## Improving electron mobility in $MoS_2$ field-effect transistors by optimizing the interface contact and enhancing the channel conductance through local structural phase transition

Zhaofang Cheng<sup>1, 2</sup>, Shaodan He<sup>1</sup>, Xiaona Han<sup>1</sup>, Xudong Zhang<sup>1</sup>, Lina Chen<sup>1</sup>, Shijun Duan<sup>1</sup>, Shimin Zhang<sup>1</sup>, and Minggang Xia <sup>1, 2, 3, \*</sup>

- <sup>1</sup> Department of Applied Physics, School of Physics, Xi'an Jiaotong University, Shaanxi 710049, People's Republic of China.
- <sup>2</sup> MOE Key Laboratory for Nonequilibrium Synthesis and Modulation of Condensed Matter, School of Physics, Xi'an Jiaotong University, 710049, People's Republic of China.
- <sup>3</sup> Laboratory of Nanostructure and Physics Properties, Key Laboratory for Quantum Information and Optoelectronic Quantum Devices of Shaanxi Province, School of Physics, Xi'an Jiaotong University, 710049, People's Republic of China.

(Some figures in this article are in color only in the electronic version.)

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

\* Address correspondence to: <u>xiamg@mail.xjtu.edu.cn</u>



Fig. S1. (a) The fabrication process of  $MoS_2$  vdW FETs. 285 nm silicon oxide (SiO<sub>2</sub>) substrate cleaned with acetone and isopropyl alcohol (IPA), the bottom is p-type heavily doped Si (p+ Si), which can be used as a back gate; two sites were etched on SiO<sub>2</sub> and 80 nm thick Au electrodes were deposited as source and drain electrodes, here there was a small gap of about 5 nm between the sample and the electrode, which facilitated the subsequent entry of oxygen plasma; About 2-3 layers of  $MoS_2$  channel are transferred onto the electrodes, where an optical microscope is used to align the  $MoS_2$  sample and electrodes for anchored transfer (b).



Fig. S2. (a) AFM spectra of  $MoS_2$  channel in  $MoS_2$  vdW device. (b) A height profile is extracted along the white line shown in panel (a). The  $MoS_2$  domain thickness is 1.17 nm, equal to 2 monolayer thickness.



Fig. S3. Raman spectra (b) acquired from different regions highlighted in optical image of  $MoS_2$  vdW devices (a) after  $O_2$  plasma treatment for 1 s. The 1T phase transition of  $MoS_2$  occurs in the region in contact with the Au electrodes firstly, which may be attributable to the catalytic effect of Au. Here Au provides free electrons in the plasma process, which can accelerate the kinetic process of the oxidation reaction, thus reducing the reaction energy barrier of oxygen doping.



Fig. S4. The impact of  $O_2$  plasma on the surface morphology of  $MoS_2$ . The optical images of fewlayer  $MoS_2$  nanosheets before (a, g) and after (d, j) being treated by oxygen plasma for 3 s. Scale bar: 10 µm. There is minimal change in color of the  $MoS_2$ , suggesting that the sample's surface did not experience significant thinning due to the plasma etching. The AFM characterizations of  $MoS_2$ nanosheets before (b, h) and after (e, k) being treated by oxygen plasm for 3 s. The samples exhibit flat surfaces and similar thicknesses before (c, i) and after (f, l) oxygen plasma treatment, indicating that our soft oxygen plasma mainly plays a role of doping on  $MoS_2$  samples, with almost no etching effect.



Fig. S5. Measurement of the leakage currents through the S or D electrodes and back gate.



Fig. S6. Electronic characteristic curves of  $MoS_2$  FET device2 after oxygen plasma exposure with 10 s. (a)  $I_{ds}$ - $V_{ds}$  characteristics up to  $V_{ds}$ =1 V and  $V_g$  ranging from -30 V to 30 V. Inset: Optical image of the  $MoS_2$  device with corresponding working principle. (b) Corresponding  $I_{ds}$ - $V_g$  characteristics, exhibiting high electron mobility.



Fig. S7. Electrical characteristic curves of  $MoS_2$  FET device3 after 5 s oxygen plasma exposure. (a)  $I_{ds}$ - $V_{ds}$  characteristics up to  $V_{ds}$ =0.5 V and  $V_g$  ranging from -30 V to 30 V. Inset: Optical image of the  $MoS_2$  device3 with corresponding working principle. (b) Corresponding  $I_{ds}$ - $V_g$  characteristic curves.



Fig. S8. XPS spectra showing S 2p core level peak regions for the pristine (a) and plasma-treated  $MoS_2$  (b-d). The fitting green and orange curves represent the contributions of 2H and 1T phases to the S 2p peaks. For the pristine  $MoS_2$ , the convoluted spectra of S 2p show two prominent peaks at 162.7 and 164.0 eV, respectively. After oxygen plasma exposure of  $MoS_2$  from 2 s to 4 s, the peak intensity of 1T-S 2p peaks gradually enhance, which indicates the increase of 1T domain concentration in  $MoS_2$ .



