Supporting Information

N/P doped MoS_2 Monolayers as Promising Materials for Controllable CO_2 Capture and separation under Reduced Electric Fields: A Theoretical Modeling

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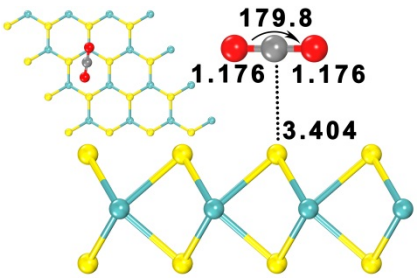
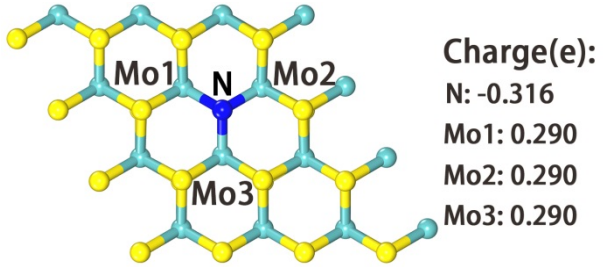
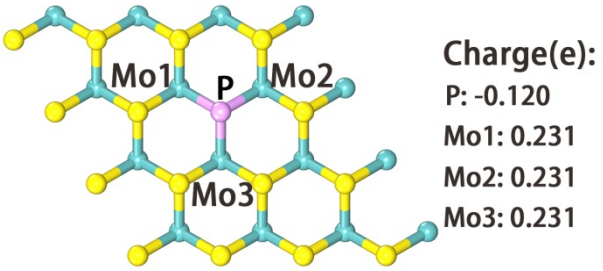


E_{ad} = 3.76 kcal/mol

Figure S1. The side and top views of the most stable configuration of CO_2 adsorbed on MoS_2.

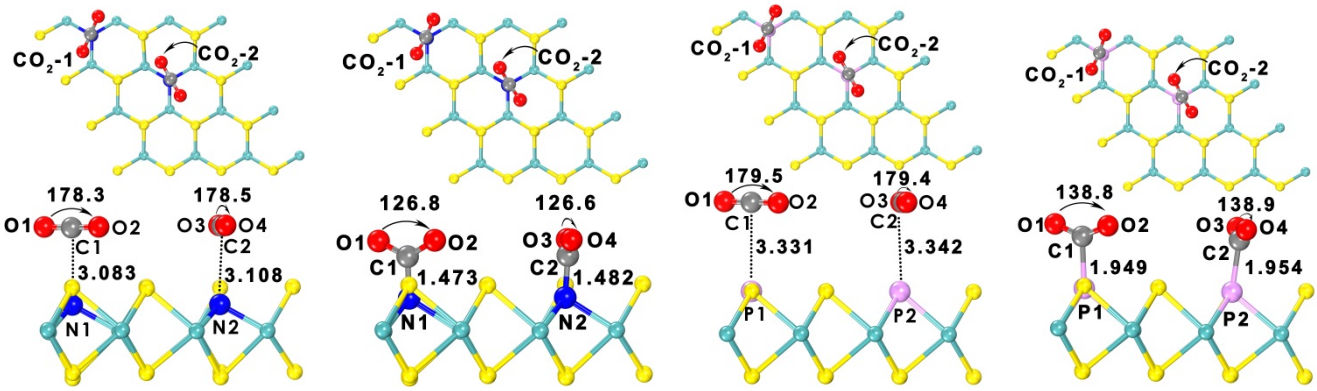


(a)



(b)

Figure S2. The charge distribution of N/P atom and its neighbor Mo atoms of (a) N-doped MoS_2 and (b) P-doped MoS_2.

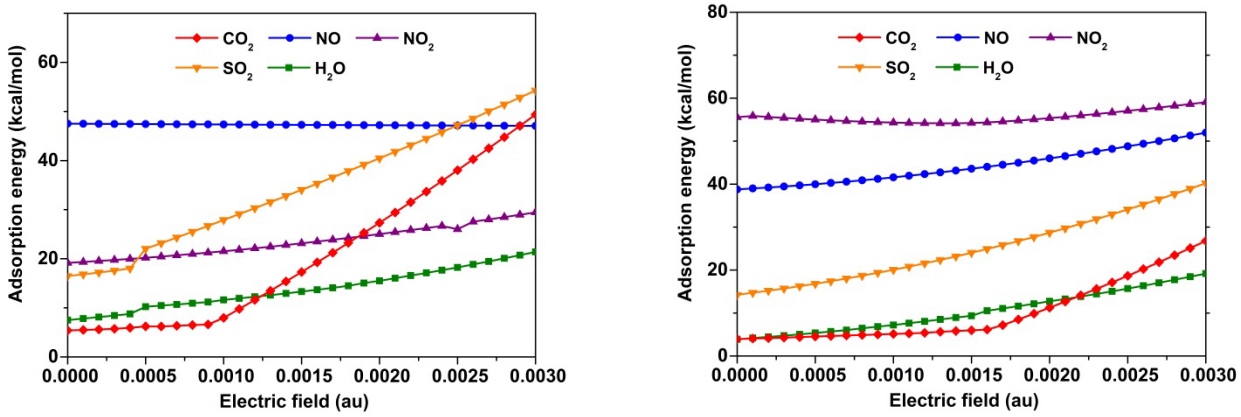


E_{ad} = 8.46 kcal/mol | E_{ad} = 25.37 kcal/mol | E_{ad} = 3.50 kcal/mol | E_{ad} = 8.90 kcal/mol

E-field: 0 au | E-field: 0.0020 au | E-field: 0 au | E-field: 0.0020 au

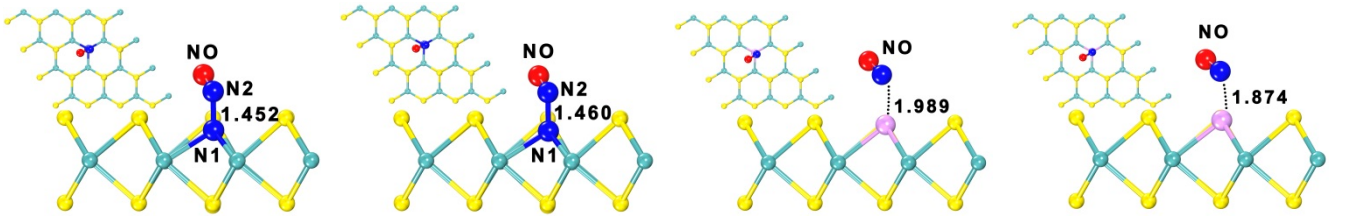
(a) (b) (c) (d)

Figure S3. The side and top views of the most stable configurations of two CO_2 molecules adsorbed on 2N/P-doped MoS_2 with the E-field of 0 au and 0.0020 au.



