PURDUE UNIVERSITY Discovery Park Birck Nanotechnology Center

Argonne NATIONAL LABORATORY

Center for Nanoscale Materials

2D Electronics with Transition Metal Dichalcogenides : Progress and Prospect

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(June 2013 – Present)

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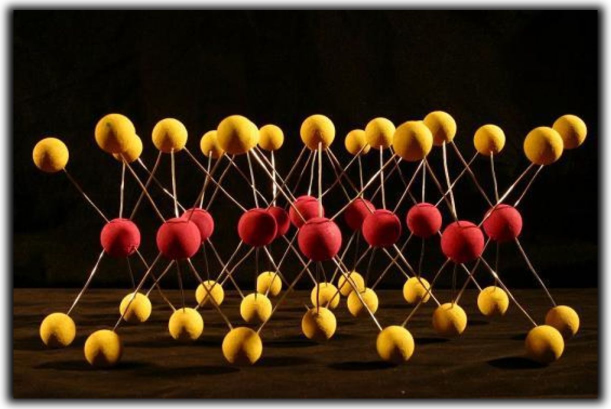
   West Lafayette, Indiana 47907

1. What is Unique about TMDs ?
2. Exploring Transistors based on TMDs
3. Tunneling Phenomenon in TMDs
4. Extreme Sensitivity of TMDs to External Forces

1. **What is Unique about TMDs ?**
2. Exploring Transistors based on TMDs
3. Tunneling Phenomenon in TMDs
4. Extreme Sensitivity of TMDs to External Forces

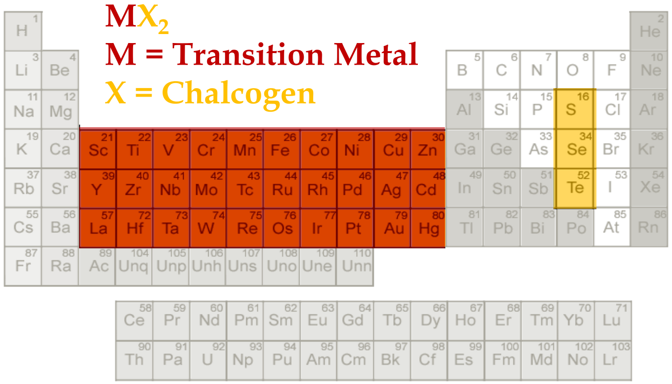
Natural 2-D System

Transition Metal Dichalcogenides



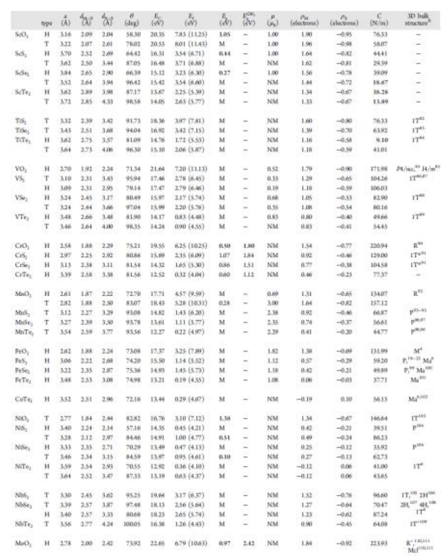
Periodic Table of Elements

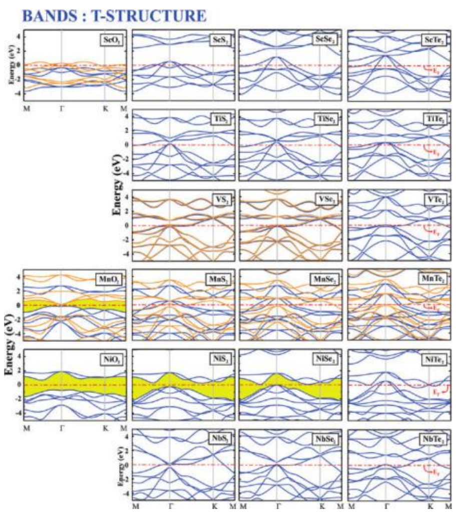
MX_2
M = Transition Metal
X = Chalcogen



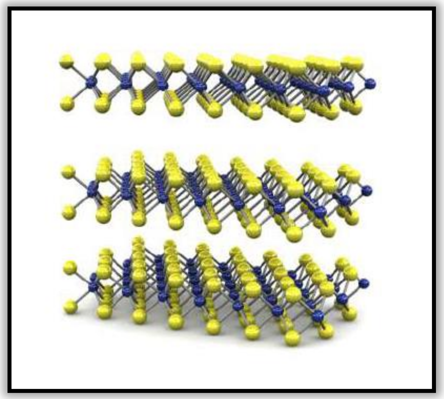
88 TMDs have been explored since 1960s

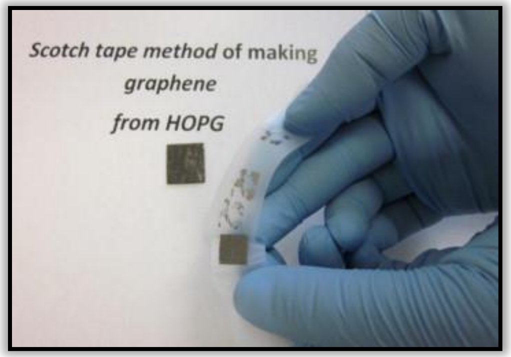
- Metals: $ScTe_2$, TaS_2 , etc.
- Semiconductors: WSe_2 , MoS_2, etc.
- Insulators: $PtSe_2$, PdS_2 , etc.
- Superconductors: VS_2 , $NbSe_2$, etc.

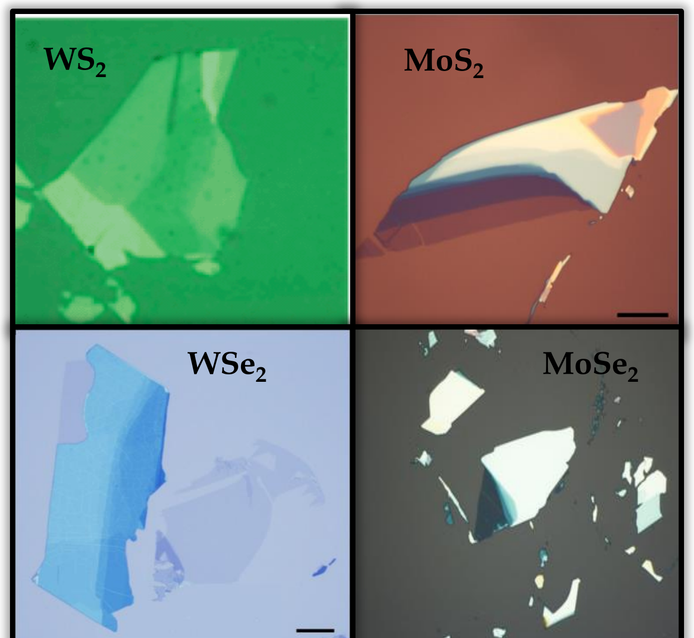




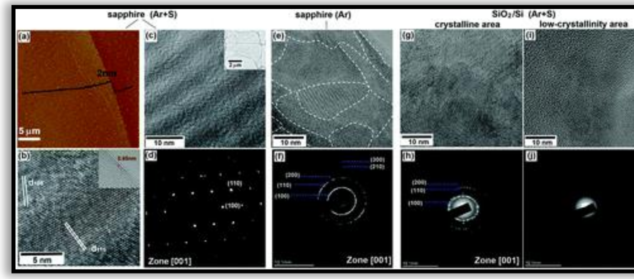
Exfoliation







Large Scale Growth



Physical Vapor Deposition

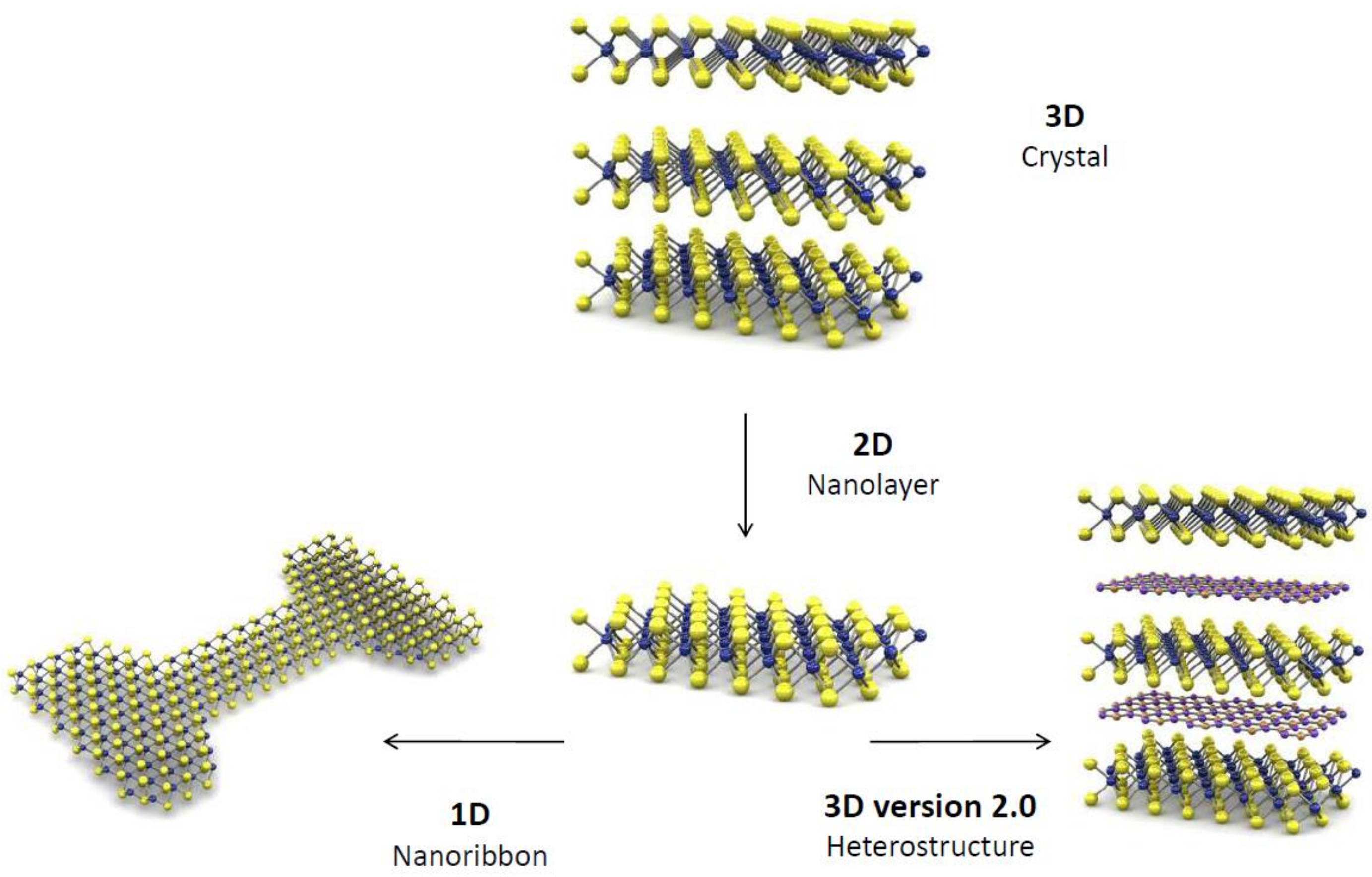
Hydrothermal Synthesis

Electrochemical Synthesis

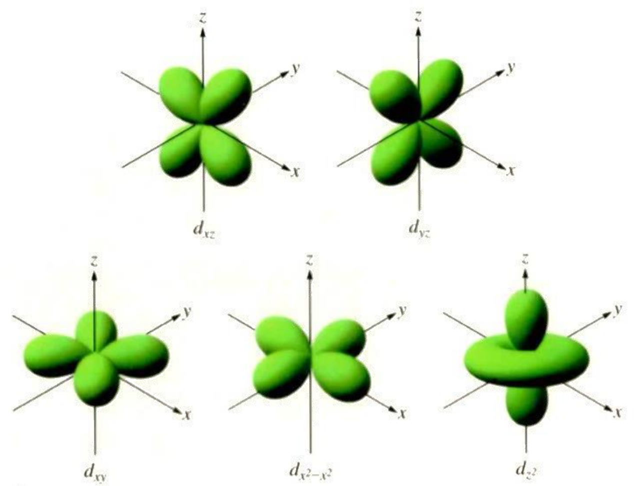
Liu, K. et al. Nano Letters, 12, 2012

Patel, P. R., et al. J.Adv.Dev.Res. 3, 2012

Layered Compounds



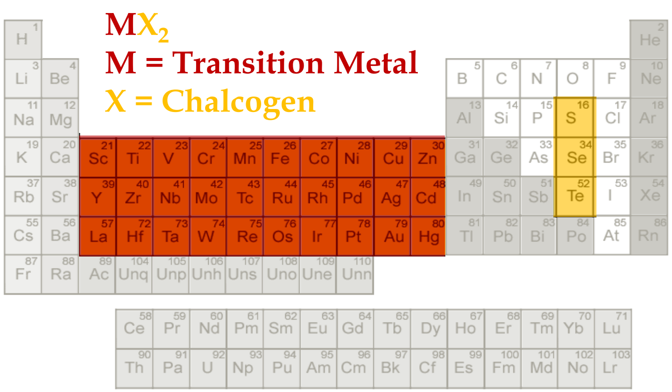
The d-orbital electronics



Mo: [Kr]. **5d⁵**.6s¹
W: [Xe].4f¹⁴.**5d⁴**.6s²

For the first time we have **Semiconductors** with conduction electrons contributed by **d-orbital**

Periodic Table of Elements

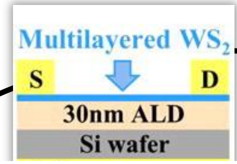


Significant Change in Band-structure due to :

- ✓Charge
- ✓Strain
- ✓Heat
- ✓Light

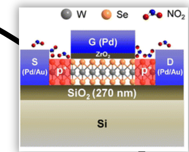
Transistors based on TMDs

WS_2



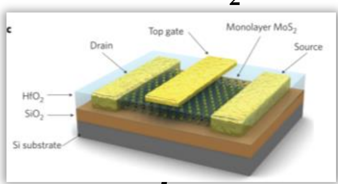
Hwang, W.S. et al.
APL, 101 (2012)

WSe_2



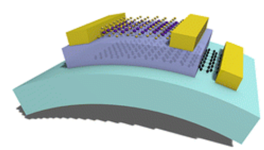
Fang, H. et al.
Nano Letters, 12, (2012).

