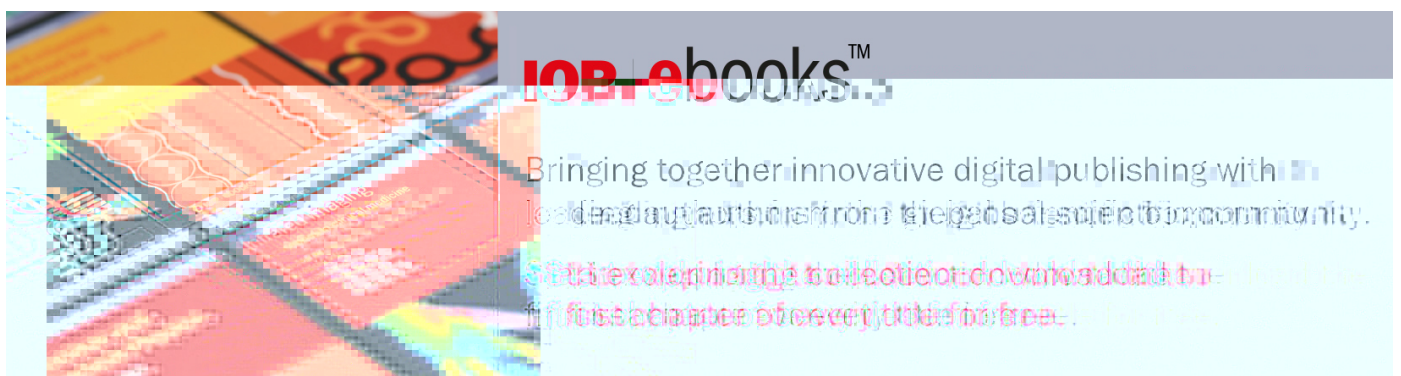


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PAPER

Evolution of calcite surface reconstruction and interface adsorption of calcite-CO₂ with temperature

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Keywords: MD simulation, surface reconstruction, CO₂ adsorption, calcite

Abstract

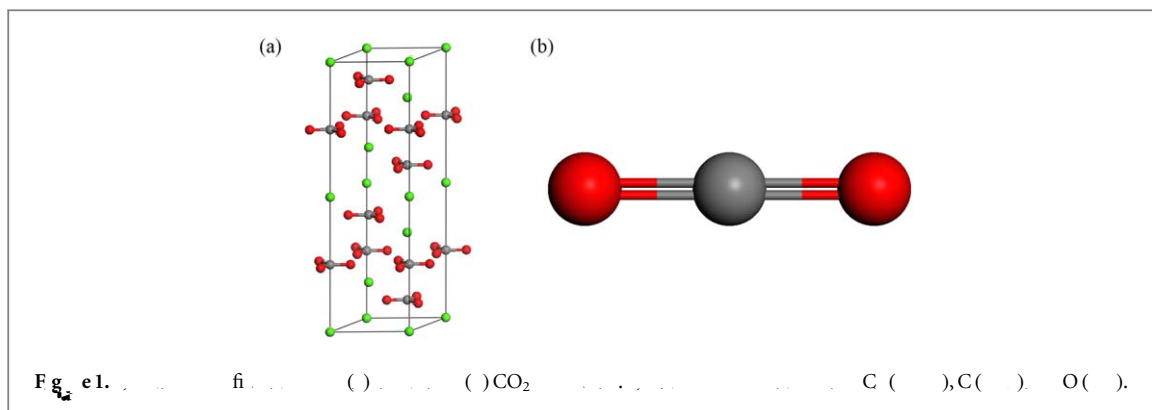
Molecular dynamics (MD) simulation was used to study the evolution of calcite surface reconstruction and interface adsorption of calcite-CO₂ with temperature. The results show that the calcite surface reconstruction is significantly affected by temperature. At low temperature, the calcite surface is relatively smooth, and the CO₂ molecules are adsorbed on the surface. As the temperature increases, the calcite surface becomes increasingly rough, and the CO₂ molecules are adsorbed on the surface. The adsorption of CO₂ molecules on the calcite surface is significantly affected by temperature. At low temperature, the adsorption of CO₂ molecules on the calcite surface is strong, and the adsorption capacity is high. As the temperature increases, the adsorption of CO₂ molecules on the calcite surface becomes weaker, and the adsorption capacity decreases. The results show that the calcite surface reconstruction and interface adsorption of calcite-CO₂ are significantly affected by temperature.

