Center for Energy Efficient Electronics Science

Synthesis and characterization of 2D Materials

towards Energy Efficient Electronics

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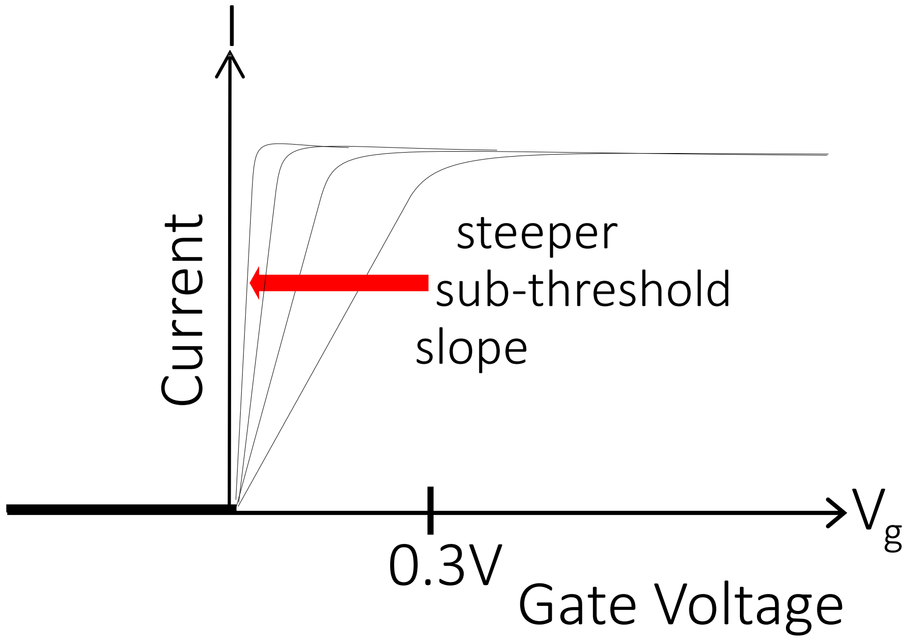
E3S Seminar

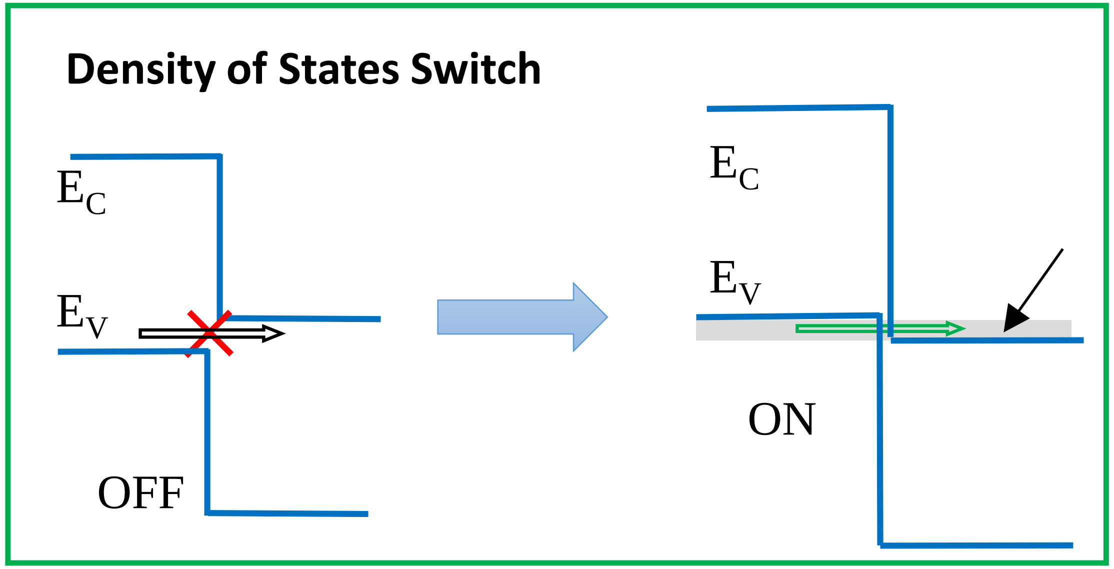
December 6, 2017

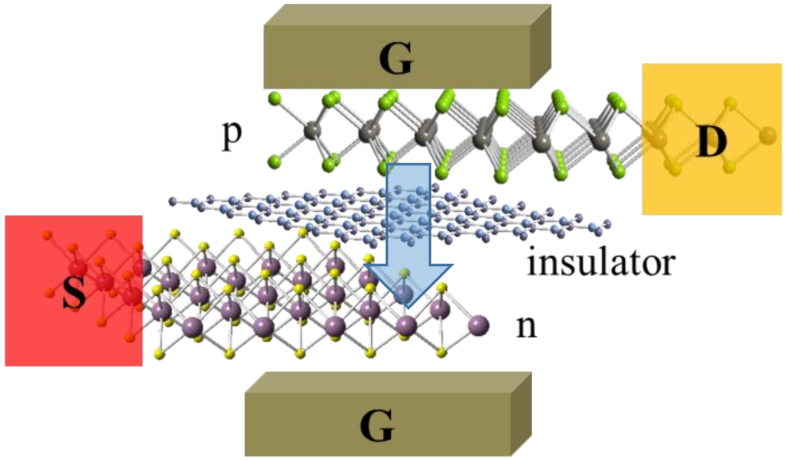
Collaborators: Eli Yablonovitch, Ali Javey, David Zubia, Jeff Bokor

A Science & Technology Center

Tunnel Transistors As a More Sensitive Electronic Switch







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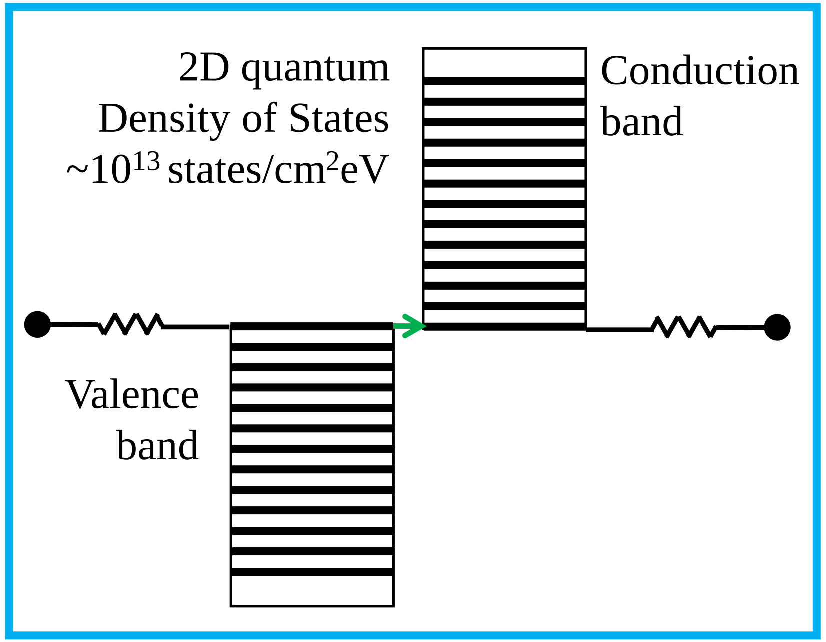
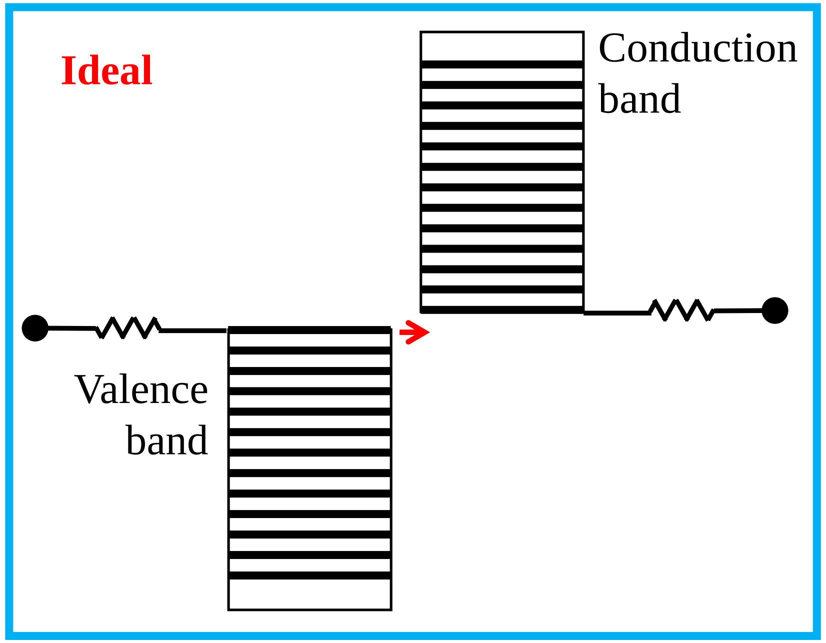
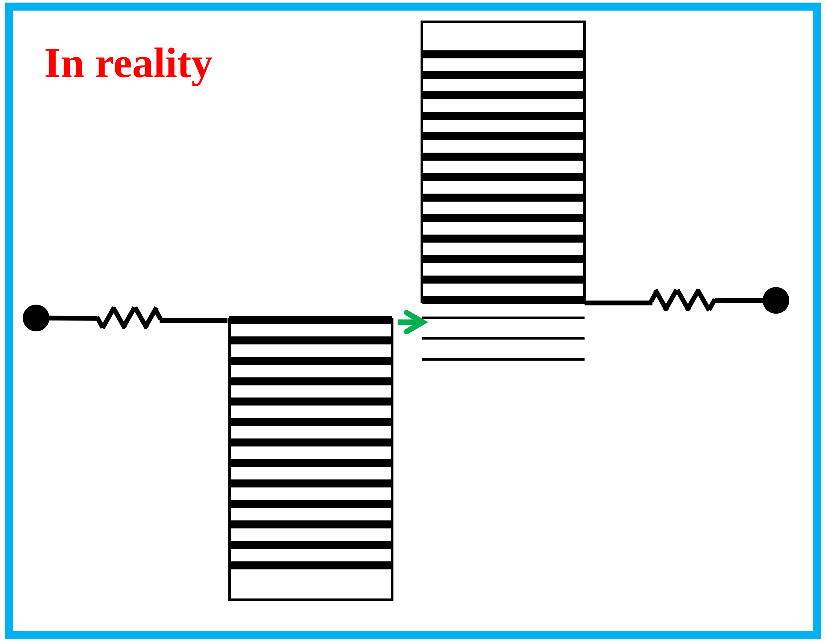
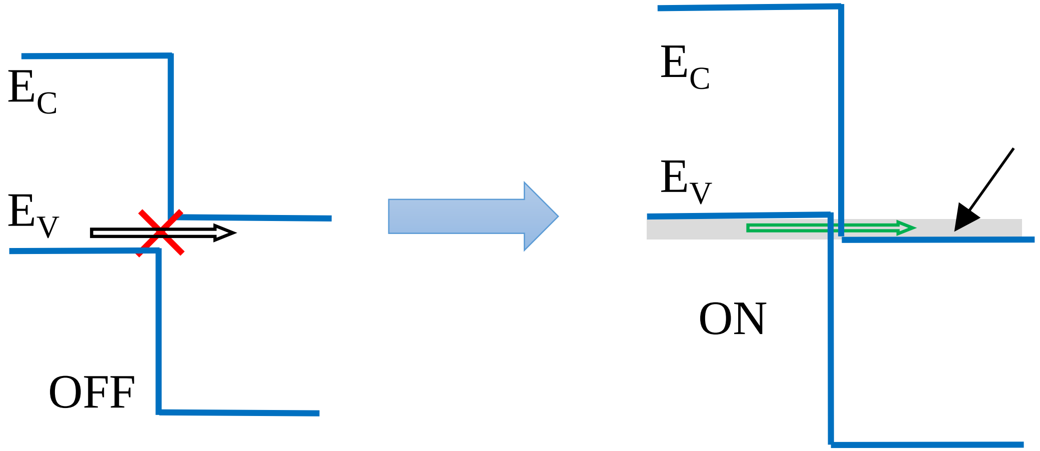
Tunnel Transistors As a More Sensitive Electronic Switch







Density of States Switch



Can we achieve 2D materials with 2D interface defect density <<10^{12} states/cm^{2}eV?

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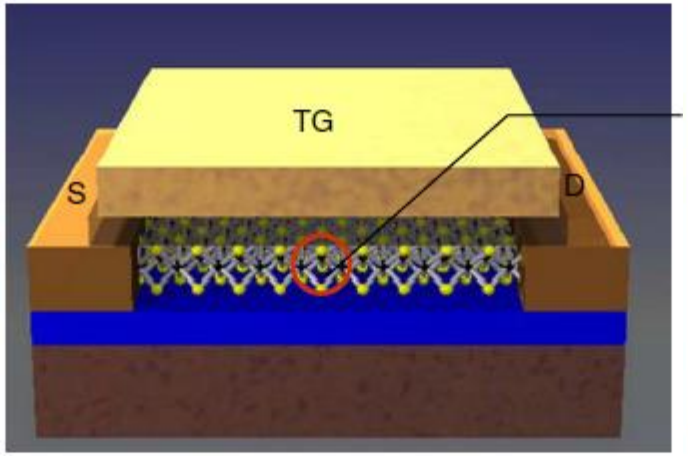
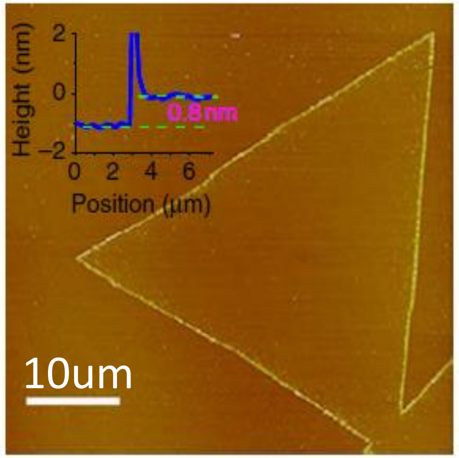
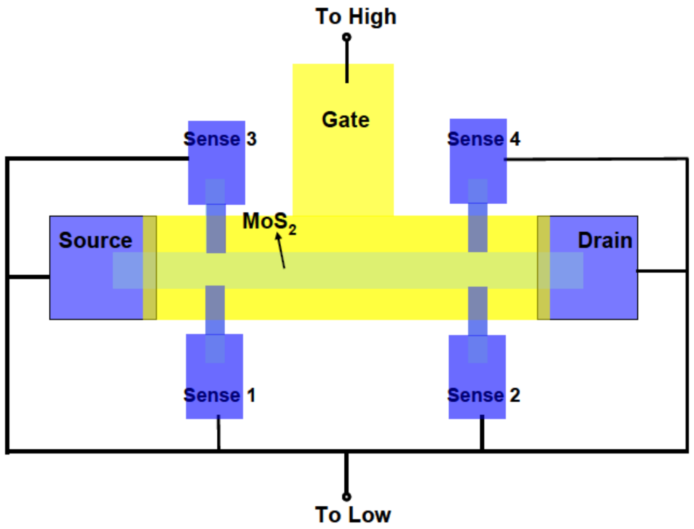
D_{it} Through Capacitance and AC Conductance Measurements



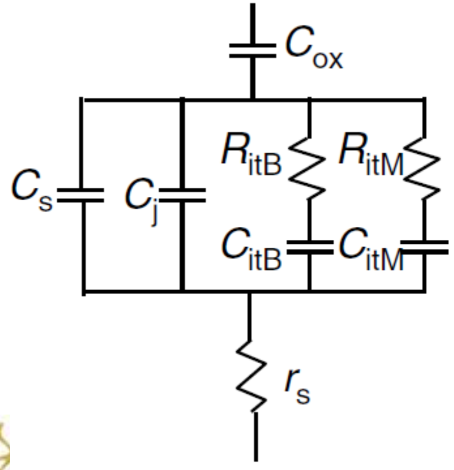




W. Zhu et. al, **Nat. Comm.** DOI: 10.1038/ncomms4087 (2014)

Device model:

$$Z = (Y_{\mathrm{itB}} + Y_{\mathrm{itM}} + i\omega C_{\mathrm{s}} + i\omega C_{\mathrm{j}})^{-1} + (i\omega C_{\mathrm{ox}})^{-1} + r_{\mathrm{s}} \qquad C_{\mathrm{ms}} = -\frac{1}{\omega * \mathrm{Im}[Z]}$$



- C_s: the quantum capacitance, C_j: the parasitic capacitance, C_{ox}: the oxide capacitance, r_s: the series resistance
- Y_{itM} and Y_{itB}: admittance of the traps ($Y_{itB}=[\tau_{itB}/C_{itB}+1/(i\omega C_{itB})]^{-1}$)

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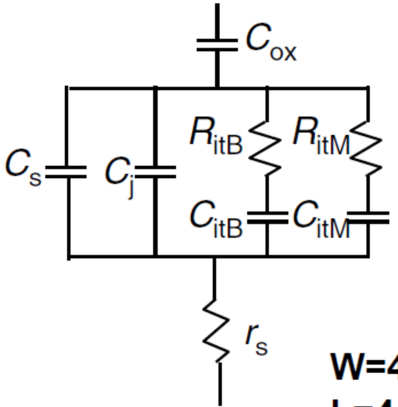
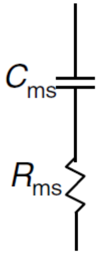
D_{it} Through Capacitance and AC Conductance Measurements

Device model: $$Z = (Y_{itB} + Y_{itM} + i\omega C_s + i\omega C_j)^{-1} + (i\omega C_{ox})^{-1} + r_s$$

