Supporting Information

Achieving Tunable Adsorption Selectivity and Sensitivity of Boridenes for Gas Detection with Surface O-termination Engineering

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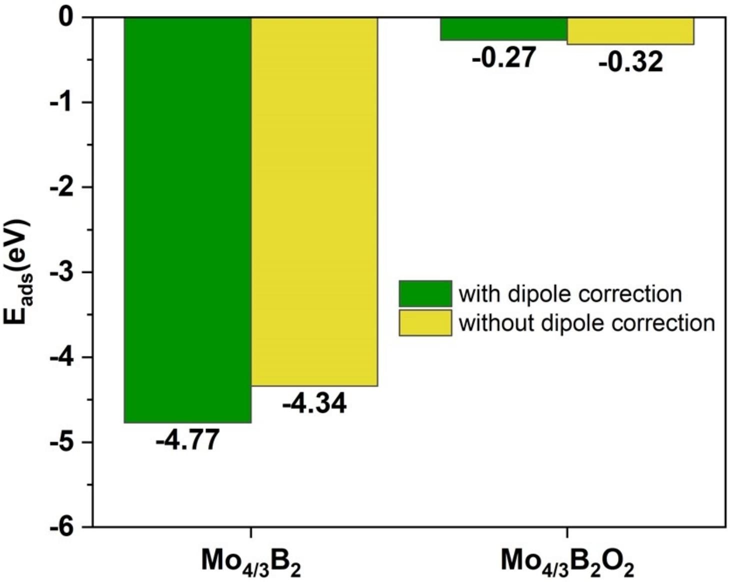

Fig. S1 Adsorption energies of NO on $Mo_{4/3}B_2$ and $Mo_{4/3}B_2O_2$ with and without dipole correction.