1. Introduction

Calcite is a common mineral in the Earth's crust, and it plays an important role in many geological processes. The surface reconstruction and interface adsorption of calcite are important factors that affect its physical and chemical properties. In recent years, there has been a lot of research on the surface reconstruction and interface adsorption of calcite. Many studies have shown that the surface reconstruction and interface adsorption of calcite are significantly affected by temperature. At low temperature, the calcite surface is relatively smooth, and the CO₂ molecules are adsorbed on the surface. As the temperature increases, the calcite surface becomes increasingly rough, and the CO₂ molecules are adsorbed on the surface. The adsorption of CO₂ molecules on the calcite surface is significantly affected by temperature. At low temperature, the adsorption of CO₂ molecules on the calcite surface is strong, and the adsorption capacity is high. As the temperature increases, the adsorption of CO₂ molecules on the calcite surface becomes weaker, and the adsorption capacity decreases. The results show that the calcite surface reconstruction and interface adsorption of calcite-CO₂ are significantly affected by temperature.

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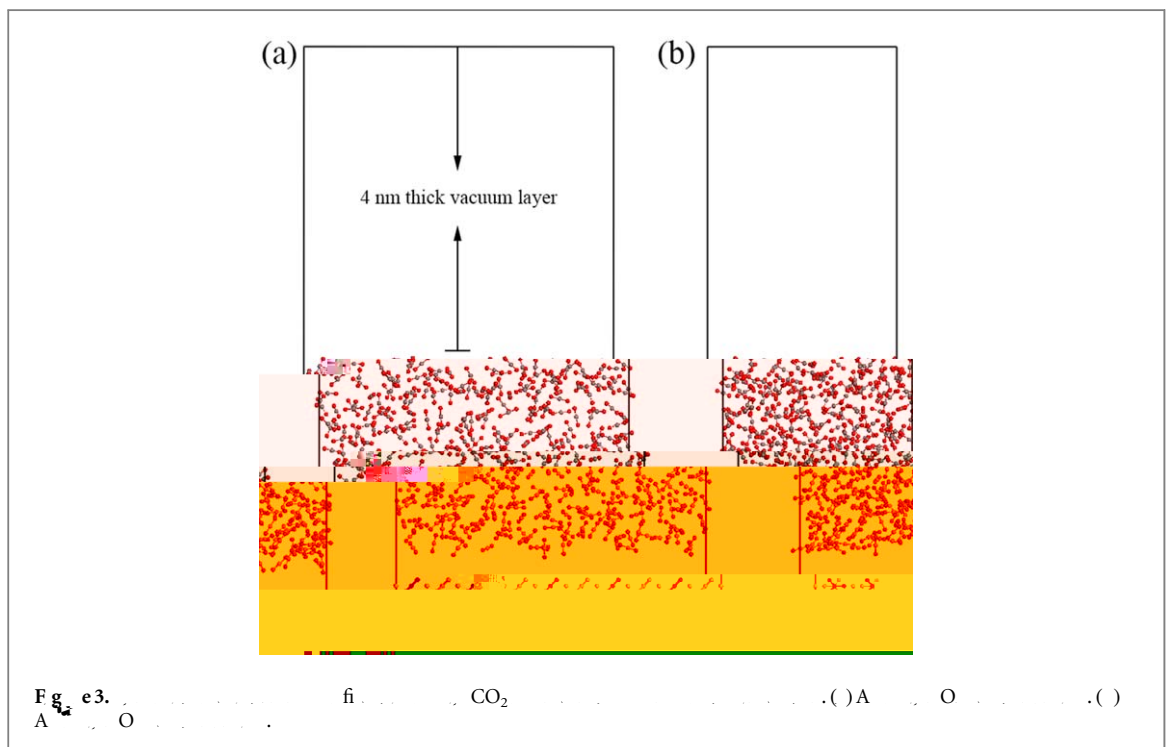
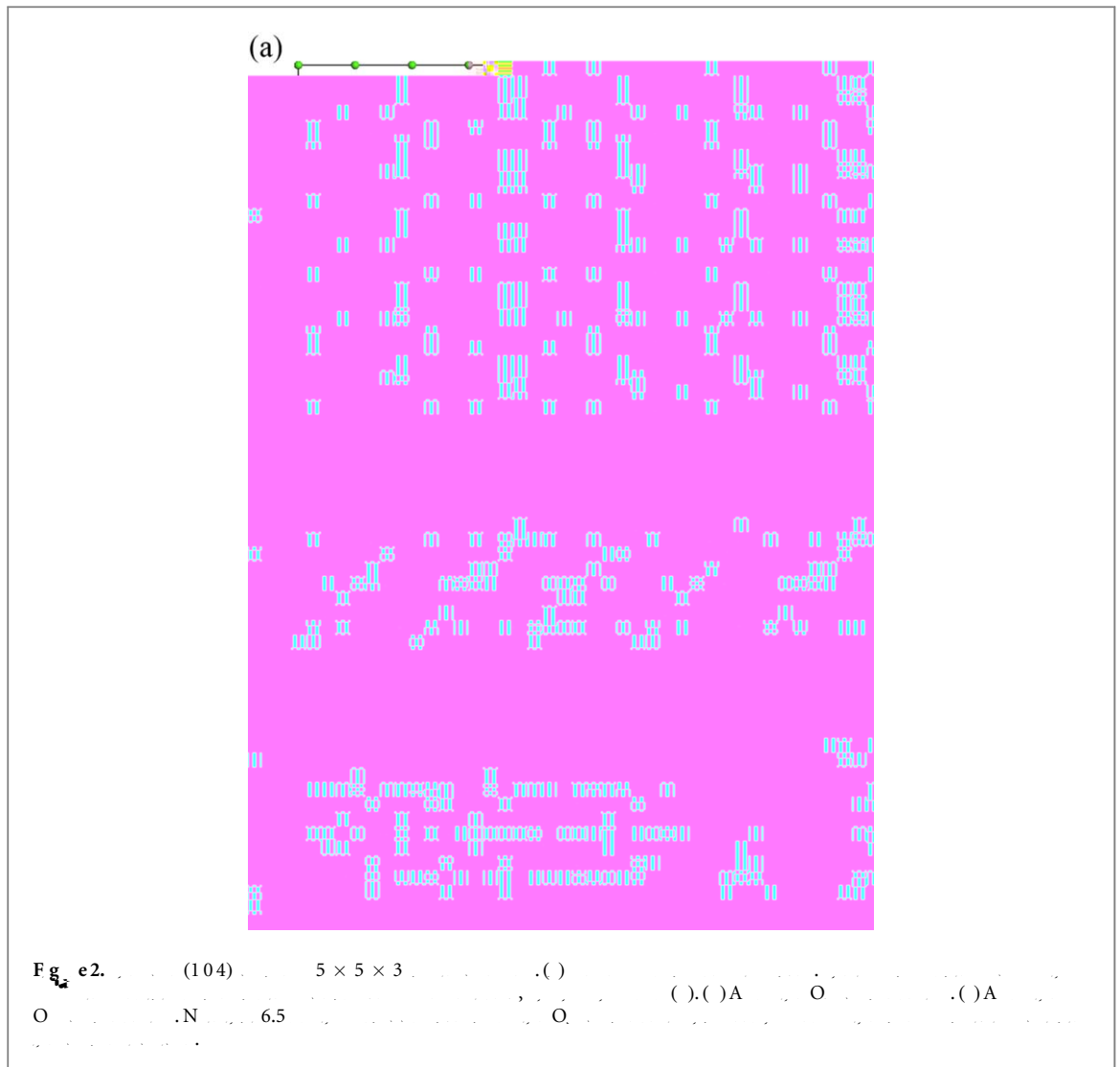
et al [28] ... CO₂ ... (110) ... MD ... (104) ... CO₂ ... MD ... 298 K ... 873 K ... CO₂ ...