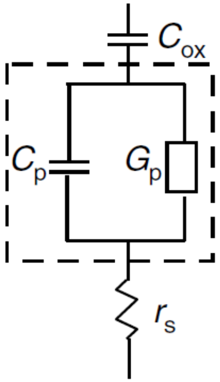


W=4μm
L=44μm

Measurement model: $$C_{ms} = -\frac{1}{\omega * \mathrm{Im}[Z]}$$



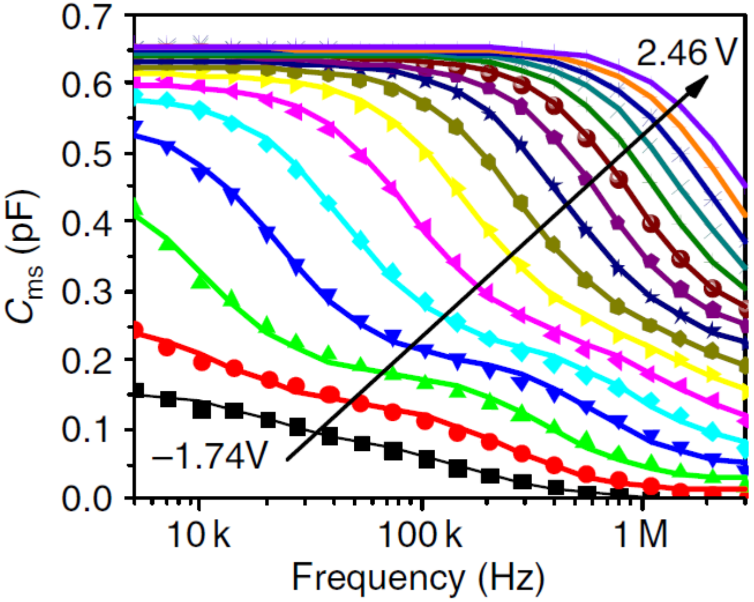
Parallel model:

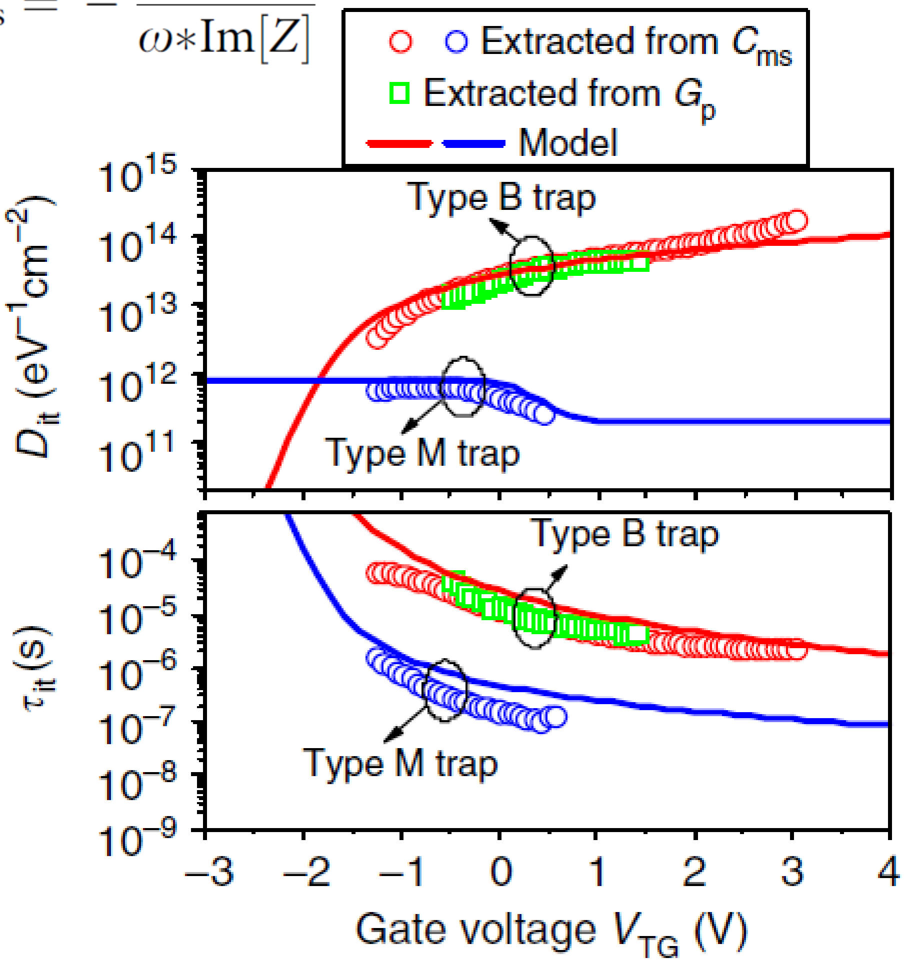


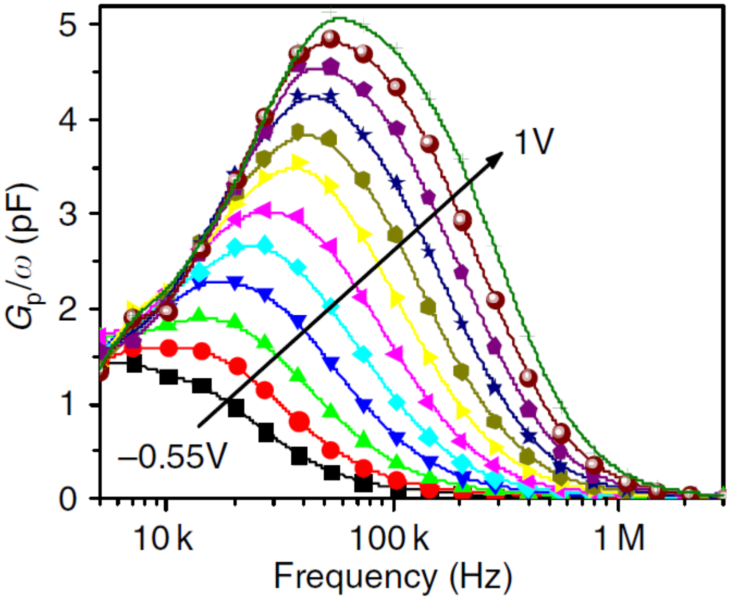
$$\frac{G_p(\omega)}{\omega} = \frac{eD_{itB}}{2\omega\tau_{itB}} \ln[1 + (\omega\tau_{itB})^2]$$

$$D_{itB} = \frac{2.5}{e}\left(\frac{G_p}{\omega}\right)_{\mathrm{peak}}$$

$$\tau_{itB} = \frac{1.98}{2 \times 3.14 \times f_0}.$$







W. Zhu et. al, **Nat. Comm.** DOI: 10.1038/ncomms4087 (2014)

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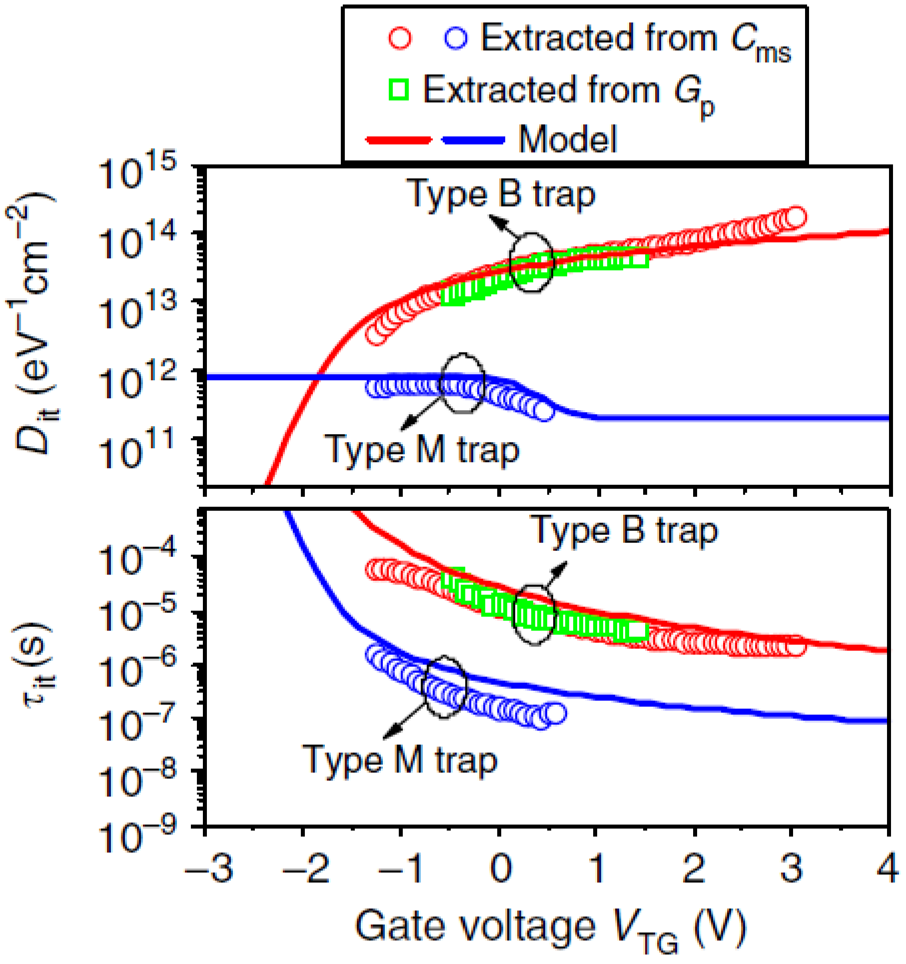
D_{it} Through Capacitance and AC Conductance Measurements



$$D_n(E) = \begin{cases} \alpha D_0 \exp\left[\frac{E-E_D}{\varphi}\right] + D_{itM}, & E_D - \frac{1}{2}E_G < E < E_D \\ D_0 - (1-\alpha) D_0 \exp\left[-\frac{E-E_D}{\varphi'}\right] + D_{itM}, & E > E_D \end{cases}$$

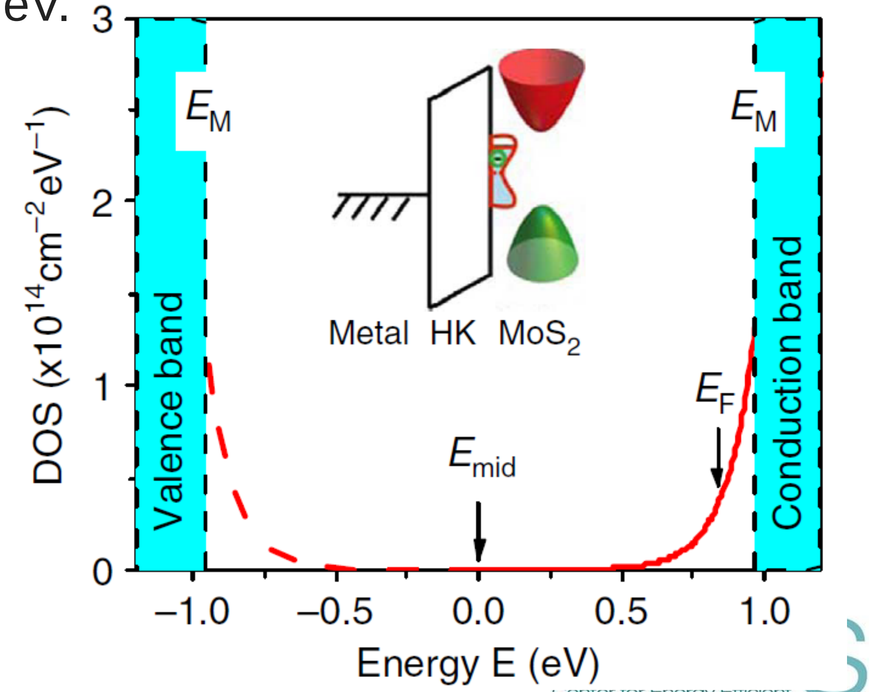
D_0 : 3.3 × 10^{14} eV^{-1}cm^{-2} (the 2D density-of-states for MoS_2)

φ : the characteristic energy width of the band tail

φ' is chosen so that the two piece-wise functions have continuous gradients at E_D

Best fit α=0.33 and φ = 100 meV.

- band tail states follow an exponentially decaying behavior
- a significantly large energy width of 100 meV



W. Zhu et. al, **Nat. Comm.** DOI: 10.1038/ncomms4087 (2014)

Improving from previous results

- Understanding of the microscopic origin of these trap states is critical for further improvement of the material’s electronic properties
  - ➢ Contribution from the substrate, processing:
    - o hBN substrate vs. SiO2
    - o Transfer process
  - ➢ Intrinsic materials quality
    - o Characterization /correlation
    - o Improve on the synthesis process

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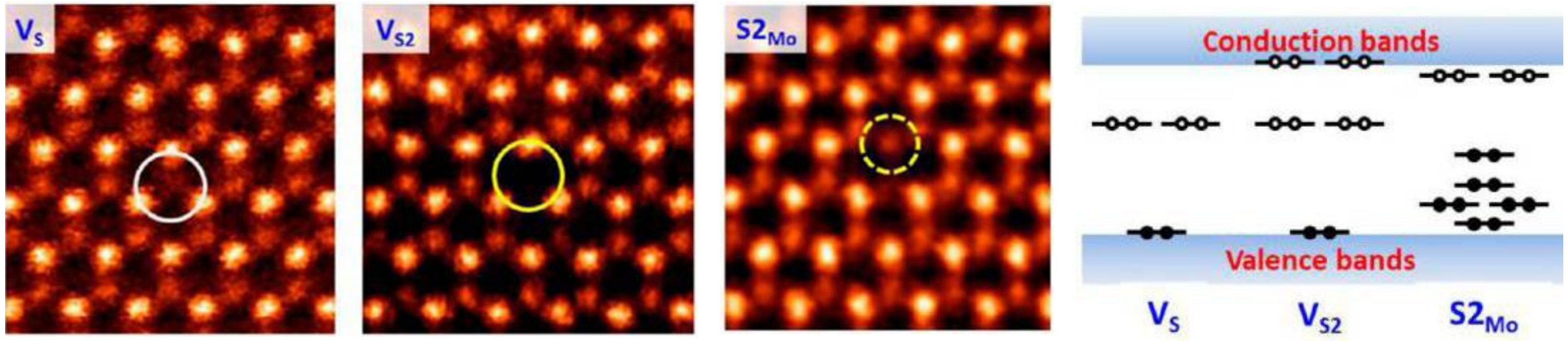
Goal: High quality 2D materials with low defect densities

- <u>Defect characterization</u>
  - ➢Various types of defects and characterization development
  - ➢Contribution to defect states



W. Zhou et. al, **Nano Letters** 13, 2615-2622, (2013)

- <u>Defect traps states characterization</u>
  - C-V and D_{it} measurement
  - Correlation with device characteristics: mobility, contact resistance
  - Correlation with optical characteristics?

MoS2 will be used as a model system
Work in Progress!

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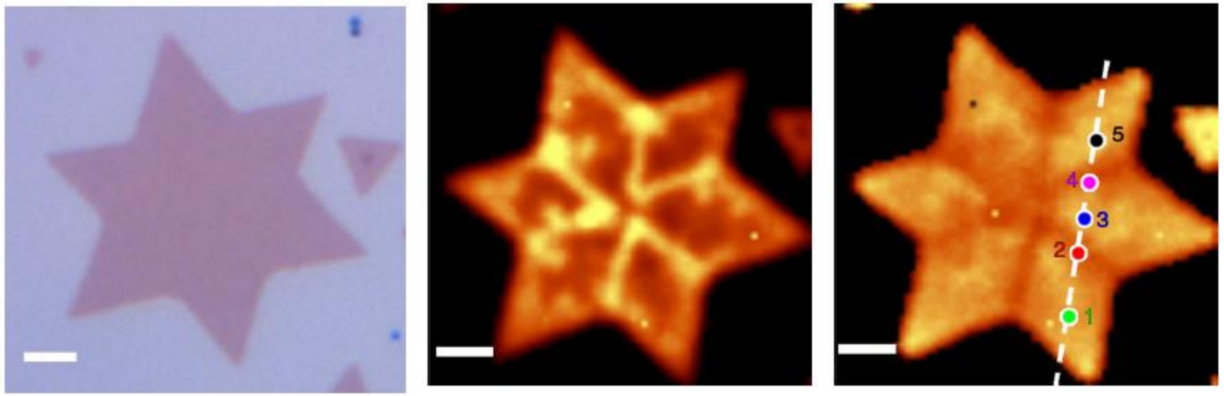
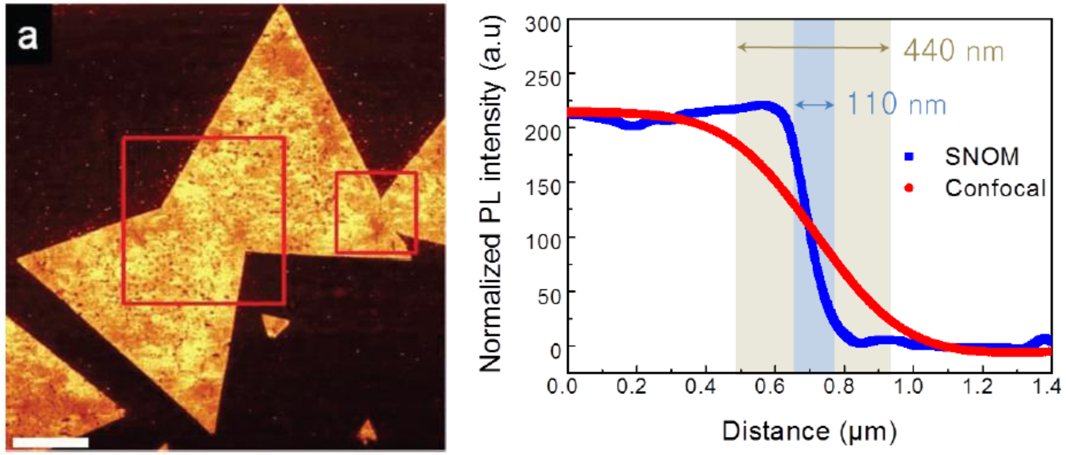
Grain boundary defect characterization

