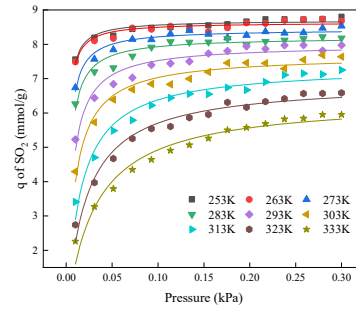
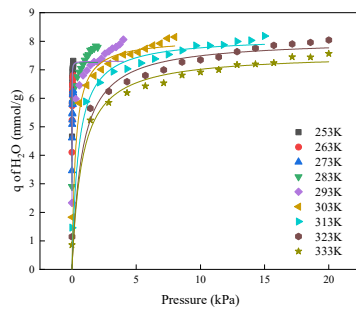
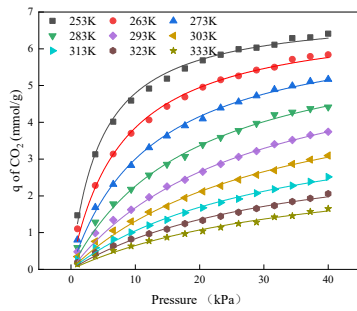


Supplementary Materials

Table S1 L-J potential function parameters

Atoms	$\epsilon(\text{kcal/mol})$	$\sigma(\text{\AA})$	Charge(e)
Si (zeolite)	0.0437	2.58175	2.4
Al (zeolite)	0.31	4.39	1.4
O (zeolite)	0.1053	3.82	-1.2
Na (zeolite)	0.5	3.144	1
Ca (zeolite)	0.05	3.472	2
C (CO ₂ -13X)	0.0595	3.081	0.6
O (CO ₂ -13X)	0.17	3.386	-0.3
H (H ₂ O-13X)	0.0152	3.195	0.335
O (H ₂ O-13X)	0.1	3.3	-0.67
S (SO ₂ -13X)	0.2899	4.063	0.328
O (SO ₂ -13X)	0.1141	3.379	-0.164
N (NO-13X)	0.1001	3.64	0
O (NO-13X)	0.1242	3.2888	0
C (CO ₂ -5A)	0.0595	3.081	0.1
O (CO ₂ -5A)	0.17	3.386	-0.05
H (H ₂ O-5A)	0.0152	3.195	0.5
O (H ₂ O-5A)	0.1	3.3	-1
S (SO ₂ -5A)	0.2899	4.063	0.4710
O (SO ₂ -5A)	0.1141	3.379	-0.2355
N (NO-5A)	0.1001	3.64	0.073
O (NO-5A)	0.1242	3.2888	-0.073
O (O ₂)	0.1	3.3	0
N (N ₂)	0.0774	3.4	0



