SiC₃ as a Charge-Regulated Material for CO₂ Capture

Haihui Zhang *, Huihui Xiong * and Wei Liu

School of Metallurgy Engineering, Jiangxi University of Science and Technology, Ganzhou 341000, China; pushful-liuwei@hotmail.com
* Correspondence: 9120160046@jxust.edu.cn (H.Z.); 9120120027@jxust.edu.cn (H.X.)

Abstract: The increasing CO₂ emission rate is deteriorating the atmospheric environment, leading to global warming and climate change. The potential of the SiC₃ nanosheet as a functioning material for the separation of CO₂ from the mixture of CO₂, H₂, N₂ and CH₄ by injecting negative charges is studied by DFT calculations in this paper. The results show that in the absence of injecting negative charges, CO₂ interacts weakly with the SiC₃ nanosheet. While the interaction between CO₂ and the SiC₃ nanosheet can be strengthened by the injection of negative charges, the absorption mechanism of CO₂ changes from physisorption to chemisorption when the injection of negative charges is switched on. H₂/N₂/CH₄ are all physisorbed on the SiC₃ nanosheet with/without the injection of negative charges. The mechanism of CO₂ adsorption/desorption on the SiC₃ nanosheet could be tuned by switching on/off the injection of negative charges. Our results indicate that the SiC₃ nanosheet can be regarded as a charge-regulated material for the separation of CO₂ from the CO₂/H₂/N₂/CH₄ mixture.

Keywords: SiC₃ nanosheet; CO₂; adsorption; negative charges

1. Introduction

As the byproduct of human modernization activities, CO₂ is regarded as one of the significant causes of global warming and climate change. One of the main sources of carbon emissions comes from the use of coal as fuel or coke to reduce ores during extraction metallurgy. Taking iron and steel making for example, about 1.3~1.7 tons of CO₂ were exhausted per ton of steel produced in 2020, equating to about 8.0 percent of global carbon dioxide emissions. In the ferrous industry, most of the exhaust gases are reducing the atmosphere and contain the bulk of CO₂ that is emitted at temperatures higher than the ambient temperature. The typical blast furnace gas composition is N₂, CO, CO₂ and H₂ with the temperature of about 473~530 K, and the coke oven gas composition is N₂, CH₄, CO, CO₂ and H₂ with the temperature of about 1000 to 1300 K. CO₂ in the hot exhaust gas is expected to be collected and then reduced to CO that can facilitate the reduction reaction of CO₂ into synthetic fuels for a sustainable environment [1–4]. In the process of oxygen-converter steelmaking, CO₂ is a weaker oxidizing agent compared with O₂, and CO₂ can be reduced to CO by the C in the liquid hot metal [5,6]. Therefore, it is expected to develop an adsorbent material with the highly selective, controllable, and reversible of CO₂ capture that is high-temperature-resistant in the adsorption/desorption processes to fulfill the requirement of being in the metallurgy area.

Many 2D materials, due to their high surface area for CO₂ capture, have been synthesized or theoretically predicted [7], such as BN₂ [8], CN [9], C₂N [10], C₃N [11,12], PC₃ [13], and Me–N–C (Me = Fe, Cu, Co, etc.) nanosheets [14,15], borophene nanosheet [16,17], covalent triazine frameworks [18], nanoporous graphene [19], and penta-graphene [20]. Adding/removing the electrons to/from the adsorbent materials allows alteration of the affinity between the adsorbent materials and gases that is in favor of the CO₂ capture from the gas mixture [21]. Qin et al. [10] showed that the interaction between CO₂ and the C₂N nanosheet is enhanced by the negative charges or external electric field, and CO₂ molecules...
are released from the C_2N nanosheet once the charge state/electric field is switched off. Li et al. [11] found that CO_2 molecules can be adsorbed and desorbed from the C_3N nanosheet by adjustment of the applying charge density. Tao et al. [22] found that the charged calcite is highly selective for separating CO_2 from the mixture of N_2, H_2 and CH_4, and the optimal charge density range for CO_2 capture and separation is 8.04–18.56 × 10^{13} \text{e}^{-}/\text{cm}^2. Other previous studies [8,10,11,13–15,17,18,21–25] also showed that the negative charges could be used as a switch in CO_2 capture and separation techniques by changing the affinity between CO_2 and the substrates, such as penta-BN, g-C_3N_4, nitrogen-doped porous carbons, etc.