2. C ... a ... a de a

C ... R3c ... D³ ... [29,30]. CA E ... [31,32] ... CO₂ ... (GGA)[33] ... (= = 0.5048 , = 1.7199), ... (= = 0.5053 , = 1.7326 [35]). A ... CO₂ ... (L_(CO2) = 0.1175) ... (L_(CO2) = 0.1163 [36]). CO₂ ... fi ... fi ... 1() ... (104) ... 2 × 2 × 1,3 × 3 × 1,4 × 4 × 1,5 × 5 × 1,6 × 6 × 1, 7 × 7 × 1,8 × 8 × 1. 9 × 9 × 1, ... 1,5 × 5 × 1 ... 4.1155 × 2.5148 × 0.7769 .F ... (104) ... fi ... 2. ... F ... MD ... F ... [37]. ... (COM A) [38] ... E ... L ... -J ... 9-6 ... [26,28,39]. CO₂ ... 350 ... CO₂ ... (104) ... A ... C C ... CO₂ ... 0.45 ... fi ... 3. ... CO₂D ... (104) ... fi [28]. fi

Table 1. ... (10³ ... / ...).

| | E ... (×) | | | | | | | |
|-------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| | 2 × 2 | 3 × 3 | 4 × 4 | 5 × 5 | 6 × 6 | 7 × 7 | 8 × 8 | 9 × 9 |
| E ... | -1.464 ± 0.012 | -1.447 ± 0.017 | -1.451 ± 0.010 | -1.445 ± 0.009 | -1.445 ± 0.013 | -1.447 ± 0.011 | -1.445 ± 0.015 | -1.446 ± 0.010 |



