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Adsorption simulation of open-ended single-walled carbon nanotubes for various gases

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ABSTRACT
In order to study the adsorption capacity of open-ended single-walled carbon nanotubes for various gases, the grand canonical Monte Carlo method is used to simulate the adsorption capacities of methane, nitrogen, water, carbon dioxide, and carbon monoxide in different types of open-ended single-walled carbon nanotubes at temperatures of 273.15 K and 298.15 K and pressures of 1 Pa–101.325 kPa. Gas adsorption isotherms under various conditions were obtained. The effects of temperature and diameter of open-ended single-walled carbon nanotubes on gas adsorption capacity were discussed. The results showed that the open-ended single-walled carbon nanotubes had a certain adsorption capacity for five kinds of gases under low pressure conditions. For a given temperature, as the diameter of the tube increased, the adsorption capacities of various gases were enhanced. Each gas exhibited different growth gradients; specifically, the growth gradients of methane and nitrogen were relatively small, while the growth gradients of water, carbon dioxide, and carbon monoxide were relatively large. With an increase in the temperature, the adsorption capacities of CH\textsubscript{4}, N\textsubscript{2}, H\textsubscript{2}O, and CO\textsubscript{2} exhibited a downward trend, while the adsorption capacity of CO was not affected by temperature, keeping a stable value. The open-ended single-walled carbon nanotube with a diameter of 10.85 Å exhibited a high adsorption capacity for CO, and it could be used as a porous material for storing or separating CO.

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I. INTRODUCTION
It has been 28 years since the first carbon nanotubes (CNTs) were discovered.\textsuperscript{1} CNTs are formed by rolled graphite sheets, of which the inner diameter starts from 7 nm up to several nm and has a length of 10–100 μm. The single-walled carbon nanotubes (SWCNTs) are formed by only one single graphite layer. At present, researchers pay much attention to SWCNTs because of their electronic and remarkable physico-chemical properties.\textsuperscript{2–9} SWCNTs are attractive materials for adsorption-related applications, such as the use of nanotubes for developing sensors of pollutant gases,\textsuperscript{10–14} storage of alternative fuels,\textsuperscript{9–11} membranes,\textsuperscript{12–22} and removal of hazardous pollutants from gas streams,\textsuperscript{22} for which the study on the characteristics of their adsorption properties are significant.

A lot of experimental research has been carried out on the adsorption of inorganic molecules (N\textsubscript{2}, CO\textsubscript{2}, Ar, Xe, and SiO\textsubscript{2})\textsuperscript{9–34} and organic vapors\textsuperscript{34–44} in different types of carbon nanotubes, such as single-walled or multi-walled carbon nanotubes and closed- or open-ended carbon nanotubes. Currently, molecular simulations of gas adsorption in carbon nanotubes\textsuperscript{33–37} have been extensively studied, including gas adsorption inside carbon nanotubes and on their external surfaces.

This research is mainly on adsorption sites, adsorption capacities of various gases, and the influence of different structural arrays of carbon nanotube bundles on external surface adsorption. However, little emphasis has been given to the adsorption on open-ended SWCNTs. CO and other gases generated by spontaneous combustion of coal seams in goafs of coal mines or the working face seriously threaten the life safety of underground workers. Although gas concentration monitoring sensors are arranged on the roadway, the CO concentration overrun problem cannot be processed well in time.