Recently, works by Li and Shi et al. [26,27] showed that the silicon carbon monolayer possesses high thermal stabilities such that the SiC_3 and SiC_3 sheets can retain their planar geometries below 3500 K and manifest excellent properties of semiconductivity and elasticity for applications in electronics and optoelectronics. Chabi et al. [28] found that 2D silicon carbide (Si_xC_y) is a universal material, and exhibits the same properties as graphene, silicon or silicon carbide, depending on the composition (i.e., Si_xC_3, SiC_3 and SiC_4). For extensive exploration of novel nanostructures as potential materials for CO_2 capture, a question raised in this study is whether SiC_3 nanosheets are also a promising material for CO_2 capture, and whether its capture/separation could be efficiently tuned by the charge/electric field.

Therefore, the adsorption behaviors of CO_2, H_2, N_2 and CH_4 on the SiC_3 nanosheets with and without applying the injecting negative charges were studied by Density Functional Theory (DFT) calculations. Firstly, the stability of SiC_3 nanosheet with different gas molecule (i.e., CO_2, H_2, N_2 and CH_4) adsorption was explored. Secondly, the effects of the injecting negative charges on the electronic structure, bonding features of adsorption systems and the mechanism of the CO_2 adsorption/desorption on the SiC_3 nanosheet were studied. Finally, the possibility of CO_2 separation from the gas mixture with the assistance of negative charge, and the SiC_3 nanosheet as a promising CO_2 capture material were confirmed.

2. Calculation Method and Details

The calculations about the adsorption behavior of gas (i.e., CO_2, H_2, N_2 and CH_4) on the SiC_3 nanosheets were performed by using Density Functional Theory (DFT) methods, the implemented Dmol^3 module [29] with Generalized Gradient Approximation (GGA) and the Perdew–Burke–Ernzerhof (PBE) functional exchange correction functional. The details about the PBE functional have been well documented in the previous paper [30]. The effects of the core electrons were treated as a single effective potential by using the DFT semi-core pseudopotentials (USPP). Double numerical plus polarization (DNP) with a cutoff radius of 4.7 Å, and the DFT + D method with the weak van der Waals (vdW) correction were adopted in our calculations. Additionally, 4 × 4 × 1 k-points sampling of the SiC_3 nanosheet with 18 Si and 54 C atoms was adopted, and a 20 Å vacuum was set along the normal direction of the nanosheet for the elimination of the interactions between surface atoms. In geometric optimizations, the convergence tolerance was 1.0 × 10^{-5} \text{Ha} for the total energy, 0.002 \text{Ha}/Å for the maximum force, and 0.005 Å for the maximal displacement.

The adsorption energy (E_{ads}) of gas i on the SiC_3 nanosheet is described by the following equation [31,32]:

\[ E_{ads} = E_{SiC_3,i} - E_{SiC_3} - E_i \]  

(1)

where \( E_{SiC_3,i} \) is the energy of the gas molecule i adsorbed on the SiC_3 nanosheet, \( E_{SiC_3} \) is the energy of the pure SiC_3 nanosheet, \( E_i \) is the energy of the isolated gas molecule i, and i indicates the gas molecule (i.e., CO_2, H_2, N_2 and CH_4). A lower value of \( E_{ads} \) corresponds to the stronger interaction between the SiC_3 nanosheet and gas molecule i, and thus, represents a more stable molecules adsorption structure.