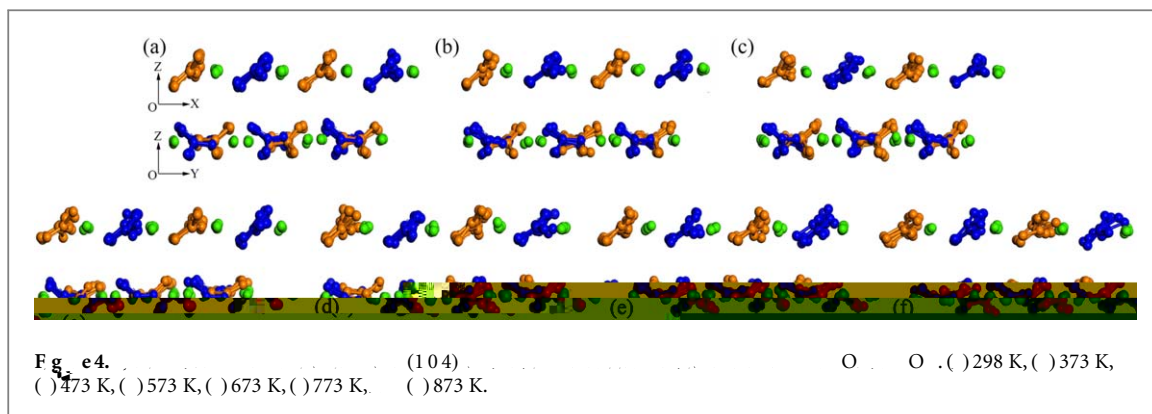


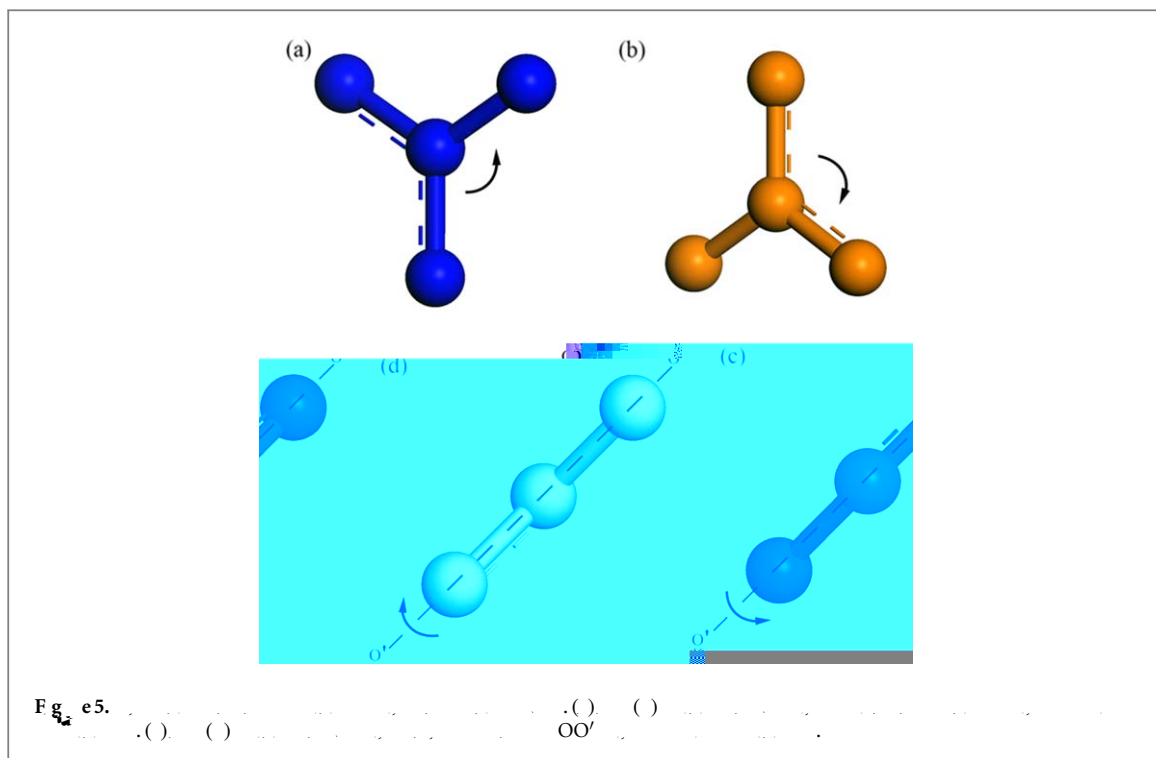
Figure 4. Molecular dynamics simulation snapshots of CO₂ adsorption on a (104) surface at various temperatures. (a) shows the crystal structure with CO₂ molecules (orange and blue spheres) and a coordinate system (x, y, z). (b), (c), (d), (e), (f), and (g) show snapshots at 298 K, 373 K, 473 K, 573 K, 673 K, 773 K, and 873 K, respectively. The legend indicates that open circles represent CO₂ at 298 K, half-filled circles represent CO₂ at 373 K, and solid circles represent CO₂ at 473 K, 573 K, 673 K, 773 K, and 873 K.

3. Results and discussion

3.1. Surface equilibrium structure

Figure 4 shows the molecular dynamics simulation snapshots of CO₂ adsorption on a (104) surface at various temperatures. The snapshots show the evolution of CO₂ molecules on the surface as the temperature increases. At 298 K, CO₂ molecules are adsorbed on the surface. As the temperature increases, the adsorption capacity of the surface decreases, and the CO₂ molecules eventually desorb from the surface. The snapshots also show the change in the surface structure of the (104) surface as the temperature increases.

Figure 5 shows the molecular dynamics simulation snapshots of CO₂ adsorption on a (104) surface at various temperatures. The snapshots show the evolution of CO₂ molecules on the surface as the temperature increases. At 298 K, CO₂ molecules are