Supporting Information

Ultrasensitive Reversible Oxygen Sensing in Liquid-Exfoliated MoS_2 Nanoparticles.

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Table S1. Effects of oxygen-deficient exposure.[1]

Oxygen concentration (% vol)	Health effects of persons at rest
19	Some adverse physiological effects occur, but they may not be noticeable.
15–19	Impaired thinking and attention. Increased pulse and breathing rate. Reduced coordination. Decreased ability to work strenuously. Reduced physical and intellectual performance without awareness.
12–15	Poor judgment. Faulty coordination. Abnormal fatigue upon exertion. Emotional upset.
10–12	Very poor judgment and coordination. Impaired respiration that may cause permanent heart damage. Possibility of fainting within a few minutes without warning. Nausea and vomiting.
below 10	Inability to move. Fainting almost immediate. Loss of consciousness. Convulsions. Death.

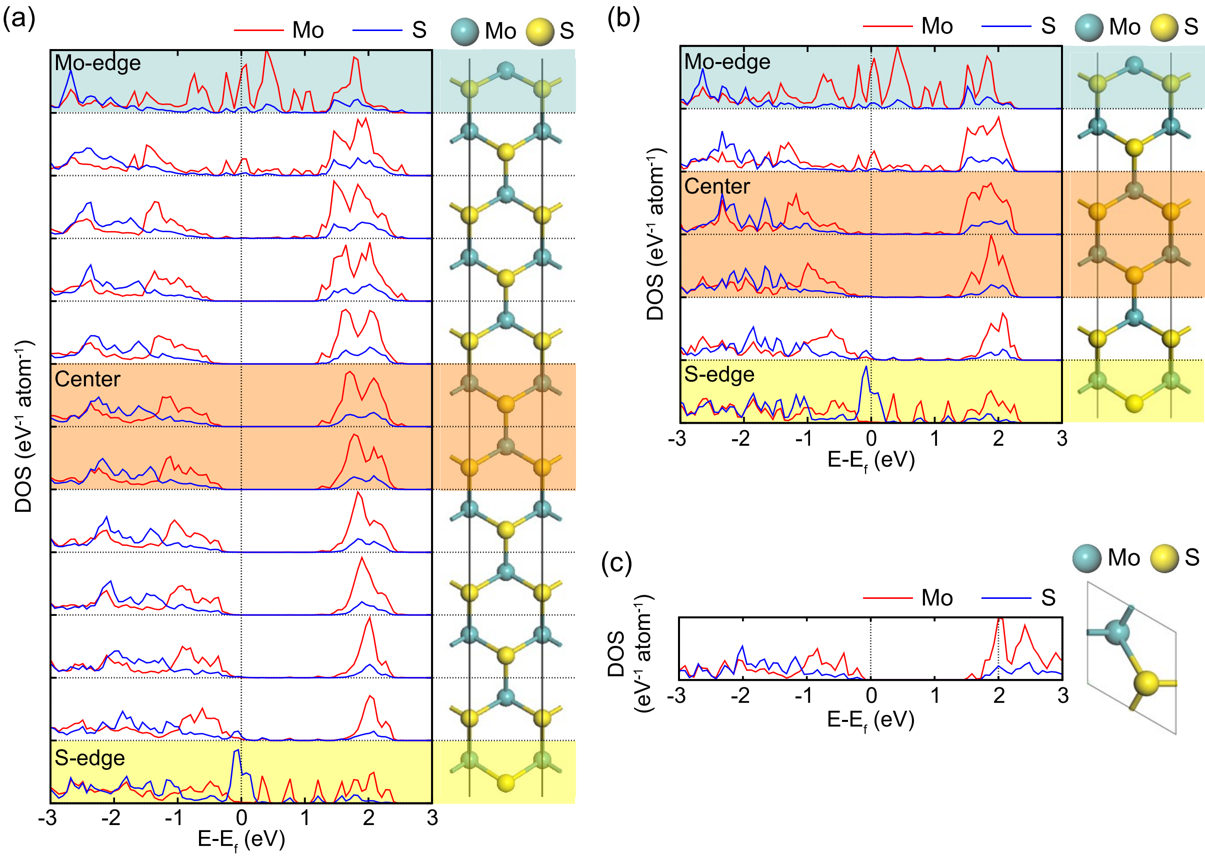

Figure S1. Density of states of each layer for MoS_2 flakes with widths of (a) 12 unit cells and (b) 6 unit cells, and (c) bulk MoS_2 layer of infinite unit cells.