(a) (b)

Figure S4. The adsorption energies of CO_2, NO, NO_2 and H_2O adsorbed on the (a) N-doped and (b) P-doped MoS_2 surfaces with different external electric fields.

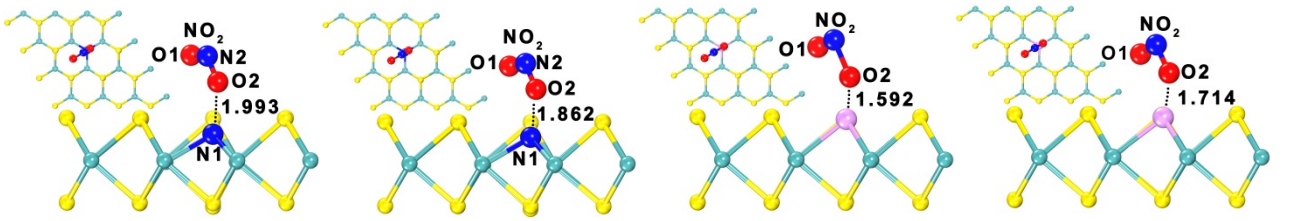


E_{ad} =47.51 kcal/mol | E_{ad} = 47.19 kcal/mol | E_{ad} = 38.76 kcal/mol | E_{ad} = 45.99 kcal/mol

E-field: 0 au | E-field: 0.0020 au | E-field: 0 au | E-field: 0.0020 au

(a) (b) (c) (d)

Figure S5. The side and top views of the most stable configurations of NO molecules adsorbed on N/P-doped MoS_2 with the E-field of 0 au and 0.0020 au.

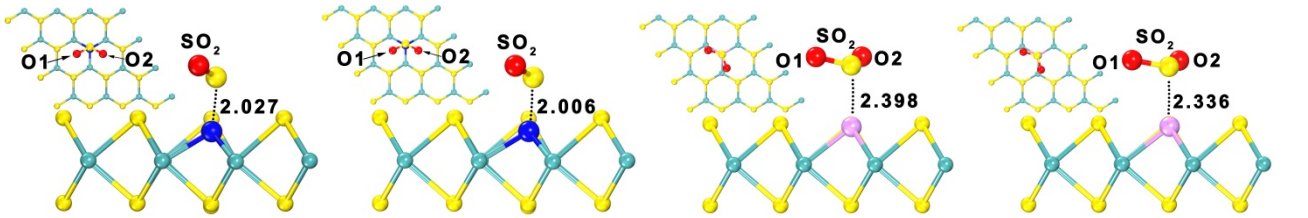


E_{ad} = 19.15 kcal/mol | E_{ad} = 25.03 kcal/mol | E_{ad} = 55.58 kcal/mol | E_{ad} = 55.36 kcal/mol

E-field: 0 au | E-field: 0.0020 au | E-field: 0 au | E-field: 0.0020 au

(a) (b) (c) (d)

Figure S6. The side and top views of the most stable configurations of NO_2 molecules adsorbed on N/P-doped MoS_2 with the E-field of 0 au and 0.0020 au.

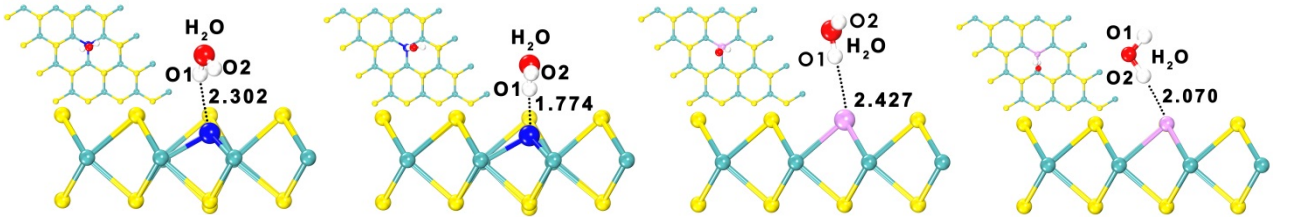


E_{ad} = 16.48 kcal/mol | E_{ad} = 40.46 kcal/mol | E_{ad} = 14.22 kcal/mol | E_{ad} = 28.69 kcal/mol

E-field: 0 au | E-field: 0.0020 au | E-field: 0 au | E-field: 0.0020 au

(a) (b) (c) (d)

Figure S7. The side and top views of the most stable configurations of SO_2 molecules adsorbed on N/P-doped MoS_2 with the E-field of 0 au and 0.0020 au.



E_{ad} = 7.50 kcal/mol | E_{ad} = 15.49 kcal/mol | E_{ad} = 3.87 kcal/mol | E_{ad} = 12.73 kcal/mol

E-field: 0 au | E-field: 0.0020 au | E-field: 0 au | E-field: 0.0020 au

(a) (b) (c) (d)

Figure S8. The side and top views of the most stable configurations of H_2O molecules adsorbed on N/P-doped MoS_2 with the E-field of 0 au and 0.0020 au.

Table S1. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from N-doped MoS_2 to CO_2, of CO_2 adsorbed on N-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)			Bond angle (°)	Electron transfer (e)
		C-N	C-O1	C-O2	O1-C-O2	Total
0	5.39	3.065	1.176	1.176	178.3	-0.022
0.0001	5.50	3.058	1.176	1.176	178.3	-0.023
0.0002	5.61	3.044	1.176	1.176	178.3	-0.024
0.0003	5.72	3.028	1.177	1.176	178.2	-0.026
0.0004	5.93	3.013	1.176	1.176	178.3	-0.027
0.0005	6.22	3.006	1.176	1.176	178.3	-0.029
0.0006	6.21	2.998	1.175	1.176	178.2	-0.030
0.0007	6.34	2.990	1.175	1.176	178.2	-0.032
0.0008	6.48	2.976	1.176	1.176	178.1	-0.033
0.0009	6.62	2.974	1.175	1.176	178.1	-0.035
0.0010	7.96	1.477	1.247	1.260	125.9	-0.393
0.0011	9.77	1.477	1.247	1.260	126.1	-0.402
0.0012	11.61	1.478	1.247	1.260	126.4	-0.411
0.0013	13.48	1.481	1.247	1.260	126.5	-0.421
0.0014	15.38	1.481	1.247	1.260	126.7	-0.430
0.0015	17.30	1.481	1.247	1.260	126.8	-0.439
0.0016	19.26	1.482	1.247	1.260	127.0	-0.448
0.0017	21.23	1.482	1.247	1.260	127.1	-0.457
0.0018	23.24	1.482	1.247	1.260	127.3	-0.466
0.0019	25.27	1.482	1.247	1.260	127.4	-0.475
0.0020	27.33	1.482	1.247	1.260	127.5	-0.484
0.0021	29.42	1.482	1.247	1.260	127.6	-0.493
0.0022	31.53	1.483	1.247	1.260	127.7	-0.502
0.0023	33.67	1.483	1.247	1.260	127.8	-0.510
0.0024	35.85	1.484	1.247	1.260	127.9	-0.519
0.0025	38.04	1.483	1.247	1.261	128.1	-0.528
0.0026	40.26	1.485	1.247	1.260	128.3	-0.536
0.0027	42.50	1.485	1.248	1.260	128.4	-0.545
0.0028	44.77	1.485	1.248	1.261	128.5	-0.553
0.0029	47.06	1.485	1.248	1.261	128.6	-0.561
0.0030	49.38	1.485	1.248	1.261	128.7	-0.570

