

# MoS<sub>2</sub> Field-Effect Transistors: Dielectric, Contacts, and Scaling

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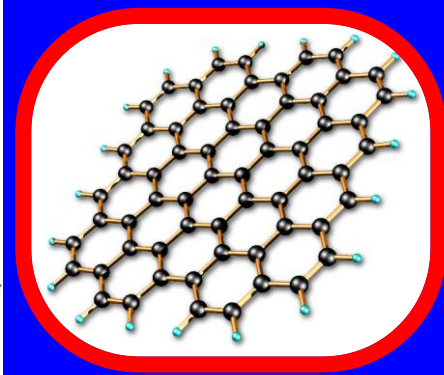
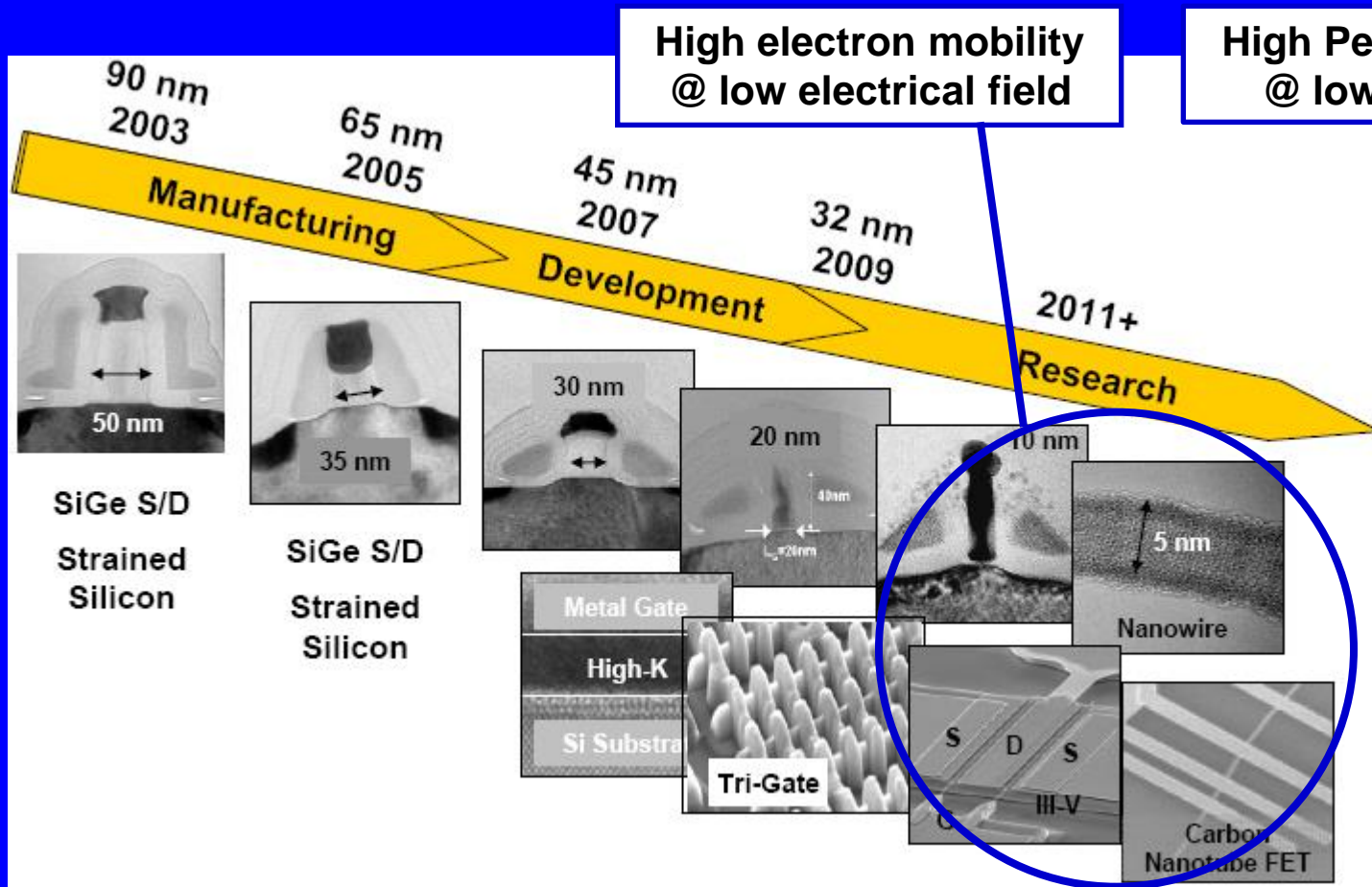
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# Outline

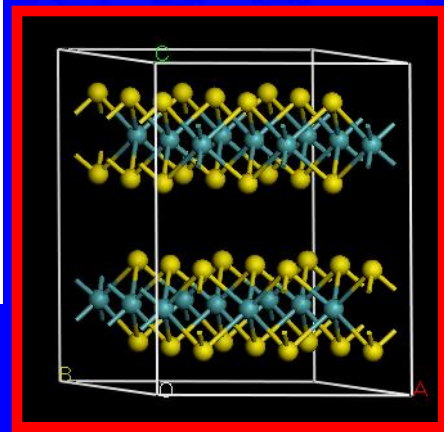
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- (1) Motivation
- (2) Fundamental properties of MoS<sub>2</sub> and others
- (3) MoS<sub>2</sub> based electronic devices
  - a. ALD high-k/MoS<sub>2</sub> integration
  - b. Metal contacts to MoS<sub>2</sub>
  - c. Device scaling factors
  - d. Doping in MoS<sub>2</sub> FETs
  - e. Transport in MoS<sub>2</sub>
- (4) Summary

# Emerging Non-Si CMOS Research



**Graphene**



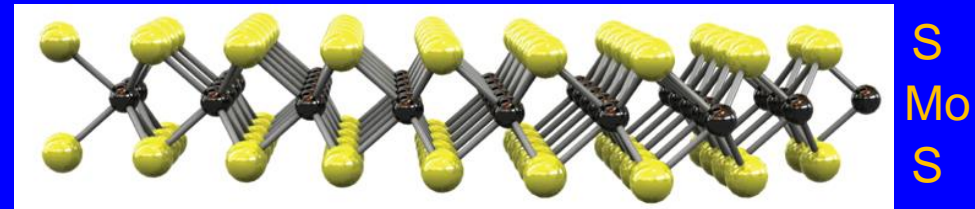
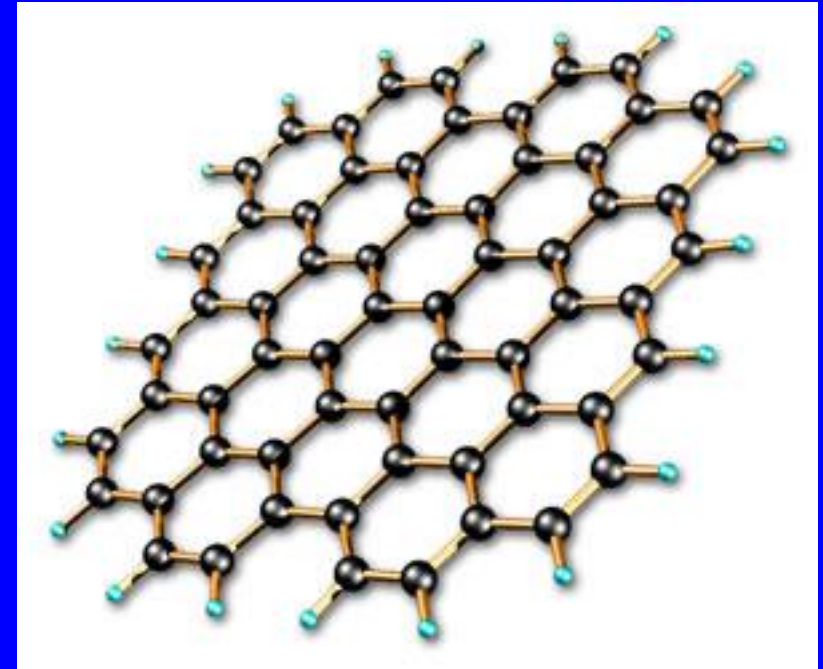
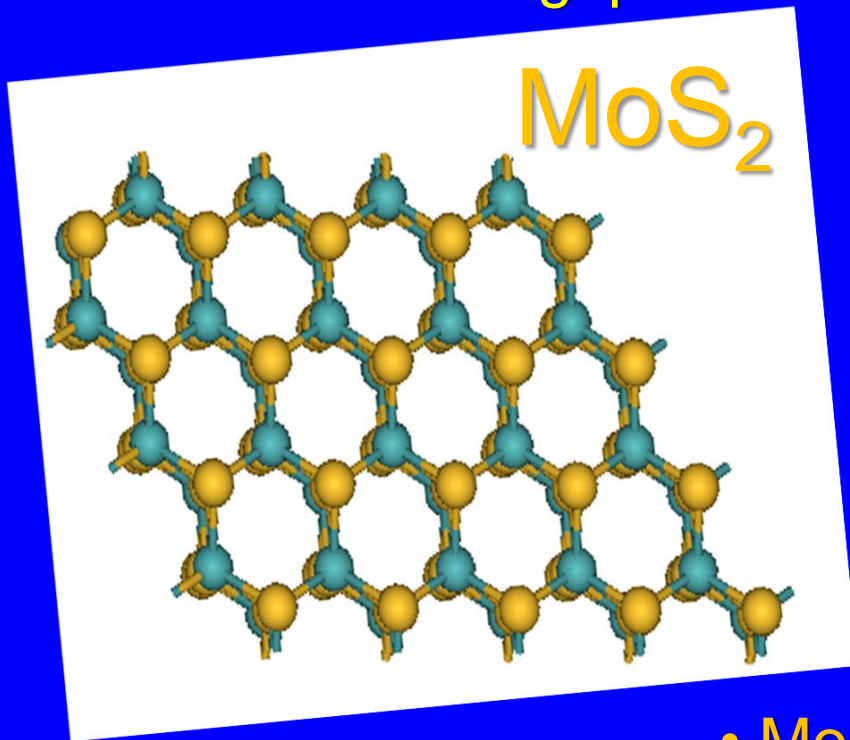
**MoS<sub>2</sub>**

**More Non-Si Elements Introduced**

Source: R. Chau, DRC 2006

# MoS<sub>2</sub> - 2D Crystal beyond Graphene

- Graphene has been actively researched for last few years
  - Zero band gap !

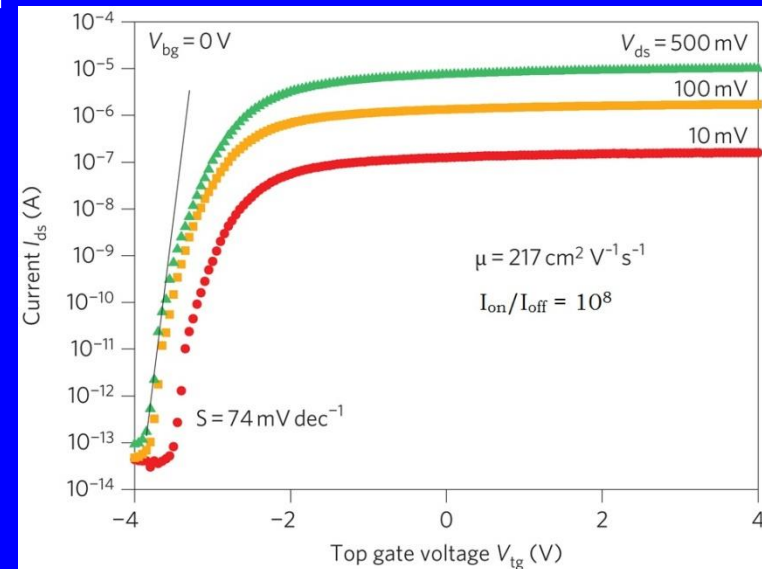
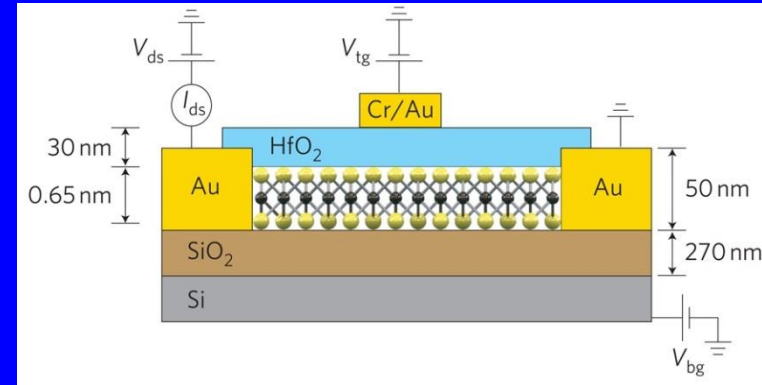


- MoS<sub>2</sub> - 2D Crystal beyond Graphene
  - Large band gap ~1.2 eV-1.8 eV
  - First MOSFET Jan 2011

# Single layer MoS<sub>2</sub> MOSFET

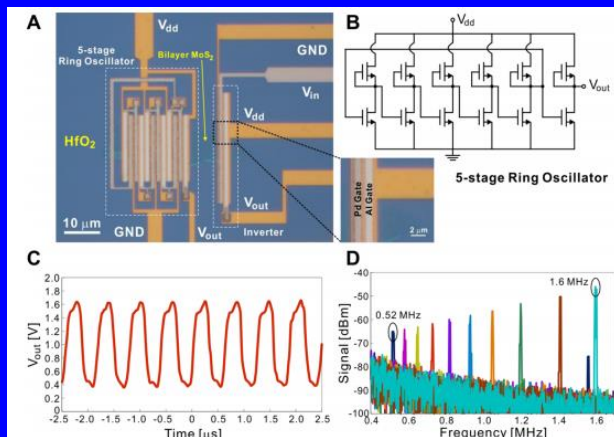
- Mechanically exfoliated
- Mobility (200 cm<sup>2</sup>/Vs)\*
- Mobility enhanced by ALD high-k
- Intrinsic direct bandgap for single layer
- Thermal stability up to 1100°C
- Thin transparent semiconductor

\* See also Hone and Fuhrer Nat. Nanotechnol. 2013



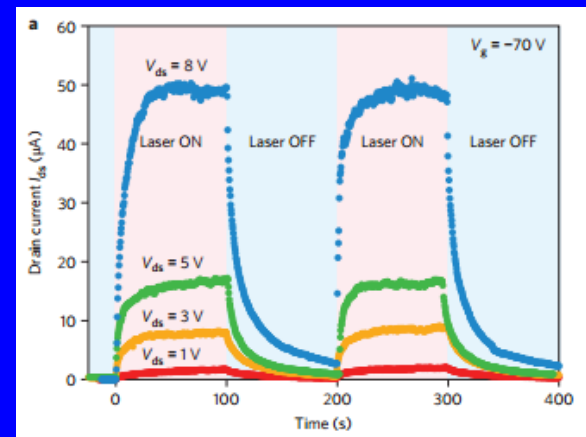
# Applications of MoS<sub>2</sub>

## Integrated Circuits



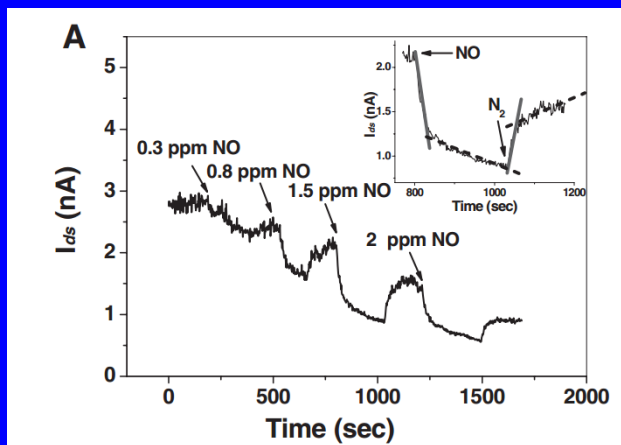
H. Wang et al. Nano Lett 2012

## Photodetectors



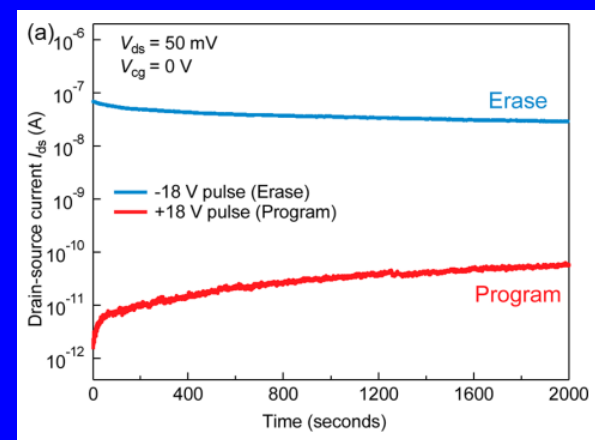
O. Lopez-Sanchez et al, Nat. Nanotechnol. 2013

## Chemical Sensor



H. Li et al. Small, 2012

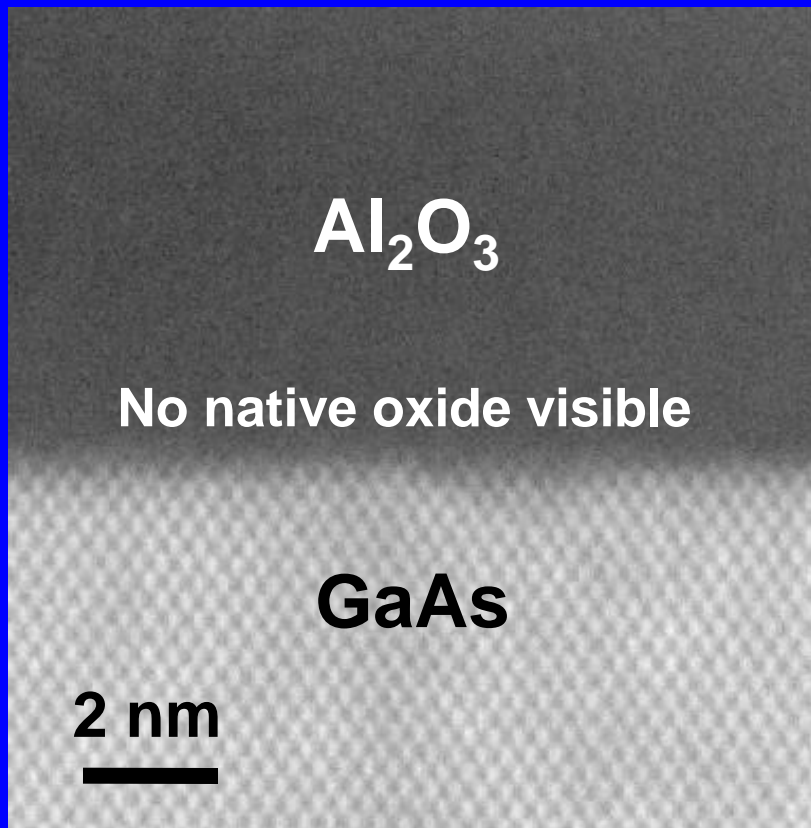
## Non-volatile Memory



S. Bertolazzi et al, ACS Nano 2013

(1) Dielectric (2) Contact Resistance (3) Channel Mobility

# Ex-situ ALD high-k on 3D substrates vs. 2D



ALD self-cleaning effect



2 ASM ALD Systems at Purdue

**3D Semiconductors: Passivation** >> Many works at Intel, IBM, SEMATECH, IMEC, AIST, Purdue, U. Tokyo, Stanford, MIT, UCB, UCSB, NUS, UT Austin, UT Dallas, many other universities

