Supplementary Information

Enhanced NH_3 and NO Sensing Performance of $Ti_3C_2O_2$ MXene by biaxial strain: Insights from First-Principles Calculations

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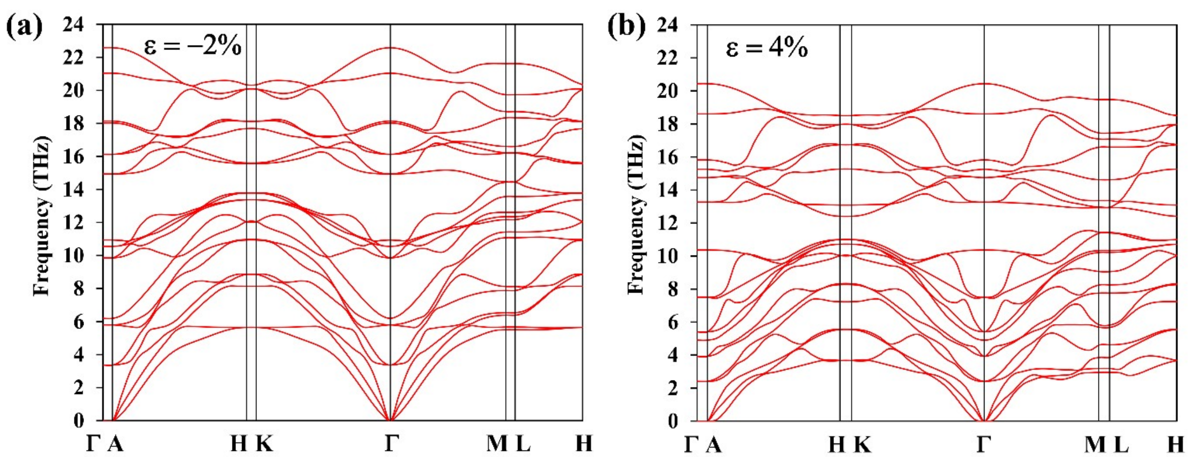

Fig. 1S Phonon dispersion curves of $Ti_3C_2O_2$ at strains of -2% and 4% represented by panel (a), and (b), respectively.

