Supporting Information

Ti_3C_2 MXene Based Sensors with High Selectivity for NH_3 Detection at Room-temperature

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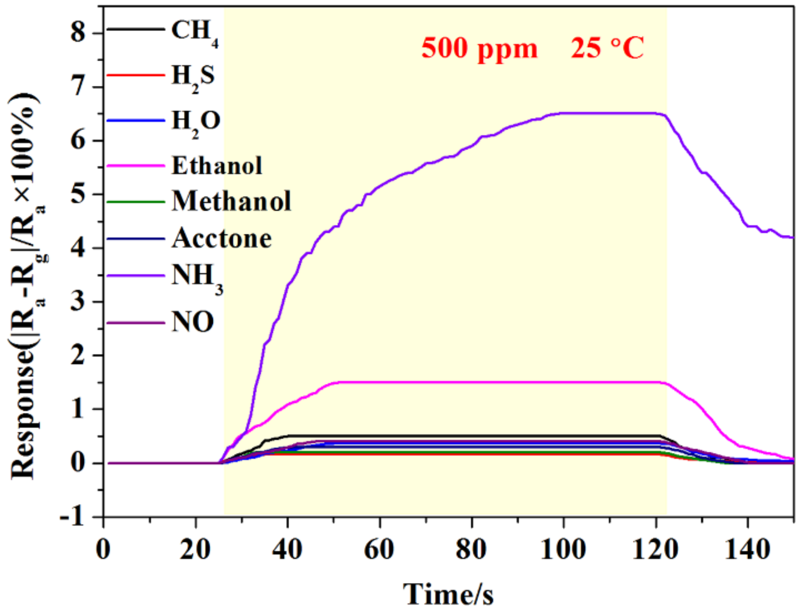


Figure S1. Real-time gas response properties of Ti_3C_2 sensors at room temperature.

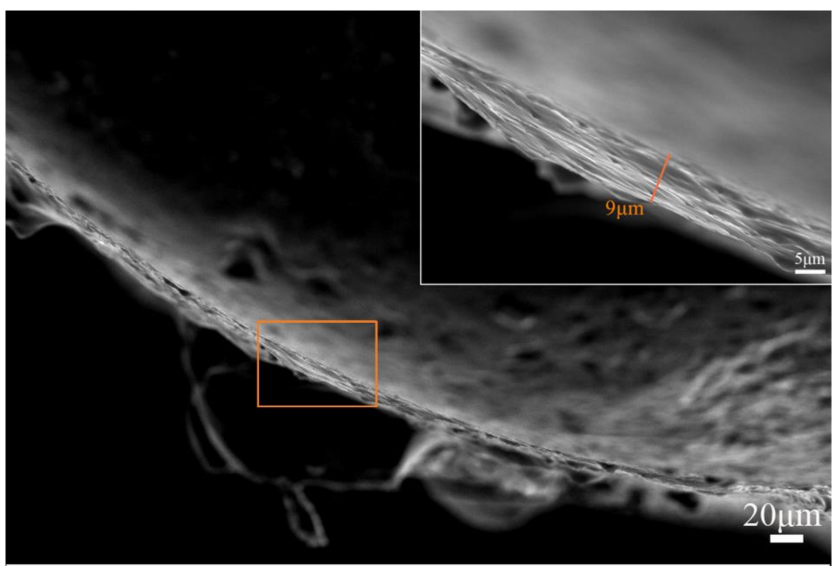


Figure S2. SEM image of single-layer SL-Ti_3C_2 on the ceramic tube.