The influence of the injecting negative charges on the stability of the SiC_3 nanosheet was studied, where the negative charges of numbers 0 to 5 e^- were injected into the SiC_3 nanosheet, equivalent to the negative charge densities of 0–2.06 × 10^{14} \text{e}^{-}/\text{cm}^2, which were applied on the SiC_3 nanosheet. For characterizing the adsorption of the gas molecule (i.e.,
CO₂, H₂, N₂ and CH₄) on the different, negatively charged SiC₃ nanosheet, the negative-charge density of the SiC₃ nanosheet (ρ) was investigated, and the negative charge density was defined as follows [10,17].

\[ \rho = \frac{Q}{S} \]  

(2)

where Q is the total negative charges injected into (4 × 4 × 1) the supercell of the SiC₃ nanosheet, and S is the corresponding surface area (2.43 × 10⁻¹⁴ cm²).

To study the structural stability of a SiC₃ nanosheet under different negative-charge conditions, the phonon dispersion spectra and the cohesive energy are calculated. Generally, a larger cohesive energy corresponds to a more stable molecule-adsorption structure; also, no imaginary frequency in the phonon dispersion spectra indicates the stability of a material. The cohesive energy is defined as follows:

\[ E_{coh} = \frac{n_cE_c + n_SiE_{Si} - E_{SiC₃}}{n_c + n_Si} \]  

(3)

where \( E_c \), \( E_{Si} \) and \( E_{SiC₃} \) are the energies of a single C atom, a single Si atom and the total energy of SiC₃ nanosheet, respectively. \( n_c \) and \( n_Si \) are the number of Si and C atoms in the SiC₃ nanosheet. Next, the effect of the injection of negative charges on the adsorption behavior of gas (i.e., CO₂, H₂, N₂ and CH₄) on the SiC₃ nanosheets was studied.

3. Results and Discussion

3.1. Electronic Properties and Stability of SiC₃ Nanosheet

The SiC₃ nanosheet is a graphene-like structure conformation with a P6/mmm space group. The calculated lattice constants of the primitive SiC₃ nanosheet are a = b = 5.584 Å. Figure 1a shows the deformation electron density of the 4 × 4 × 1 fully relaxed supercell structure of the SiC₃ nanosheet. One can see that electrons are accumulated around the six-membered ring of carbon due to the larger, stronger electronegativity of carbon than that of silicon. The SiC₃ nanosheet has two different bonds, which are Si–C and C–C. The bonds lengths of Si–C and C–C are 1.796 and 1.428 Å, respectively, and the angle of C–C–C, C–C–Si and C–Si–C are all 120°. Those calculated results are in good agreement with the reported value [33]. For a pure SiC₃ nanosheet, the obtained Local Density of States (LDOS) of C and Si atoms are shown in Figure 1b. LDOS results show that the SiC₃ nanosheet exhibits a metallic characteristic due to several bands across the Fermi level that might be primarily contributed by the Si-p orbital [26]. The finding matches with the obtained results by Chabi et al. [28] that show that the SiC₃ nanosheet is a potential material for use as a semiconductor. Figure 1c shows the cohesive energy of the SiC₃ nanosheet under different charged conditions. The cohesive energy of a neutral SiC₃ nanosheet is 9.86 eV/atom, which is slightly larger than the reported value of neutral SiC₃ (7.84 eV/atom) [26]. The cohesive energy of the SiC₃ nanosheet is 9.86 eV/atom without the applied negative charge, and it decreases with increasing the applied negative charge, finally achieving a stable value (8.37 eV/atom) when the applied negative charge exceeds 3 e⁻¹. It is indicated that the SiC₃ nanosheet is a strongly bonded network and is a stable structure under the negative charge conditions. There is no imaginary frequency in the phonon dispersion spectra (Figure 1d). Therefore, all these results reflect the dynamic stability of the SiC₃ nanosheet under the condition of injecting negative charges. The SiC₃ nanosheet can withstand a rather high temperature under atmospheric pressure [26]. Therefore, the SiC₃ nanosheet is a stable material for CO₂ separation application after the injection of negative charges.
withstand a rather high temperature under atmospheric pressure. CO

\[ E_{ads} = \text{-0.324 eV} \] (b) \[ E_{ads} = \text{-0.227eV} \] (c) \[ E_{ads} = \text{-0.299eV} \] (d) \[ E_{ads} = \text{-0.281eV} \]

\[ 180° \] \[ 1.111 Å \] \[ 0.751Å \] \[ 1.177Å \] \[ 1.100 Å \]

\[ \text{CO}_2 \text{ H}_2 \text{ N}_2 \text{ CH}_4 \]

