Supporting Information

Few-Layered α-$MoTe_2$ Schottky Junction for High Sensitive Chemical-Vapour Sensor

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KEYWORDS: α-$MoTe_2$, Schottky diode, gas sensing, two-dimensional materials

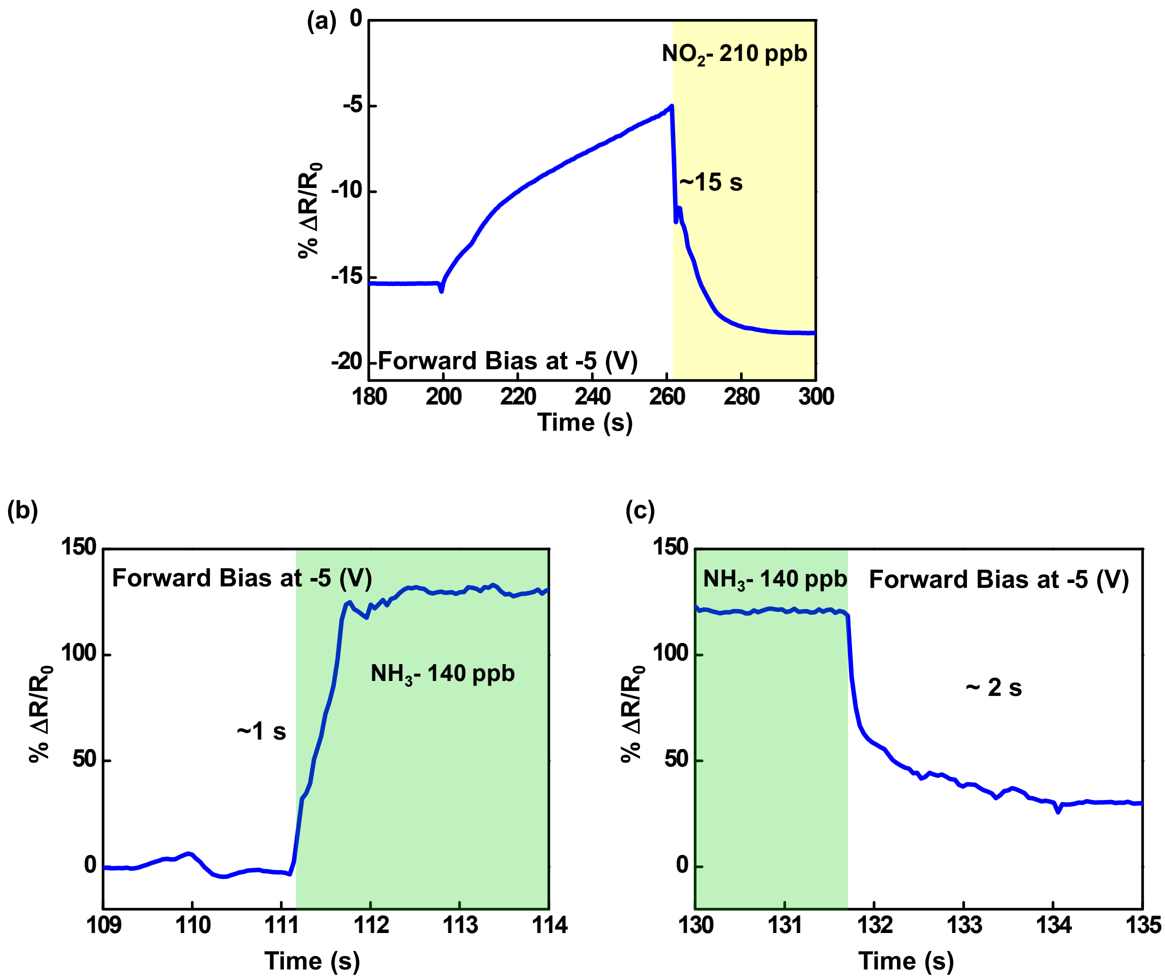

Figure S1. (a) Magnified third cycle in Figure 4b, showing the SD responses under exposure to 210-ppb NO_2. The response time of NO_2 was ~15 s. A forward-bias voltage of −5 V was applied across the device. (b, c) Magnified second cycle in Figure 4d, showing the response and recovery behaviour of the SD under exposure to 140-ppb NH_3. At a forward bias of −5 V, the response time was ~1 s and the recovery time was ~2 s.

