Supporting Information

Electric Field Controlled CO_2 Capture and CO_2/N_2 Separation on MoS_2 Monolayer

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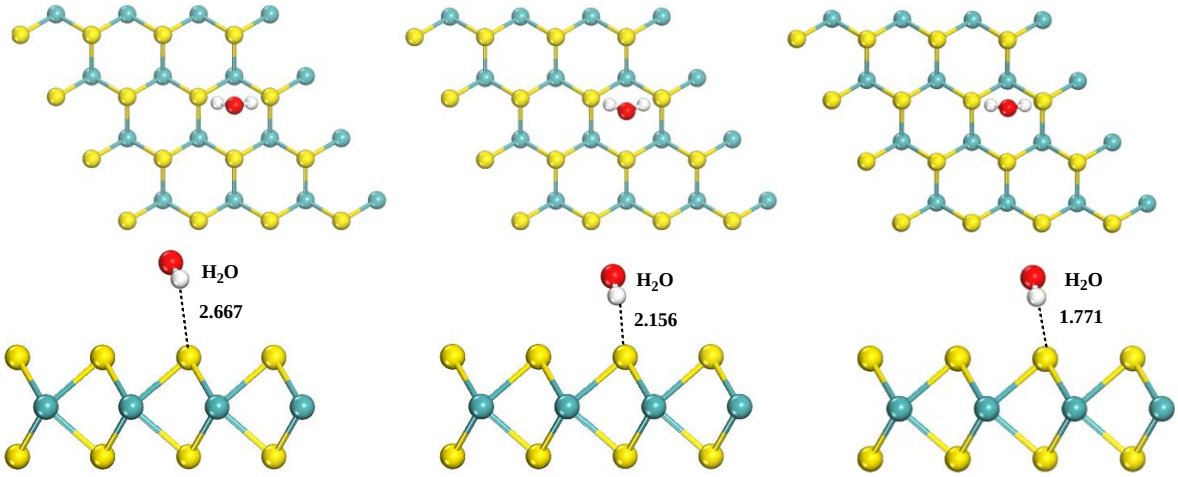


E_{ad} =4.54 kcal/mol
Without electric field
(a)

E_{ad} =12.88 kcal/mol
Electric field=0.0020 a.u.
(b)

E_{ad} = 41.75 kcal/mol
Electric field=0.0050 a.u.
(c)

Figure S1. Top and side views of H_2O adsorption on the surface of MoS_2 monolayer without an electric field, and with the electric fields of 0.0020 a.u. and 0.0050 a.u..

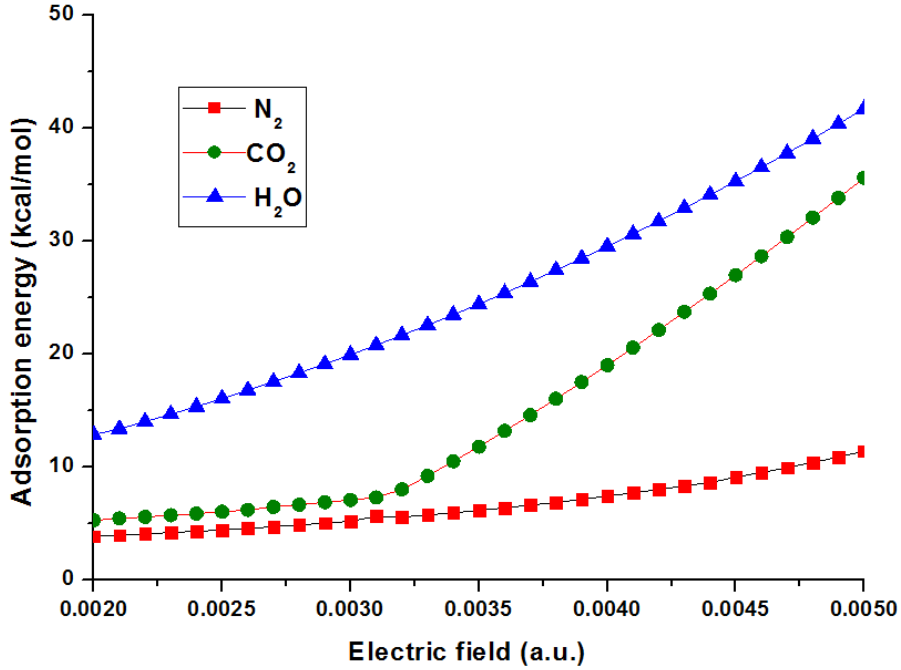
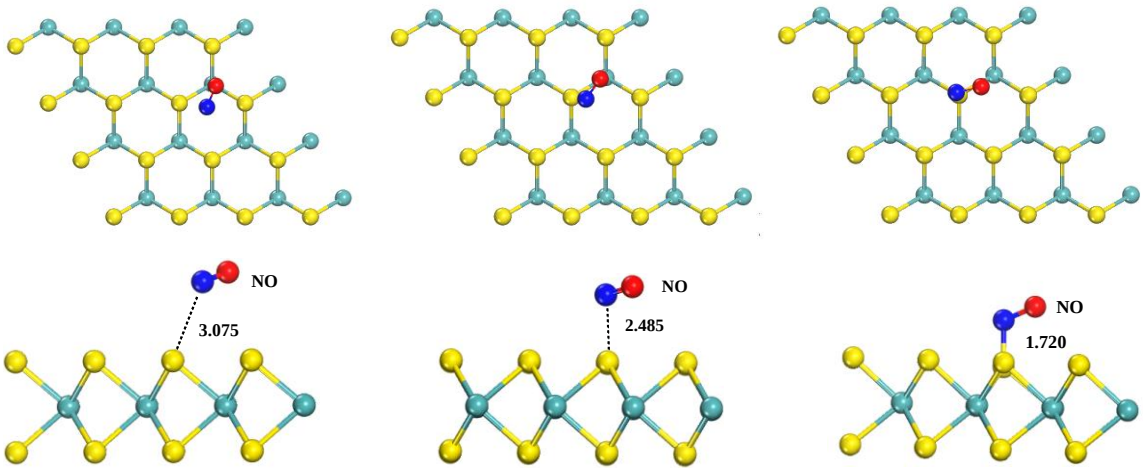