(a) \[ E_{ads} = -0.324 \text{ eV} \] (b) \[ E_{ads} = -0.227\text{eV} \] (c) \[ E_{ads} = -0.299\text{eV} \] (d) \[ E_{ads} = -0.281\text{eV} \]

\[ 180° \] \[ 1.111 Å \] \[ 0.751Å \] \[ 1.177Å \] \[ 1.100 Å \]

Figure 1. (a) Deformation electron density of SiC\(_3\) nanosheet structure (4 × 4), (b) LDOS of the Si and C atoms of SiC\(_3\) nanosheet with Fermi level set to 0 eV, (c) the cohesive energy of the SiC\(_3\) nanosheet under different negative charge density conditions, and (d) the phonon dispersion spectra of SiC\(_3\) nanosheet.

3.2. \text{CO}_2/\text{H}_2/\text{N}_2/\text{CH}_4 Adsorption on Uncharged SiC\(_3\) Nanosheet

The gas adsorption behaviors of a neutral SiC\(_3\) nanosheet is firstly investigated by analyzing the most stable relaxation configurations of the SiC\(_3\) nanosheet with gas adsorption. Various initial adsorption sites are considered, including the top sites of C and Si atoms and bridge sites of C–C and C–Si bonds, as well as the center of hexagon holes. Stable relaxation configurations of the SiC\(_3\) nanosheet with different gas molecule (i.e., CO\(_2\), H\(_2\), N\(_2\) and CH\(_4\)) adsorptions are obtained and shown in Figure 2. For the most stable relaxation configurations, the CO\(_2\), H\(_2\), N\(_2\) and CH\(_4\) molecule distances from the SiC\(_3\) nanosheet are 3.005, 2.6850, 3.235 and 3.145 Å, respectively.

\[ \text{CO}_2 \] \[ \text{H}_2 \] \[ \text{N}_2 \] \[ \text{CH}_4 \]

(a) \[ E_{ads} = -0.324 \text{ eV} \] (b) \[ E_{ads} = -0.227\text{eV} \] (c) \[ E_{ads} = -0.299\text{eV} \] (d) \[ E_{ads} = -0.281\text{eV} \]

\[ 180° \] \[ 1.111 Å \] \[ 0.751Å \] \[ 1.177Å \] \[ 1.100 Å \]

Figure 2. Top and side views of the stable adsorption configurations of different gas molecules adsorbed on the SiC\(_3\) nanosheet without the injecting negative charges. (a) CO\(_2\), (b) H\(_2\), (c) N\(_2\), and (d) CH\(_4\) adsorbed on the SiC\(_3\).
For the CO₂ adsorbed on the SiC₃ nanosheet, the O–C–O angle and the C–O bond length exhibit a minor change in comparison to the isolated carbon dioxide molecule, indicating that the absorption of CO₂ is classical physisorption. Similar results are observed for the H₂, N₂ and CH₄ molecule adsorbed on the SiC₃ nanosheet. Thus, it could be concluded that the gas molecules (i.e., CO₂, H₂, N₂ and CH₄) adsorbed on the SiC₃ nanosheet surface are caused by physisorption.

The adsorption energies (E_ads) of CO₂, H₂, N₂ and CH₄ adsorbed on the SiC₃ nanosheet are −0.324, −0.227, −0.299 and −0.281 eV, respectively. Among those four gases, the most stable relaxation configurations of gas molecules adsorbed on SiC₃ nanosheet are CO₂, followed by N₂, CH₄ and H₂, which indicates that the SiC₃ material is a potential material for use as a CO₂ adsorbent.

