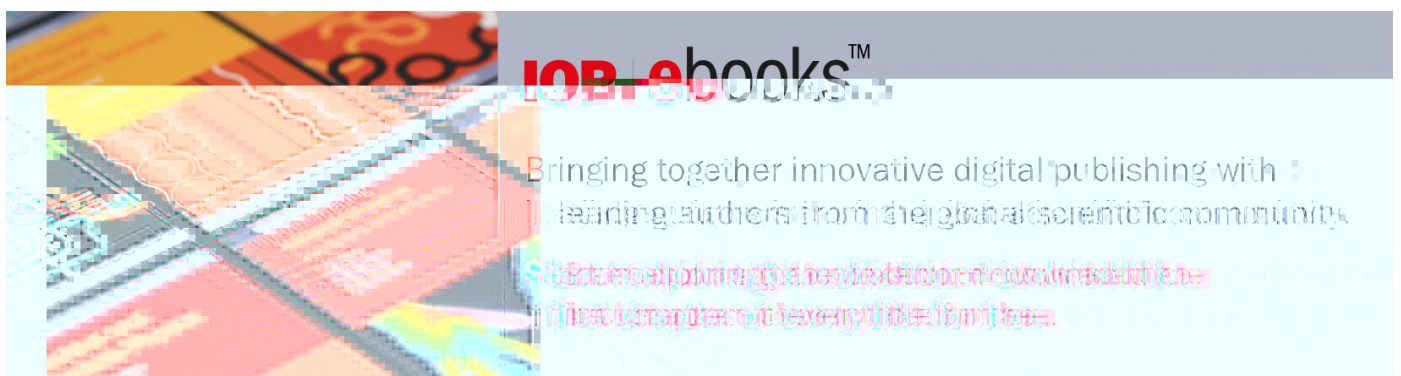


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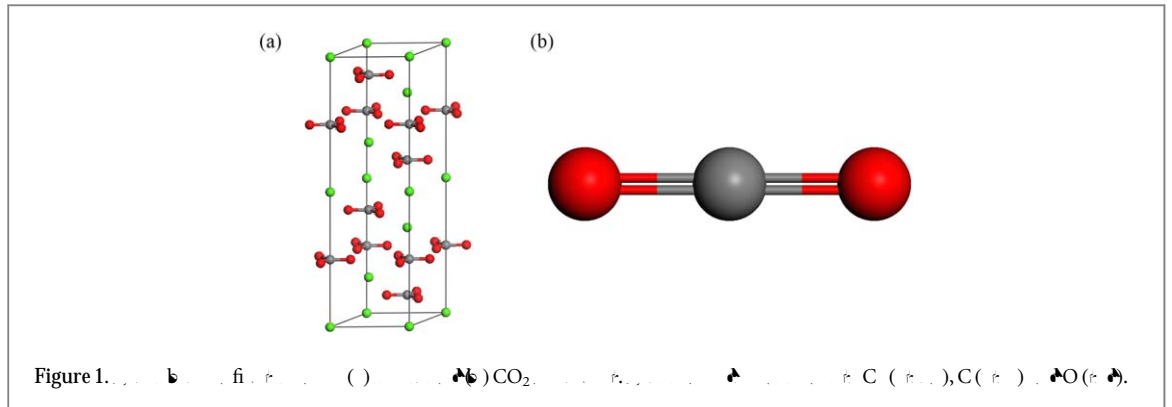
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