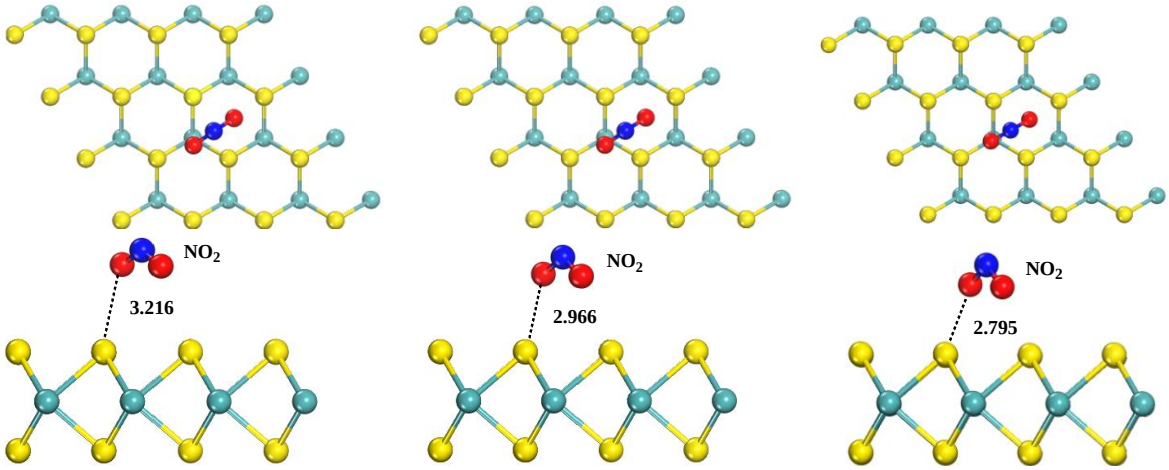
Figure S2. The adsorption energies (kcal/mol) of H_2O, N_2 and CO_2 adsorbed on the surface of MoS_2 monolayer with the applied electric fields in the range of 0.0020 ～ 0.0050 a.u..



E_{ad} =3.22 kcal/mol
Without electric field
(a)

E_{ad} =8.27 kcal/mol
Electric field=0.0020 a.u.
(b)

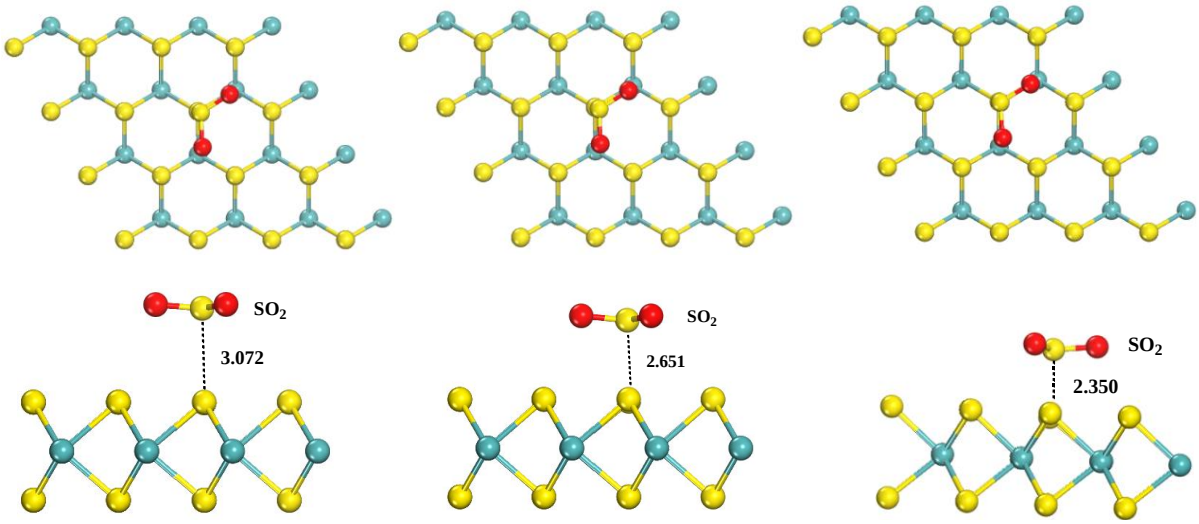
E_{ad} = 41.39 kcal/mol
Electric field=0.0050 a.u.
(c)