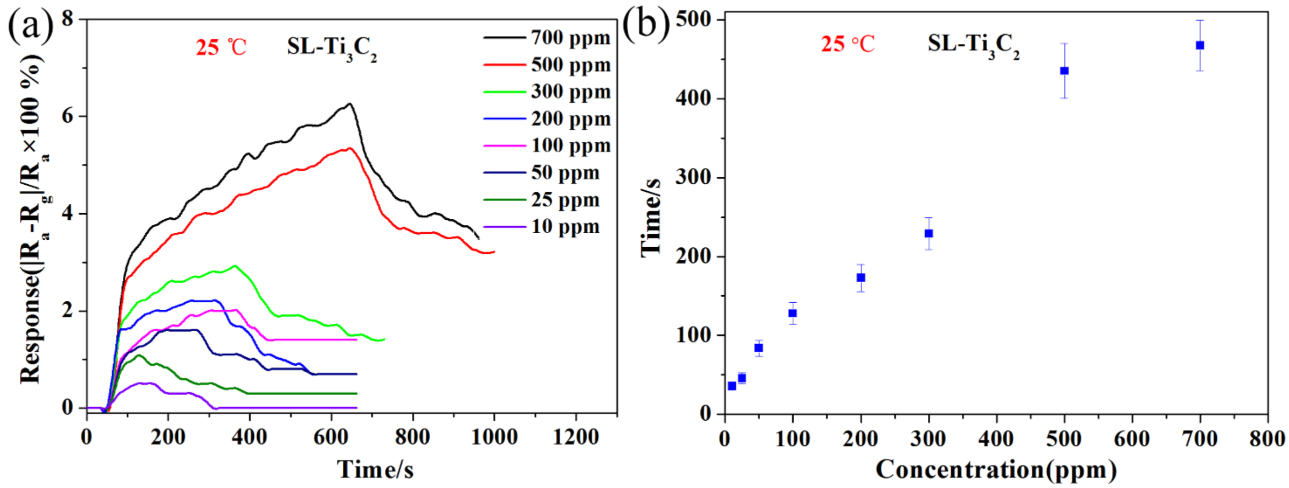


Figure S3. (a) Response/recovery curves and (b) Response time of ammonia with different