In this article, a series of molecular simulations of various gas adsorption capacities inside the tubes of open-ended SWCNTs were carried out, and the results were analyzed. The various gas...
adsorption capacities in the tube of the open-ended SWCNTs were determined by the grand canonical Monte Carlo (GCMC) simulation method. In molecular simulation, the influence of temperatures and diameters of open-ended SWCNTs on adsorption capacity was taken into account. The open-ended SWCNTs with the diameters of 8.14, 9.49 and 10.85 Å selected for calculation were the ones determined by manufactured in this study. The results indicated that temperature had a serious influence on the adsorption capacity of \( \text{H}_2\text{O} \) but had no influence on the adsorption capacity of \( \text{CO} \). Under different pressure and temperature conditions, the adsorption capacities of \( \text{CH}_4 \), \( \text{N}_2 \), \( \text{H}_2\text{O} \), \( \text{CO}_2 \), and \( \text{CO} \) were affected by the pore diameter of the open-ended SWCNTs. Not all gas adsorption capacities would increase as the diameters of SWCNTs grow. For \( \text{CH}_4 \), \( \text{N}_2 \), \( \text{H}_2\text{O} \), and \( \text{CO}_2 \), their adsorption capacities in a certain pressure range did not increase with the increase in the pore diameters. In contrast to this, the adsorption capacity of \( \text{CO} \) in the range of 1–101.325 kPa was positively related to the diameter of the open-ended SWCNTs. As the diameter of the open-ended SWCNTs increased, the open-ended SWCNTs showed a higher adsorption capacity for \( \text{CO} \). In view of this, open-ended SWCNTs can be used as a porous material for storing \( \text{CO} \).

II. MODELS AND SIMULATIONS

A. The model of open-ended SWCNTs and adsorbates

Open-ended SWCNTs with three different diameters are shown in Fig. 1. The molecular structures of adsorbates are shown in Fig. 2. The open-ended SWCNT diameter \( d \), which is defined as the internuclear distance between diametrically opposed carbon atoms on the external surface of a nanotube, and the length \( L \) define the geometry of the model. The parameters of the supercell we have established are shown in Table I. The supercell is composed of three unit cells.

B. Simulations

The grand canonical (constant chemical potential, volume, and temperature) Monte Carlo method was used to simulate the adsorption of gases (\( \text{CH}_4 \), \( \text{N}_2 \), \( \text{H}_2\text{O} \), \( \text{CO}_2 \), and \( \text{CO} \)) in SWCNTs at 273.15 K and 289.15 K. In the study, \( \text{CH}_4 \) and \( \text{N}_2 \) used the TraPPE model, \( \text{H}_2\text{O} \) adopted the extended simple point charge (SPC-E) model, \( \text{CO}_2 \) adopted the EPM2 [EPM2 is obtained by rescaling the potential parameters of the elementary physical model (EPM)] model, and the Lennard-Jones (LJ) parameters of linear molecules of \( \text{CO} \) was calculated by Bohn. It was assumed that the SWCNTs and each fluid molecule were rigid and remained electrically neutral during the simulations. \( \text{CH}_4 \) and \( \text{N}_2 \) are non-polar molecules. Although \( \text{CO}_2 \) is a polar molecule, due to the feedback \( \pi \) bond, the polarity of the molecule is very weak and can be negligible. Therefore, the interaction of these three molecules with the combined atoms of SWCNTs did not require consideration of the long-range charge Coulomb force, and only the short-range van der Waals force was needed to be considered. For them, the interaction between the carbon atoms of nanotubes and each adsorbate molecule is modeled using the LJ potential, expressed as

\[
    u_{ij}(r) = 4\varepsilon_{ij} \left( \frac{\sigma_{ij}}{r} \right)^{12} - \left( \frac{\sigma_{ij}}{r} \right)^{6},
\]

where \( r \) is the intermolecular distance.

\( \text{CO}_2 \) and \( \text{H}_2\text{O} \) are polar molecules that carry a charge; hence, the effect of the long-range charge Coulomb force needs to be considered when interacting with carbon atoms of nanotubes. The LJ potential is expressed as

\[
    u_{ij}(r) = 4\varepsilon_{ij} \left( \frac{\sigma_{ij}}{r} \right)^{12} - \left( \frac{\sigma_{ij}}{r} \right)^{6} + \frac{q_i q_j}{4\pi\varepsilon_0 r},
\]

where \( r \) is the intermolecular distance.
TABLE I. Parameters of the supercell.

| SWCNTs | a (Å) | b (Å) | c (Å) | α (deg) | β (deg) | γ (deg) | Diameter (Å) | Volume (Å³) |
|--------|-------|-------|-------|--------|--------|--------|-------------|-------------|
| (6,6)  | 11.48 | 11.48 | 14.76 | 90     | 90     | 120    | 8.14        | 1685.16     |
| (7,7)  | 12.84 | 12.84 | 14.76 | 90     | 90     | 120    | 9.49        | 2106.65     |
| (8,8)  | 14.20 | 14.20 | 14.76 | 90     | 90     | 120    | 10.85       | 2575.15     |