E_{ad} =4.86 kcal/mol
Without electric field
(d)

E_{ad} =9.89 kcal/mol
Electric field=0.0020 a.u.
(e)

E_{ad} = 48.63 kcal/mol
Electric field=0.0050 a.u.
(f)



E_{ad} =5.33kcal/mol
Without electric field
(g)

E_{ad} =13.45 kcal/mol
Electric field=0.0020 a.u.
(h)

E_{ad} = 46.79 kcal/mol
Electric field=0.0050 a.u.
(i)

Figure S3. Top and side views of NO, NO_2 and SO_2 adsorbed on the surface of MoS_2 monolayer without an electric field, and with the electric fields of 0.0020 a.u. and 0.0050 a.u..

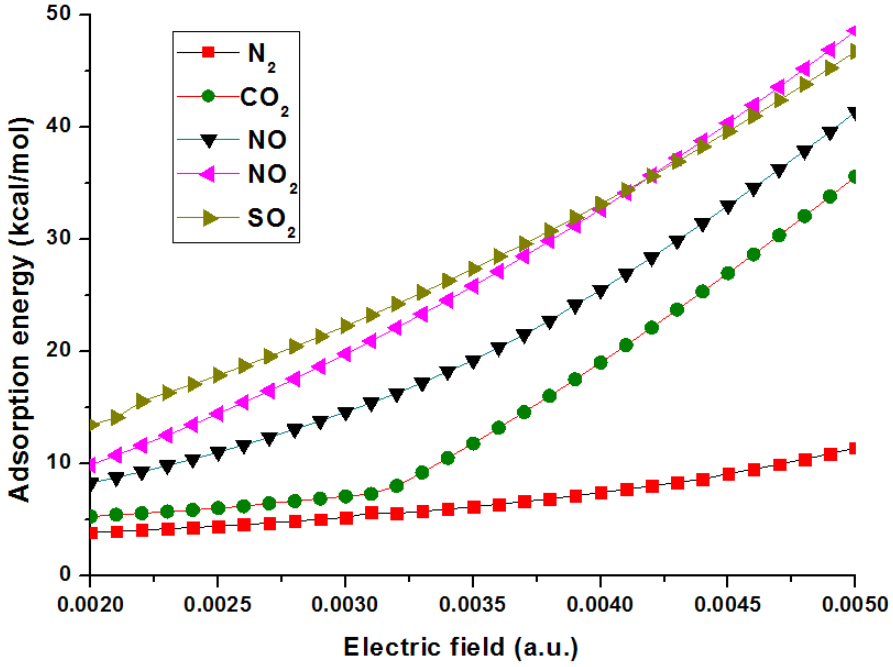


Figure S4. The adsorption energies (kcal/mol) of NO, NO_2, SO_2, CO_2 and N_2 adsorbed on the surface of MoS_2 monolayer with the applied electric fields in the range of 0.0020 ~ 0.0050 a.u..

Table S1. The important structural parameters, such as bond distance (Å) and bond angle (°), adsorption energies (kcal/mol) and electron transfer (e^-) from MoS_2 surface to CO_2, of CO_2 adsorbed on the surface of MoS_2 monolayer with different electric fields.