adsorbed on the surface. As the temperature increases, the adsorption capacity of the surface decreases, and the CO₂ molecules eventually desorb from the surface. The snapshots also show the change in the surface structure of the (104) surface as the temperature increases.



Tab e2.E

| (K) | R (Å) | | | | O-C-O (°) | | D (Å) | | ∠CO ₃ ²⁻ (°) | D (Å) | Δ _{surface} (Å) |
|-----|-----------------------------|-----------------------------|-------------------------------|-------------------------------|---------------------------------|---------------------------------|--------------------------------|--------------------------------|------------------------------------|-------|--------------------------|
| | R _C ^B | R _C ^Y | R _{OO'} ^B | R _{OO'} ^Y | ∠ _{O-C-O} ^B | ∠ _{O-C-O} ^Y | D _{Ca-O} ^B | D _{Ca-O} ^Y | | | |
| 298 | 18.5 | 19.4 | 14.2 | 14.7 | 122.7 | 122.8 | 0.194 | 0.194 | 39.4 | | 0.0669 |
| 373 | 19.3 | 19.1 | 15.1 | 14.3 | 123.0 | 122.9 | 0.194 | 0.195 | 39.3 | | 0.0727 |
| 473 | 20.0 | 20.8 | 15.3 | 15.4 | 123.0 | 122.9 | 0.196 | 0.196 | 39.0 | | 0.0721 |
| 573 | 22.6 | 21.1 | 16.6 | 16.1 | 123.3 | 123.0 | 0.197 | 0.196 | 38.9 | | 0.0736 |
| 673 | 24.2 | 24.0 | 18.1 | 18.3 | 123.5 | 123.5 | 0.198 | 0.198 | 38.4 | | 0.0715 |
| 773 | 24.3 | 24.7 | 18.6 | 18.7 | 123.6 | 123.5 | 0.198 | 0.198 | 38.3 | | 0.0748 |
| 873 | 24.7 | 24.5 | 18.5 | 18.4 | 123.5 | 123.6 | 0.198 | 0.199 | 38.4 | | 0.0771 |