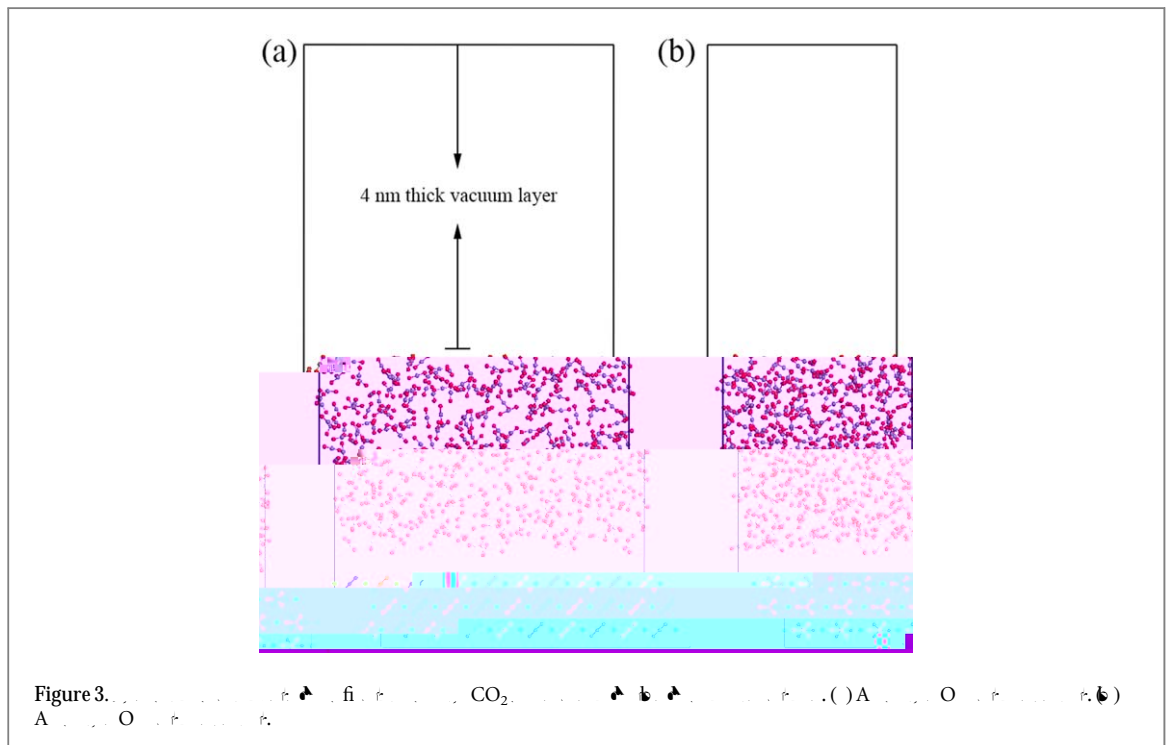
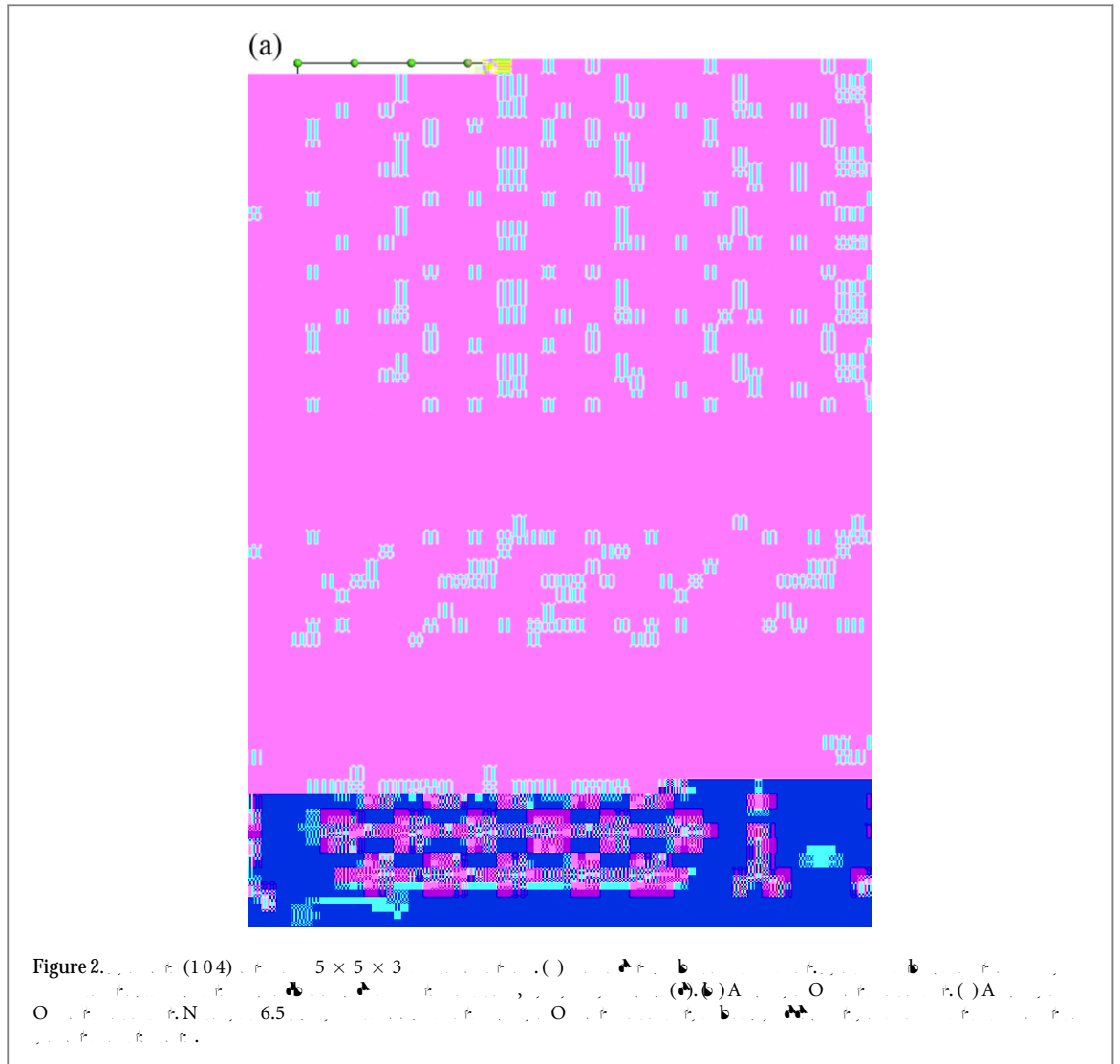
et al [28] ... MD ... CO₂ ... (1 1 0) ... MD ... CO₂ ... (104) ... MD ... 298 K - 873 K ... CO₂ ...