Figure S1 shows the density of states (DOS) of each layer for MoS_2 flakes with widths of 12 unit cells (uc) and 6 uc, and bulk MoS_2 layer of infinite uc. 12 uc and 6 uc models have the Mo-terminated edge on the top, the S-terminated edge on the bottom and bulk-like uc at the center. The DOS of Mo- and S-terminated edges of 12 uc and 6 uc models are exactly same. Also the center uc of 12 uc and 6 uc models are almost same electronic structure as the bulk. Therefore, we suggest that 6 uc model is enough to investigate the sensing mechanism.

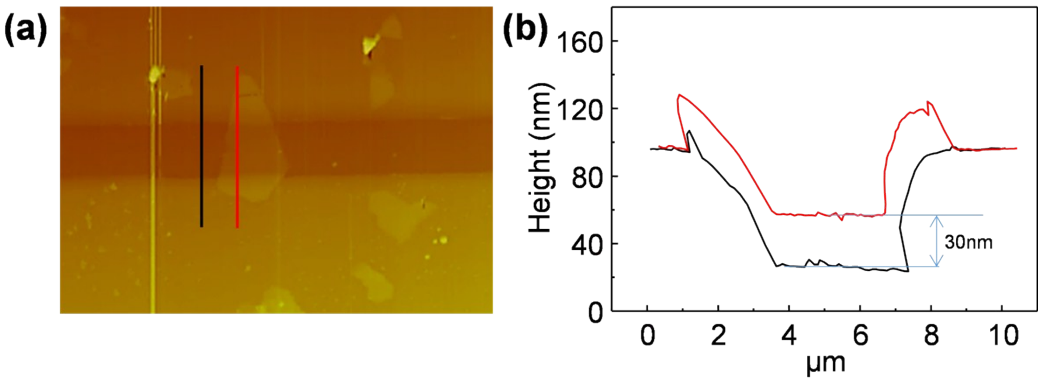

Figure S2. (a) AFM image and (b) height profiles of mechanically exfoliated MoS_2 microflake deposited between Pt IDEs (red line) and Pt IDEs without the MoS_2 microflakes (black line).

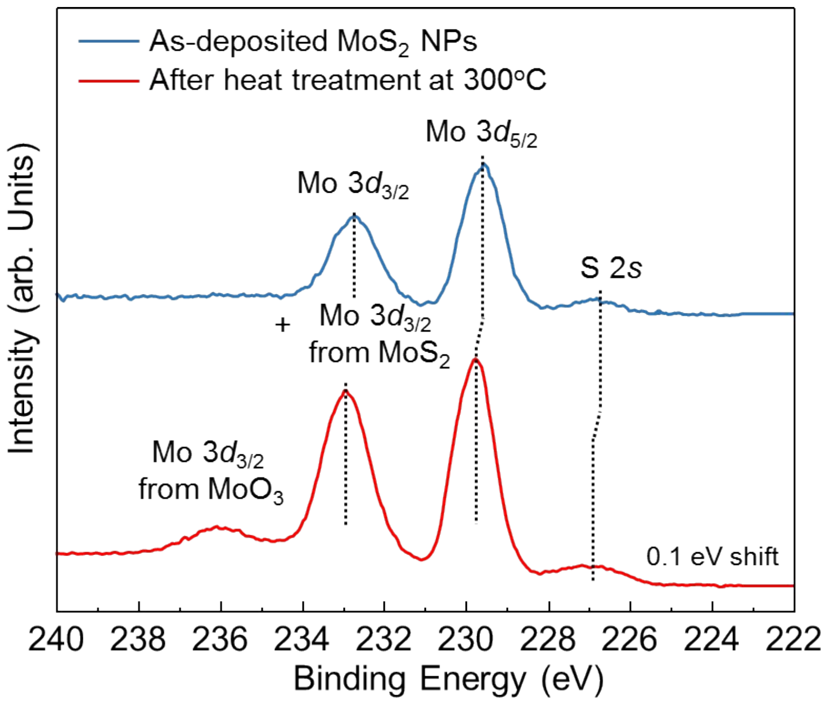

Figure S3. X-ray photoemission spectroscopy of as-deposited and after heat treatment liquid-exfoliated MoS_2.