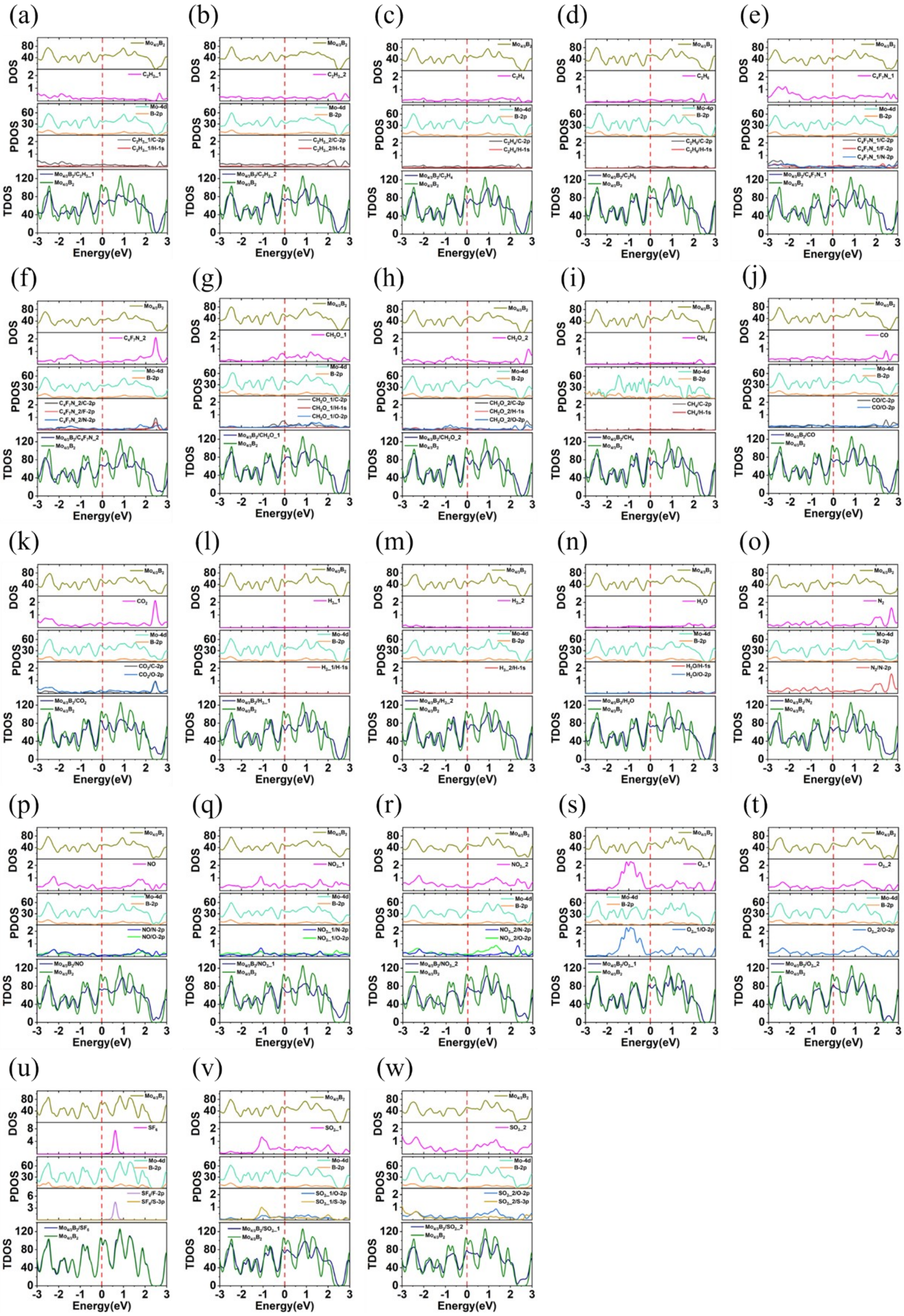

Fig. S2 The calculated partial density of states (PDOS) and total density of states (TDOS) for the stable adsorption structures of the bare $Mo_{4/3}B_2$ monolayer: (a): C_2H_2_1; (b): C_2H_2_2; (c): C_2H_4; (d): C_2H_6; (e): C_4F_7N_1; (f): C_4F_7N_2; (g): CH_2O_1; (h): CH_2O_2; (i): CH_4; (j): CO; (k): CO_2; (l): H_2_1; (m): H_2_2; (n): H_2O; (o): N_2; (p): NO; (q): NO_2_1; (r): NO_2_2; (s): O_2_1; (t): O_2_2; (u): SF_6; (v): SO_2_1; (w): SO_2_2.

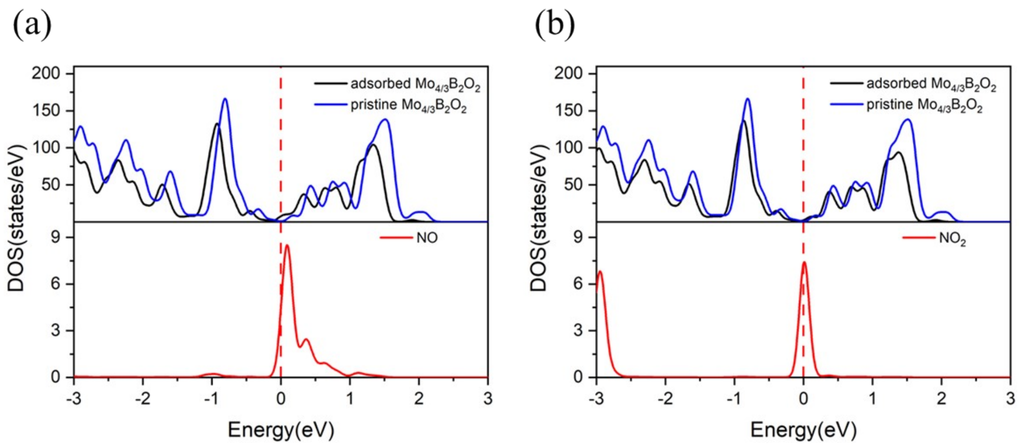

Fig. S3 TDOS of the $Mo_{4/3}B_2O_2$ substrate with and without the gas adsorbates and the gas molecule along: (a): NO; (b): NO_2.