- Photoluminescence mapping (Intensity, peak position): 440nm resolution



Z. Liu et. al, **Nat. Comm** 5, 5346 (2014)

- SNOM PL mapping: 110nm resolution



Y. Lee et. al, **Nanoscale** 7, 11909 (2015)

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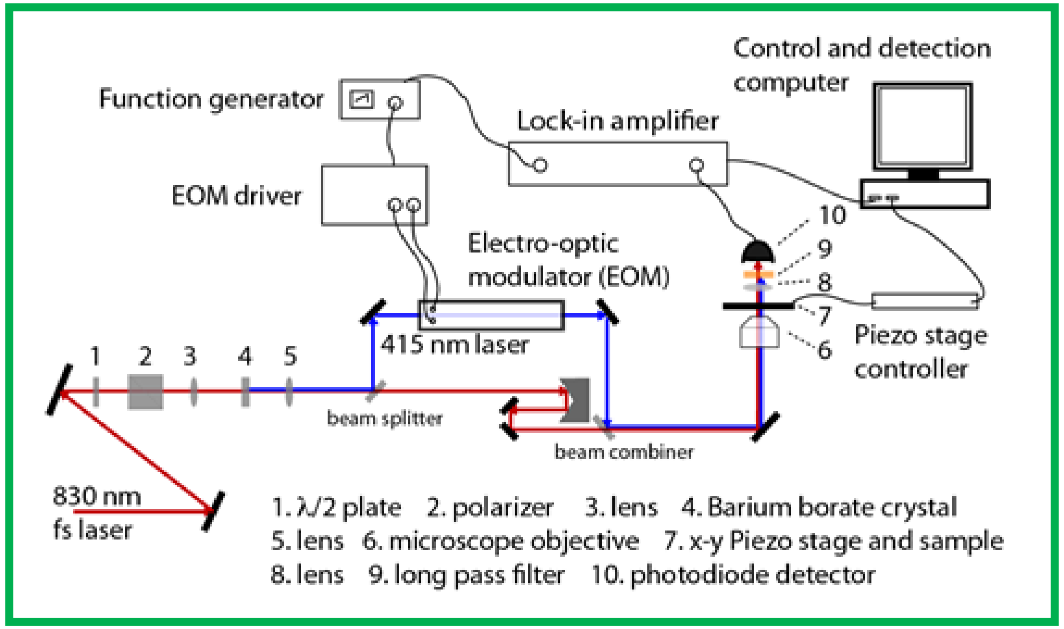
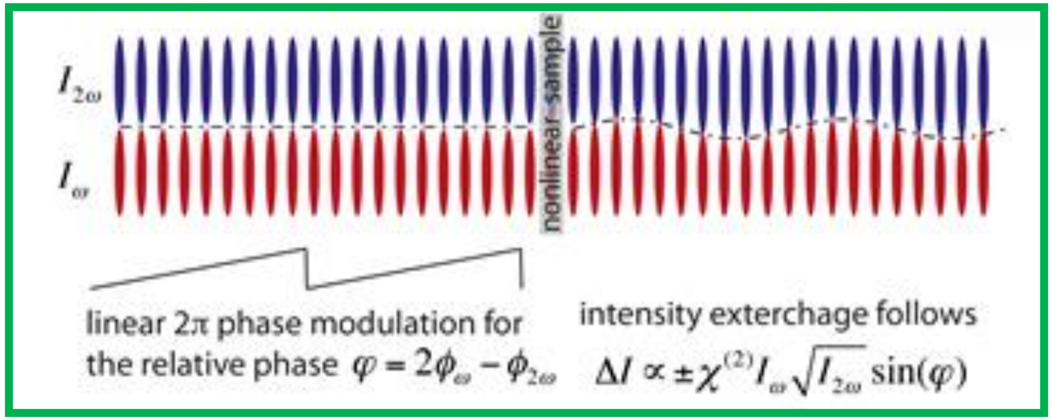
Phase-Modulated Optical Parametric Amplification Imaging

- EOM: modulates the relative optical phase between the two fields (1 MHz to a depth of 2π) according to a saw tooth waveform
- the two fields exchange intensity according to the phase modulation and the sample's nonlinear response
- Advantages over SHG:
  - Much easier
    - No need for single photon detector
    - Normal room lighting
  - Capture phase of the input signal in addition to its magnitude





Y. Gao et. al., manuscript in preparation

Collaboration with William Tisdale group in Chem E at MIT

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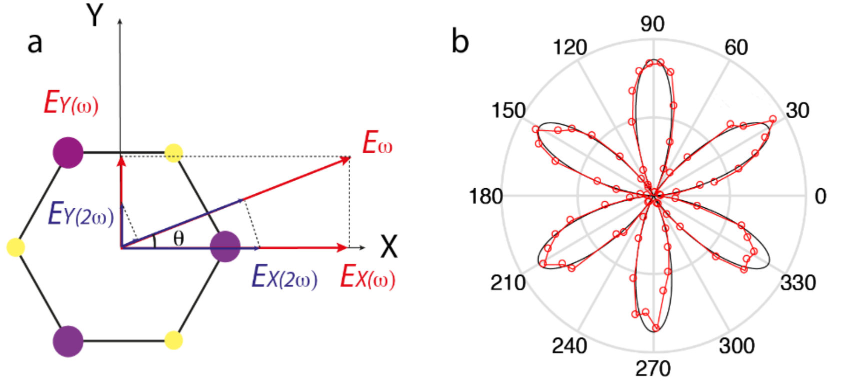
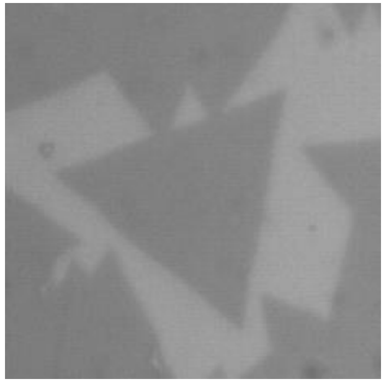
MoS_2 Grain Orientation

- Second harmonic generation (SHG) in monolayer MoS2

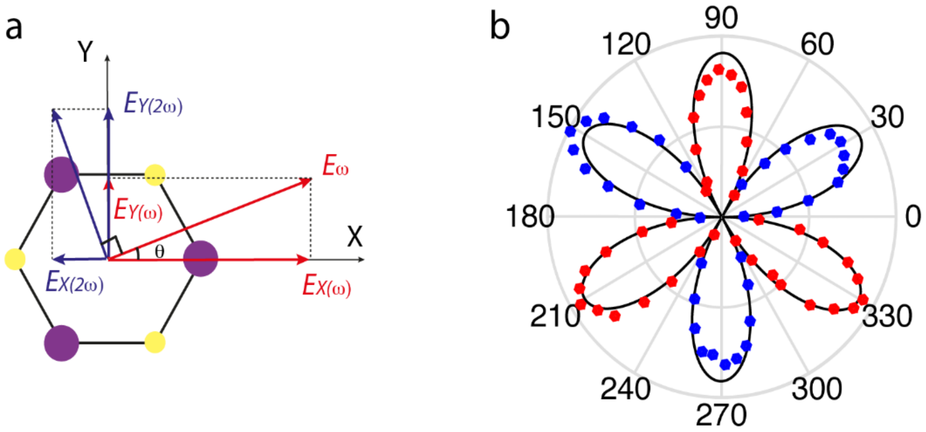


$$E_{\perp}^{2\omega} \propto -\chi_{xxx} \sin 3\theta \qquad I_{\perp}^{2\omega} \propto (\chi_{xxx} \sin 3\theta)^2$$

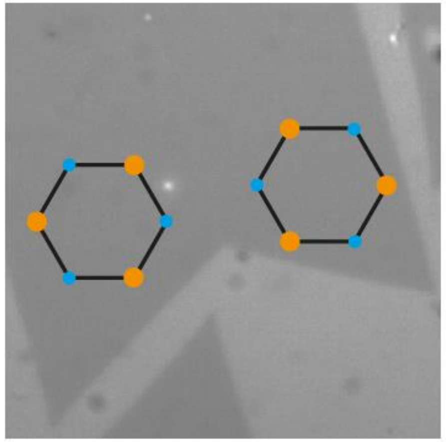


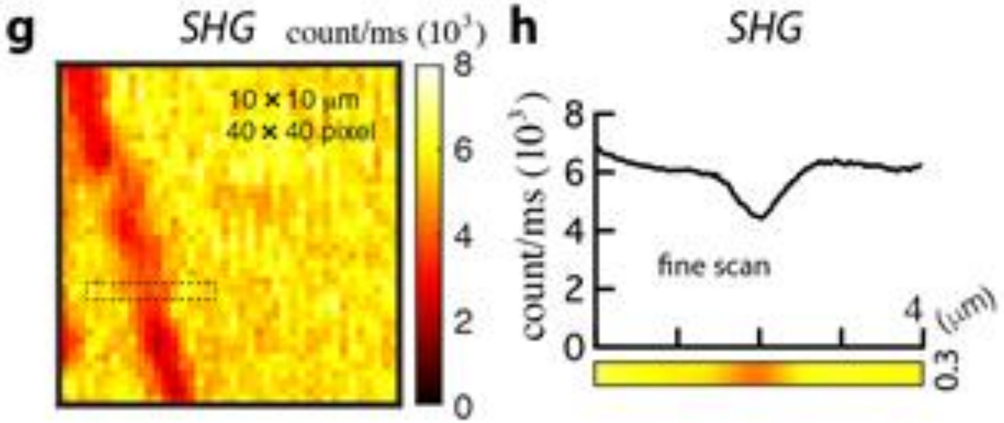
θ: orientation of monolayer MoS_2 triangle relative to the field polarizations

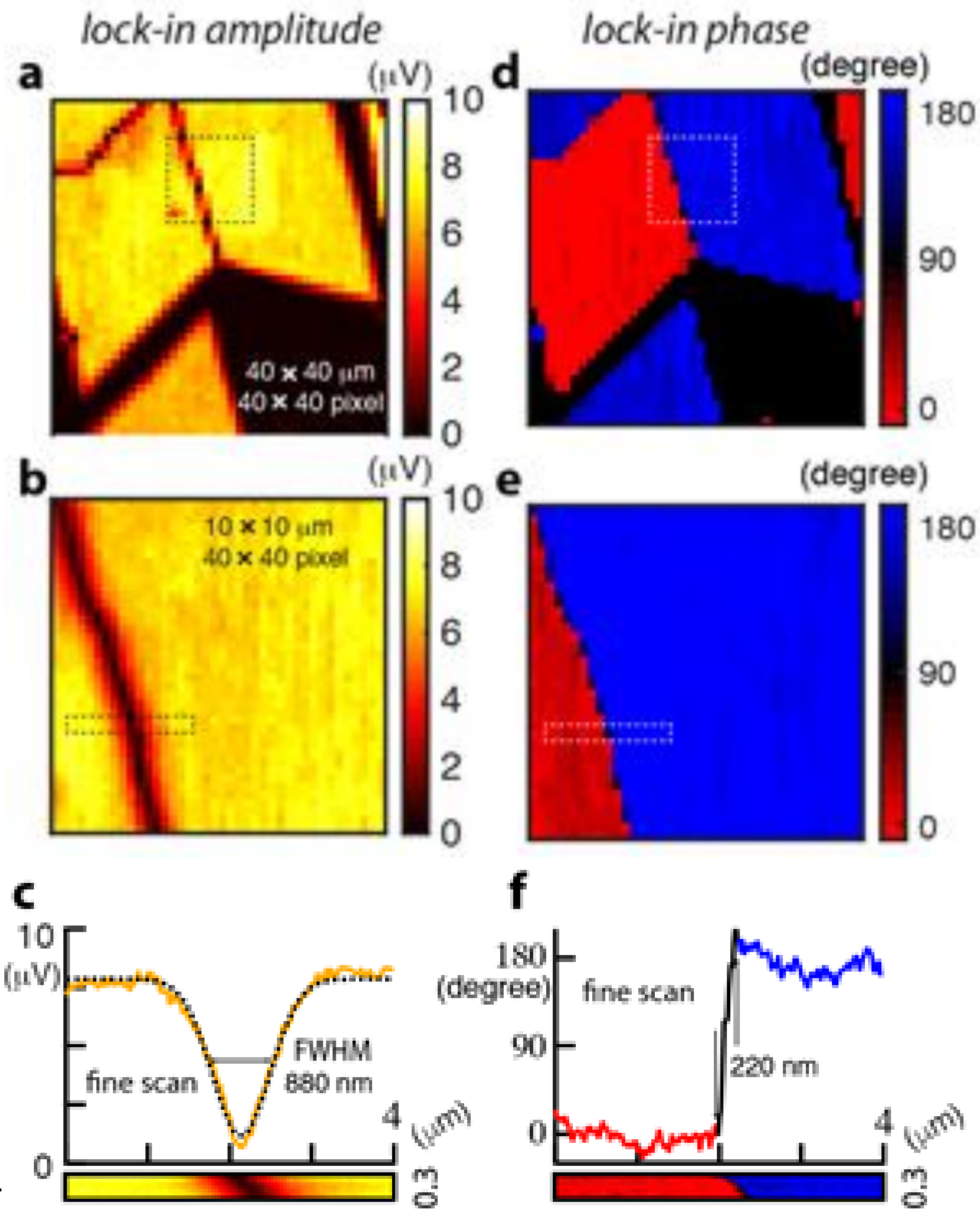
- pOPA signals in monolayer MoS2



MoS_2 Grain Characterization







- Grains with mirror symmetry distinguished
- Better contrast and higher resolution

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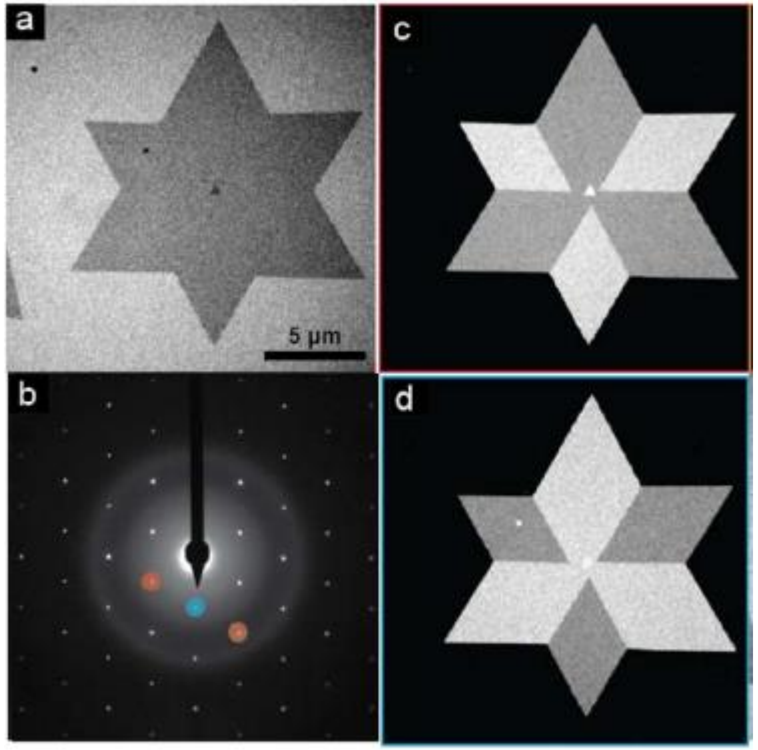
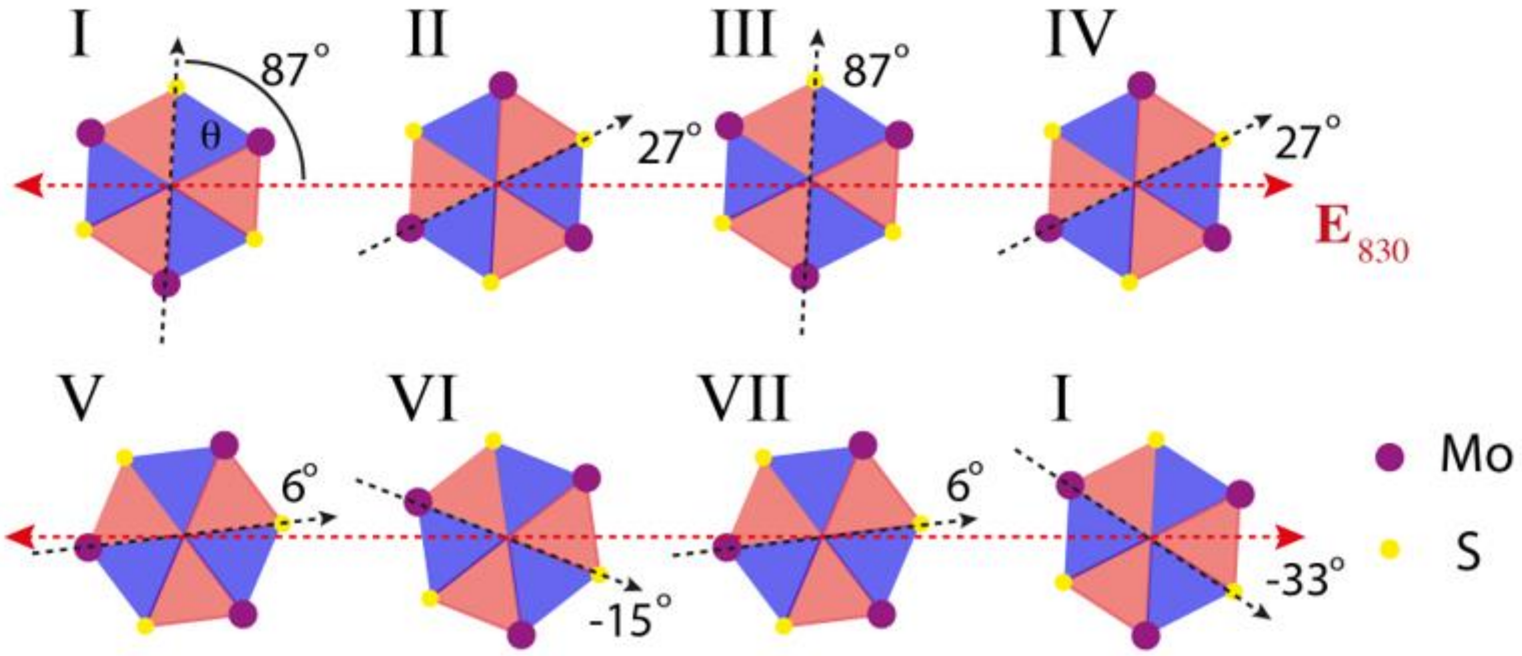
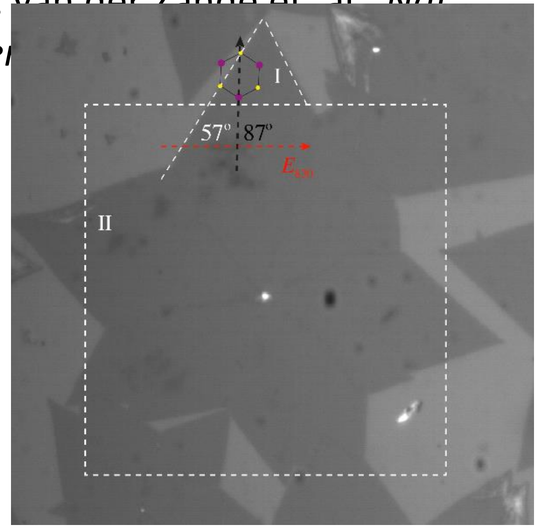
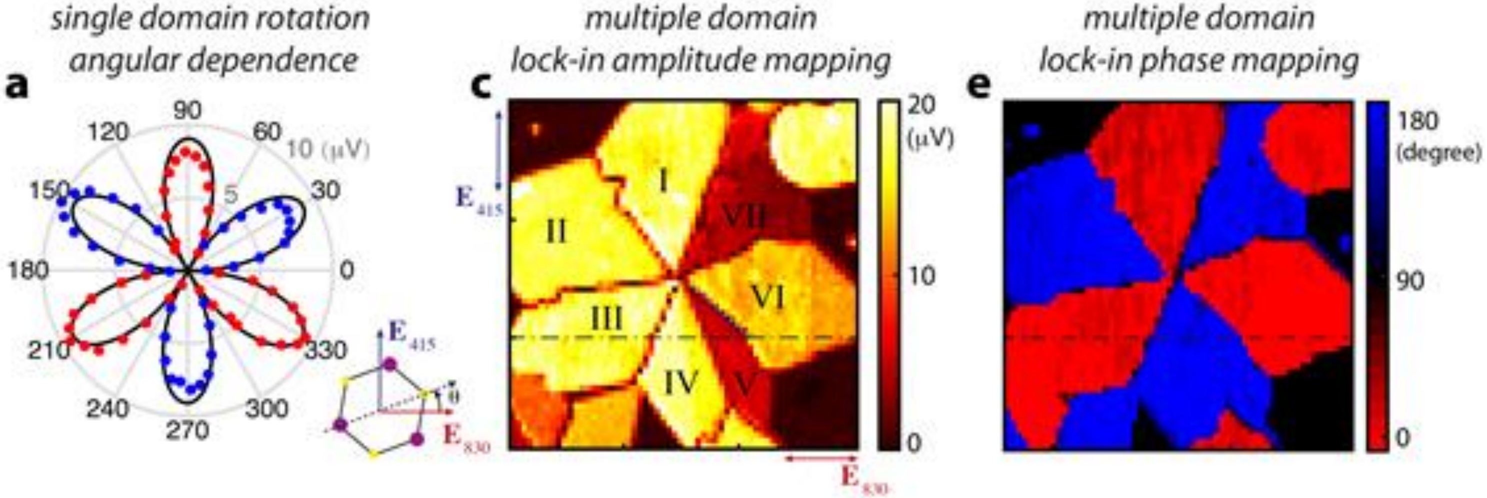
MoS_2 Grain Characterization



