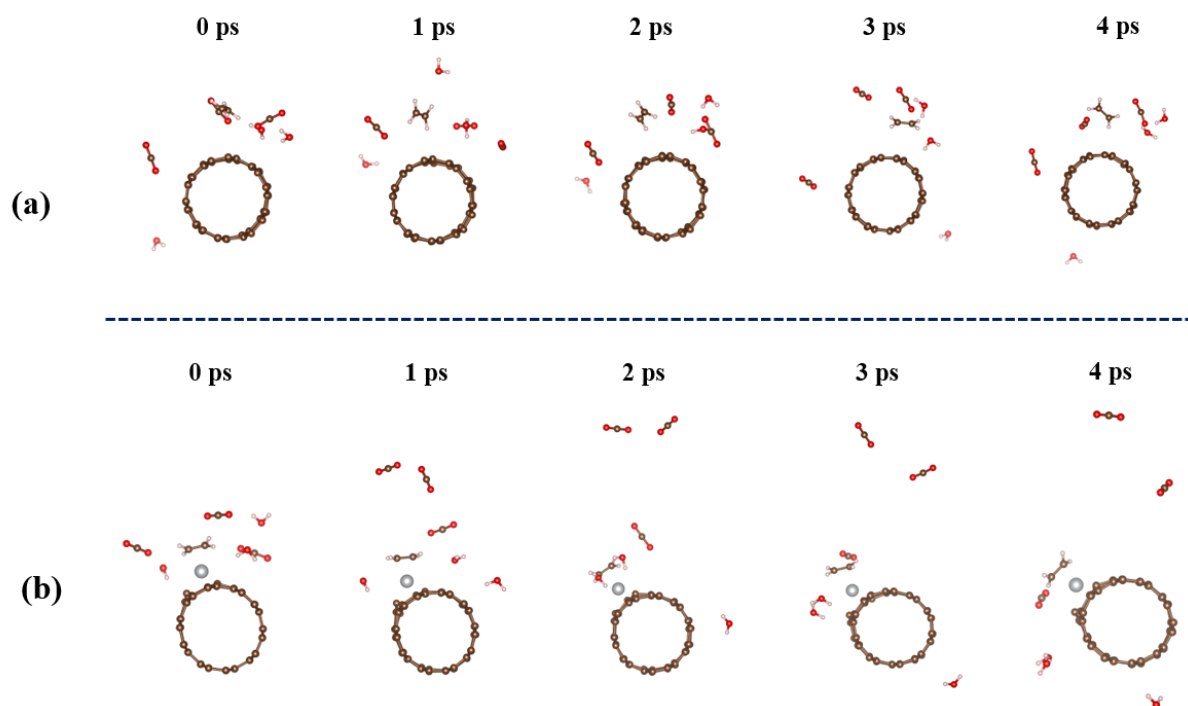


Figure 5. Representative snapshots from ab initio molecular dynamics (AIMD) simulations showing the dynamics of C_2H_4 , H_2O , and CO_2 molecules near the sidewall of (a) pristine SWCNT and (b) Ag-doped SWCNT over a simulation time of 4 ps. Snapshots are shown at 0, 1, 2, 3, and 4 ps. In the pristine SWCNT system, gas molecules diffuse freely around the nanotube surface, whereas in the Ag-doped SWCNT system, the C_2H_4 molecule remains localized near the Ag active site, indicating selective trapping.