MoS_2



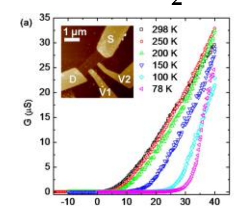
Radisavljevic, B. et al.
Nature Nanotechnology, 6, (2011)

Graphene/h-BN/MoS_2



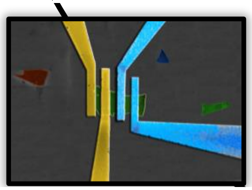
Lee, G. H. et al.
ACS Nano, 7, (2013).

$MoSe_2$



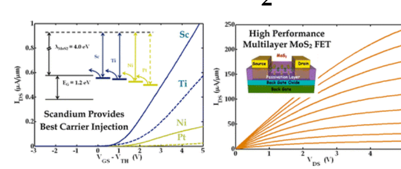
Larentis, S. et al.
APL, 101, (2012).

WSe_2



Das, S. et al.
APL, 103, (2013).

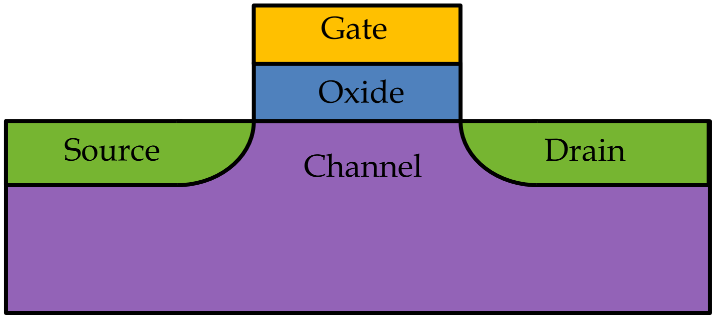
MoS_2

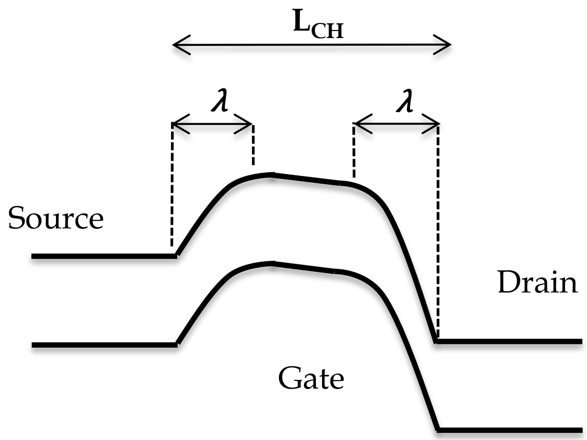


Das, S. et al.
Nano Letters, 13, (2013).

Going Beyond Silicon CMOS

Field Effect Transistor





Screening Length

$$\lambda = \sqrt{\frac{t_{OX}}{\epsilon_{OX}} t_{BODY} \epsilon_{BODY}}$$

$$L_{CH} > 3\lambda$$

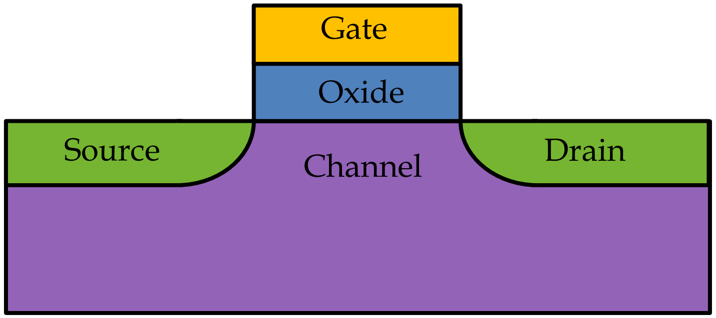
<u>Scaling oxide thickness</u>
Increase in gate leakage current

<u>High-k gate oxide</u>
Limited choice and complex integration

<u>Scaling the body thickness</u>
ON-state performance is impacted

Going Beyond Silicon CMOS

Field Effect Transistor



Screening Length

$$\lambda = \sqrt{\frac{t_{OX}}{\epsilon_{OX}} t_{BODY} \epsilon_{BODY}}$$

$$L_{CH} > 3\lambda$$

Alternative Channel (body) Materials

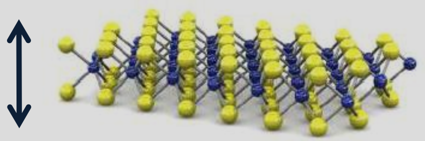
Ultra thin body

High mobility (diffusive) / High effective mass (ballistic)

Small in-plane dielectric constant

Molybdenum Disulphide: MoS_2

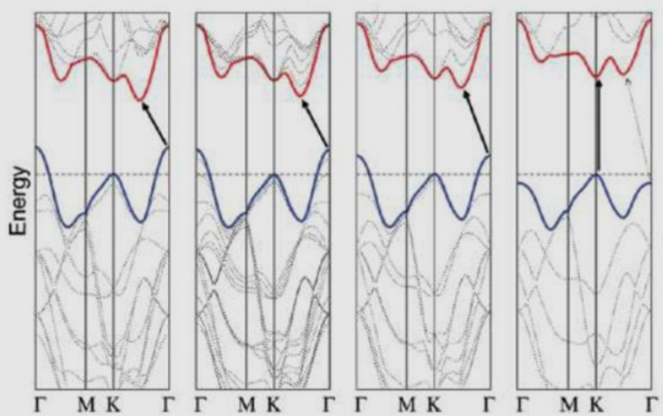
t_{MoS2} = 0.65 nm



Kumar, A. et al., Physica B, 407, (2012)		
MoS_2	$\varepsilon_{BODY}^{\perp}$	$\varepsilon_{BODY}^{\parallel}$
Monolayer	4.8	3.0
Bilayer	6.9	4.4
6-layers	9.8	6.4
Bulk	12.8	8.9

Multi-layer
$E_{G\text{-}MoS2}$ = 1.2eV
$m^* = 0.57m_0$

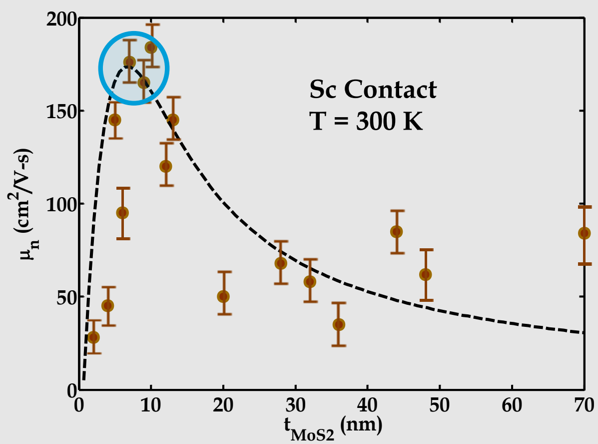
Mono-Layer
$E_{G\text{-}MoS2}$ = 1.8eV
$m^* = 0.42m_0$



Bulk 3- Layers 2 Layers 1-Layer

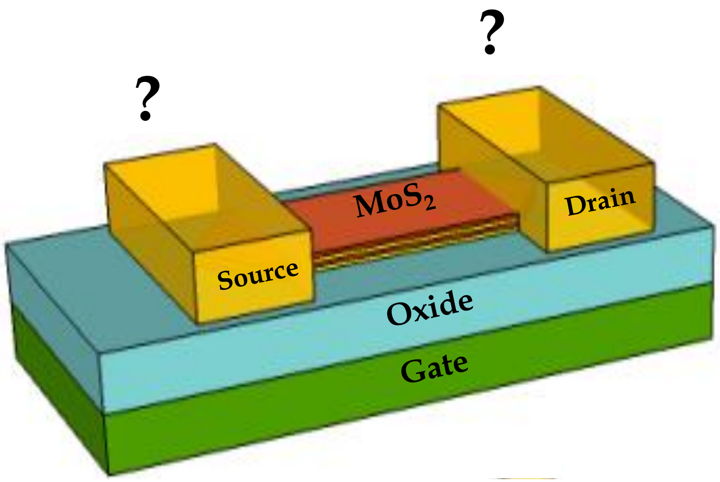
Splendiani et al., Nano Lett. 10, (2010)

μ_{MoS2} ~ 200 cm^2/V-s
(multi-layer systems)



Saptarshi Das, et al., Nano Letters, 13 (1), 100-105, 2013

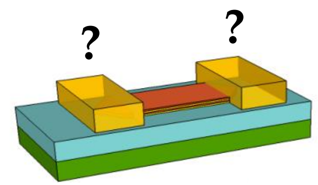
Transistor Optimization: Contact



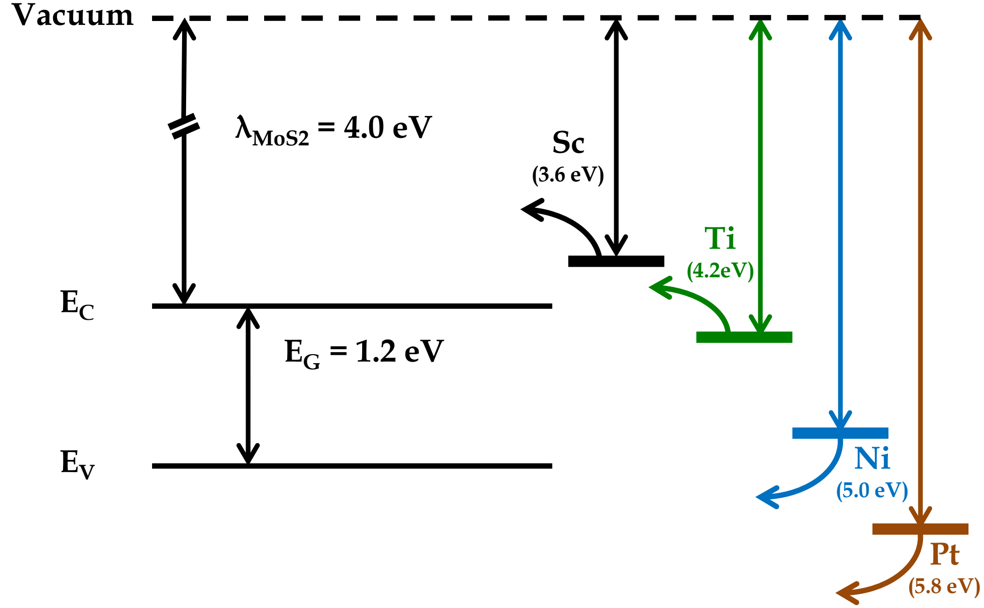
$$R_{TOTAL} = R_{CONTACT} + R_{CHANNEL}$$