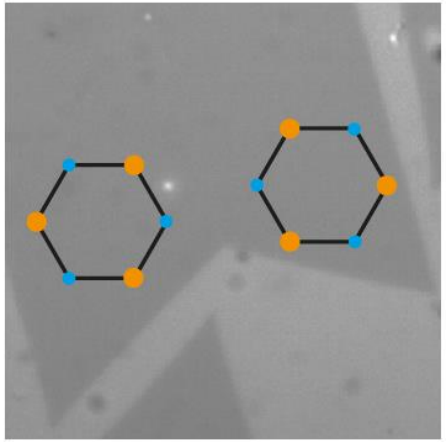


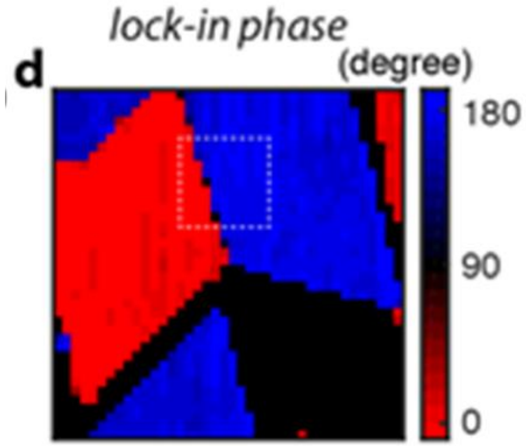
A. M. van der Zande et. al., *Nat. Mater*

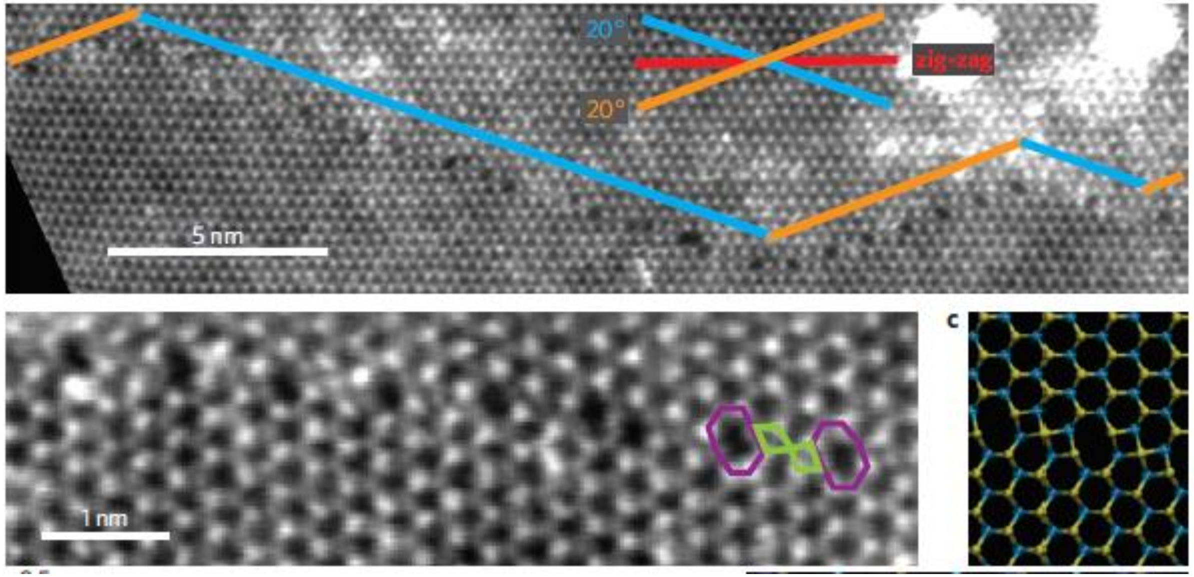




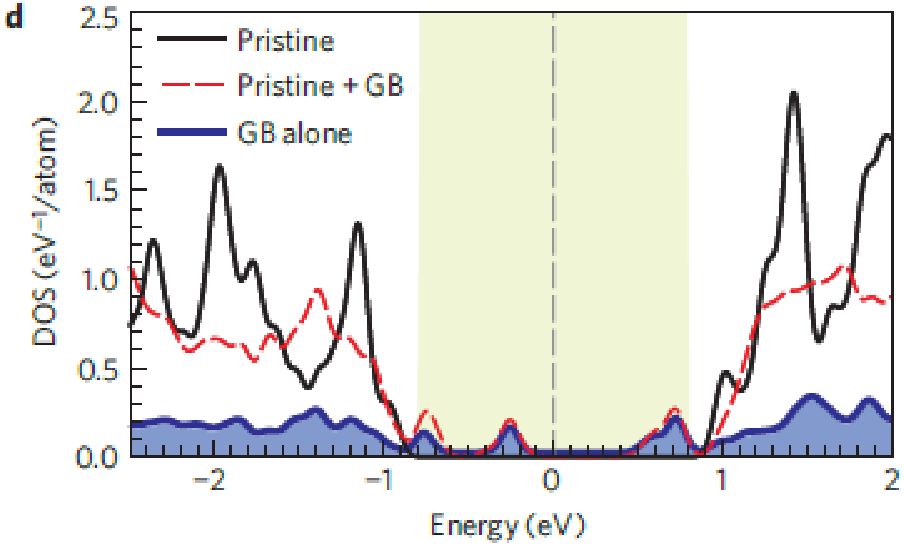
MoS_2 Grain Characterization







- Various types of grain boundaries contribute to midgap states or even metallic conduction
- Need to avoid these via growth of much larger single crystalline domains



Y. Gao et. al., manuscript in preparation

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A. M. van der Zande et. al., *Nat Mater* **12**, 554-561 (2013)

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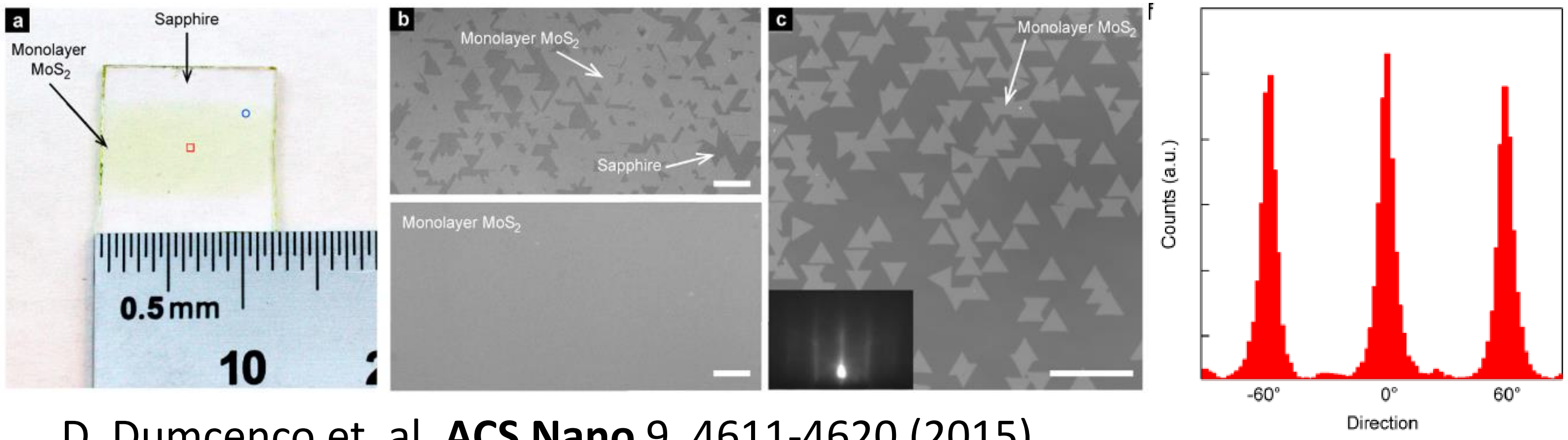
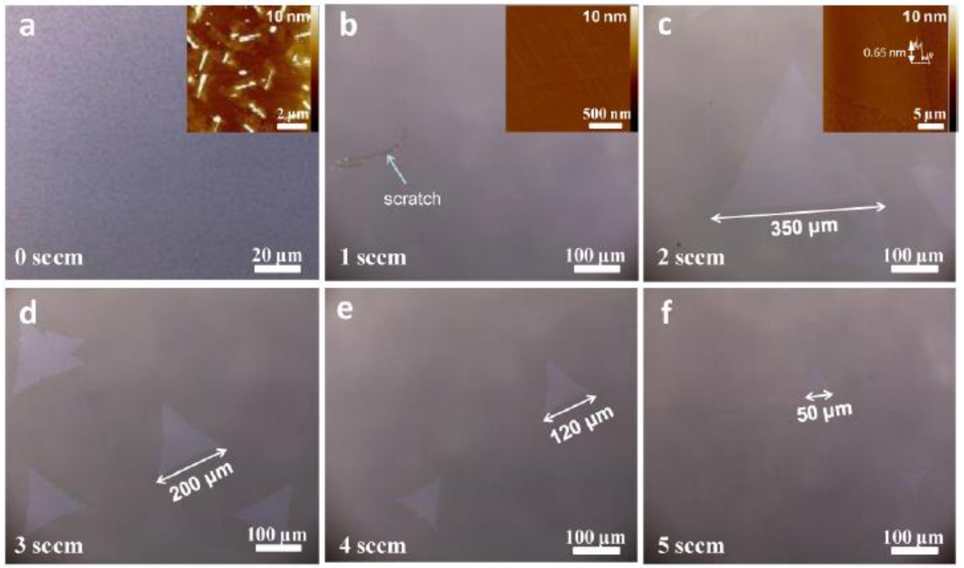
Moving forward: large single crystal grains in MoS_2

- single crystalline Sapphire growth substrate



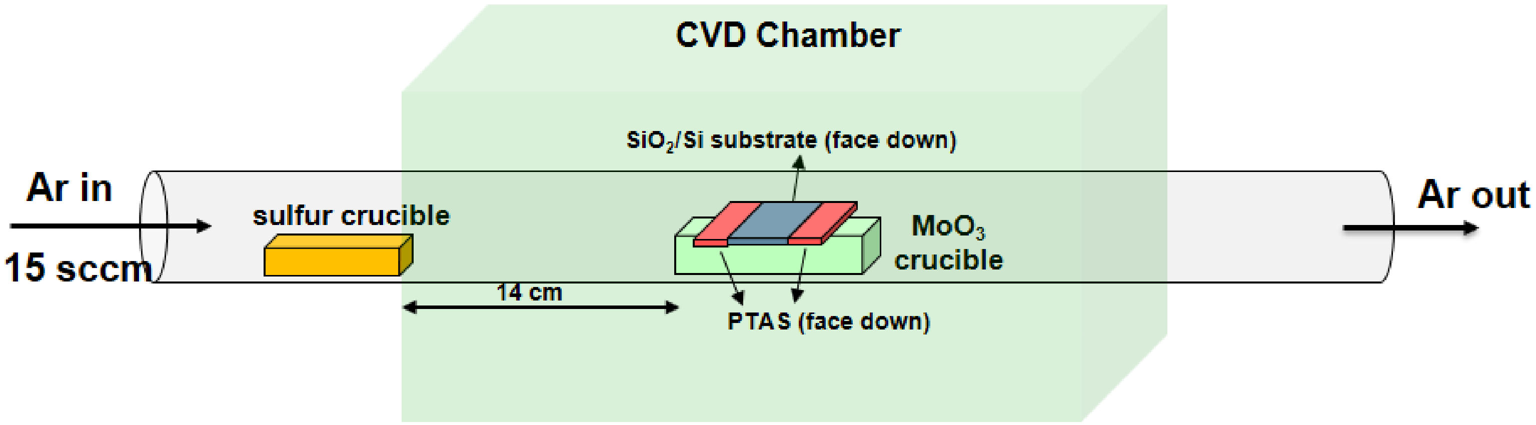
D. Dumcenco et. al, **ACS Nano** 9, 4611-4620 (2015)

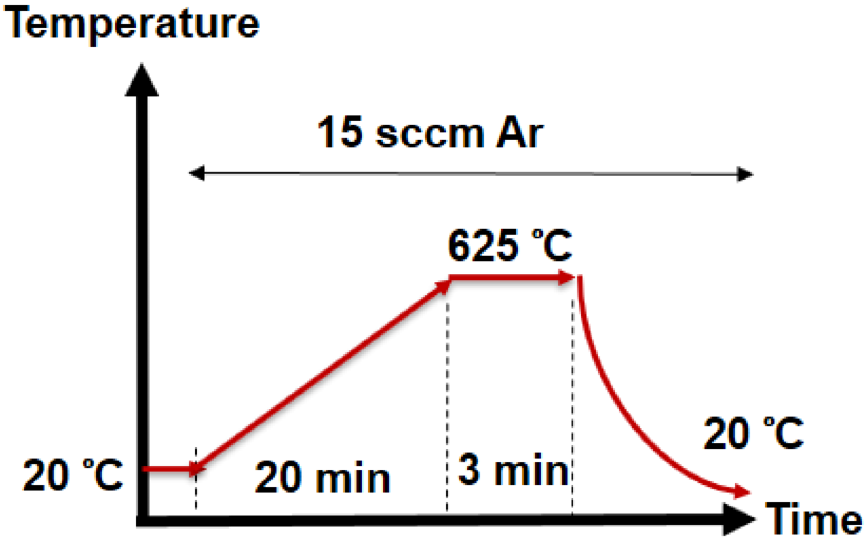
- Oxygen assisted CVD

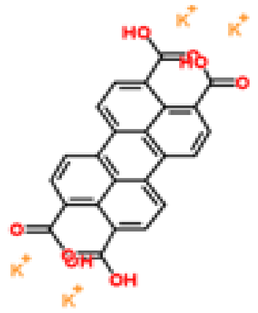


W. Chen et. al, **JACS** 137, 15632 (2015)

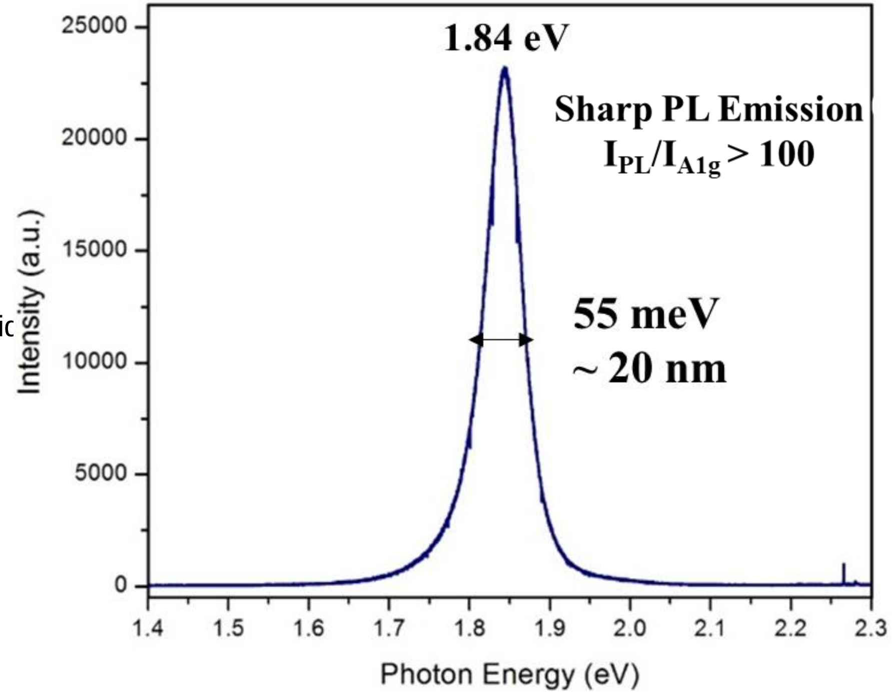
Improvement on the synthesis and transfer







perylene-3,4,9,10-tetracarboxylic acid tetrapotassium salt (PTAS)

