Simulation of the VOC Adsorption Mechanism on Activated Carbon Surface by Nitrogen-Containing Functional Groups

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Abstract: In this paper, the physical adsorption of volatile organic compounds (VOCs) such as methyl chloride (CH₃Cl), carbon disulfide (CS₂), dimethyl sulfide (C₂H₆S), and benzene (C₆H₆) by three models of activated carbon (without a functional group, with a pyridine-containing functional group, and with a pyrrole-containing functional group) was simulated. The surface electrostatic potential (ESP), physical adsorption energy, and non-covalent interaction between activated carbon and VOC molecules were analyzed based on the density functional theory (DFT). The effect mechanism of nitrogen-containing functional groups on VOC adsorption by activated carbon was determined. Our simulations showed that nitrogen-containing functional groups can change the surface ESP and polarity of activated carbon. The pyrrole functional group is conducive to CH₃Cl and CS₂ adsorption on the activated carbon plane, while the pyridine functional group is relatively small or even unfavorable for CH₃Cl and CS₂ adsorption on the activated carbon plane. The promotional effect of the pyrrole functional group on the adsorption of C₂H₆S is more significant than that of the pyridine functional group. The adsorption of C₆H₆ on activated carbon occurs through parallel-displaced π–π stacking interactions, in which functional groups have little influence on it. The adsorption energy of VOCs on the activated carbon plane is higher than that at the edge, so VOCs are more likely to be adsorbed on the activated carbon plane.

Keywords: activated carbon; functional group; VOC; DFT; adsorption

1. Introduction

Methyl chloride (CH₃Cl), carbon disulfide (CS₂), dimethyl sulfide (C₂H₆S), and benzene (C₆H₆) are typical volatile organic compounds (VOCs), with CH₃Cl being the most abundant long-lived chlorinated organic compound in the atmosphere, accounting for 17% of the stratospheric chlorine load and having an important impact on stratospheric ozone depletion [1]. Chemical production, industrial combustion, biomass combustion, and solvent use serve as crucial sources of CH₃Cl [1,2]. The rapid growth of the chemical industry, using CH₃Cl as a raw material, has driven the increase in its production and consumption [3]. A range of industrial processes, such as the Klaus process, sticky fiber production, and coal and biomass gasification, release sulfur compounds like CS₂. CS₂ is extremely unstable under ultraviolet irradiation, and it can be oxidized to form SO₂ and other substances, leading to the formation of acid fog and acid rain that pose serious environmental harm [4]. In addition, CS₂ has cytotoxic effects on human systems, especially in the nervous system, cardiovascular system, and reproductive system [5–8]. In addition to the petroleum and chemical industries, notable sources of C₂H₆S emissions include marine
activities, biomass combustion processes, landfill sites, and sewage treatment facilities. This gas has an unpleasant odor and can cause symptoms such as nausea and dizziness when inhaled in small quantities. \( \text{C}_6\text{H}_6 \) primarily originates from petrochemical industries, transportation sources, and indoor air pollution. It not only exhibits high toxicity but also serves as a potential precursor for the formation of PM2.5 and \( \text{O}_3 \). Therefore, appropriate measures should be implemented to mitigate its emissions and pollution.