concentrations for Ti_3C_2 sensors at room temperature.

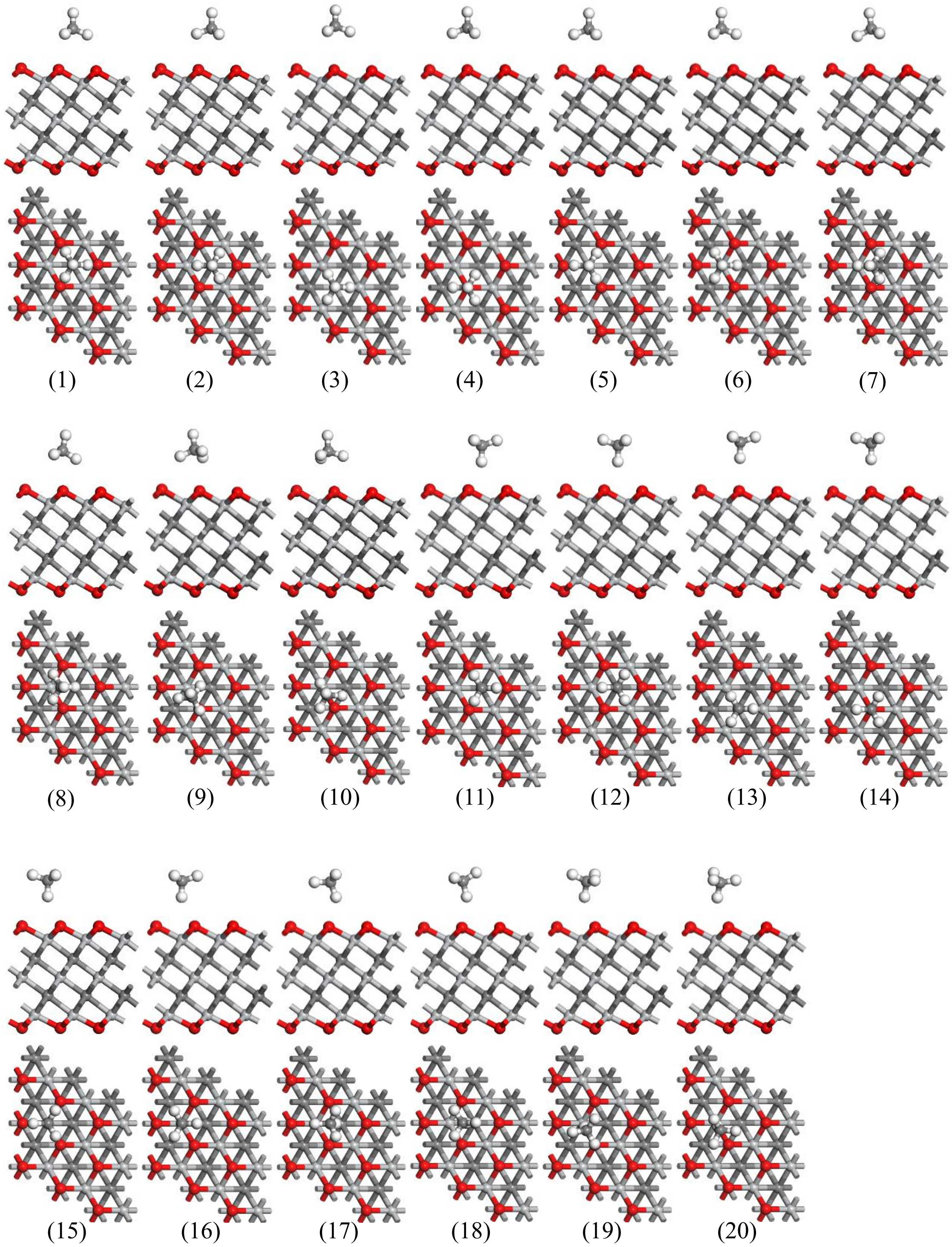
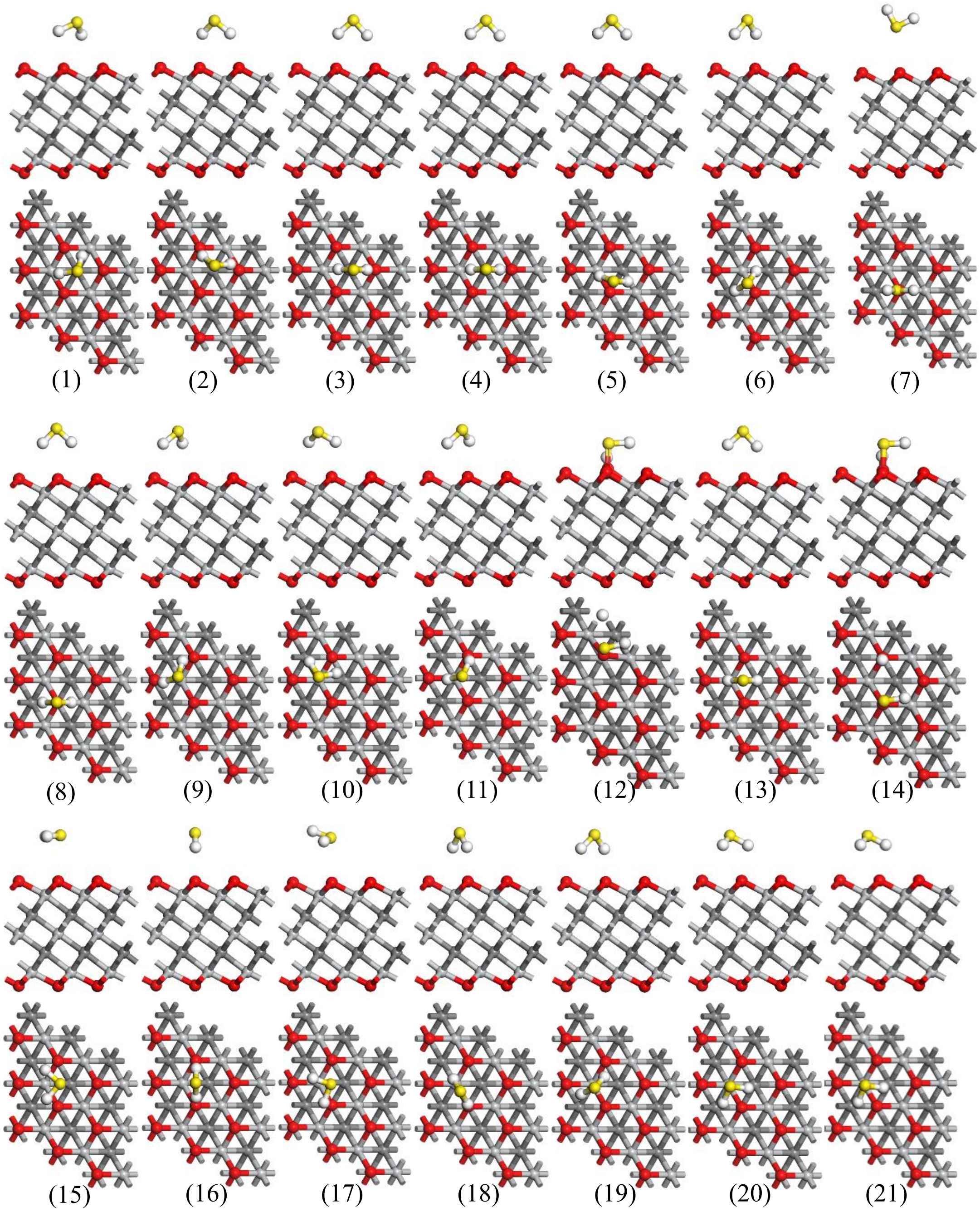