Table S2. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from P-doped MoS_2 to CO_2, of CO_2 adsorbed on P-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)			Bond angle (°)	Electron transfer (e)
		C-P	C-O1	C-O2	O1-C-O2	Total
0	3.95	3.544	1.176	1.177	179.5	-0.030
0.0001	4.06	3.544	1.176	1.177	179.5	-0.031
0.0002	4.17	3.543	1.176	1.177	179.5	-0.032
0.0003	4.28	3.543	1.176	1.177	179.5	-0.033
0.0004	4.39	3.542	1.176	1.177	179.5	-0.034
0.0005	4.53	3.542	1.176	1.177	179.5	-0.035
0.0006	4.64	3.541	1.176	1.177	179.0	-0.036
0.0007	4.76	3.541	1.176	1.176	179.0	-0.037
0.0008	4.88	3.540	1.176	1.177	178.9	-0.038
0.0009	5.01	3.538	1.177	1.177	178.8	-0.039
0.0010	5.13	3.537	1.177	1.177	179.0	-0.040
0.0011	5.25	3.540	1.176	1.176	179.3	-0.041
0.0012	5.38	3.535	1.176	1.176	179.3	-0.042
0.0013	5.62	3.534	1.176	1.177	179.3	-0.043
0.0014	5.81	3.534	1.176	1.177	179.1	-0.044
0.0015	5.97	1.988	1.230	1.236	140.0	-0.469
0.0016	6.14	1.975	1.231	1.238	139.4	-0.488
0.0017	7.17	1.964	1.233	1.240	138.9	-0.499
0.0018	8.50	1.954	1.234	1.241	138.4	-0.513
0.0019	9.84	1.937	1.236	1.243	137.8	-0.530
0.0020	11.24	1.934	1.237	1.244	137.5	-0.541
0.0021	12.66	1.925	1.238	1.245	137.1	-0.554
0.0022	14.12	1.917	1.239	1.246	136.8	-0.567
0.0023	15.60	1.911	1.240	1.248	136.5	-0.579
0.0024	17.13	1.904	1.241	1.249	136.1	-0.591
0.0025	18.67	1.898	1.242	1.250	135.9	-0.602
0.0026	20.24	1.892	1.243	1.251	135.6	-0.614
0.0027	21.84	1.887	1.244	1.251	135.3	-0.625
0.0028	23.46	1.882	1.245	1.252	135.1	-0.635
0.0029	25.11	1.877	1.246	1.253	134.8	-0.646
0.0030	26.78	1.873	1.247	1.254	134.6	-0.656

Table S3. The calculated adsorption energies (kcal/mol), C-O bond lengths (Å), C…N/P distances (Å), CO_2 bond angles (°) and Mulliken charge transfers (e) from 2N/P-doped MoS_2 to CO_2 molecule with applied electric field of 0 au and 0.0020 au of CO_2 adsorption on 2N/P-doped MoS_2.

N-doped MoS_2			
E-field (au)		0	0.0020
Adsorption energy (kcal/mol)		5.52	25.37
Bond distance (Å)	C1-N1	3.083	1.473
	C2-N2	3.108	1.482
	C1-O1	1.176	1.258
	C1-O2	1.176	1.252
	C2-O3	1.176	1.251
	C2-O4	1.176	1.257
Bond angle (°)	O1-C1-C2	178.3	126.6
	O3-C2-O4	178.5	126.8
Electron transfer (e)	C1O1O2	-0.020	-0.444
	C2O3O4	-0.020	-0.443

P-doped MoS_2			
E-field (au)		0	0.0020
Adsorption energy (kcal/mol)		3.50	8.90
Bond distance (Å)	C1-P1	3.331	1.949
	C2-P2	3.342	1.954
	C1-O1	1.176	1.237
	C1-O2	1.176	1.237
	C2-O3	1.176	1.234
	C2-O4	1.176	1.238
Bond angle (°)	O1-C1-C2	179.5	138.8
	O3-C2-O4	179.4	138.9
Electron transfer (e)	C1O1O2	-0.027	-0.486
	C2O3O4	-0.028	-0.479

Table S4. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from N-doped MoS_2 to N_2, of N_2 adsorbed on N-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)			Bond angle (°)		Electron transfer (e)
		N1-N2	N1-N3	N2-N3	N1-N2-N3	N1-N2-S	Total
0	4.19	2.855	3.342	1.109	106.4	53.4	-0.021
0.0001	4.28	2.855	3.342	1.109	106.4	53.4	-0.022
0.0002	4.37	2.855	3.342	1.109	106.4	53.4	-0.023
0.0003	4.46	2.854	3.342	1.109	106.4	52.3	-0.024
0.0004	4.55	2.854	3.341	1.109	106.4	53.4	-0.025
0.0005	4.65	2.853	3.341	1.109	106.5	52.3	-0.026
0.0006	4.74	2.845	3.334	1.109	106.5	53.5	-0.027
0.0007	4.84	2.836	3.326	1.109	106.5	53.6	-0.029
0.0008	4.95	2.827	3.318	1.109	106.6	53.7	-0.030
0.0009	5.06	2.818	3.310	1.109	106.6	53.8	-0.032
0.0010	5.17	2.808	3.301	1.109	106.6	53.9	-0.034
0.0011	5.28	2.798	3.292	1.109	106.7	54.1	-0.035
0.0012	5.40	2.787	3.284	1.109	106.8	54.2	-0.037
0.0013	5.53	2.777	3.275	1.109	106.8	54.3	-0.039
0.0014	5.65	2.768	3.268	1.110	106.9	54.4	-0.041
0.0015	5.78	2.751	3.249	1.110	106.7	54.6	-0.044
0.0016	5.90	2.702	3.312	1.110	107.3	55.3	-0.050
0.0017	6.05	2.689	3.206	1.110	107.7	55.5	-0.053
0.0018	6.22	2.687	3.205	1.110	107.8	55.5	-0.055
0.0019	6.38	2.683	3.204	1.111	107.9	55.6	-0.057
0.0020	6.56	2.682	3.203	1.111	107.9	55.6	-0.059
0.0021	6.73	2.680	3.202	1.110	108.0	55.6	-0.061
0.0022	6.91	2.687	3.201	1.110	108.1	55.6	-0.063
0.0023	7.10	2.675	3.200	1.110	108.1	55.7	-0.066
0.0024	7.29	2.668	3.194	1.110	108.2	55.7	-0.069
0.0025	7.55	2.602	3.120	1.111	107.4	56.7	-0.078
0.0026	7.78	2.586	3.118	1.112	108.2	56.8	-0.084
0.0027	8.02	2.570	3.116	1.112	108.4	57.0	-0.090
0.0028	8.28	2.553	3.093	1.112	108.6	57.3	-0.096
0.0029	8.55	2.536	3.080	1.113	108.7	57.5	-0.102
0.0030	8.83	2.520	3.067	1.113	108.9	57.7	-0.108