E-field (a.u.)	Adsorption energy (kcal/mol)	Bond distance (Å)	Bond distance (Å)	Bond distance (Å)	Bond angle (°)	CT
		C-S	O1-C	O2-C	OCO	total
0.0020	5.29	3.093	1.177	1.177	178.8	-0.036
0.0021	5.44	3.092	1.190	1.190	178.8	-0.038
0.0022	5.58	3.091	1.176	1.176	178.7	-0.040
0.0023	5.73	3.090	1.176	1.176	178.7	-0.041
0.0024	5.88	3.089	1.177	1.177	178.6	-0.042
0.0025	6.04	3.088	1.177	1.180	178.6	-0.045
0.0026	6.20	3.072	1.177	1.177	178.0	-0.047
0.0027	6.46	3.012	1.177	1.177	177.6	-0.057
0.0028	6.66	2.984	1.177	1.177	177.2	-0.061
0.0029	6.87	2.948	1.178	1.177	176.9	-0.066
0.0030	7.08	2.917	1.178	1.221	176.1	-0.074
0.0031	7.30	2.916	1.180	1.178	175.8	-0.077
0.0032	8.01	2.048	1.221	1.265	144.2	-0.527
0.0033	9.21	1.995	1.225	1.223	142.5	-0.577
0.0034	10.51	1.99	1.226	1.225	142.1	-0.589
0.0035	11.81	1.959	1.180	1.180	172.6	-0.623
0.0036	13.19	1.954	1.230	1.228	140.7	-0.634
0.0037	14.60	1.938	1.233	1.230	140.0	-0.656
0.0038	16.04	1.918	1.236	1.233	139.2	-0.680
0.0039	17.52	1.914	1.236	1.233	139.0	-0.694
0.0040	19.03	1.904	1.237	1.235	138.6	-0.711
0.0041	20.57	1.901	1.238	1.255	138.4	-0.724
0.0042	22.14	1.889	1.240	1.237	137.9	-0.743
0.0043	23.74	1.882	1.241	1.238	137.6	-0.758
0.0044	25.36	1.872	1.242	1.239	137.2	-0.776
0.0045	27.01	1.864	1.243	1.240	136.9	-0.792
0.0046	28.68	1.857	1.250	1.241	136.6	-0.807
0.0047	30.37	1.853	1.245	1.242	136.4	-0.821
0.0048	32.10	1.845	1.247	1.243	136.0	-0.832
0.0049	33.84	1.835	1.248	1.245	135.7	-0.854
0.0050	35.62	1.833	1.249	1.245	135.6	-0.865

Table S2. The important structural parameters, such as bond distance (Å) and bond angle ( ), adsorption energies (kcal/mol) and electron transfer (e^-) from MoS_2 surface to N_2, of N_2 adsorbed on the surface of MoS_2 monolayer with different electric fields.

E-field (a.u.)	Adsorption energy (kcal/mol)	Bond distance (Å)	Bond distance (Å)	Bond angle ( )	Bond angle ( )	CT
		N1-S1	N1-N2	S1N1N2	S1N1S2	total
0.0020	3.85	3.329	1.109	108.1	57.2	-0.027
0.0021	3.96	3.320	1.109	108.1	57.3	-0.029
0.0022	4.08	3.296	1.109	108.3	57.8	-0.032
0.0023	4.20	3.296	1.109	108.2	57.8	-0.033
0.0024	4.31	3.281	1.109	108.9	58.1	-0.037
0.0025	4.41	3.210	1.109	108.6	59.5	-0.044
0.0026	4.56	3.209	1.109	108.6	59.6	-0.046
0.0027	4.71	3.208	1.110	108.6	59.6	-0.048
0.0028	4.87	3.207	1.110	108.7	59.6	-0.051
0.0029	5.03	3.207	1.110	108.7	59.6	-0.053
0.0030	5.20	3.206	1.110	108.7	59.6	-0.056
0.0031	5.65	3.175	1.111	108.8	60.2	-0.065
0.0032	5.56	3.162	1.111	108.8	60.5	-0.067
0.0033	5.75	3.161	1.111	108.8	60.5	-0.070
0.0034	5.95	3.146	1.111	108.9	60.8	-0.075
0.0035	6.16	3.132	1.111	109.1	61.2	-0.082
0.0036	6.39	3.116	1.112	109.2	61.5	-0.088
0.0037	6.62	3.097	1.112	109.5	62.0	-0.097
0.0038	6.87	3.063	1.113	109.6	62.7	-0.106
0.0039	7.13	3.052	1.113	109.3	62.8	-0.115
0.0040	7.42	3.051	1.113	109.1	62.8	-0.115
0.0041	7.71	3.048	1.114	109.5	62.9	-0.124
0.0042	8.01	3.046	1.114	109.5	63.0	-0.130
0.0043	8.32	3.043	1.115	109.6	63.0	-0.136
0.0044	8.63	3.04	1.115	109.7	63.1	-0.143
0.0045	9.11	2.948	1.117	110.4	65.4	-0.173
0.0046	9.52	2.943	1.118	110.7	65.7	-0.185
0.0047	9.95	2.903	1.118	110.8	66.6	-0.199
0.0048	10.41	2.883	1.119	110.9	67.1	-0.213
0.0049	10.89	2.862	1.120	111.1	67.7	-0.227
0.0050	11.41	2.840	1.121	111.3	68.3	-0.243