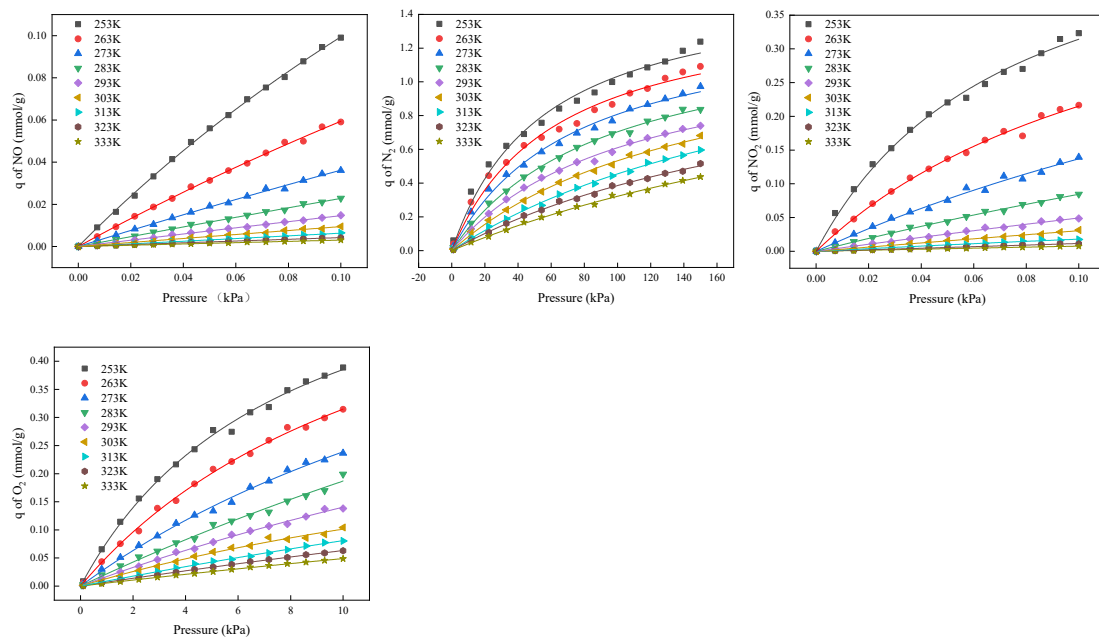


Figure S1. Isotherms of pure components on 13X

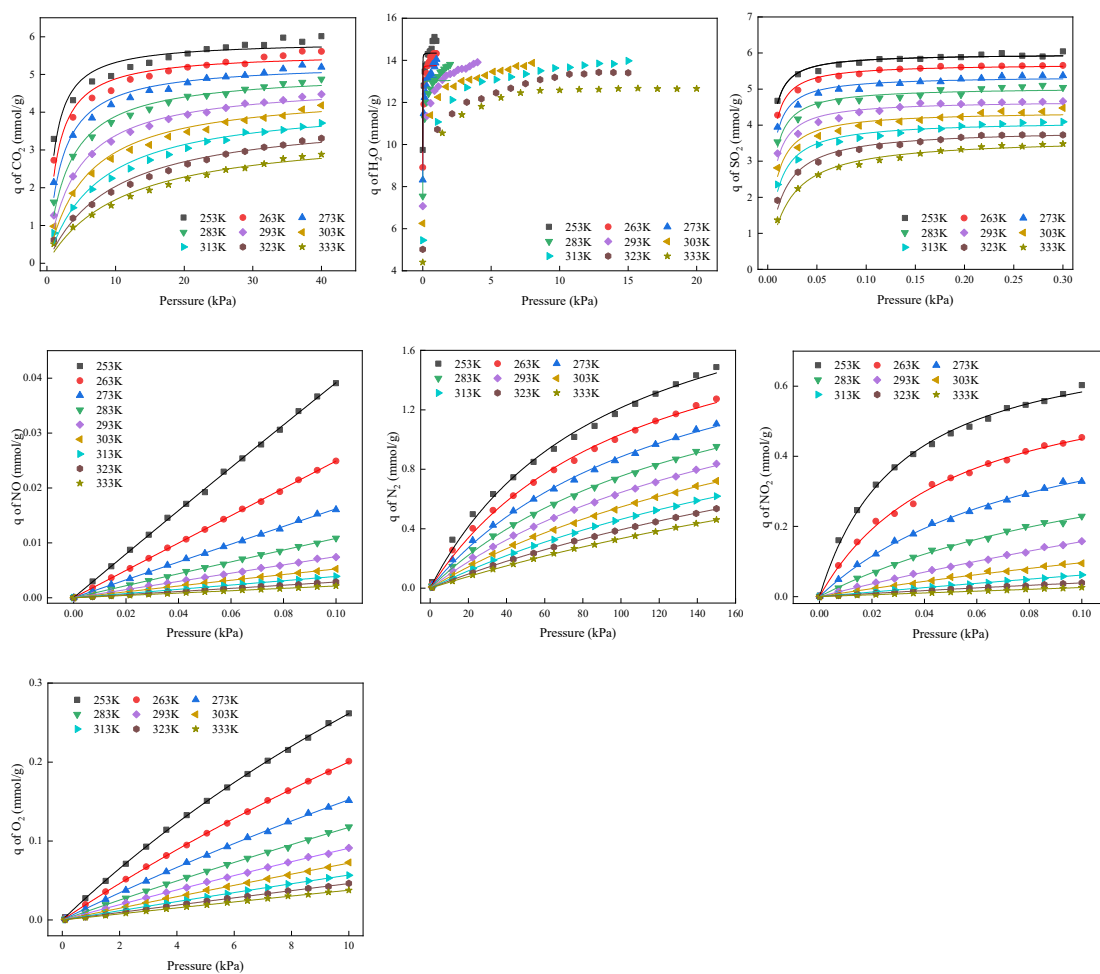


Figure S2. Isotherms of pure components on 5A.

