Supporting Information

Iodide Substitution Induced Phase Transition of Chemical Vapor Deposited MoS_2

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1. AFM image for MoS_2 before and after KI treatment.

The AFM image for MoS_2 after treatment was almost identical to that before treatment, which shows almost no extra contamination residual was introduced to the surface of MoS_2 as well as the excellent integrity of sample.

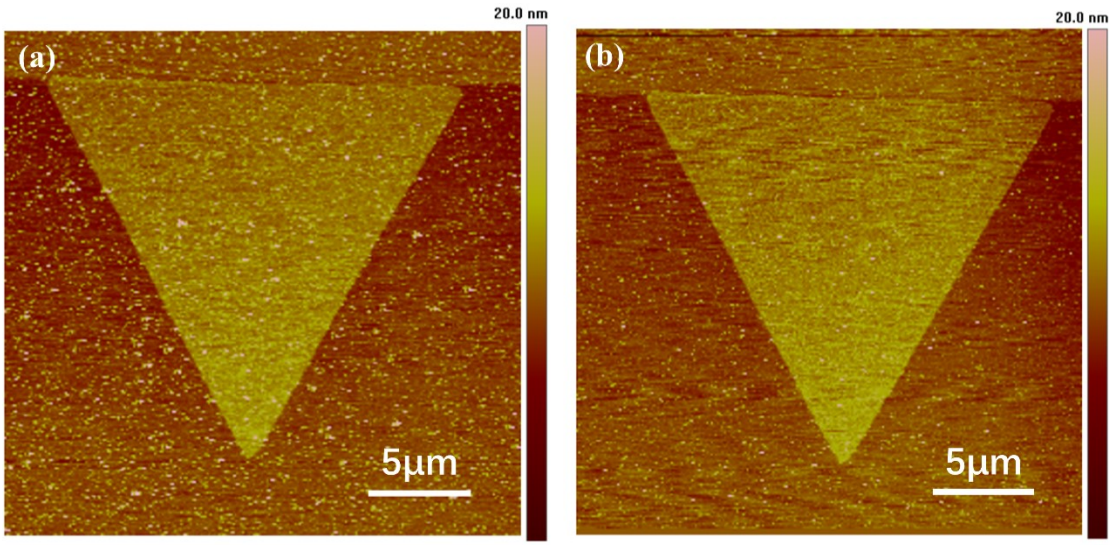

Fig. S1. (a) AFM image of CVD-grown MoS_2 before KI treatment. (b) AFM image of same MoS_2 after KI treatment.

2.Raman spectra for MoS_2 soaked in KI solution for 2 days

The experiment of soaking MoS_2 into KI solution for 2 days was carried, and then Raman analysis was implemented. The Raman spectra is shown below. It is almost identical with spectra of MoS_2 dipped for 20 mins.

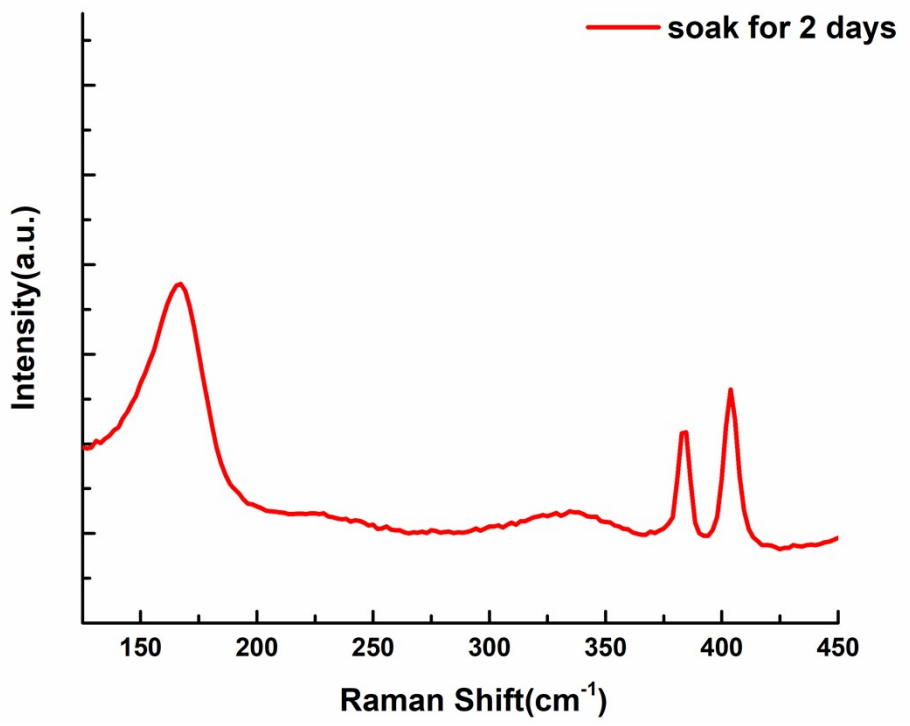

Fig. S2. Raman spectra of the MoS_2 soaked into KI solution for 2 days.

3. Stability of MoS_2 undergone the phase transition by KI treatment.

Raman spectra of MoS_2 was acquired after being treated with KI, and J_1, J_2 and J_3 were observed. Then same sample was placed in air and tested 5 days, 10 days and 30 days later respectively. The results showing that J_1, J_2 and J_3 were clear and almost identical even placed under ambient condition for one month. This result shows good stability of MoS_2 treated with KI treatment.