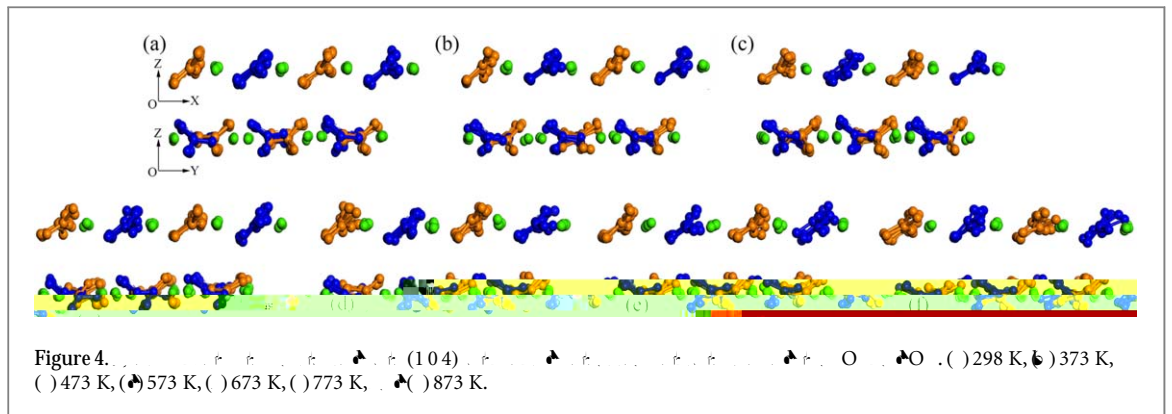
2. Computational details

C ... R³ ... D ... [29, 30] ... CA ... E ... [31, 32] ... CO₂ ... (GGA) [33] ... (91) [34] ... (=b = 0.5048, = 1.7199), ... (=b = 0.5053, = 1.7326 [35]). A ... CO₂ ... (L_{CO2}) = 0.1175 ... (L_{CO2}) = 0.1163 [36]. ... CO₂ ... (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. ... (104) ... MD ... [37] ... (COM A) [38] ... E ... L ... J ... 9-6 ... [26, 28, 39]. ... CO₂ ... 350 ... CO₂ ... (104) ... CO₂ ... 0.45 ... 3. ... CO₂ ... D ... (104) ... [28]. ...