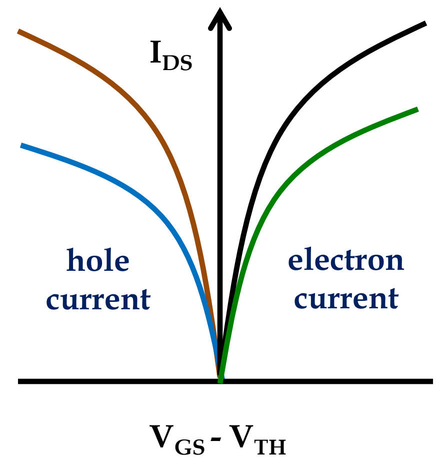
$$= R_{CONTACT} + R_0 L_{CH}$$

Transistor Optimization: Contact



Center for Nanoscale Materials

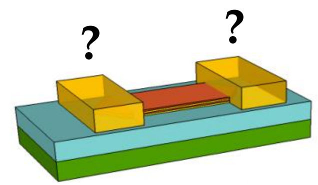


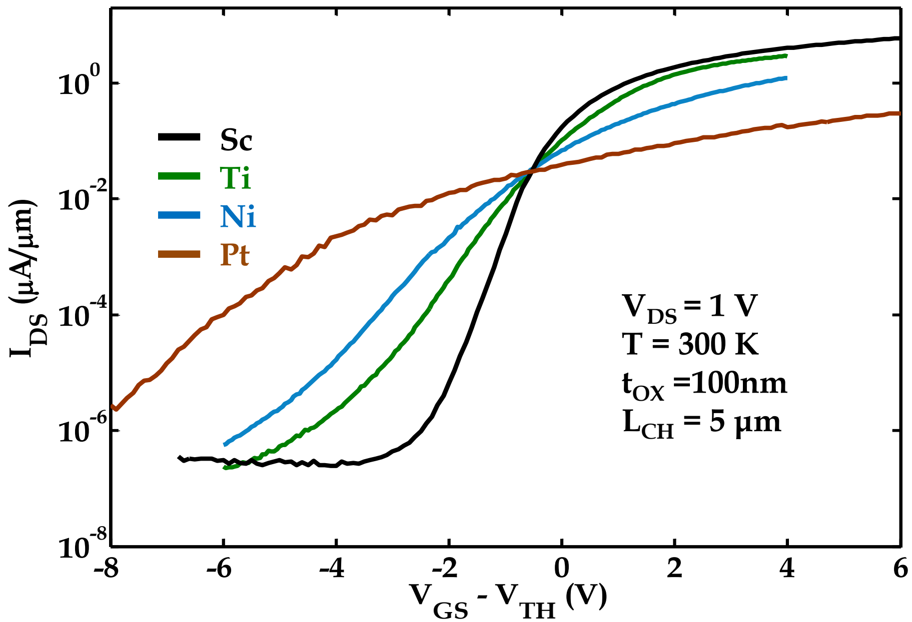


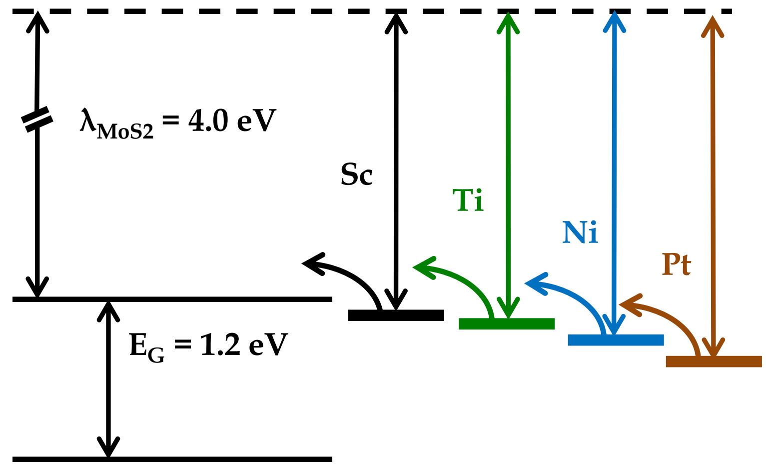
Ti : n-FET (Qiu et al.)
Ni : n-FET (Liu et al.)
Au : n-FET (Radisavljevic et al.)
Pd : n-FET (Neal et al.)

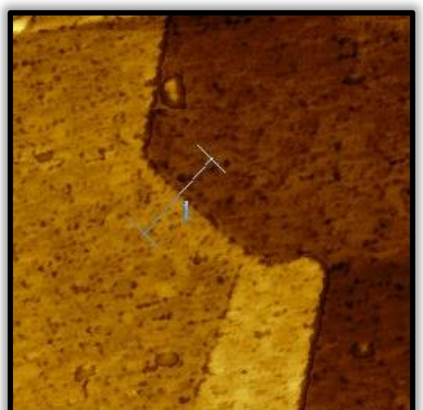
Ohmic Contact !!!!
No Fermi level pinning !!!

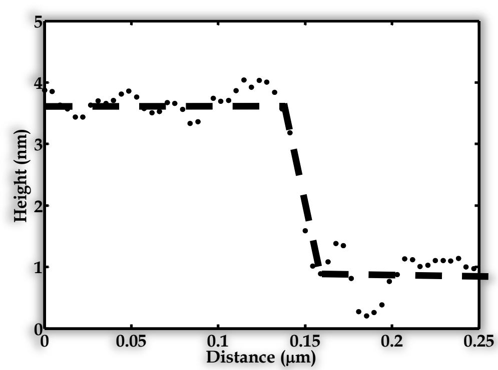
Transistor Optimization: Contact

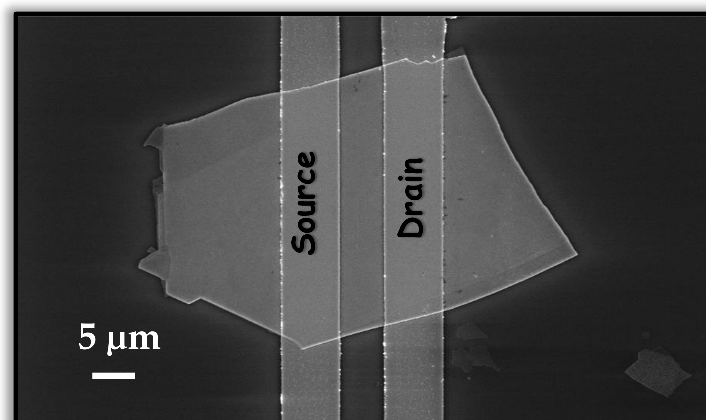




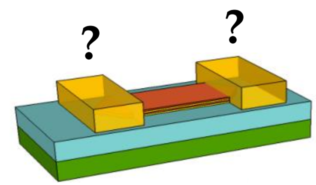






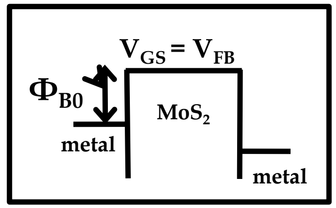


Transistor Optimization: Contact

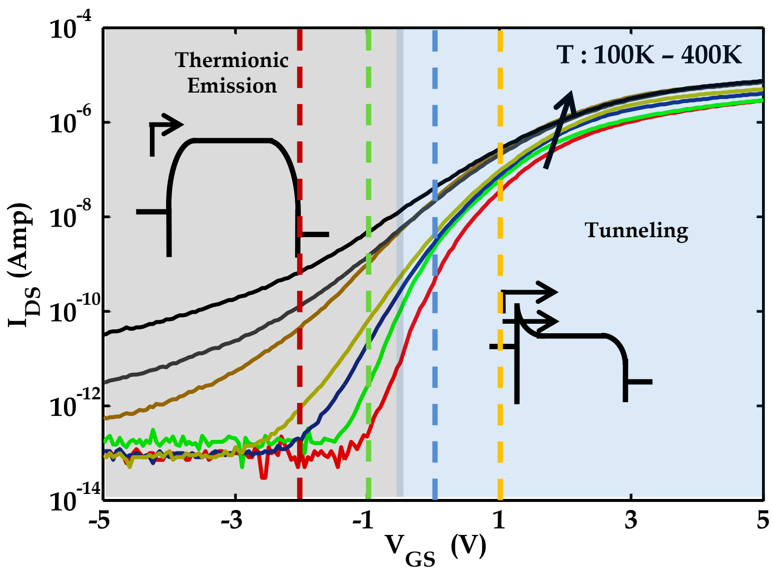


$$I_{DS} \propto AT^2 \exp\left(-\frac{q\Phi_B}{k_B T}\right)$$

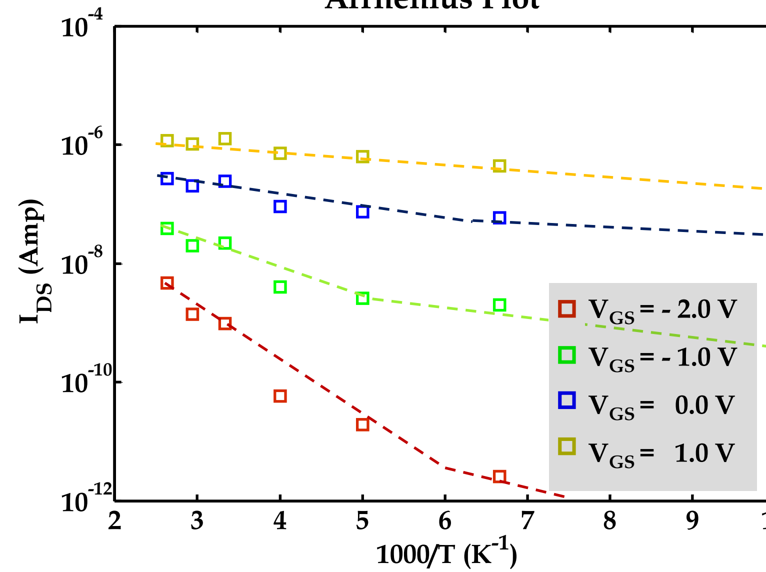
$$\frac{d\ln(I_{DS})}{d(1000/T)} \approx -\frac{q\Phi_B}{k_B}(\text{meV})$$

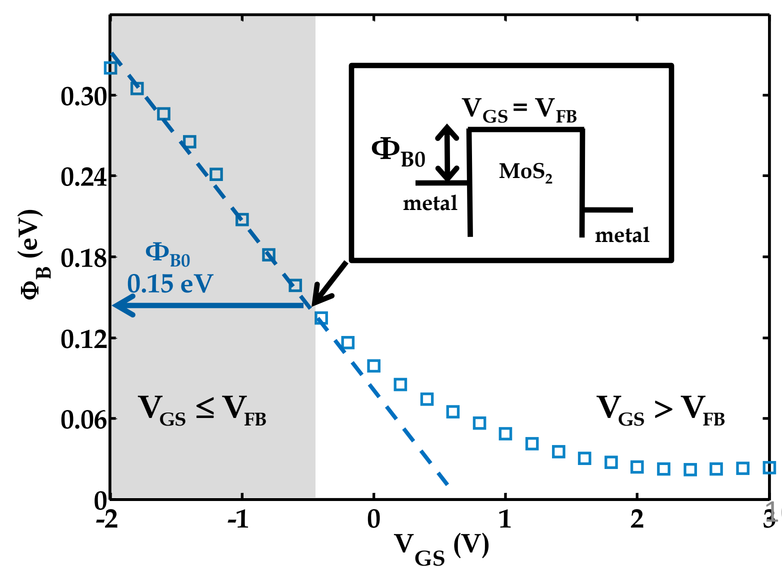


Transfer Characteristics : Ni Contact ($V_{DS} = 1$ V)



Arrhenius Plot

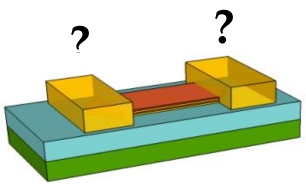


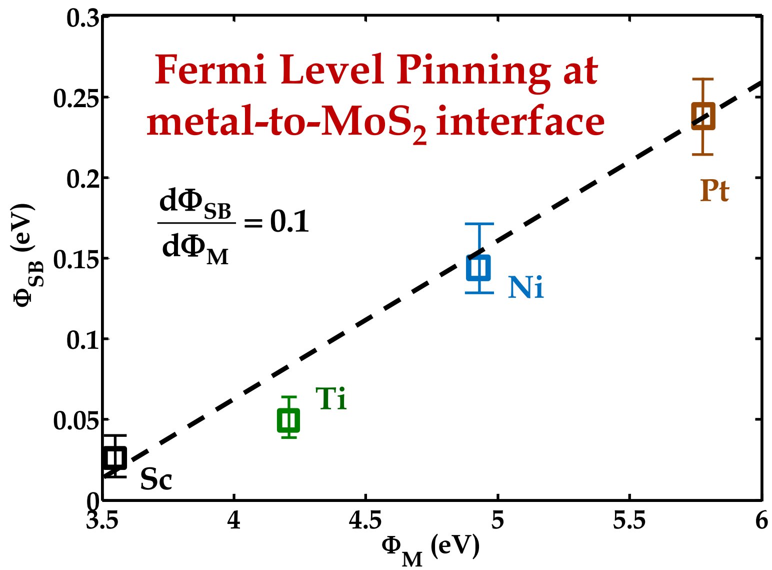


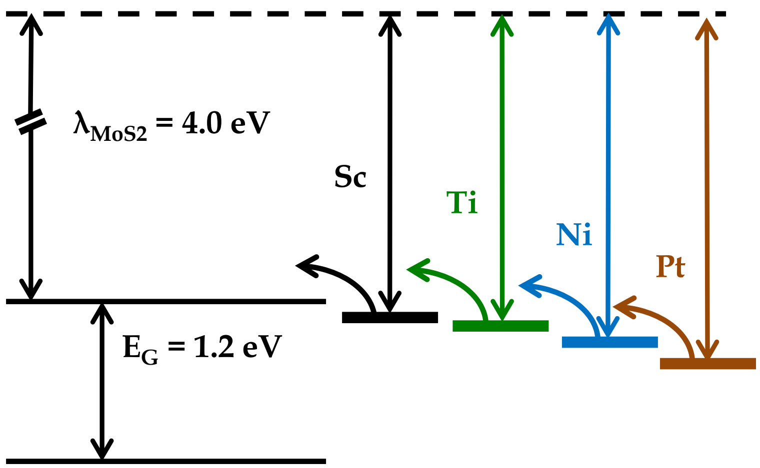
$\Phi_B = \Phi_{B0} + \gamma(V_{FB} - V_{GS})$ for $V_{GS} \le V_{FB}$