Table S2. Gas sensing properties of different resistive oxygen gas sensors in the literatures.[2-6]

Sensing material	Synthesis method	Oxygen conc.	Response (S)	T_{sens} (°C)	Ref.
MoS_2	Ultrasonication	100%	63.73	300	This study
ZrO_2-doped CeO_2	Wet-chemical precipitation	100%	~ 1.1	800	2
CeO_2	Spray-pyrolysis	100%	~3	800	3
Ga_2O_3	Sputtering	60%	~4.5	900	4
TiO_2	Sputtering	6000 ppm	~0.3	500	5
$RBaCo_2O_5$	Solid state reaction	100%	~2	600	6

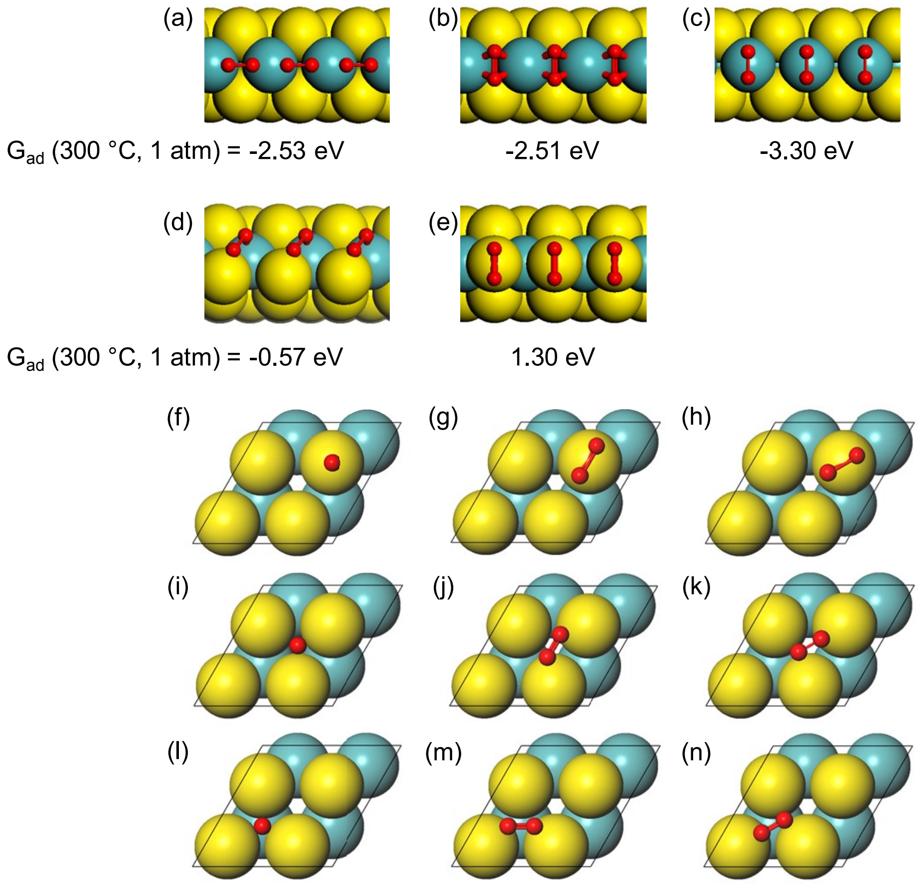

Figure S4. (a-e) Stable sites of O_2 adsorption.(a), (b) and (c) show locally stable configurations of O_2 adsorbed on clean Mo-edge. (d) and (e) show O_2 adsorption on Mo-edge with S monomer. The adsorption free energy at 300 °C and 1 atm [G_{ad}(300 °C, 1 atm)] is displayed under each figure. (f-n) Considered O_2 adsorption configurations on MoS_2 clean surface: (f) vertical O_2, (g) O_2 parallel to *a* axis, and (h) O_2 parallel to *a*+*b* axis on S top, (i) vertical O_2, (j) O_2 parallel to *a* axis, and (k) O_2 parallel to *a*+*b* axis on FCC center and (l) vertical O_2, (m) O_2 parallel to *a* axis, and (n) O_2 parallel to *a*+*b* axis on HCP center.