Table 1. Error of the χ^2 fit (in 10^3 / deg^2).

E _γ (keV)	E _γ bin width (keV)							
	2 × 2	3 × 3	4 × 4	5 × 5	6 × 6	7 × 7	8 × 8	9 × 9
1447	-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





... [40]. I... CO_2 ... F... 6.5...
 ... [41, 42]. A... (N...)
 ... N... [43]. B...
 ... MD...
 ... 298 K, 373 K, 473 K, 573 K, 673 K, 773 K, 873 K, ...

3. Results and discussion

3.1. Pure surface reconstruction

F... 4...
 ... C... 2...
 ... O...
 ... B...
 ... O, C...
 ... (104)...
 ... A... MD...
 ...
 ... [6, 16, 17]... [18, 44]. H...
 ...
 ... F... R_C^B $R_{OO'}^B$...
 ... C... OO' ... R_C $R_{OO'}$...
 ... \angle_{O-C-O} \angle_{O-C-O} ...
 ... O-C-O... O...
 ... F... D_C^B D_C ...
 ... C... O...
 ... (104)... F... Δ_{surface} ... (104)...
 ... 100... 1... 2...
 ... 2...
 ... N... (298 K), R_C^B R_C ...
 ... $(R_C = 0^\circ)$... *etal*[16]...
 ... 17° ... A...