$\Phi_B = \Phi_{B0} - \Delta$ for $V_{GS} > V_{FB}$

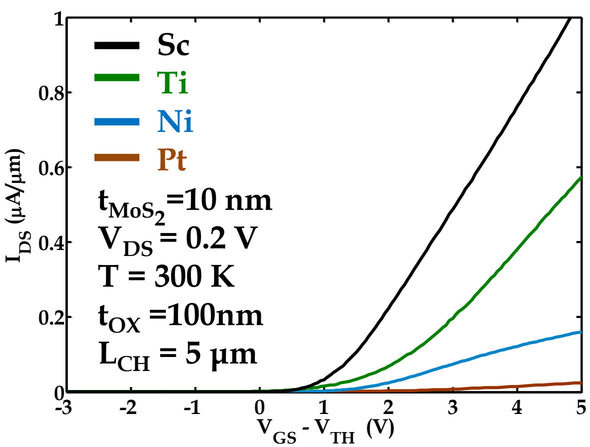
Transistor Optimization: Contact



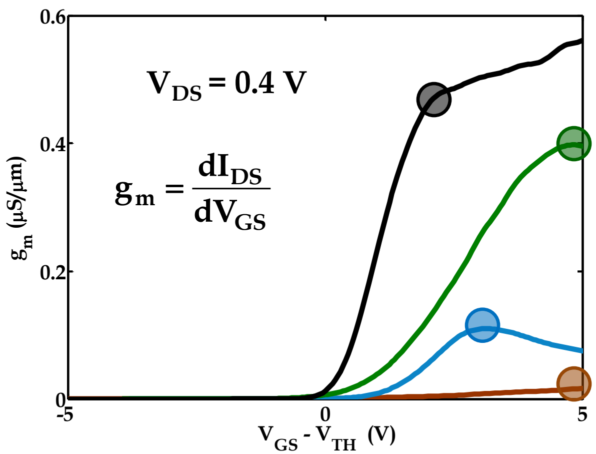




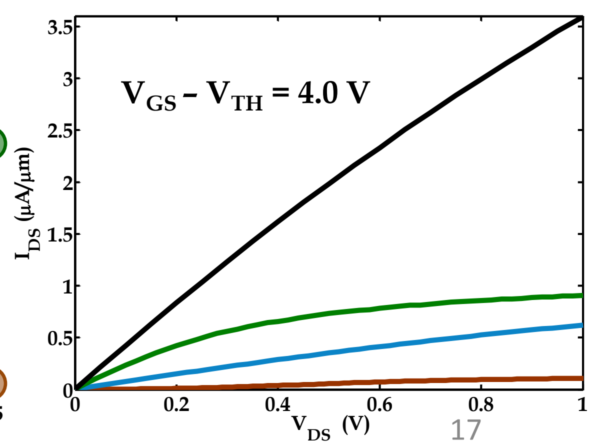
Transfer Characteristics



Trans-Conductance



Output Characteristics



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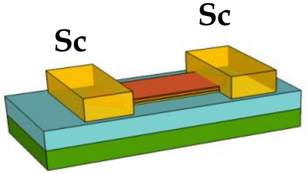
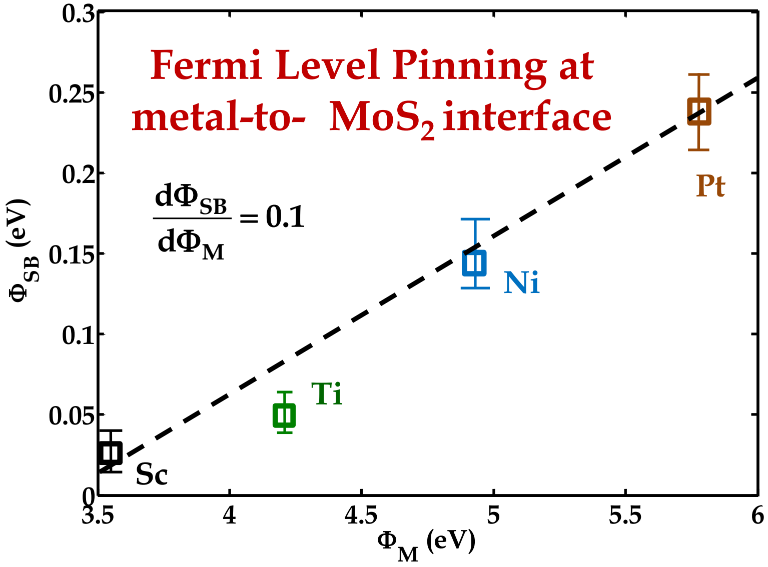
Transistor Optimization: Contact





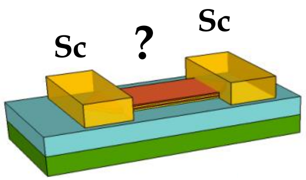
$g_m = \mu_n C_{OX}(W/L)V_{DS}$

μ_n= 184 cm²/V-s (Sc)
μ_n= 125 cm²/V-s (Ti)
μ_n= 36 cm²/V-s (Ni)
μ_n= 21 cm²/V-s (Pt)

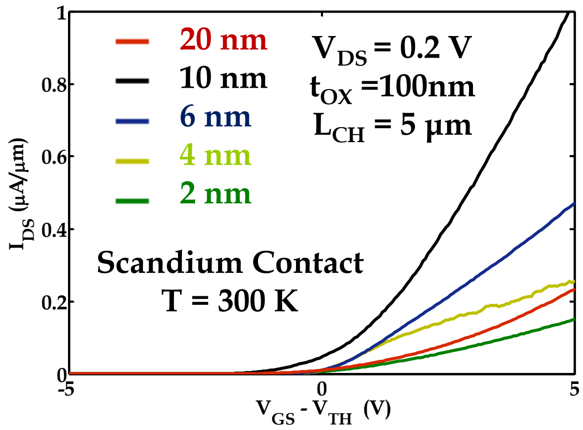
Scandium is the best metal Contact

Saptarshi Das, et al., "High Performance Multi Layer MoS_2 Transistor with Scandium Contacts", **Nano Letters** 13 (1), 100-105**, 2013.**

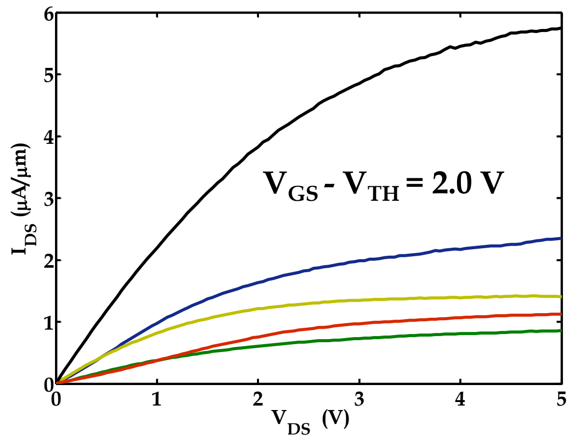
Transistor Optimization: Flake Thickness

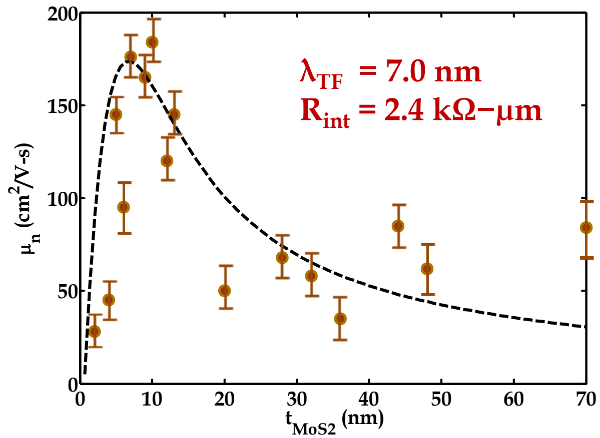


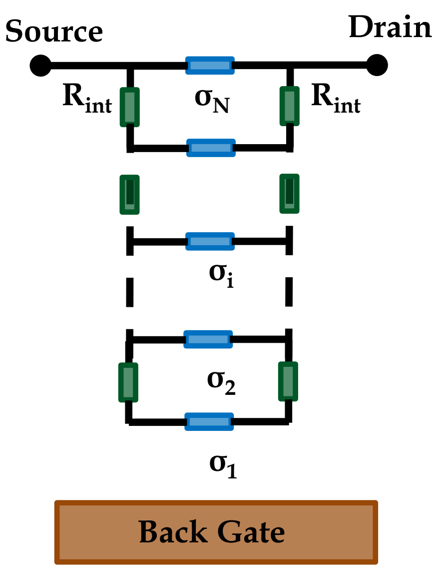
Transfer Characteristics



Output Characteristics







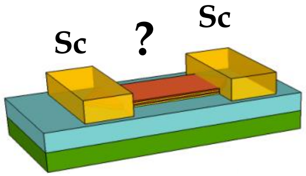
Thomas - Fermi Screening

$$Q_i = \frac{1}{t_{OX}+r_i}\exp\left(-\frac{t_{OX}+r_i}{\lambda_{TF}}\right)$$

Inter-layer Coupling Conductance

R_{int}

Transistor Optimization: Flake Thickness



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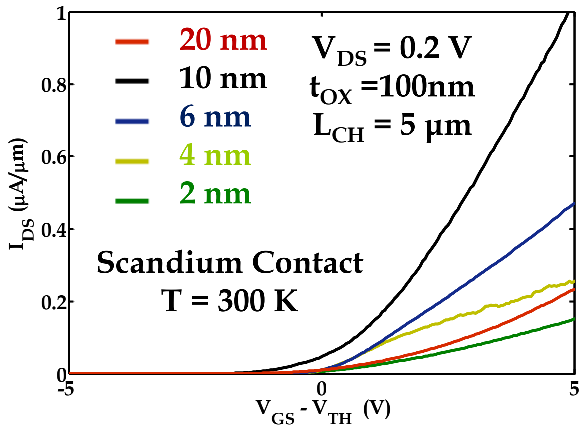
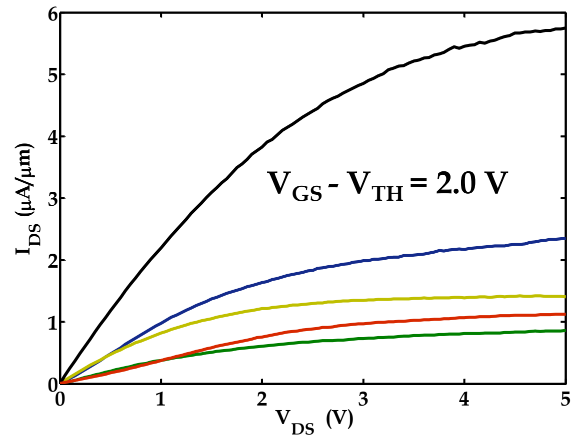
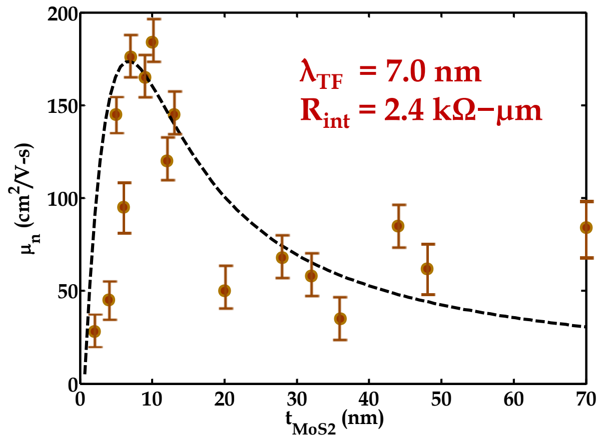


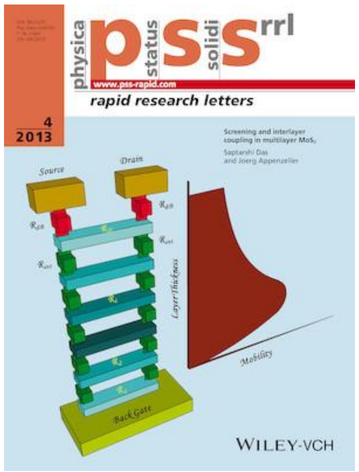




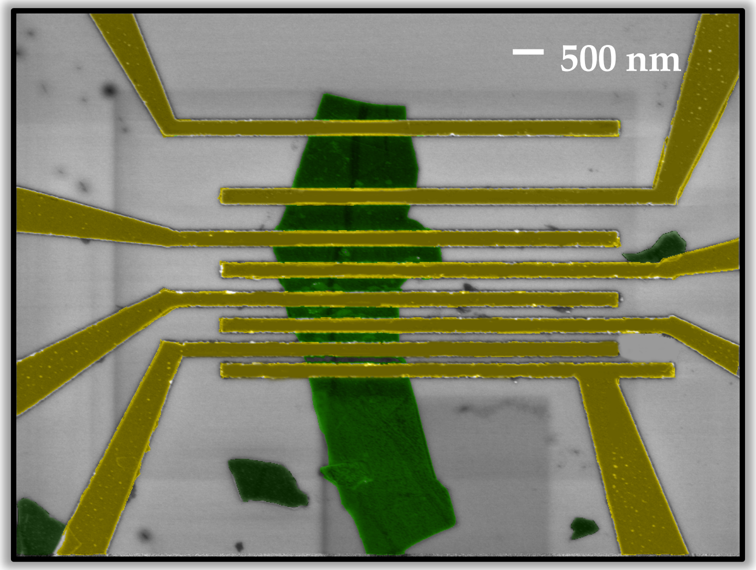
6-10nm Flake is optimum for high mobility channel

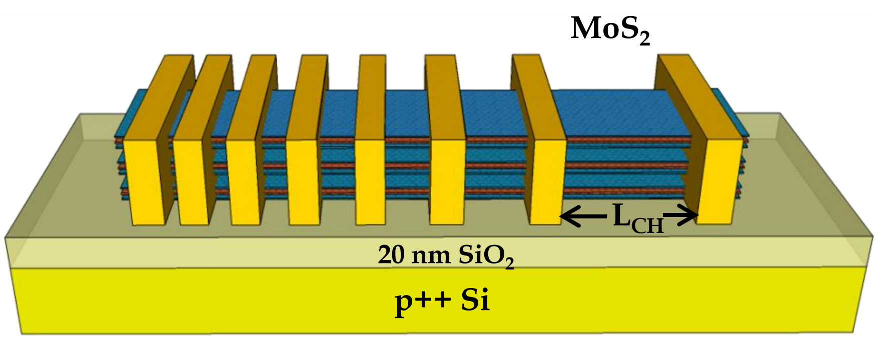
Cover Article

Saptarshi Das, et al., Screening and Interlayer Coupling in Multilayer MoS_2, **Physica Status Solidi, RRL**, 7 (4), 268-273, **2013.**