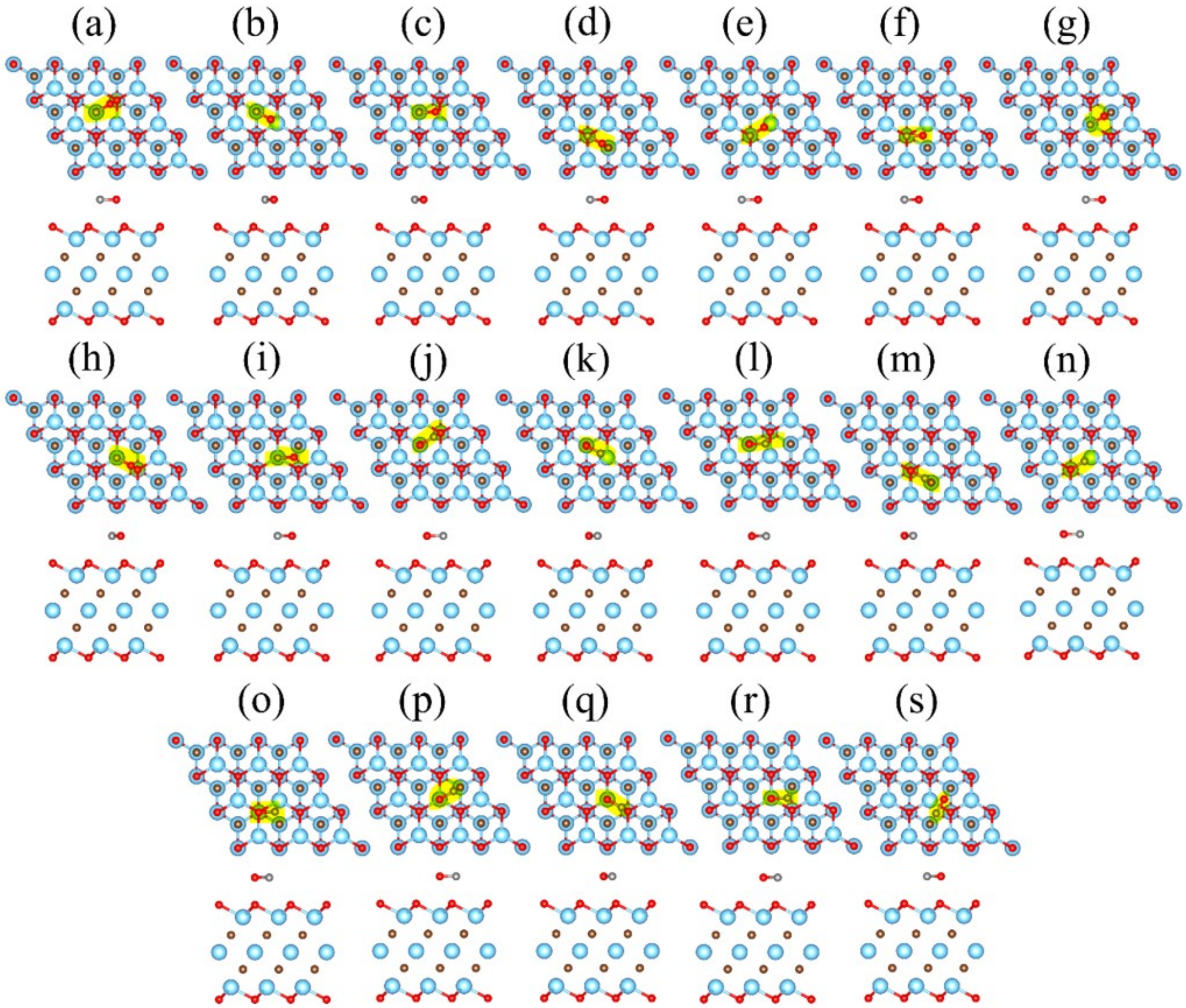

Fig. 2S Top and side views of the possible adsorption sites of CO and NO on $Ti_3C_2O_2$. The azure, brown, red, and grey balls represent the Ti, C, O, and C or N of gases, respectively. The yellow-highlighted area in the top view clearly indicates the position of the gases.