**2D Semiconductors: No dangling bonds**

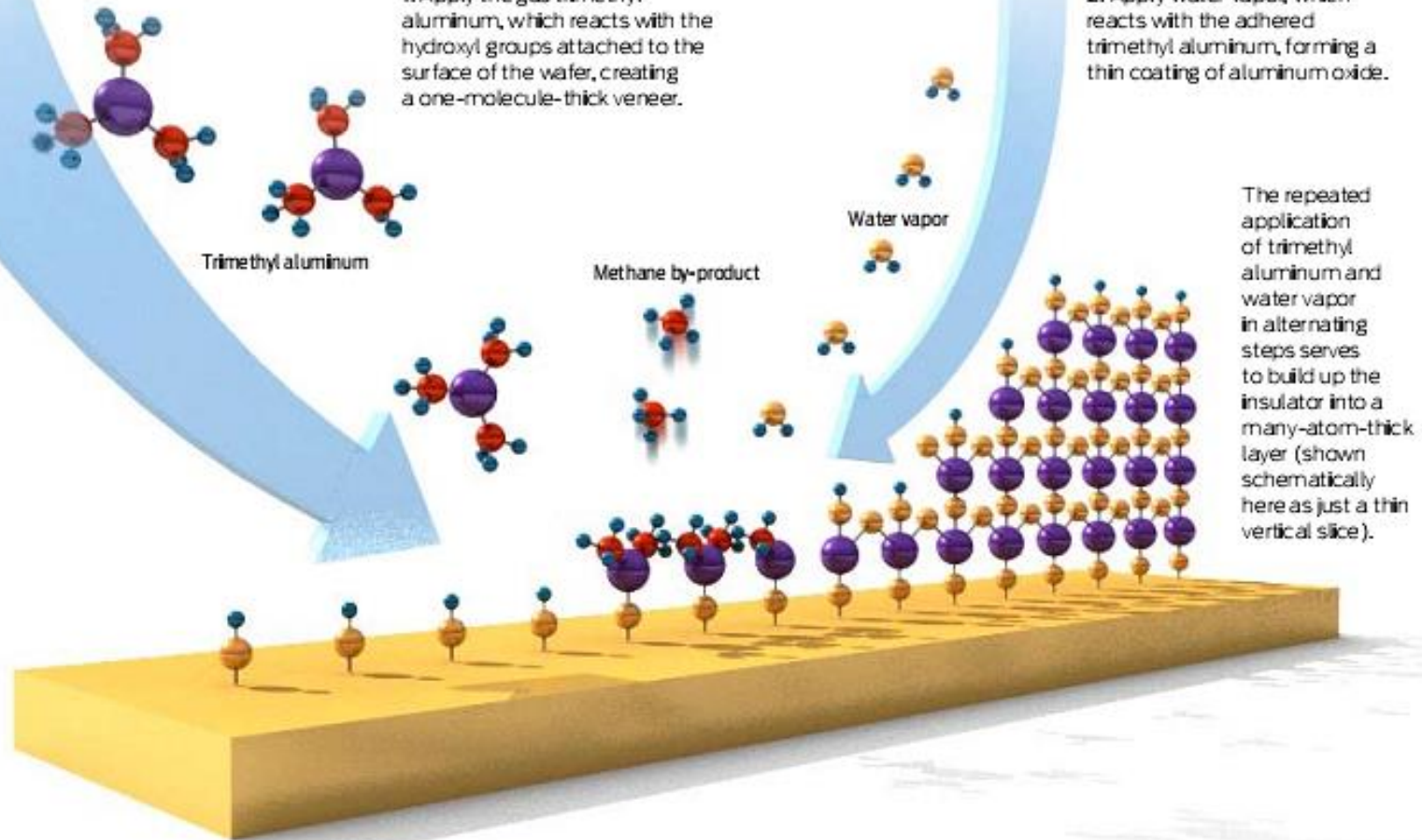
Yoon et al. Nano Letters 2011

# ALD $\text{Al}_2\text{O}_3$ Process with TMA and $\text{H}_2\text{O}$

**A** TOMIC-LAYER DEPOSITION provides one means for coating a semiconductor wafer with a high-k aluminum oxide insulator. The benefit of this technique is that it offers atomic-scale control of the coating thickness without requiring elaborate equipment.

1. Apply the gas trimethyl aluminum, which reacts with the hydroxyl groups attached to the surface of the wafer, creating a one-molecule-thick veneer.

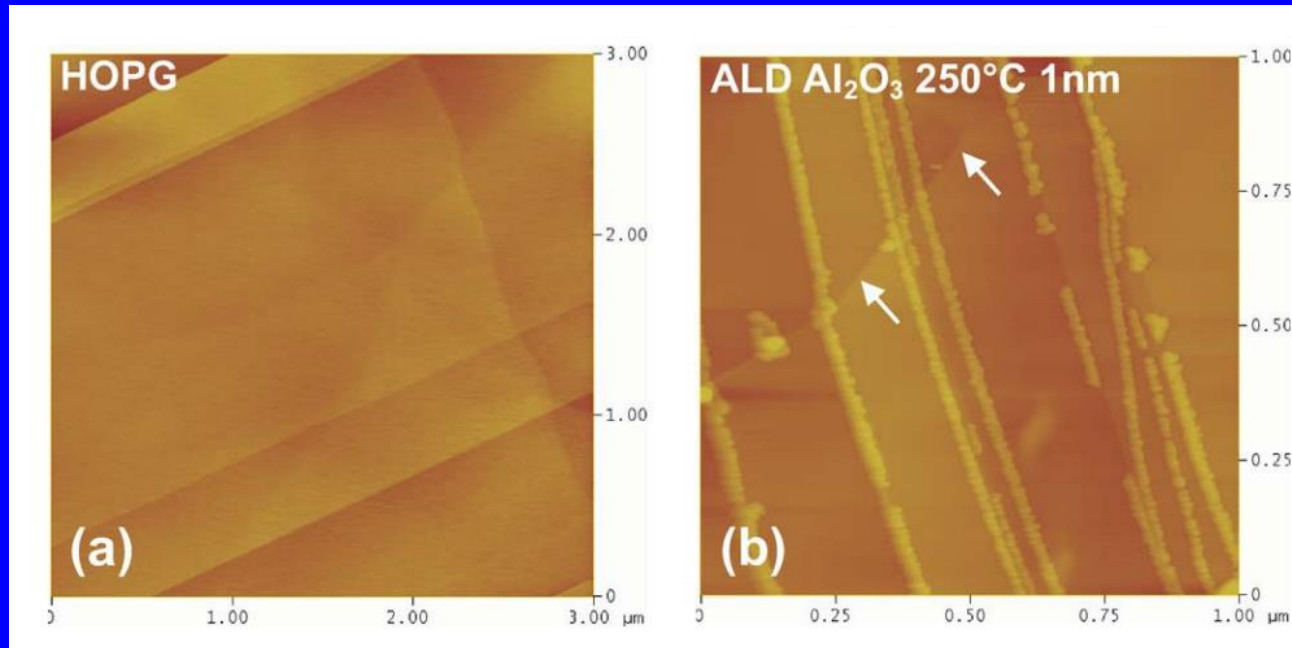
2. Apply water vapor, which reacts with the adhered trimethyl aluminum, forming a thin coating of aluminum oxide.

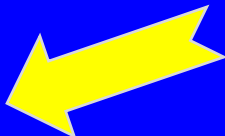




# ALD Cannot Simply Grow on Graphene

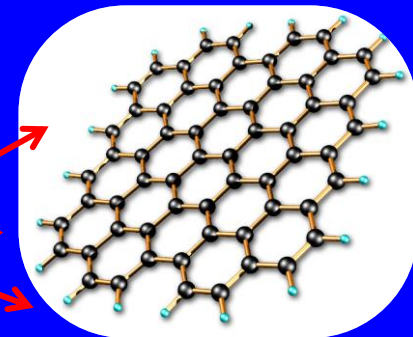
If we do not have dangling bonds....



  
No Al<sub>2</sub>O<sub>3</sub> on  
basal plane

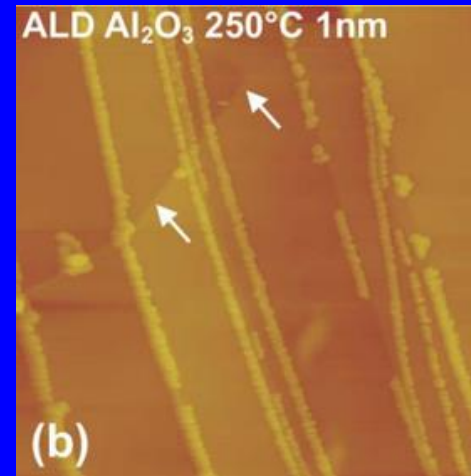
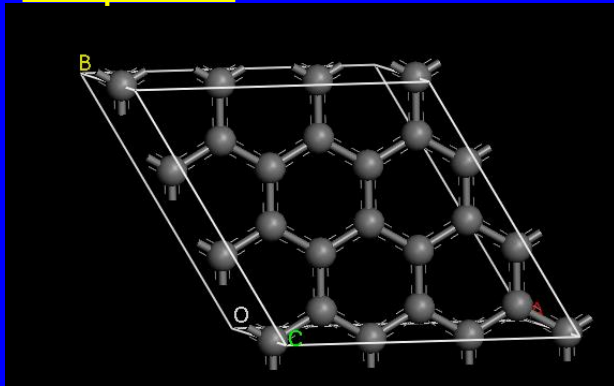
***the graphene case...***

Al<sub>2</sub>O<sub>3</sub> on edges

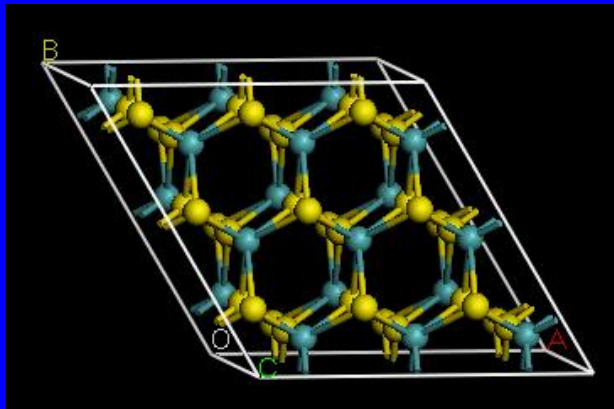


# ALD on MoS<sub>2</sub> 2D Crystal

## Graphene

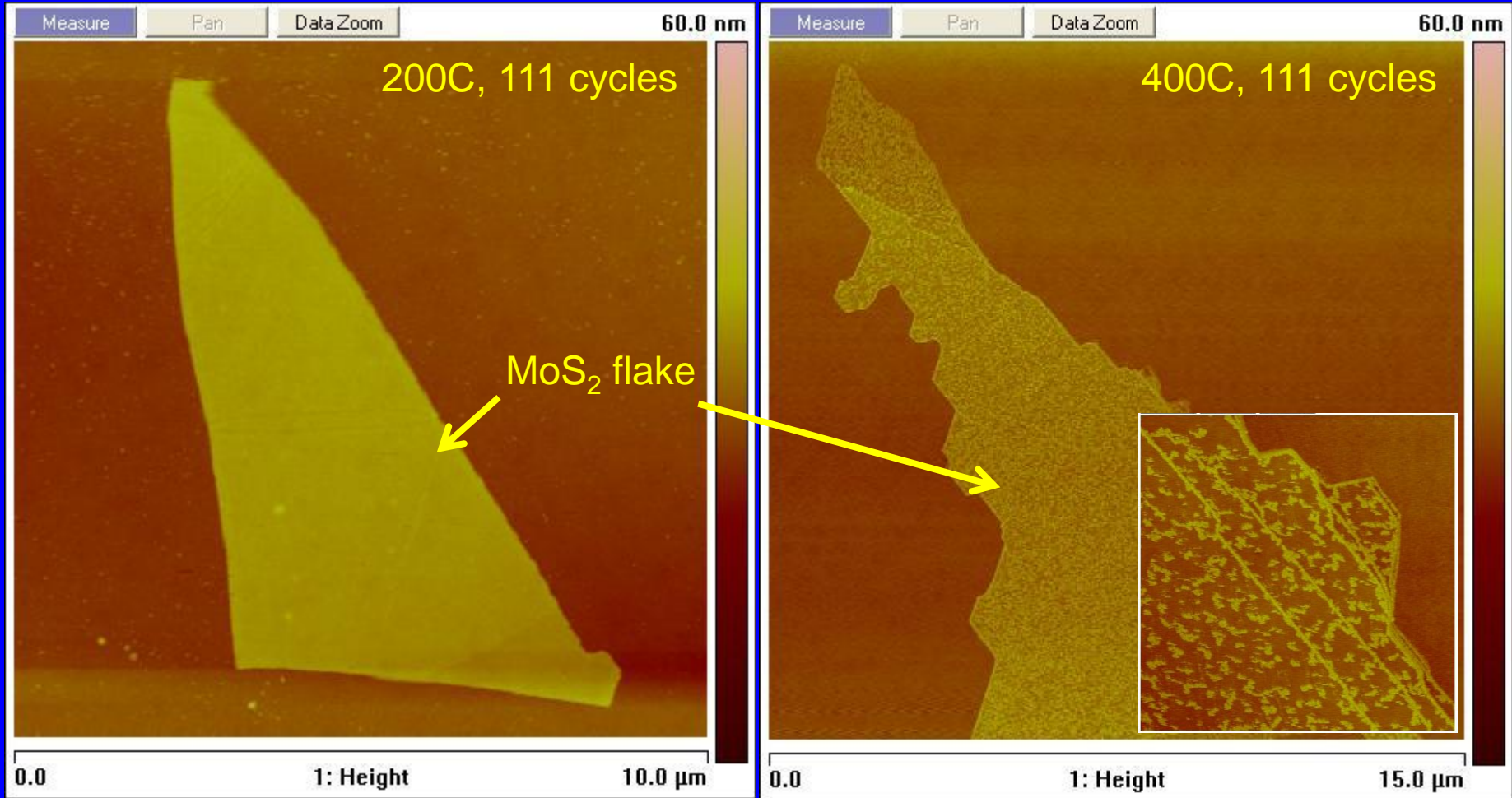


## MoS<sub>2</sub>

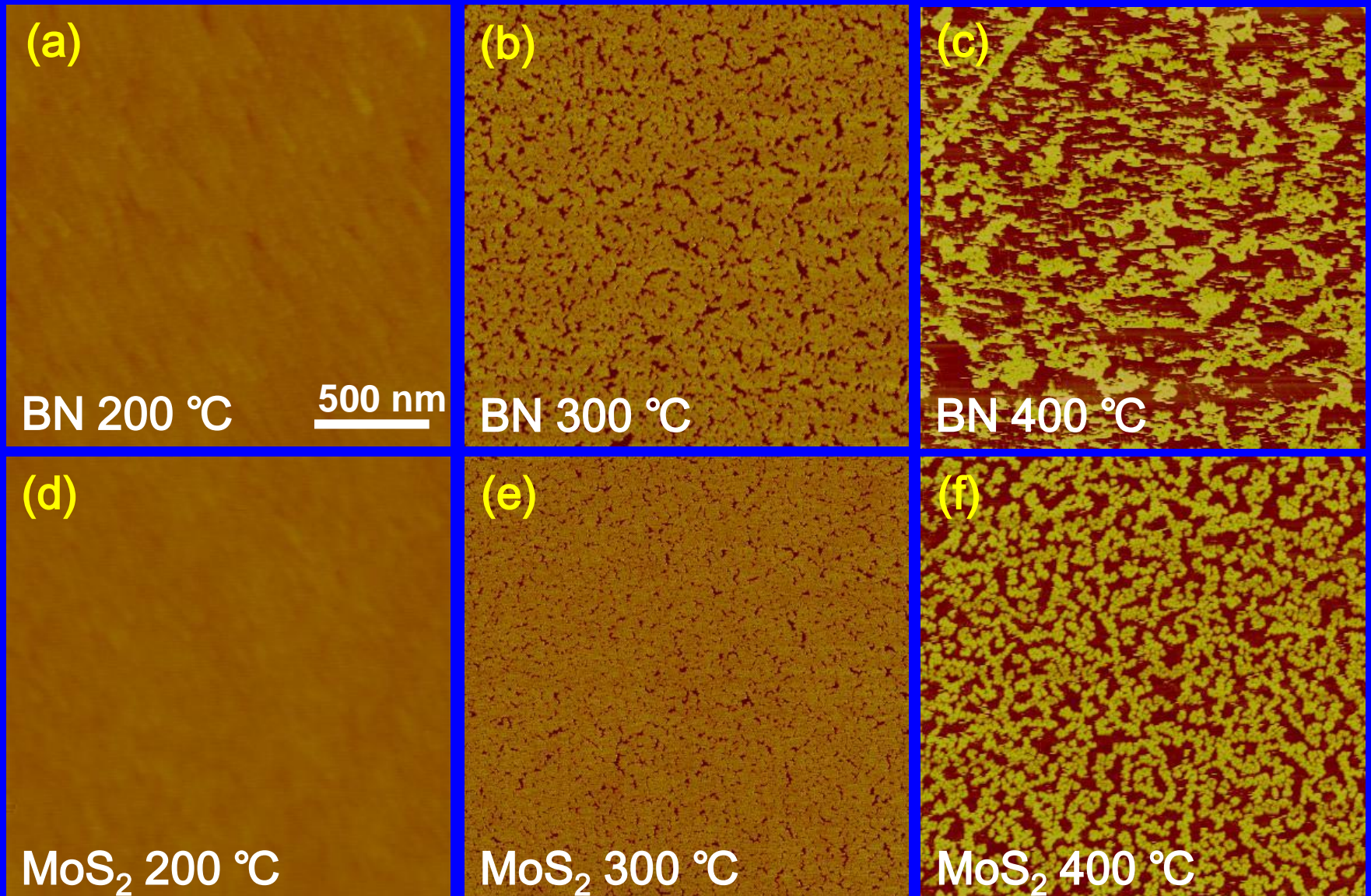


Q: Can we realize ALD growth on other 2D crystals?

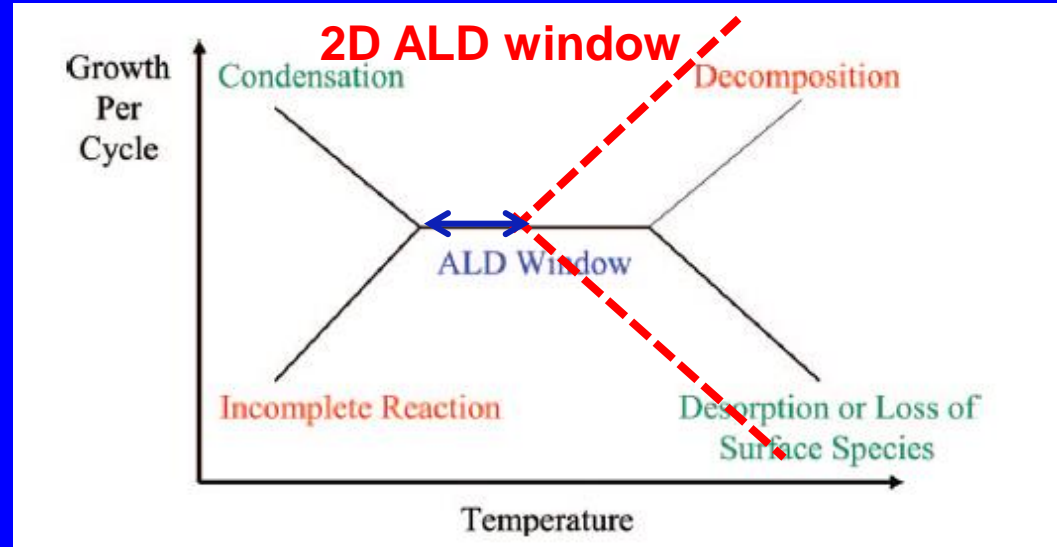
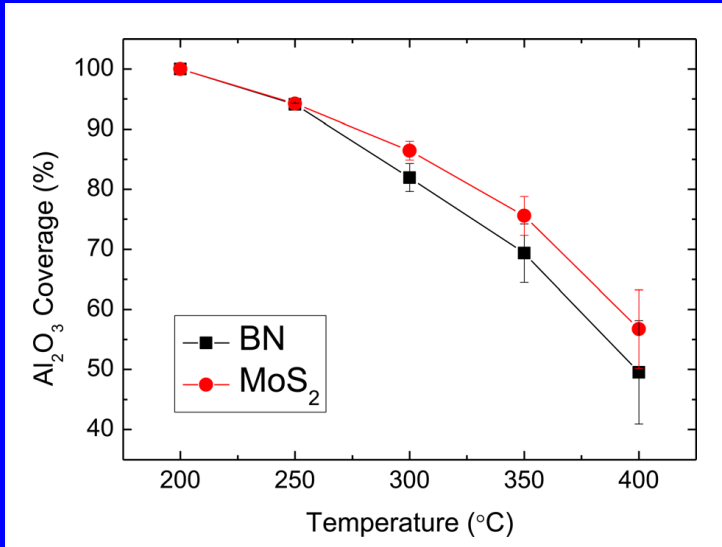
# ALD on MoS<sub>2</sub> 2D Crystal