Figure S4. Different adsorption configurations of CH_4 molecules on $Ti_3C_2O_2$ surfaces.



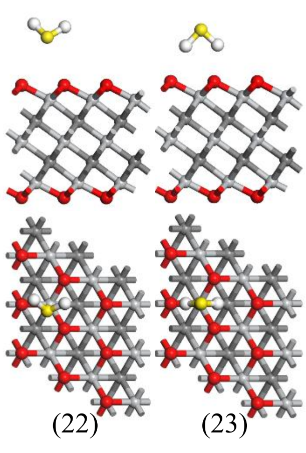


Figure S5. Different adsorption configurations of H_2S molecules on $Ti_3C_2O_2$ surfaces.

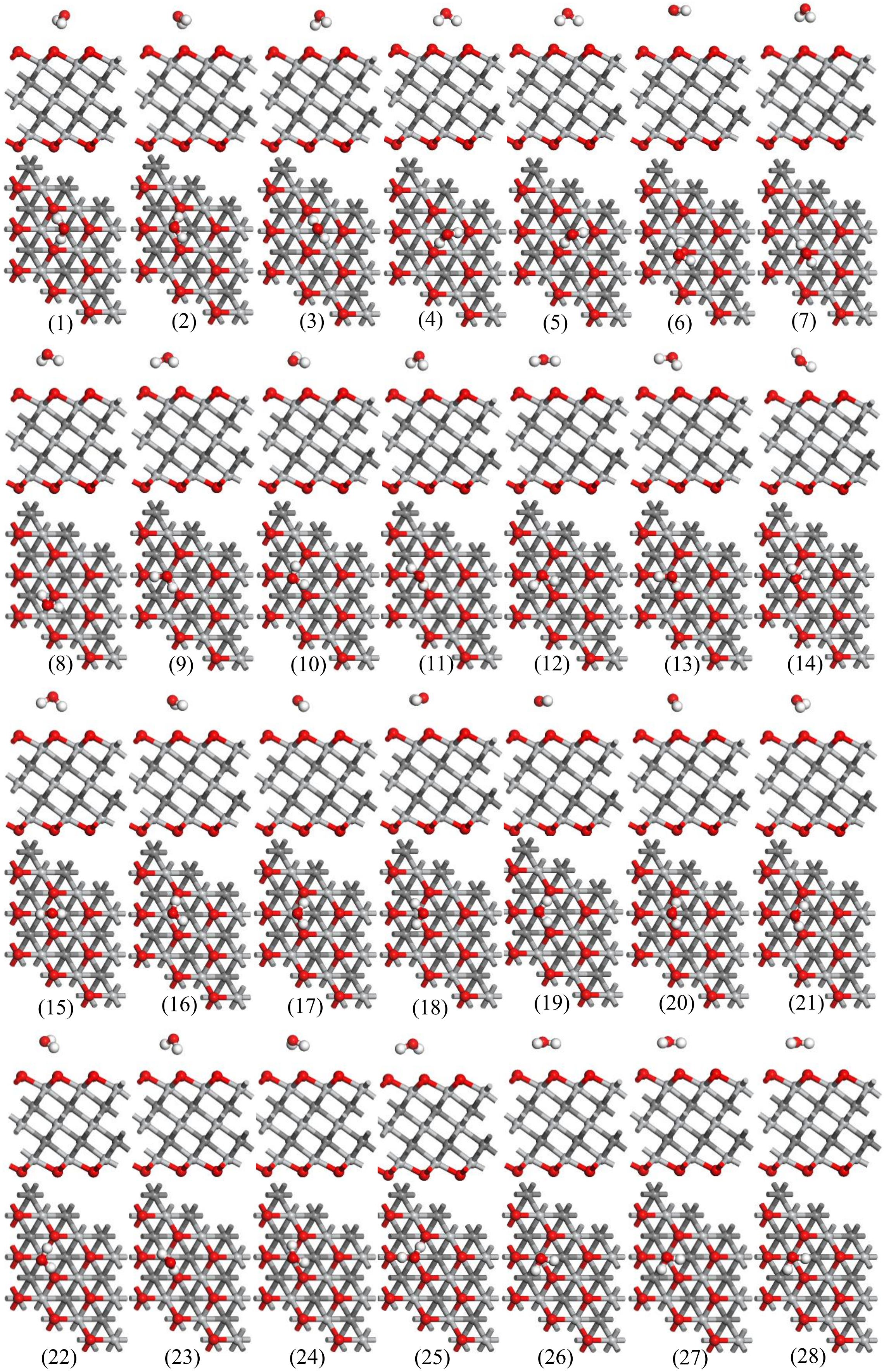


Figure S6. Different adsorption configurations of H_2O molecules on $Ti_3C_2O_2$ surfaces.