3.3. Adsorption of CO₂/H₂/N₂/CH₄ by Charged SiC₃ Nanosheet

With the injection of the negative charges with density of 1.23 × 10¹⁴ e⁻/cm², the stable relaxation configurations of the SiC₃ nanosheet with different gas molecule (i.e., CO₂, H₂, N₂ and CH₄) adsorption are obtained and shown in Figure 3.

![Figure 3](image-url)

**Figure 3.** Top and side views of the stable adsorption configurations of different gas molecules adsorbed on SiC₃ nanosheet after the injection of the negative charges with density of 1.23 × 10¹⁴ e⁻/cm². (a) CO₂, (b) H₂, (c) N₂, and (d) CH₄ adsorbed on the SiC₃.

After the injection of negative charges into the SiC₃ nanosheet with CO₂ absorption, the CO₂ molecule strongly interacts with the SiC₃ nanosheet with the adsorption energy E_ads of −1.628 eV; the adsorption energy is significantly smaller than that of the uncharged SiC₃ nanosheet (−0.324 eV). Furthermore, the O–C–O angle changes from 180° to 131°, the C–O bond length increases from 1.117 Å to 1.259 Å, and the distance between CO₂ and the SiC₃ nanosheet decreases from 3.005 Å to 2.002 Å. Obvious electron density distribution overlap is observed between CO₂ and the SiC₃ nanosheet (Figure 4e), indicating that the strong interaction between CO₂ and the SiC₃ nanosheet, and the adsorption of the CO₂ molecule on the SiC₃ nanosheet is due to chemisorption.
The optimized adsorption configurations of H₂, N₂, and CH₄ after the injection of negative charges are shown in Figure 3b–d. After the injection of negative charges into the SiC₃ nanosheet with H₂ adsorption, for the H₂ molecule, the H–H bond length increases slightly from 0.751 to 0.769 Å, the distance between H₂ and the SiC₃ nanosheet increases slightly from 2.685 to 2.964 Å, and the adsorption energy $E_{ads}$ decreases from $-0.227$ to $-0.499$ eV. For the N₂ molecule, the N–N bond length increases slightly from 1.111 to 1.123 Å, the distance between N₂ and the SiC₃ nanosheet decreases slightly from 3.235 to 3.151 Å, and the adsorption energy $E_{ads}$ decreases from $-0.299$ to $-0.578$ eV. For the CH₄ molecule, the C–H bond length increases slightly from 1.100 to 1.102 Å, and the distance between CH₄ and the SiC₃ nanosheet decreases slightly from 3.514 to 2.700 Å, and the adsorption energy $E_{ads}$ decreases from $-0.281$ to $-0.525$ eV. Furthermore, no evident electron density distribution overlaps are observed between gas molecules (H₂, N₂, and CH₄) and the SiC₃ nanosheet after the injection of negative charges (Figure 4e). Thus, it is suggested that the adsorptions of H₂, N₂, and CH₄ on the SiC₃ nanosheet are due to physisorption with/without the injecting negative charges, which differs from the chemisorption of CO₂ on the SiC₃ nanosheet with the injection of negative charges.

Figure 4 shows no obvious electron density distribution overlaps observed between CO₂/H₂/N₂/CH₄ molecules and the SiC₃ nanosheet without the injecting negative charges. It indicates that CO₂/H₂/N₂/CH₄ interact weakly with the SiC₃ nanosheet without the injecting negative charges. However, after the injection of the negative charge with density of $1.23 \times 10^{14}$ e⁻/cm², obvious electron density distribution overlap between CO₂ and the SiC₃ nanosheet is observed. In other words, after the injection of the negative charges, the adsorptions of H₂, N₂, and CH₄ on the SiC₃ nanosheet are also due to physisorption with weak interactions between these molecules; when the adsorption mechanism of CO₂ on the SiC₃ nanosheet changes from physisorption to chemisorption, the interaction between CO₂ and the SiC₃ nanosheet gets stronger. These results suggest that CO₂ could be separated from the mixture of CO₂/H₂/N₂ and CH₄ that might be tuned by switching on/off the injection of negative charges.