# ALD on h-BN and MoS<sub>2</sub> 2D Crystal



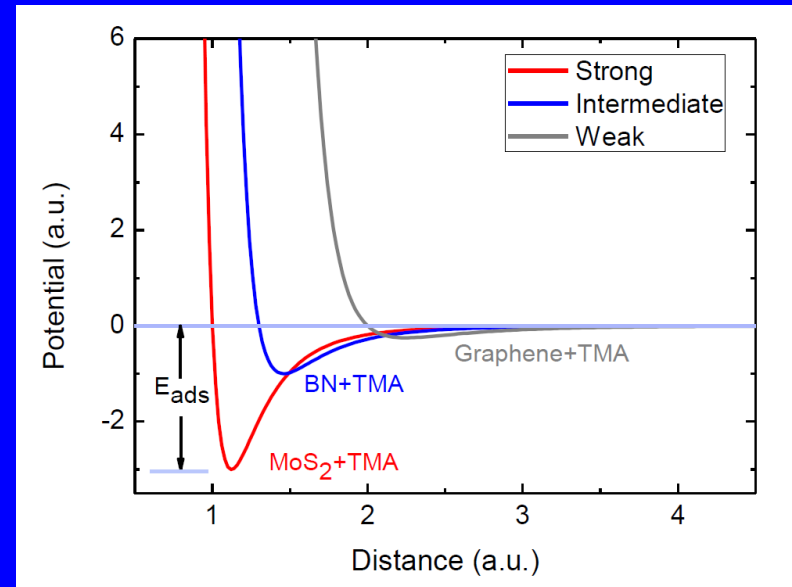
# ALD on h-BN and MoS<sub>2</sub> 2D Crystal



## Lennard-Jones Potential Model

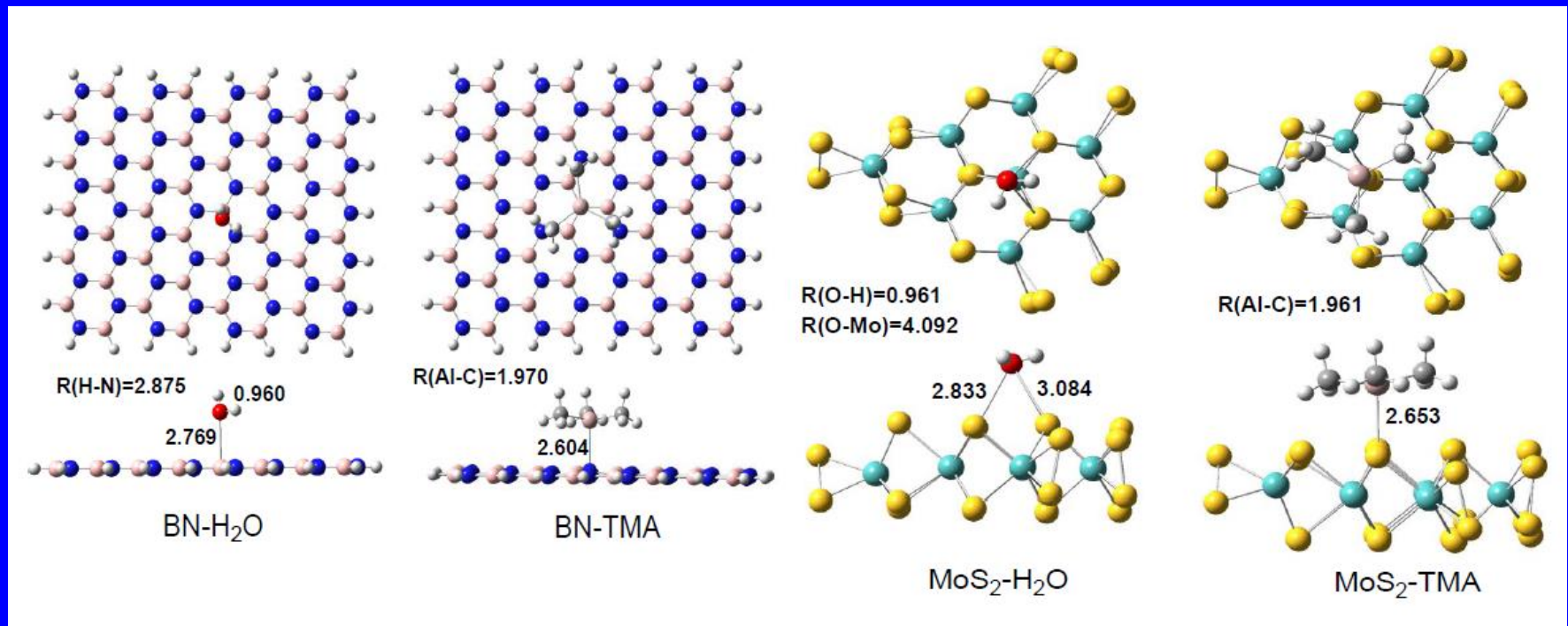
$$V_{LJ} = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

$$= \epsilon \left[ \left( \frac{r_m}{r} \right)^{12} - 2 \left( \frac{r_m}{r} \right)^6 \right]$$

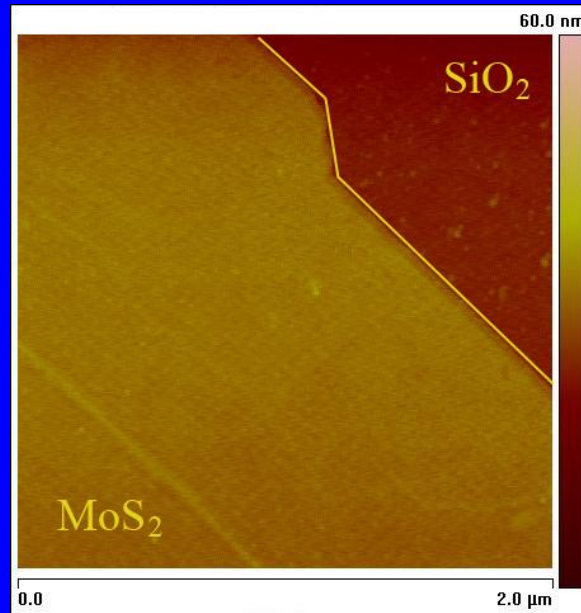
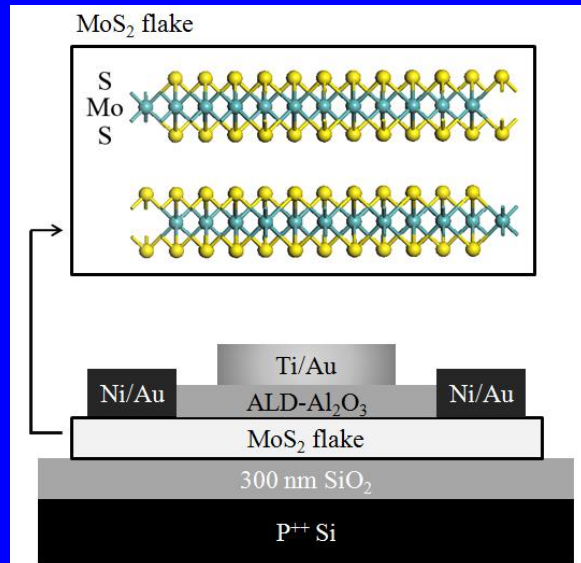


# ALD on h-BN and MoS<sub>2</sub> 2D Crystal

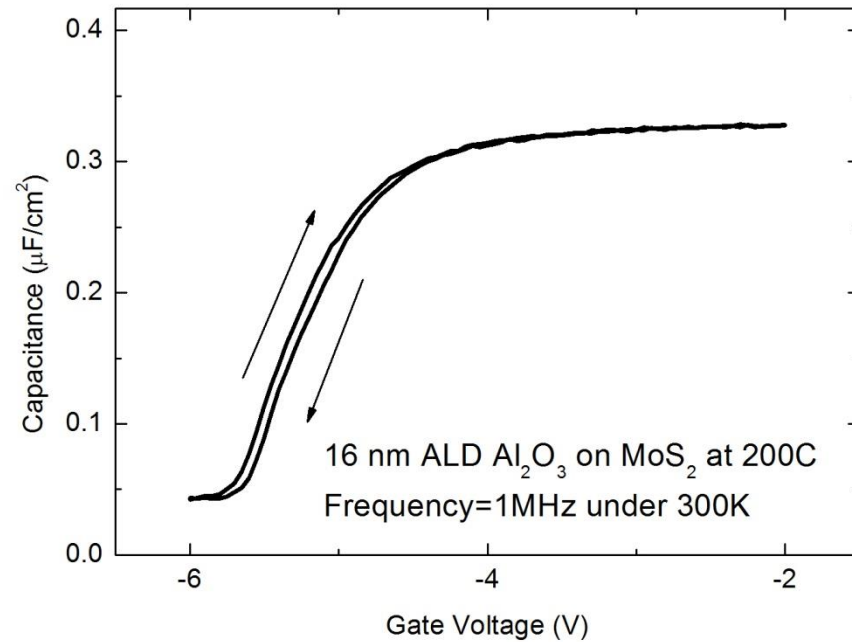
## *Ab initio* DFT calculations:



# ALD high-k/MoS<sub>2</sub> dual-gate MOSFET

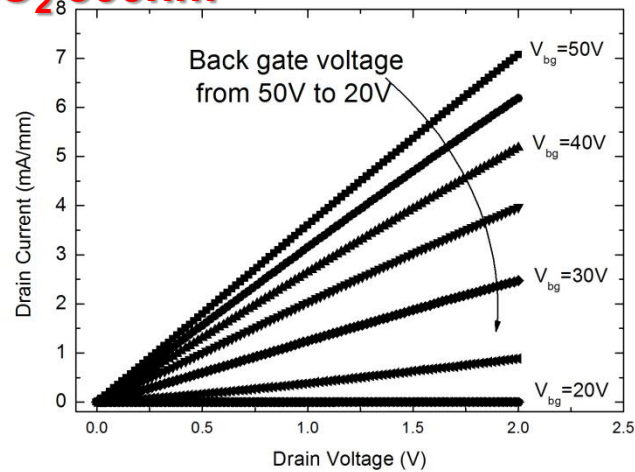


## Few-layer MoS<sub>2</sub>

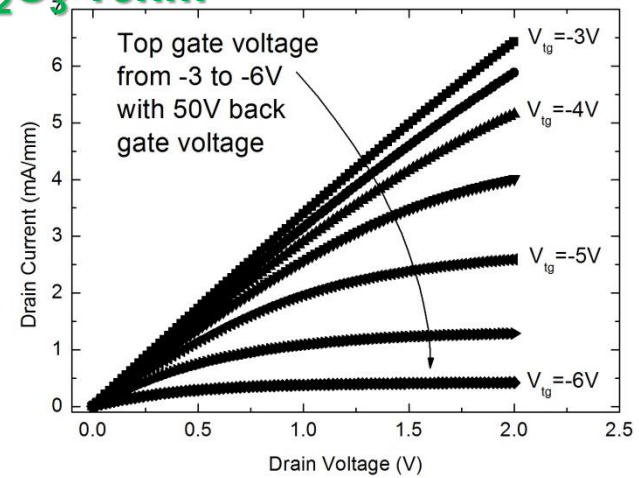


# ALD high-k/MoS<sub>2</sub> dual-gate MOSFET

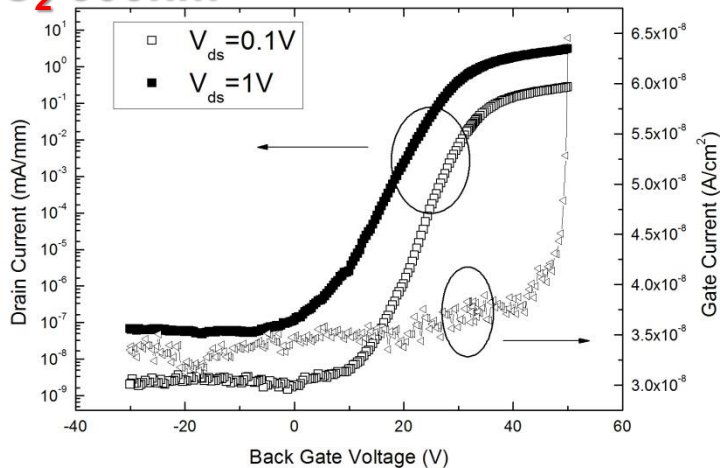
## SiO<sub>2</sub> 300nm



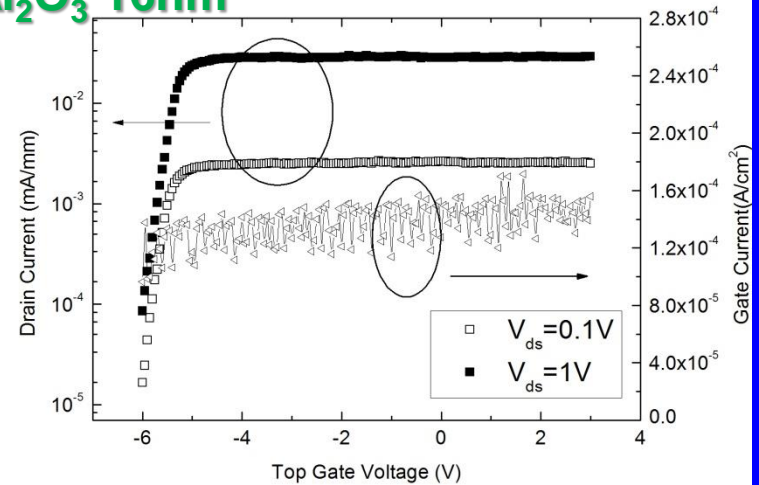
## Al<sub>2</sub>O<sub>3</sub> 16nm



## SiO<sub>2</sub> 300nm

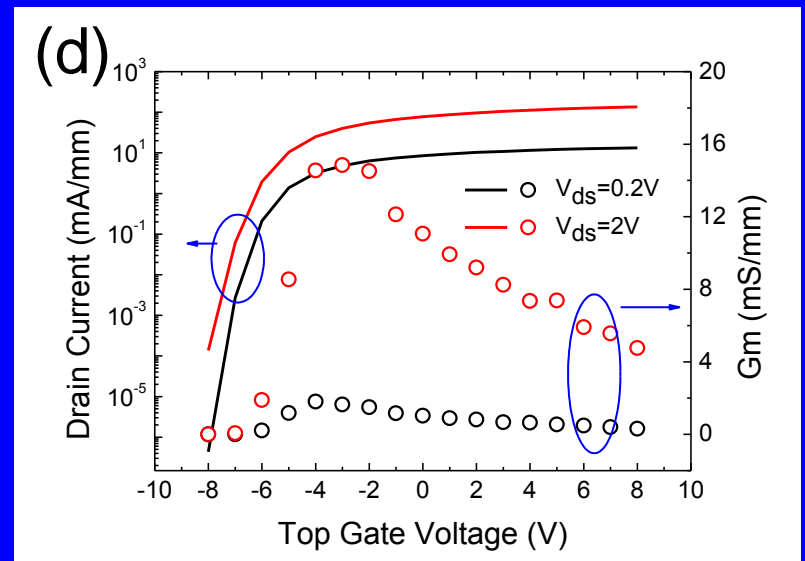
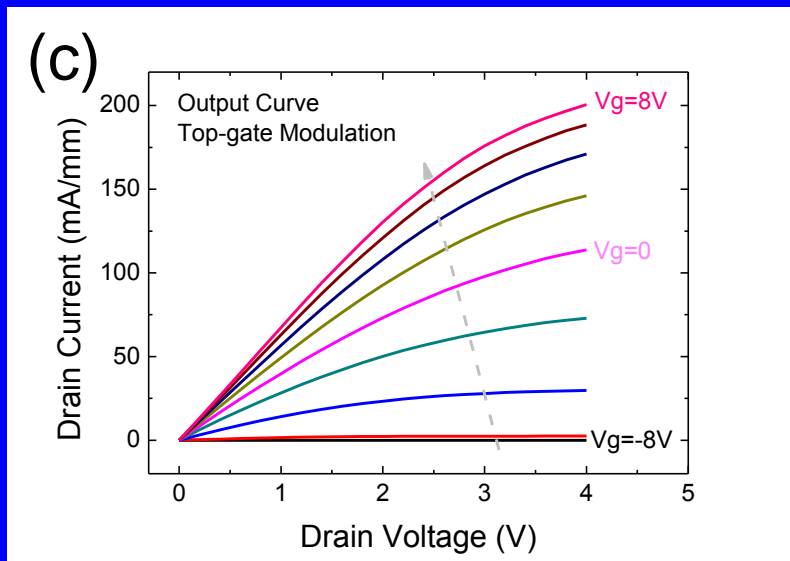
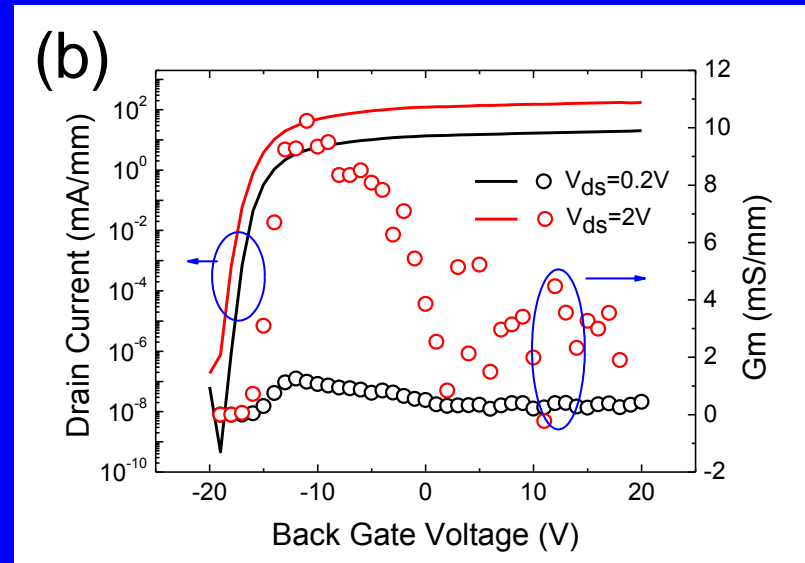
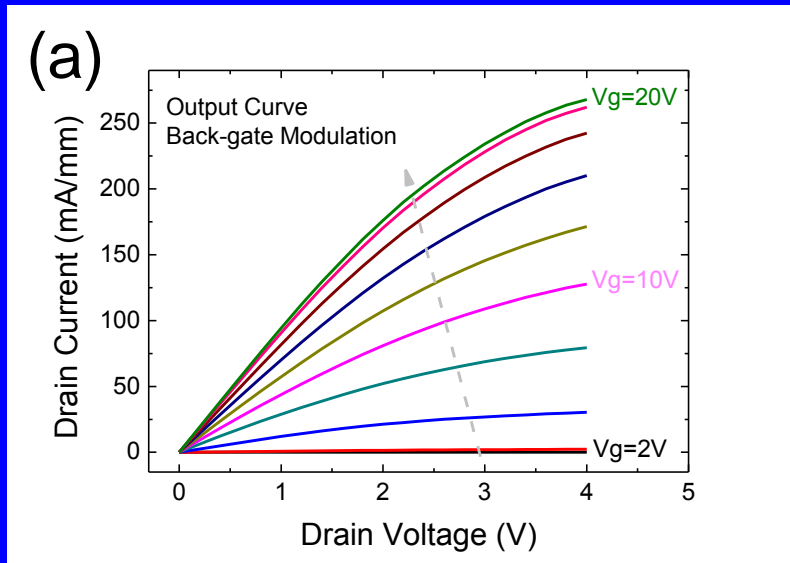