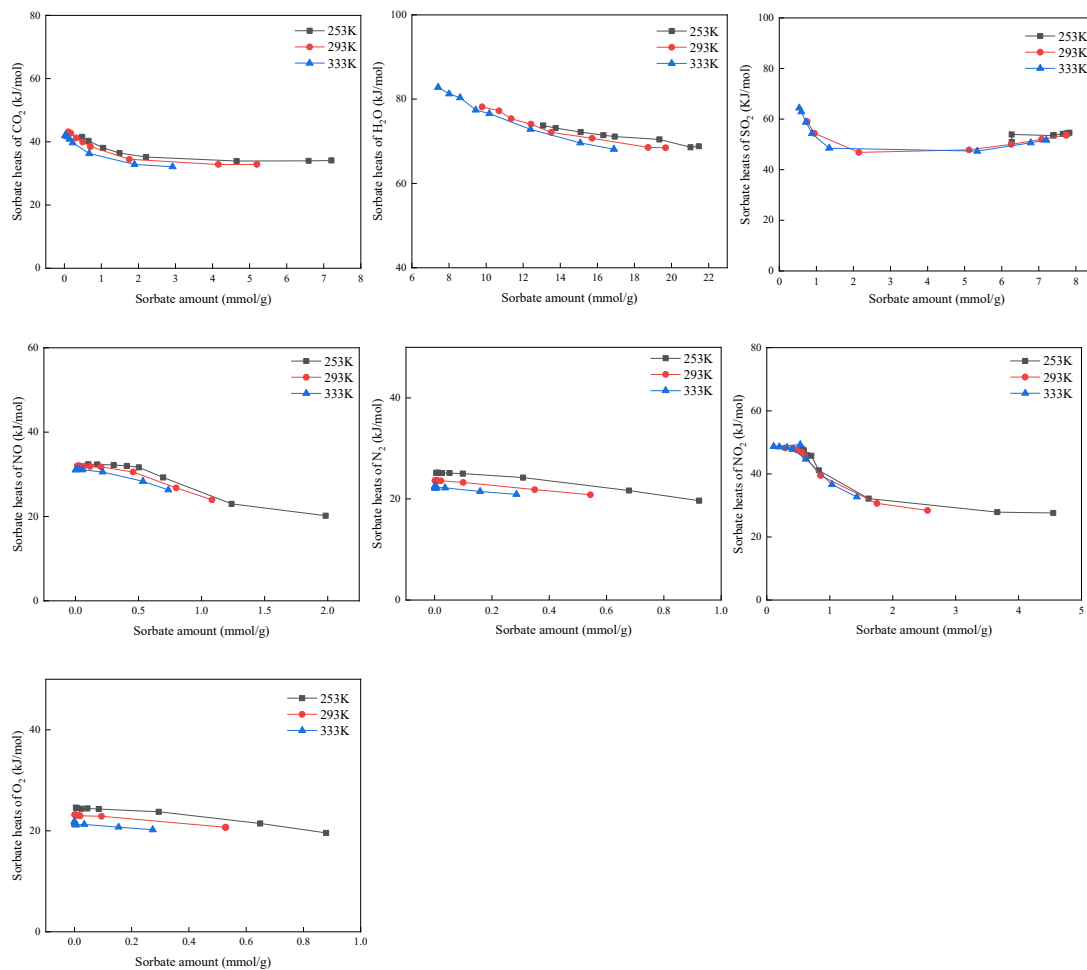
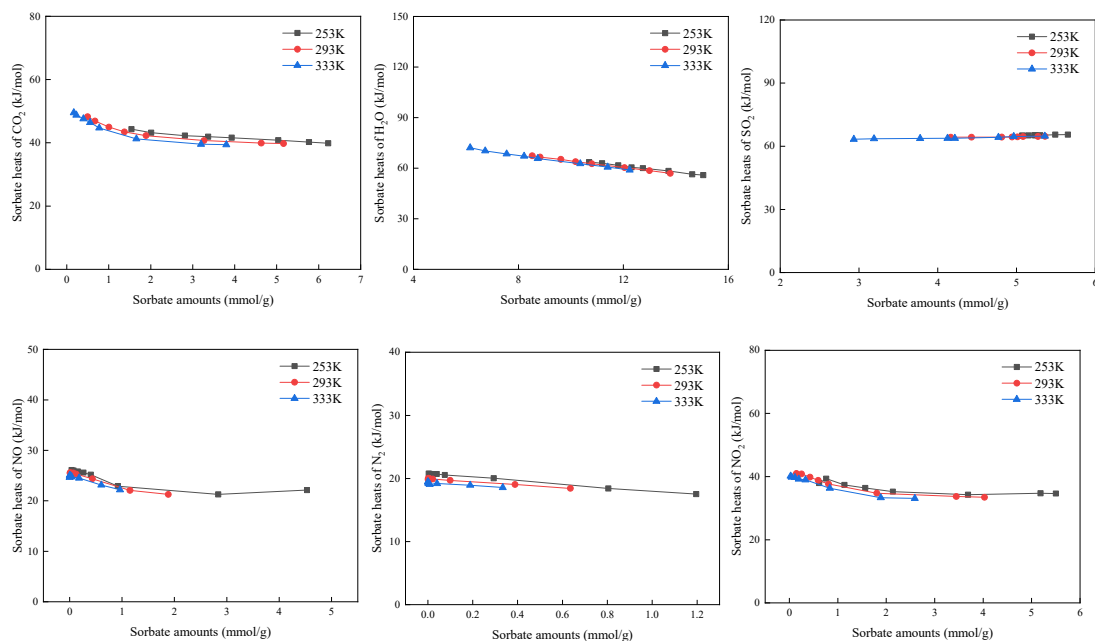