Table S5. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from P-doped MoS_2 to N_2, of N_2 adsorbed on P-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)			Bond angle (°)		Electron transfer (e)
		P-N1	P-N2	N1-N2	P-N1-N2	P-N-S	Total
0	2.02	3.332	3.903	1.109	113.1	39.4	-0.010
0.0001	2.06	3.332	3.903	1.109	113.1	39.4	-0.011
0.0002	2.11	3.332	3.903	1.109	113.1	39.4	-0.046
0.0003	2.16	3.332	3.903	1.109	113.1	39.4	-0.012
0.0004	2.21	3.331	3.902	1.109	113.1	39.4	-0.012
0.0005	2.28	3.331	3.902	1.109	113.2	39.4	-0.013
0.0006	2.33	3.321	3.893	1.109	113.2	39.5	-0.014
0.0007	2.39	3.311	3.883	1.109	113.2	39.5	-0.015
0.0008	2.45	3.301	3.874	1.109	113.2	39.6	-0.016
0.0009	2.51	3.290	3.863	1.109	113.2	39.7	-0.017
0.0010	2.57	3.282	3.854	1.109	113.1	39.8	-0.011
0.0011	2.64	3.264	3.840	1.109	113.3	39.9	-0.019
0.0012	2.71	3.247	3.824	1.109	113.3	40.1	-0.021
0.0013	2.76	3.206	3.774	1.110	112.6	40.5	-0.023
0.0014	2.84	3.192	3.761	1.109	112.6	40.6	-0.024
0.0015	2.91	3.164	3.743	1.109	112.2	40.9	-0.027
0.0016	3.00	3.142	3.732	1.110	112.9	41.1	-0.029
0.0017	3.09	3.127	3.725	1.110	114.4	41.2	-0.032
0.0018	3.20	3.122	3.723	1.111	114.5	41.2	-0.033
0.0019	3.30	3.121	3.722	1.111	114.6	41.3	-0.035
0.0020	3.41	3.119	3.722	1.110	114.7	41.3	-0.037
0.0021	3.53	3.117	3.721	1.110	114.8	41.3	-0.039
0.0022	3.64	3.114	3.720	1.111	114.9	41.3	-0.041
0.0023	3.77	3.112	3.719	1.111	115.0	41.3	-0.043
0.0024	3.89	3.106	3.718	1.111	115.2	41.4	-0.046
0.0025	4.02	3.103	3.716	1.111	115.3	41.4	-0.049
0.0026	-4.18	3.063	3.690	1.112	116.1	41.7	-0.055
0.0027	4.39	2.984	3.601	1.113	115.1	42.3	-0.065
0.0028	4.59	2.943	3.568	1.114	115.6	42.7	-0.072
0.0029	4.79	2.911	3.540	1.115	115.8	42.9	-0.079
0.0030	5.02	2.878	3.511	1.115	115.9	43.2	-0.087

Table S6. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from N-doped MoS_2 to CH_4, of CH_4 adsorbed on N-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)	Bond angle (°)	Electron transfer (e)
		C-N	N-C-S	Total
0	5.33	2.968	53.3	-0.113
0.0001	5.39	2.968	53.3	-0.114
0.0002	5.44	2.967	53.3	-0.116
0.0003	5.49	2.967	53.3	-0.117
0.0004	5.53	2.967	53.3	-0.119
0.0005	5.58	2.966	53.3	-0.120
0.0006	5.62	2.950	53.5	-0.124
0.0007	5.68	2.934	53.7	-0.127
0.0008	5.73	2.919	53.9	-0.131
0.0009	5.79	2.905	54.1	-0.134
0.0010	5.86	2.891	54.3	-0.138
0.0011	5.93	2.878	54.5	-0.142
0.0012	6.01	2.865	54.6	-0.145
0.0013	6.06	2.881	54.4	-0.143
0.0014	6.04	2.775	55.8	-0.163
0.0015	6.17	2.774	55.8	-0.165
0.0016	6.30	2.773	55.8	-0.167
0.0017	6.43	2.773	55.8	-0.169
0.0018	6.56	2.772	55.8	-0.171
0.0019	6.69	2.771	55.8	-0.174
0.0020	6.81	2.770	55.8	-0.176
0.0021	6.94	2.769	55.9	-0.178
0.0022	7.07	2.768	55.9	-0.180
0.0023	7.19	2.767	55.9	-0.182
0.0024	7.31	2.766	55.9	-0.184
0.0025	7.43	2.764	55.9	-0.186
0.0026	7.71	2.702	57.0	-0.201
0.0027	7.89	2.692	57.1	-0.206
0.0028	8.07	2.683	57.3	-0.210
0.0029	8.26	2.674	57.4	-0.214
0.0030	8.45	2.665	57.5	-0.219