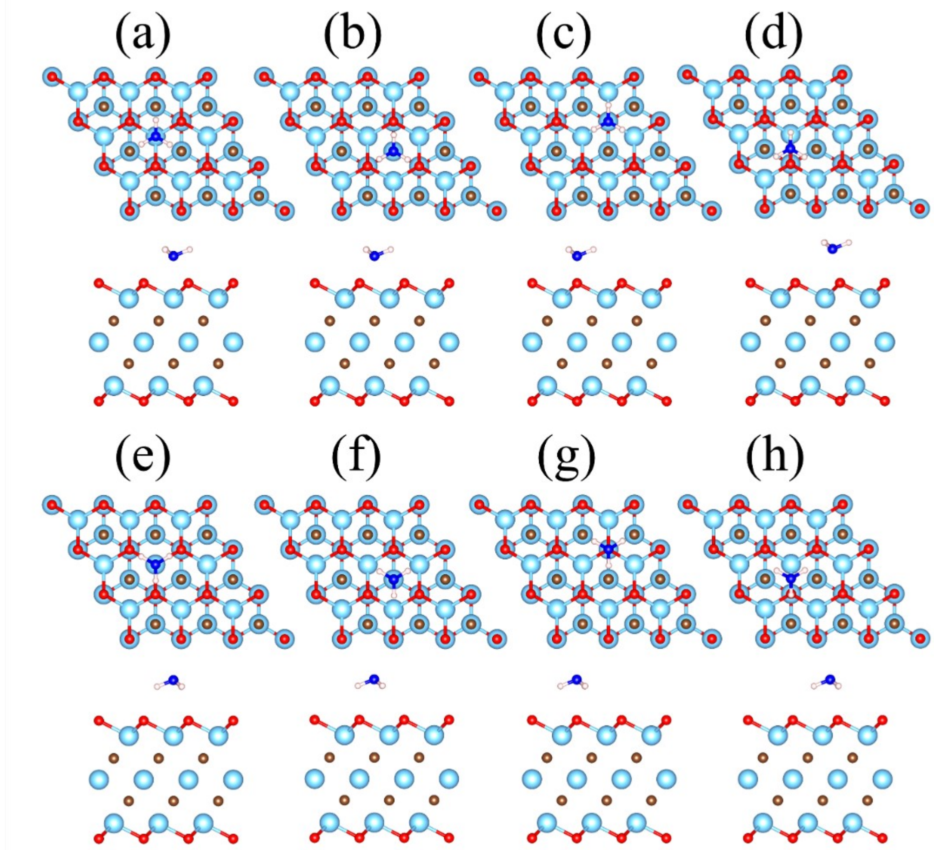

Fig. 3S Top and side views of the possible adsorption sites of NH_3 on $Ti_3C_2O_2$. adsorption site configuration on $Ti_3C_2O_2$ surface. The azure, brown, red, blue, and pink balls represent the Ti, C, O, N, and H, respectively.

Tabel 1S The Mulliken charge analysis of CO, NH_3, and NO before and after adsorption on $Ti_3C_2O_2$.

	Gases	Species	States		Charge (e)
			s	p	
Before	**CO**	C	1.68	1.90	0.42
		O	1.84	4.57	-0.42
	NH_3	N	1.75	4.49	-1.23
		H	0.59	-	0.41
		H	0.59	-	0.41
		H	0.59	-	0.41
	NO	N	1.80	3.07	0.13
		O	1.84	4.29	-0.13
After	**CO**	C	1.66	1.95	0.39
		O	1.84	4.53	-0.37
	NH_3	N	1.68	4.32	-1.00
		H	0.65	-	0.35
		H	0.65	-	0.35
		H	0.65	-	0.35
	NO	N	1.79	2.97	0.24
		O	1.84	4.20	-0.05