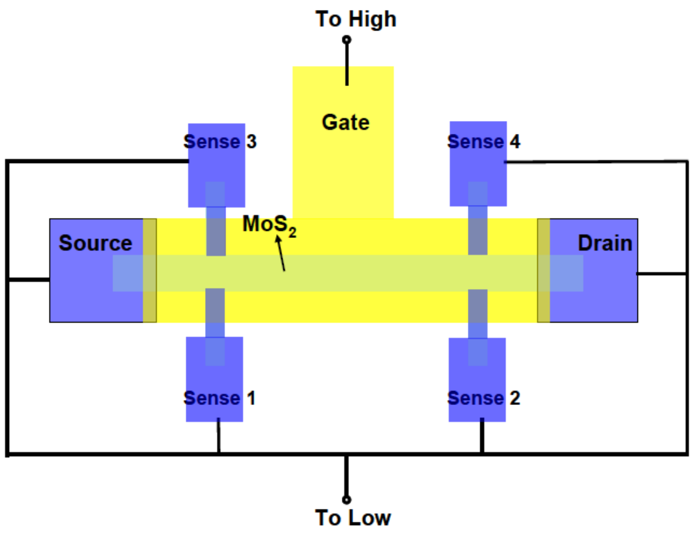


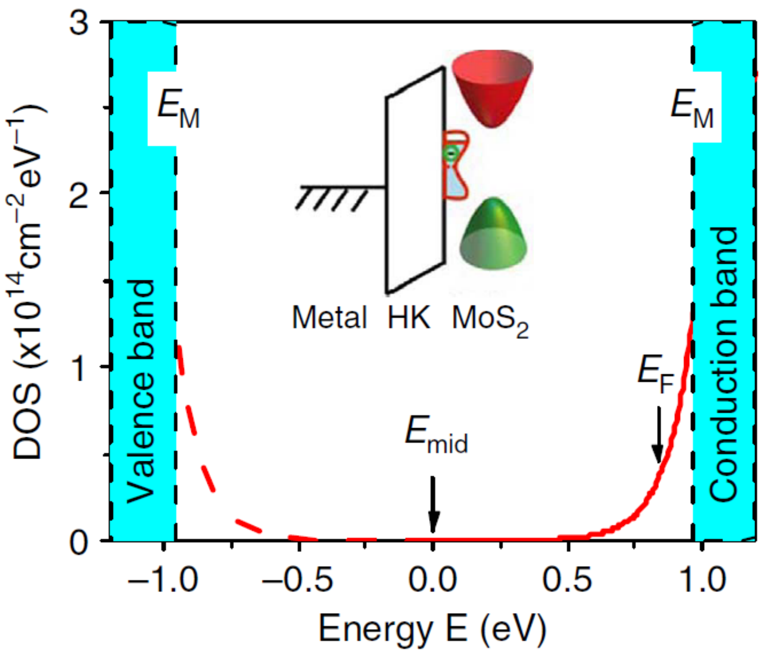
- Simpler PL features instead of PL quantum yield?
- Surface passivation with superacid treatment:
  - Significant impact in optoelectronic applications
  - Effect of passivation on electronic or defect states?

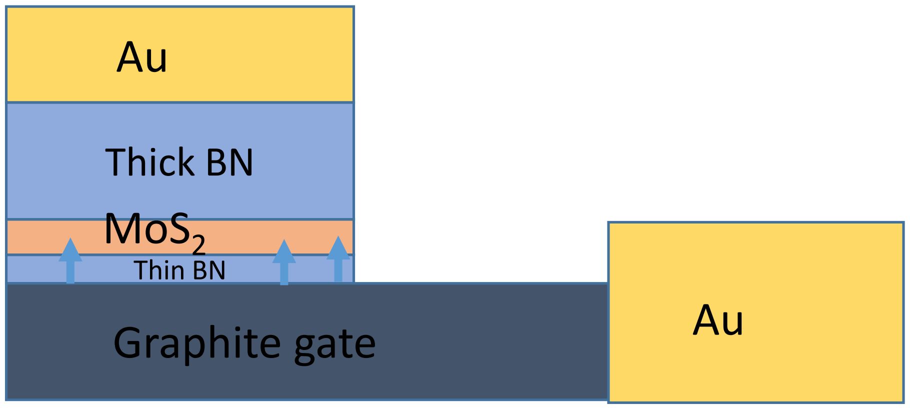
Moving forward: Correlating optical with electrical characterizations

- C-V measurement and device characterizations on MoS2 with various PL characteristics
  - ➢ Superacid treated MoS_2

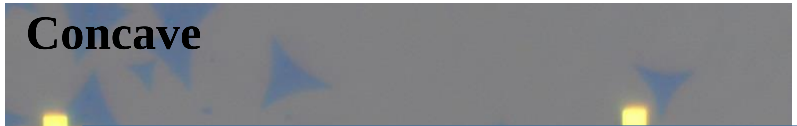
- Capacitance measurement through “vertical” devices instead of “lateral”: (collaboration with Prof. Ray Ashoori group at MIT)

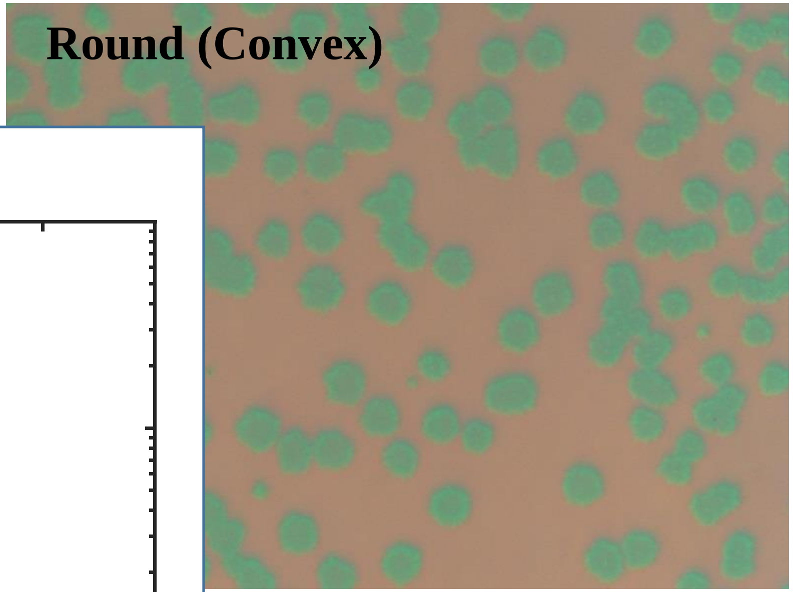


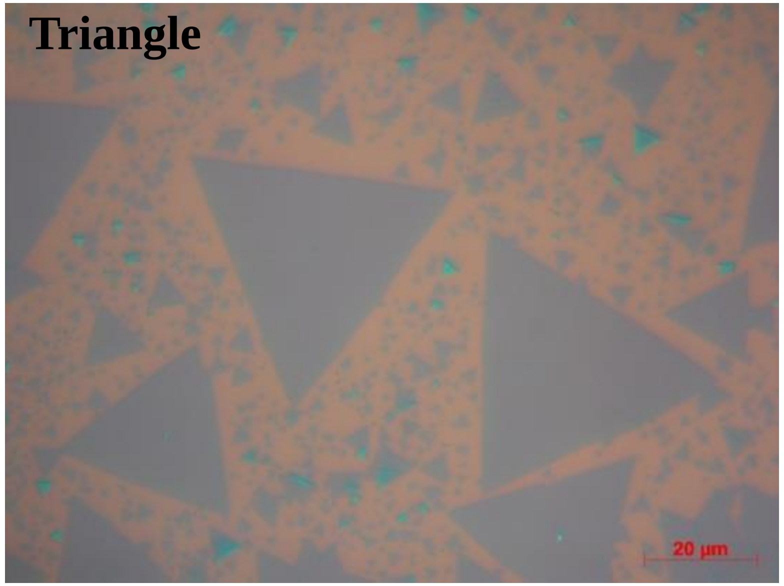


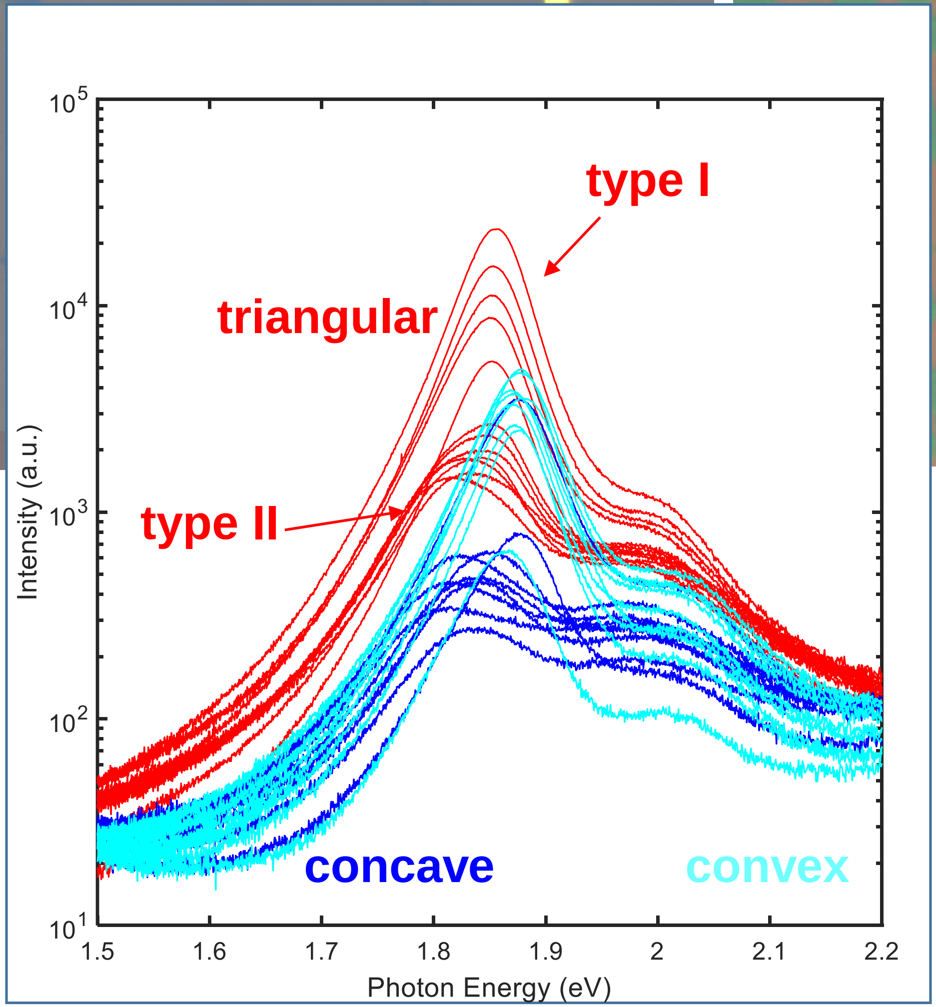


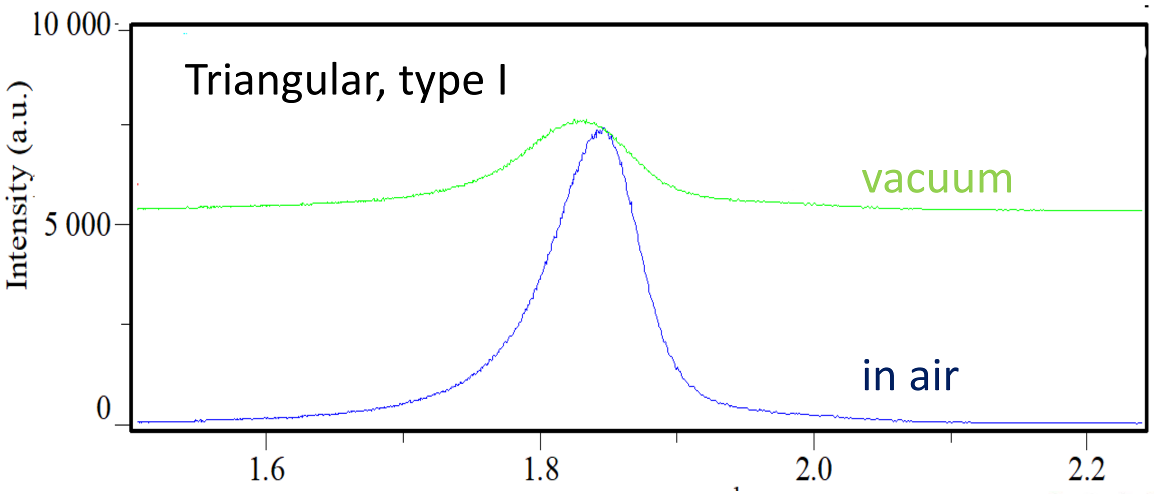
Optical characterizations with various shapes of MoS_2











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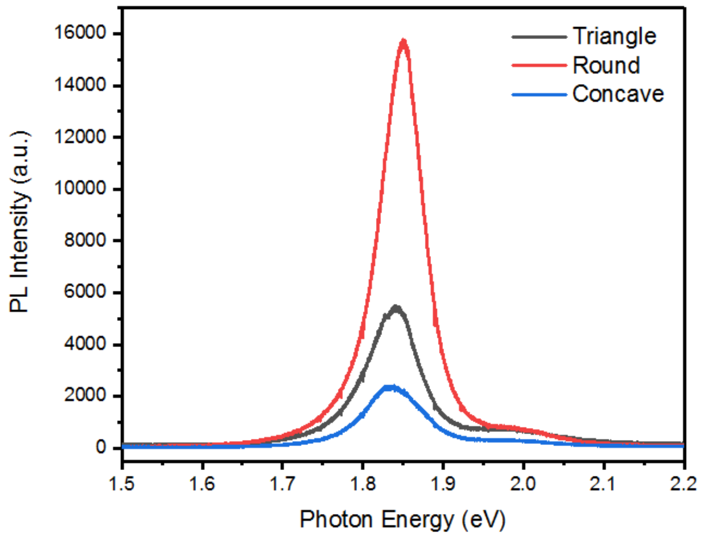
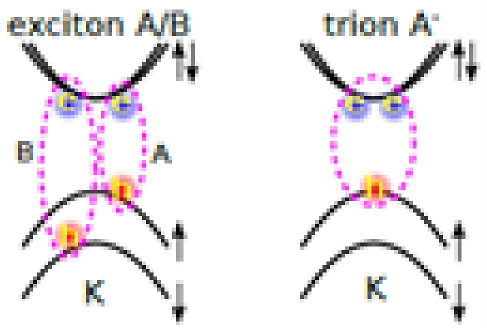
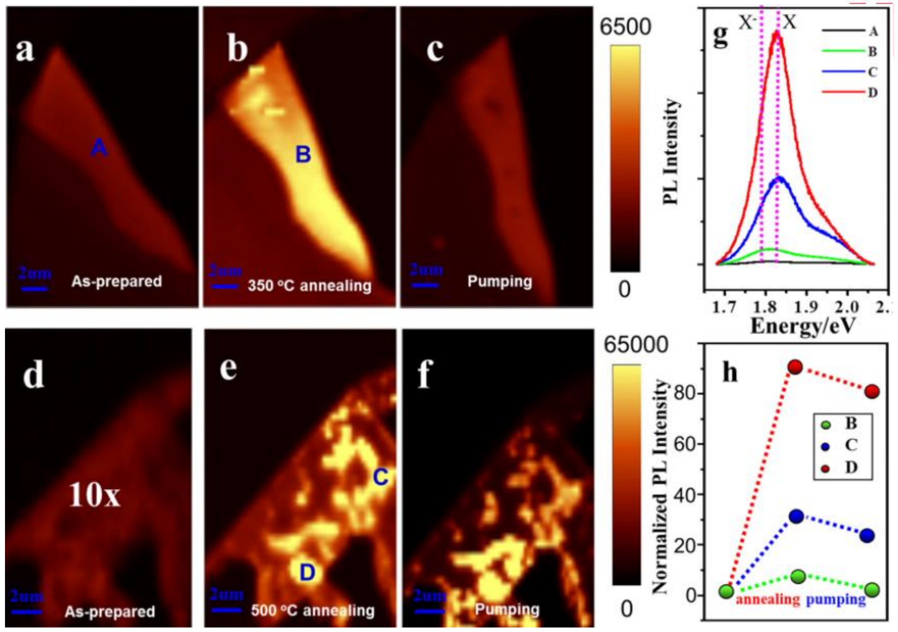
PL Fitting for Exciton and Trion Transitions