## Al<sub>2</sub>O<sub>3</sub> 16nm



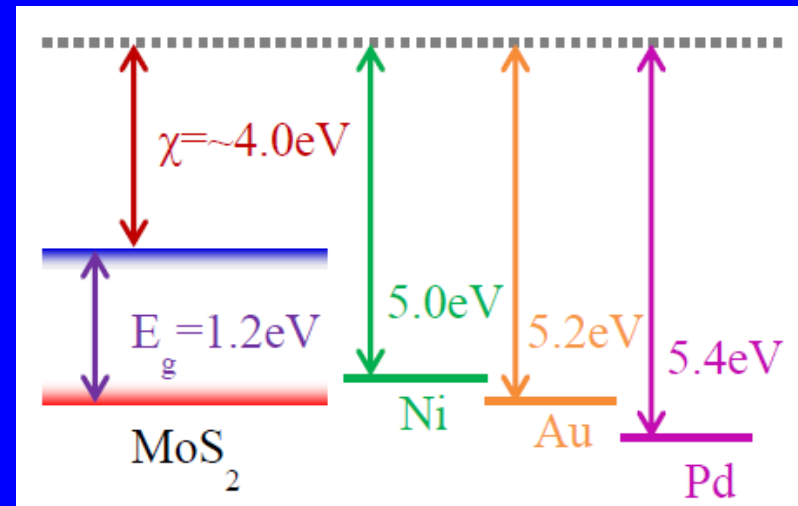
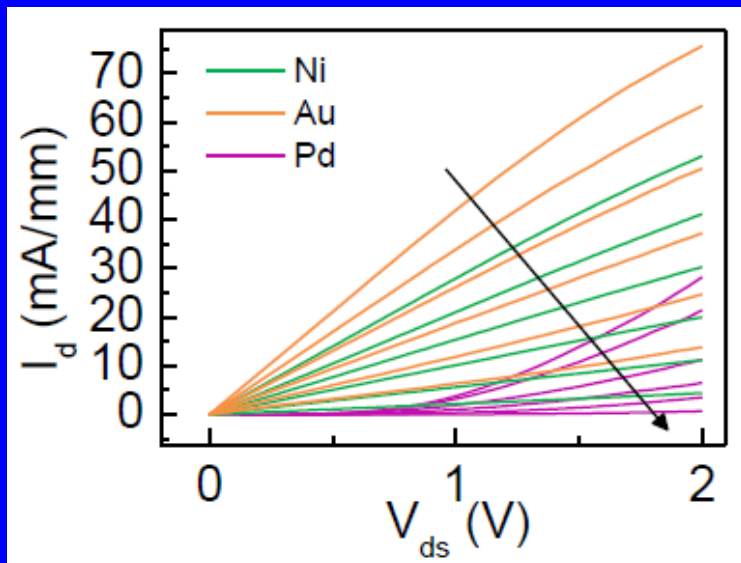
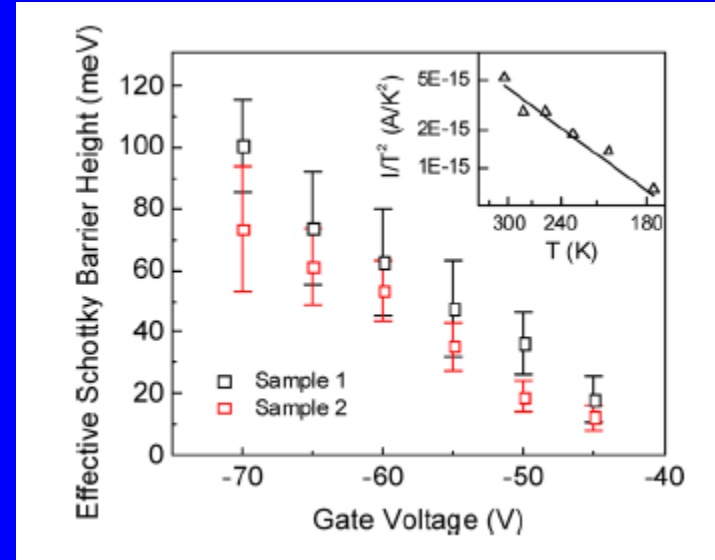
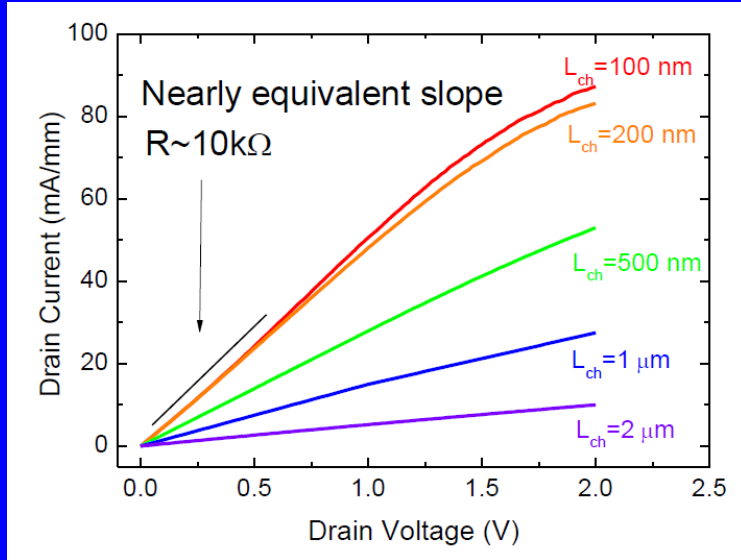


# Low Work-function Metal (Ti) for MoS<sub>2</sub> NFET

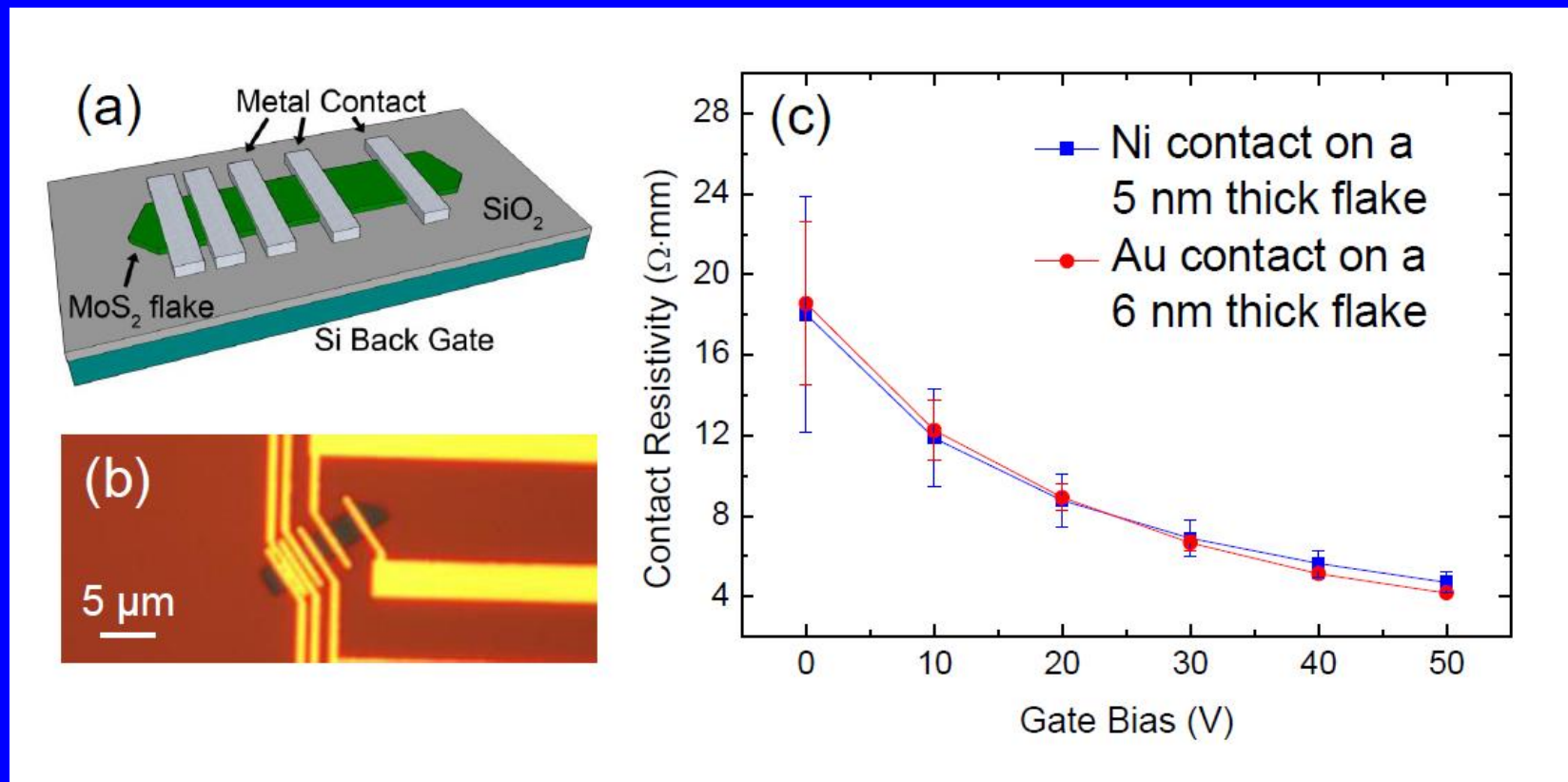


Drain current ~ 300 mA/mm starts encouraging as transistors

# MoS<sub>2</sub> MOSFET Contacts

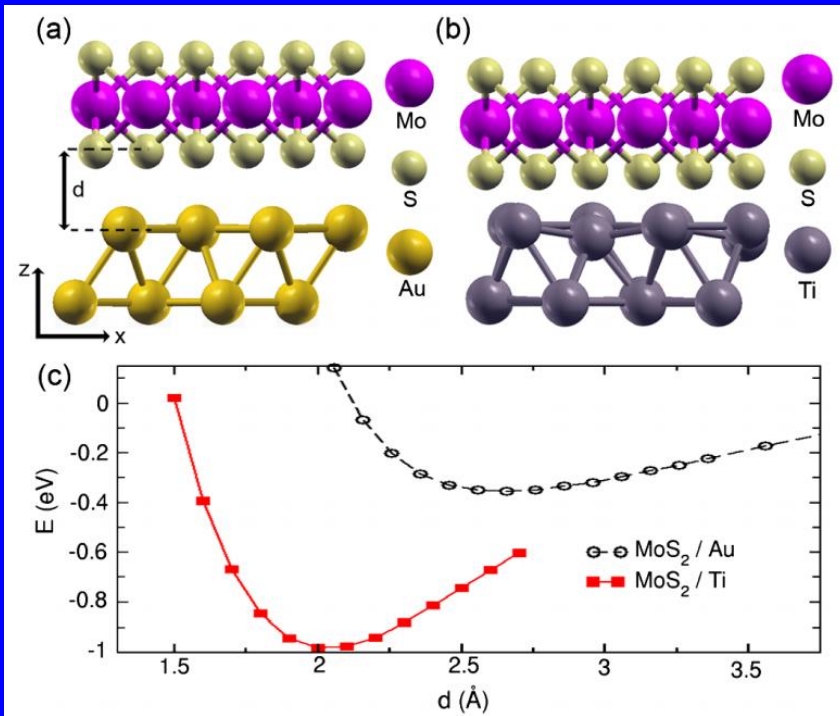


# $R_c$ of MoS<sub>2</sub> MOSFETs by TLM

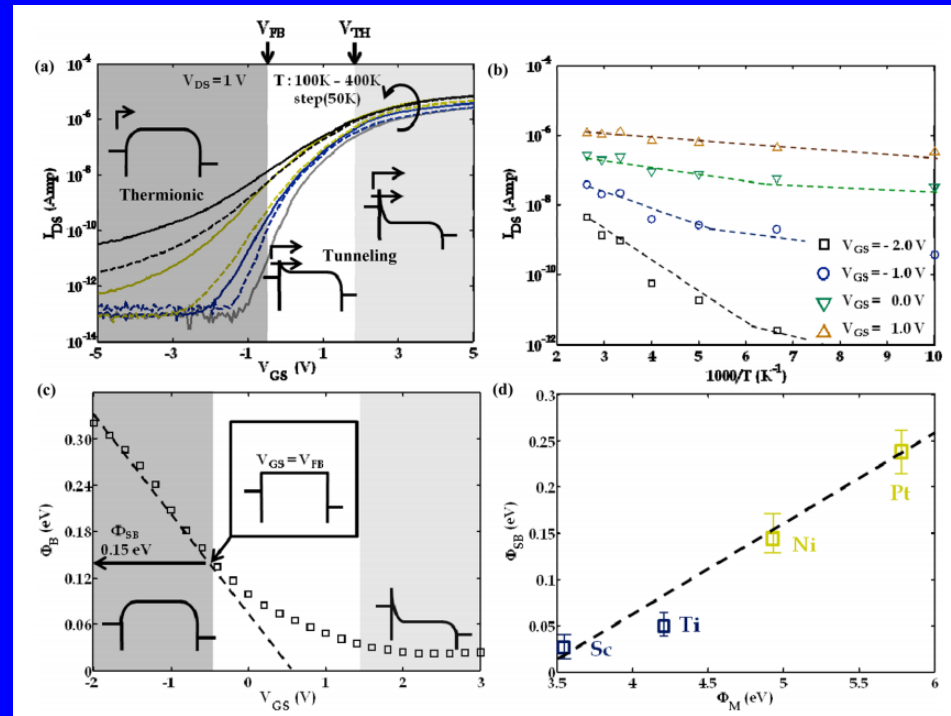


Contact Resistance: 5 Ω·mm (too large!)

# Metal Contacts on MoS<sub>2</sub>



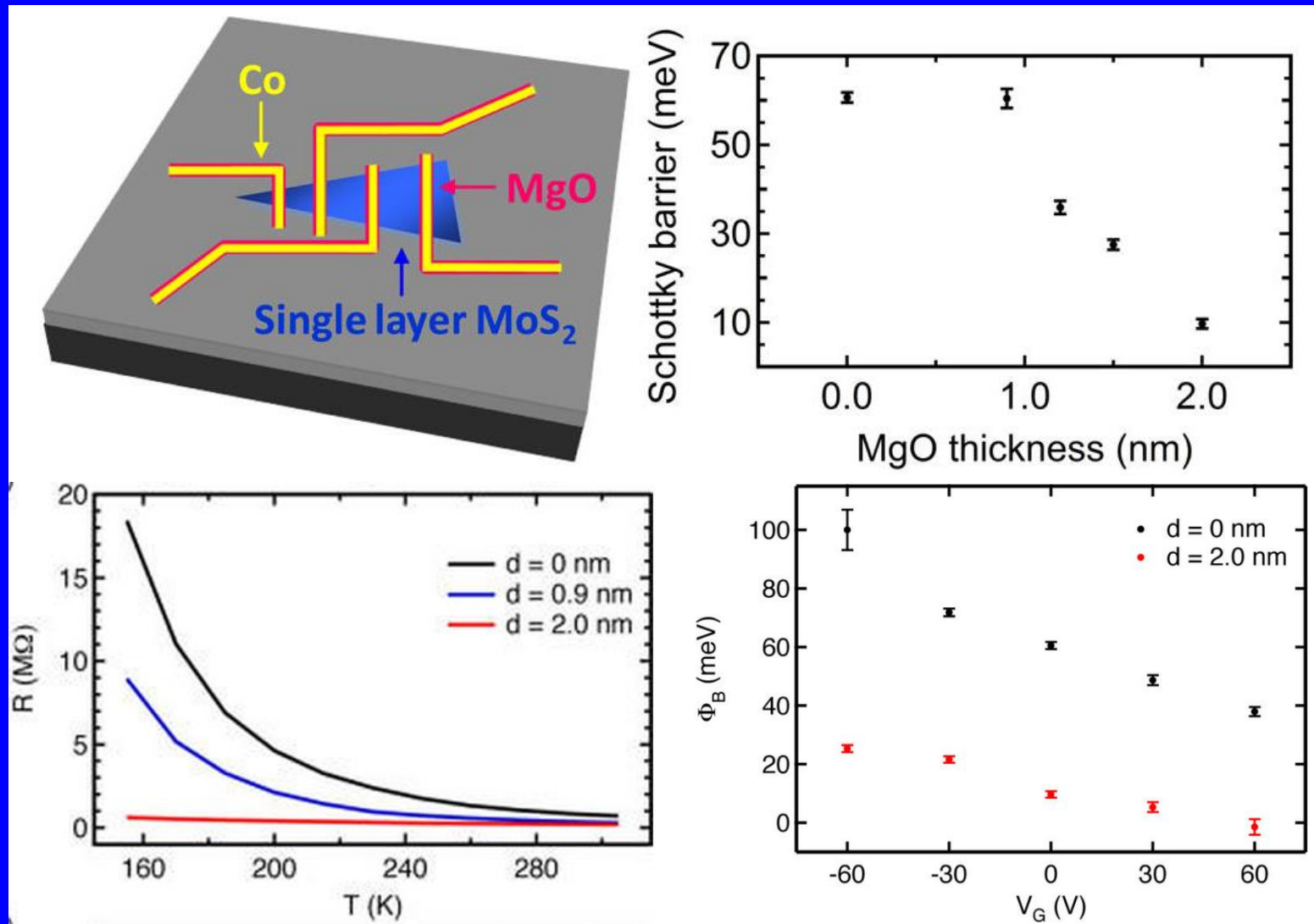
I. Popov et al, PRL 2012



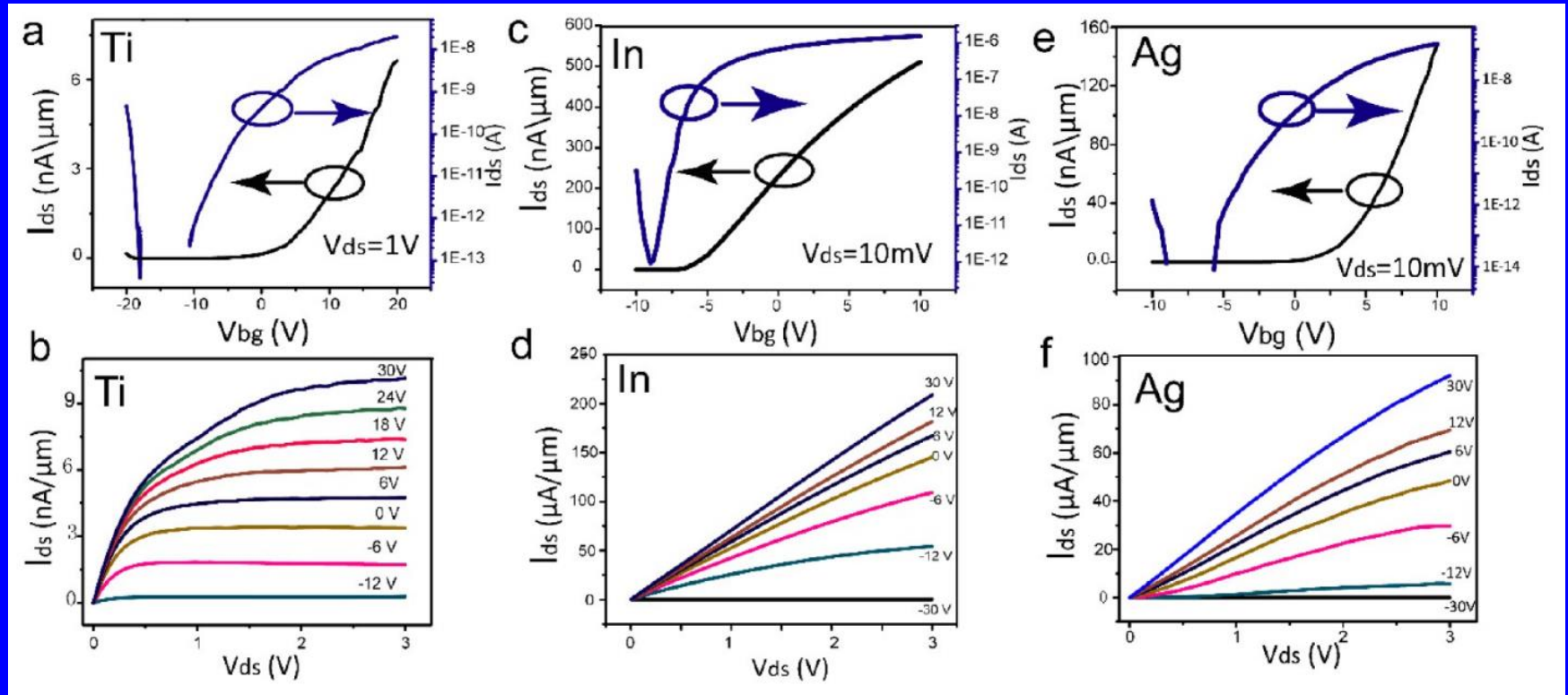
S. Das et al, Nano Lett. 2012

**Much more work on contact engineering is needed:**  
 **$R_c < 0.1 \Omega \cdot \text{mm}$  at least**      **For ITRS 10nm  $\rho_c = 1 \times 10^{-9} \Omega \text{cm}^2$**