Table S7. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from P-doped MoS_2 to CH_4, of CH_4 adsorbed on P-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)	Bond angle (°)	Electron transfer (e)
		C-P	P-C-S	Total
0	3.20	3.299	43.8	-0.046
0.0001	3.06	3.299	43.8	-0.047
0.0002	2.93	3.299	43.8	-0.048
0.0003	2.79	3.299	43.8	-0.049
0.0004	2.64	3.299	43.8	-0.050
0.0005	2.49	3.299	43.8	-0.052
0.0006	2.35	3.284	43.9	-0.053
0.0007	2.20	3.269	44.1	-0.055
0.0008	2.06	3.255	44.2	-0.056
0.0009	1.91	3.242	44.3	-0.058
0.0010	1.76	3.230	44.4	-0.060
0.0011	1.50	3.123	45.7	-0.065
0.0012	2.53	3.123	45.7	-0.066
0.0013	2.46	3.123	45.7	-0.068
0.0014	2.39	3.122	45.7	-0.069
0.0015	2.32	3.122	45.7	-0.071
0.0016	2.25	3.121	45.7	-0.072
0.0017	2.50	3.121	45.7	-0.073
0.0018	2.13	3.120	45.7	-0.075
0.0019	2.42	3.120	45.7	-0.076
0.0020	2.04	3.120	45.7	-0.078
0.0021	2.36	3.119	45.7	-0.079
0.0022	2.17	3.119	45.7	-0.080
0.0023	2.23	3.118	45.7	-0.082
0.0024	2.20	3.117	45.7	-0.083
0.0025	2.14	3.117	45.7	-0.085
0.0026	2.20	3.116	45.7	-0.086
0.0027	1.90	3.043	46.3	-0.093
0.0028	2.06	3.033	46.4	-0.096
0.0029	2.27	3.024	46.5	-0.098
0.0030	2.31	3.014	46.6	-0.101

Table S8. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from N-doped MoS2 to H_2, of H_2 adsorbed on N-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)			Bond angle (°)		Electron transfer (e)
		H1-N	H2-N	H1-H2	N-H1-H2	S-H-N	Total
0	2.65	2.333	3.072	0.755	166.2	53.9	-0.061
0.0001	2.71	2.332	3.070	0.755	166.0	53.9	-0.061
0.0002	2.79	2.331	3.068	0.755	165.9	53.9	-0.062
0.0003	2.87	2.239	3.067	0.755	165.8	54.0	-0.063
0.0004	2.96	2.328	3.065	0.755	165.6	54.0	-0.063
0.0005	3.05	2.313	3.048	0.755	165.0	54.3	-0.064
0.0006	3.21	2.195	2.937	0.757	166.4	56.5	-0.073
0.0007	3.29	2.264	2.999	0.757	164.1	54.9	-0.069
0.0008	3.43	2.187	2.922	0.757	164.1	56.3	-0.075
0.0009	3.54	2.223	2.946	0.757	160.3	55.5	-0.073
0.0010	3.66	2.214	2.946	0.758	162.5	55.2	-0.075
0.0011	3.79	2.214	2.933	0.757	158.9	55.0	-0.076
0.0012	3.92	2.165	2.893	0.760	160.6	55.6	-0.079
0.0013	4.07	2.189	2.889	0.758	154.8	55.3	-0.079
0.0014	4.24	2.189	2.869	0.759	155.2	55.2	-0.080
0.0015	4.43	2.189	2.895	0.758	155.1	55.4	-0.081
0.0016	4.61	2.185	2.886	0.759	154.0	55.5	-0.082
0.0017	4.79	2.185	2.886	0.759	154.0	55.5	-0.082
0.0018	5.01	2.126	2.852	0.760	159.1	56.4	-0.088
0.0019	5.20	2.124	2.845	0.761	158.3	56.6	-0.087
0.0020	5.41	2.142	2.867	0.760	159.7	56.7	-0.087
0.0021	5.60	2.157	2.872	0.760	157.1	55.7	-0.088
0.0022	5.83	2.102	2.838	0.762	162.5	62.9	-0.092
0.0023	6.06	2.132	2.835	0.761	158.3	56.3	-0.091
0.0024	6.29	2.083	2.818	0.763	162.0	58.3	-0.096
0.0025	6.54	2.059	2.792	0.766	160.4	58.6	-0.097
0.0026	6.85	1.952	2.665	0.768	154.4	58.2	-0.113
0.0027	7.13	1.951	2.665	0.768	154.4	58.2	-0.114
0.0028	7.41	1.950	2.664	0.769	154.3	58.2	-0.115
0.0029	7.70	1.950	2.664	0.769	154.2	58.3	-0.116
0.0030	8.01	1.948	2.662	0.769	154.3	58.3	-0.117

Table S9. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from P-doped MoS_2 to H_2, of H_2 adsorbed on P-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)			Bond angle (°)		Electron transfer (e)
		H1-P	H2-P	H1-H2	P-H1-H2	S-H-P	Total
0	1.21	2.797	3.551	0.755	178.6	46.1	-0.038
0.0001	1.34	2.796	3.551	0.755	178.6	46.2	-0.039
0.0002	1.48	2.795	3.550	0.755	178.7	46.2	-0.039
0.0003	1.61	2.795	3.549	0.755	178.7	46.2	-0.040
0.0004	1.74	2.794	3.549	0.755	178.7	46.2	-0.041
0.0005	1.88	2.793	3.548	0.755	178.7	46.2	-0.042
0.0006	2.02	2.767	3.522	0.755	178.8	46.4	-0.043
0.0007	2.17	2.740	3.495	0.755	178.9	46.6	-0.045
0.0008	2.32	2.713	3.468	0.756	179.1	46.9	-0.047
0.0009	2.48	2.689	3.445	0.756	179.2	47.1	-0.050
0.0010	2.65	2.662	3.418	0.757	179.2	47.3	-0.052
0.0011	2.82	2.628	3.385	0.757	179.2	47.6	-0.055
0.0012	3.01	2.599	3.356	0.758	179.3	47.9	-0.057
0.0013	3.21	2.573	3.331	0.758	179.3	48.1	-0.060
0.0014	3.41	2.545	3.304	0.759	179.2	48.4	-0.062
0.0015	3.63	2.567	3.325	0.758	179.2	48.3	-0.057
0.0016	3.86	2.464	3.225	0.761	179.1	48.3	-0.070
0.0017	4.06	2.371	3.134	0.763	178.9	50.9	-0.077
0.0018	4.33	2.370	3.134	0.764	178.8	50.9	-0.078
0.0019	4.61	2.369	3.117	0.764	178.8	50.9	-0.080
0.0020	4.89	2.350	3.115	0.765	178.9	51.1	-0.084
0.0021	5.18	2.347	3.113	0.766	178.9	51.1	-0.086
0.0022	5.47	2.346	3.112	0.766	178.9	51.2	-0.086
0.0023	5.76	2.328	3.096	0.768	178.9	51.3	-0.092
0.0024	6.14	2.250	3.021	0.771	178.6	51.7	-0.099
0.0025	6.48	2.231	3.004	0.773	178.6	51.9	-0.103
0.0026	6.83	2.204	2.978	0.775	178.6	52.1	-0.108
0.0027	7.20	2.177	2.954	0.777	178.6	52.4	-0.113
0.0028	7.59	2.160	2.939	0.779	178.6	52.6	-0.117
0.0029	7.98	2.148	2.929	0.781	178.6	52.2	-0.120
0.0030	8.40	2.147	2.928	0.781	178.5	52.2	-0.125