Channel Length Scaling





Sc Contacts

8nm MoS2 Flake

$L_{CH\text{-}min}$ = 50nm

$L_{CH\text{-}max}$ = 1μm

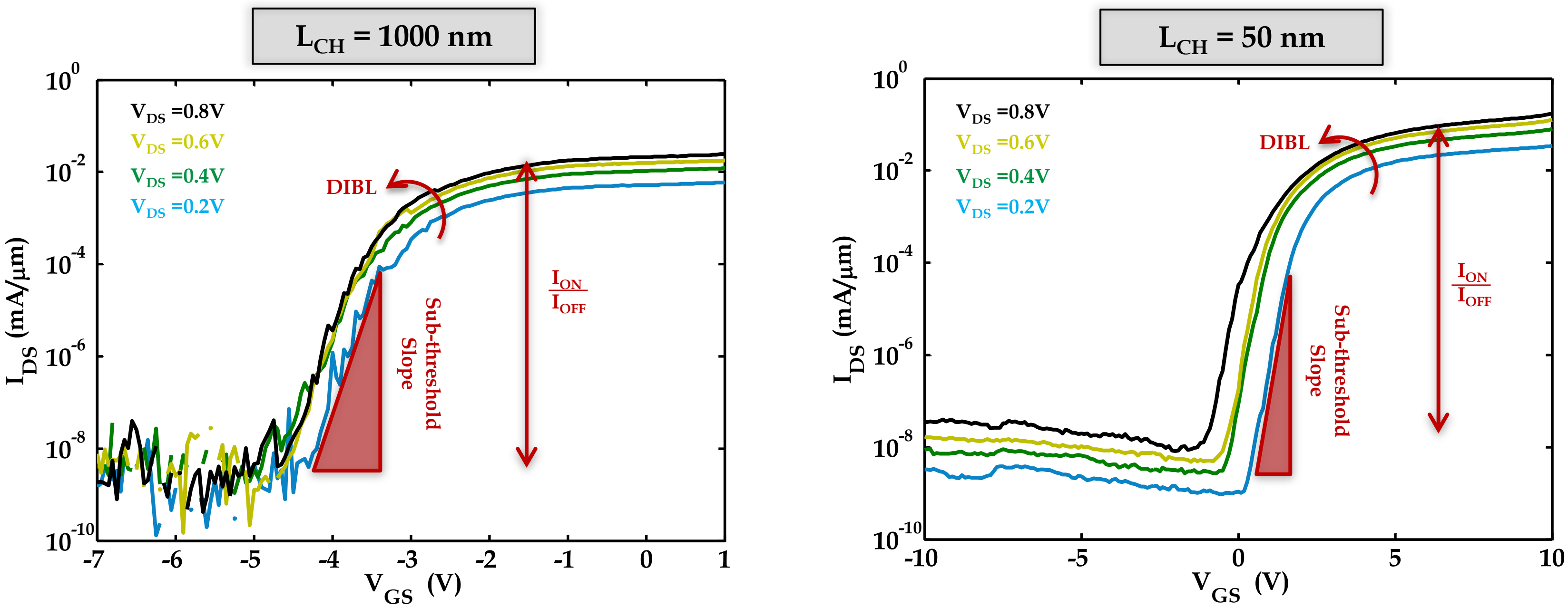
t_{OX} = 20nm SiO_2

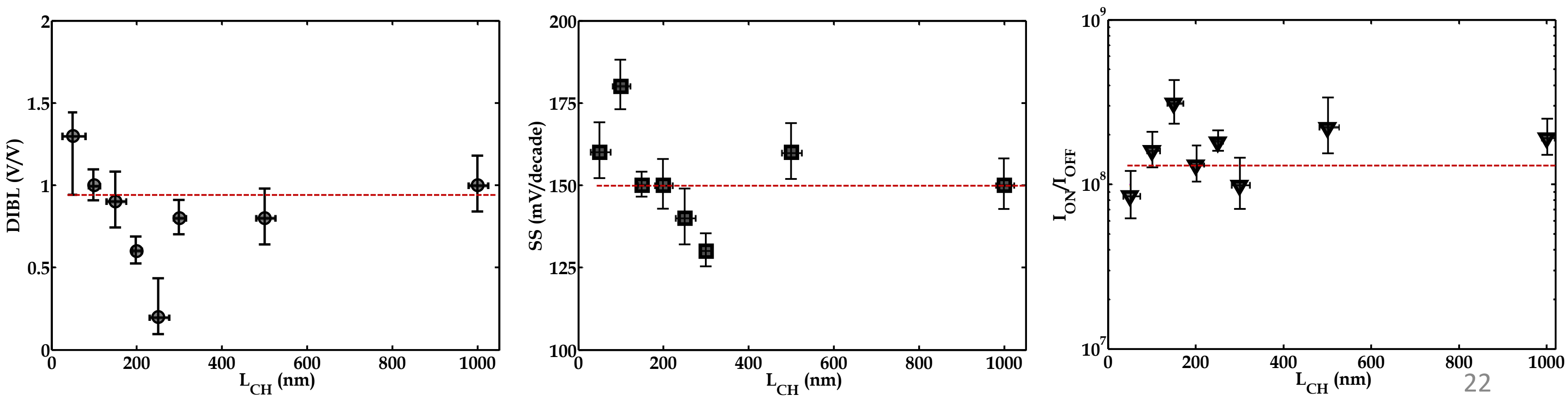
✓15 times better gate control compared to 300nm oxide.

✓Reduces the possibility of short channel effect.

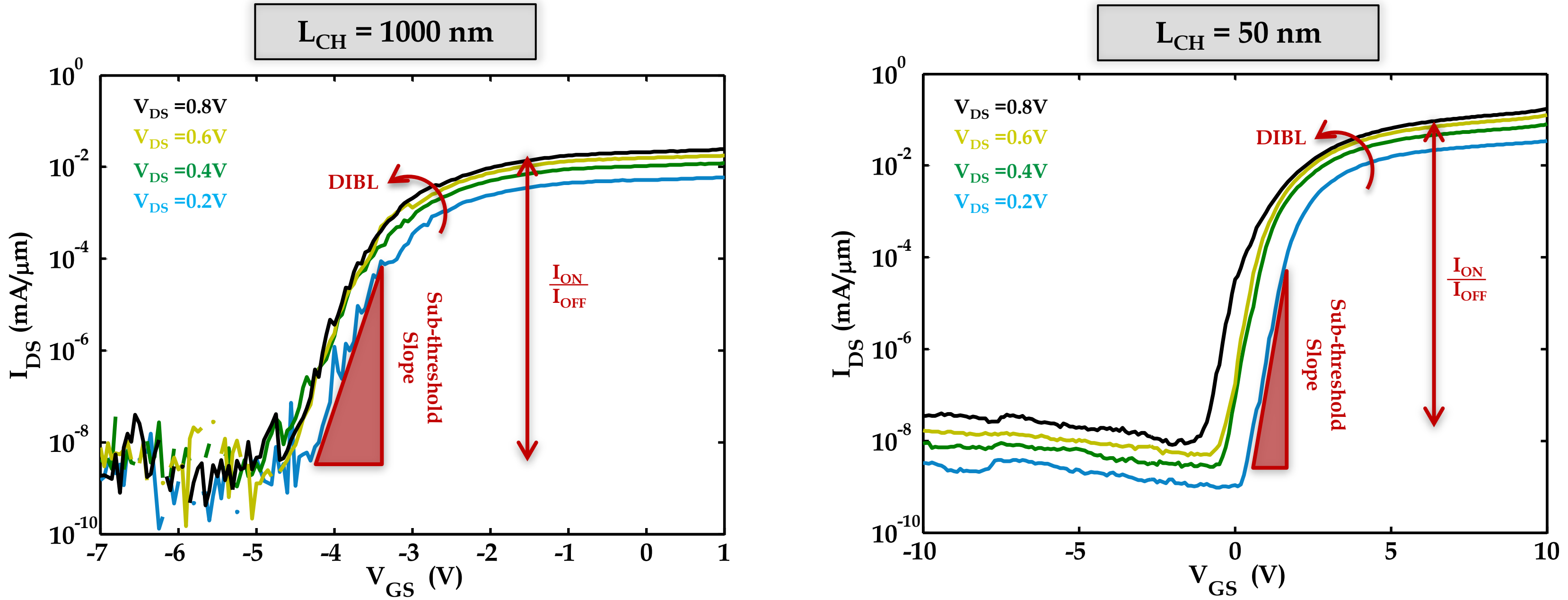
$$\lambda = \sqrt{\frac{t_{OX}}{\epsilon_{OX}} t_{BODY} \epsilon_{BODY}}$$

Channel Length Scaling





Channel Length Scaling



Saptarshi Das, et al., "Evaluating the Scalability of Multilayer MoS_2 Transistors", **Device Research Conference , 2013.**

"Contact Resistance"

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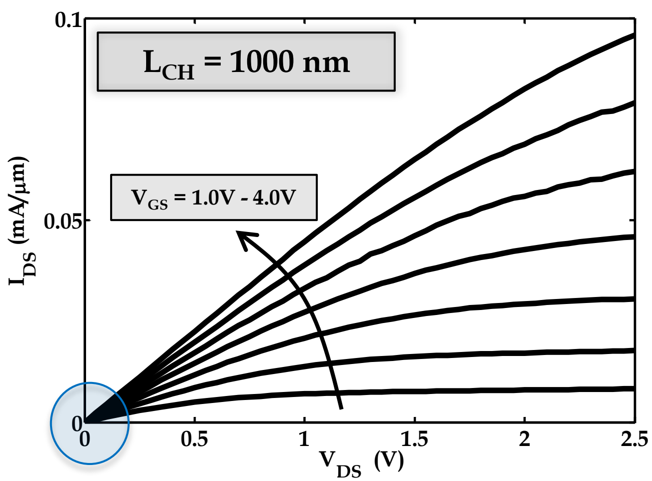
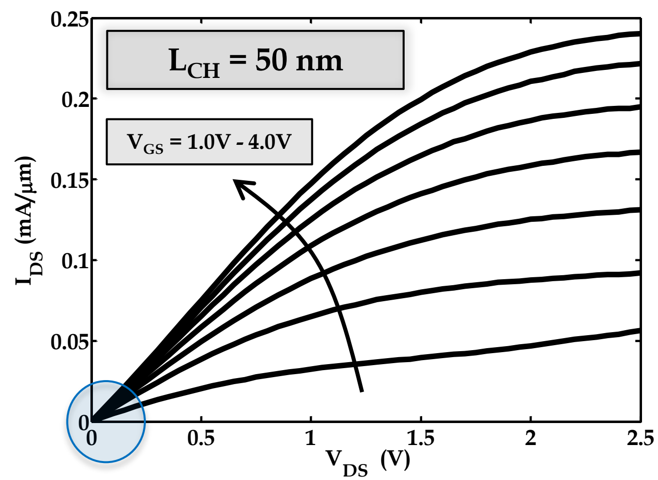
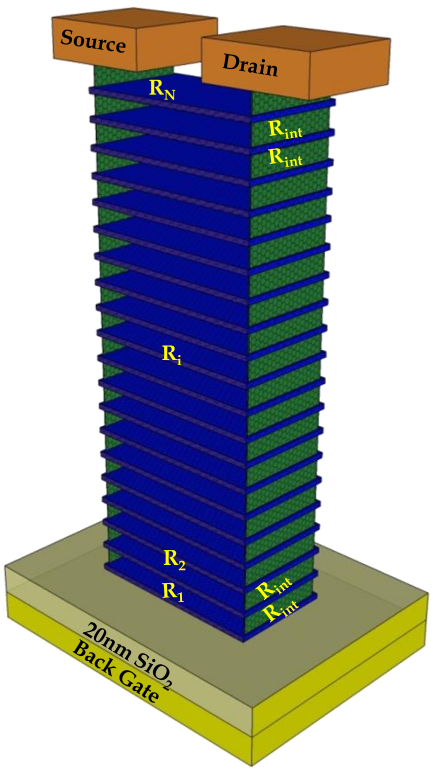
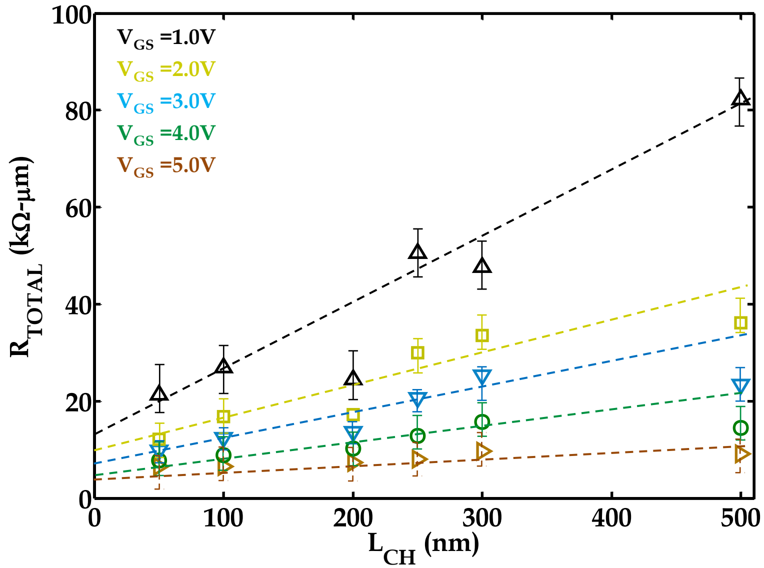








$$\frac{V_{DS}}{I_{DS}} = R_{TOTAL}$$

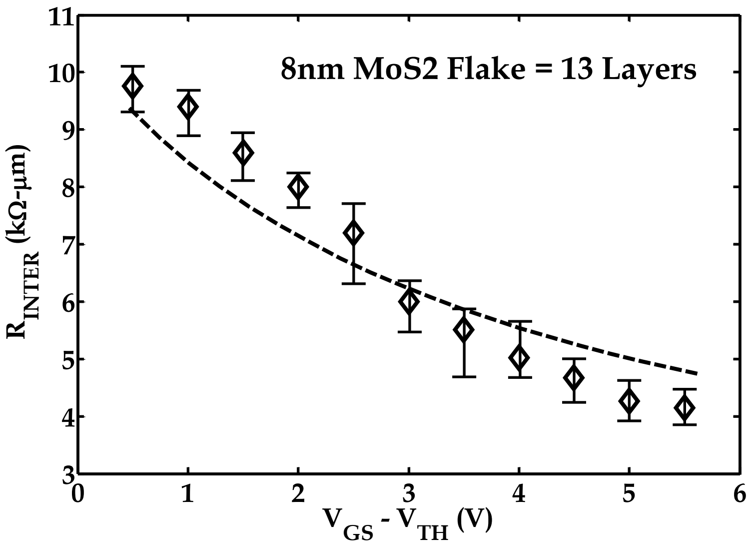
$$= R_{CONTACT} + R_{CHANNEL}$$

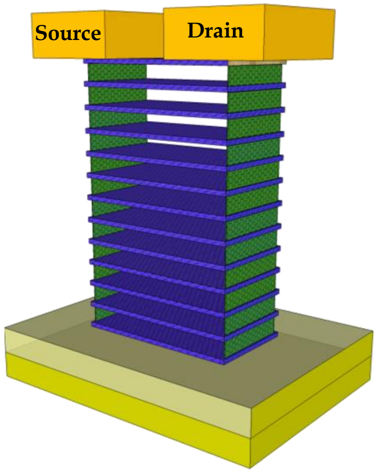
$$= (R_{INTER} + R_{SB}) + R_0 L_{CH}$$

0

R_{SB}=0.65kΩ-μm (Sc-MoS_2 Contact @ V_T)