In recent years, there has been a growing scholarly focus on the study of functional materials, which have a prominent position in the realm of high-tech. With their distinctive properties and extensive advantages, these functional materials exhibit significant potential in terms of catalysis, photocatalysis, sensor design, and adsorption fields [9]. Altering the chemical compositions of material surfaces through acid-base modification [10], doping metal [11], etc., is a approach commonly used to achieve functionalization. This method substantially enhances the adsorption sites and gas molecule adsorption capabilities on the surfaces of functional materials [12]. Activated carbon materials are evolving from conventional carbon-based porous substances to high-performance and highly functional materials that find widespread application in treating industrial VOCs [13]. The mechanism driving interactions between VOCs and porous carbon materials primarily involves physical adsorption [14]. Apart from factors like the adsorption device, the concentration, pressure, humidity, surface structure, and functional group of activated carbon significantly influence its adsorption capacity. During the process of the preparation of activated carbon, non-C elements such as N, O, and H can bond with C to form surface functional groups. Among these functional groups containing nitrogen atoms are mainly pyridine and pyrrole functional groups [15,16]. Graphene is a monolayer of carbon atoms, bonded in a trigonal sp2 configuration, forming a perfectly flat structure with microscopic ripples [17]. It serves as an ideal model for investigating the adsorption properties of activated carbon. By adjusting its chemical composition and other parameters, one can simulate the adsorption and removal processes of various gas pollutants. Remarkable advancements have been achieved by utilizing graphene as an activated carbon model. Studies have demonstrated that the interaction and adsorption energy between an adsorbate and an activated carbon model can be deeply explored by constructing a monolayer graphene model embedded with functional groups, thereby revealing the molecular adsorption mechanism [18,19].

Density functional theory (DFT) is a computational method based on the principles of quantum mechanics. By describing and solving the electron density, it can predict the structure, energy and various physical and chemical properties of materials. The development of hybrid DFT, such as B3LYP [20], brought to the desktop of experimental chemists a tool that allows the calculation of fairly accurate chemical structures and properties in reasonable timeframes [21]. Due to its excellent balance between computational cost and accuracy, this method has been widely used to investigate the atomic-scale adsorption properties of activated carbon [22,23]. Furthermore, with the introduction of the DFT-D dispersion correction method [24,25], DFT has become a very suitable method for calculating all kinds of non-covalent interactions. The independent gradient model based on the Hirshfeld partition (IGMH) proposed by Lu et al. [26] is a novel method for the visual analysis of noncovalent interactions. In comparison to the more popular independent gradient model (IGM) often used in recent years [27], the IGMH approach exhibits significantly superior graphical effects and a more rigorous physical background, thus being adopted by numerous scholars [28] since its inception. Guo et al. [29] conducted an IGMH study and found that the hydrogen bonding and \( \pi-\pi \) interactions can synergize to significantly improve the adsorption by increasing the \( \pi \)-electron density and shortening the distance of aromatic rings; thus, dyes with H-donors show significantly better adsorption capacities. Tang et al. [30] assessed the roles of oxygen-containing functional groups in uranium adsorption by aged polystyrene microplastics through IGMH analysis, revealing that the hydrogen bond formed by oxygen-containing functional groups is major driving force in interactions between uranyl and aged polystyrene microplastics.
The primary objective of this study is to investigate the impact of nitrogen-containing functional groups on the adsorption of VOCs by activated carbon using DFT. Specifically, by analyzing electrostatic potential (ESP), adsorption energy, and non-covalent interactions, we have gained a comprehensive understanding of how pyridine and pyrrole functional groups influence the adsorption of VOCs by activated carbon. These findings can provide valuable guidance for designing and synthesizing high-quality activated carbon with enhanced VOC adsorption capabilities.

2. Models and Methods

2.1. Calculation Models

The impacts of pyridine and pyrrole functional groups on the adsorption behavior of VOCs were investigated using activated carbon models, as depicted in Figure 1a–c, where Figure 1a represents a comparison model without any functional groups, referred to as NF. The activated carbon model containing the pyridine functional group is denoted as PD in Figure 1b, while the one with the pyrrole functional group is denoted as PR in Figure 1c. Models for CH₃Cl, CS₂, C₂H₆S, and C₆H₆ are illustrated in Figure 1d–g, respectively. The typical bond length data for the molecular models is provided in Figure S1.

Figure 1. Molecular models of activated carbon and volatile organic compounds (VOCs): (a) NF, (b) PD, (c) PR, (d) methyl chloride (CH₃Cl), (e) carbon disulfide (CS₂), (f) dimethyl sulfide (C₂H₆S), and (g) benzene (C₆H₆). NF is a comparative model devoid of any functional groups, while PD and PR denote activated carbon models featuring the pyridine and pyrrole functional groups, respectively.