# Tunneling Barrier on MoS<sub>2</sub>



# Metal contacts on WSe<sub>2</sub>



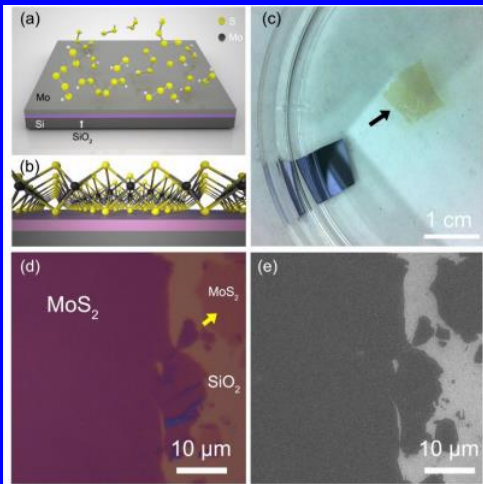
W. Liu et al, Nano Lett. 2013

**Different material sources**  
**Different laboratories**  
**Different students**  
**Different time**



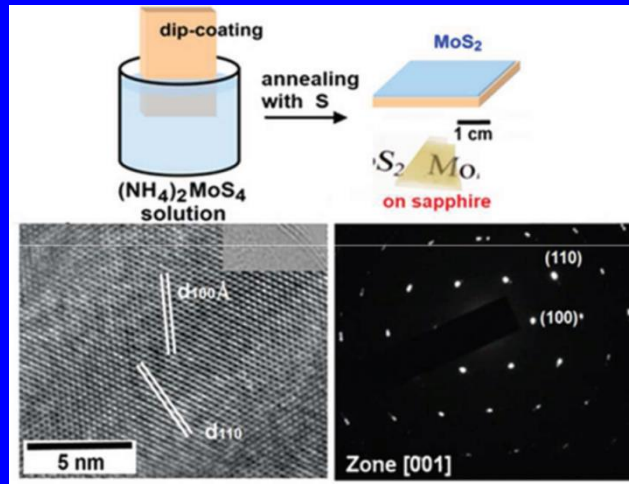
**Same starting materials**  
**Hundreds of devices**

# MoS<sub>2</sub>: CVD Synthesis



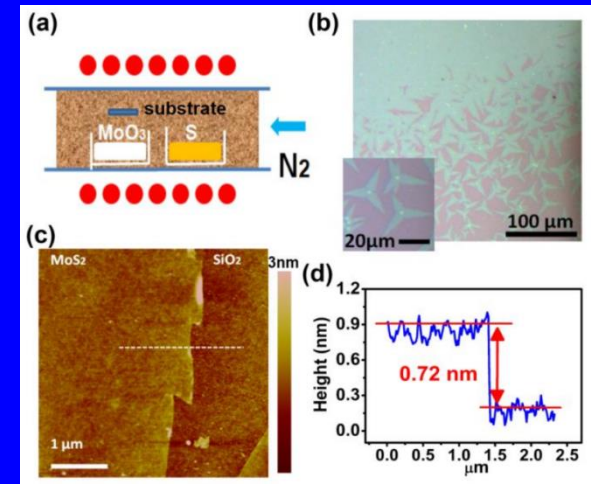
Direct  
Sulfurization of  
Mo layer

Y. Zhan et al, Small, 8, 966 (2012)



Sulfurization of Mo  
Compound (NH<sub>4</sub>)<sub>2</sub>MoS<sub>4</sub>

K.K. Liu et al, Nano Lett. 12, 1538 (2012)

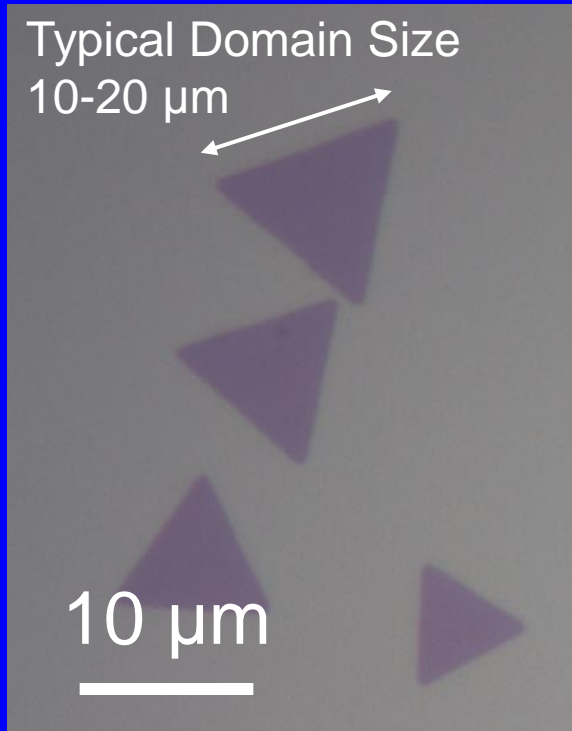


Sulfurization of  
MoO<sub>3</sub>

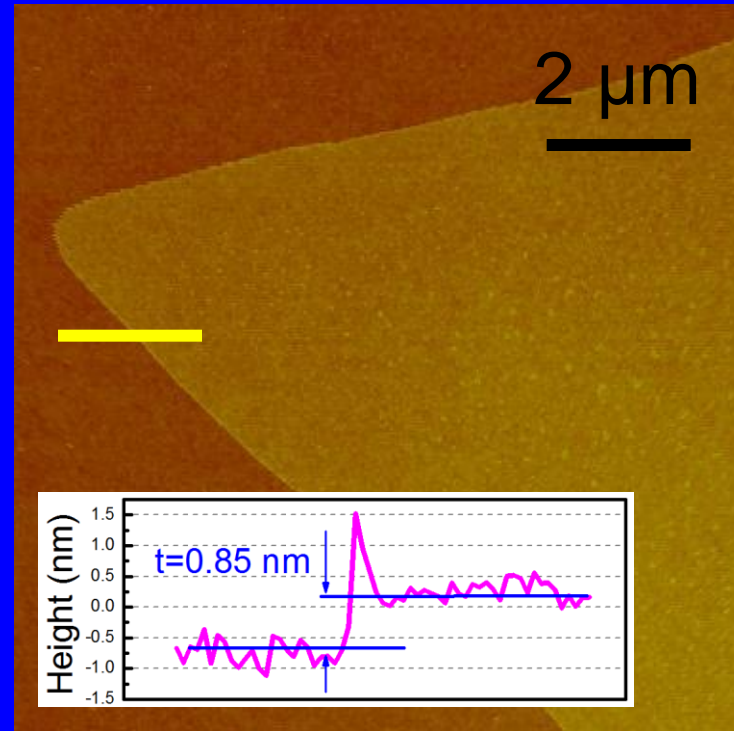
Y.H. Lee et al, Adv. Mater. 24, 2320(2012)

# CVD Monolayer MoS<sub>2</sub>

## Optical Micrograph



## Atomic Force Microscope



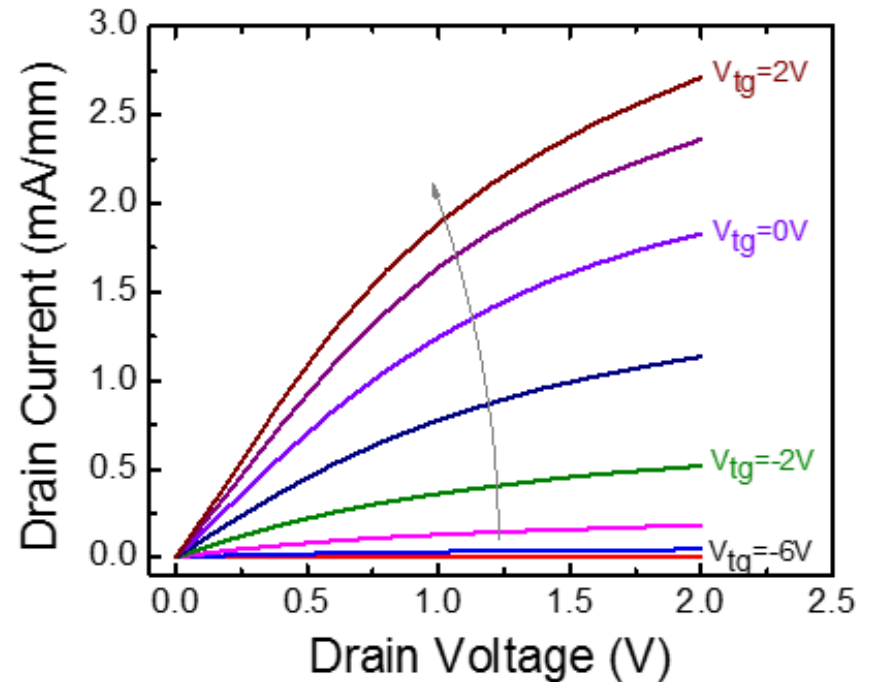
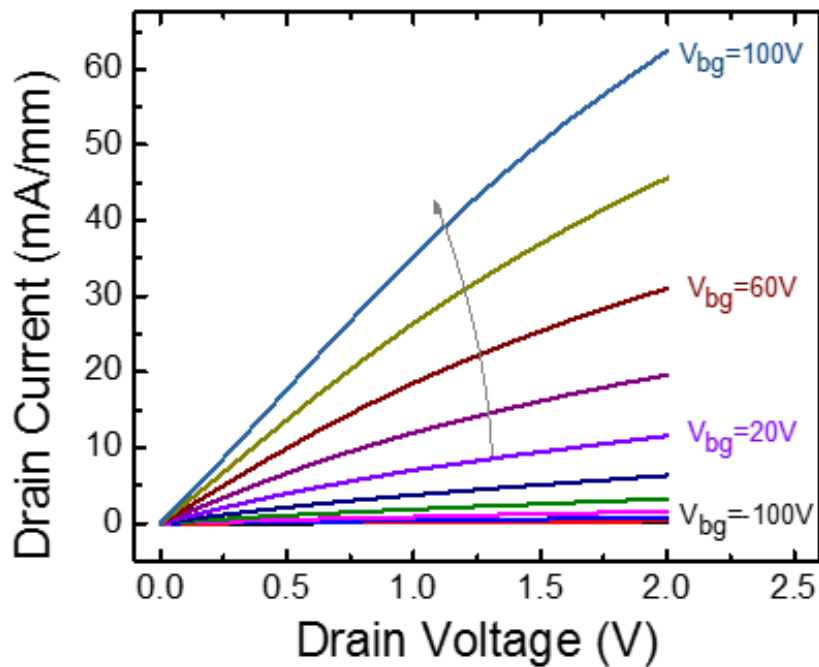
H. Liu et al. Nano Lett., 13, 2640 (2013)

In collaborations with Jun Lou and P.M. Ajayan's groups at Rice University



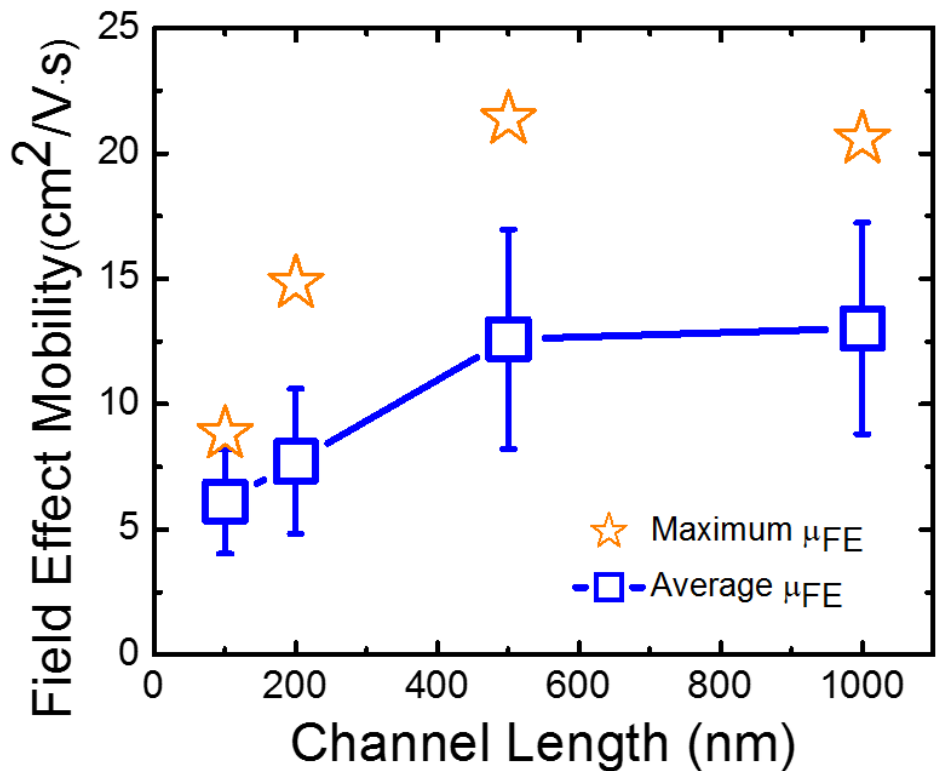
# Transistor: Output Behavior

$L_{ch}=100$  nm



The difference between Top/Back Gate modulation mostly comes from  $R_C$ .

# Field-Effect Mobility

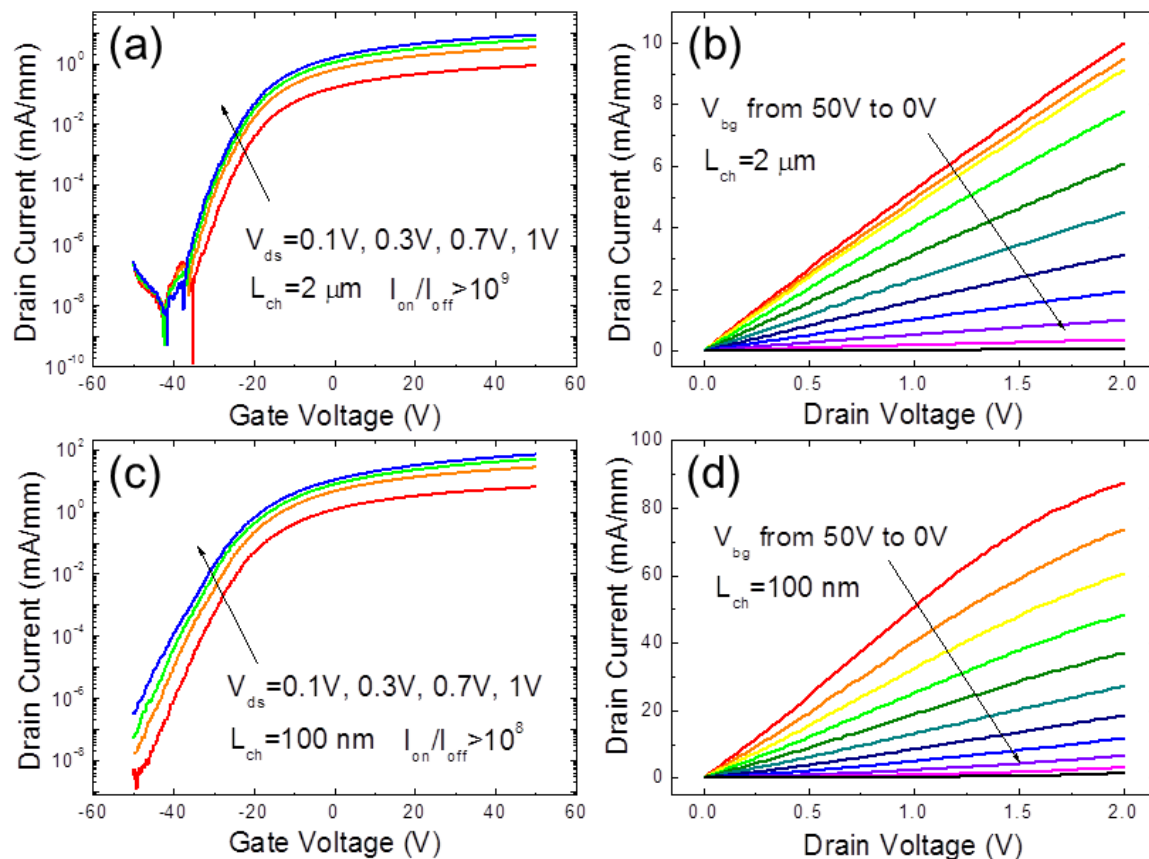


$$g_m = \frac{\partial I_{ds}}{\partial V_{gs}} = \mu_{FE} C_{ox} \frac{W}{L} V_{ds}$$

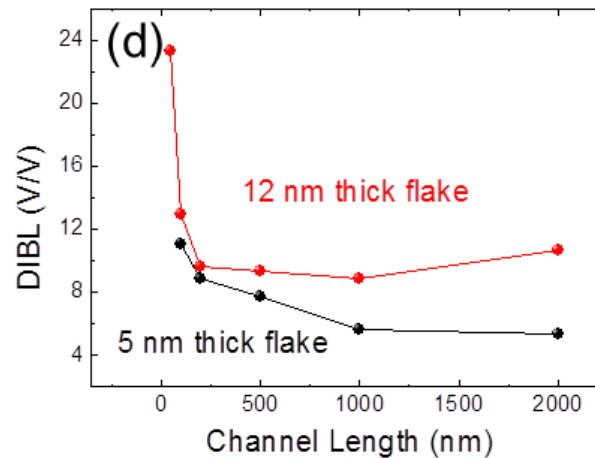
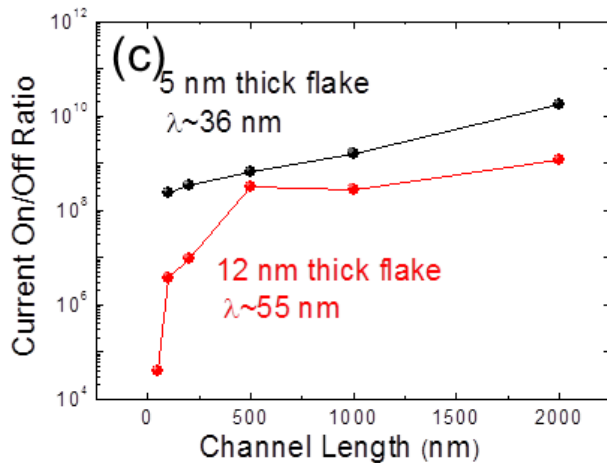
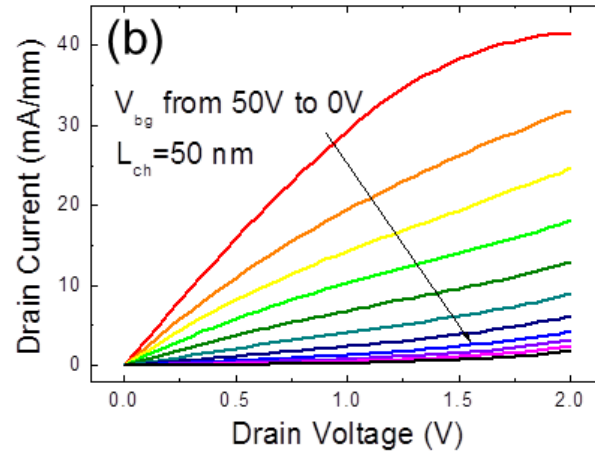
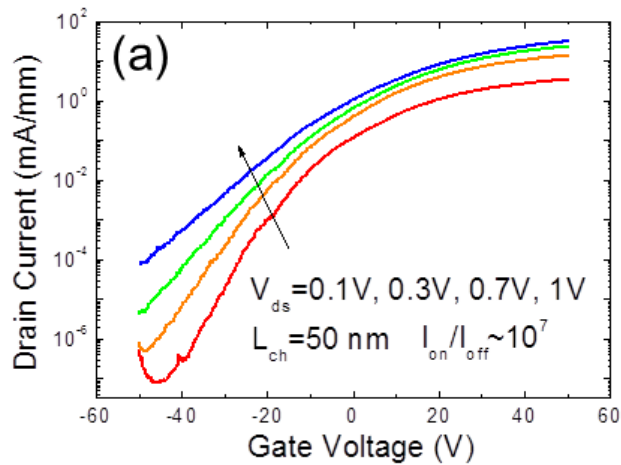
$$\mu' = \mu \left( \frac{R_{ch}}{R_{tot}} \right)^{-1} = \mu \left( 1 - \frac{2R_c}{R_{tot}} \right)^{-1}$$

$L_{ch}$	$\mu_{FE,mean}$ (cm <sup>2</sup> /V·s)	$\mu_{FE,max}$ (cm <sup>2</sup> /V·s)
100 nm	6.10	8.82
200 nm	7.71	14.8
500 nm	12.6	21.6
1 $\mu$ m	13.0	20.6