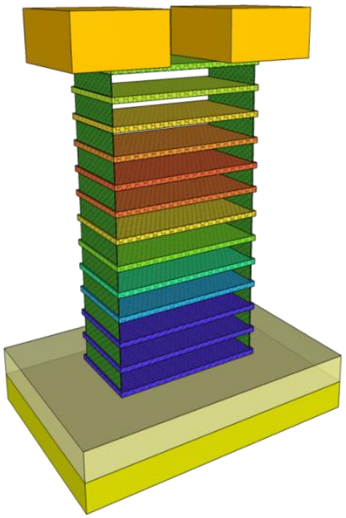
"Contact Resistance"

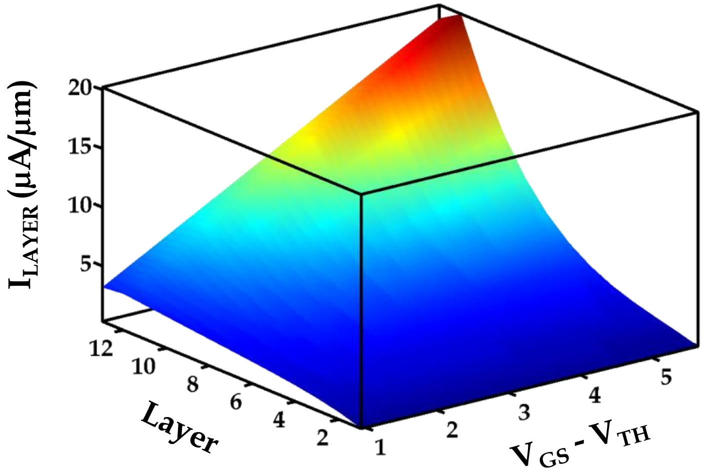




Different numbers of interlayer resistors are involved in the current flow for different gate biases.

"HOT-SPOT"

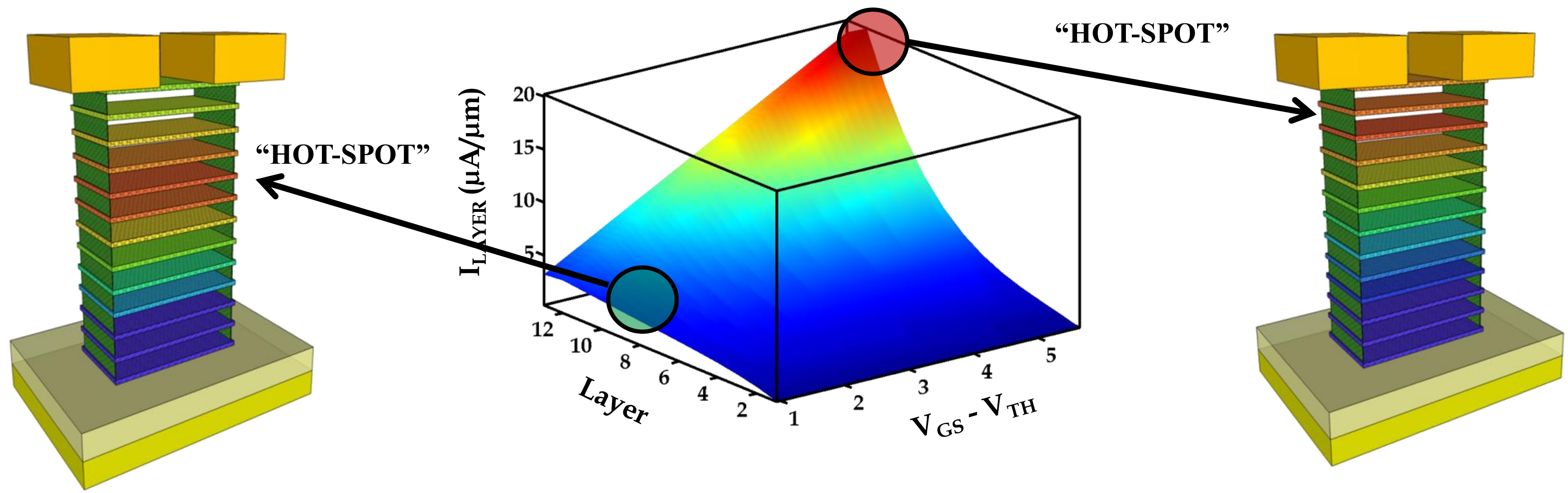


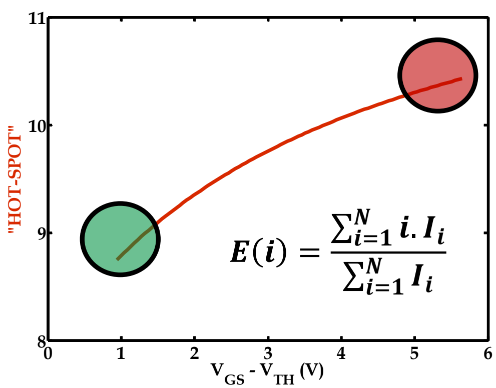


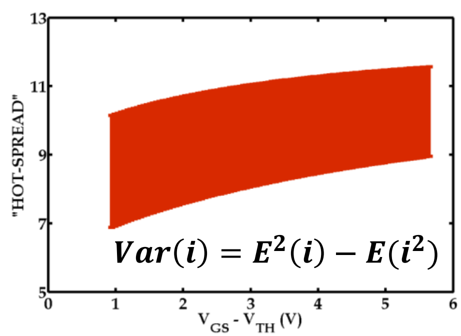
Thomas-Fermi charge screening: $\lambda_{TF}= 7nm$

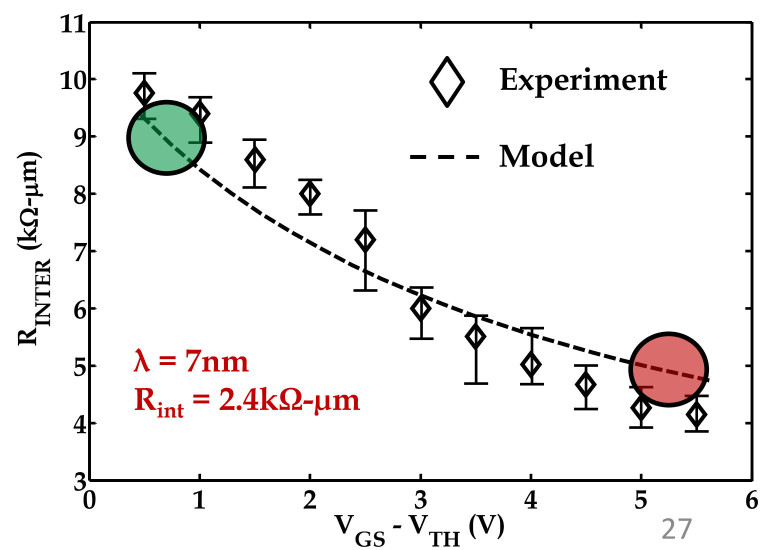
Inter-layer resistive coupling: $R_{int}= 2.4k\Omega-\mu m$

“HOT-SPOT”


“HOT-SPOT”
“HOT-SPOT”
I_LAYER (µA/µm)
20
15
10
5
12
10
8
6
4
2
1
Layer
2
3
4
5
V GS - V TH

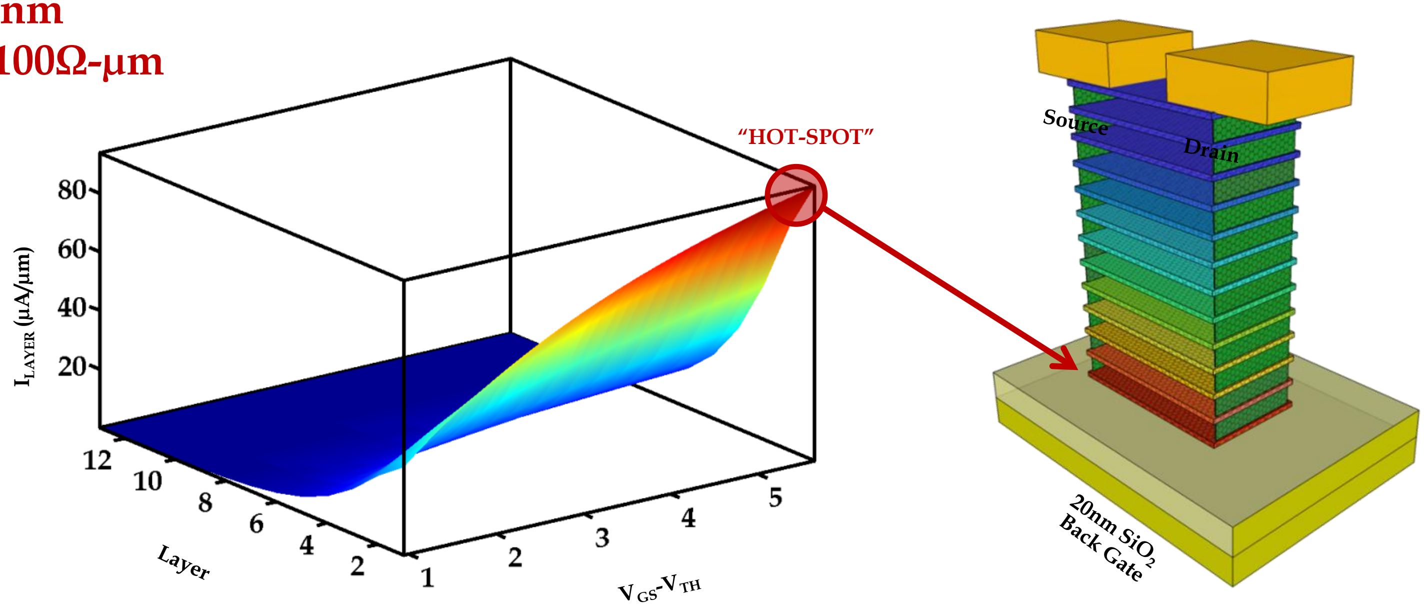

"HOT-SPOT"
11
10
9
8
0
1
2
3
4
5
6
$E(i) = \frac{\sum_{i=1}^{N} i.I_i}{\sum_{i=1}^{N} I_i}$
V_GS - V_TH (V)


"HOT-SPREAD"
13
11
9
7
5
0
1
2
3
4
5
6
$Var(i) = E^2(i) - E(i^2)$
V_GS - V_TH (V)


Experiment
Model
R_INTER (kΩ-µm)
11
10
9
8
7
6
5
4
3
λ = 7nm
R_int = 2.4kΩ-µm
0
1
2
3
4
5
6
V_GS - V_TH (V)

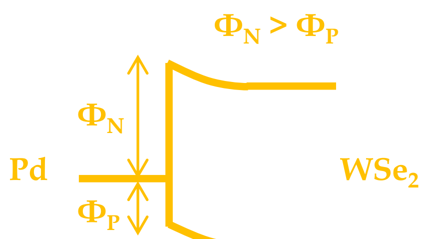
Graphene

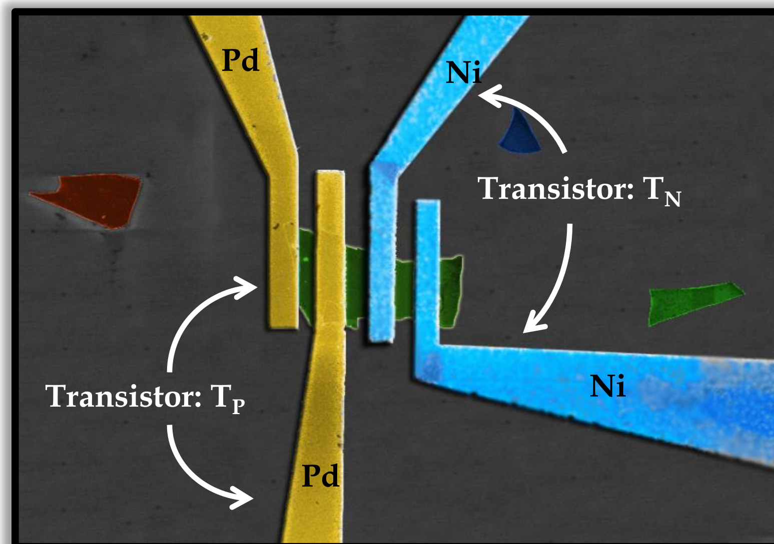
$\lambda = 0.7nm$
$R_{int} = 100\Omega\text{-}\mu m$

