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

B doped 2D-InSe as a bifunctional catalyst for CO_2/CH_4 separation under the regulation of external electric field

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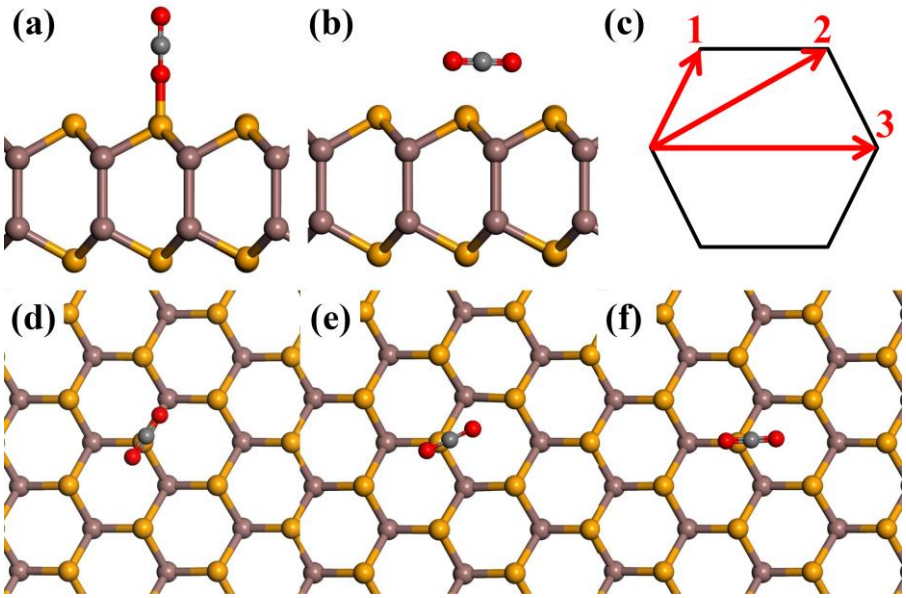

Fig. S1 The side view of (a) vertical and (b) parallel adsorption of CO_2; (c) indicates the schematic diagram of different orientation; (d), (e), and (f) denote the top view of CO_2 parallel adsorption with C-O bond pointing to different atoms in the hexagonal unit.

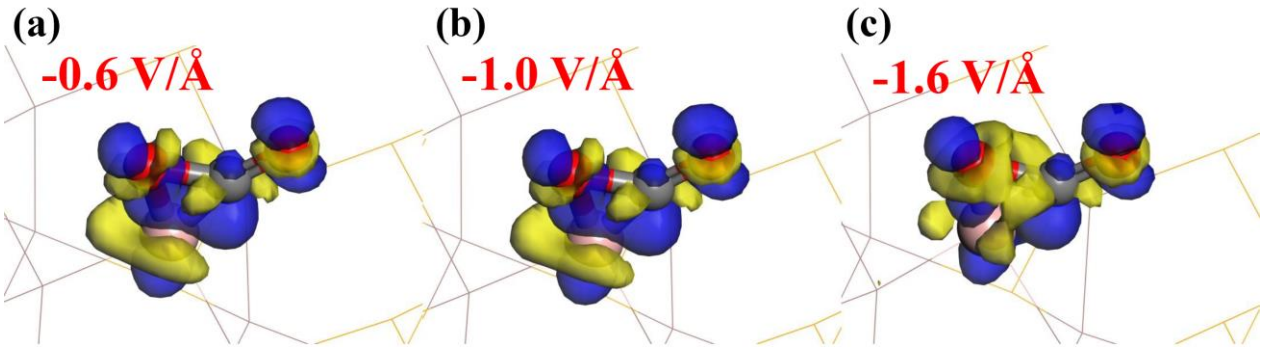

Fig. S2 The charge density difference of CO_2-B@2DInSe complex at electric fields of (a) -0.6, (b) -1.0, and (c) -1.6 V/Å respectively.

Tab. S1 The adsorption energies of CO_2 ($E_{ad}[CO_2]$) in different manners on 2D InSe, v-2DInSe, and B@2DInSe surfaces respectively with various manners. The serial numbers for the parallel manners corresponds to the numbers in Fig. S1 (c). The values labeled in red denote the optimal situations for each system.

	$E_{ad}[CO_2]$ (eV)			
	Vertical	Parallel 1	Parallel 2	Parallel 3
2D InSe	0.00	-0.02	-0.05	-0.03
v-2DInSe	-0.16	-0.07	-0.08	-0.09
B@2DInSe	-0.13	-0.50	-0.47	-0.52

Tab. S2 The adsorption energies of CO_2 ($E_{ad}[CO_2]$) and CH_4 ($E_{ad}[CH_4]$) at different electric field (EF)

EF(V/Å)	2D InSe (eV)		v-2DInSe (eV)		B@2DInSe (eV)	
	$E_{ad}[CO_2]$	$E_{ad}[CH_4]$	$E_{ad}[CO_2]$	$E_{ad}[CH_4]$	$E_{ad}[CO_2]$	$E_{ad}[CH_4]$
-2		-0.27	0.54	0.31		0.16
-1.9		-0.45				
-1.8			-0.02	-0.23	0.70	-0.30
-1.7		-0.82		-0.49	0.38	
-1.6		-0.92	-0.38	-0.60	0.02	-0.64
-1.5	0.07		-0.56		-0.25	-0.66
-1.4	-0.10		-0.55		-0.46	-0.74
-1.3	-0.18	-0.70	-0.58		-0.64	-0.67
-1.2	-0.20	-0.52	-0.55	-0.51	-0.76	-0.52
-1.1	-0.10					
-1.0	-0.04	-0.15	-0.27	-0.23	-0.79	
-0.9					-0.78	
-0.8	-0.04	-0.02	-0.08	-0.06	-0.77	-0.08
-0.7	-0.02					
-0.6	-0.03		-0.10		-0.68	
-0.5	-0.01		-0.10			
-0.4	-0.01	-0.02	-0.11	-0.13	-0.73	-0.12
-0.3						
-0.2	-0.03		-0.12		-0.61	
-0.1						
0.0	-0.05	-0.03	-0.16	-0.16	-0.52	-0.13
0.1						
0.2	-0.03		-0.13		-0.47	
0.3						
0.4	-0.04	-0.08	-0.13	-0.19	-0.39	-0.15
0.5						
0.6	-0.03		-0.14		-0.35	
0.7						
0.8	-0.01	-0.09	-0.16	-0.19	-0.34	-0.20
0.9	0.00		-0.16		-0.31	
1.0	0.01		-0.16		-0.28	
1.1						
1.2	0.20	-0.03	0.08	-0.10	0.00	-0.13
1.3	0.48	0.11	0.35	0.06	0.31	0.05
1.4	0.87	0.41		0.40		0.38
1.5		0.79				