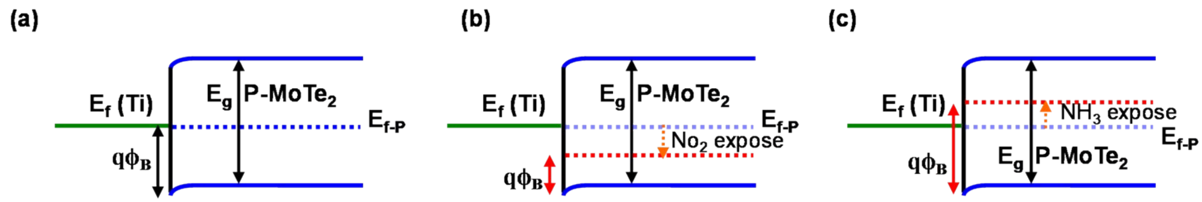

Figure S2. Energy-band diagram of the α-$MoTe_2$ SD in three different conditions: (a) before gas exposure; (b) under NO_2 gas exposure, showing the reduction of the Fermi level; and (c) under NH_3 gas exposure, indicating the increase of the Schottky-barrier height compared with the pre-exposure condition.

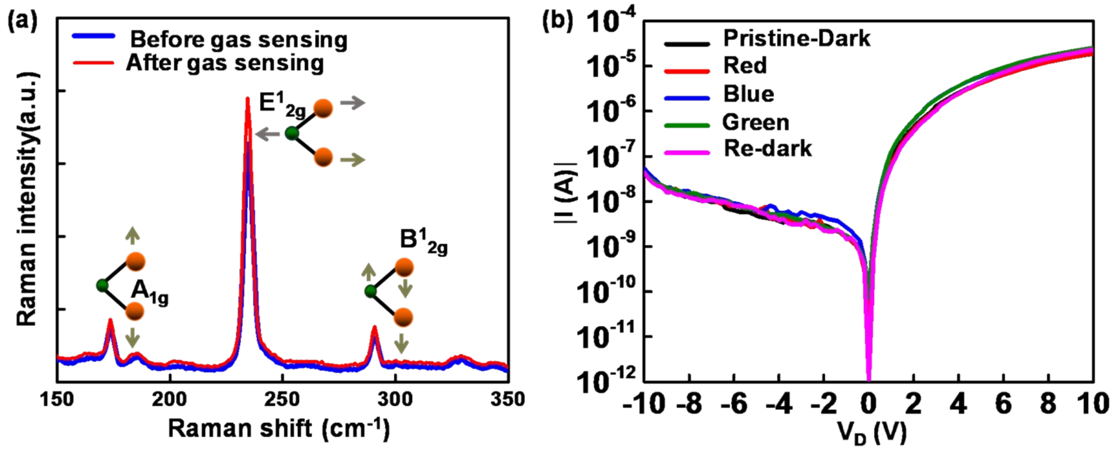

Figure S3. (a) Raman spectra of $MoTe_2$ before (blue) and after (red) gas sensing in NO_2 and NH_3. The Raman spectra confirms the stability of the $MoTe_2$ sensors after sensing. (b) The I–V curves of the SD under irradiation from red, green and blue light-emitting diodes (LEDs). The SD is insensitive to the visible light.