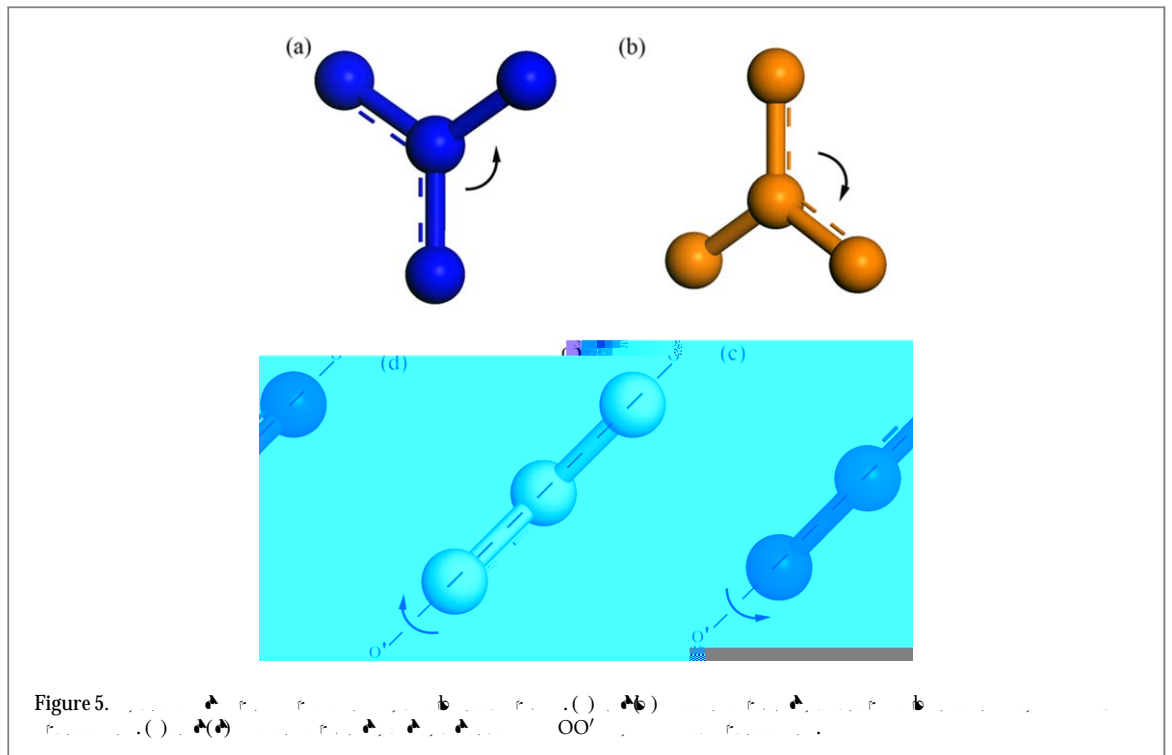


Figure 5. Snapshots of CO₂ adsorption on a surface. (a) Top view of a CO₂ molecule (blue spheres) with a rotation arrow. (b) Top view of a CO₂ molecule (orange spheres) with a rotation arrow. (c) Side view of a CO₂ molecule (blue spheres) near a surface, with a rotation arrow. (d) Side view of a CO₂ molecule (blue spheres) near a surface, with a rotation arrow.

Table 2. E structural parameters of CO₂ adsorption on a surface.

T (K)	C-O bond length (Å)				O-C-O angle (°)		D _{C-O} (Å)		∠CO ₃ ²⁻ (°)	D _{C-O} (Å)	Δ _{surface} (Å)
	R _C ^B	R _C	R _{OO'} ^B	R _{OO'}	∠ _{O-C-O} ^B	∠ _{O-C-O}	D _{C-O} ^B	D _{C-O}			
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	

Figure 5. Snapshots of CO₂ adsorption on a surface. (a) Top view of a CO₂ molecule (blue spheres) with a rotation arrow. (b) Top view of a CO₂ molecule (orange spheres) with a rotation arrow. (c) Side view of a CO₂ molecule (blue spheres) near a surface, with a rotation arrow. (d) Side view of a CO₂ molecule (blue spheres) near a surface, with a rotation arrow.

Table 2. E structural parameters of CO₂ adsorption on a surface.

Table 2. E structural parameters of CO₂ adsorption on a surface. The table lists structural parameters for CO₂ adsorption on a surface at various temperatures (298 K to 873 K). The parameters include C-O bond lengths (R_C^B, R_C, R_{OO'}^B, R_{OO'}), O-C-O angles (∠_{O-C-O}^B, ∠_{O-C-O}), D_{C-O} distances (D_{C-O}^B, D_{C-O}), ∠CO₃²⁻ angle, and Δ_{surface}.

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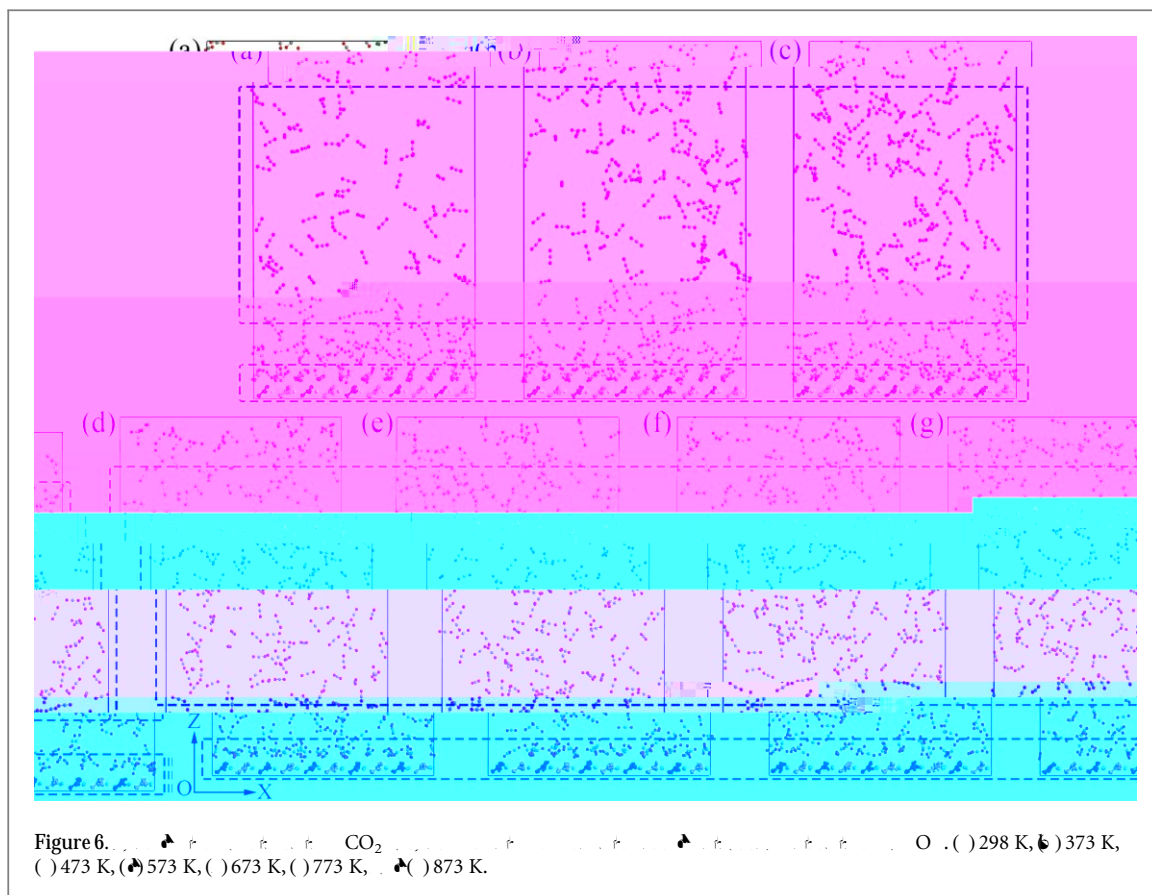