Table S10. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from N-doped MoS_2 to NO, of NO adsorbed on N-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)		Bond angle (°)	Electron transfer (e)
		N1-N2	N2-O	N1-N2-O	Total
0	47.51	2.302	0.974	102.0	-0.030
0.0001	47.49	2.300	0.974	101.9	-0.030
0.0002	47.48	2.299	0.974	101.8	-0.030
0.0003	47.46	2.298	0.974	101.8	-0.029
0.0004	47.44	2.297	0.974	101.8	-0.028
0.0005	47.42	1.784	0.994	103.1	-0.028
0.0006	47.41	1.783	0.995	103.0	-0.027
0.0007	47.40	1.778	0.997	102.9	-0.026
0.0008	47.38	1.770	1.000	102.8	-0.026
0.0009	47.36	1.766	1.001	102.8	-0.025
0.0010	47.35	1.769	0.999	102.3	-0.023
0.0011	47.33	1.784	1.000	102.2	-0.024
0.0012	47.31	1.775	1.002	102.1	-0.023
0.0013	47.30	1.753	1.004	101.8	-0.022
0.0014	47.28	1.749	1.006	101.7	-0.022
0.0015	47.27	1.747	1.006	101.7	-0.018
0.0016	47.25	1.745	1.008	101.7	-0.018
0.0017	47.24	1.742	1.010	101.6	-0.017
0.0018	47.22	1.734	1.013	101.5	-0.017
0.0019	47.20	1.778	1.008	100.7	-0.016
0.0020	47.19	1.774	1.011	100.5	-0.014
0.0021	47.19	1.774	1.011	100.4	-0.013
0.0022	47.17	1.771	1.012	100.3	-0.013
0.0023	47.16	1.767	1.013	100.2	-0.011
0.0024	47.14	1.763	1.015	100.0	-0.010
0.0025	47.12	1.764	1.016	99.7	-0.010
0.0026	47.11	1.754	1.019	99.7	-0.009
0.0027	47.10	1.750	1.020	99.6	-0.008
0.0028	47.08	1.745	1.022	99.4	-0.006
0.0029	47.07	1.740	1.023	99.3	-0.005
0.0030	47.05	1.733	1.027	99.2	-0.004

Table S11. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from P-doped MoS_2 to NO, of NO adsorbed on P-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)		Bond angle (°)	Electron transfer (e)
		P-O	N-O	P-N-O	Total
0	38.76	1.989	1.180	114.9	0.019
0.0001	38.99	1.980	1.183	114.2	0.009
0.0002	39.21	1.973	1.184	114.1	0.002
0.0003	39.44	1.966	1.186	114.0	-0.005
0.0004	39.70	1.959	1.187	113.9	-0.012
0.0005	39.96	1.949	1.190	113.7	-0.019
0.0006	40.26	1.946	1.191	113.7	-0.026
0.0007	40.56	1.939	1.192	113.6	-0.032
0.0008	40.88	1.930	1.194	113.7	-0.040
0.0009	41.22	1.925	1.196	113.6	-0.047
0.0010	41.58	1.921	1.197	113.4	-0.052
0.0011	41.94	1.914	1.199	113.4	-0.055
0.0012	42.33	1.909	1.200	113.3	-0.066
0.0013	42.72	1.897	1.202	113.2	-0.076
0.0014	43.15	1.895	1.203	113.1	-0.080
0.0015	43.58	1.895	1.204	113.0	-0.085
0.0016	44.03	1.895	1.205	112.9	-0.089
0.0017	44.50	1.893	1.206	112.7	-0.094
0.0018	44.98	1.884	1.208	112.6	-0.102
0.0019	45.48	1.881	1.210	112.5	-0.108
0.0020	45.99	1.874	1.212	112.5	-0.115
0.0021	46.52	1.870	1.212	112.4	-0.120
0.0022	47.06	1.867	1.214	112.3	-0.126
0.0023	47.62	1.864	1.215	112.2	-0.132
0.0024	48.19	1.861	1.217	112.1	-0.138
0.0025	48.79	1.855	1.219	112.0	-0.145
0.0026	49.39	1.852	1.220	112.0	-0.150
0.0027	50.01	1.848	1.222	111.9	-0.157
0.0028	50.65	1.844	1.223	111.7	-0.163
0.0029	51.30	1.841	1.225	111.6	-0.168
0.0030	51.97	1.837	1.226	111.6	-0.174

Table S12. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from N-doped MoS_2 to NO_2, of NO_2 adsorbed on N-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)			Bond angle (°)	Electron transfer(e)
		N1-O	N2-O1	N2-O2	O1-N2-O2	Total
0	19.15	1.993	1.243	1.205	126.6	-0.025
0.0001	19.34	1.987	1.244	1.206	129.3	-0.033
0.0002	19.54	1.981	1.244	1.207	129.0	-0.042
0.0003	19.75	1.974	1.245	1.208	128.7	-0.050
0.0004	19.97	1.968	1.246	1.209	128.4	-0.058
0.0005	20.20	1.962	1.247	1.211	128.1	-0.066
0.0006	20.45	1.954	1.248	1.211	127.8	-0.073
0.0007	20.70	1.947	1.249	1.212	127.5	-0.081
0.0008	20.97	1.940	1.250	1.213	127.2	-0.089
0.0009	21.25	1.933	1.251	1.215	126.9	-0.096
0.0010	21.54	1.927	1.252	1.216	126.7	-0.104
0.0011	21.80	1.867	1.261	1.216	125.7	-0.110
0.0012	22.13	1.867	1.261	1.217	125.6	-0.117
0.0013	22.45	1.862	1.261	1.217	125.3	-0.123
0.0014	22.80	1.862	1.261	1.218	125.2	-0.129
0.0015	23.15	1.860	1.262	1.219	125.0	-0.136
0.0016	23.50	1.862	1.261	1.221	125.0	-0.143
0.0017	23.87	1.972	1.261	1.223	131.0	-0.149
0.0018	24.24	1.863	1.264	1.223	124.7	-0.155
0.0019	24.62	1.863	1.260	1.224	124.6	-0.162
0.0020	25.03	1.862	1.259	1.225	124.2	-0.167
0.0021	25.42	1.866	1.258	1.227	124.1	-0.176
0.0022	25.83	1.866	1.257	1.227	124.1	-0.183
0.0023	26.25	1.868	1.257	1.229	123.9	-0.189
0.0024	26.67	1.867	1.257	1.232	123.6	-0.196
0.0025	27.13	1.869	1.257	1.233	123.4	-0.203
0.0026	27.55	1.872	1.256	1.235	123.3	-0.210
0.0027	28.01	1.876	1.255	1.236	123.1	-0.217
0.0028	28.47	1.880	1.254	1.238	122.9	-0.224
0.0029	28.95	1.877	1.255	1.239	122.7	-0.230
0.0030	29.45	1.875	1.254	1.240	122.4	-0.235