2.2. Calculation Methods

The adsorption of CH₃Cl, CS₂, C₂H₆S, and C₆H₆ on activated carbon was simulated using Gaussian software [31]. The B3LYP method was employed for structural optimization and wavefunction generation at the 6-311+G** [24] basis set level. To address the inadequate description of dispersion interactions using functional methods, DFT-D3 (BJ) [25] dispersion correction was incorporated into the simulation. In order to enhance computational accuracy, DFT-D3 [32] dispersion correction was performed at the M062X/jun-cc-pVTZ [33–35] level for single-point energy calculations after geometry optimization. The optimized wavefunctions were analyzed using Multiwfn software [36] for van der Waals (vdW) surface ESP and IGMH analysis, while isosurface plots were generated using VMD software [37]. The physical adsorption energy $E_{Ads}$ was defined as follows:

$$E_{Ads} = E_{Pro} - (E_{AC} + E_{VOC})$$  \hspace{1cm} (1)$$

where $E_{Pro}$, $E_{AC}$, and $E_{VOC}$ represent the single-point energies of the physical adsorbate, activated carbon, and small molecule VOCs (CH₃Cl, CS₂, C₂H₆S and C₆H₆), respectively.
In the IGMH analysis, Lu et al. proposed using $\delta\rho_{\text{inter}}$ iso-surfaces to visualize the regions of interaction. Furthermore, they employed a color-scale bar of the $\text{sign}(\lambda_2)\rho$ function onto these surfaces to demonstrate both the type and strength of the interactions, as depicted in Figure 2. Here, $\lambda_2$ represents the second largest eigenvalue of the electron density ($\rho$) Hessian matrix, and $\text{sign}(\lambda_2)$ represents taking a sign of $\lambda_2$. The $\delta\rho_{\text{atom}}$ defined by Lu et al. was utilized for quantitatively measuring atomic contributions to the interactions between fragments.

\begin{equation}
\rho > 0 \quad \text{sign}(\lambda_2)\rho \text{ decreases} \quad \rho \approx 0 \quad \text{sign}(\lambda_2)\rho \text{ increases} \quad \rho > 0
\end{equation}

$\lambda_2 < 0 \quad \lambda_2 \approx 0 \quad \lambda_2 > 0$

-0.05 a.u. 0.05 a.u.

- bond with nonnegligible covalency (H-bond, halogen-bond...), and purely ionic bond
- prominent attractive weak interaction
- van der Waals interaction
- prominent repulsive interaction (steric effect in ring and cage...)

**Figure 2.** Common interpretation of coloring method of mapped function $\text{sign}(\lambda_2)\rho$ in the independent gradient model based on the Hirshfeld partition (IGMH) maps [38].

### 3. Results and Discussion

#### 3.1. ESP Analysis

The distribution of surface ESP in Figure 3a is relatively uniform. The ESP near to the H-atom is positive, while that above the C-atom is negative, reflecting a rich $\pi$ electron cloud. Comparing Figure 3a–c, it becomes evident that the absolute value of surface ESP on the plane of the activated carbon molecule without functional groups surpasses that with a pyridine functional group and is lower compared to that with a pyrrole functional group. This disparity has implications for the adsorption behavior of VOCs on activated carbon planes. In Figure 3b, incorporating a pyridine functional group alters the ESP distribution of the activated carbon model, with negative ESP being present around the dopd N-atom as an electron donor [39,40]. In Figure 3c, adding a pyrrole functional group causes an increase in ESP around the H-atom connected to the N-atom, where the highest ESP functions as an electron acceptor [39,40]. In summary, introducing nitrogen-containing groups can modify both the surface ESP distribution and molecular polarity characteristics of the activated carbons.