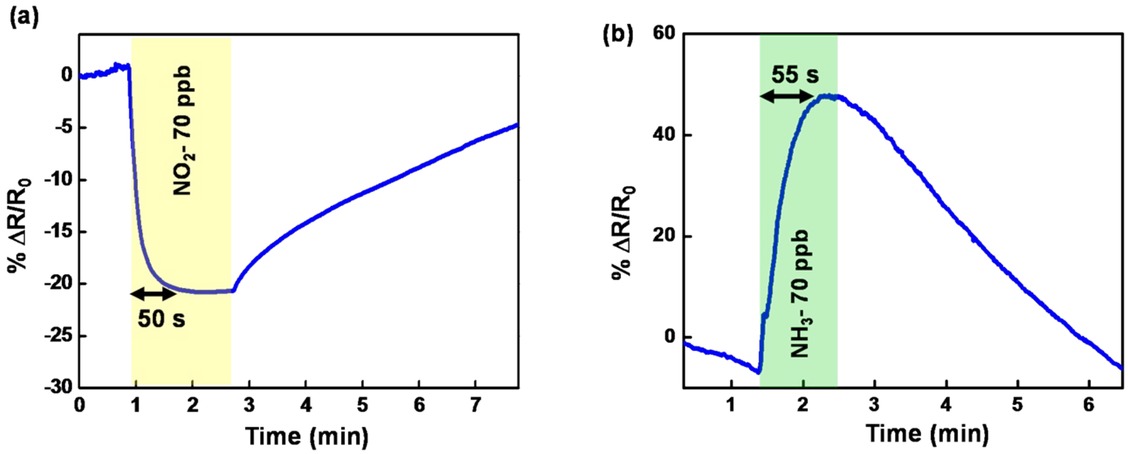

Figure S4. Magnified first cycles in (a) Figure 6a and (b) Figure 6b, showing the relative resistance change of the $MoTe_2$ FET under exposure to 70-ppb NO_2 and 70-ppb NH_3, respectively.