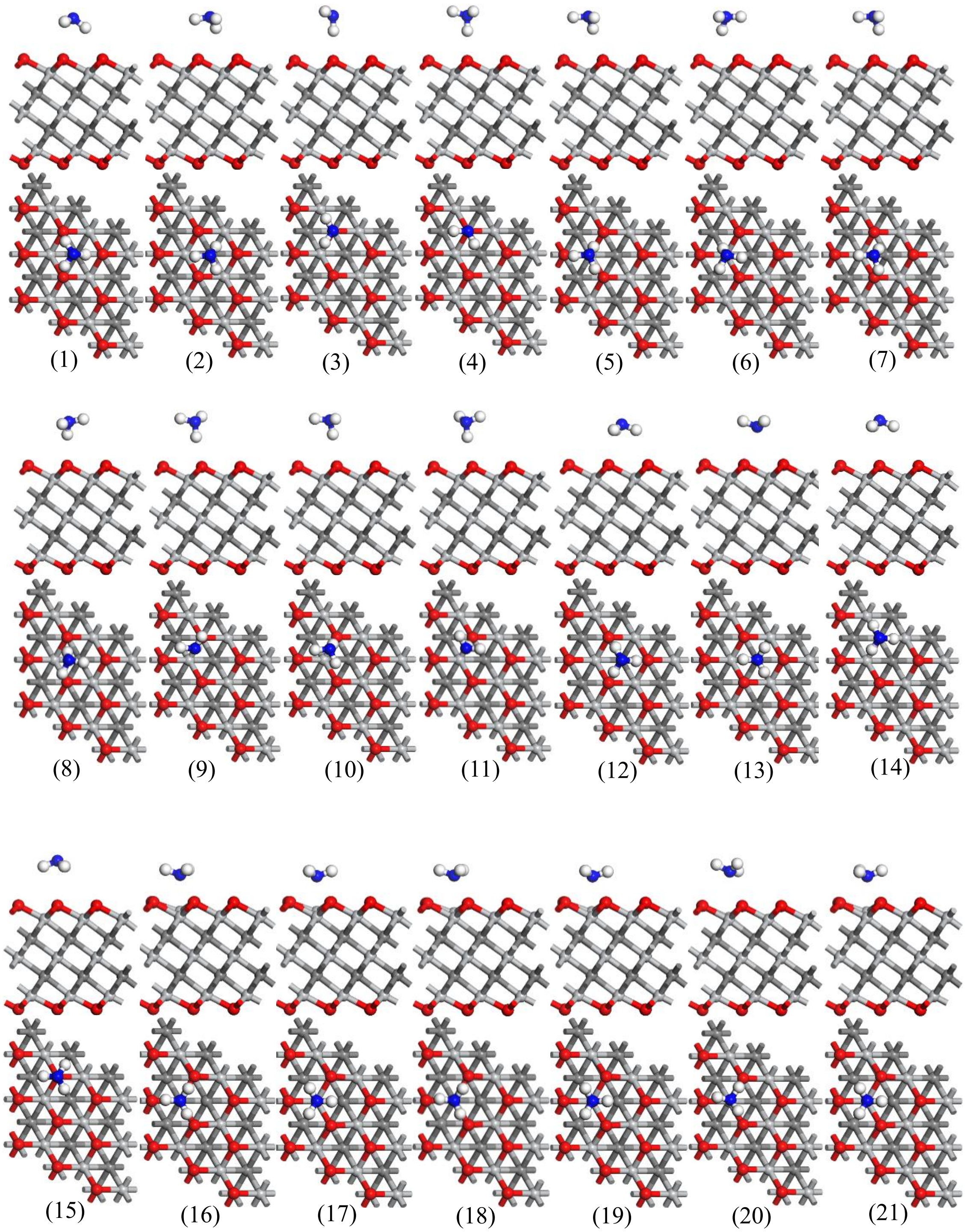


Figure S7. Different adsorption configurations of NH_3 molecules on $Ti_3C_2O_2$ surfaces.