OO' fl. 5.I R_{OO'}^B R_{OO'}^Y

.B ∠_{O-C-O}^B ∠_{O-C-O}^Y

[16] O-C-O O

C-O 3° C-O [1,17]. [45].

(298 K). I (104)

fl. G et al[46]M fl. (104)

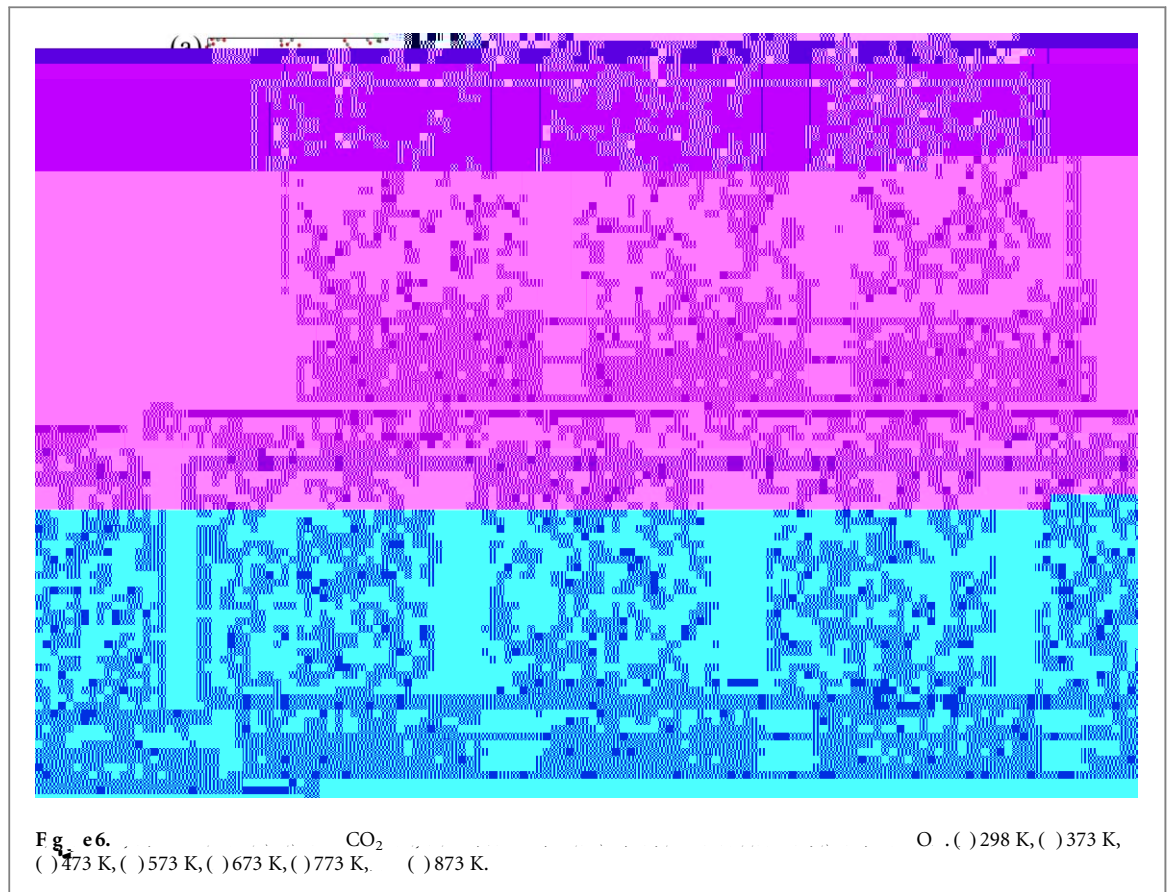
.N [47,48],

[1]. C O.