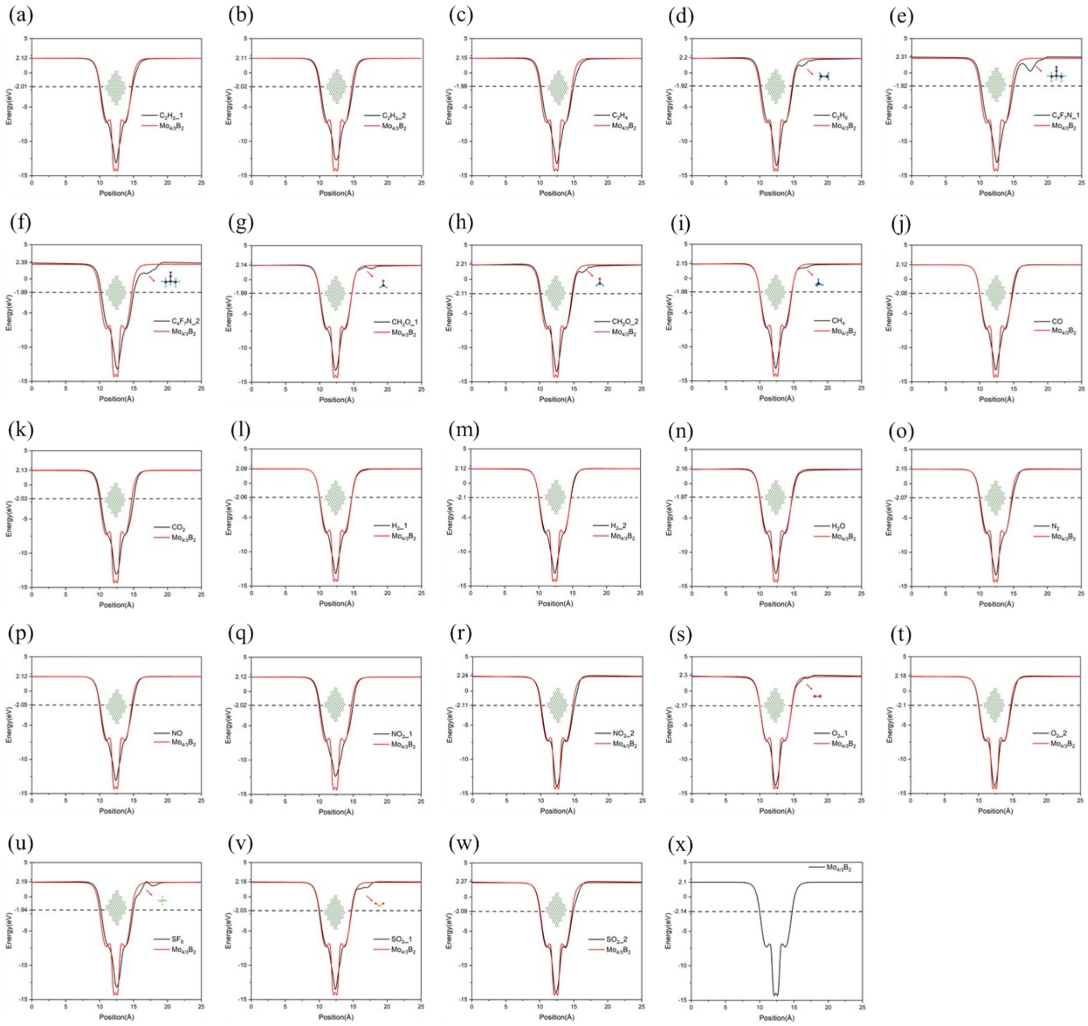

Fig. S4 Electrostatic potential profiles for the stable gas adsorption structures of $Mo_{4/3}B_2$: (a): C_2H_2_1; (b): C_2H_2_2; (c): C_2H_4; (d): C_2H_6; (e): C_4F_7N_1; (f): C_4F_7N_2; (g): CH_2O_1; (h): CH_2O_2; (i): CH_4; (j): CO; (k): CO_2; (l): H_2_1; (m): H_2_2; (n): H_2O; (o): N_2; (p): NO; (q): NO_2_1; (r): NO_2_2; (s): O_2_1; (t): O_2_2; (u): SF_6; (v): SO_2_1; (w): SO_2_2, (x) bare $Mo_{4/3}B_2$.