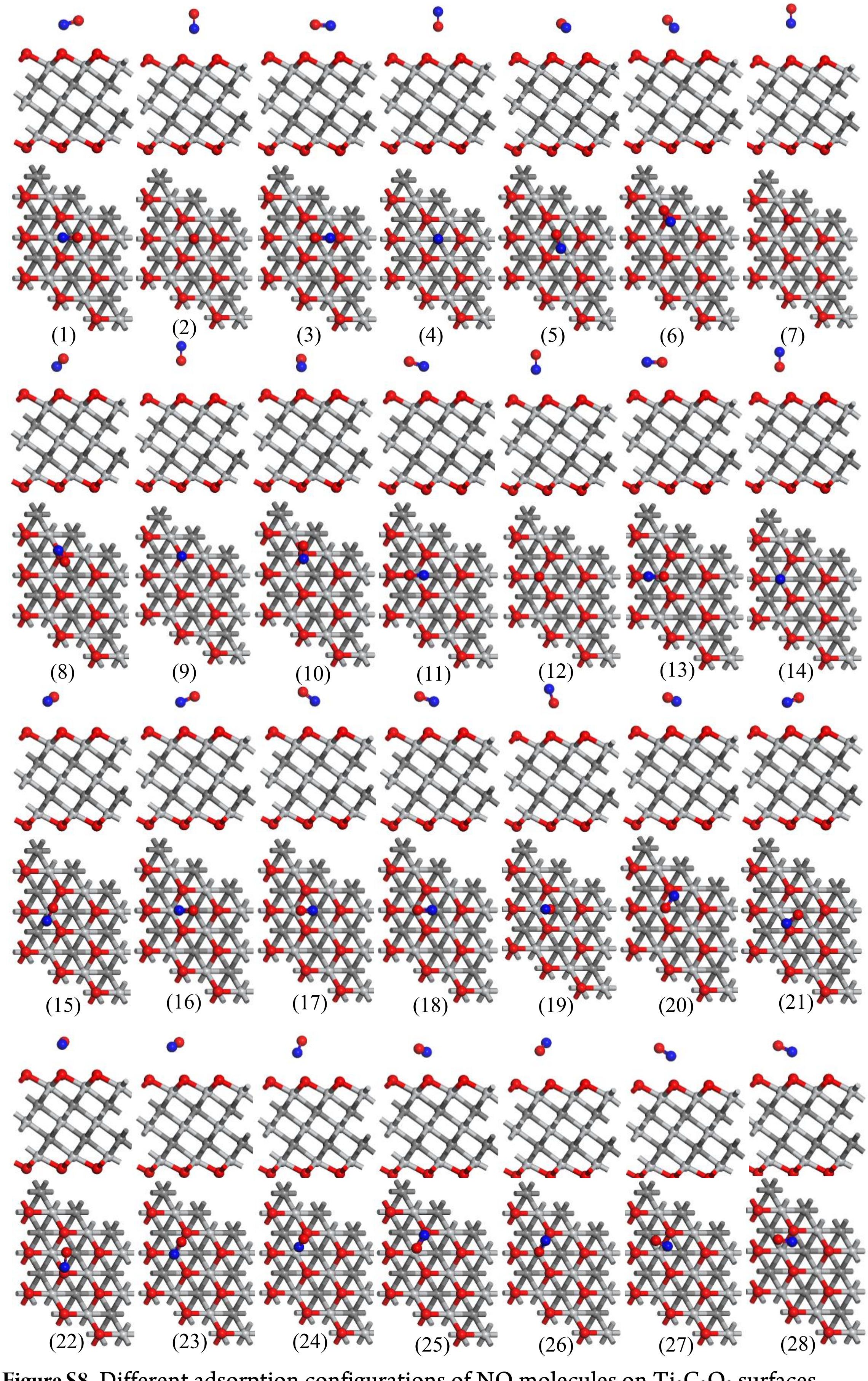


Figure S8. Different adsorption configurations of NO molecules on $Ti_3C_2O_2$ surfaces.

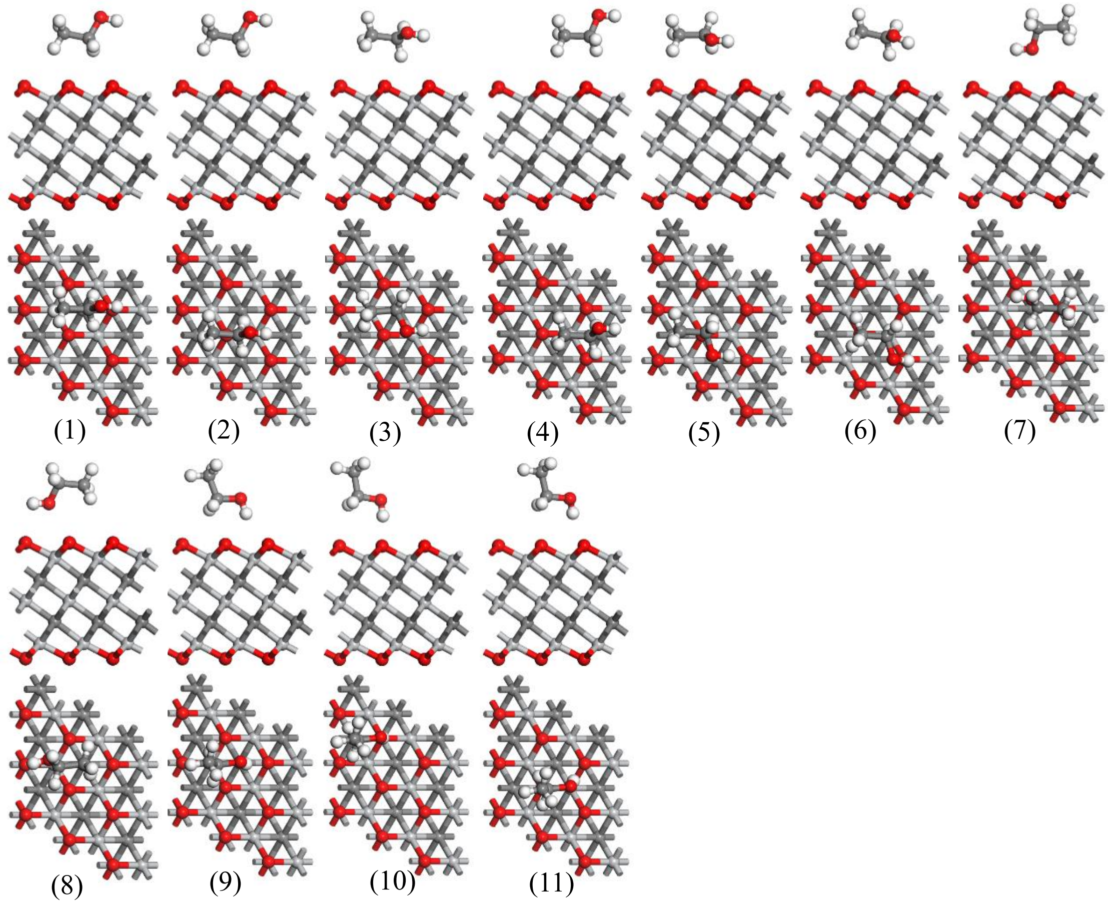


Figure S9. Different adsorption configurations of ethanol molecules on $Ti_3C_2O_2$ surfaces.