# MoS<sub>2</sub> MOSFET Length Scaling

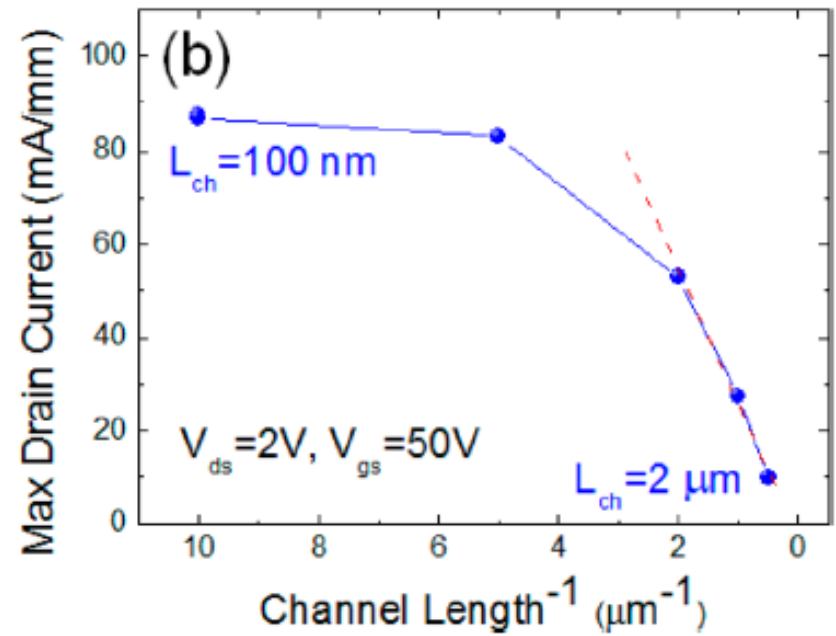
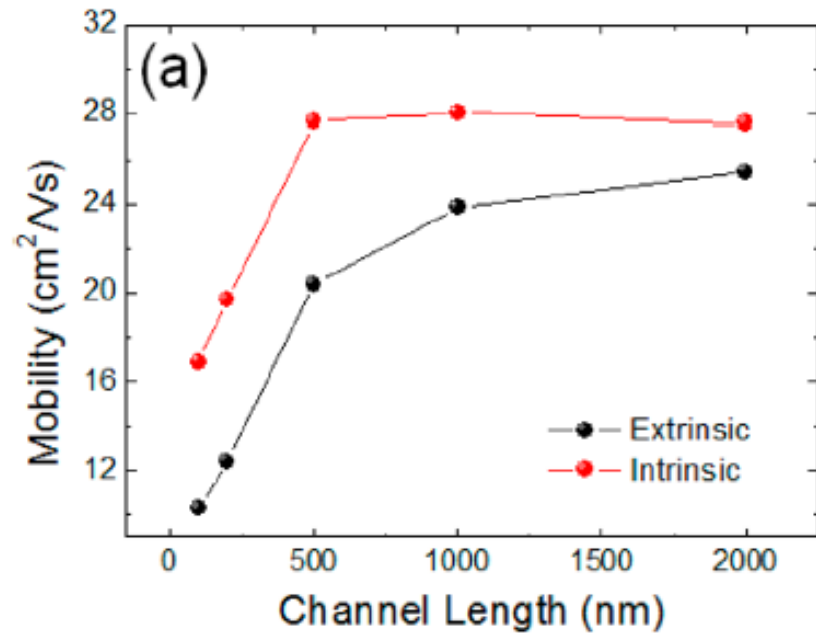


# MoS<sub>2</sub> MOSFET Length Scaling

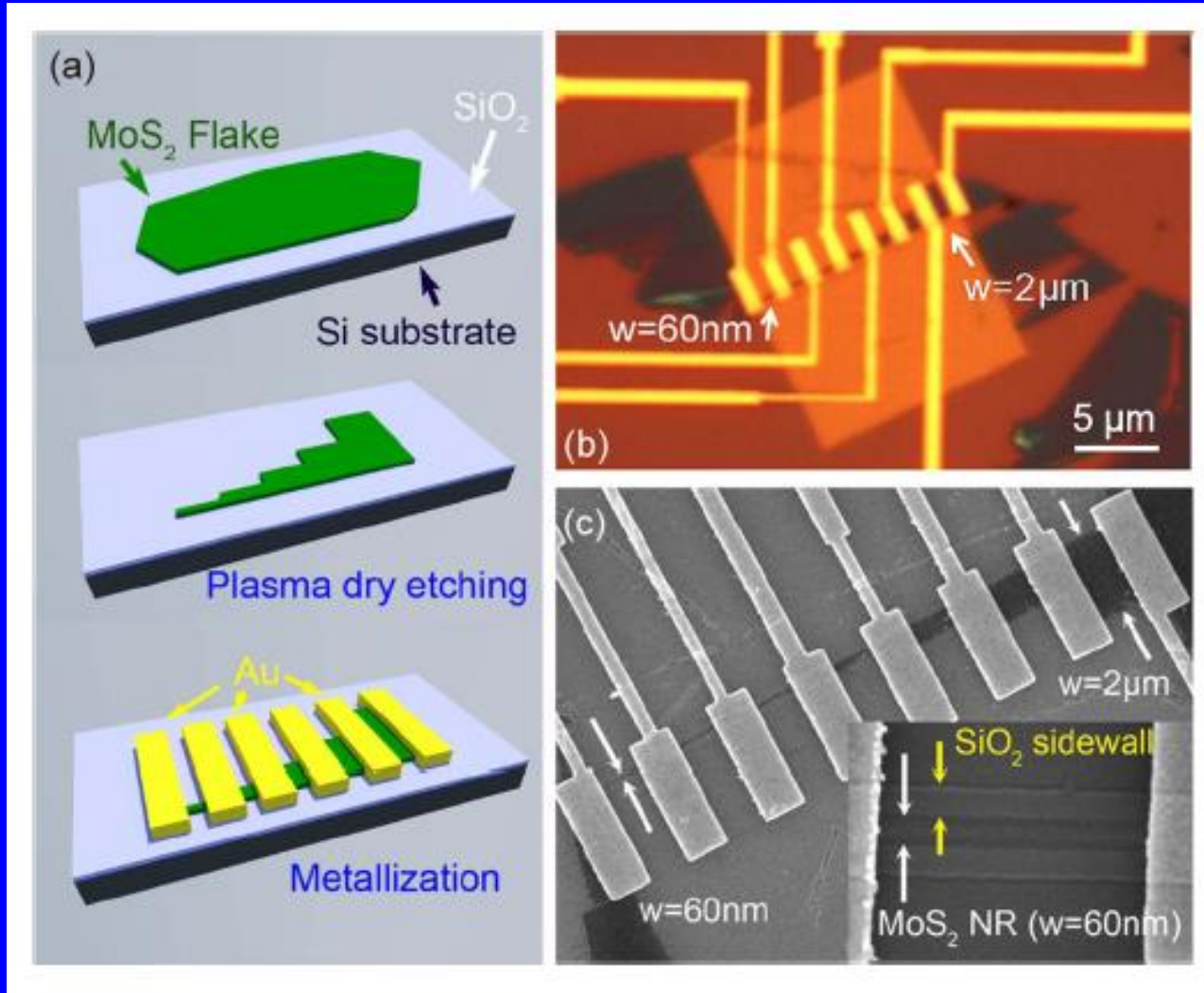


Evident short-channel effects at 12nm thick MoS<sub>2</sub> and  $L_{ch} = 50 \text{ nm}$

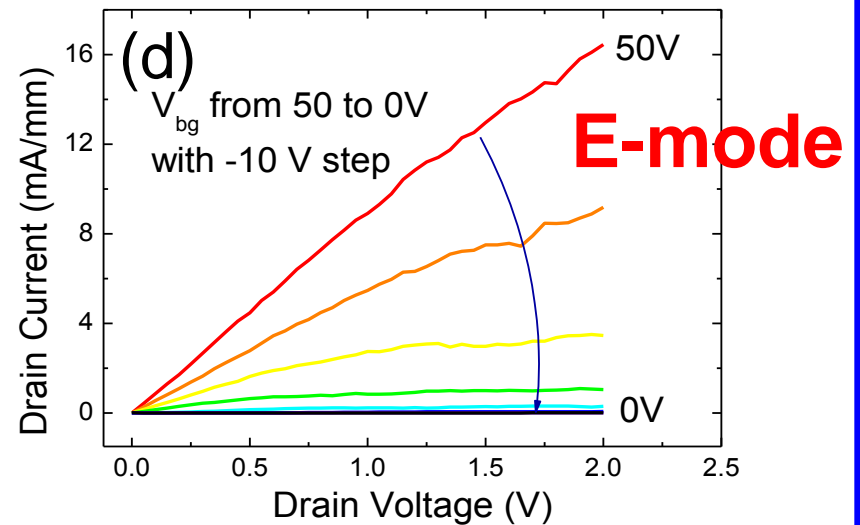
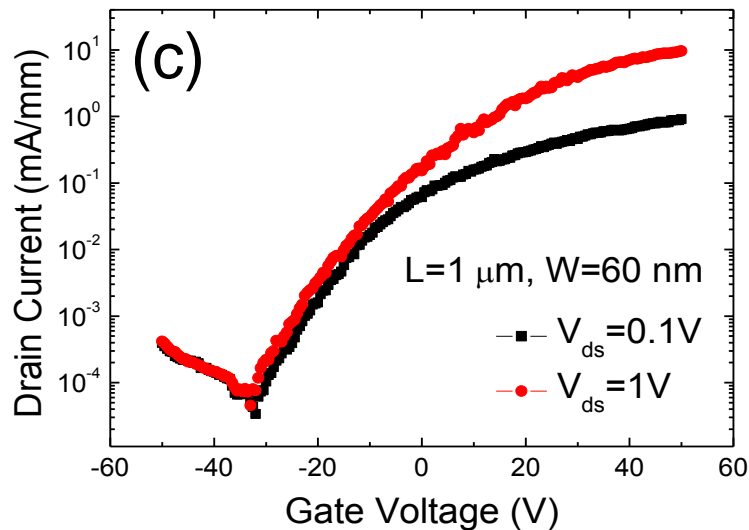
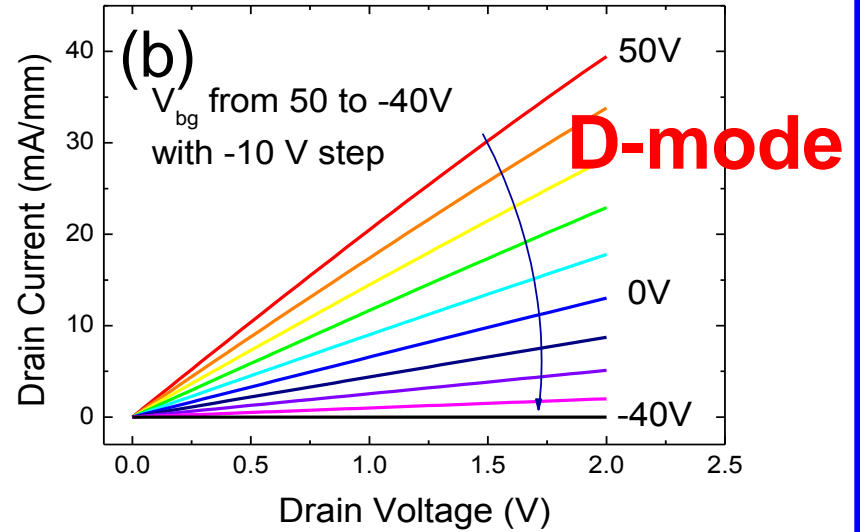
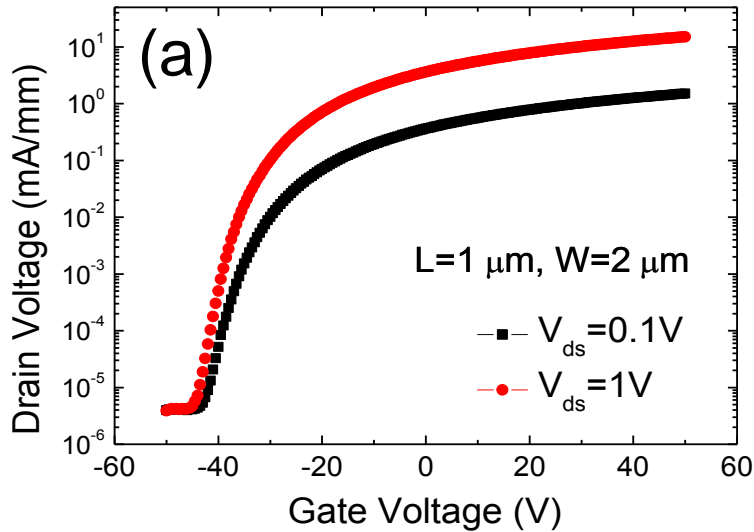
# MoS<sub>2</sub> MOSFET Length Scaling



# MoS<sub>2</sub> MOSFET Width Scaling

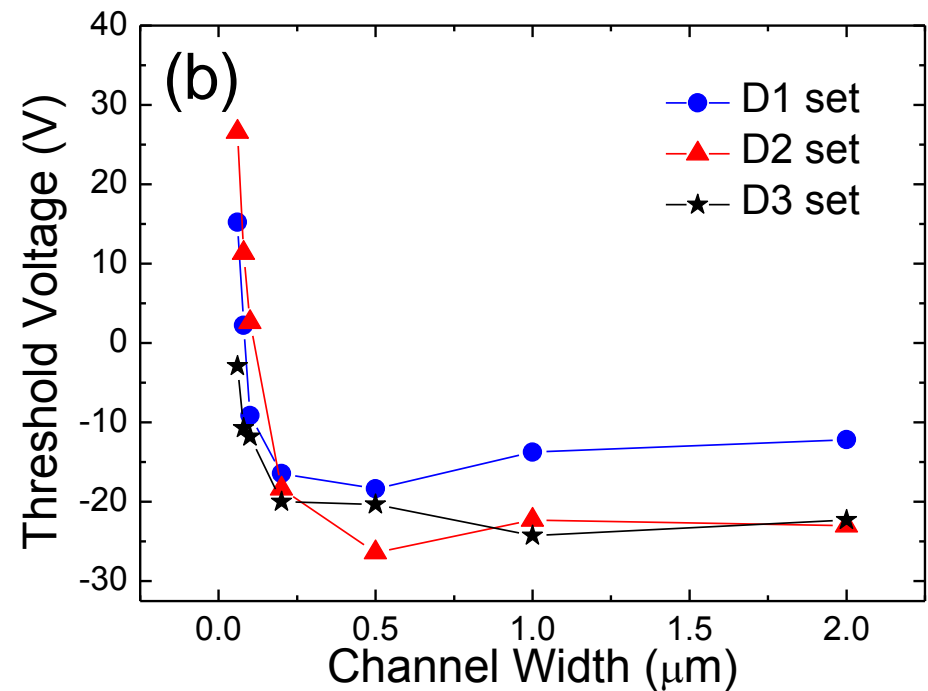
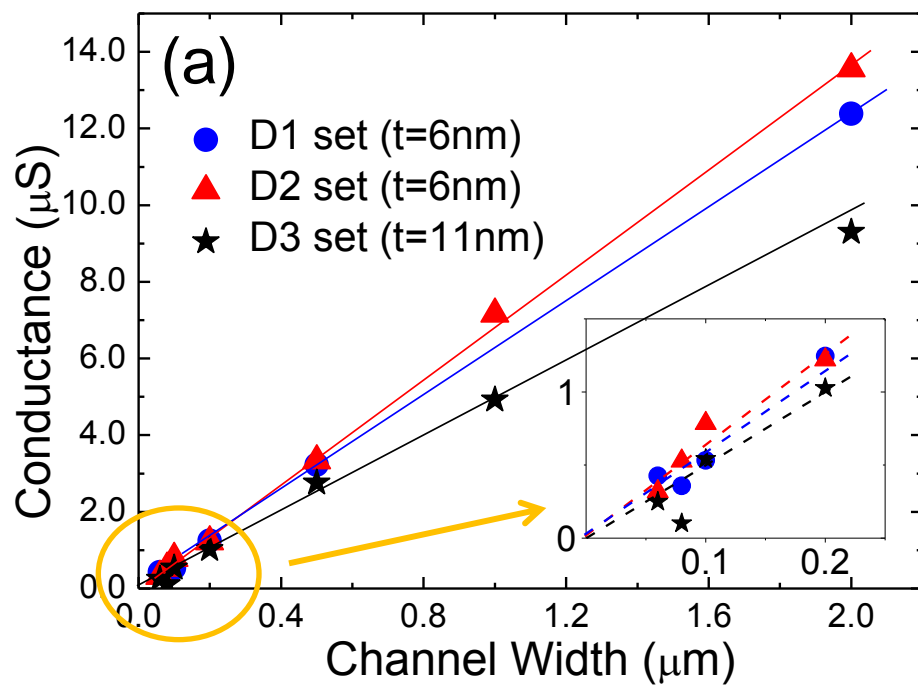


# MoS<sub>2</sub> MOSFET Width Scaling



# MoS<sub>2</sub> MOSFET Width Scaling

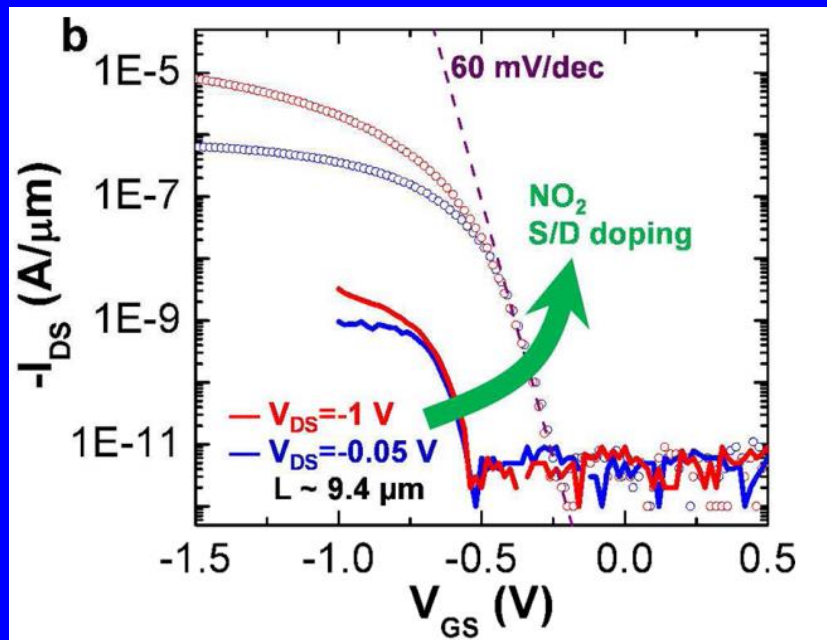
D-mode to E-mode transition by simple width trimming



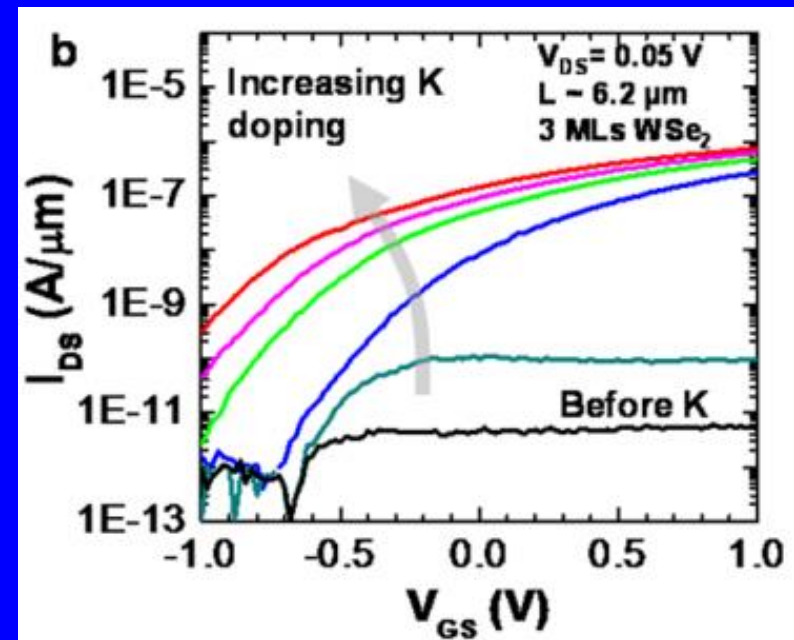


# Chemical Doping on 2D Crystals

## Gaseous Doping ( $\text{NO}_2$ )



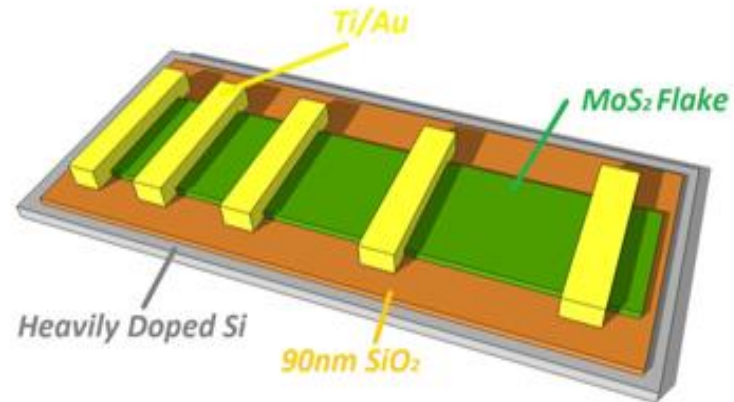
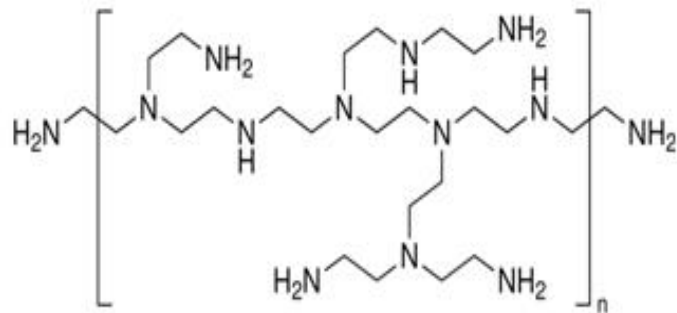
## Solid Doping (K)