**Figure 3.** The surface electrostatic potential (ESP) of activated carbon models on the van der Waals (vdW) surface: (a) NF, (b) PD, (c) PR, and (d) a color scale bar.

Figure 4a–d illustrate the surface ESP distributions of the $\text{CH}_3\text{Cl}$, $\text{CS}_2$, $\text{C}_2\text{H}_6\text{S}$, and $\text{C}_6\text{H}_6$ molecular models. For $\text{CH}_3\text{Cl}$, the ESP surrounding the three H-atoms exhibits a positive charge, rendering it an electron acceptor that can be adsorbed onto activated carbon planes and around pyridine nitrogen sites. Conversely, the ESP around the Cl-atom...
displays a negative charge, signifying its role as an electron donor. The ESP distribution on the surface of the CS₂ molecular model exhibits a relatively homogeneous pattern, characterized by small absolute values. Notably, the ESP maximums are situated at both ends and in the middle region. The presence of negative ESP surrounding the S atom in C₂H₆S indicates its electron-donating properties and ability to form hydrogen bonds with the H atom at the edge of the activated carbon model. Conversely, the positive ESP near the H atom in C₂H₆S suggests its electron-accepting characteristics and capacity to engage in hydrogen bonding with the C atom and pyridine N atom of the activated carbon model. These predictions are subsequently validated. The ESP of C₆H₆ is similar to that of NF in that its π-electron cloud is rich, allowing it to perform π–π stacking interactions with other benzene rings.

![Figure 4](image.png)

**Figure 4.** The surface ESP of VOCs on the vdW surface: (a) CH₃Cl, (b) CS₂, (c) C₂H₆S, (d) C₆H₆, and (e) a color scale bar.

### 3.2. Physical Adsorption of CH₃Cl by Activated Carbon

There are two adsorption configurations of CH₃Cl on the activated carbon plane, as depicted in Figure 5a–f. The green isosurfaces in Figure 5a–c reveal that the interaction between CH₃Cl and activated carbon primarily involves dispersion and hydrogen bonding, predominantly caused by the C- and H-atoms of CH₃Cl. The physical adsorption energy of CH₃Cl on the activated carbon plane depends on the ESP of the activated carbon plane, resulting in a physical adsorption energy order of PR plane > NF plane > PD plane, as shown in Table 1. Notably, no significant variation is observed in the physical adsorption energy among these three configurations, indicating the minimal influence of functional groups on the physical adsorption behavior of CH₃Cl on the activated carbon plane.

### Table 1. Physical adsorption energy (eV) of CH₃Cl₂ on the plane and edge of activated carbon.

<table>
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<tr>
<th></th>
<th>NF</th>
<th>PD</th>
<th>PR</th>
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<tbody>
<tr>
<td>Plane</td>
<td>−0.216 (−0.221)</td>
<td>−0.201 (−0.223)</td>
<td>−0.229 (−0.265)</td>
</tr>
<tr>
<td>Edge</td>
<td>−0.115</td>
<td>—</td>
<td>—</td>
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Another adsorption configuration of CH₃Cl on the activated carbon plane is depicted in Figure 5d–f. The interaction between CH₃Cl and activated carbon involves dispersion forces, halogen bonds, and hydrogen bonds, primarily contributed by the C, Cl, and H atoms of CH₃Cl. Table 1 shows that the promotion effect of the pyrrole functional group on CH₃Cl adsorption by activated carbon is more pronounced compared to that of the pyridine functional group. Figure 5d,f reveal similar adsorption configurations and interactions of CH₃Cl on the planes of NF and PR. However, due to the higher absolute value of ESP on the PR plane than that on NF plane, the interaction strength and physical adsorption energy for CH₃Cl adsorbed by PR are greater than those by NF. This is supported by the electron density values at the bond critical points shown in Figure S2. Despite having a lower ESP value than NF, PD exhibits slightly higher adsorption energy for CH₃Cl because its Cl atom’s adsorption site lies in the middle of the PD plane and has a larger action area.
CH$_3$Cl selectively adsorbs onto the PD edge, primarily through vdW forces and hydrogen bonding, resulting in a relatively weak physical adsorption energy of $-0.115$ eV. In comparison to edge adsorption, CH$_3$Cl demonstrates a higher affinity for the activated carbon plane.