Figure S3. The variation of adsorption heat of pure components on 13X zeolite with adsorption capacity.



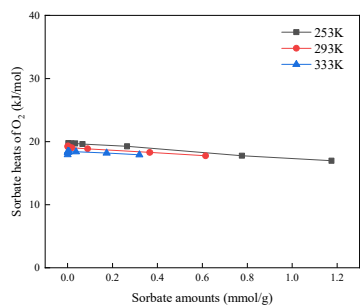


Figure S4. The variation of adsorption heat of pure components on 5A zeolite with adsorption capacity.

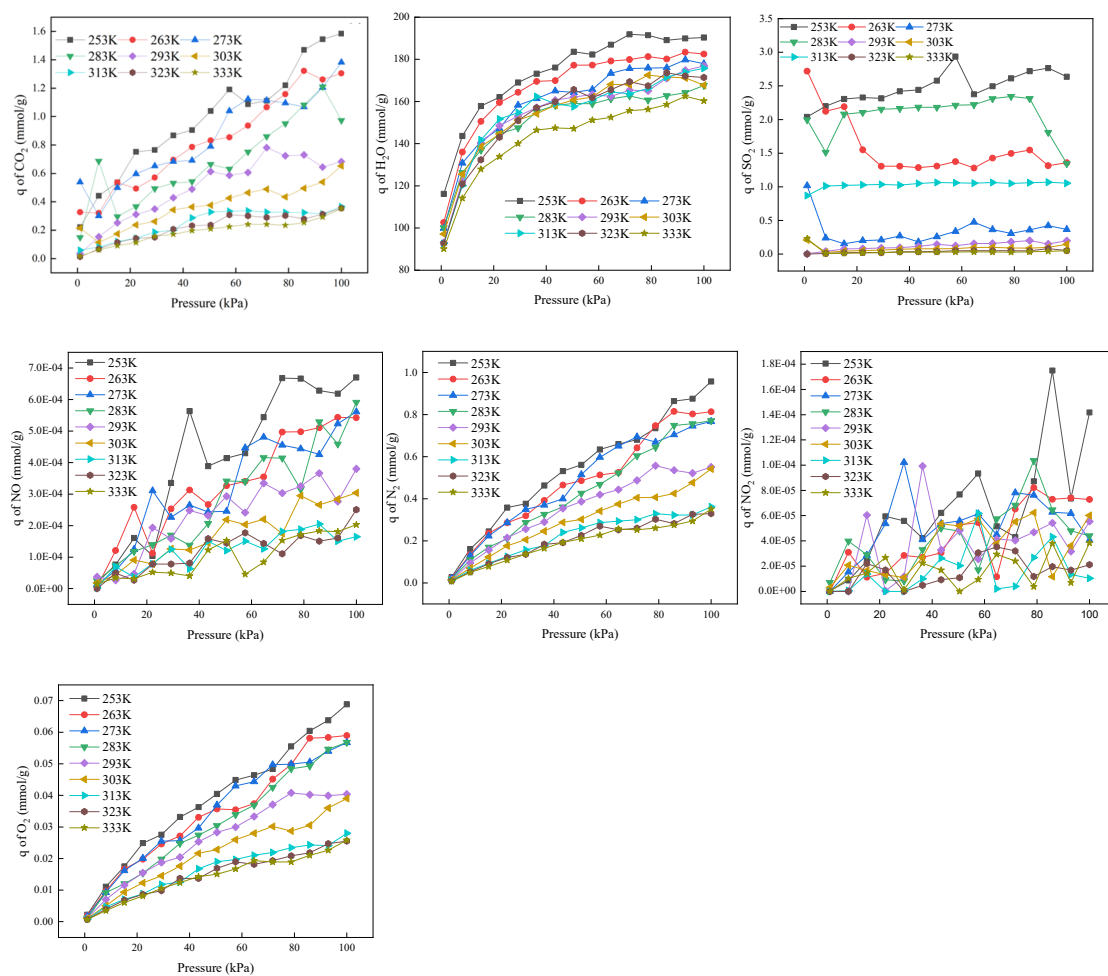
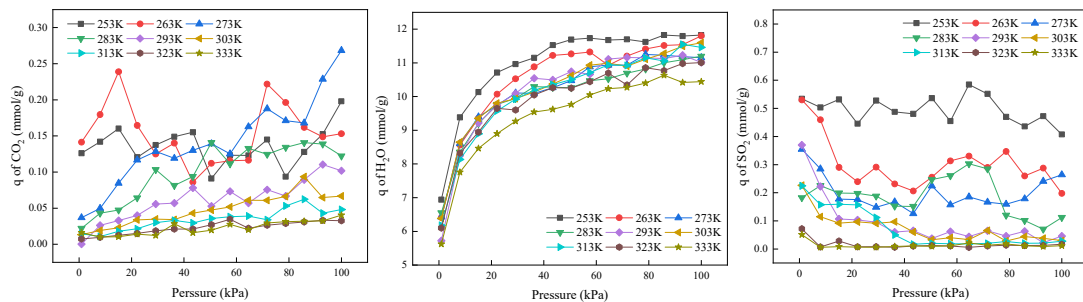


Figure S5. Isotherms of mixture on 13X.



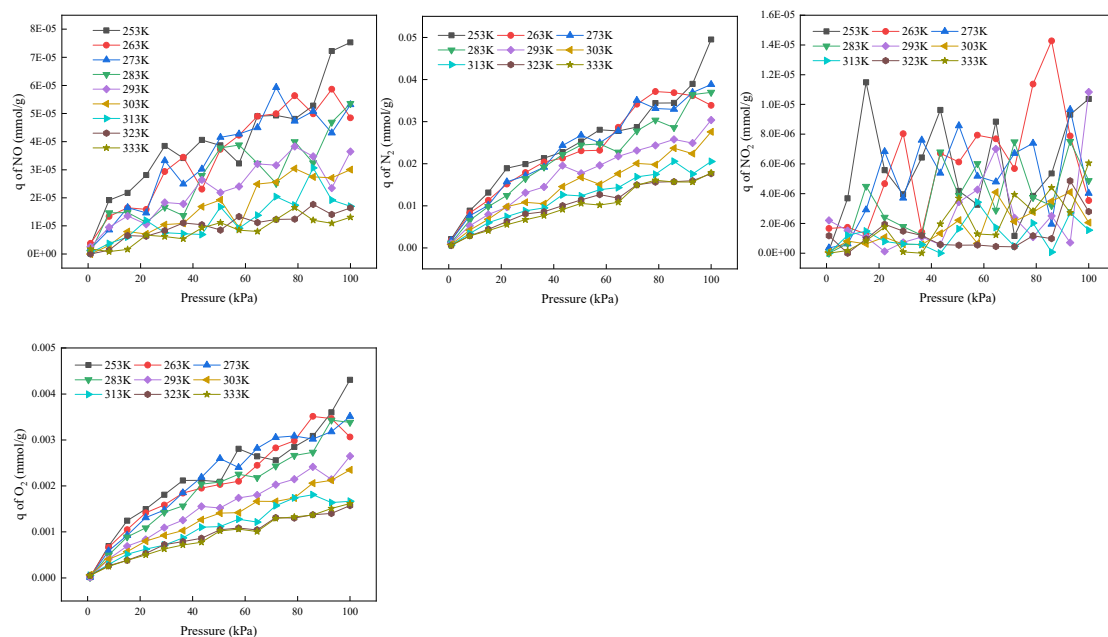


Figure S6. Isotherms of mixture on 5A.