TABLE II. Lennard-Jones potential parameters.

| Substance | Type of atom | ε/k_B (K) | σ_1 (Å) | q/ε |
|-----------|--------------|-----------|--------|-----|
| SWCNTs    | C            | 28.0      | 3.40   | 0   |
| CH_4      | CH_4         | 148.1     | 3.73   | 0   |
| H_2O      | H            | 0         | 3.17   | 0.4238 |
|           | O            | 78.18     | 3.17   | -0.8476 |
| CO_2      | C            | 28.13     | 2.76   | 0.6512 |
|           | O            | 80.51     | 3.03   | -0.3256 |
| N_2       | N            | 36        | 0.33   | 0   |
| CO        | CO           | 42.28     | 3.27   | 0   |

TABLE III. Parameters in simulation.

| Forcefield | Dreiding Equilibration steps | 10^6 |
|------------|-----------------------------|------|
| Charges    | Use current Production steps | 2 × 10^6 |
| Electrostatic | Ewald Exchange               | 0.39 |
| Ewald accuracy | 0.001 kcal/mol Conformer | 0.20 |
| van der Waals | Atom based Rotate | 0.20 |
| Cutoff distance | 0.5a nm Translate | 0.20 |

where q_i and q_j are the atomic charge, ε_0 is the dielectric constant, ε_i/k_B is the well depths, k_B is the Boltzmann constant, and σ_i is the collision diameters.

The parameters are listed in Table I. Cross-terms are obtained using the standard Lorenz-Berthelot combining rules, represented by the following equations:

ε_{ij} = \sqrt{ε_i ε_j}, \quad (3)

σ_{ij} = (σ_i + σ_j)/2. \quad (4)

This potential is applicable to gas adsorption inside the tube of SWCNTs. Periodic boundary conditions were employed in the calculation of adsorbate interactions beyond the simulation cell. The Lennard-Jones potential parameters are listed in Table II.

The construction and optimization of open-ended SWCNTs and adsorbent molecules were completed by the Forcite module of the Materials Studio software. Simulations were performed by the Sorption module, of which the calculation process was based on the GCMC method. In the simulation, both the van der Waals and electrostatic potential were considered as the intermolecular forces. It was impossible to take the forces between all molecules into account during calculation. At the same time, in order to reduce the calculation time, a truncation radius was introduced (that is, the interaction between molecules mainly comes from truncation within the radius; hence, the force outside the range was small and could be ignored). The truncation radius of the vdW force in this paper was half of the minimum side length of the supercell (equal to 0.5a). The summation method of the van der Waals force was Ewald based, of which the accuracy was 0.001 kcal/mol. For the purpose of making the simulation results more credible, the equilibrium steps and production steps were set to one million and two million, respectively, and the adsorption isotherm of each gas was simulated three times. Finally, the average value was taken as the adsorption amount. The parameter settings in GCMC simulations were listed in Table III, and all of them had been verified in the literature.44

III. RESULTS AND DISCUSSION

A. Adsorption in the tube of open-ended single-walled carbon nanotubes

For open-ended single-walled carbon nanotubes, gas adsorption only took place in its tubes. The space available to the adsorptive molecules and the adsorption potential are dependent on the diameter, d. Figures 3(a)–3(f) show the adsorption isotherms of different gases adsorbed on open-ended SWCNTs (6,6), (7,7), and (8,8) with diameters of 8.14 Å, 9.49 Å, and 10.85 Å, respectively, at 273.15 K and 298.15 K. According to the classification about pores of the International Union of Pure and Applied Chemistry (IUPAC), the tubes may be regarded as supermicropore (7 < d < 20 Å) with strongly enhanced interaction potentials, resulting in type I shape isotherms in each case. The interstitial space available to the adsorptive molecules was enhanced with the increase in d, which in turn resulted in an increase in the adsorption amount.