**Figure 5.** IGMH analysis diagram depicting the adsorption of CH$_3$Cl on different activated carbon surfaces: (a,d) NF plane, (b,e) PD plane, (c,f) PR plane, and (g) PD edge. Atoms are colored by $\delta G_{\text{atom}}$. Bond critical points (orange spheres) and bond paths (brown lines) are also shown.

### 3.3. Physical Adsorption of CS$_2$ by Activated Carbon

The adsorption configuration of CS$_2$ on the activated carbon plane is illustrated in Figure 6a–c. The green interface between CS$_2$ and activated carbon represents vdW forces, which are influenced by the ESP of the activated carbon plane. Consequently, the physical adsorption energy order of CS$_2$ on the activated carbon plane can be observed as PR plane > NF plane > PD plane, as depicted in Table 2. Compared to the results calculated by Bhattarai et al. [41], our findings indicate a higher adsorption energy of CS$_2$ on the PD plane, i.e., $-0.231$ eV. This discrepancy can be attributed to our utilization of a larger activated carbon model, which effectively enhances the interaction area with CS$_2$. 
The above description implies that the presence of the pyridine functional group enhances the adsorption of CH$_3$Cl and CS$_2$ on the activated carbon edge, whereas the pyrrole functional group contributes to their adsorption on the activated carbon plane. This finding offers a pathway for designing highly efficient activated carbon materials tailored for CH$_3$Cl and CS$_2$ adsorption. Research has demonstrated that melamine [40], urea-formaldehyde resin [43], nitric acid [44], and ammonia [16,45] modifications enrich activated carbon surfaces with pyridine and pyrrole functional groups. Therefore, these modification methods can be used to enhance the adsorption effectiveness of CH$_3$Cl and CS$_2$ on activated carbon.
3.4. Physical Adsorption of C$_2$H$_6$S by Activated Carbon

The adsorption configuration of C$_2$H$_6$S on the activated carbon plane is illustrated in Figure 7a–c. The interaction between C$_2$H$_6$S and the three established activated carbon models exhibits similarity, showcasing a V-shaped green isosurface that encompasses three distinct regions of interaction. Specifically, the isosurface on both sides represents the hydrogen bond and dispersion interaction formed by the H and C atoms of C$_2$H$_6$S with the activated carbon plane, while the isosurface in the middle corresponds to the dispersion interaction formed by the S atoms of C$_2$H$_6$S with the activated carbon plane. It can be easily determined by the atomic color that the S atom makes the greatest contribution to the physical adsorption. Referring to Table 3 for adsorption energy, both pyridine and pyrrole functional groups have a positive effect on the adsorption of C$_2$H$_6$S on the activated carbon plane, augmenting its adsorption energy by 0.024 and 0.031 eV, respectively.

![Figure 7](image)

**Figure 7.** IGMH analysis diagram depicting the adsorption of C$_2$H$_6$S on different activated carbon surfaces: (a) NF plane, (b) PD plane, (c) PR plane, (d) NF edge, (e) PD edge, and (f) PD edge. Atoms are colored by $\delta G_{\text{atom}}$. Bond critical points (orange spheres) and bond paths (brown lines) are also shown.