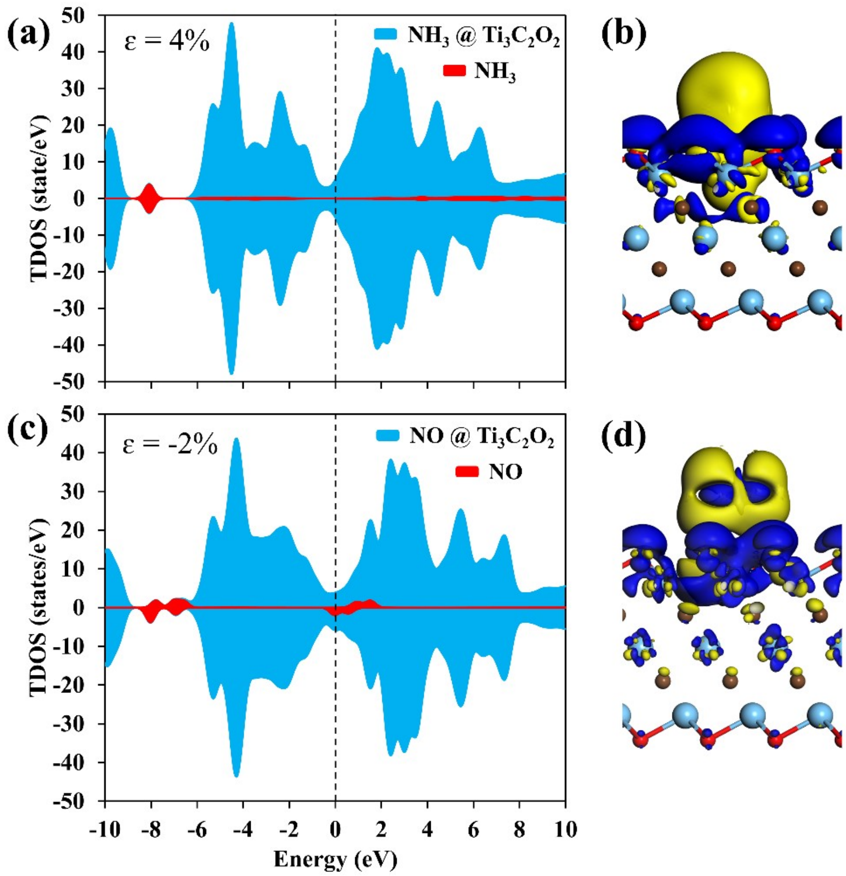

Fig. 4S Electronic density of state (TDOS) and electron differences density (EDD) of (a, b) NH_3 adsorbed on $Ti_3C_2O_2$ at 4% strain and (c, d) NO adsorbed on $Ti_3C_2O_2$ at -2% strain.

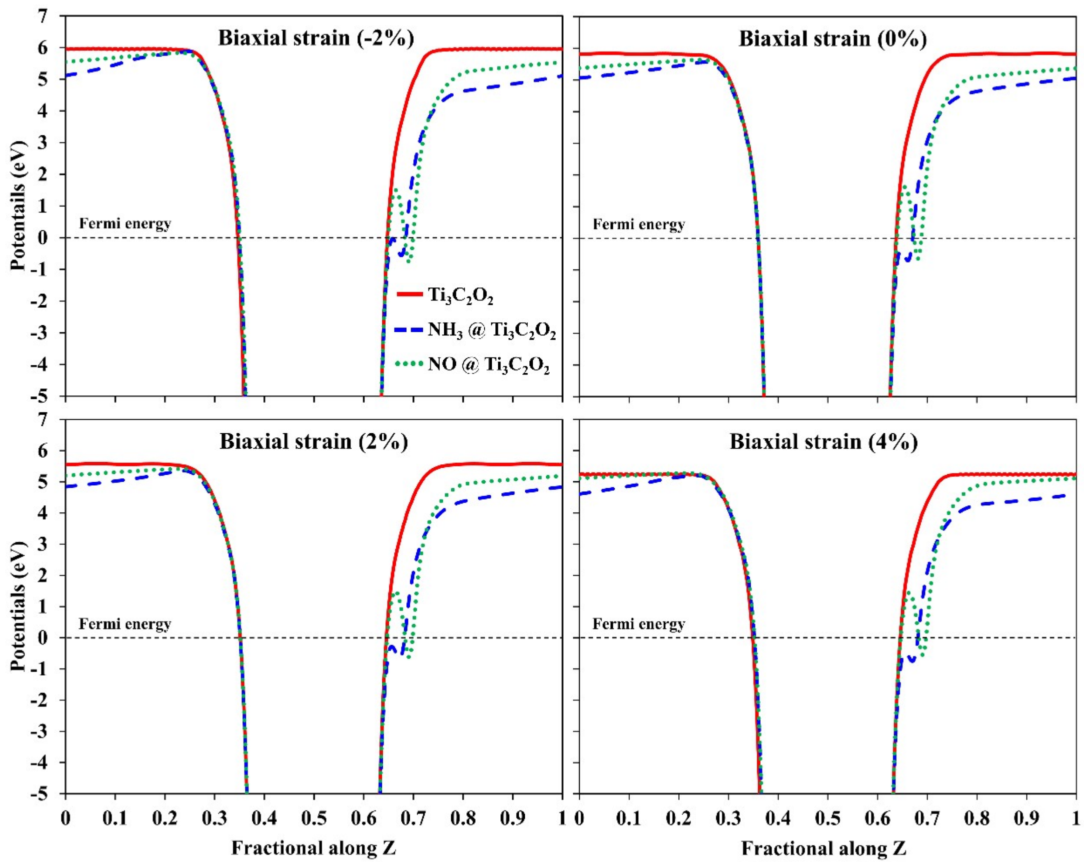

Fig. 5S Electrostatic potentials of toxic gas molecules adsorption on $Ti_3C_2O_2$ under biaxial strain -2% to 4%.