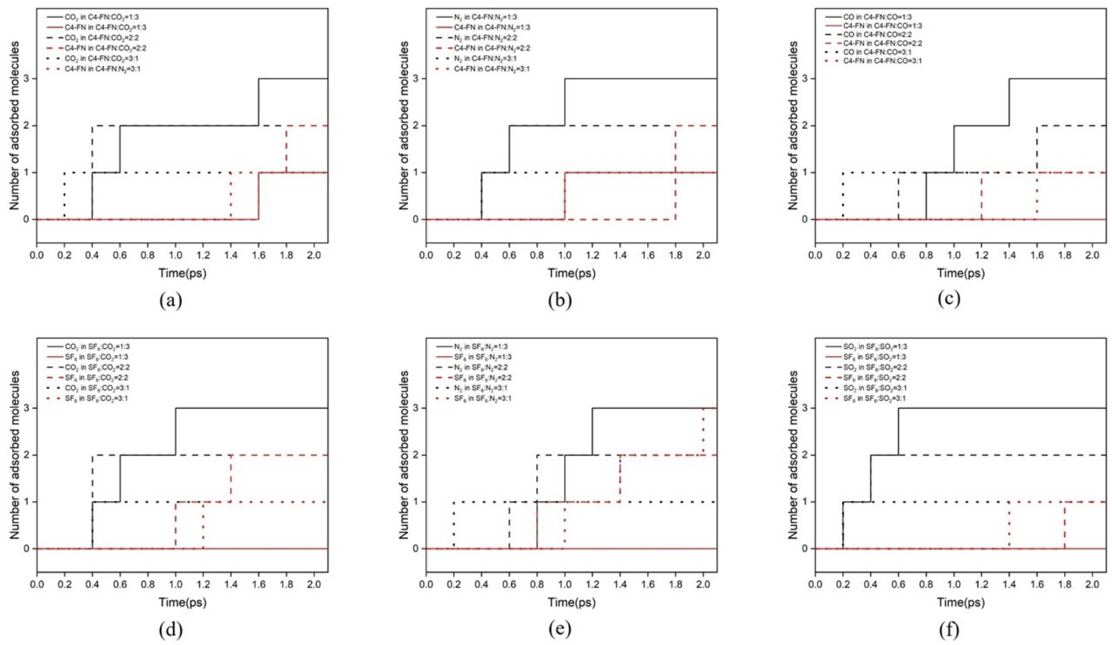

Fig. S5 Tracking the adsorbed molecules in FPMD simulations at 300 K for insulating gases: (a): CO_2/C_4F_7N; (b): N_2/C_4F_7N; (c): CO/C_4F_7N; (d): CO_2/SF_6; (e): N_2/SF_6; (f): SO_2/SF_6.