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<th>NF</th>
<th>PD</th>
<th>PR</th>
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<tbody>
<tr>
<td>Plane</td>
<td>−0.302</td>
<td>−0.326</td>
<td>−0.333</td>
</tr>
<tr>
<td>Edge</td>
<td>−0.107</td>
<td>−0.196</td>
<td>−0.283</td>
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</table>

The adsorption of C$_2$H$_6$S on the activated carbon edge exhibits a common characteristic, namely, the formation of a hydrogen bond between the S atom of C$_2$H$_6$S and the H atom of the activated carbon models. This interaction is illustrated as a disc-shaped isosurface in the figure. Among these interactions, the H atom connected to the N atom in PR displays the highest electrostatic potential, resulting in its strongest hydrogen bonding with the S atom. The corresponding bond critical point density reaches 0.01705 a.u., significantly surpassing that of 0.01032 and 0.01093 a.u. in NF and PD, respectively, as illustrated in Figure S4. Consequently, this leads to the PR edge having the highest adsorption energy for C$_2$H$_6$S, reaching −0.283 eV. In Figure 7d, a weak dispersion force is observed between the two H atoms of C$_2$H$_6$S and the
H atom of NF, resulting in the formation of an isosurface with a small region. In Figure 7e, a larger region exhibits an isosurface formed between the two H atoms of C₂H₆S and the N atom of PD, indicating a stronger interaction characterized by hydrogen bonding. This leads to an increase in adsorption energy. Consequently, it can be inferred that the pyridine functional group facilitates the adsorption of C₂H₆S at the edge of activated carbon.

Based on Table 3 and the above analysis, it becomes evident that, comparatively speaking, the pyrrole functional group is more favorable for C₂H₆S adsorption than the pyridine functional group. Furthermore, it can be observed that C₂H₆S is more readily adsorbed onto the activated carbon plane rather than its edge.

3.5. Physical Adsorption of C₆H₆ by Activated Carbon

No physical adsorption configuration of C₆H₆ at the edge of activated carbon was observed in this study, despite multiple attempts at geometric optimization. This suggests that the adsorption of C₆H₆ at the edge of activated carbon is challenging to achieve.

Figure 8 illustrates the adsorption configuration of C₆H₆ on the activated carbon plane, revealing noticeable parallel-displaced π–π stacking interactions between C₆H₆ and the activated carbon models. The distances from the center of C₆H₆ to the marked C atom (as depicted in Figure 8) on NF, PD, and PR are 3.331 a.u., 3.329 a.u., and 3.371 a.u., respectively. Consequently, it can be concluded that pyridine does not exert a significant influence on this distance while pyrrole functional groups lead to its increase. By comparing the electron density of the bond critical points numbered 1, 2, and 3 in Figure 8a–c, it is evident that the bond critical point formed by C₆H₆ and PR has the lowest electron density, while the bond critical point formed by C₆H₆ and PD demonstrates the highest electron density (excluding bond critical point 3 in PD). This implies that the presence of the pyridine functional group enhances the π–π stacking interaction between C₆H₆ and C atoms connected to the marked C atom, whereas the pyrrole functional group diminishes this interaction. Regarding bond critical point 4, the electron density follows the order of PR > NF > PD. In other words, the pyrrole functional group strengthens interactions in proximity to bond critical point 4, while the pyridine functional group weakens them. According to the adsorption energy values given in Table 4, a comprehensive assessment can be made regarding the π–π stacking interaction between C₆H₆ and activated carbon models. It is evident that C₆H₆ exhibits similar adsorption energy values on PR and NF, indicating that pyrrole functional groups have minimal impact on the adsorption of C₆H₆ onto the activated carbon plane. However, it is noteworthy that C₆H₆ demonstrates a higher adsorption energy (−0.0379 eV) on PD, surpassing its value on NF by 0.01 eV. Hence, it can be inferred that pyridine functional groups weakly enhance the adsorption process of C₆H₆ onto the activated carbon plane.

![Figure 8](image-url)

**Figure 8.** IGMH analysis diagram depicting the adsorption of C₆H₆ on different activated carbon surfaces: (a) NF plane, (b) PD plane, and (c) PR plane. Atoms are colored by δG^atom. Bond critical points (orange spheres) and bond paths (brown lines) are also shown. Parts of bond critical points are labeled in red, while the electron density at these points is depicted in black.
Table 4. Physical adsorption energy (eV) of $C_6H_6$ on the plane of activated carbon.