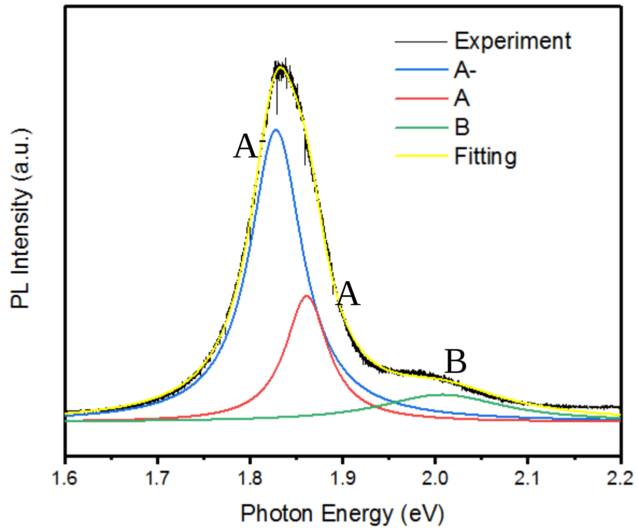




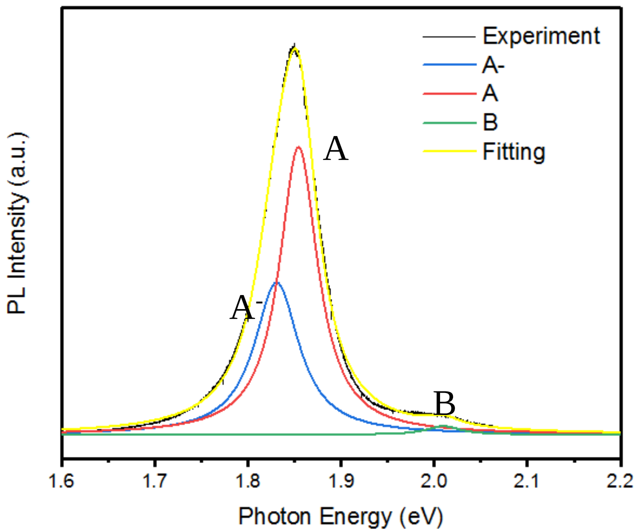


H. Nan et al. *ACS nano* 8.6 (2014): 5738-5745

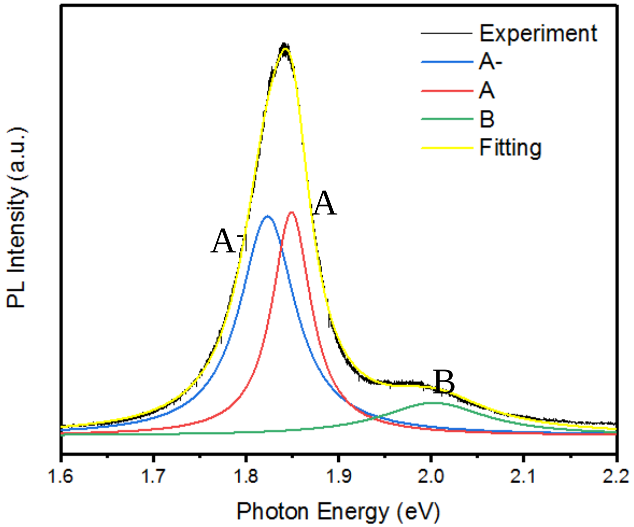
Concave



Round (convex)

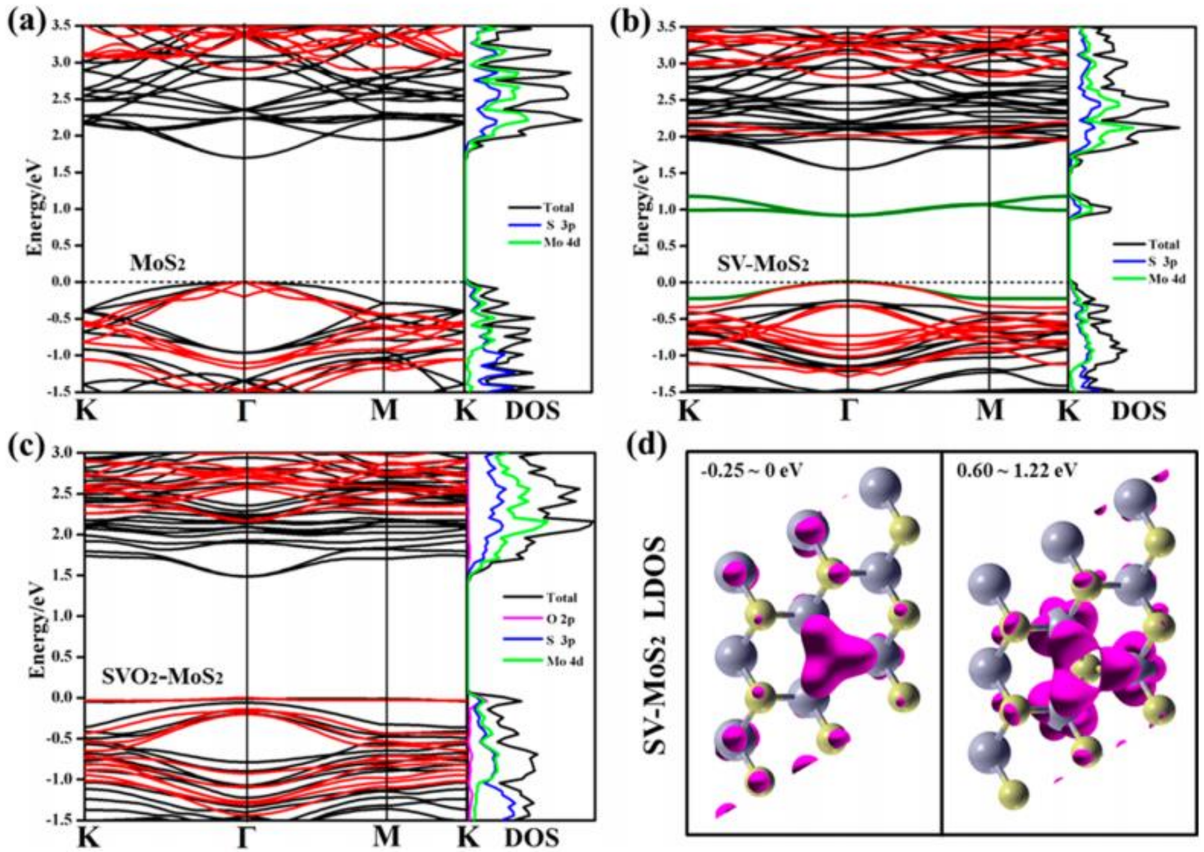


Triangle



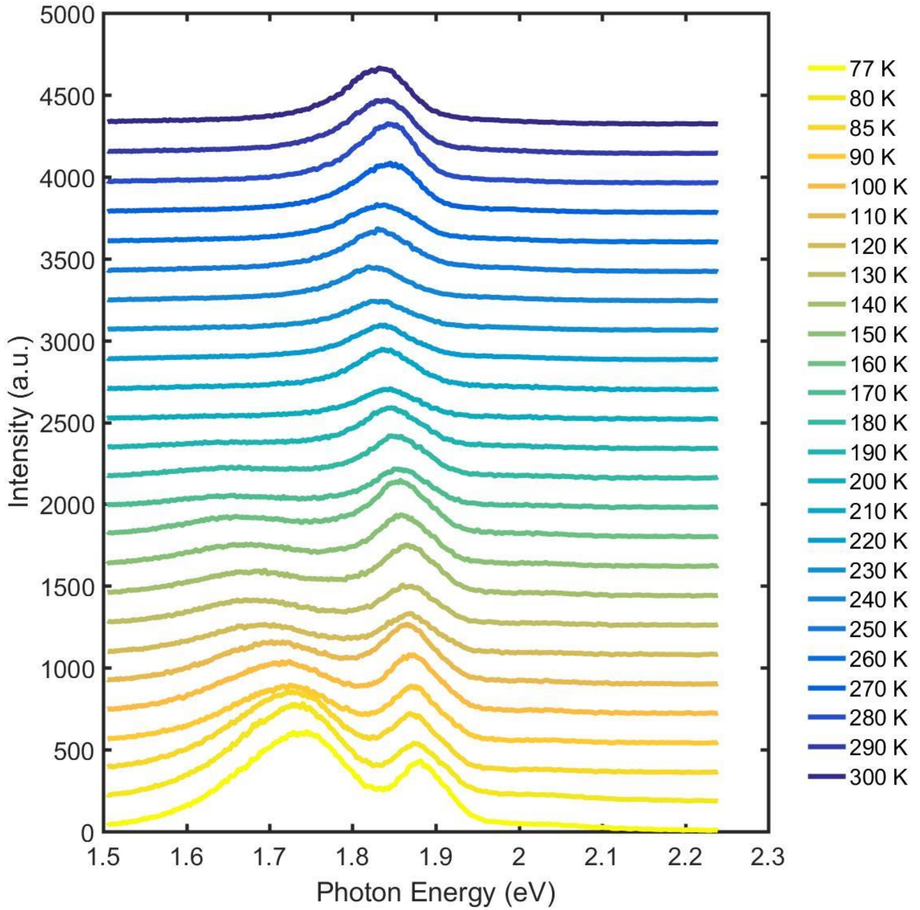
Oxygen passivation and enhanced optical absorption of MoS_2

- Sulfur vacancy: one shallow localized state around VBM, two others midgap
- Oxygen passivation: shallow localized state -> a flat "molecular state" 0.015eV above VBM

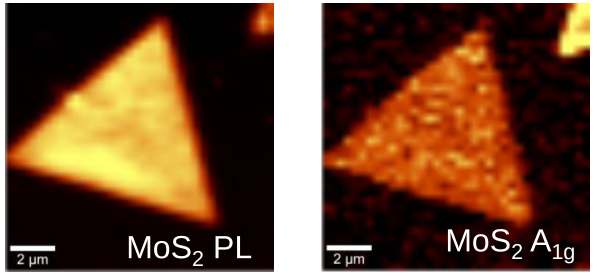


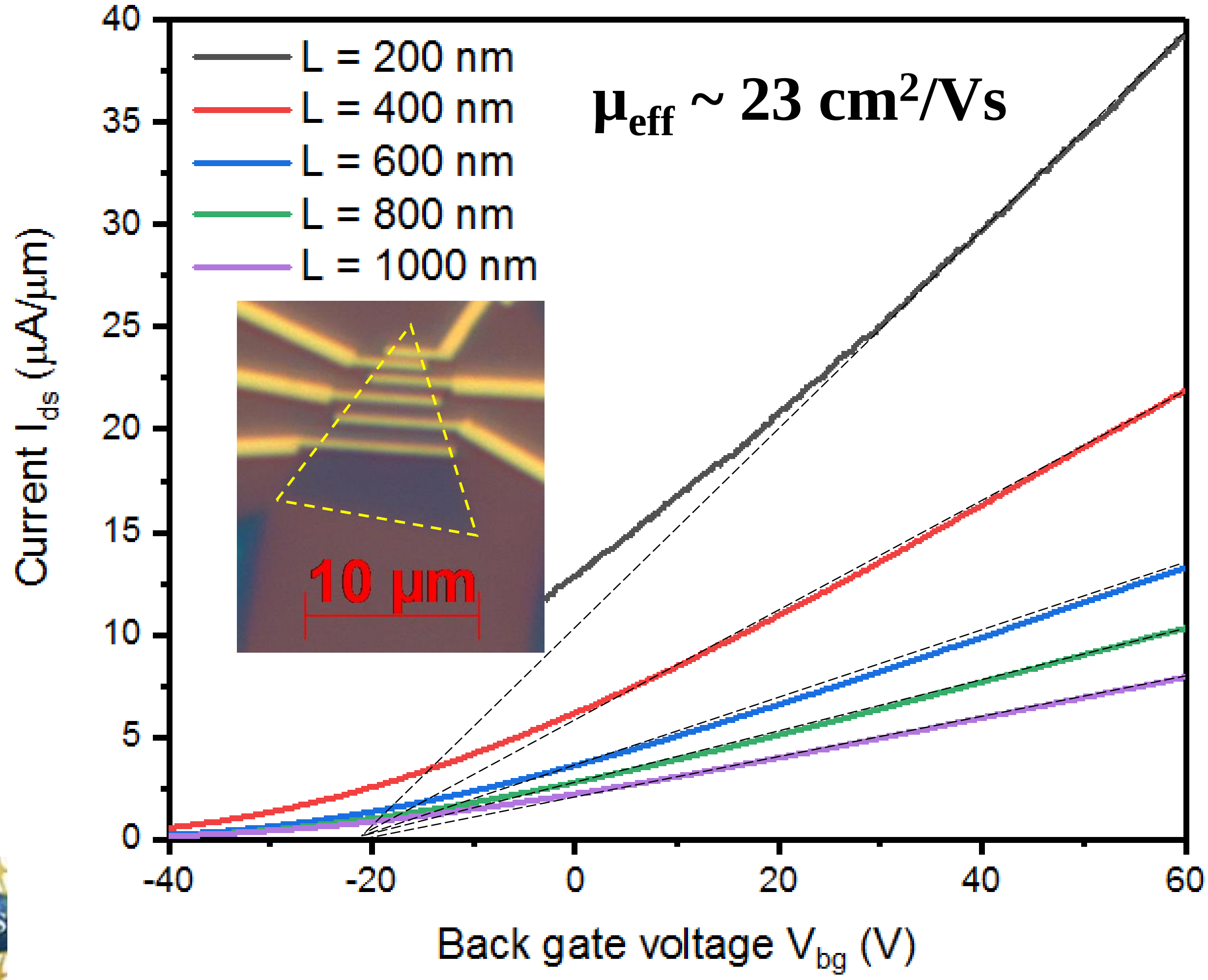
H. Shu et. al., ACS Appl. Mater. Interfaces 2016, 8, 13150−13156

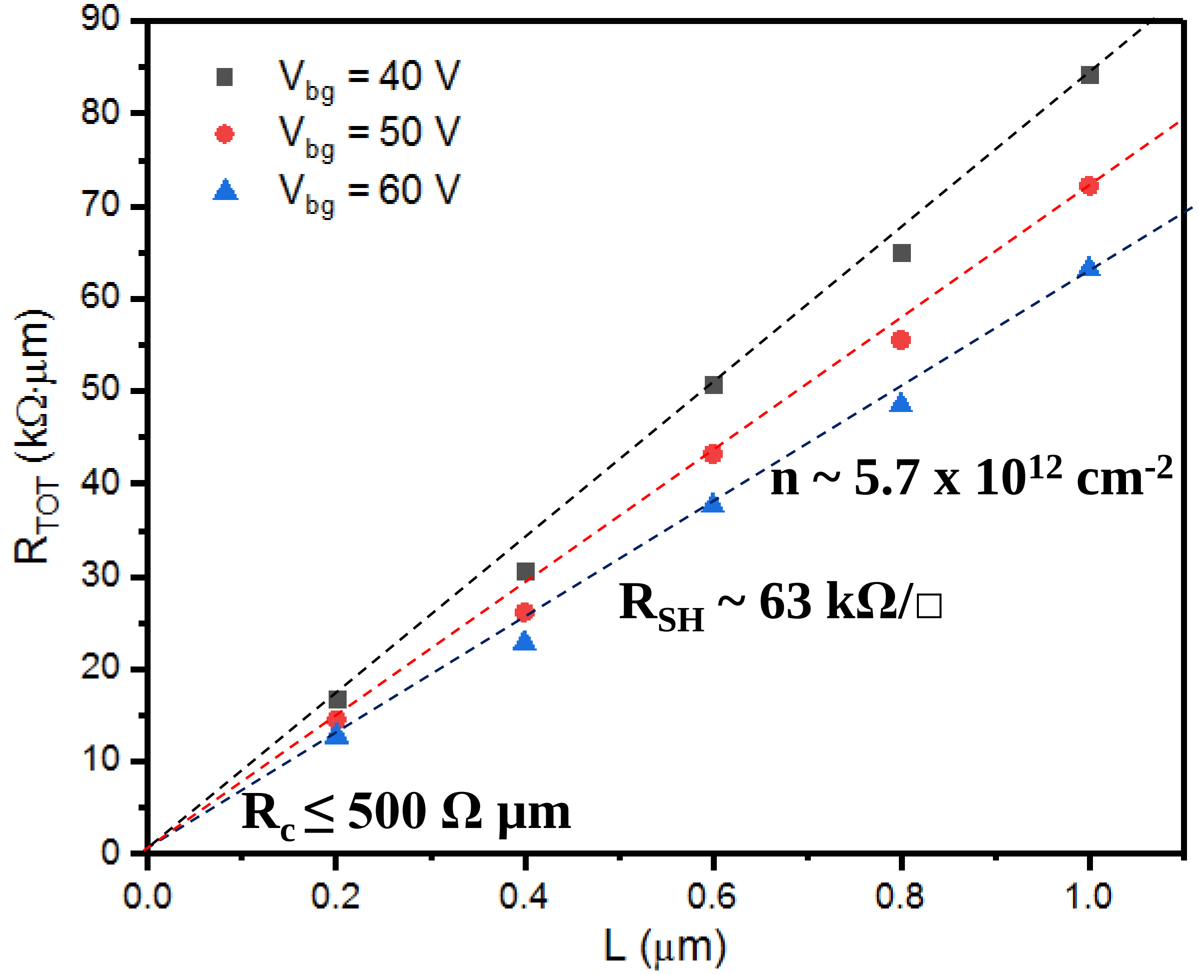
Triangular type I (convex similar)



Low-Contact- Resistance Monolayer MoS_2 Transistors







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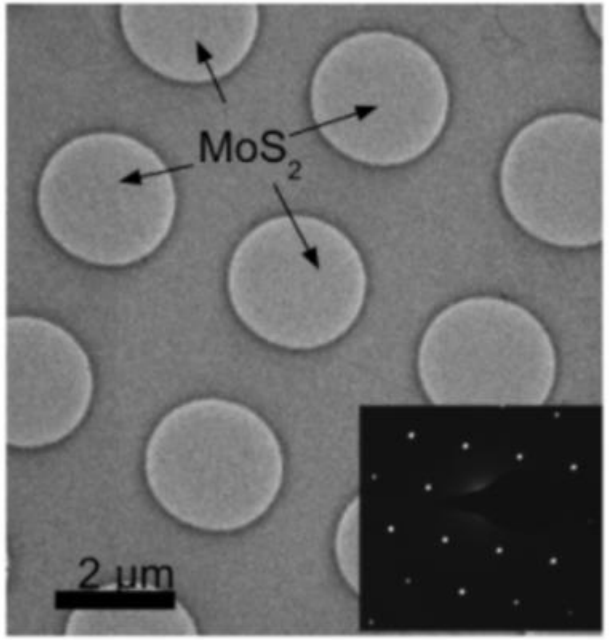
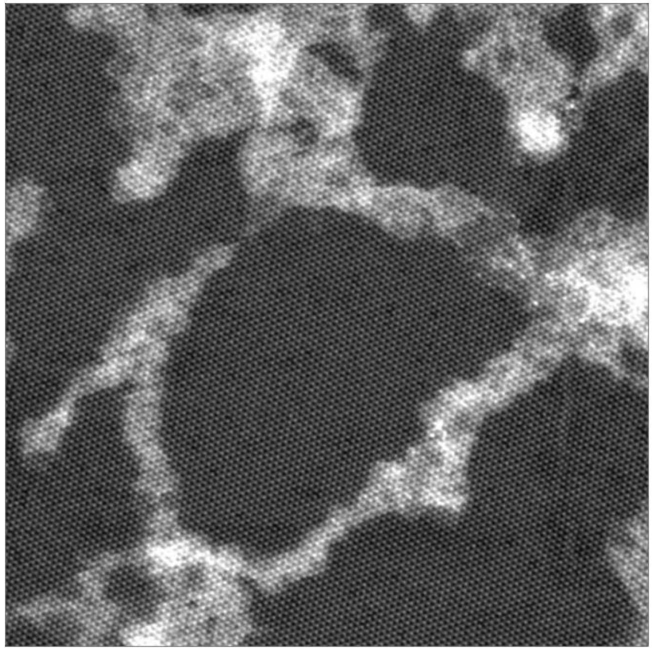
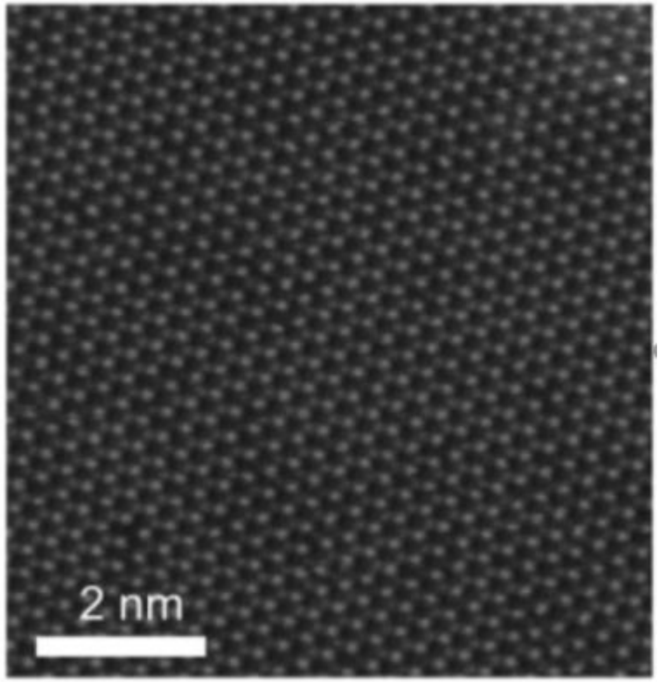
Improvement on the synthesis and transfer