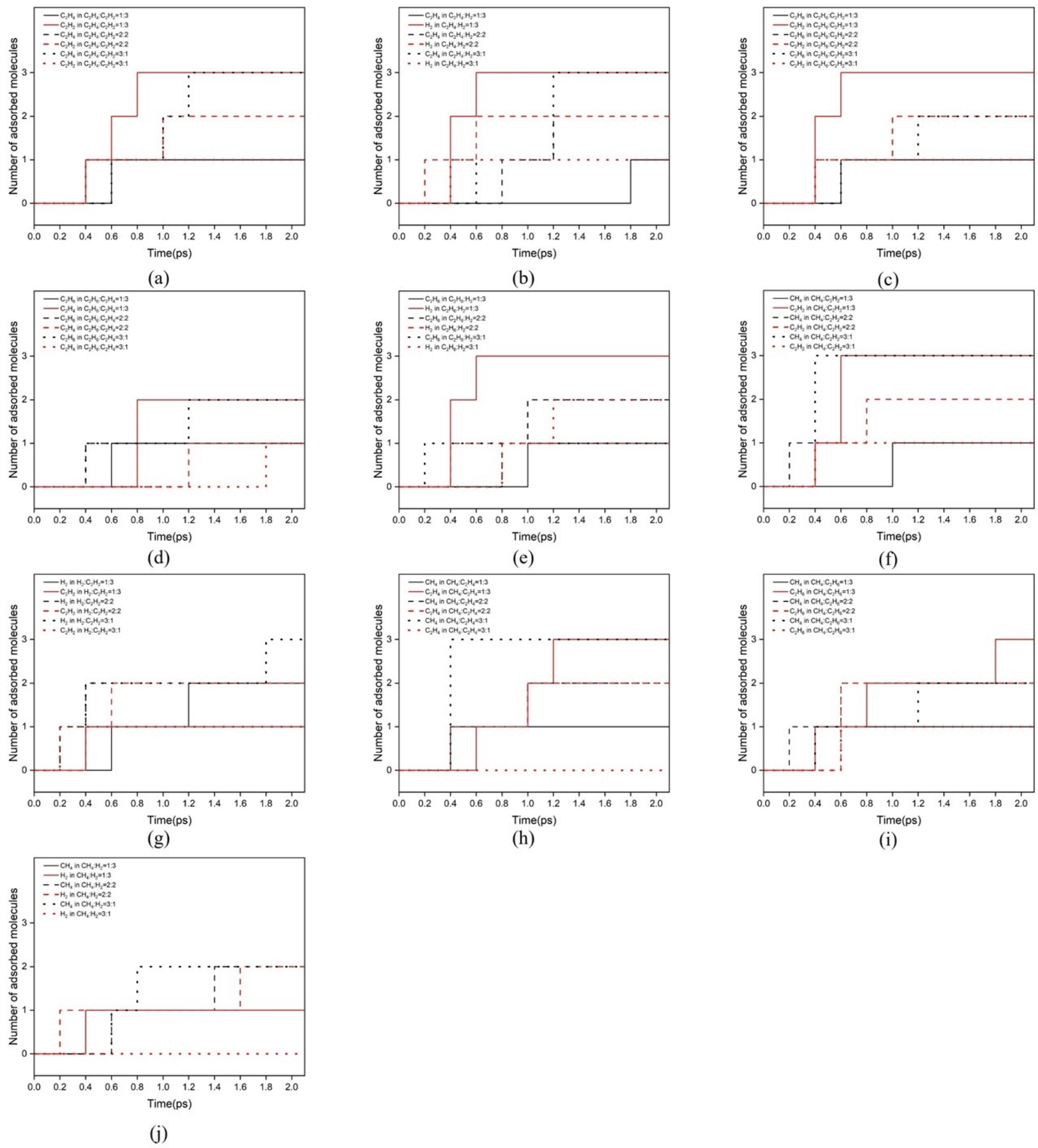

Fig. S6 Tracking the adsorbed molecules for characteristic decomposition gases of insulating oils from FPMD simulations at 300 K: (a): C_2H_4/C_2H_2; (b): C_2H_4/H_2; (c): C_2H_6/C_2H_2; (d): C_2H_6/C_2H_4; (e): C_2H_6/H_2; (f): CH_4/C_2H_2; (g): H_2/C_2H_2; (h): CH_4/C_2H_4; (i): CH_4/C_2H_6; (j): CH_4/H_2.