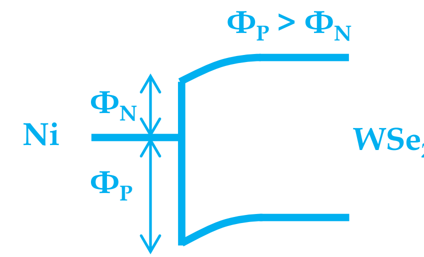


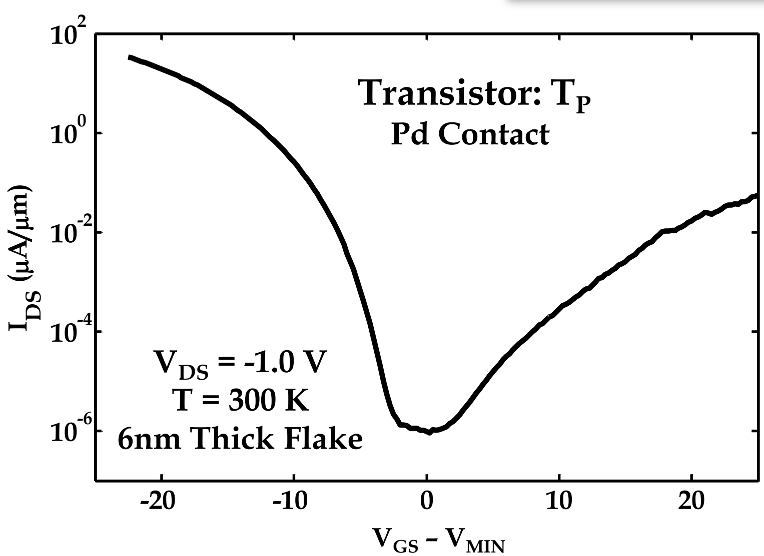
Saptarshi Das, et al., "Where does the Current Flow in the Two Dimensional Layered Systems", **Nano Letters** 13 (7), 3396-3402**, 2013.**

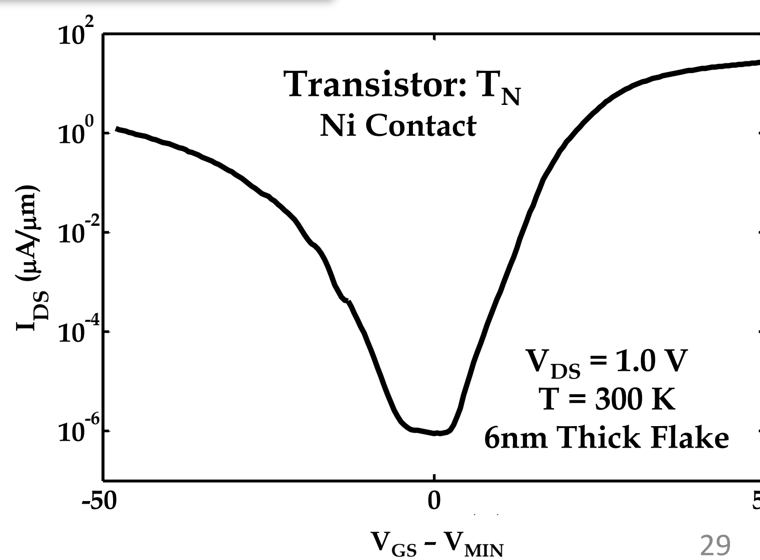
Tungsten Diselenide: WSe_2











Tungsten Diselenide: WSe_2

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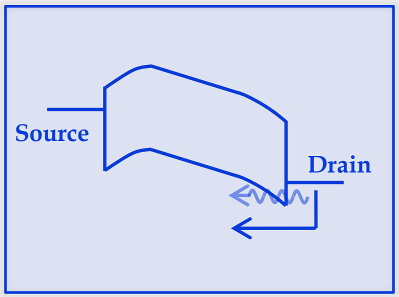
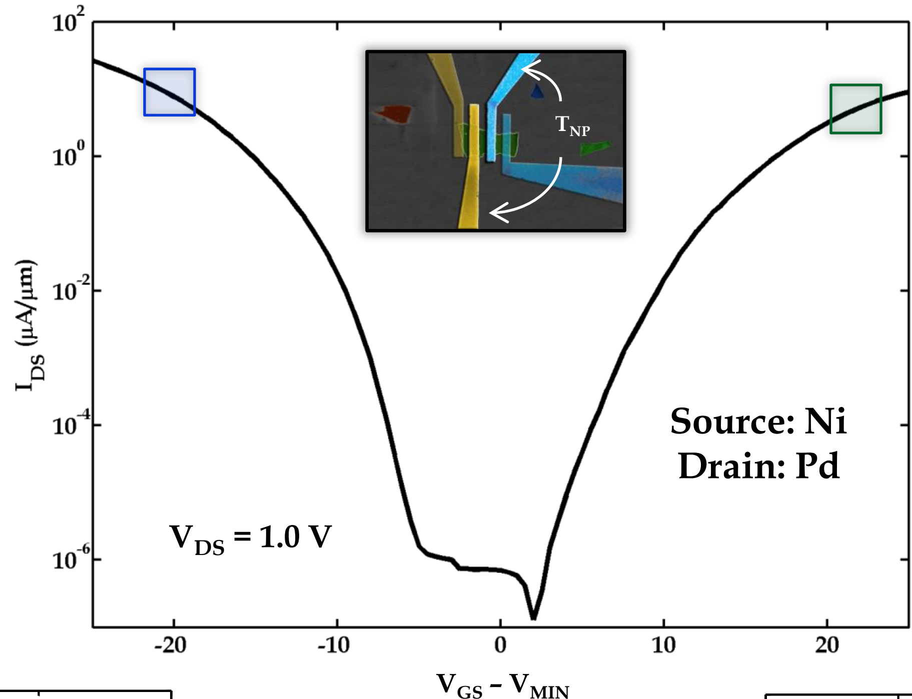
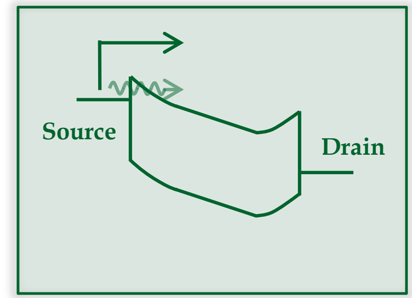
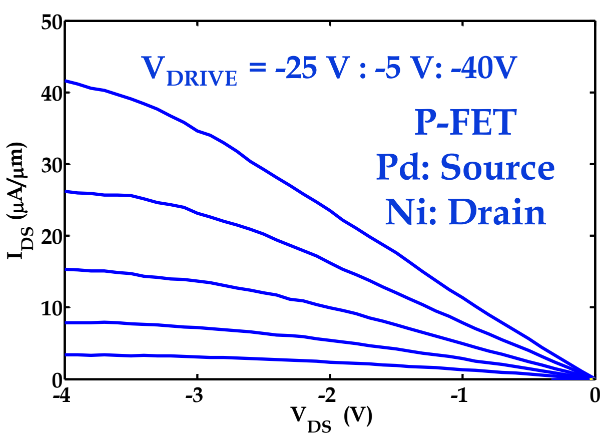
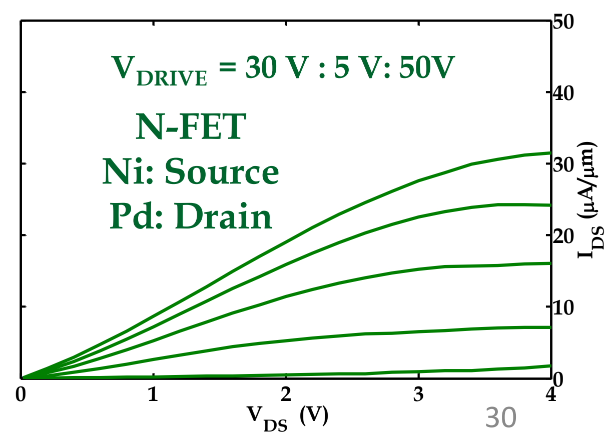


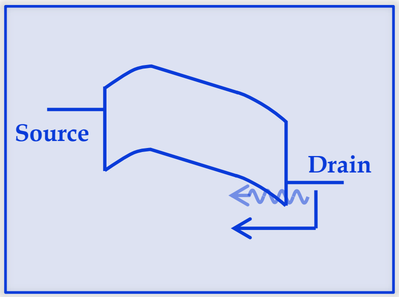


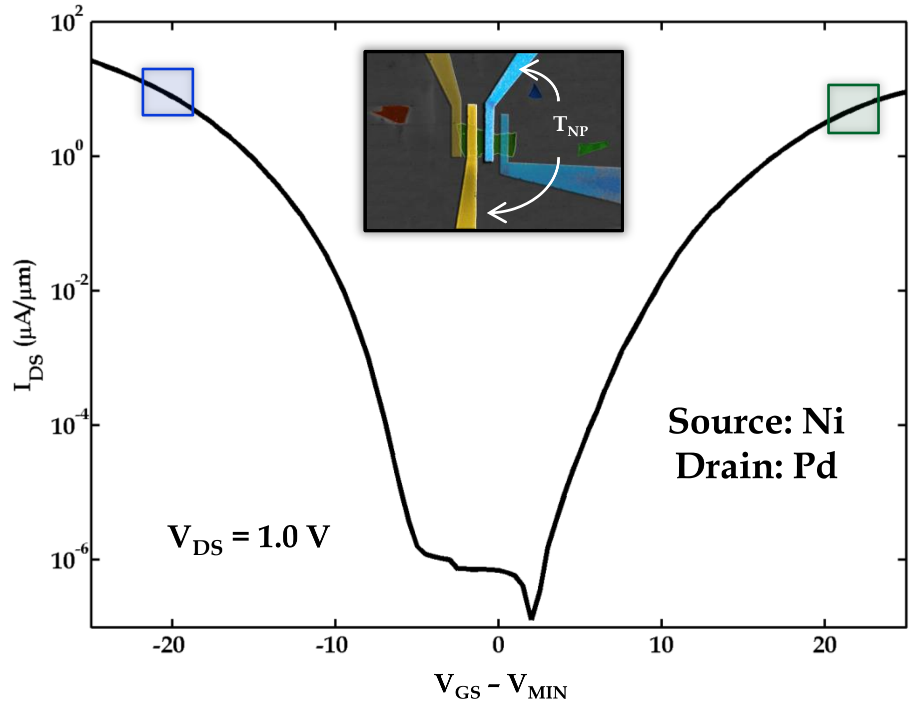


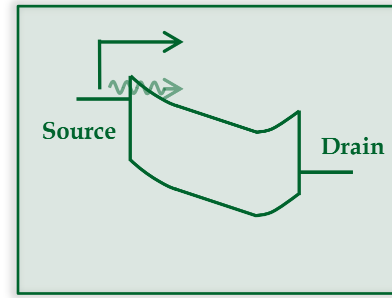




Tungsten Diselenide: WSe_2



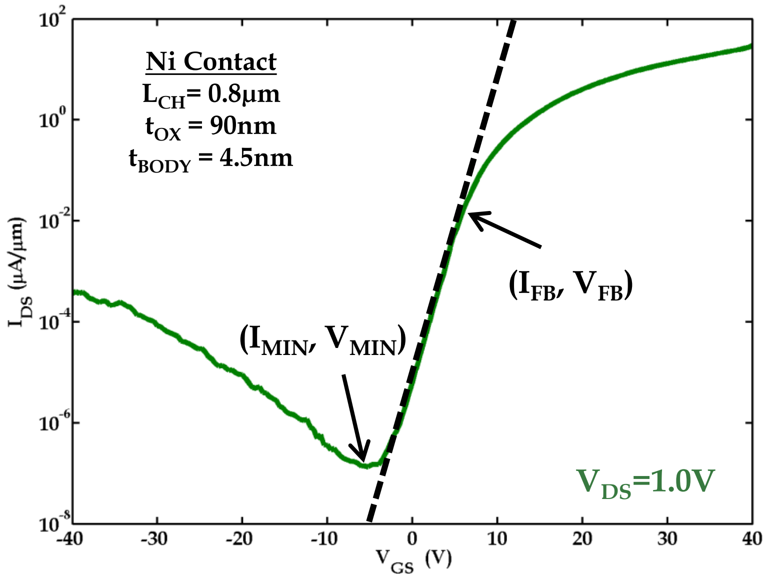


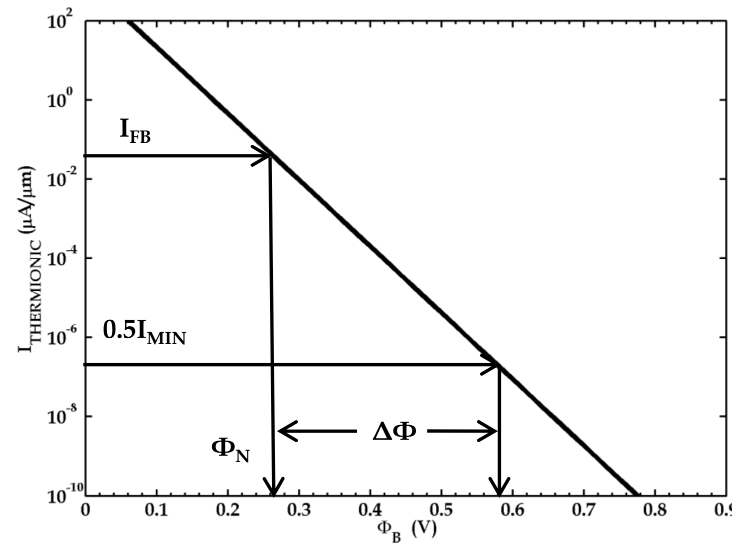


Work Function Engineering for CMOS Compatibility

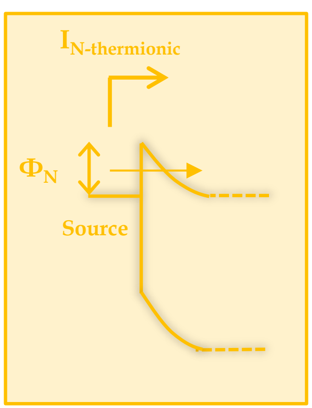
Saptarshi Das , et al., "WSe2 Field Effect Transistor with Enhanced Ambipolar Characteristics", **Applied Physics Letters**, 103 (10), 103501-5, **2013**