Fig. S9. XPS characterizations of Mo 3d (a-d) and S 2p (e-h) core level peak regions for the  $MoS_2$  after  $O_2$  plasma treatment with time varying from 6-25 s. We observed that the 1T phase concentrations continue to increase from 25% to 89% as the plasma treatment time increased.



Fig. S10. I-V characteristic curve of  $MoS_2$  device4 with plasma treatment time exceeding 6 s. (a) Optical image of  $MoS_2$  device4. Here, the channel length (L) and width (W) are 2.8 µm and 6.5 µm, respectively. (b-c) Output (b) and transfer (c) characteristics of  $MoS_2$  device4 with plasma treatment time exceeding 6 s.

Device	method	Contact Resistance	Conductivity	Mobility	On/off	Ref
		(kΩ μm)	(S m <sup>-1</sup> )	(cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> )	ratio	
MoS <sub>2</sub>	vdW	430	4.2	44	107	[1]
FET	contacts, Pt					
MoS <sub>2</sub>	vdW	2.3	~140	-	107	[2]
FET	contacts, Ag					
MoS <sub>2</sub>	vdW	3±0.3(monolayer)	20	167±20	-	[3]
FET	contacts, In	0.8±0.2(few layers)				
MoS <sub>2</sub>	1T contacts	0.2-0.3	85	50	>107	[4]
FET						
MoS <sub>2</sub>	1T contacts	0.2	~20	56	-	[5]
FET						
MoS <sub>2</sub>	Bi contacts	123	100-373	20	>107	[6]
FET						
MoS <sub>2</sub>	vdW	115	~5	35	>108	[7]
FET	contacts,					
	Graphene					
MoS <sub>2</sub>	Au contacts	6.5	~140	20	-	[8]
FET						
MoS <sub>2</sub>	Re doping	26.65	0.7	-	-	[9]
FET						
MoS <sub>2</sub>	vdW	2-20	~1	40-120	-	[10]
FET	contacts,					
	Graphene					
MoS <sub>2</sub>	vdW	1.8	~30	73	-	[11]
FET	contacts		(V <sub>G</sub> =40V)			
	BN/Au					
MoS <sub>2</sub>	Au /Al <sub>2</sub> O <sub>3</sub> /	5.4	~5	-	-	[12]
FET	TiO <sub>2</sub>					
MoS <sub>2</sub> F	Thiol-	25.2	$\sim 10 (V_G = 40$	-	-	[13]
ET	Molecules		V )			
MoS <sub>2</sub>	Cl-doped	0.5	~160 (V <sub>G</sub> =4	60	4*10 <sup>6</sup>	[14]
FET			5V)			
MoS <sub>2</sub>	Mo/Au	2	$\sim 35 (V_G = 30$	27	-	[15]
FET			V)			
MoS <sub>2</sub>	vdW 1T	4	83.8	237	104	This
FET	contacts					work

Table S1 Literature survey of electrical performance of  $MoS_2 \ devices$ 

	Property	Contact Resistances	Transconductance	Mobility	On/off
MoS <sub>2</sub> FETs		(kΩ)	(µA/V)	(cm <sup>2</sup> /V s)	ratio
Device1	Before plasma treatment	477.2	0.1	7	~10 <sup>2</sup>
(L=3µm)	O <sub>2</sub> plasma 3s	4.0	4.3	237	~104
Device2 (L=4.8µm)	O <sub>2</sub> plasma 10s		3.1	202	~10 <sup>3</sup>
Device3 (L=4.8µm)	O <sub>2</sub> plasma 5s		4.3	179	~10 <sup>3</sup>
Device4 (L=2.8µm)	Before plasma treatment		0.2	7	~10 <sup>2</sup>
	O <sub>2</sub> plasma 2s		0.9	55	~103
	O <sub>2</sub> plasma 4s		2.6	185	~104

Table S2 Comparison of MoS<sub>2</sub> FETs before and after plasma treatment

## References

[1] Y. Wang, J.C. Kim, Y. Li, K.Y. Ma, S. Hong, M. Kim, H. S. Shin, H.Y. Jeong, M. Chhowalla, P-type electrical contacts for 2D transition-metal dichalcogenides, Nature 610 (2022) 61-66.

X. Yang, J.Li, R. Song, B. Zhao, J. Tang, L. Kong, H. Huang, Z. Zhang, L. Liao, Y. Liu, X. Duan,
 X. Duan, Highly reproducible van der Waals integration of two-dimensional electronics on the wafer scale, Nat. Nanotechnol. 18 (2023) 471.