- Clean transfer avoiding polymer residue





30x30nm



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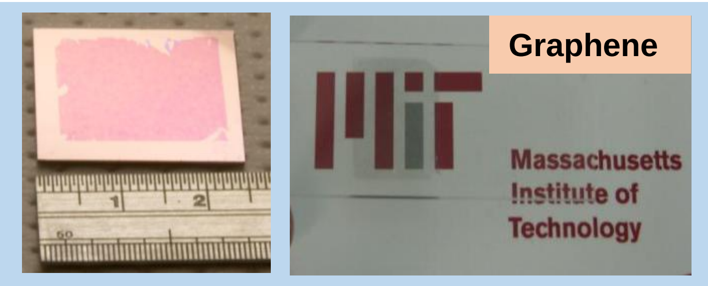
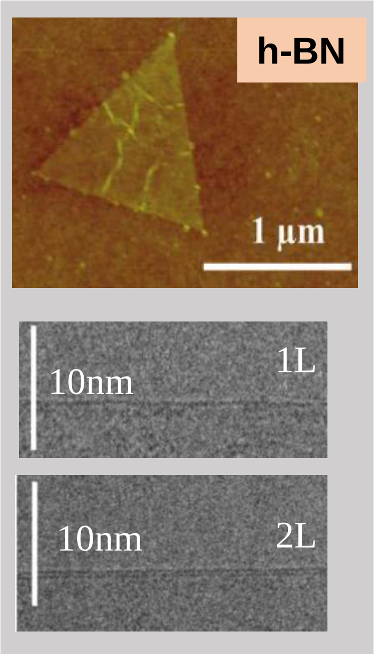
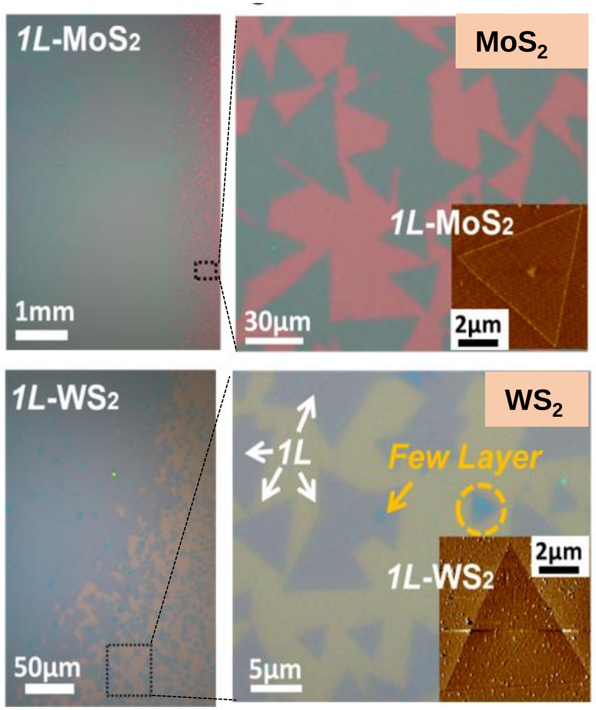
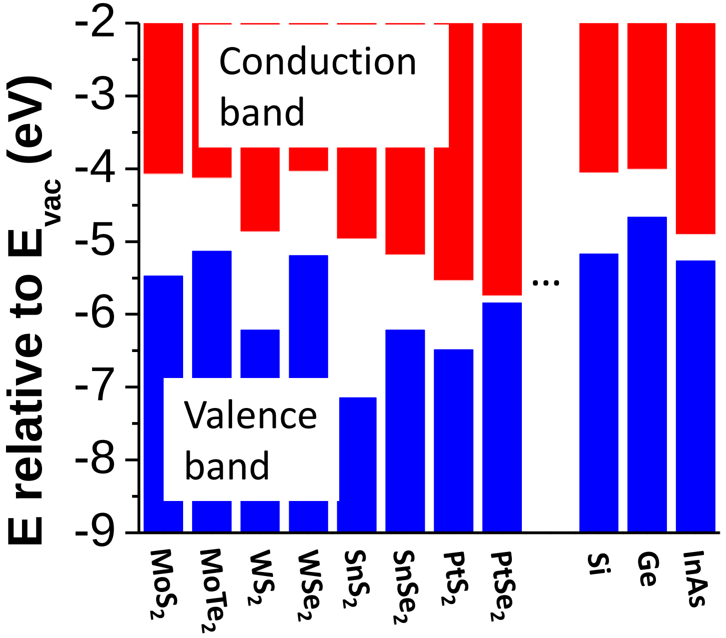
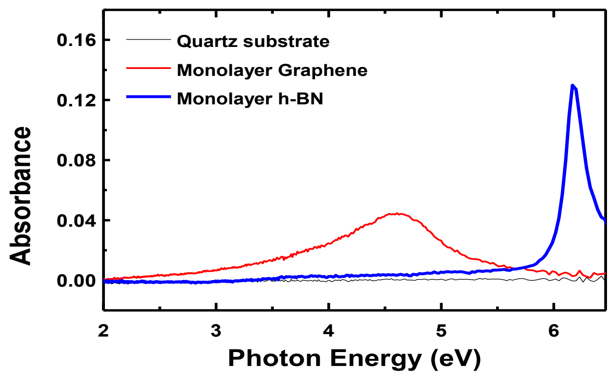
Synthesis of other 2D materials

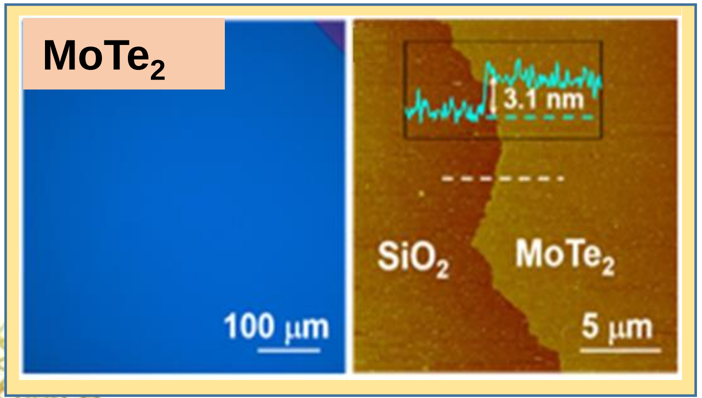


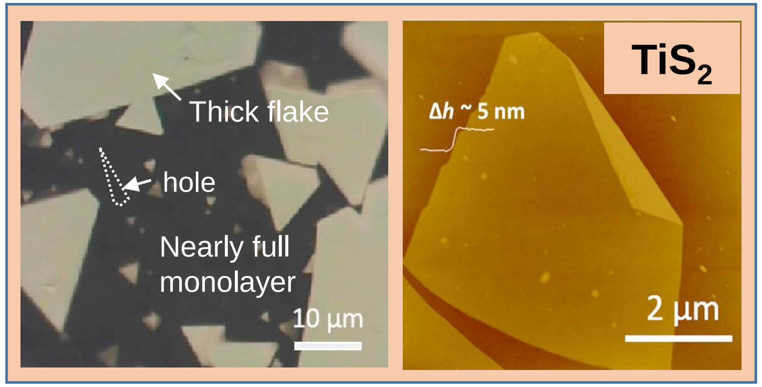


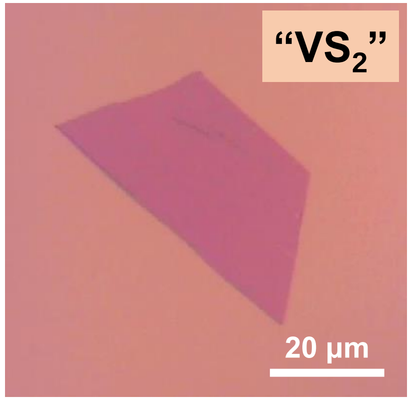


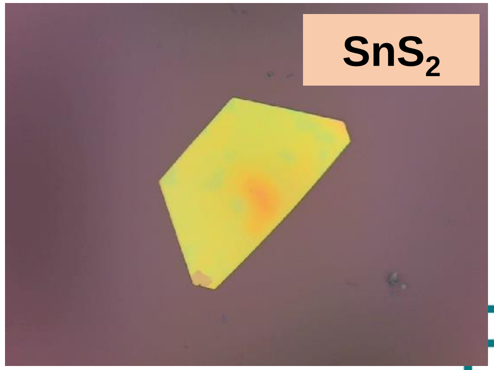




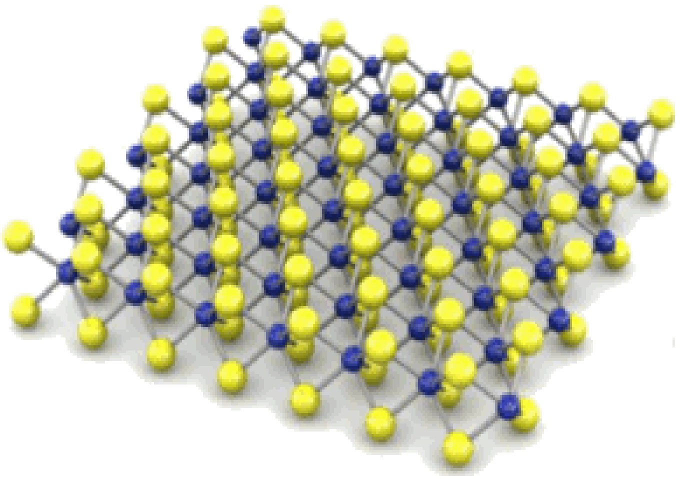


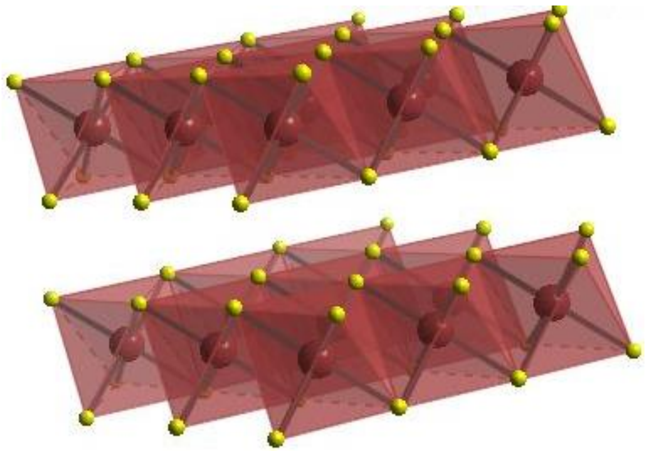


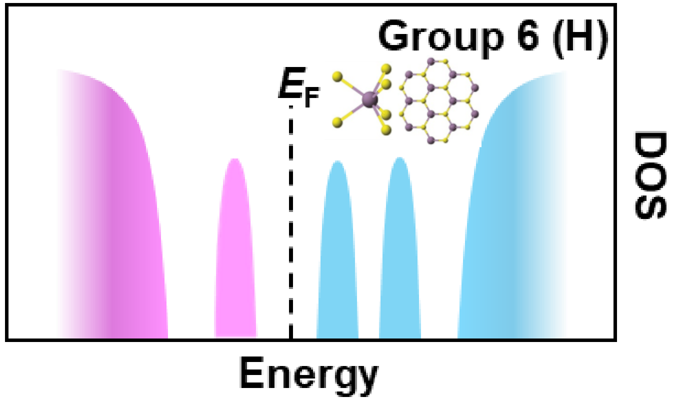


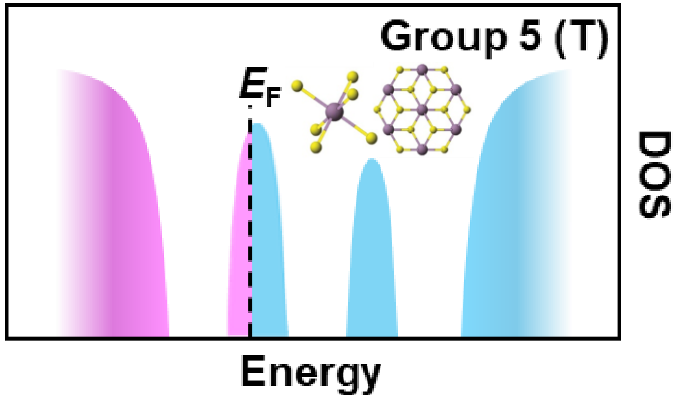


VS_2 vs. MoS_2: similar structures, complementary properties









Mater.	Stable phase	periodicity	Layer distance	bandgap
MoS_2	2H	0.316 nm	0.61 nm	1.8 eV (1L)
VS_2	1T	0.322 nm	0.58 nm	metal

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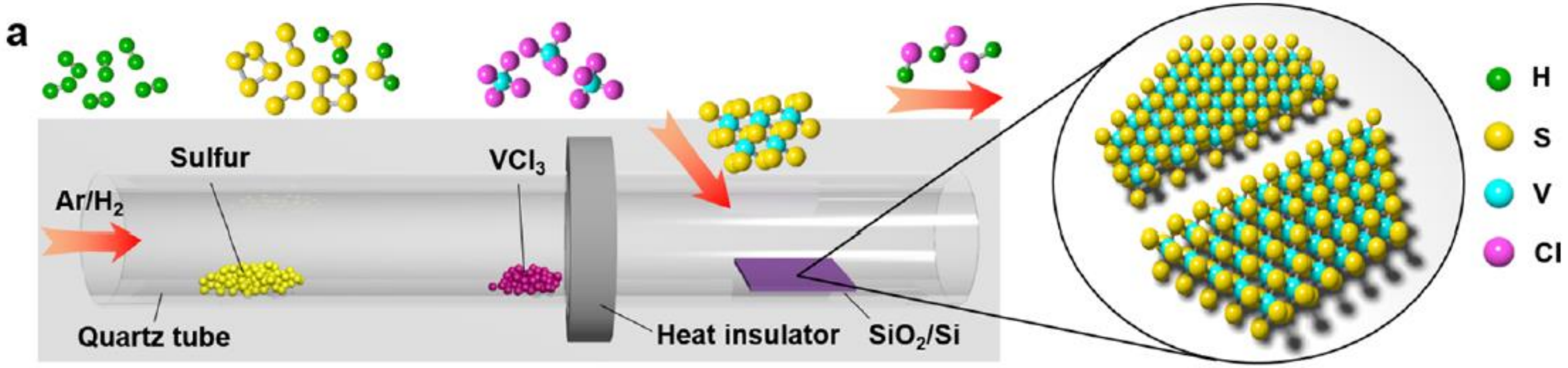
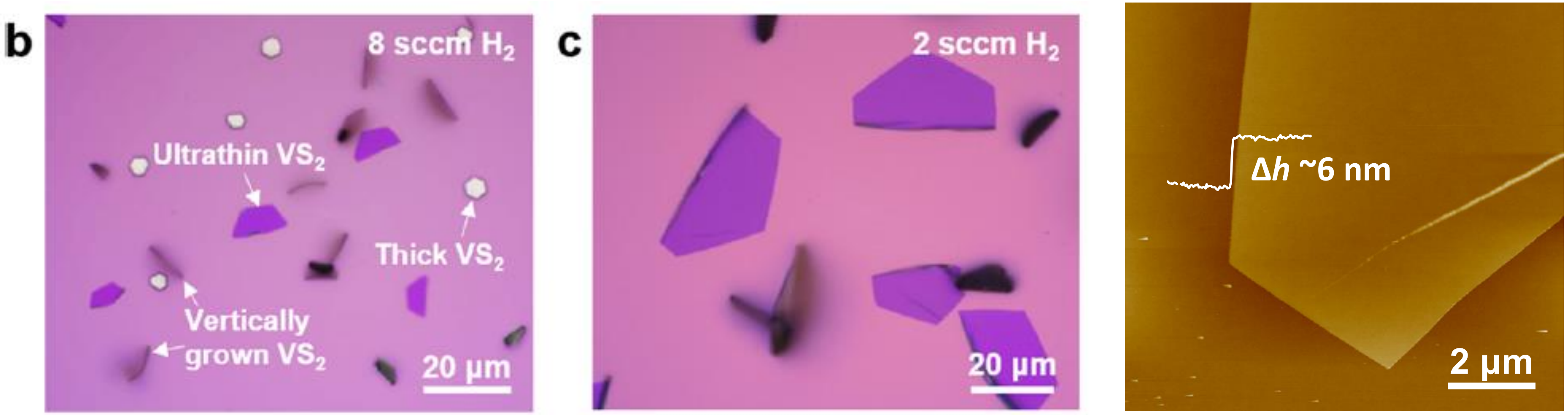
Multilayer "VS_2" flakes