$\text{WSe}_2$

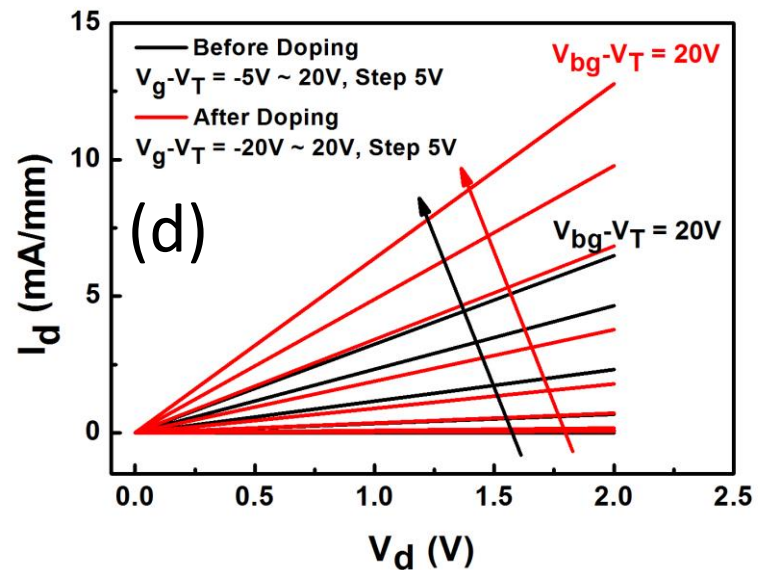
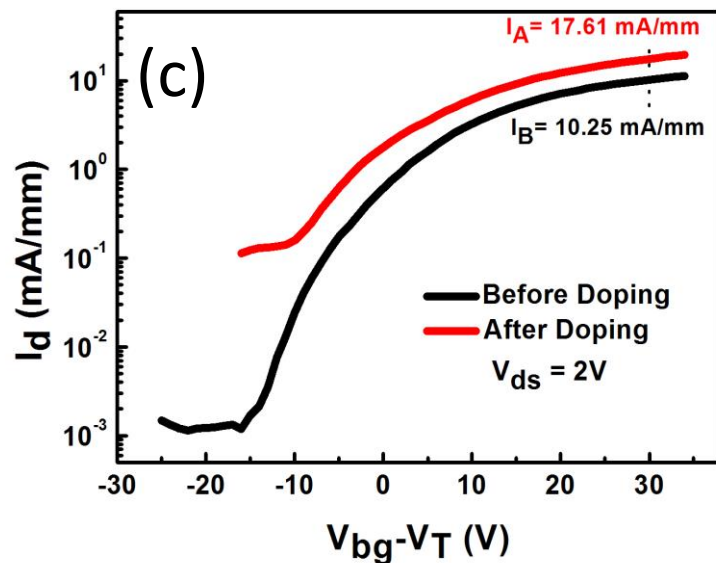
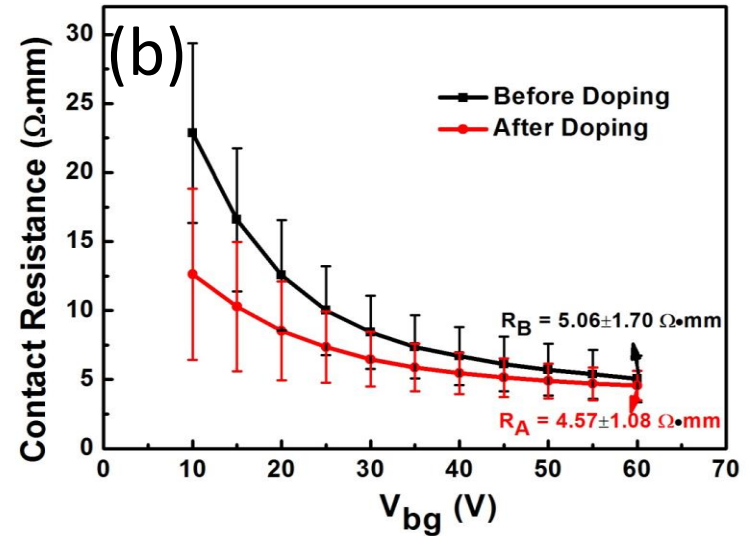
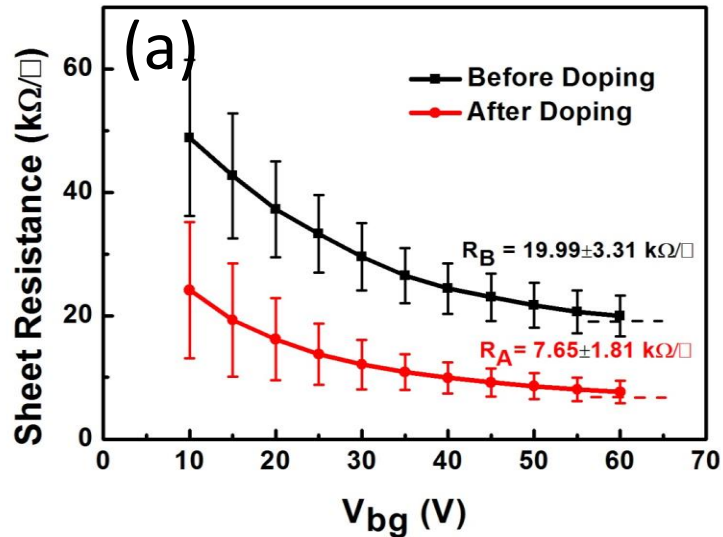
H. Fang et al. Nano Lett 2012  
H. Fang et al. Nano Lett 2013

# MoS<sub>2</sub> Molecular Doping

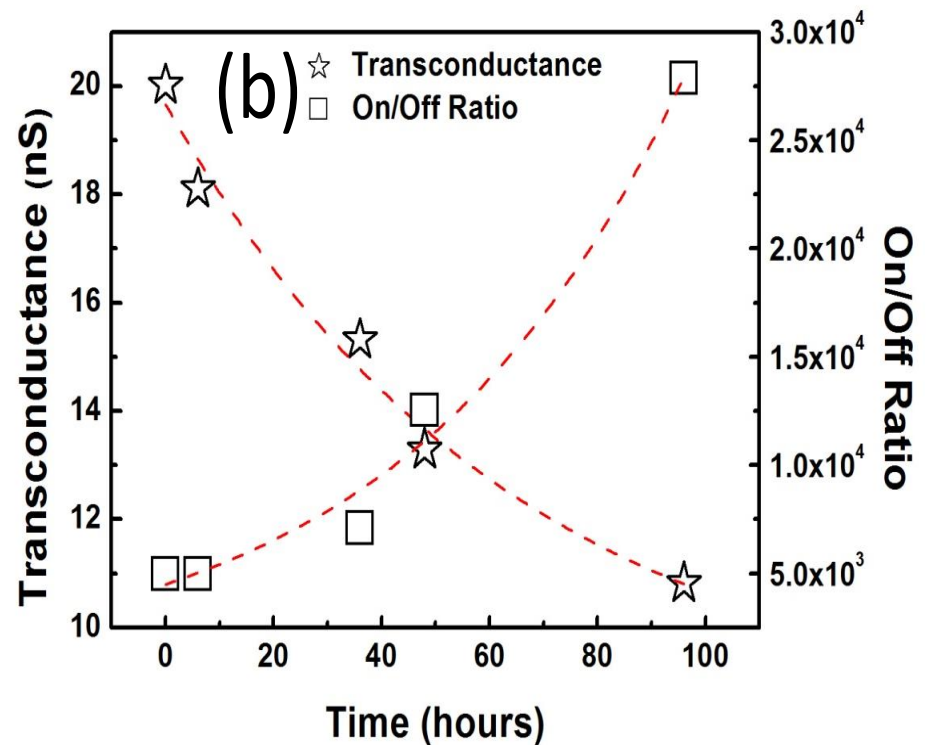
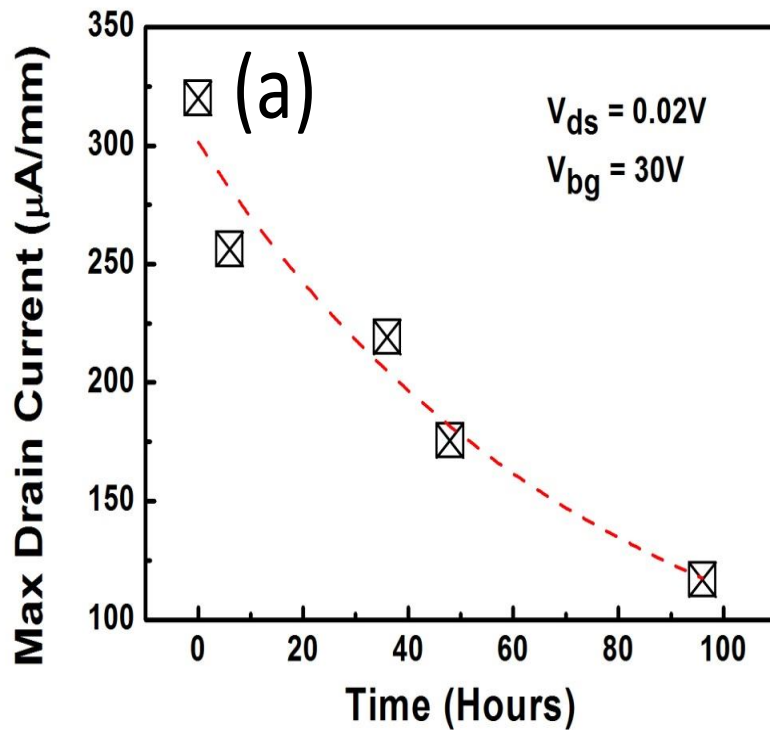


**Strong n-type dopant:  
Polyethylenimine (PEI)**

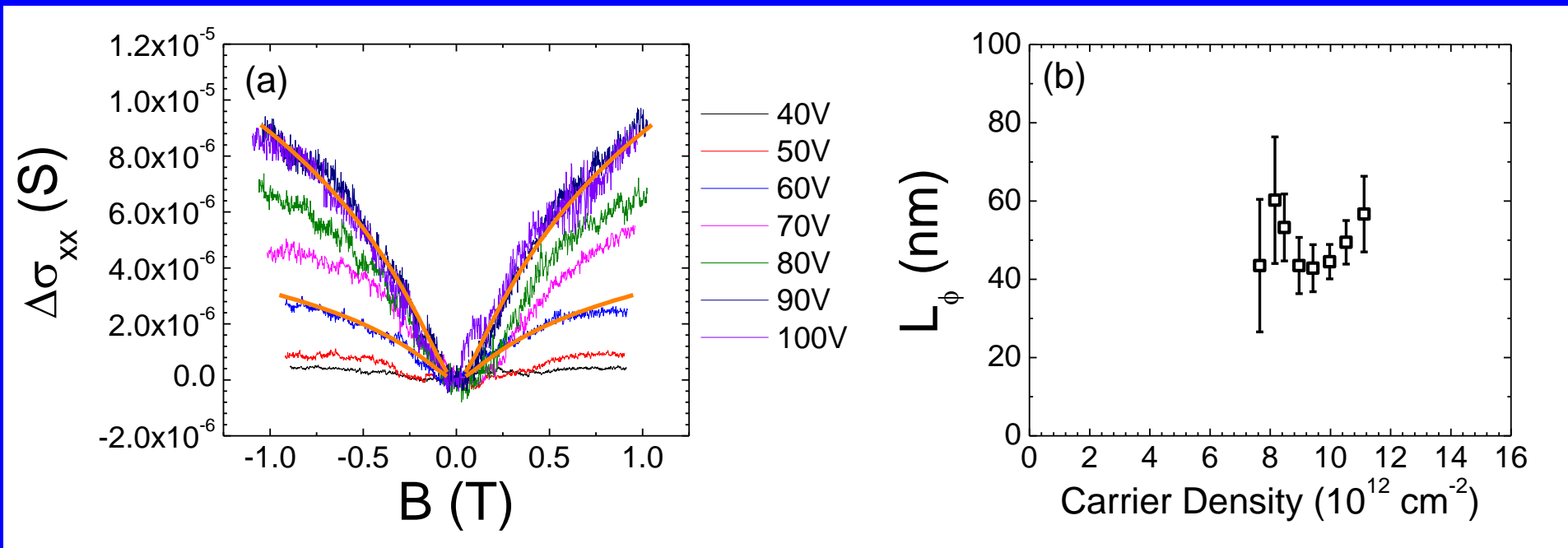
# MoS<sub>2</sub> Molecular Doping



# MoS<sub>2</sub> Molecular Doping



# Electron Phase Coherence in MoS<sub>2</sub>



$$\Delta\sigma = \sigma(B) - \sigma(B = 0) = \alpha \frac{e^2}{4\pi^2 \hbar} F\left(\frac{B}{B_\phi}\right)$$

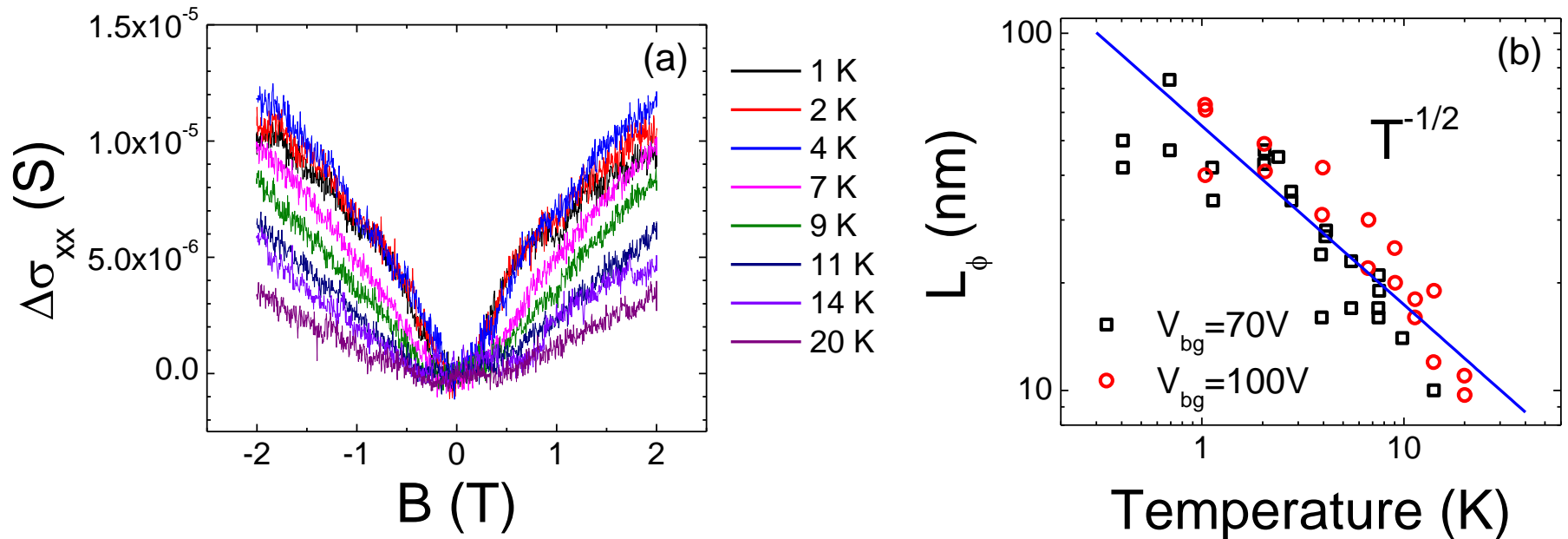
$$F(z) = \psi\left(\frac{1}{2} + \frac{1}{z}\right) - \ln(z),$$

$$B_\phi = \frac{\hbar}{4eL_\phi^2}$$

$L_\phi \sim 50 \text{ nm}$

$T = 400 \text{ mK}$

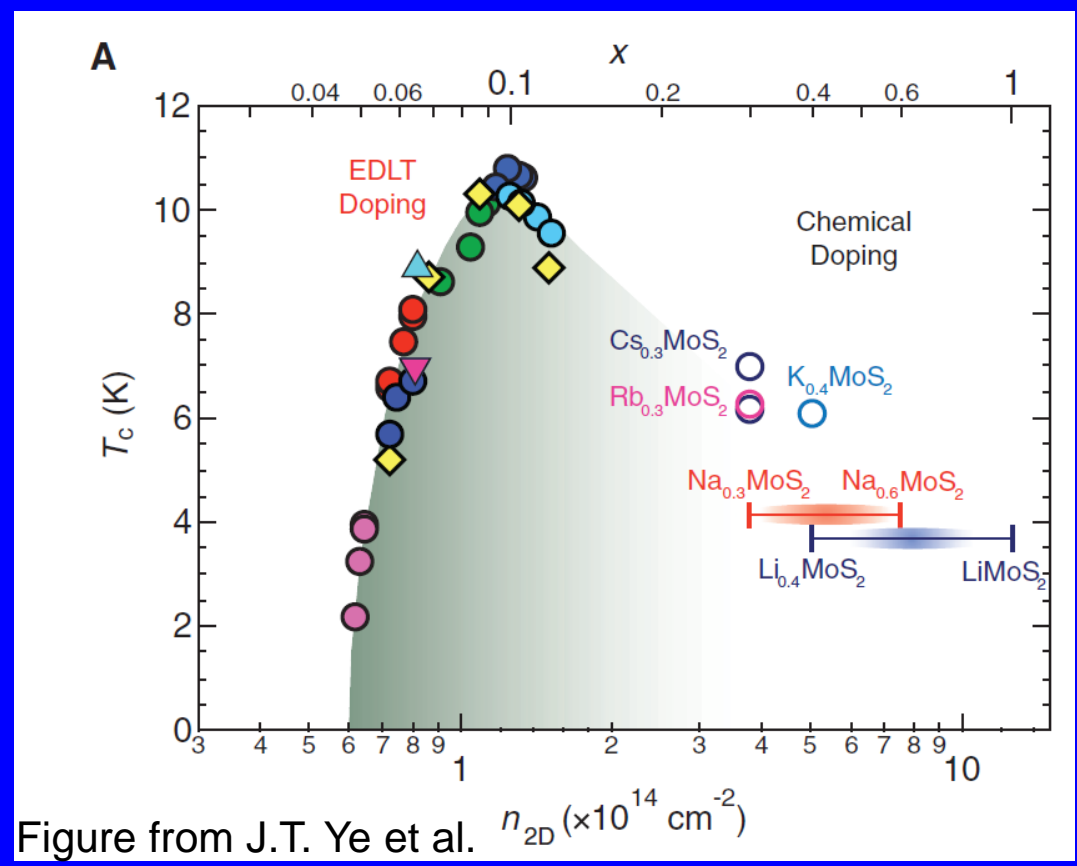
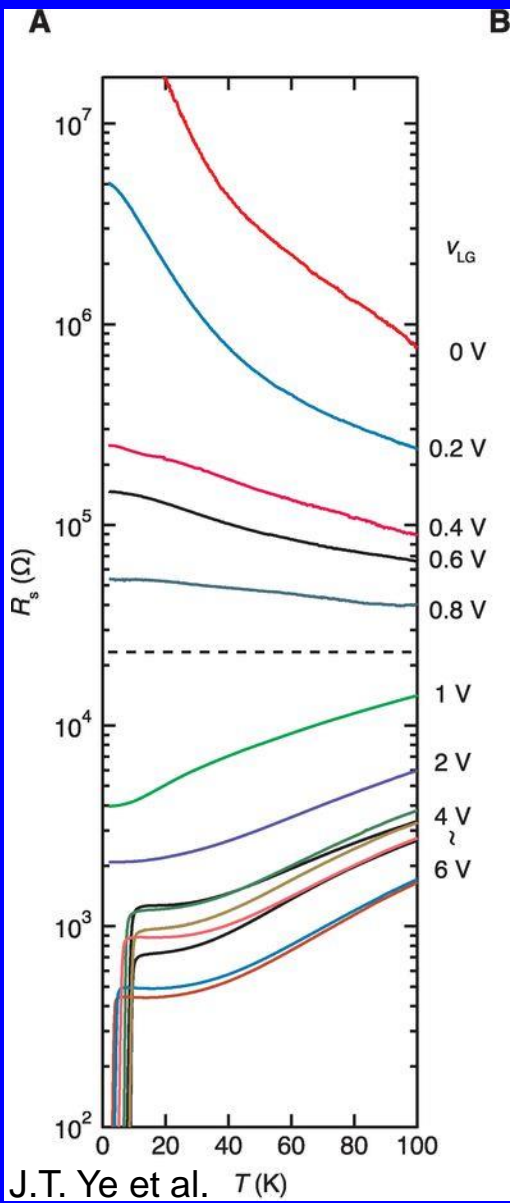
# $L_\phi$ vs. Temperature



$L_\phi$  decreases as  $T^{-1/2}$

Indicates electron-electron scattering responsible for dephasing

# MoS<sub>2</sub> Superconductivity



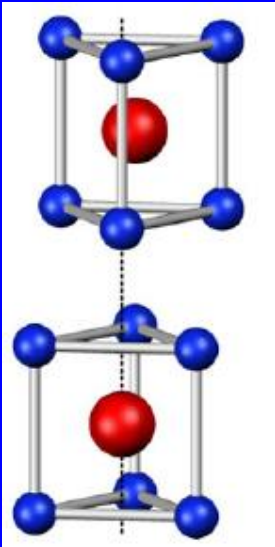
Maximum  $T_c \sim 11\text{K}$   $n \sim 1.3 \times 10^{14} \text{ cm}^{-2}$   
via ionic liquid gating

Taniguchi et al. APL 101, 042603, (2012).