Table S3. Adsorption free energy of oxygen molecule on MoS_2 clean surface

	(f)	(g)	(h)
G_{ads} (300°C, 1atm) (eV)	3.21	1.72	1.73

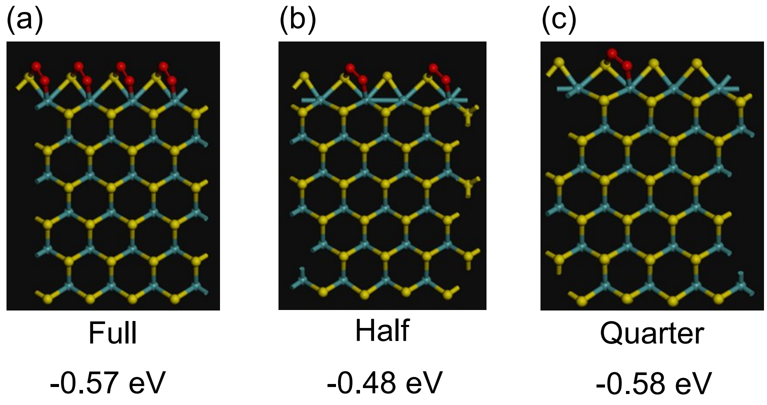

Figure S5. O_2 adsorption energy on Mo-S bridge sites of Mo-edges with S monomer: (a) full, (b) half and(c) quarter O_2 coverage.

O_2 adsorption energy on Mo-S bridge sites of Mo-edge with S monomer was calculated depending on O_2 coverage, defined as the ratio of the number of adsorbed oxygen to available adsorption sites. The adsorption free energy at 300 °C, 1 atm for O_2 coverage of 1, 0.5, and 0.25 are -0.57, -0.48 and -0.58 eV, respectively. This simulation demonstrates the adsorption free energies are hardly affected by O_2 coverage. Therefore, the concentration of O_2 does not influence on the linear relationship in large oxygen concentration.

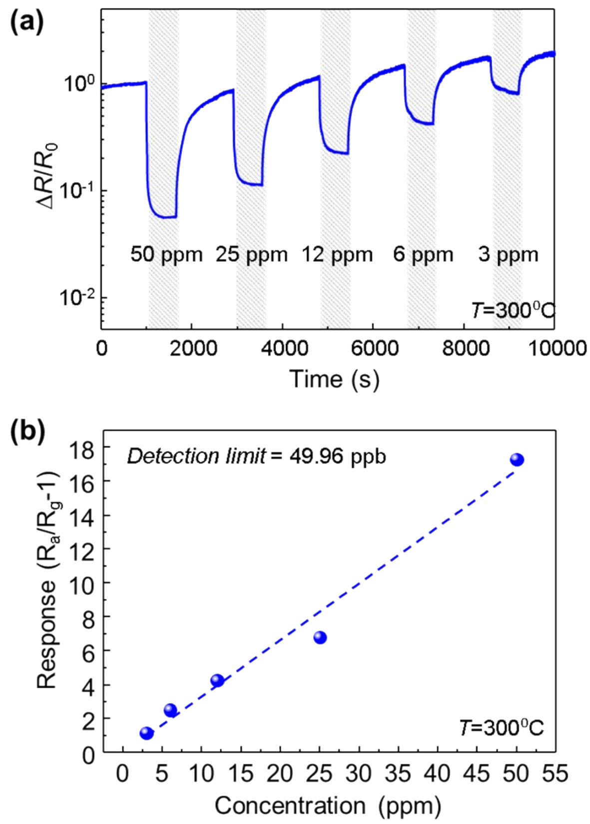

Figure S6. (a) Gas sensing transients of liquid-exfoliated MoS_2 to different C_2H_5OH concentration at 300ºC. (b) Linear fit of responses as a function of C_2H_5OH concentration at 300ºC.

Reference

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