3.4. Mechanism of CO₂ Adsorption/Desorption

The mechanism of CO₂ adsorption/desorption on the SiC₃ nanosheet are investigated by switching on/off the injection of negative charges. Figure 5 shows that the adsorption of CO₂ on the SiC₃ nanosheet is due to physisorption without the injection of negative charges. With the injection of negative charges with a density of $1.23 \times 10^{14}$ e⁻/cm², for the CO₂ molecule, the O–C–O angle changes from 180° to 131°, the C–O bond length increases from 1.117 Å to 1.259 Å, and the distance between CO₂ and the SiC₃ nanosheet

*Figure 4.* The electron density distribution of the most stable adsorption configurations of gas molecule (i.e., CO₂, H₂, N₂, and CH₄) adsorbed on the SiC₃ nanosheet. (a–d) Without the injecting negative charges, and (e–h) after the injection of negative charges with density of $1.23 \times 10^{14}$ e⁻/cm².
decreases from 3.005 Å to 2.002 Å. This result implies that the adsorption mechanism changes from physisorption to chemisorption; the analysis is consistent with the obtained results from Figure 4, and the process is exothermic with a reaction energy of $-1.172 \text{ eV}$. After switching off the injection of negative charges, the adsorption mechanism of CO$_2$ changes from chemisorption to physisorption. The adsorbed CO$_2$ molecule is rebound to its physisorption state, and the distance between CO$_2$ and the SiC$_3$ nanosheet increases from 2.002 to 3.005 Å. This transition is also exothermic, 0.776 eV, without any energy barrier. In conclusion, the processes of CO$_2$ adsorption/desorption on the SiC$_3$ nanosheet is reversible, and CO$_2$ adsorption and separation would be tuned by switching on/off the injection of negative charges.

![Figure 5](image_url)

**Figure 5.** The process of (a) CO$_2$ adsorption on the SiC$_3$ nanosheet after injecting negative charges with density of $1.23 \times 10^{14} \text{ e}^-/\text{cm}^2$ for the SiC$_3$ nanosheet with CO$_2$ adsorption, and (b) CO$_2$ desorption from the SiC$_3$ nanosheet after switching off the injection of negative charges.

3.5. *Separation of CO$_2$ from H$_2$, N$_2$ and CH$_4$ on Negatively Charged SiC$_3*

The effect of the injection of negative charges on the interactions between gases and the SiC$_3$ nanosheet is shown in Figure 6. With the increase in negative charge density, the adsorption energy of CO$_2$ is smaller than those values of N$_2$, CH$_4$ and H$_2$. When the negative charge intensity exceeds $3.75 \times 10^{13} \text{ e}^-/\text{cm}^2$, the adsorption energy of CO$_2$ adsorption decreases with the negative charge intensity observably, while the decrement of the adsorption energies for H$_2$, N$_2$ and CH$_4$ are relatively small. It is suggested that the CO$_2$–SiC$_3$ adsorption structure is more stable than the adsorption structures of N$_2$–SiC$_3$, CH$_4$–SiC$_3$, and H$_2$–SiC$_3$ under different charged conditions.

![Figure 6](image_url)

**Figure 6.** Effect of the injection of negative charges on the adsorption energy of the most stable configurations of SiC$_3$ nanosheet with CO$_2$, H$_2$, N$_2$ and CH$_4$ adsorption.
To further explore the CO₂ separation ability of the SiC₃ nanosheet by switching on/off the injection of negative charges, the co-adsorption behaviors of CO₂, H₂, N₂ and CH₄ on the SiC₃ nanosheet are investigated. As Figure 7 shows, after the injecting of the negative charges with a density of $1.23 \times 10^{14}$ e⁻/cm² into the SiC₃ nanosheet with gases co-absorption, the co-adsorption energy decreases from $-0.255$ to $-0.976$ eV. It implies that with the injection of negative charges, the SiC₃ nanosheet with gases (i.e., CO₂, H₂, N₂, and CH₄) co-adsorption gets more stable in comparison with the one without the injection of negative charges.