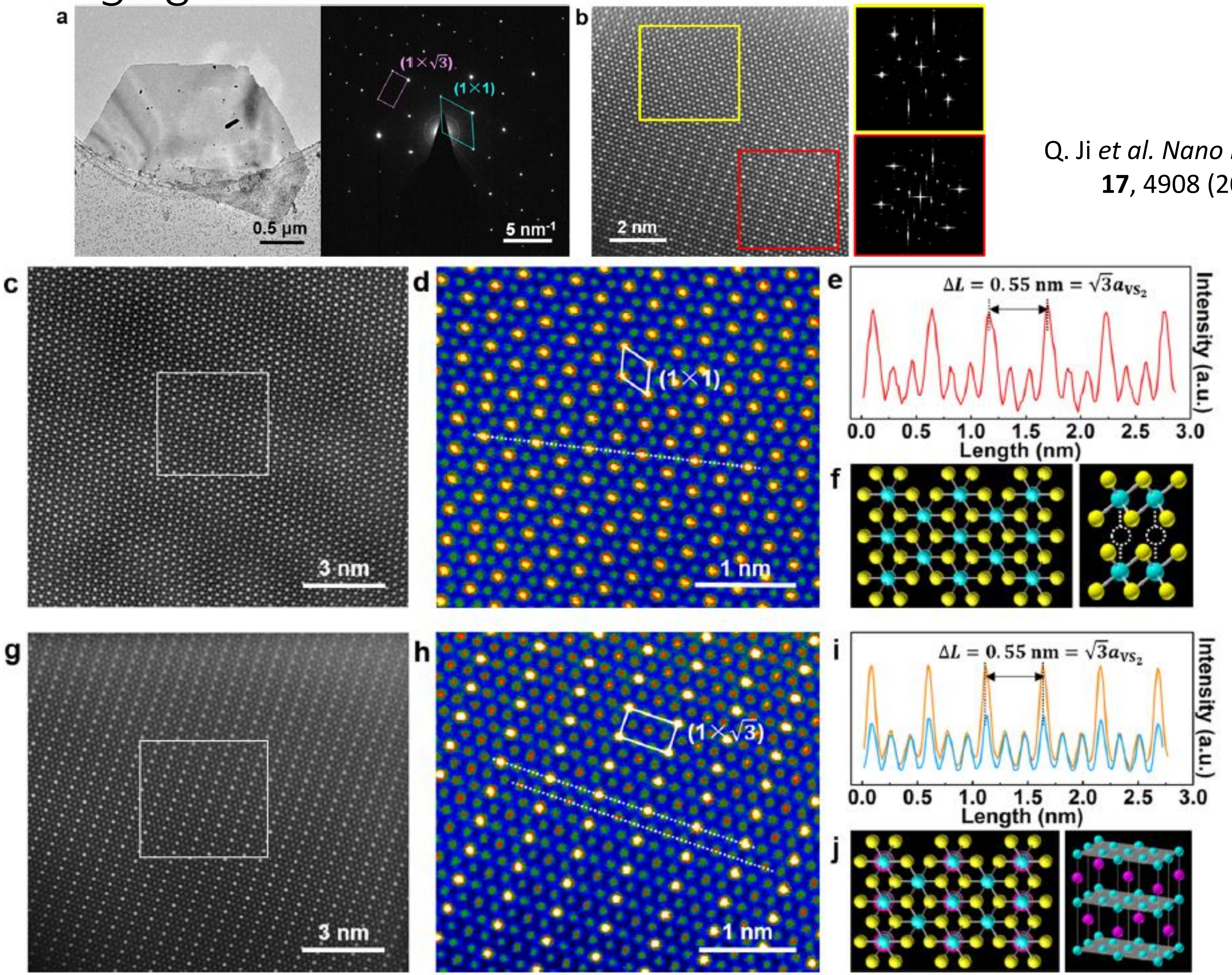


Q. Ji *et al.* *Nano Lett.* **17**, 4908 (2017)

$$2VCl_3(s) \rightarrow VCl_4(g) + VCl_2(s);\;\; VCl_4(g) + 2H_2(g) + 2S(g) \rightarrow VS_2(s) + 4HCl(g)$$



VS_2 and V_5S_8 domains



Q. Ji *et al. Nano Lett.* **17**, 4908 (2017)

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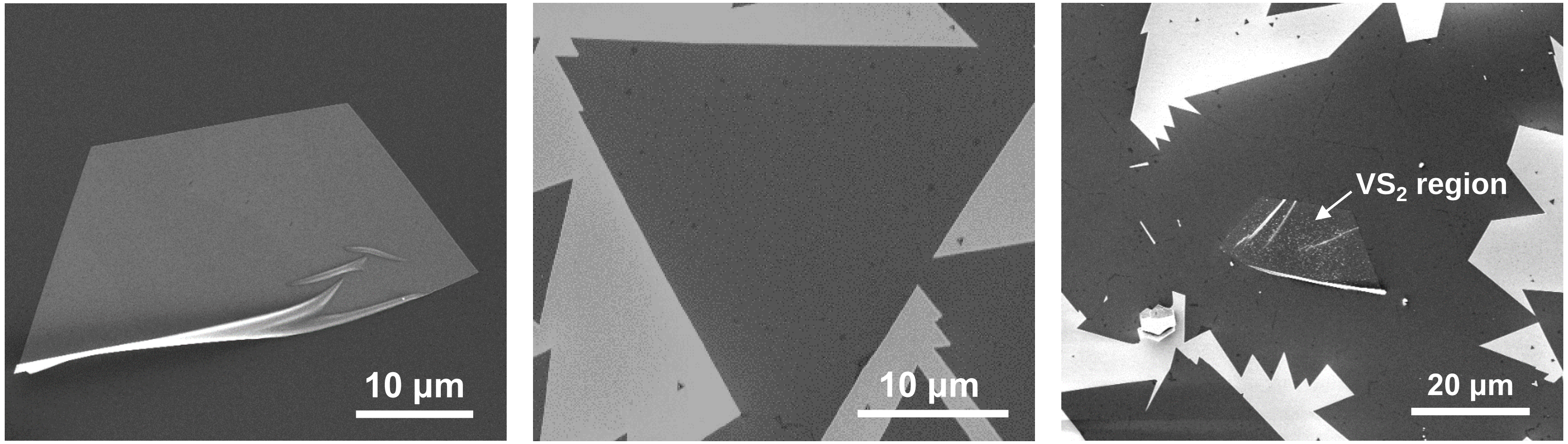
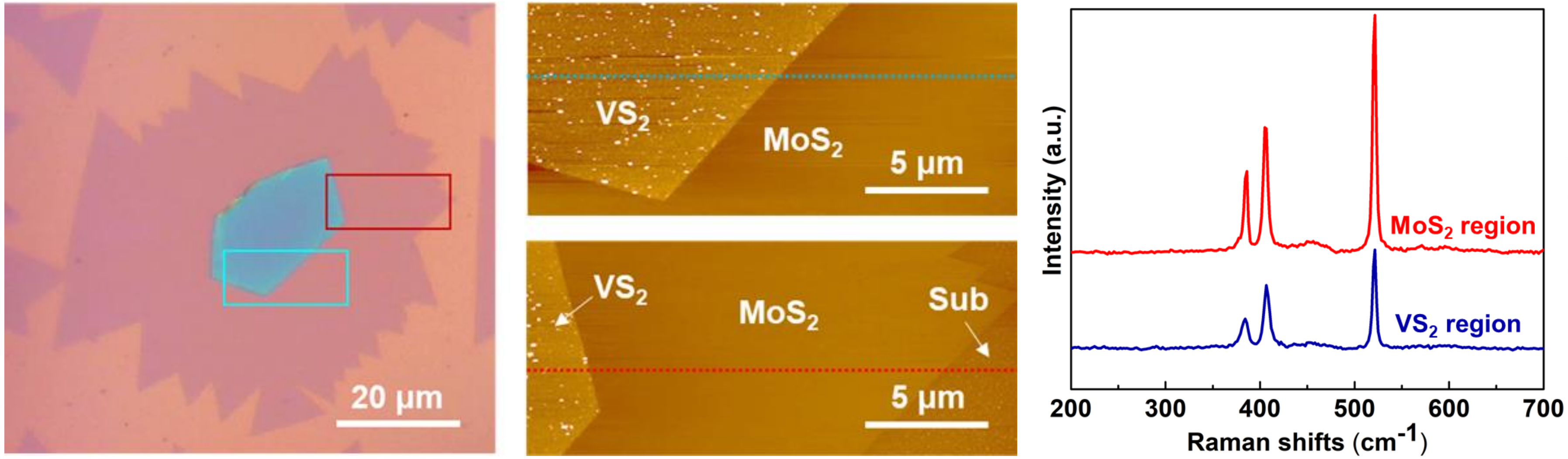
Two step CVD growth for hetero-structure

"VS_2" is first grown/transferred, and MoS2 grows adjacent to "VS_2" flakes





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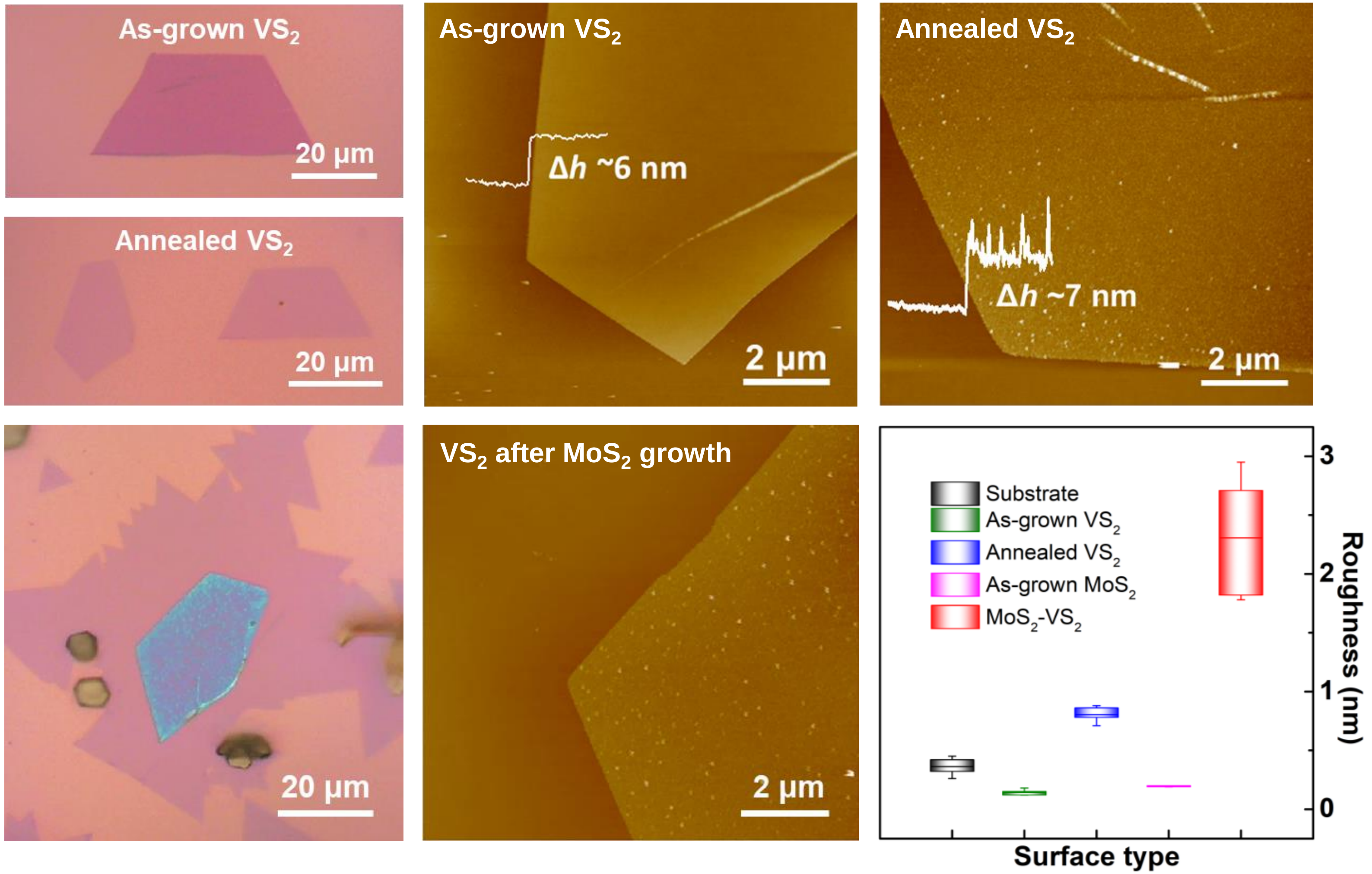
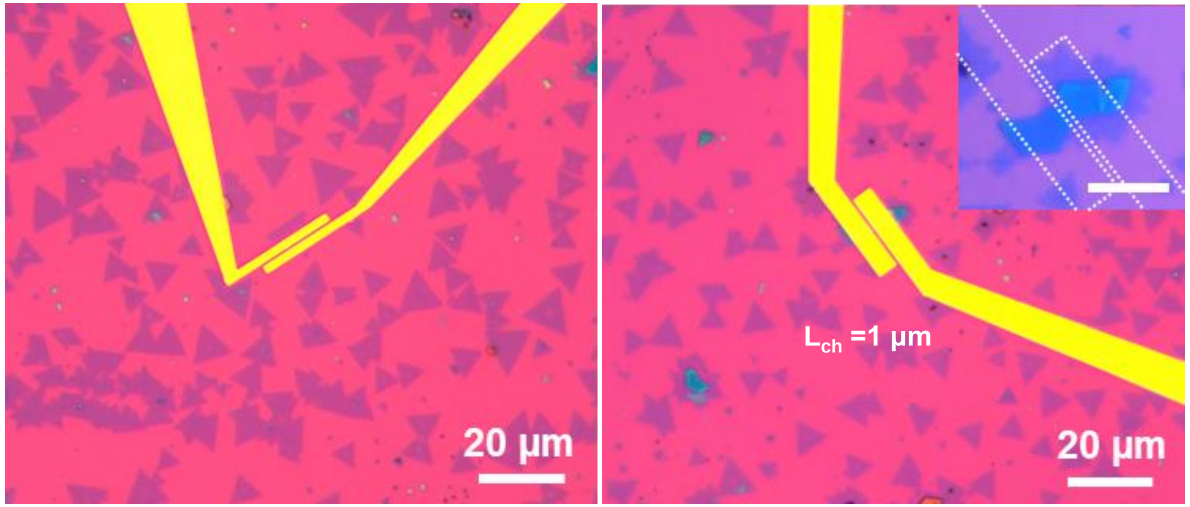
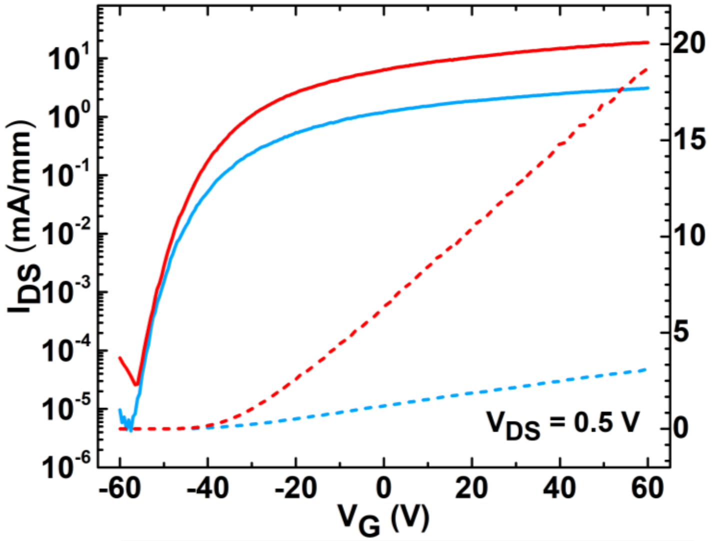
Roughening of the “VS_2” regions

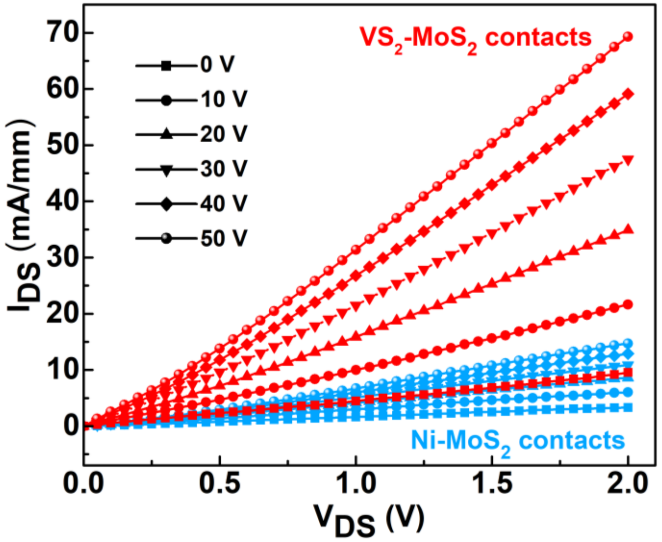


“VS_2” electrical contacts





Properties	Ni contacts	VS_2 contacts
On currents ($\mu A\ \mu m^{-1}$)	3.0	18.7
Transconductance ($\mu S\ \mu m^{-1}$)	0.033	0.21
Mobility ($cm^2\ V^{-1}\ s^{-1}$)	5.5	35
On/off ratio	~10^6	~10^6
Subthreshold swing ($V\ dec^{-1}$)	2.6	2.5



- Preliminary results indicate better contact with “VS_2”

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- Other Kong group members: Angyu Lu, Jiyuan Zhao, Mahomed Mehdi Goulamaly, Seong Soon Jo, JiHoon Park, Haozhe Wang, Luda Wang, Giovanni Azzellino, Mohammadmahdi Tavakoli, Hongzhang Geng, Luiz Gustavo Pimenta Martins, Nannan Mao, Lin Zhou, Xiaoyan Zhu, Jin Niu, Bingnan Han
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Thank you very much!

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