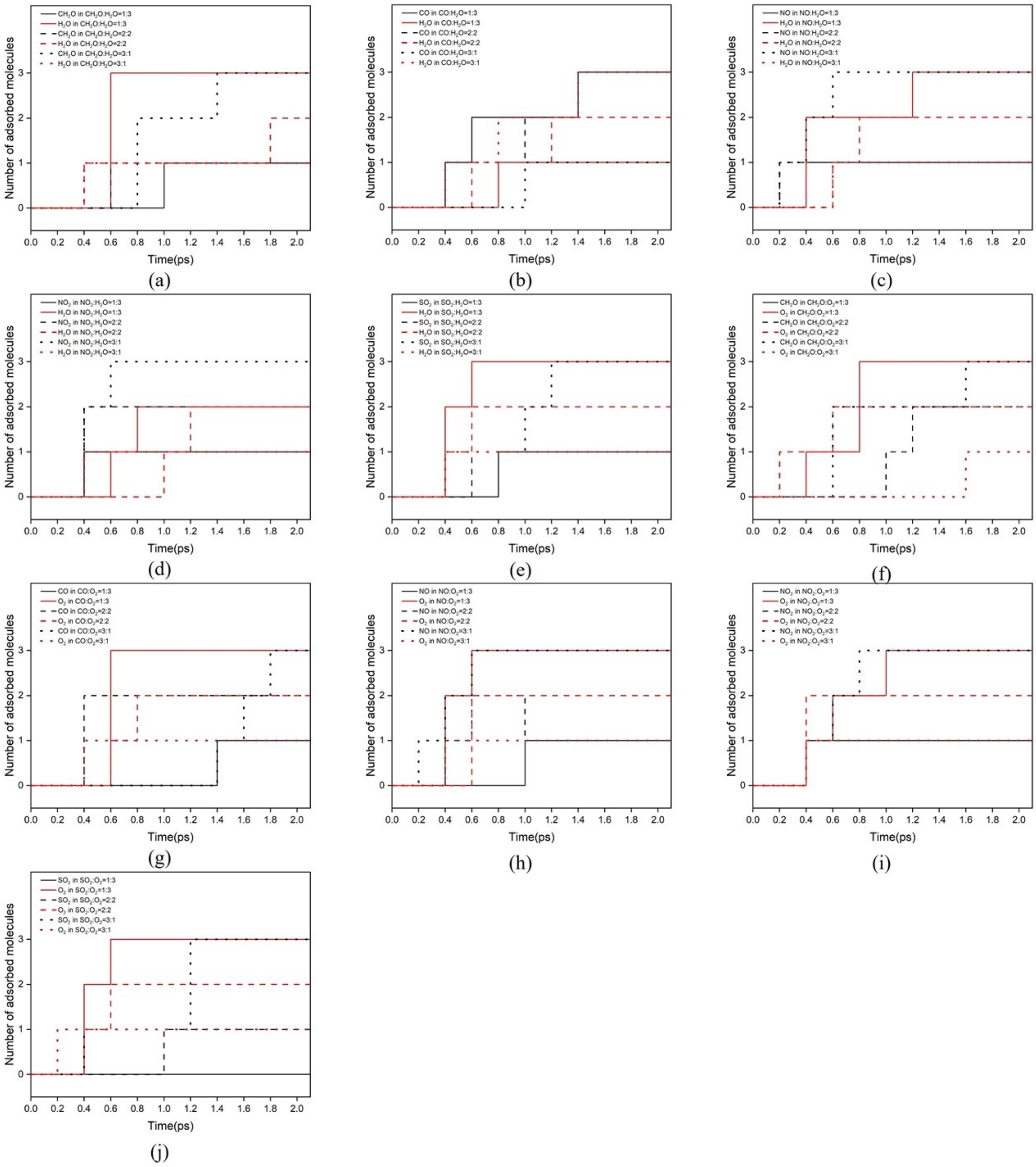

Fig. S7 Tracking the adsorbed molecules for pollutant gases from FPMD simulations at 300 K: (a): CH_2O/H_2O; (b): CO/H_2O; (c): NO/H_2O; (d): NO_2/H_2O; (e): SO_2/H_2O; (f): CH_2O/O_2; (g): CO/O_2; (h): NO/O_2; (i): NO_2/O_2; (j): SO_2/O_2.