Ye, J.T. et al. Science 338 1193–1196 (2012)

# Spin-Valley coupling in MoS<sub>2</sub>

Bulk TMD unit cell



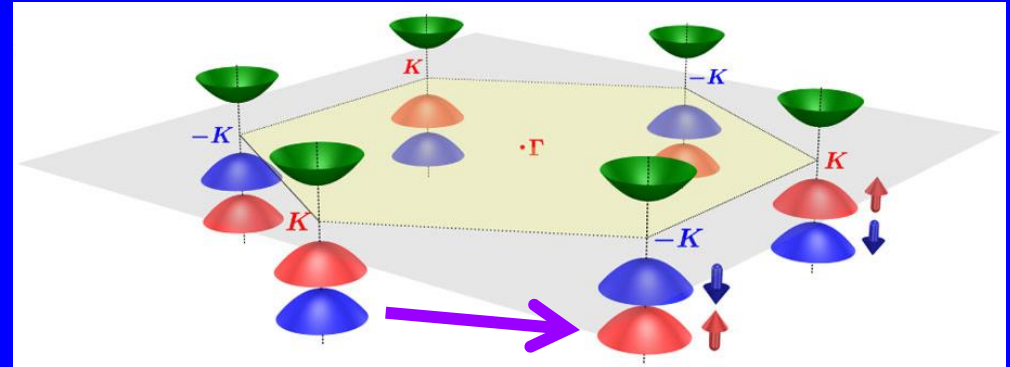
spin orbit coupling  
+  
broken inversion  
symmetry for odd  
layer number



Monolayer TMD

low-energy band structure

large valence band spin splitting



graphics from Xiao et al.

	MoS <sub>2</sub>	MoSe <sub>2</sub>	WS <sub>2</sub>	WSe <sub>2</sub>	III-V's
Predicted monolayer spin splitting from [1]	148 meV	183 meV	426 meV	456 meV	Typically <30 meV

Spin scattering requires intervalley scattering

Enhanced spin lifetime predicted [2]

[1] Zhu et al. Phys. Rev. B **84**, 153402 (2011)

[2] Xiao et al. Phys. Rev. Letters **108**, 196802 (2012)



# Optically induced valley polarization in MoS<sub>2</sub>

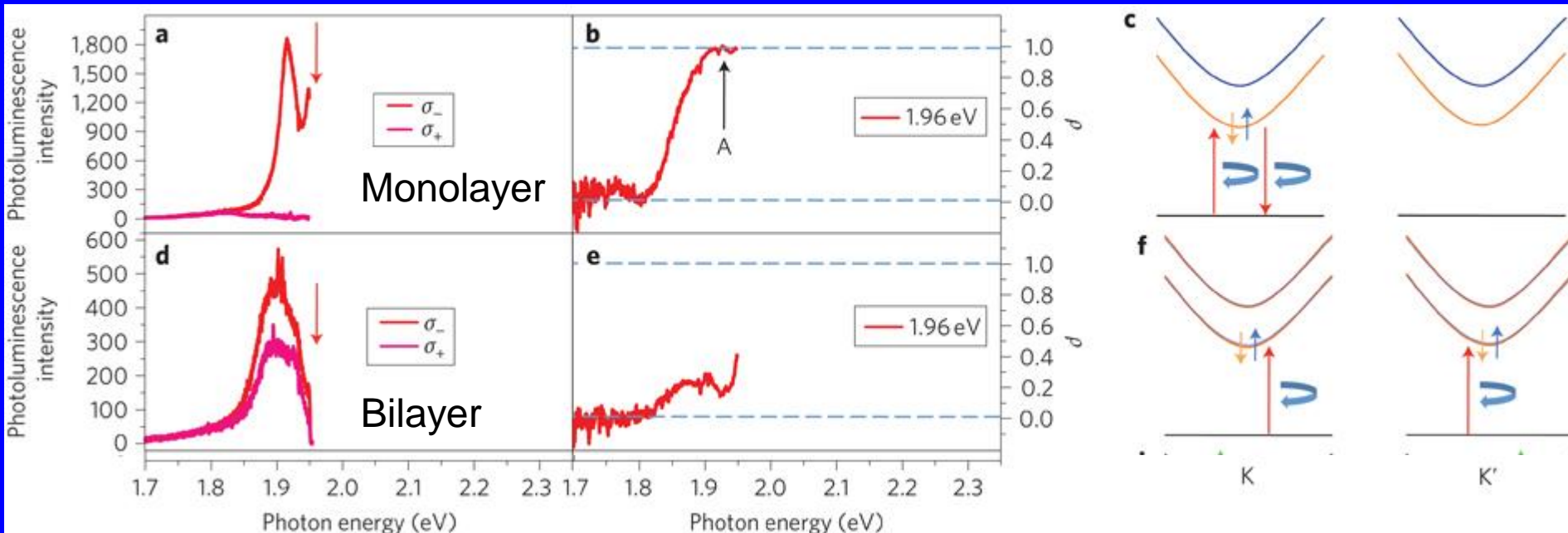


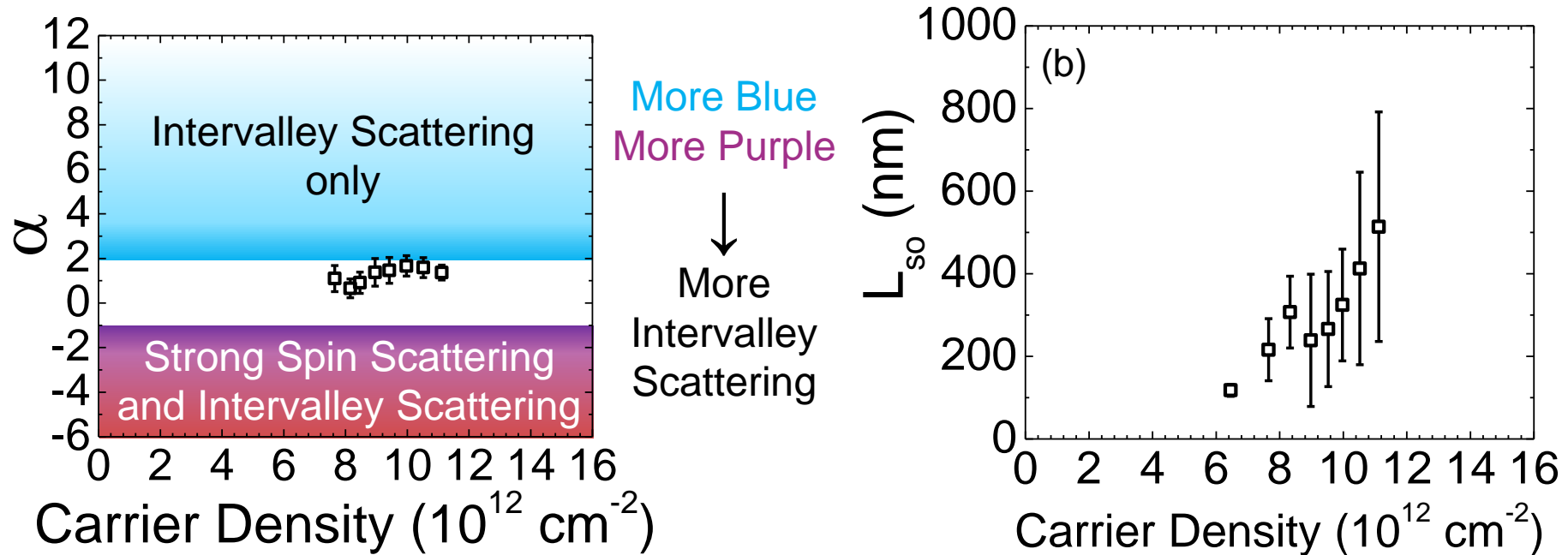
Figure from Mak et al.

Valley polarization induced by optical pumping with circularly polarized light in monolayer MoS<sub>2</sub>

Hole spin-valley  
lifetime  $>1$  ns observed

Mak et al. *Nat. Nanotechnol.* 7, 494–498 (2012)  
Zeng et al. *Nat. Nanotechnol.* 7, 490–493 (2012)  
Cao et al. *Nat. Commun.* 3, 887 (2012)

# Spin-orbit and Intervalley scattering in MoS<sub>2</sub>



$$0 < \alpha < 2$$

$\Downarrow \Rightarrow$

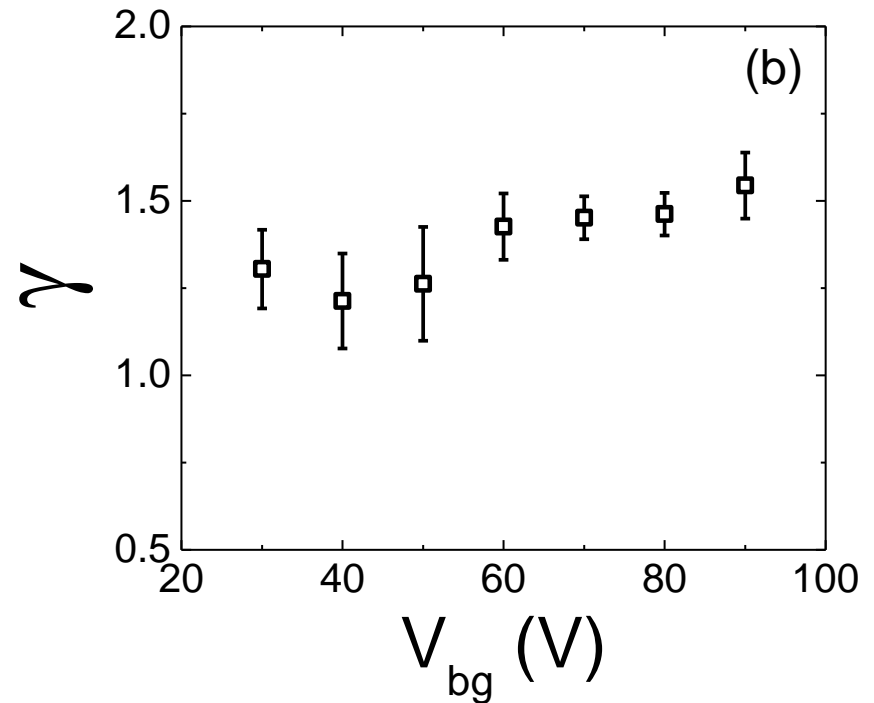
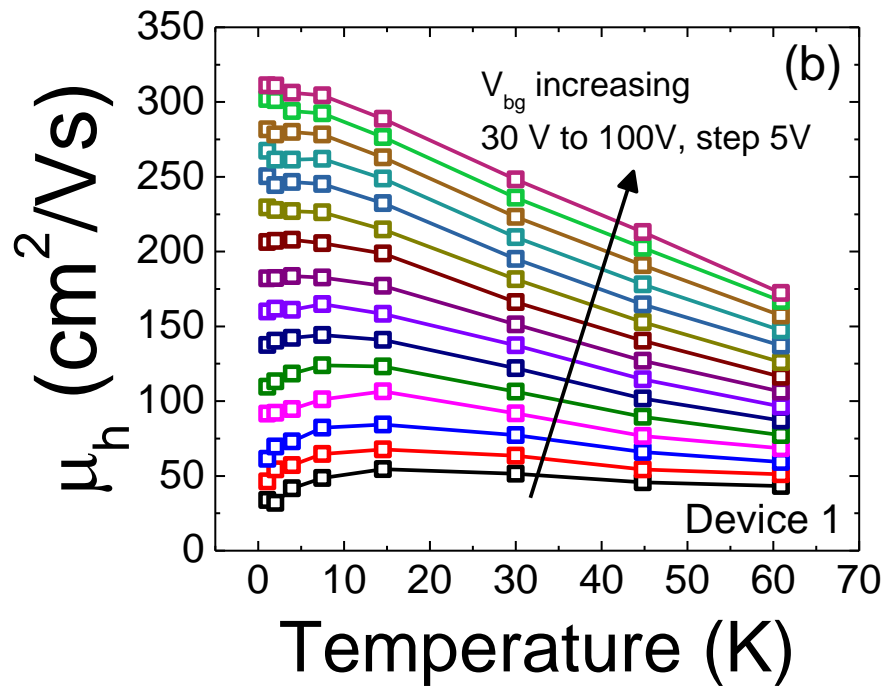
Strong Intervalley Scattering  
Weak Spin Scattering

$$\Delta\sigma = n_s \frac{e^2}{4\pi^2 \hbar} \left( F\left(\frac{B}{B_\phi + B_{so}}\right) + \frac{-1}{n_s} \left( F\left(\frac{B}{B_\phi}\right) - F\left(\frac{B}{B_\phi + 2B_{so}}\right) \right) \right)$$

$$B_* = \frac{\hbar}{4eL_*^2}, \quad * = \phi, so$$

$L_{so}$  as high as 500nm, T=400mK

# Low temperature MoS<sub>2</sub> Mobility

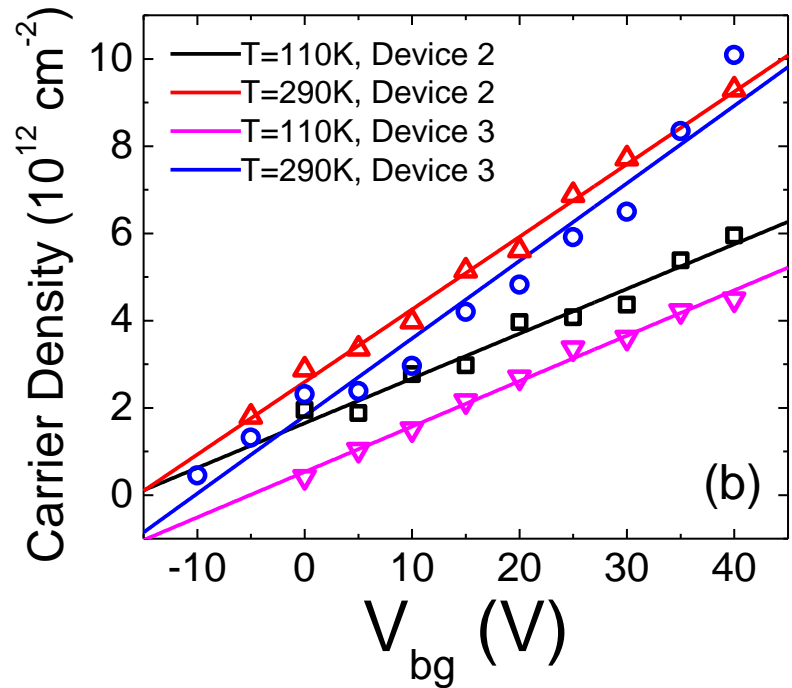
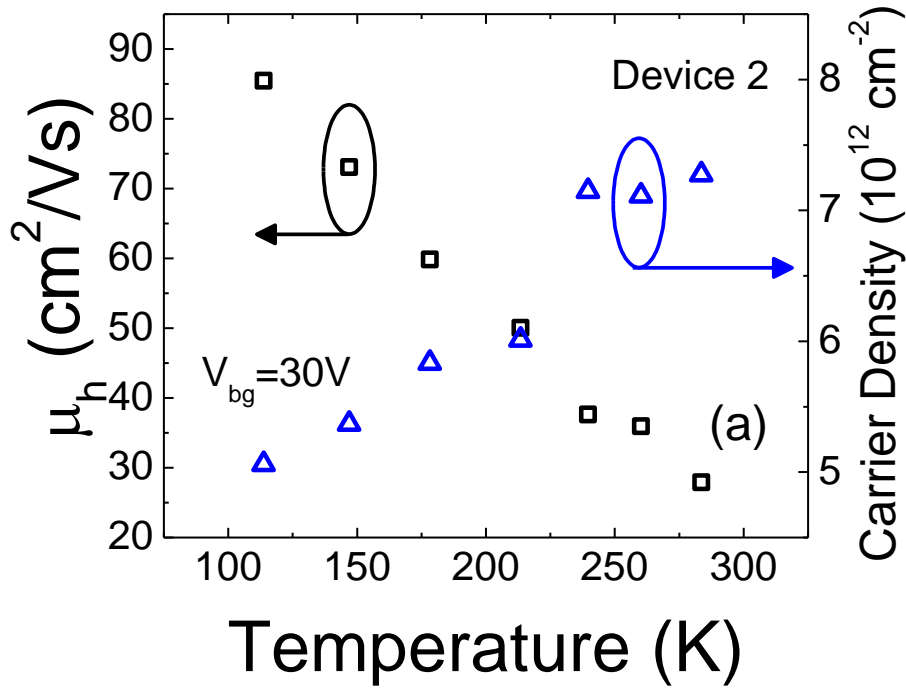


$\mu_h$  decreases as  $T^{-\gamma}$   $\gamma \sim 1.5$ ,  $T=10\text{K}$  to  $60\text{K}$

$\mu_H > 300 \text{ cm}^2/\text{Vs}$  at LT

Adam T. Neal et al. submitted to ACS Nano  
Kaasbjerg et al. *PRB*, 85, 115317 (2012).  
Kaasbjerg et al. *arXiv:1206.2003v1* (2012).

# Hall Factor of MoS<sub>2</sub>



$$\frac{dn_h}{dV_g} = \frac{r_h C_{gate}}{q}, \text{ accumulation} \Rightarrow C_{gate} = C_{ox}$$

$$r_h = 1.35, T = 1K$$

$$r_h = 2.4, T = 290K$$

$$\mu_{drift} = r_h \mu_h = 420 \text{ cm}^2/\text{Vs} @ T = 1K, 56 \text{ cm}^2/\text{Vs} @ T = 290K$$

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# Summary

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- 1) We demonstrated direct **ALD high-k integration** on MoS<sub>2</sub> and other 2D crystals.
- 2) **Low work-function metals, i.e. Ti**, lead to high-performance MoS<sub>2</sub> MOSFETs.
- 3) We studied **vertical layers** (CVD monolayer), **channel length and channel width scaling** (down to 50-60nm). We observe a **D-mode to E-mode transition** by scaling width, meanwhile length scaling shows **dominate contact resistance**.
- 4) **Hall Factor ~2.4**, T=290K, multilayer MoS<sub>2</sub>. Needed for accurate determination of drift mobility from Hall effect
- 5) Electron spin orbit scattering length **L<sub>so</sub> as high as 500nm** in few layer MoS<sub>2</sub>, indicating potential for spintronics applications.

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