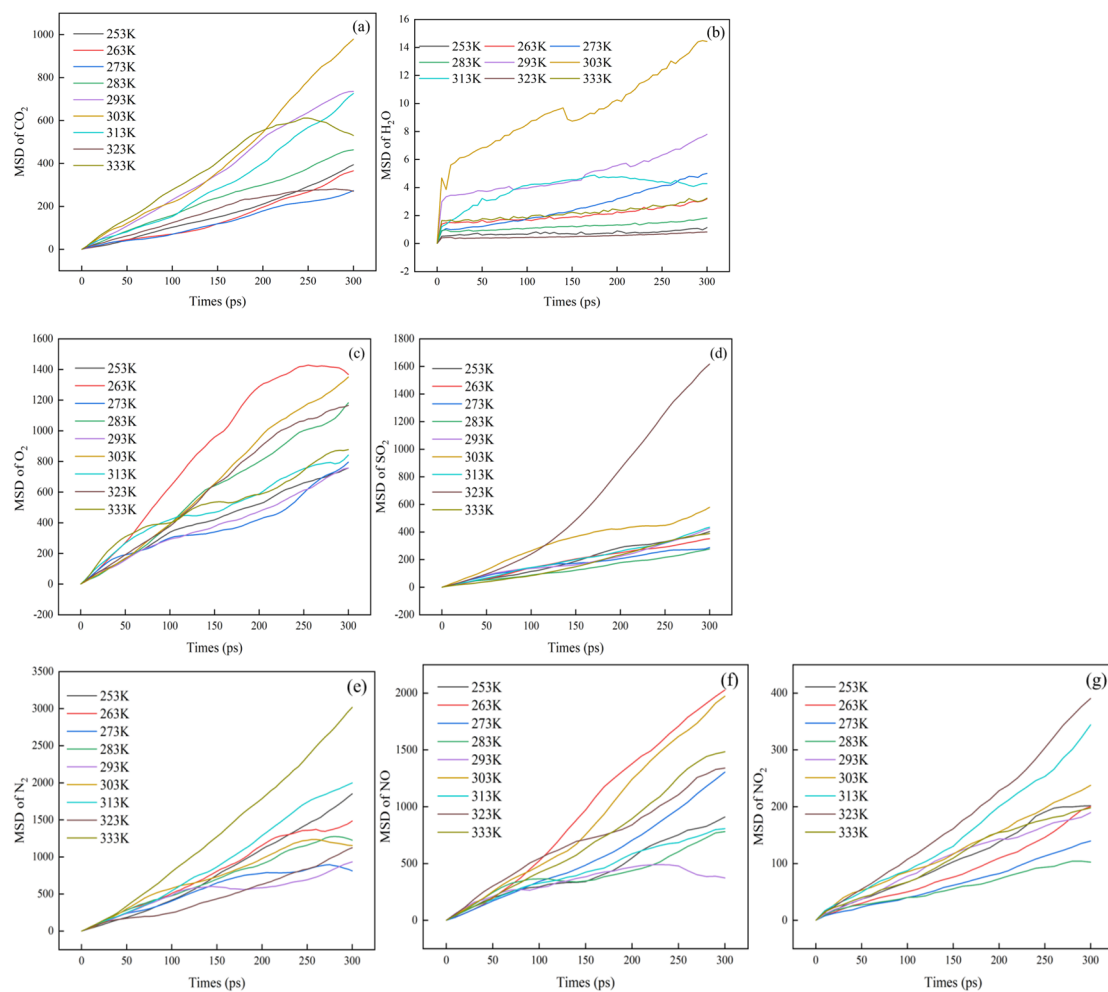


Figure S7. The variation of diffusion coefficients with temperature of (a) CO₂ (b) H₂O (c) SO₂ (d) O₂ (e) N₂ (f) NO (g) NO₂ on 13X.