Table S13. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from P-doped MoS_2 to NO_2, of NO_2 adsorbed on P-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)			Bond angle (°)	Electron transfer (e)
		P-O	N-O1	N-O2	O1-N-O2	Total
0	55.58	1.592	1.812	1.136	116.8	0.020
0.0001	55.86	1.592	1.814	1.136	116.8	0.013
0.0002	55.63	1.592	1.805	1.137	116.7	0.005
0.0003	55.41	1.595	1.765	1.139	116.7	-0.002
0.0004	55.21	1.598	1.785	1.140	116.6	-0.010
0.0005	55.02	1.600	1.774	1.142	116.6	-0.017
0.0006	54.84	1.602	1.762	1.144	116.5	-0.025
0.0007	54.67	1.605	1.747	1.145	116.4	-0.033
0.0008	54.54	1.608	1.736	1.147	116.3	-0.041
0.0009	54.42	1.612	1.721	1.149	116.2	-0.049
0.0010	54.32	1.615	1.705	1.151	116.2	-0.059
0.0011	54.24	1.620	1.685	1.154	116.0	-0.067
0.0012	54.18	1.626	1.662	1.157	115.9	-0.076
0.0013	54.16	1.634	1.633	1.161	115.7	-0.087
0.0014	54.14	1.660	1.551	1.172	115.5	-0.111
0.0015	54.24	1.660	1.548	1.173	115.5	-0.117
0.0016	54.34	1.661	1.546	1.174	115.4	-0.123
0.0017	54.56	1.692	1.466	1.187	115.3	-0.148
0.0018	54.79	1.701	1.445	1.192	115.3	-0.158
0.0019	55.06	1.708	1.430	1.196	115.3	-0.166
0.0020	55.36	1.714	1.418	1.199	115.3	-0.174
0.0021	55.65	1.719	1.409	1.202	115.2	-0.181
0.0022	55.98	1.724	1.400	1.205	115.3	-0.188
0.0023	56.32	1.729	1.392	1.207	115.3	-0.194
0.0024	56.67	1.732	1.386	1.209	115.2	-0.200
0.0025	57.05	1.735	1.380	1.211	115.2	-0.206
0.0026	57.42	1.739	1.375	1.213	115.1	-0.212
0.0027	57.81	1.742	1.370	1.215	115.1	-0.217
0.0028	58.22	1.744	1.365	1.217	115.1	-0.223
0.0029	58.63	1.747	1.361	1.219	115.0	-0.229
0.0030	59.08	1.748	1.358	1.221	115.0	-0.234

Table S14. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from N-doped MoS_2 to SO_2, of SO_2 adsorbed on N-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)			Bond angle (°)	Electron transfer (e)
		N-S	S-O1	S-O2	O-S-O	Total
0	16.48	2.027	1.492	1.492	116.3	-0.152
0.0001	16.82	2.027	1.493	1.493	116.2	-0.164
0.0002	17.19	2.027	1.493	1.493	116.1	-0.177
0.0003	17.59	2.027	1.494	1.494	116.0	-0.188
0.0004	18.02	2.027	1.494	1.494	115.9	-0.199
0.0005	22.03	2.006	1.492	1.492	116.0	-0.167
0.0006	23.17	2.007	1.492	1.492	115.9	-0.170
0.0007	24.33	2.007	1.493	1.492	116.0	-0.172
0.0008	25.50	2.007	1.492	1.492	116.0	-0.175
0.0009	26.69	2.006	1.492	1.492	116.1	-0.176
0.0010	27.89	2.005	1.492	1.492	116.0	-0.179
0.0011	29.09	2.006	1.492	1.492	116.1	-0.181
0.0012	30.31	2.007	1.492	1.492	116.0	-0.184
0.0013	31.54	2.007	1.492	1.492	116.1	-0.185
0.0014	32.78	2.007	1.492	1.492	116.2	-0.187
0.0015	34.04	2.009	1.492	1.492	116.1	-0.190
0.0016	35.30	2.005	1.493	1.491	116.0	-0.194
0.0017	36.58	2.008	1.492	1.491	116.2	-0.194
0.0018	37.86	2.006	1.492	1.492	116.2	-0.196
0.0019	39.16	2.007	1.492	1.492	116.3	-0.198
0.0020	40.46	2.006	1.493	1.491	116.0	-0.203
0.0021	41.79	2.005	1.492	1.492	116.1	-0.203
0.0022	43.11	2.007	1.491	1.491	116.3	-0.204
0.0023	44.45	2.008	1.491	1.491	116.3	-0.206
0.0024	45.81	1.996	1.492	1.491	116.2	-0.210
0.0025	47.17	2.007	1.491	1.491	116.4	-0.210
0.0026	48.55	2.009	1.491	1.491	116.5	-0.212
0.0027	50.03	1.998	1.492	1.492	115.9	-0.219
0.0028	51.43	1.996	1.492	1.492	115.9	-0.221
0.0029	52.83	1.996	1.492	1.492	116.1	-0.223
0.0030	54.24	1.994	1.492	1.492	116.0	-0.225

