Supporting Information

Dual selective gas sensing characteristics of 2D α -MoO_{3-x}, via a facile transfer process

Fahmida Rahman,^{*b} Ali Zavabeti, ^{b§} Md. Ataur Rahman,^a Aram Arash,^a Aishani Mazumder,^b Sumeet Walia,^b Sharath Sriram,^a Madhu Bhaskaran^a and Sivacarendran Balendhran^{*bc}

^aFunctional materials and Microsystem Research group and Micro Nano Research facility, RMIT University, Melbourne, Victoria 3000, Australia. E-mail: fahmida.rahman@gmail.com.

^bSchool of Engineering, RMIT University, Melbourne, Victoria 3000, Australia.

^cSchool of Physics, The University of Melbourne, Parkville, Victoria 3010, Australia.

Corresponding Authors

*E-mail: fahmida.rahman@gmail.com (F.R.).

*E-mail: sbalendhran@unimelb.edu.au (S.B.).

S1. The transfer of MoO_{3-x} on PDMS and Kapton substrates:

The transfer process can be applied to realize pristine MoO_{3-x} on any arbitrary substrate. As a proof of concept, we have transferred the materials onto flexible substrates such as PDMS and Kapton. The optical images of the transferred MoO_{3-x} on PDMS and Kapton are presented in Figure S1a and b. Raman spectroscopy was utilized to confirm the compositional integrity of the transferred material. Raman spectra (Figure S1c and d) show the 820 cm⁻¹ and 996 cm⁻¹ characteristic Raman peaks of as-grown MoO_{3-x} .



Figure S1. Transferred MoO_{3-x} on (a) PDMS and (b) Kapton substrates. Raman spectra of the transferred material on (b) PDMS and (d) Kapton. Raman peaks corresponding to PDMS and Kapton substrates are denoted by * and # respectively.

S2. Schematic illustration of the transfer process:



Figure S2. Schematic illustrating the method used to transfer the as-grown MoO_{3-x} crystals from mica to SiO₂.(a) CVD grown MoO_{3-x} on mica substrate (b) spin coating PDMS on $MoO_{3-x}/mica$ (c) cured PDMS layer on top of $MoO_{3-x}/mica$ layer (d) mica/PDMS/MoO_{3-x} layer submerged in to DI water (e) peeling off PDMS/MoO_{3-x} from mica (f) PDMS/MoO_{3-x} pressing on to SiO₂ for transferring MoO_{3-x} (g) transferred MoO_{3-x} on SiO₂

Table S1: NO₂ and H₂S sensing performance reports on various 2D materials in comparison to our work.

Structure	Synthesis	Concentration/ ppm	Operating Temperature/ ⁰ C	% Sensitivity $S = \frac{ R_a - R_g }{R_a} \times 100\%$	Reference
2D MoS ₂	CVD	10 ppm NO ₂	100	16	S1
2D WS ₂	ALD	25 ppm NO ₂	RT	10	S2
2D SnS ₂ - rGO	Thermal reduction and wet chemical	11.9 ppm NO ₂	80	56.8	\$3
2D MoO _{3-x}	CVD	10 ppm NO ₂	250	56	Our work
quasi-2D Cu ₂ O/SnO ₂	Electroche mical	50 ppm H ₂ S	RT	45	S4
2D MoO _{3-x}	CVD	50 ppm H ₂ S	250	81	Our work

S3. Response and recovery of the devices at various concentrations of NO₂ and H₂S gases:

The gas sensing performance of the MoO_{3-x} sensor was assessed towards NO_2 and H_2S gases with concentrations ranging from 0.5 ppm to 10 ppm and 1 ppm to 50 ppm respectively, at the optimum temperature of 250 ^{0}C .



Figure S3. Gas sensing response with different concentration of (a) NO_2 and (b) H_2S gas.

S4. Long-term performance stability of the sensors:

Figure S4 presents the cyclic stability of the MoO_{3-x} based sensors tested over an extended period of time.



Figure S4. Long-term stability of the MoO_{3-x} based sensors towards (a) 10 ppm (b) and (c) 50 ppm of H₂S at 250 °C.

References

- (S1) Cho, B.; Hahm, M. G.; Choi, M.; Yoon, J.; Kim, A. R.; Lee, Y.-J.; Park, S.-G.; Kwon, J.-D.;
 Kim, C. S.; Song, M.; Jeong, Y.; Nam, K.-S.; Lee, S.; Yoo, T. J.; Kang, C. G.; Lee, B. H.;
 Ko, H. C.; Ajayan, P. M.; Kim, D.-H., Charge-Transfer-Based Gas Sensing using Atomic-Layer MoS₂. *Sci Rep* 2015, *5*, 8052.
- (S2) Ko, K. Y.; Song, J.-G.; Kim, Y.; Choi, T.; Shin, S.; Lee, C. W.; Lee, K.; Koo, J.; Lee, H.; Kim, J.; Lee, T.; Park, J.; Kim, H., Improvement of Gas-Sensing Performance of Large-Area Tungsten Disulfide Nanosheets by Surface Functionalization. ACS Nano 2016, 10 (10), 9287-9296.
- (S3) Shafiei, M.; Bradford, J.; Khan, H.; Piloto, C.; Wlodarski, W.; Li, Y.; Motta, N., Low-Operating Temperature NO₂ Gas Sensors Based on Hybrid Two-Dimensional SnS₂-Reduced Graphene Oxide. *Appl. Surf. Sci.* **2018**, *462*, 330-336.
- (S4) Cui, G.; Zhang, M.; Zou, G., Resonant Tunneling Modulation in Quasi-2DCu₂O/SnO₂ p-n Horizontal-Multi-Layer Heterostructure for Room Temperature H₂S Sensor Application. *Sci. Rep.* 2013, *3*, 1250.