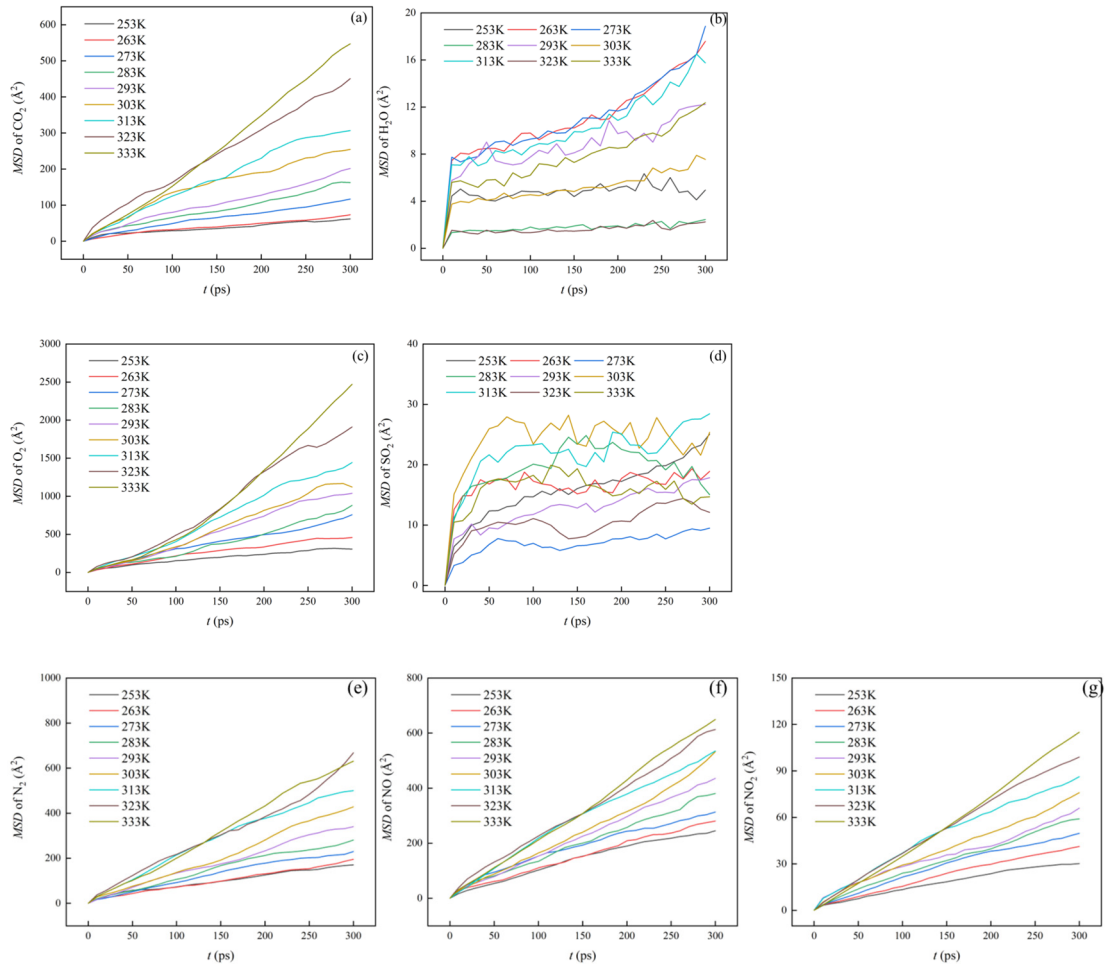


Figure S8. The variation of diffusion coefficients with temperature of (a) CO₂ (b) H₂O (c) SO₂ (d) O₂ (e) N₂ (f) NO (g) NO₂ on 5A.