Table S15. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from P-doped MoS_2 to SO_2, of SO_2 adsorbed on P-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)			Bond angle (°)	Electron transfer (e)
		P-S	S-O1	S-O2	O-S-O	Total
0	14.22	2.398	1.494	1.494	119.8	-0.163
0.0001	14.71	2.379	1.495	1.495	119.9	-0.176
0.0002	15.19	2.377	1.496	1.496	119.7	-0.188
0.0003	15.70	2.375	1.496	1.496	119.7	-0.200
0.0004	16.24	2.373	1.497	1.497	119.6	-0.212
0.0005	16.79	2.384	1.498	1.498	119.2	-0.224
0.0006	17.40	2.370	1.499	1.499	119.3	-0.237
0.0007	18.03	2.368	1.500	1.499	119.2	-0.249
0.0008	18.68	2.366	1.501	1.500	119.0	-0.262
0.0009	19.36	2.364	1.501	1.501	118.9	-0.274
0.0010	20.05	2.369	1.502	1.502	118.7	-0.286
0.0011	20.80	2.359	1.503	1.503	118.8	-0.299
0.0012	21.56	2.358	1.504	1.503	118.6	-0.311
0.0013	22.35	2.355	1.505	1.504	118.5	-0.324
0.0014	23.17	2.354	1.506	1.505	118.3	-0.337
0.0015	24.02	2.354	1.506	1.506	118.1	-0.349
0.0016	24.90	2.352	1.508	1.507	118.0	-0.363
0.0017	25.81	2.350	1.509	1.508	117.9	-0.375
0.0018	26.73	2.349	1.510	1.509	117.8	-0.388
0.0019	27.69	2.348	1.511	1.510	117.6	-0.400
0.0020	28.69	2.336	1.512	1.511	117.5	-0.413
0.0021	29.72	2.329	1.512	1.512	117.5	-0.427
0.0022	30.77	2.326	1.513	1.513	117.4	-0.439
0.0023	31.85	2.323	1.514	1.514	117.3	-0.452
0.0024	32.96	2.319	1.515	1.514	117.3	-0.465
0.0025	34.10	2.316	1.516	1.515	117.2	-0.477
0.0026	35.27	2.312	1.517	1.516	117.1	-0.490
0.0027	36.47	2.308	1.518	1.517	117.0	-0.503
0.0028	37.69	2.305	1.519	1.518	117.0	-0.516
0.0029	38.93	2.302	1.520	1.519	116.9	-0.529
0.0030	40.21	2.298	1.521	1.520	116.8	-0.541

Table S16. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from N-doped MoS_2 to H_2O, of H_2O adsorbed on N-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)			Bond angle (°)	Electron transfer (e)
		N-H	H-O1	H-O2	H-O-H	Total
0	7.50	2.30	0.97	0.97	101.96	-0.118
0.0001	7.81	2.30	0.97	0.97	101.86	-0.121
0.0002	8.13	2.30	0.97	0.97	101.83	-0.123
0.0003	8.44	2.30	0.97	0.97	101.79	-0.125
0.0004	8.76	2.30	0.97	0.97	101.76	-0.126
0.0005	10.22	1.78	0.99	0.97	103.05	-0.157
0.0006	10.45	1.78	1.00	0.97	103.00	-0.160
0.0007	10.69	1.78	1.00	0.97	102.94	-0.162
0.0008	10.94	1.77	1.00	0.97	102.85	-0.166
0.0009	11.19	1.77	1.00	0.97	102.82	-0.176
0.0010	11.62	1.77	1.00	0.97	102.31	-0.180
0.0011	11.92	1.78	1.00	0.97	102.16	-0.184
0.0012	12.25	1.78	1.00	0.97	102.05	-0.188
0.0013	12.58	1.75	1.00	0.97	101.79	-0.196
0.0014	12.94	1.75	1.01	0.97	101.71	-0.199
0.0015	13.31	1.75	1.01	0.97	101.70	-0.201
0.0016	13.69	1.75	1.01	0.97	101.65	-0.204
0.0017	14.08	1.74	1.01	0.97	101.61	-0.207
0.0018	14.48	1.73	1.01	0.97	101.47	-0.211
0.0019	15.06	1.78	1.01	0.98	100.66	-0.224
0.0020	15.49	1.77	1.01	0.98	100.54	-0.227
0.0021	16.04	1.77	1.01	0.98	100.39	-0.233
0.0022	16.57	1.77	1.01	0.98	100.27	-0.238
0.0023	17.11	1.77	1.01	0.98	100.18	-0.242
0.0024	17.66	1.76	1.02	0.98	100.02	-0.247
0.0025	18.22	1.76	1.02	0.98	99.72	-0.252
0.0026	18.84	1.75	1.02	0.98	99.72	-0.257
0.0027	19.45	1.75	1.02	0.98	99.59	-0.262
0.0028	20.08	1.75	1.02	0.98	99.45	-0.267
0.0029	20.74	1.74	1.02	0.98	99.32	-0.272
0.0030	21.40	1.73	1.03	0.98	99.16	-0.275

Table S17. The important information, such as adsorption energies (kcal/mol), bond distances (Å), bond angles (°) and electron transfers (e) from P-doped MoS_2 to H_2O, of H_2O adsorbed on P-doped MoS_2 with different electric fields.

E-field (au)	Adsorption energy (kcal/mol)	Bond distance (Å)			Bond angle (°)	Electron transfer (e)
		P-H	H-O1	H-O2	H-O-H	Total
0	3.87	2.427	0.978	0.971	103.7	-0.099
0.0001	4.19	2.438	0.978	0.972	103.4	-0.095
0.0002	4.44	2.368	0.981	0.972	103.5	-0.105
0.0003	4.72	2.318	0.982	0.972	103.5	-0.114
0.0004	5.04	2.316	0.982	0.972	103.5	-0.116
0.0005	5.36	2.314	0.982	0.972	103.6	-0.119
0.0006	5.69	2.312	0.983	0.972	103.6	-0.120
0.0007	6.03	2.295	0.985	0.972	103.6	-0.124
0.0008	6.44	2.239	0.986	0.972	103.7	-0.132
0.0009	6.83	2.218	0.988	0.972	103.8	-0.136
0.0010	7.19	2.214	0.988	0.972	103.6	-0.140
0.0011	7.63	2.184	0.990	0.972	103.8	-0.145
0.0012	8.05	2.169	0.992	0.972	103.9	-0.150
0.0013	8.49	2.154	0.993	0.972	103.9	-0.154
0.0014	8.94	2.140	0.994	0.972	103.9	-0.158
0.0015	9.35	2.132	0.994	0.972	103.6	-0.163
0.0016	10.54	2.131	0.994	0.972	103.4	-0.162
0.0017	11.06	2.117	0.996	0.972	103.4	-0.167
0.0018	11.59	2.103	0.997	0.972	103.4	-0.171
0.0019	12.13	2.090	0.999	0.972	103.4	-0.176
0.0020	12.73	2.070	1.003	0.972	103.4	-0.181
0.0021	13.26	2.061	1.003	0.972	103.4	-0.185
0.0022	13.84	2.042	1.007	0.972	103.5	-0.191
0.0023	14.44	2.020	1.008	0.972	103.4	-0.197
0.0024	15.05	1.998	1.011	0.972	103.4	-0.203
0.0025	15.68	1.990	1.014	0.972	103.5	-0.209
0.0026	16.35	1.986	1.015	0.972	103.6	-0.212
0.0027	17.04	1.966	1.019	0.972	103.5	-0.219
0.0028	17.74	1.953	1.021	0.972	103.5	-0.225
0.0029	18.45	1.942	1.022	0.972	103.6	-0.230
0.0030	19.17	1.934	1.026	0.972	103.7	-0.236