The growth gradient is calculated by

\[ \text{Growth gradient} = \frac{Q_i - Q_j}{d_i - d_j} (i = 2, 3; j = 1, 2). \quad (5) \]

The maximum amount of the different gases adsorbed in the tubes of open-ended SWCNTs is listed in Tables IV and V.

The density of N_2 in open-ended SWCNTs (6,6), (7,7), and (8,8) at 298.15 K are 0.002 078, 0.001 613, and 0.001 668 molecules/Å³, respectively, which have the same order of magnitude of the density of N_2 0.002 462 molecules/Å³, in the literature.66 The relative errors are 15.60%, 34.48%, and 32.25%. The densities
FIG. 3. Adsorption isotherms [a), (c), and (e) are SWCNTs (6,6), (7,7), and (8,8), respectively, at 273.15 K; and (b), (d), and (f) are SWCNTs (6,6), (7,7), and (8,8), respectively, at 298.15 K].
of CH₄, H₂O, CO₂, and CO are of the same order of magnitude as that of N₂, as shown in Table VI. The adsorption simulation of SWCNT (9,9) is studied in the literature. We find that the densities of CH₄, CO₂, and CO, shown in Table VI, are of an order of magnitude smaller than that in the literature. This is because in the simulation, the gas is only adsorbed on the tube of open-ended SWCNTs, and gas adsorption does not occur outside the tube. At the same time, the unit cell established is a hexagonal structure, leaving free space at the corners. This free volume participates in the calculation of the densities, so the densities we obtained are smaller than the true values. The computational model in the literature is SWCNT (10,10). Comparing it with the adsorption amount of H₂O we obtained from the simulation, the relative errors are 23%, 27.33%, and 23%, respectively. Through this analysis, we can make sure that the established model and simulation are correct.

**B. Effect of the pore diameter of open-ended SWCNTs on adsorption capacity**

Figures 4(a) and 4(b) show that the amount of CH₄ adsorbed on the tube of open-ended SWCNTs is enhanced progressively with an increase in d for a given temperature, especially at the pressure of 10 kPa. For open-ended SWCNT (8,8), the adsorption amount of CH₄ is obviously larger than that of the other two open-ended SWCNTs for pressures more than 10 kPa.

Figures 4(c) and 4(d) show that the amount of N₂ adsorbed on the tubes of open-ended SWCNT (6,6) and SWCNT (7,7) nearly overlap for a given temperature. The amount of N₂ adsorbed on the tube of SWCNT (8,8) is less than that of the others less than 20 kPa at 273.15 K or 50 kPa at 298.15 K.

Figures 4(e) and 4(f) show the adsorption isotherms of H₂O at the temperature of 273.15 K and 298.15 K. From Fig. 4(e), it can be obviously observed that the diameters of open-ended SWCNTs are smaller and the pressures at which the adsorption starts are lower. The adsorption amount of SWCNT (6,6) is quick to reach the maximum under strong adsorption potential. The intersection point of three curves, as shown in Fig. 4(e), is at a pressure of about 35 kPa; after that, the adsorption amount of H₂O in open-ended SWCNT (8,8) is enhanced rapidly. The adsorption isotherms of these three open-ended SWCNTs at 298.15 K are different from those at 273.15 K. The pressure at which the adsorption starts tends to be larger than that at 273.15 K. The intersection point of three curves, as shown in Fig. 4(f), is at a pressure of about 92 kPa. The adsorption amounts of open-ended SWCNT (6,6) and SWCNT (7,7) are similar, and that of SWCNT (8,8) is the greatest at 101.325 kPa due to its largest tube volume.