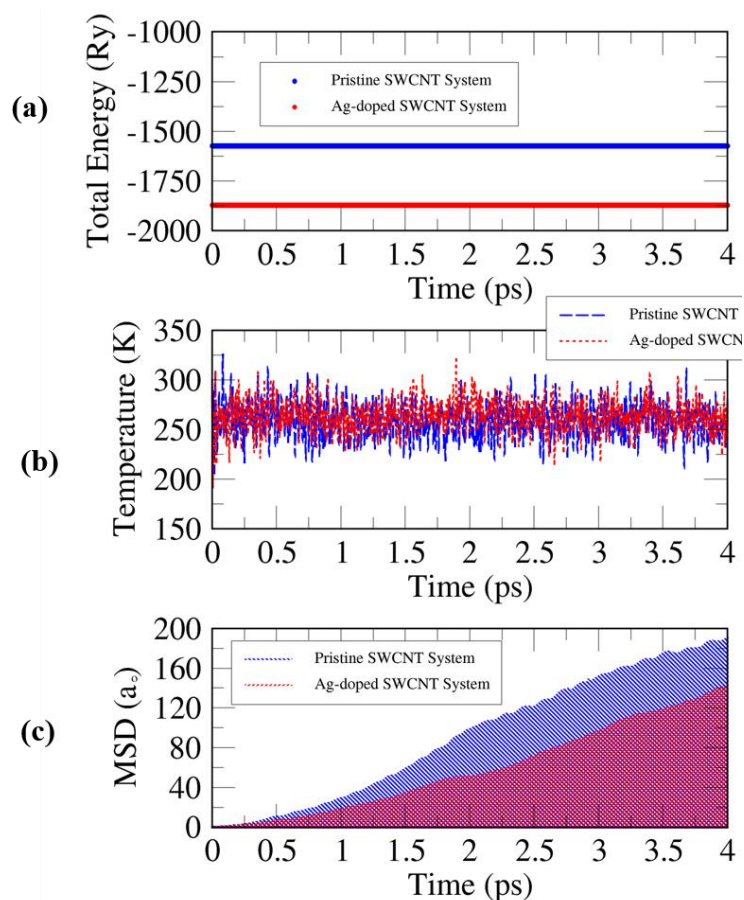


Figure 6. Time evolution of the (a) total energy, (b) temperature, and (c) mean-squared displacement (MSD) obtained from ab initio molecular dynamics simulations of pristine and Ag-doped SWCNT systems interacting with C_2H_4 , CO_2 , and H_2O molecules during a 4 ps trajectory.

The dynamical stability of the systems was further analyzed by tracking the evolution of total energy, temperature, and mean-squared displacement. The total energy remains nearly constant during the simulations (Figure 6a), confirming the stability of the AIMD trajectories. The instantaneous temperature fluctuates around 300 K (Figure 6b), indicating that the systems are properly equilibrated at room temperature conditions. The MSD analysis (Figure 6c) reveals a rapid increase for C₂H₄ on pristine SWCNT, showing high surface mobility and weak adsorption. Meanwhile, the significantly smaller MSD observed for C₂H₄ on the Ag-doped SWCNT demonstrates restricted diffusion near the dopant site, consistent with the selective trapping behavior observed in the AIMD snapshots (Figure 5).

4. Conclusions

This work investigates the adsorption of C₂H₄ on pristine and Ag-doped SWCNTs at the atomic level. The results reveal that C₂H₄ interacts weakly with pristine SWCNT via physisorption, characterized by low-magnitude adsorption energies (< 0.5 eV). Introducing an Ag dopant strengthens the interaction between the SWCNT and C₂H₄, resulting in bonding with covalent character. Electronic structure analysis reveals strong hybridization between the Ag(4d) and C(2p) states of C₂H₄, in agreement with the charge redistribution and electron localization observed at the adsorption site. Moreover, a single Ag-doped SWCNT active site can trap multiple C₂H₄ molecules without a substantial loss of adsorption strength. Ab initio molecular dynamics simulations at 300 K show that C₂H₄ remains trapped near the Ag dopant throughout the simulated period, even in the presence of competing volatile molecules such as H₂O and CO₂. These results suggest that Ag-doped SWCNTs could be used to control C₂H₄ levels in postharvest technologies and warrant further investigation of metal-doped carbon nanotubes for this purpose.

The present work predicts the ethylene-trapping capability of Ag-doped SWCNTs. Their adsorption performance has not yet been verified experimentally, either in the laboratory or under postharvest storage conditions. In practice, ethylene adsorption efficiency may be influenced by nanotube structure, surface properties, Ag loading, temperature, relative humidity, and ethylene concentration. Future studies should also investigate Ag dopant clustering and its impact on the adsorbent performance through theoretical and experimental approaches. Lastly, adsorption isotherms, isosteric heat measurements, and performance tests in sealed fruit chambers are also needed to fully evaluate the adsorption properties and practical effectiveness of the developed materials under realistic storage conditions.

Author Contributions

Conceptualization, A.A.Z.M. and C.B.M.; methodology, A.A.Z.M., C.B.M., D.L.H., R.N.N.G., R.M.R.H.; software, A.A.Z.M., C.B.M. and R.M.R.H.; validation; formal analysis, R.M.R.H.; investigation, A.A.Z.M. and C.B.M.; resources, A.A.Z.M., C.B.M. and R.M.R.H.; data curation, R.M.R.H.; writing—original draft preparation, A.A.Z.M.; writing—review and editing, A.A.Z.M., A.Q.L.J., C.B.M., D.L.H., R.N.N.G., R.M.R.H. and J.A.S.L; visualization, D.L.H., R.N.N.G.; supervision, A.A.Z.M.; project administration, A.A.Z.M.; All authors have read and agreed to the published version.

Institutional Review Board Statement

Not applicable.

Informed Consent Statement

Not applicable.

Data Availability Statement

Data supporting the findings of this study are available upon reasonable request from the corresponding author.

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Conflicts of Interest

The authors declare no conflict of interest.

Artificial Intelligence Disclosure

Artificial intelligence-based tools were used solely for language editing.

Abbreviations

The following abbreviations are used in this manuscript:

Abbreviation	Definition
Ag	Silver
Ag-doped SWCNT	Silver-doped Single-Walled Carbon Nanotube
AIMD	Ab Initio Molecular Dynamics
C ₂ H ₄	Ethylene
CDD	Charge Density Difference
CO ₂	Carbon Dioxide
DFT	Density Functional Theory
DOS	Density of States
ELF	Electron Localization Function
H ₂ O	Water
MSD	Mean-squared Displacement
PDOS	Partial Density of States
SWCNT	Single-Walled Carbon Nanotube

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