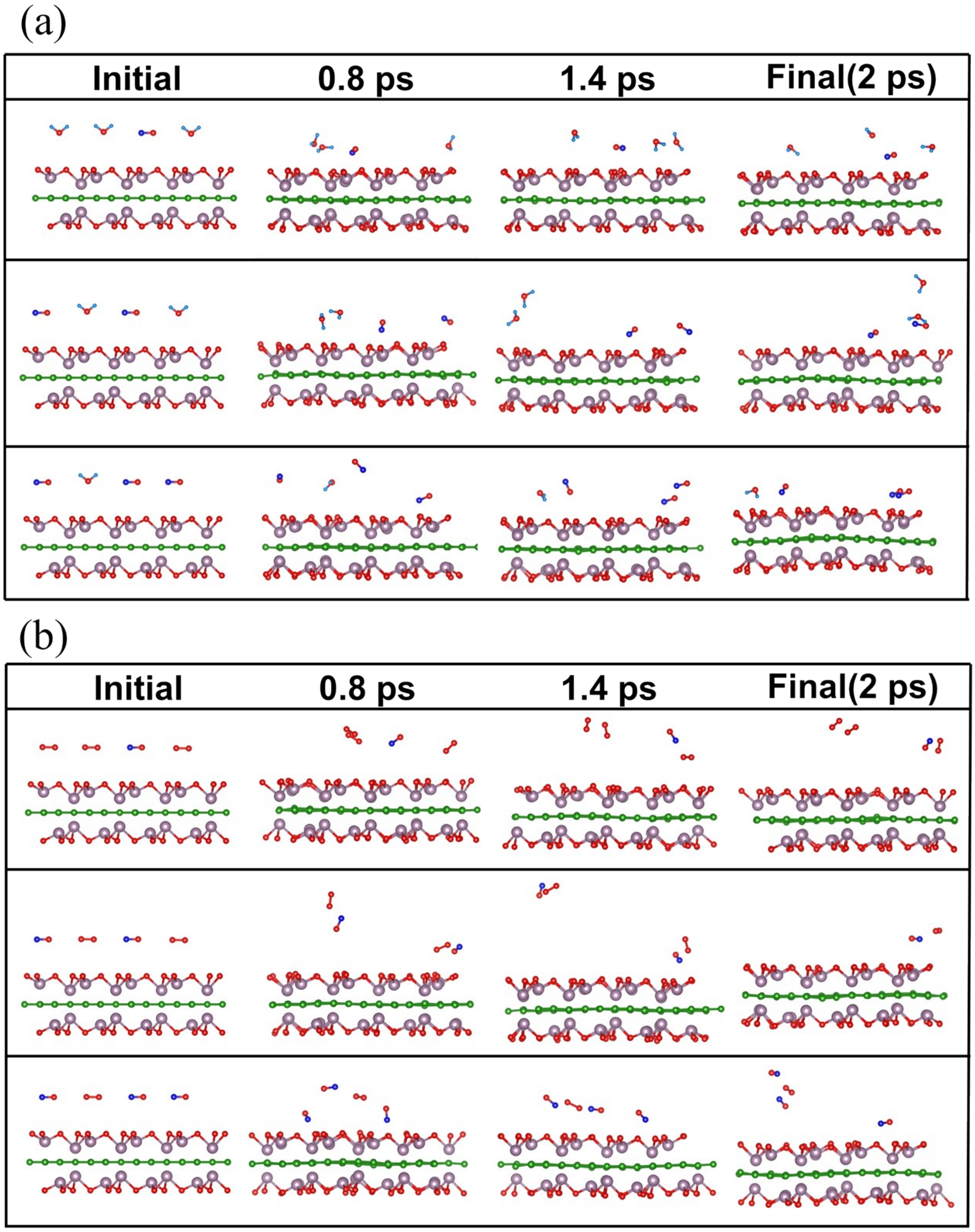

Fig. S8 Molecular dynamics sampling of NO adsorption configurations on $Mo_{4/3}B_2O_2$ in gas mixtures with different molecular ratios (1:3, 1:1 and 3:1) at 300 K and different times: (a):NO-H_2O; (b): NO-O_2.

Table. S1 Average DOS values or band gaps of $Mo_{4/3}B_2$ or $Mo_{4/3}B_2O_2$ before and after adsorption of various gas species.

Gas species	$Mo_{4/3}B_2$(average DOS: states/eV.cell)	$Mo_{4/3}B_2O_2$(band gap: eV)
substrate(before adsorption)	98.72	0.324
C_2H_2(_1)	65.74	0.333
C_2H_2_2	71.62	
C_2H_4	68.65	0.324
C_2H_6	78.58	0.333
C_4F_7N(_1)	67.75	0.324
C_4F_7N_2	61.07	
CH_2O(_1)	79.31	0.333
CH_2O_2	74.81	
CH_4	70.06	0.333
CO	70.3	0.333
CO_2	78.62	0.333
H_2(_1)	65.31	0.333
H_2_2	68.41	
H_2O	72.37	0.333
N_2	64.22	0.333
NO	71.55	0
NO_2(_1)	70.67	0.09
NO_2_2	77.8	
O_2(_1)	78.55	0.333
O_2_2	82.38	
SF_6	96.7	0.333
SO_2(_1)	72.92	0.333
SO_2_2	77.44	

Table. S2 Gas sensing-properties of $Mo_{4/3}B_2$ and $Mo_{4/3}B_2O_2$.