Figures 4(g) and 4(h) show that the adsorption amount of CO₂ is enhanced with the increased diameter of the tube of open-ended SWCNTs at a given temperature. The adsorption amount of CO₂ inside the tube of open-ended SWCNT (6,6) is about 1.8–2.8

| TABLE IV. Maximum adsorption amount at 273.15 K. |
|-----------------|----------------|-----------------|-----------------|-----------------|-----------------|
| SWCNTs          | CH₄/molecules  | N₂/molecules    | H₂O/molecules   | CO₂/molecules   | CO/molecules    |
| (6,6)           | 3.6            | 3.8             | 5               | 4               | 4               |
| (7,7)           | 3.9            | 3.8             | 8               | 5.6             | 6               |
| (8,8)           | 5.3            | 5.5             | 14.6            | 9.4             | 18              |
| Growth gradient | 0.22/1.03      | 0/1.25          | 2.22/4.85       | 1.19/2.79       | 1.48/8.82       |

| TABLE V. Maximum adsorption amount at 298.15 K. |
|-----------------|----------------|-----------------|-----------------|-----------------|-----------------|
| SWCNTs          | CH₄/molecules  | N₂/molecules    | H₂O/molecules   | CO₂/molecules   | CO/molecules    |
| (6,6)           | 3.3            | 3.5             | 5               | 4               | 4               |
| (7,7)           | 3.7            | 3.4             | 5.2             | 4.4             | 6               |
| (8,8)           | 4.6            | 4.3             | 7.3             | 8.5             | 18              |
| Growth gradient | 0.30/0.66      | −0.07/0.66      | 0.15/1.54       | 0.30/3.01       | 1.48/8.82       |

| TABLE VI. Density of each gas at 298.15 K. |
|-----------------|----------------|-----------------|-----------------|-----------------|-----------------|
| SWCNTs          | CH₄/molecules cell⁻¹ | H₂O/m mol g⁻¹ | CO₂/molecules cell⁻¹ | CO/molecules cell⁻¹ |
| (6,6)           | 0.0023          | 2.31            | 0.0024           | 0.0024           |
| (7,7)           | 0.0018          | 2.18            | 0.0027           | 0.0028           |
| (8,8)           | 0.0021          | 3.69            | 0.0037           | 0.0070           |
|                 | 0–0.041         | 3               | 0–0.047          | 0–0.026          |
| Literature      | (Lithoxoos, 2010) | (Mao, 2006)     | (Lithoxoos, 2010) | (Lithoxoos, 2010) |
FIG. 4. Adsorption isotherms of different adsorbates at a temperature of 273.15 K and 298.15 K [(a), (c), (e), (g), and (i) are the adsorption isotherms of CH$_4$, N$_2$, H$_2$O, CO$_2$, and CO, respectively, at 273.15 K; and (b), (d), (f), (h), and (j) are the adsorption isotherms of CH$_4$, N$_2$, H$_2$O, CO$_2$, and CO, respectively, at 298.15 K].
molecules per supercell at the original point; however, the adsorption amounts inside open-ended SWCNT (7,7) and SWCNT (8,8) are nearly zero due to their adsorption potential not being strong enough to adsorb CO$_2$ molecules, which indicates that the adsorption potential in the tube of open-ended SWCNT (6,6) is the strongest. Furthermore, the adsorption amount of open-ended SWCNT (8,8) is about twice that of open-ended SWCNT (6,6) and SWCNT (7,7).

Figures 4(i) and 4(j) show that the adsorption amounts of CO in the tubes of open-ended SWCNTs increase progressively with increasing $d$ at a given temperature. The adsorption isotherms of CO have the same trend at 273.15 K and 298.15 K. Taking the adsorption isotherms at 273.15 K as an example, we find that the adsorption amounts of CO in open-ended SWCNTs (6,6), (7,7), and (8,8) at the original point are about 3, 4.5, and 12 molecules per supercell, respectively, which is different from those of the other adsorbates in the tubes of open-ended SWCNTs. It can be concluded that open-ended SWCNTs have strong adsorption sensitivity and adsorption capacity for CO.

