Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Theoretical analysis of the absorption of CO_2 and CO on pristine and Al-doped C_3B

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Table S1 The change in lattice constant

Material	Lattice constants calculated using PBE	Lattice constants calculated using PBEsol
C3B	a = b = 10.355 Å	a = b = 10.321 Å
Al-doped C3B	a = b = 10.536 Å	a = b = 10.501 Å

Note 1 From the results in **Table S1**, we can find that the lattice constant slightly increases after the introduction of Al doping in the PBE function calculations. It is due to the fact that the atomic radius of the AL element is larger than that of the B element and the stretching lattice strain occurs during doping, such a phenomenon is also observed in the al-doped BN.[1] Moreover, since the PBEsol function is more accurate in the calculation of the structural parameters, we used PBEsol to re-optimize both structures. The obtained lattice parameters showed no significant difference from the results of the PBE function and also show a trend of increasing lattice constants after al-doping.

Table S2 Atomic coordinates in C3B

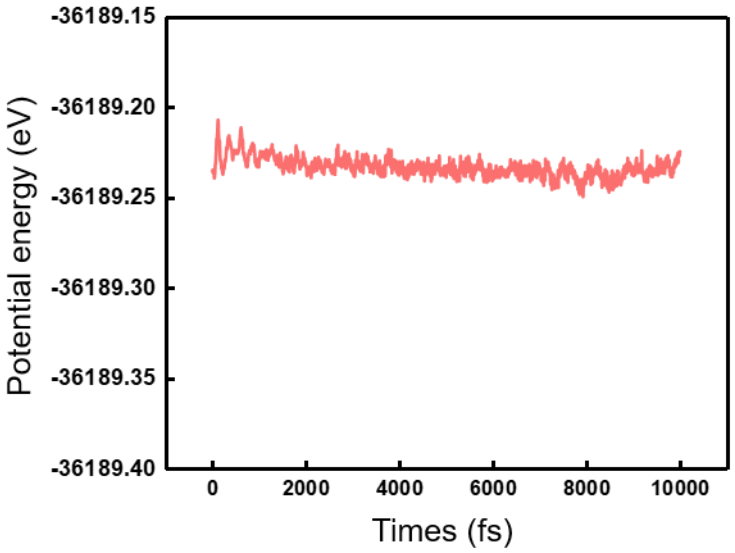
	Atom	X(Å)	Y(Å)	Z(Å)
1	C	2.577564	3.045200	8.521425
2	C	1.229125	0.709636	8.521425
3	C	3.926002	0.709636	8.521425
4	C	0.000000	1.419272	8.521425
5	C	1.348438	3.754835	8.521425
6	C	-1.348438	3.754835	8.521425
7	B	2.577564	1.488157	8.521425
8	B	0.000000	2.976314	8.521425
9	C	7.732691	3.045200	8.521425
10	C	6.384252	0.709636	8.521425
11	C	9.081129	0.709636	8.521425
12	C	5.155127	1.419272	8.521425
13	C	6.503566	3.754835	8.521425
14	C	3.806689	3.754835	8.521425
15	B	7.732691	1.488157	8.521425
16	B	5.155127	2.976314	8.521425
17	C	0.000000	7.509671	8.521425
18	C	-1.348438	5.174107	8.521425
19	C	1.348438	5.174107	8.521425
20	C	-2.577564	5.883743	8.521425
21	C	-1.229125	8.219306	8.521425
22	C	-3.926002	8.219306	8.521425
23	B	0.000000	5.952628	8.521425
24	B	-2.577564	7.440785	8.521425
25	C	5.155127	7.509471	8.521425
26	C	3.806689	5.174107	8.521425
27	C	6.503566	5.174107	8.521425
28	C	2.577564	5.883743	8.521425
29	C	3.926002	8.219306	8.521425
30	C	1.229125	8.219306	8.521425
31	B	5.155127	5.952628	8.521425
32	B	2.577564	7.440785	8.521425

Table S3 Atomic coordinates in Al-doped C3B

	Atom	X(Å)	Y(Å)	Z(Å)
1	C	2.547358	3.138213	5.189144
2	C	1.244877	0.718730	5.189144
3	C	3.991451	0.636970	5.189144
4	C	0.000000	1.442694	5.189144
5	C	1.326657	3.857980	5.189144
6	C	-1.326657	3.857890	5.189144
7	B	2.619867	1.512581	5.189144
8	B	0.000000	3.045603	5.189144
9	C	7.989070	3.138213	5.189144
10	C	6.544977	0.636970	5.189144
11	C	9.291551	0.718730	5.189144
12	C	5.268214	1.235204	5.189144
13	C	6.832603	3.944805	5.189144
14	C	3.703825	3.944805	5.189144
15	B	7.916561	1.512581	5.189144
16	Al	5.268214	3.041605	5.189144
17	C	0.000000	7.652142	5.189144
18	C	-1.358736	5.298743	5.189144
19	C	1.358736	5.298743	5.189144
20	C	-2.590433	6.046905	5.189144
21	C	-1.263776	8.344742	5.189144
22	C	-4.018804	8.403467	5.189144
23	B	0.000000	6.083209	5.189144
24	B	-2.630644	7.602013	5.189144
25	C	5.268214	7.687354	5.189144
26	C	3.824121	5.349631	5.189144
27	C	6.712307	5.349631	5.189144
28	C	2.590433	6.046905	5.189144
29	C	4.018804	8.403467	5.189144
30	C	1.263776	8.344742	5.189144
31	B	5.268214	6.099652	5.189144
32	B	2.630644	7.602013	5.189144

Table S4 Comparison of adsorption energy

Ref	Material	Eads(CO)	Eads(CO2)
[2]	B-N@Graphene	-0.110 eV	-0.120 eV
[3]	MoS_2-nanotubes	-0.440 eV	-0.120 eV
[4]	Au-doped VO_2	-0.450 eV	+0.030 eV
[5]	β-SnSe	-0.202 eV	-0.175 eV
[6]	In-doped SnO_2	-0.346 eV	/
[7]	SiGe monolayer	-0.241 eV	-0.200 eV
[8]	SnP_3 sheets	-0.338 eV	-0.221 eV
[9]	$PtSe_2$ monolayer	-0.141 eV	-0.182 eV
Our work	Al-doped C_3B	-0.401 eV	-0.590 eV



. **Fig. S1.** Energy fluctuation of monolayer Al-C_3B in molecular dynamics simulations at 300K

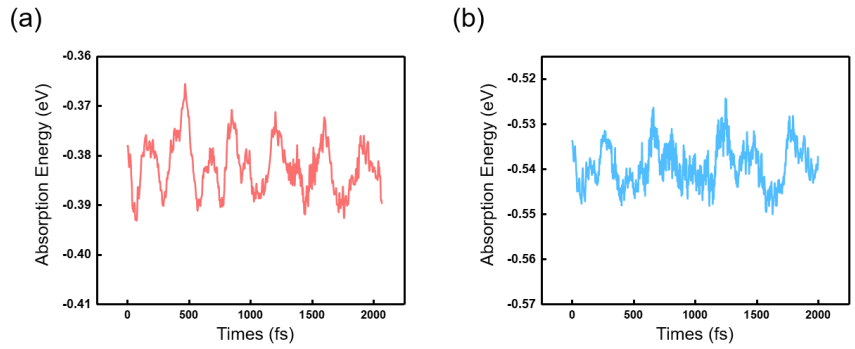


Fig.S2 Fluctuation of adsorption energy at room temperature (300 K) for (a)CO/Al-C_3B system (b) CO_2/Al-C_3b system.

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