Figure 6. Snapshots of CO₂ adsorption on a surface at various temperatures: (a) 298 K, (b) 373 K, (c) 473 K, (d) 573 K, (e) 673 K, (f) 773 K, (g) 873 K.

Table 3. E_{ads} and D_{CO₂} of CO₂ adsorption on a surface.

T (K)	E _{ads} (eV)				O-C-O angle (°)		D _{CO₂} (Å)		∠CO ₃ ²⁻ (°)	D _{surface} (Å)
	R _C ^B	R _C	R _{OO'} ^B	R _{OO'}	∠ _{O-C-O} ^B	∠ _{O-C-O}	D _{C-o} ^B	D _{C-o}		
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 CO₂ adsorption on a surface at 673 K. The snapshots show the CO₂ molecule (red and black) interacting with the surface atoms (grey and white). The O-C-O angle and the distance between the carbon atom and the surface oxygen atom (D_{C-o}) are indicated.

3.2. CO₂ adsorption behavior

The adsorption energy (E_{ads}) and the diffusion coefficient (D_{CO₂}) of CO₂ on a surface are calculated. The adsorption energy (E_{ads}) is defined as the energy difference between the adsorbed state and the gas phase state. The diffusion coefficient (D_{CO₂}) is calculated using the Einstein relation. The adsorption energy (E_{ads}) and the diffusion coefficient (D_{CO₂}) are shown in Table 3. The adsorption energy (E_{ads}) increases with temperature, while the diffusion coefficient (D_{CO₂}) decreases. The adsorption energy (E_{ads}) is higher than the activation energy (E_p) for the diffusion of CO₂ on a surface.

Table 4. The values of the activation energy (E_a) and pre-exponential factor (E_p) for the degradation of the polymer (10^3 / s⁻¹).

	Temperature (K)						
	298	373	473	573	673	773	873
E_p	$-109\ 451 \pm 75$	$-109\ 411 \pm 81$	$-109\ 313 \pm 84$	$-109\ 237 \pm 78$	$-109\ 199 \pm 85$	$-109\ 101 \pm 92$	$-109\ 005 \pm 95$
E_a	$-109\ 442 \pm 72$	$-109\ 424 \pm 77$	$-109\ 309 \pm 80$	$-109\ 228 \pm 79$	$-109\ 203 \pm 88$	$-109\ 086 \pm 97$	$-108\ 997 \pm 94$