C. Effect of temperature on adsorption capacity

Figure 5 shows the adsorption amounts of open-ended SWCNTs with different diameters at 273.15 K and 298.15 K. For open-ended SWCNT (6,6), no matter what the temperature is, 273.15 K or 298.15 K, the maximum adsorption amounts of H$_2$O, CO$_2$, and CO are the same, and the adsorption amounts of CH$_4$ and N$_2$ are very close. At 273.15 K, the adsorption amounts of gases on average are slightly larger than those at 298.15 K. After analysis, we can conclude that temperature is not the main effect on the adsorption amount of open-ended SWCNT (6,6) with the diameter of 8.14 Å. Due to hydrogen bonds between H$_2$O molecules, it is easier to interact with the adsorption potential in the tube of open-ended SWCNTs, resulting in the amount of H$_2$O adsorbed on the tube of SWCNT (6,6) being the most. When the diameter of open-ended SWCNTs reaches 9.49 Å, the adsorption amounts of H$_2$O and CO$_2$ in open-ended SWCNT (7,7) decrease with the increase in temperature, and the difference in the amount is obvious. The changes in the adsorption amount of H$_2$O and CO$_2$ are 2.8 and 1.2 molecules per supercell, respectively, with $\Delta T = 25$ K. However, the adsorption amounts of CH$_4$, N$_2$, and CO are still not affected by temperature obviously. For open-ended SWCNT (8,8), temperature has a significant effect on the maximum adsorption amount of H$_2$O. The adsorption amount of H$_2$O in the tube of open-ended SWCNT (8,8) at 273.15 K is twice that of at 298.15 K. However, temperature has little effect on the amounts of CH$_4$, N$_2$, and CO$_2$. From Fig. 5, it can be concluded that the amount of CO adsorbed on the tubes...
of open-ended SWCNTs is not affected by temperature and remains equal.

In the simulations, we researched on the adsorption sites of CH\(_4\), N\(_2\), H\(_2\)O, and CO\(_2\) in the tubes of open-ended SWCNT (6,6) and SWCNT (7,7), as shown in Fig. 6, which indicates that gas adsorption takes place primarily inside the tube of open-ended SWCNTs under the given simulation conditions. However, the adsorption sites of CO are not all inside the tube of open-ended SWCNT (8,8). A few of the CO molecules are adsorbed on the external surface of open-ended SWCNT (8,8), and most of the CO molecules exist in the tube of open-ended SWCNT (8,8). This is related to the size of the CO molecule. The volume of the simulation box, which is made of three vectors, OA, OB, and OC, is 2577.47 Å\(^3\), and that of open-ended SWCNT (8,8) is 502.86 Å\(^3\), so the free volume is 2574.7 = 2074.61 Å\(^3\). Since open-ended SWCNT (8,8) is at the center of the simulation box, there exists 1037.305 Å\(^3\) free volume on both sides of open-ended SWCNT (8,8). The sagittal plane formed by the vectors OA and OB is a parallelogram with an angle of 120° and a length of 14.2 Å, so the length of vector AB is 24.60 Å. The diameter of the carbon atom is 1.82 Å, so the length of the free space on the corner of open-ended SWCNT (8,8) is (24.60 – 10.85 – 1.82)/2 = 5.965 Å.

The diameter of the oxygen atom is 1.32 Å, which is smaller than the diameter of the carbon atom. Combined with the adsorption form of CO shown in Fig. 7, the distance of available space is 5.965 – 1.82 = 4.145 > 3.76 Å (van der Waals radius), so the residual volume in the simulation box can provide adsorption space for CO.

IV. CONCLUSIONS

1. For a given temperature, the adsorption amounts of CH\(_4\), N\(_2\), H\(_2\)O, CO\(_2\), and CO are enhanced with the increase in the diameter of the open-ended SWCNTs. The growth gradients of CH\(_4\) and N\(_2\) are not obvious with the increase in diameter, while the growth gradients of H\(_2\)O, CO\(_2\), and CO exhibit a significant increase in diameter.

2. The adsorption amount of CO is enhanced exponentially with an increase in the diameter of the open-ended SWCNTs, regardless of temperature. In contrast to this, the adsorption amounts of CH\(_4\), N\(_2\), H\(_2\)O, and CO\(_2\) decrease apparently with the increase in temperature.

3. Under the conditions of 298.15 K and 101.325 kPa, open-ended SWCNT (8,8) presents a high adsorption capacity for CO and can be considered as a kind of porous material for storing CO to reduce environmental pollution.

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