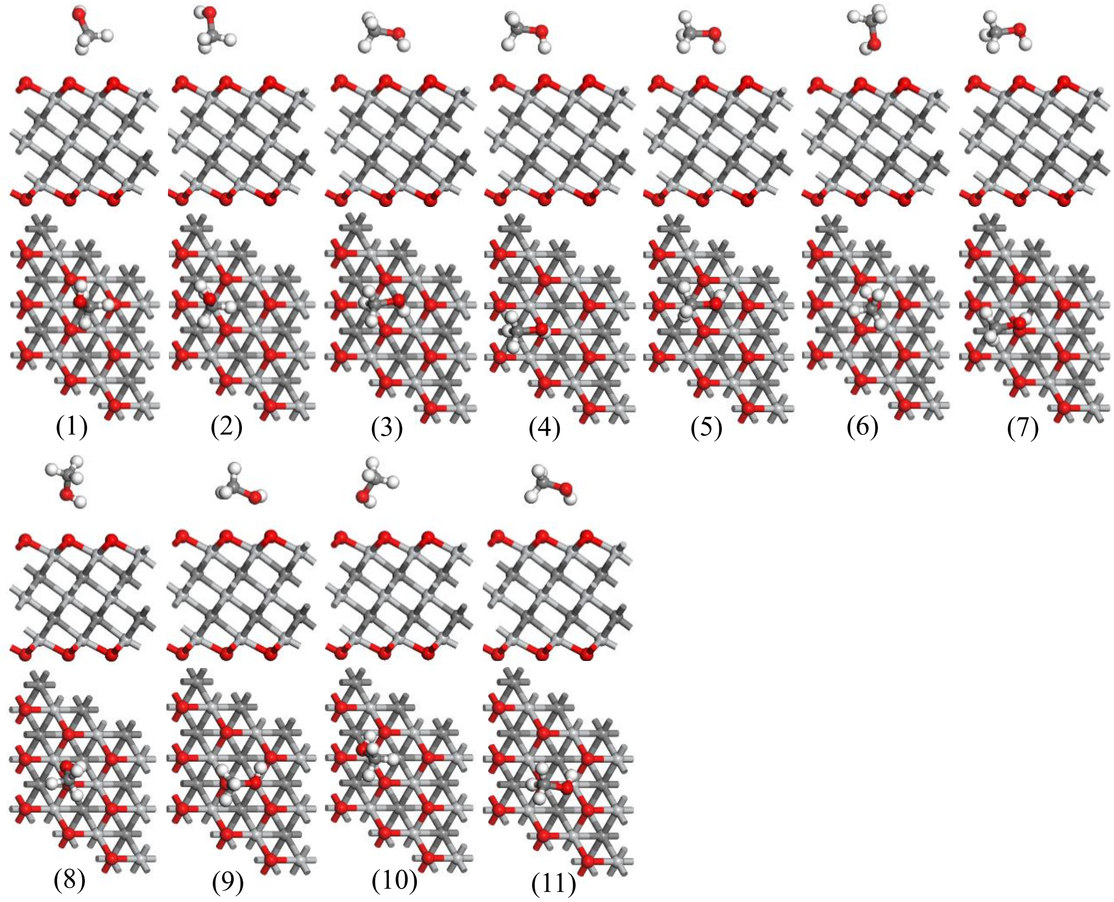


Figure S10. Different adsorption configurations of methanol molecules on $Ti_3C_2O_2$ surfaces.