Y. Wang, J.C. Kim, R.J. Wu, J. Martinez, X. Song, J. Yang, F. Zhao, K.A. Mkhoyan, H.Y. Jeong,
 M. Chhowalla, Van der Waals contacts between three-dimensional metals and two-dimensional semiconductors, Nature 568 (2019) 70.

[4] R. Kappera, D.Voiry, S.E.Yalcin, B. Branch, G. Gupta, A.D. Mohite, M. Chhowalla, Phaseengineered low-resistance contacts for ultrathin MoS<sub>2</sub> transistors, Nat. Mater. 13 (2014) 1128-1134.

[5] R. Kappera, D. Voiry, S.E. Yalcin, W. Jen, M. Acerce, S. Torrel, B. Branch, S. Lei, W. Chen, S. Najmaei, J. Lou, P.M. Ajayan, G. Gupta, A.D. Mohite, M. Chhowalla, Metallic 1T phase source/drain electrodes for field effect transistors from chemical vapor deposited MoS<sub>2</sub>, Apl Mater. 2 (2014) 092516.
[6] P.-C. Shen, C. Su, Y. Lin, A.-S. Chou, C.-C. Cheng, J.-H. Park, M.-H. Chiu, A.-Y. Lu, H.-L. Tang, M.M. Tavakoli, G. Pitner, X. Ji, Z. Cai, N. Mao, J. Wang, V. Tung, J. Li, J. Bokor, A. Zettl, C.-I. Wu, T. Palacios, L.-J. Li, J. Kong, Ultralow contact resistance between semimetal and monolayer semiconductors, Nature 593 (2021) 211.

[7] S.-S. Chee, D. Seo, H. Kim, H. Jang, S. Lee, S.P. Moon, K.H. Lee, S.W. Kim, H. Choi, M.-H. Ham, Lowering the schottky barrier height by graphene/Ag electrodes for high-mobility MoS<sub>2</sub> field-effect transistors, Adv. Mater. 31 (2019) 1804422.

[8] K.K.H. Smithe, C.D. English, S.V. Suryavanshi, E. Pop, Intrinsic electrical transport and performance projections of synthetic monolayer  $MoS_2$  devices, 2D Mater. 4(2017) 011009.

[9] J. Gao, Y.D. Kim, L. Liang, J.C. Idrobo, P. Chow, J. Tan, B. Li, L. Li, B.G. Sumpter, T.-M. Lu, V. Meunier, J. Hone, N. Koratkar, Transition-metal substitution doping in synthetic atomically thin

semiconductors, Adv. Mater. 28 (2016) 9735.

[10] X. Cui, G.-H. Lee, Y.D. Kim, G. Arefe, P.Y. Huang, C.-H. Lee, D.A. Chenet, X. Zhang, L. Wang, F. Ye, F. Pizzocchero, B.S. Jessen, K. Watanabe, T. Taniguchi, D.A. Muller, T. Low, P. Kim, J. Hone, Multi-terminal transport measurements of MoS<sub>2</sub> using a van der Waals heterostructure device platform, Nat. Nanotech. 10 (2015) 534-540.

[11] J. Wang, Q. Yao, C.-W. Huang, X. Zou, L. Liao, S. Chen, Z. Fan, K. Zhang, W. Wu, X. Xiao, C. Jiang, W.-W. Wu, High mobility MoS<sub>2</sub> transistor with low schottky barrier contact by using atomic thick h-BN as a tunneling layer, Adv. Mater. 28 (2016) 8302-8308.

[12] W. Park, Y. Kim, S.K. Lee, U. Jung, J.H. Yang, C. Cho, Y.J. Kim, S.K. Lim, I.S. Hwang, H.-B.-R. Lee, B.H. Lee, Contact Resistance Reduction using Fermi Level De-pinning Layer for MoS<sub>2</sub> FETs, 2014 IEEE International Electron Devices Meeting, San Francisco, CA, USA (2014) 5.1.1-5.1.4.

[13] K. Cho, J. Pak, J.-K. Kim, K. Kang, T.-Y. Kim, J. Shin, B.Y. Choi, S. Chung, T. Lee, Contactengineered electrical properties of MoS<sub>2</sub> field-effect transistors via electively deposited thiol-molecules, Adv. Mater. 30 (2018) 1705540.

[14] L. Yang, K. Majumdar, H. Liu, Y. Du, H. Wu, M. Hatzistergos, P.Y. Hung, R. Tieckelmann, W. Tsai, C. Hobbs, P.D. Ye, Chloride molecular doping technique on 2D materials: WS<sub>2</sub> and MoS<sub>2</sub>, Nano Lett. 14 (2014) 6275-6280.

[15] J. Kang, W. Liu, K. Banerjee, High-performance  $MoS_2$  transistors with low-resistance molybdenum contacts, Appl. Phys. Lett. 104 (2014) 093106.