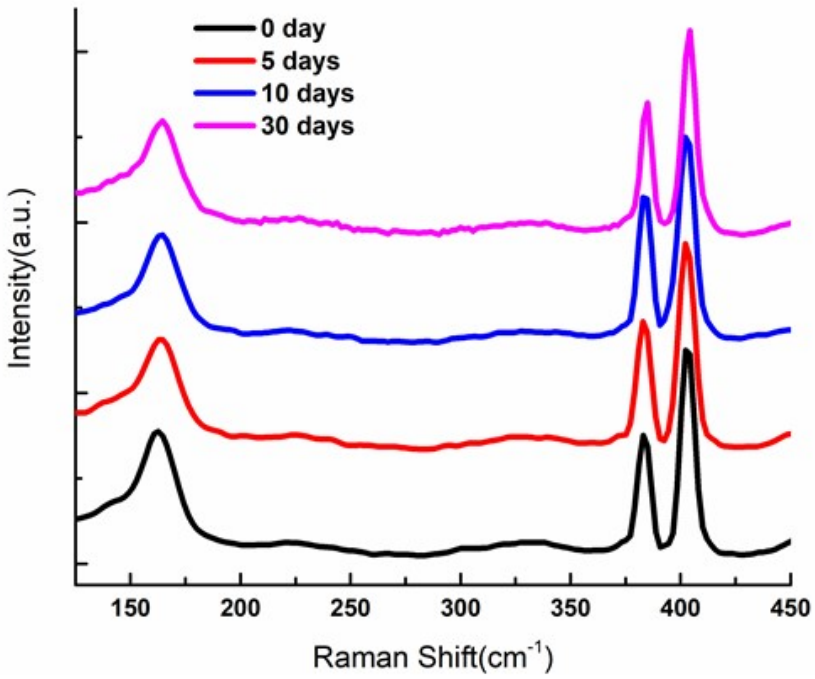

Fig. S3. Raman spectra of same MoS_2 under ambient condition 5 days, 10 days and 30 days after KI treatment.

4. Calculation method

All calculations are done using the calculation tool vasp[1] based on density functional theory. A 6×6×1 k grid mesh is used in the calculation. The Perdew–Burke–Ernzerhof form generalized gradient approximation is used to consider the exchange correlation energy between electrons. The cutoff energy of the plane wave basis set is always set to 530eV. In order to consider the single-layer problem, there is a vacuum layer of at least 15Å in the c direction to ensure that the interaction between the layers is negligible. The atom and the lattice are fully optimized until the force on the atom is less than 0.1 eV/Å. The calculated energy band of the undoped 2H phase MoS2 under similar parameters is consistent with the previous results[3], which also proves the reliability of the calculation.

5. Optical microscope image of the MoS_2 transistors.

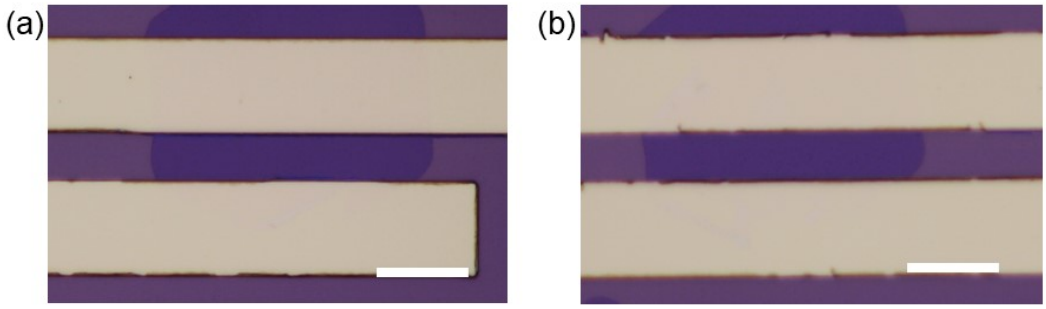

Fig. S4. (a) Normal MoS_2 transistor fabricated with standard process. (b) MoS_2 transistor with selected-area phase transition treatment. Scale bars in both figures was 20 μm.

6. Contact resistance extraction of the MoS_2 transistors.

The contact resistance of MoS_2 transistor with and without KI treatment were extracted respectively. The simplified I-V equation can be expressed as[2]

$$I_D = \frac{\mu_0}{1 + \theta(V_{gs} - V_{th})} C_0 V_{ds} \frac{W}{L} (V_{gs} - V_{t} \quad (1)$$

.

With $\theta \approx \mu_o C_o R_c W/L$, R_c can be extracted from the strong inversion region. The low-field mobility (μ_o) and threshold voltage (V_{th}) here can be extracted via Y-function method with the simplified expression

$$Y = \frac{I_d}{\sqrt{g_m}} = \sqrt{\mu_0 C_0 V_d \frac{W}{L}} (V_{gs} - V_{th}) \quad (2)$$

.

The g_m here is the transconductance defined as dI_d/dV_{gs}, C_o is the gate capacitance per unit area. From the linear fit in the strong inversion region, V_{th} and μ_o can be extracted from the intercept and the slope, respectively. Then substitute them into Eq 1, value of θ can be acquired as well as that of R_c. Using this method, μ_o of MoS_2 FET treated with KI and normal MoS_2 FET were extracted as 3.51 and 0.32 cm^2/Vs respectively, and the contact resistance R_c were 59 and 1.94×10^4 $k\Omega\cdot\mu m$, respectively. The substantially reduction of contact resistance was just caused by KI treatment.

Reference

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3. The Materials, P. Materials Data on MoS2 (SG:164) by Materials Project. The Materials Project 2017. https://materialsproject.org/materials/mp-1023939/ (accessed Oct 8, 2021).