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<tr>
<th>Plane</th>
<th>NF</th>
<th>PD</th>
<th>PR</th>
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<tr>
<td>Plane</td>
<td>$-0.369$</td>
<td>$-0.379$</td>
<td>$-0.371$</td>
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</table>

4. Conclusions

In this study, we investigated the mechanism for the adsorption of CH$_3$Cl, CS$_2$, C$_2$H$_6$S, and C$_6$H$_6$ onto activated carbon modified with pyridine and pyrrole functional groups by analyzing ESP and non-covalent interactions. The polarity of the activated carbon surface is enhanced through the incorporation of nitrogen-containing functional groups. Upon the introduction of the pyridine functional group, a negative ESP surrounds the pyridine nitrogen, leading to a decrease in the absolute ESP on the activated carbon plane. Conversely, when incorporating the pyrrole functional group, a positive ESP is observed on the hydrogen atom connected to the pyrrole nitrogen, resulting in an increase in absolute ESP on the activated carbon plane.

The physical adsorption of CH$_3$Cl and CS$_2$ on the activated carbon plane is influenced by the ESP of the activated carbon plane. The presence of a pyrrole functional group enhances the adsorption capacity of CH$_3$Cl and CS$_2$ on the activated carbon plane, whereas the pyridine functional group has limited or even unfavorable effects. The S atom in C$_2$H$_6$S plays a crucial role in the adsorption process by forming dispersion interactions with C atoms on the activated carbon plane and hydrogen bonds with H atoms at the edges. Both pyridine and pyrrole functional groups positively impact the adsorption of C$_2$H$_6$S, with pyrrole exhibiting a more significant promotion effect than pyridine. The adsorption of C$_6$H$_6$ onto activated carbon occurs through parallel-displaced π–π stacking interactions, where the influence of the pyrrole functional group is minimal while the pyridine functional group weakly promotes it. Moreover, it should be noted that VOCs exhibit higher adsorption energy on the activated carbon plane compared to that at its edges, indicating a greater propensity for their adsorption onto it.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/app14051793/s1, Figure S1: Molecular models of activated carbon and volatile organic compounds (VOCs): (a) NF, (b) PD, (c) PR, (d) CH$_3$Cl, (e) CS$_2$, (f) C$_2$H$_6$S, and (g) C$_6$H$_6$. Typical bond lengths (Å) have been marked with text; Figure S2: IGMH analysis diagram depicting the adsorption of CH$_3$Cl on different activated carbon surfaces: (a,d) NF plane, (b,e) PD plane, (c,f) PR plane, and (g) PD edge. Atoms are colored by $\delta^{\text{atom}}$. Bond critical points (orange spheres) and bond paths (brown lines) are also shown. Electron density values (a.u.) at the bond critical points are indicated by texts. Figure S3: IGMH analysis diagram depicting the adsorption of CS$_2$ on different activated carbon surfaces: (a) NF plane, (b) PD plane, (c) PR plane, (d) NF edge, and (e) PD edge. Atoms are colored by $\delta^{\text{atom}}$. Bond critical points (orange spheres) and bond paths (brown lines) are also shown. Electron density values (a.u.) at the bond critical points are indicated by texts. Figure S4: IGMH analysis diagram depicting the adsorption of C$_2$H$_6$S on different activated carbon surfaces: (a) NF plane, (b) PD plane, (c) PR plane, (d) NF edge, (e) PD edge, and (f) PD edge. Atoms are colored by $\delta^{\text{atom}}$. Bond critical points (orange spheres) and bond paths (brown lines) are also shown. Electron density values (a.u.) at the bond critical points are indicated by texts.

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Conflicts of Interest: The authors declare no conflicts of interest.


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