C O. I

(C CO₃)₂ [50]. C CO₃ [51]

C CO₃ [22].



Tab e 3. E. Parameters of ZnO for CO2 adsorption at various temperatures.

| (K) | θ (°) | | | | O-C-O (°) | | D (Å) | | $\angle CO_3^{2-}$ (°) | D (Å) | $\Delta_{surface}$ (Å) |
|-----|--------------|---------|-------------|-------------|--------------------|--------------------|--------------|--------------|------------------------|--------|------------------------|
| | R_C^B | R_C^Y | $R_{OO'}^B$ | $R_{OO'}^Y$ | \angle_{O-C-O}^B | \angle_{O-C-O}^Y | D_{Ca-O}^B | D_{Ca-O}^Y | | | |
| 298 | 18.5 | 19.4 | 14.4 | 14.7 | 122.6 | 122.7 | 0.193 | 0.194 | 39.6 | 0.0670 | |
| 373 | 19.4 | 19.2 | 15.1 | 14.3 | 123.0 | 122.9 | 0.194 | 0.196 | 38.7 | 0.0722 | |
| 473 | 20.1 | 20.9 | 15.4 | 15.4 | 123.1 | 123.0 | 0.196 | 0.196 | 39.0 | 0.0734 | |
| 573 | 22.6 | 21.4 | 16.6 | 16.1 | 123.3 | 123.0 | 0.197 | 0.197 | 38.9 | 0.0740 | |
| 673 | 24.1 | 23.8 | 18.0 | 17.9 | 123.5 | 123.4 | 0.198 | 0.197 | 38.1 | 0.0720 | |
| 773 | 24.3 | 24.4 | 18.2 | 18.1 | 123.6 | 123.5 | 0.198 | 0.198 | 37.8 | 0.0748 | |
| 873 | 24.5 | 24.6 | 18.3 | 18.4 | 123.5 | 123.6 | 0.197 | 0.198 | 37.9 | 0.0769 | |

A. MD simulation of ZnO surface adsorption of CO2 at 673 K. The figure shows the molecular structure of ZnO and the adsorption of CO2 molecules on the surface. The O-C-O angle is indicated as 123.5 degrees.

3.2. CO2 adsorption behavior

The adsorption of CO2 on ZnO is studied using molecular dynamics (MD) simulation. The figure shows the adsorption of CO2 molecules on the ZnO surface at different temperatures. The adsorption energy is calculated as E_{Ads} and compared with the pure ZnO energy E_{Pure} . The adsorption energy is found to be negative, indicating that the adsorption of CO2 on ZnO is exothermic. The adsorption energy increases with increasing temperature, which is consistent with the experimental results.

Tab e4. ... (10³ ... / ...).

| | ... (K) | | | | | | |
|------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| | 298 | 373 | 473 | 573 | 673 | 773 | 873 |
| E_{Pure} | -109 451 ± 75 | -109 411 ± 81 | -109 313 ± 84 | -109 237 ± 78 | -109 199 ± 85 | -109 101 ± 92 | -109 005 ± 95 |
| E_{Ads} | -109 442 ± 72 | -109 424 ± 77 | -109 309 ± 80 | -109 228 ± 79 | -109 203 ± 88 | -109 086 ± 97 | -108 997 ± 94 |

fi CO₂ ...
 A fi 6, CO₂ ... [26]. CO₂ ...
 C ... CO₂ ...
 A CO₂ ...
 CO₂ ... F ... CO₂ ...

$$E_{Ads} = E_{Sur} + E_{Gas} - E_{Tot} \tag{1}$$

E_{Tot} , E_{Sur} , E_{Gas} ... CO₂ ...
 A fi 7 ... CO₂ ...
 fi 6.

CO₂ ... E ... (873 K), ...
 CO₂ ...
 D *etal* [52]. G ... CO₂ ...

4. C

I ... MD ... (104) ...
 CO₂ ...
 673 K, ... O ...
 W ... I ... CO₂ ...
 A ... CO₂ ... CO₂ ...
 N e ... fi ...

Accepted Article

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Reference

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