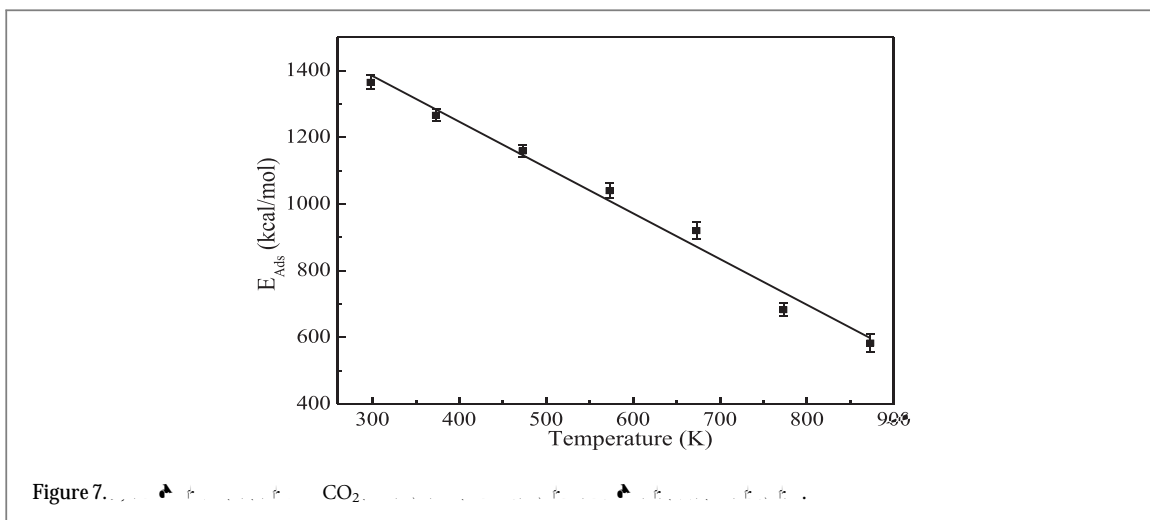


Figure 7. Relationship between E_{Ads} and Temperature for CO_2 .

Figure 6 shows the relationship between E_{Ads} and Temperature for CO_2 . The data points are fitted with a linear regression line, showing a negative correlation. The equation of the line is $E_{Ads} = -1.5T + 1350$, where T is Temperature (K) and E_{Ads} is Adsorption Energy (kcal/mol). The correlation coefficient is $R^2 = 0.98$. The data points are as follows:

Temperature (K)	E_{Ads} (kcal/mol)
300	1350
350	1250
450	1150
550	1050
650	950
750	850
850	750
900	650

$$E_A = E_{S_s} + E_G - E_T \tag{1}$$

where E_T , E_{S_s} , and E_G are the adsorption energy, surface energy, and gas energy, respectively. The adsorption energy E_A is the energy released when a gas molecule is adsorbed on a solid surface. The surface energy E_{S_s} is the energy required to create a new surface area. The gas energy E_G is the energy of the gas molecule in the gas phase. The adsorption energy E_A is the difference between the surface energy E_{S_s} and the gas energy E_G . The adsorption energy E_A is a function of the adsorption temperature T . The adsorption energy E_A decreases as the adsorption temperature T increases. The adsorption energy E_A is a function of the adsorption temperature T . The adsorption energy E_A decreases as the adsorption temperature T increases. The adsorption energy E_A is a function of the adsorption temperature T . The adsorption energy E_A decreases as the adsorption temperature T increases.

4. Conclusion

In this study, the adsorption of CO_2 on MD was investigated. The adsorption capacity of MD for CO_2 was found to be 104 mg/g at 273 K. The adsorption capacity of MD for CO_2 decreased as the adsorption temperature increased. The adsorption capacity of MD for CO_2 was found to be 673 mg/g at 273 K. The adsorption capacity of MD for CO_2 decreased as the adsorption temperature increased. The adsorption capacity of MD for CO_2 was found to be 673 mg/g at 273 K. The adsorption capacity of MD for CO_2 decreased as the adsorption temperature increased. The adsorption capacity of MD for CO_2 was found to be 673 mg/g at 273 K. The adsorption capacity of MD for CO_2 decreased as the adsorption temperature increased.

Notes

The authors have no competing financial interests.

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