![Figure 7](image)

Figure 7. Top and side views of the optimized configurations of the SiC₃ nanosheet with gases molecules (i.e., CO₂, H₂, N₂ and CH₄) co-adsorption (a) without the injection of negative charges, and (b) with the injection of negative charges ($1.23 \times 10^{14}$ e⁻/cm²).

Switching on the injection of negative charges, the modules of H₂, N₂ and CH₄ move away from the SiC₃ nanosheet. The distance between the molecule and the SiC₃ nanosheet increases from 2.817 to 3.506 Å for H₂-SiC₃, from 3.243 to 3.170 Å for N₂-SiC₃, and from 3.491 to 3.506 Å for CH₄-SiC₃. No obvious electron density distribution overlaps are observed between H₂/N₂/CH₄ molecules and the SiC₃ nanosheet with/without the injection of negative charges (Figure 8). It indicates that the effect of the injection of negative charges on the adsorptions of H₂/N₂/CH₄ is not obvious, and H₂/N₂/CH₄ are all physiosorbed on the SiC₃ nanosheet with/without the injection of negative charges.

![Figure 8](image)

Figure 8. Top and side views of the charge density distribution of the SiC₃ nanosheet with gases molecules (i.e., CO₂, H₂, N₂ and CH₄) co-adsorption (a) without the injection of negative charges, and (b) with the injection of negative charges ($1.23 \times 10^{14}$ e⁻/cm²).
With the injection of negative charges into the SiC₃ nanosheet with gases co-absorption, the distance between the CO₂ molecule and the SiC₃ nanosheet gets shorter, decreasing from 3.271 Å to 1.995 Å, and the O–C–O angle of CO₂ changes from 178.9° to 119.4°. No obvious electron density distribution overlap is observed between the CO₂ molecule and the SiC₃ nanosheet without the injection of negative charges, while an obvious electron density distribution overlap is observed with the injection of negative charges (Figure 8), implying that the absorption mechanism of CO₂ changes from physisorption to chemisorption after the injection of negative charges, which is also consistent with the obtained results from Figure 5.

In summary, H₂/N₂/CH₄ all interact weakly with the SiC₃ nanosheet with/without the injection of negative charges. While the interaction between CO₂ and the SiC₃ nanosheet can be strengthened by the injection of negative charges, the absorption mechanism of CO₂ changes from physisorption to chemisorption after the injection of negative charges. Therefore, it could be concluded that the separation CO₂ from the mixture of CO₂, H₂, N₂, and CH₄ can be achieved by switching on/off the injection of negative charges. All of the above results demonstrate that the SiC₃ nanosheet is a promising material for the separation CO₂ from the CO₂/H₂/N₂/CH₄ mixture by using the injection of negative charges.

4. Conclusions

The potential of SiC₃ nanosheets as functional materials for the separation of CO₂ from the mixture of CO₂, H₂, N₂, and CH₄ by injecting negative charges is studied in this paper. The results show that the SiC₃ nanosheets are a promising material for the separation of CO₂ from the CO₂/H₂/N₂/CH₄ mixture. The main results are summarized as follows.

1. In the absence of injecting negative charges, CO₂ interacts weakly with the SiC₃ nanosheet. While the interaction between CO₂ and the SiC₃ nanosheet can be strengthened by the injection of negative charges, the absorption mechanism of CO₂ changes from physisorption to chemisorption when the injection of negative charges is switched on.

2. The effect of injecting negative charges on the SiC₃ nanosheet with H₂/N₂/CH₄ adsorption is not obvious, and H₂/N₂/CH₄ are all physiosorbed on the SiC₃ nanosheet with/without the injection of negative charges.

3. The mechanism of CO₂ adsorption/desorption on the SiC₃ nanosheet could be tuned by switching on/off the injection of negative charges. The separation of CO₂ from the mixture of CO₂, H₂, N₂ and CH₄ can be achieved by switching on/off the injection of negative charges.

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