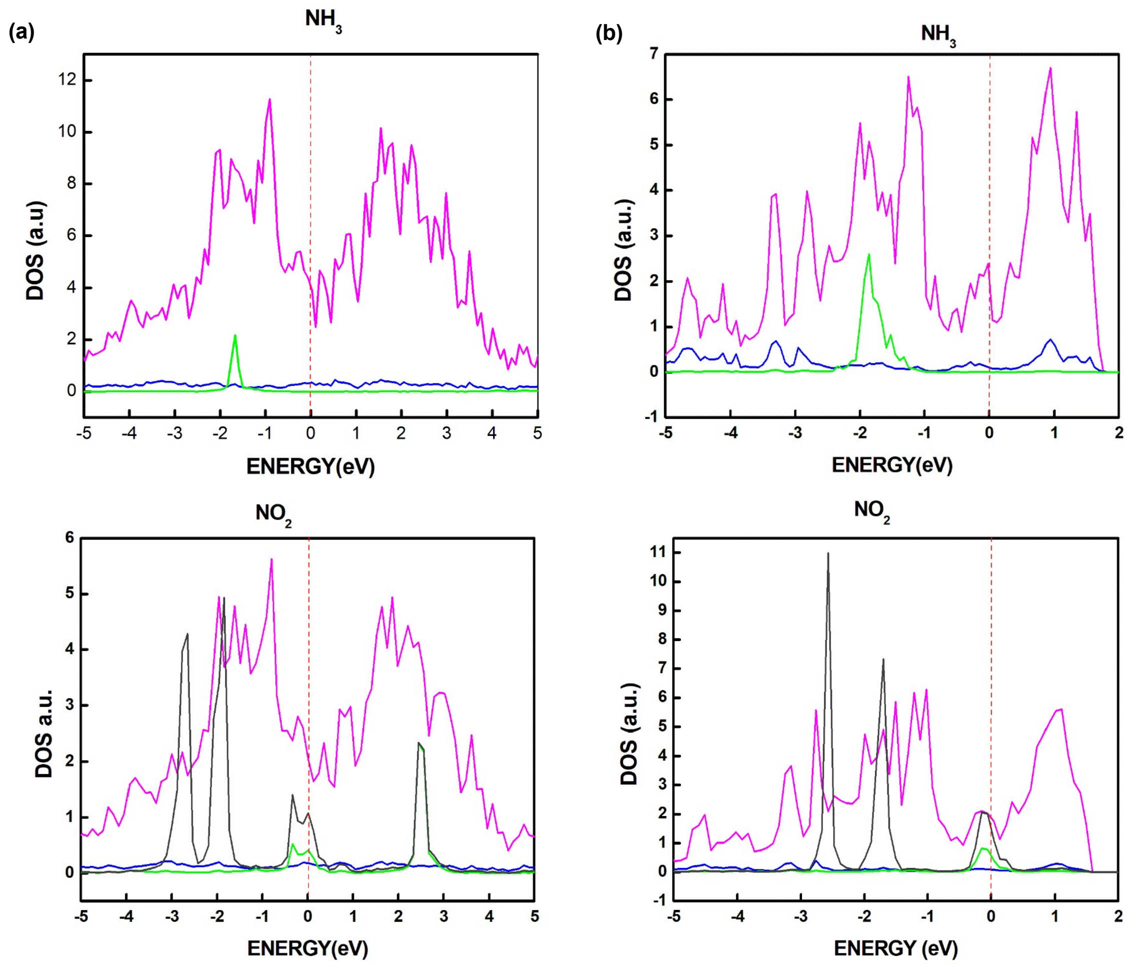

Figure S5. Partial Density of States (PDOS) of the $MoTe_2$ with adsorbed gas molecules in (a) Pt surface and (b) Ti. Note that the Fermi level is fitted at 0 eV. Colour code used for the PDOS is Mo-d (magenta), Te-s (blue), N-p (green) and O-p (Dark grey) respectively.

Table S1.

Ref.	2D material	Type of device	Chemical	Gas concentration	Response time	ΔR/R or ΔG/G	Note
This study	**$MoTe_2$**	**Schottky diode**	**NO_2**	**70 ppb**	**~ 15 s**	**13%**	**Room temperature**
			NH_3	**70 ppb**	**~ 1 s**	**112%**	
		FET	**NO_2**	**70 ppb**	**~50 s**	**22 %**	
			NH_3	**70 ppb**	**~55 s**	**61%**	
1	BP	FET	NO_2	5 ppb	280 s	2.9 %[1]	Room temperature
2	Graphene/MoS_2	Heterostructure	NO_2	1.2 ppm	~10 min	3 %	150 ^{O}C
			NH_3	5 ppm	~10 min	1.5 %	150 ^{O}C
3	h-BN Capped MoS_2	FET	ethanol, acetonitrile, toluene, chloroform, methanol	No data	100-400 s	~500%	150 ^{O}C
4	MoS_2-Decorated TiO2 nanotube	p-n heterojunction	ethanol	100 ppm	~20 s	400 %	150 ^{O}C
5	Graphene/Silicon Heterojunction [2]	Schottky Diode	NO_2	20 ppm	10 min	75%	Room temperature
			NH_3	50 ppm	6 min	60%	Room temperature
6	$MoTe_2$ Gate bias (-60 and 20 V)	FET	NO_2	100-1000 ppb	~ 7 min	100%	Room temperature
			NH_3	2-100 ppm	~7 min	32%	Room temperature

[1] In this report, the authors reported relative conductance change instead of relative resistance change.
[2] The relative conductance change is reported.

Table S2: Adsorption energy (eV), Bond length Å, and charge transfer (e) value for the studied complex.

Metal	Gas Molecule	E_{Ads} (eV)	Bond length (Å)	Charge Transfer e
Pt	NH_3 (B)	-0.150	1.02 (1.02)[1]	0.068
	NH_3 (H)	-0.149	1.02	0.067
	NO_2 (B)	*		
	NO_2 (H)	-0.153	1.25 (1.21) 1.24	0.070
Ti	NH_3 (B)	-0.124	1.02 (1.02)	0.071
	NH_3 (H)	-0.124	1.02	0.071
	NO_2 (B)	-0.129	1.25 (1.21) 1.26	0.074
	NO_2 (H)	-0.129	1.25 1.26	0.074

[1] Denotes the monomer value
*Structure not converged

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