Molecules	$Mo_{4/3}B_2$				$Mo_{4/3}B_2O_2$			
	E_{ads} (eV)	△q (e)	S (%)	τ (s)	E_{ads} (eV)	△q (e)	S (%)	τ (s)
C_2H_2(_1)	-4.42	-0.79	33.41	1.36×10^{62}	0.037	0.04	2.78	2.4×10^{-13}
C_2H_2_2	-5.45	-1.55	27.45	2.56×10^{79}				
C_2H_4	-3.23	-0.76	30.46	1.49×10^{42}	-0.028	0.05	0	2.95×10^{-12}
C_2H_6	-1.2	-0.09	20.4	1.34×10^{8}	-0.046	0.01	2.78	5.91×10^{-12}
C_4F_7N(_1)	-1.89	-2.23	38.14	5.01×10^{19}	-0.078	0	0	2.03×10^{-11}
C_4F_7N_2	-7.84	-1.39	31.37	3.12×10^{119}				
CH_2O(_1)	-3.54	-0.29	19.66	2.36×10^{47}	0.052	0.07	2.78	1.34×10^{-13}
CH_2O_2	-4.86	-1.66	24.22	3.26×10^{69}				
CH_4	-0.89	-0.02	29.03	8.46×10^{2}	0.073	0.01	2.78	5.97×10^{-14}
CO	-2.79	-0.96	28.79	6.23×10^{34}	0.122	0.01	2.78	8.99×10^{-15}
CO_2	-7.41	-1.31	20.36	1.91×10^{112}	0.107	0	2.78	1.6×10^{-14}
H_2(_1)	-0.41	-0.04	33.85	7.53×10^{-6}	0.155	0.01	2.78	2.51×10^{-15}
H_2_2	-2.75	-0.88	30.7	1.33×10^{34}				
H_2O	-1.74	-0.11	26.69	1.53×10^{17}	0.076	0.02	2.78	5.31×10^{-14}
N_2	-1.11	-1.11	34.95	4.14×10^{6}	0.086	0	2.78	3.61×10^{-14}
NO	-4.77	-1.1	27.52	1.01×10^{68}	-0.27	0.38	100	3.38×10^{-8}
NO_2(_1)	-10.14	-2.76	28.41	1.17×10^{158}	0.059	0.09	72.22	1.02×10^{-13}
NO_2_2	-13.67	-1.43	21.18	1.89×10^{217}				
O_2(_1)	-3.81	-0.72	20.43	7.98×10^{51}	0.175	0.06	2.78	1.16×10^{-15}
O_2_2	-10.82	-1.82	16.55	2.98×10^{169}				
SF_6	1.33	-0.05	2.04	4.93×10^{-35}	0.039	-0.01	2.78	2.22×10^{-13}
SO_2(_1)	-5.43	-0.85	26.13	1.18×10^{79}	0.021	0.01	2.78	4.44×10^{-13}
SO_2_2	-10.38	-2.5	21.55	1.24×10^{162}				

Table. S3 Gas sensing-properties of $Mo_{4/3}B_2O_{2/3}$ and $Mo_{4/3}B_2O_{4/3}$.

Molecules	$Mo_{4/3}B_2O_{2/3}$				$Mo_{4/3}B_2O_{4/3}$			
	E_{ads} (eV)	$\triangle$q (e)	S (%)	τ (s)	E_{ads} (eV)	$\triangle$q (e)	S (%)	τ (s)
C_2H_2	-0.986	-0.51	11.3	3.45×10^{4}	-0.607	0.13	8.74	1.52×10^{-2}
C_2H_4	-0.991	-0.35	11.87	4.18×10^{4}	-0.55	0.14	34.05	1.68×10^{-3}
C_2H_6	0.149	-0.01	9.28	3.17×10^{-15}	-0.353	0.06	37.71	8.33×10^{-7}
C_4F_7N	-0.035	-0.33	9.42	3.86×10^{-12}	-0.651	0.03	35.74	8.29×10^{-2}
CH_2O	-0.665	-0.22	17.59	1.42×10^{-1}	-0.848	0.08	38.37	1.67×10^{2}
CH_4	0.3	0.04	8.96	9.3×10^{-18}	-0.262	0.03	33.44	2.48×10^{-8}
CO	-0.787	-0.34	13.57	15.8	-0.447	-0.04	37.86	3.14×10^{-5}
CO_2	0.002	-0.01	10.99	9.26×10^{-13}	-0.467	0.01	37.55	6.8×10^{-5}
H_2(_1)	0.443	-0.01	0.79	3.71×10^{-20}	-0.189	0.03	42.51	1.48×10^{-9}
H_2_2	-1.018	-0.66	18.89	1.19×10^{5}				
H_2O	-0.932	0.1	9.08	4.28×10^{3}	-1.163	0.11	43.27	3.21×10^{7}
N_2	-0.31	-0.22	18.87	1.58×10^{-7}	-0.382	-0.01	33.12	2.55×10^{-6}
NO	-1.594	-0.89	8.02	5.43×10^{14}	-1.006	-0.26	23.14	7.46×10^{4}
NO_2	-3.212	-1.4	11.28	7.45×10^{41}	-1.213	-0.45	8.87	2.21×10^{8}
O_2(_1)	-2.795	-0.71	14.55	7.55×10^{34}	-1.326	-0.52	0.78	1.74×10^{10}
O_2_2	-7.992	-1.68	26.99	1.1×10^{122}				
SF_6	0.411	-0.01	0.03	1.28×10^{-19}	-0.282	-0.02	30.26	5.37×10^{-8}
SO_2	-1.847	-0.81	9.76	9.51×10^{18}	-0.647	-0.04	29.38	7.11×10^{-2}