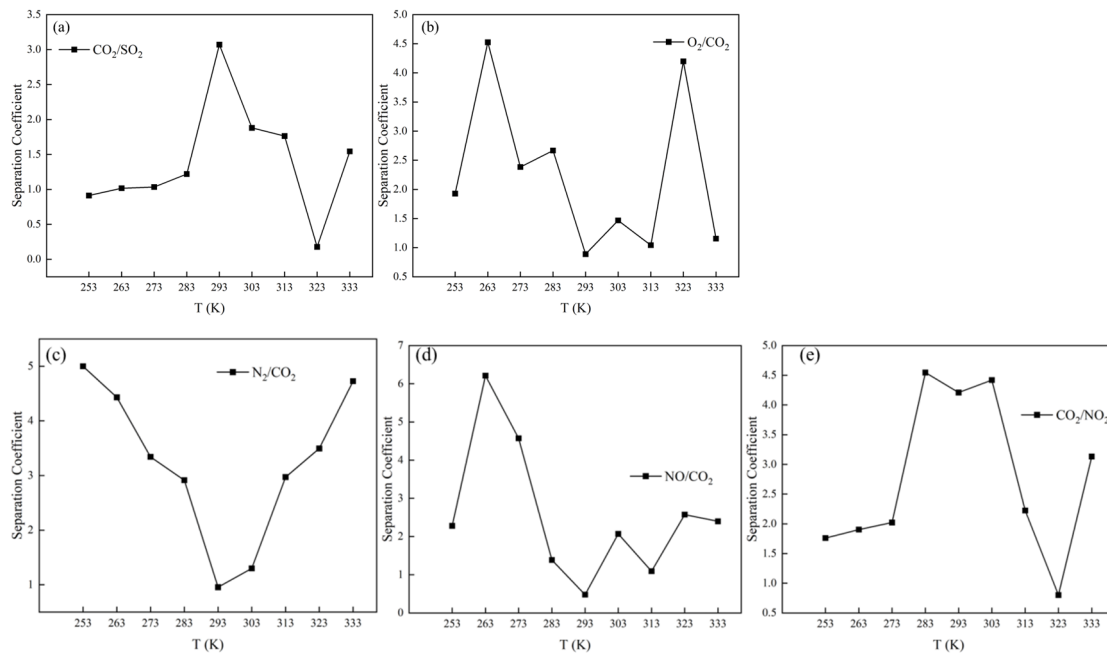


Figure S9. Adsorption kinetics selectivity of (a) SO₂ (b) O₂ (c) N₂ (d) NO (e) NO₂ from CO₂ on 13X.

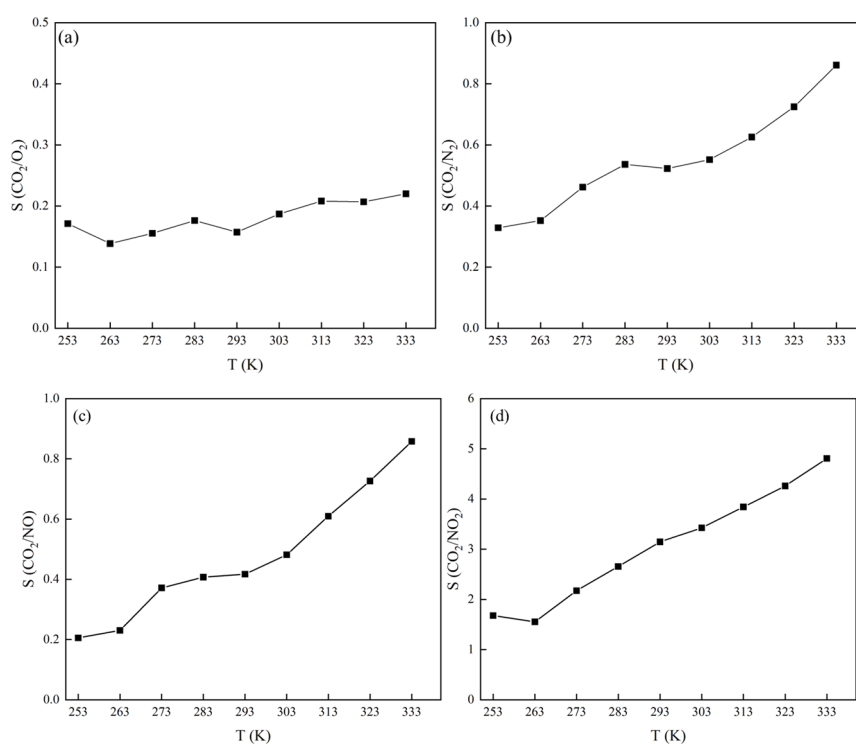


Figure S10. Adsorption kinetics selectivity of (a) O₂ (b) N₂ (c) NO (d) NO₂ from CO₂ on 5A.