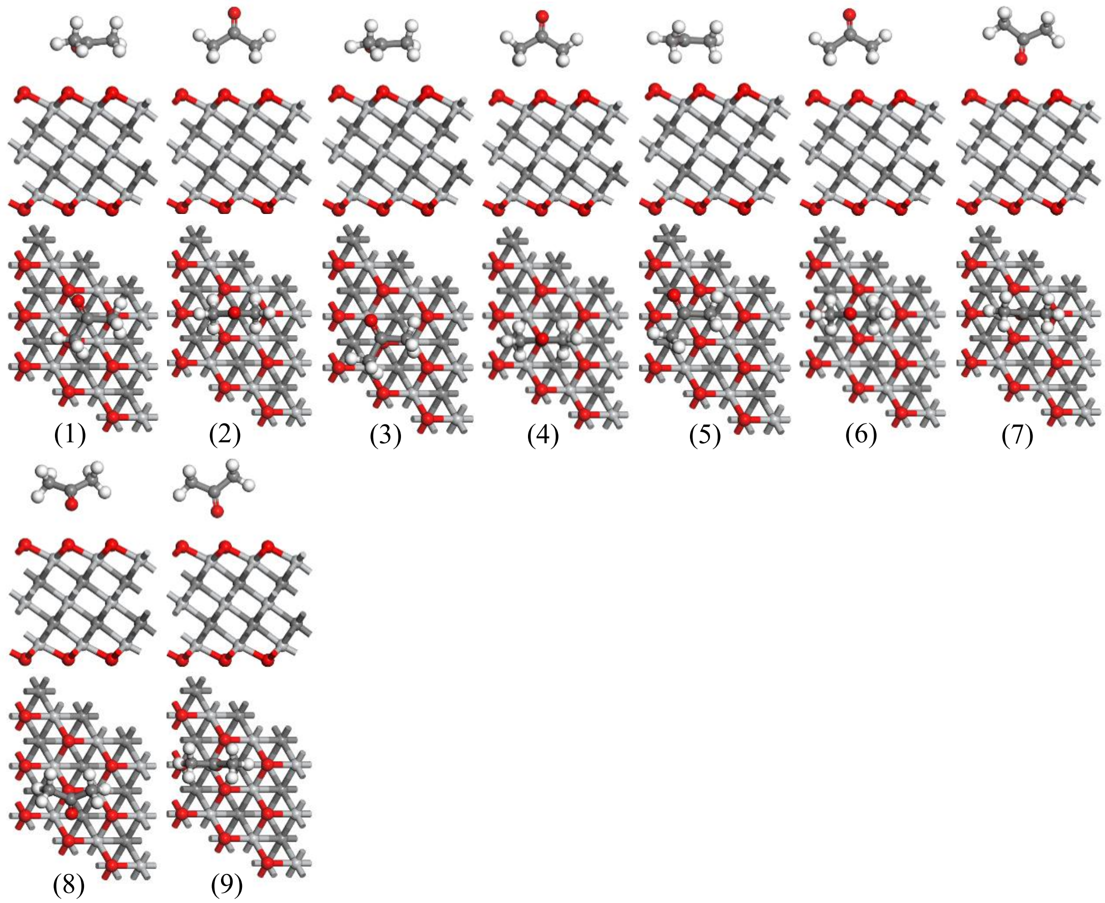


Figure S11. Different adsorption configurations of acetone molecules on $Ti_3C_2O_2$ surfaces.

Table S1. The corresponding calculated adsorption energies (eV/molecule) for different models given in Figure S4-S11.

Model No.	Adsorption energy (E_{ads}) of different gases							
	CH_4	H_2S	H_2O	NH_3	NO	Ethanol	Methanol	Acetone
1	-0.107	-0.113	-0.133	-0.138	-0.478	-0.178	-0.165	-0.275
2	-0.100	-0.136	-0.141	-0.110	-0.357	-0.180	-0.125	-0.233
3	-0.089	-0.125	-0.116	-0.094	-0.491	-0.222	-0.231	-0.326
4	-0.085	-0.121	-0.137	-0.094	-0.333	-0.182	-0.221	-0.249
5	-0.110	-0.101	-0.069	-0.122	-0.482	-0.239	-0.235	-0.299
6	-0.109	-0.110	-0.053	-0.106	-0.523	-0.216	-0.180	-0.247
7	-0.097	-0.078	-0.073	-0.112	-0.280	-0.170	-0.216	-0.131
8	-0.098	-0.099	-0.088	-0.115	-0.519	-0.225	-0.152	-0.144
9	-0.104	-0.136	-0.150	-0.091	-0.286	-0.223	-0.259	-0.145
10	-0.096	-0.124	-0.125	-0.113	-0.521	-0.235	-0.204	
11	-0.085	-0.131	-0.120	-0.092	-0.462	-0.167	-0.216	
12	-0.090	0.667	-0.123	-0.139	-0.392			
13	-0.064	-0.115	-0.137	-0.109	-0.445			
14	-0.060	0.505	-0.107	-0.067	-0.346			
15	-0.075	-0.108	-0.079	-0.072	-0.462			
16	-0.075	-0.140	-0.132	-0.248	-0.473			
17	-0.090	-0.107	-0.146	-0.311	-0.436			
18	-0.085	-0.119	-0.104	-0.249	-0.441			
19	-0.073	-0.131	-0.139	-0.310	-0.334			
20	-0.077	-0.125	-0.145	-0.178	-0.503			
21		-0.124	-0.144	-0.299	-0.528			
22		-0.103	-0.140		-0.504			
23		-0.128	-0.122		-0.422			
24			-0.124		-0.448			
25			-0.145		-0.517			
26			-0.116		-0.367			
27			-0.115		-0.484			
28			-0.117		-0.511			