Molybdenum Diselenide: $MoSe_2$

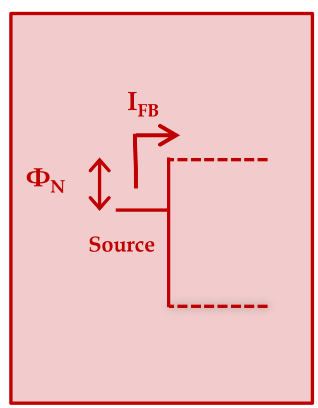




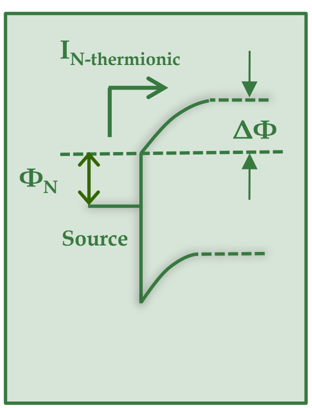
Band Position at the Source end for $V_{GS} > V_{FB}$



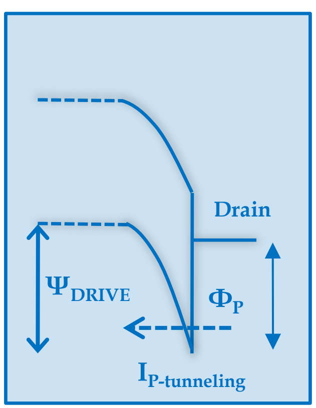
Band Position at the Source end for $V_{GS} = V_{FB}$



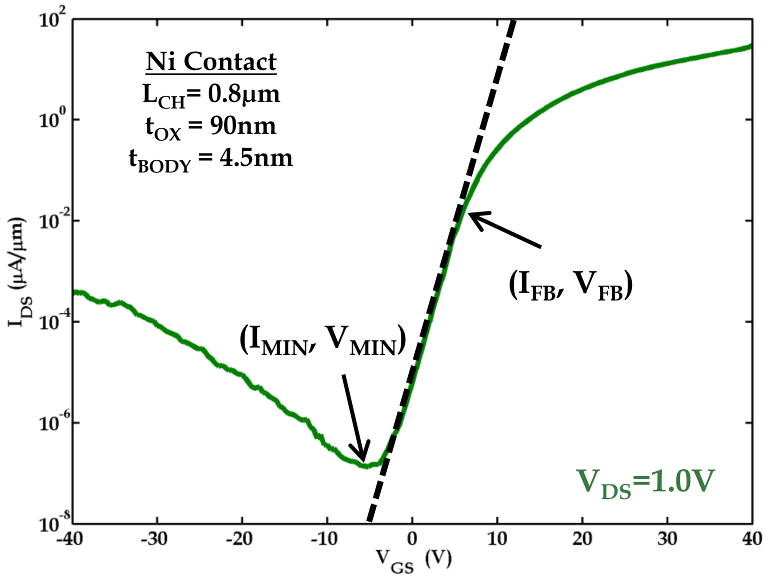
Band Position at the Source end for $V_{GS} = V_{MIN}$

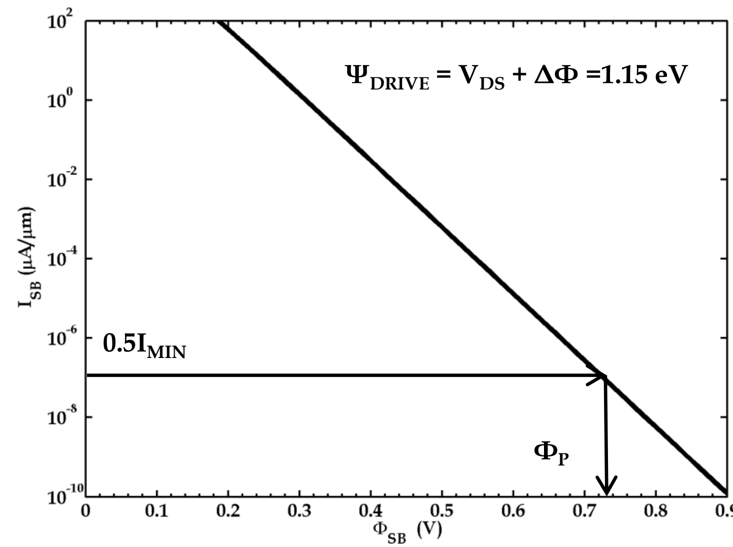


Band Position at the Drain end for $V_{GS} = V_{MIN}$

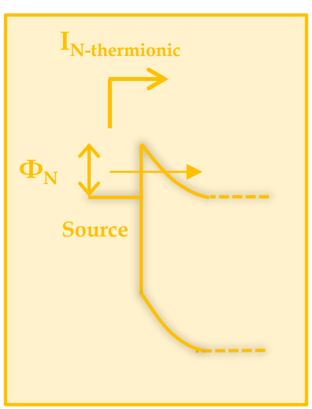


Molybdenum Diselenide: $MoSe_2$

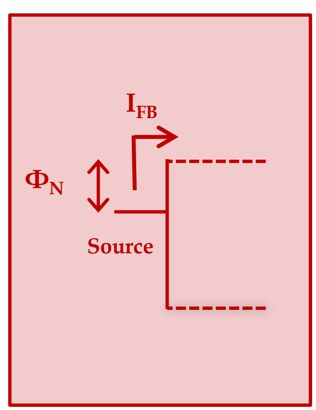




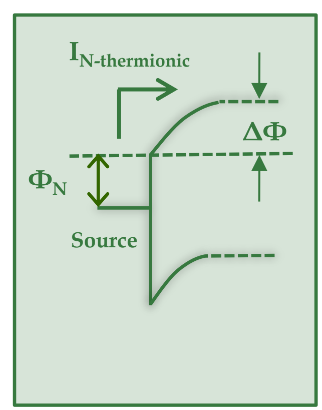
Band Position at the Source end for $V_{GS} > V_{FB}$



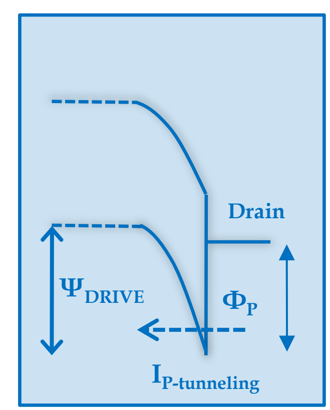
Band Position at the Source end for $V_{GS} = V_{FB}$



Band Position at the Source end for $V_{GS} = V_{MIN}$

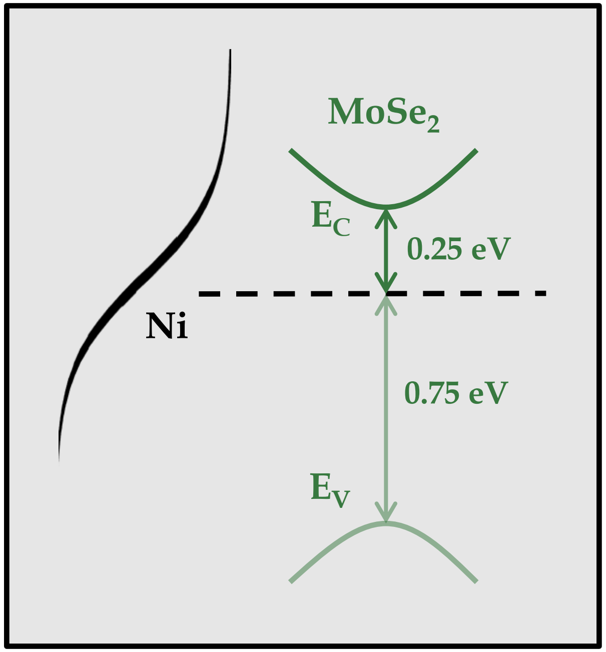


Band Position at the Drain end for $V_{GS} = V_{MIN}$



Molybdenum Diselenide: $MoSe_2$

Band Alignment of Ni with the Band-Structure of $MoSe_2$

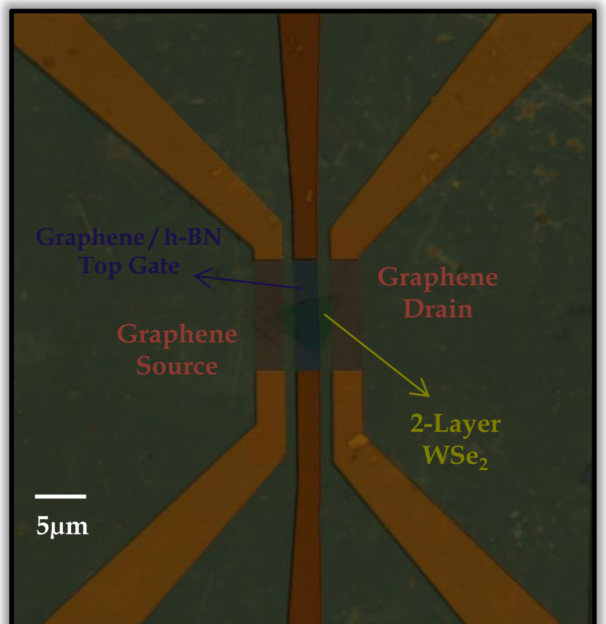


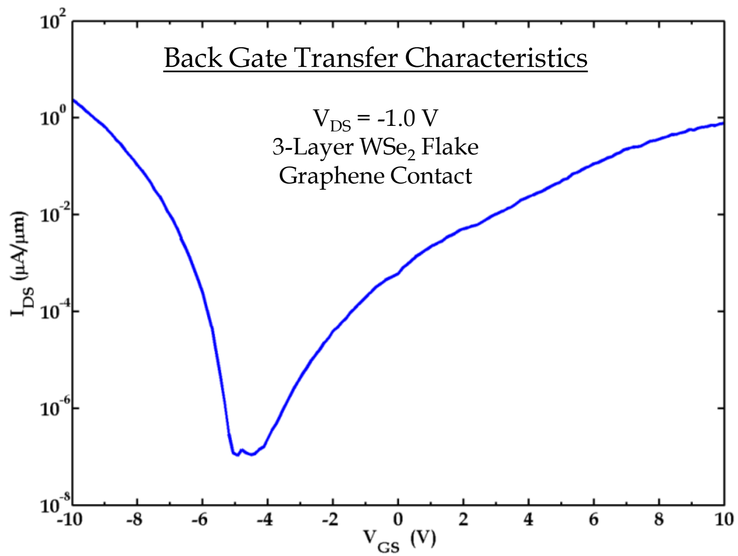
$$E_G = \Phi_N + \Phi_P$$

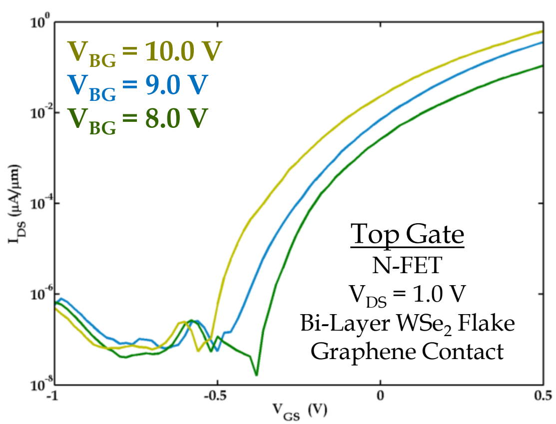
Electronic Bandgap Extraction

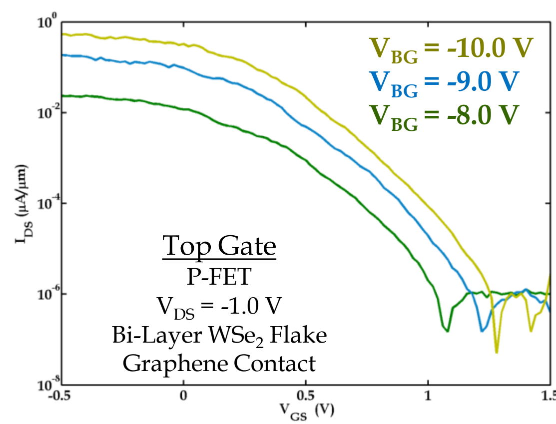
Saptarshi Das , et al., "Electronic Bandgap and Band Alignment of Transition Metal Dichalcogenides", **submitted**, **2014**

All 2D Transistor









Flexible Transparent Transistor

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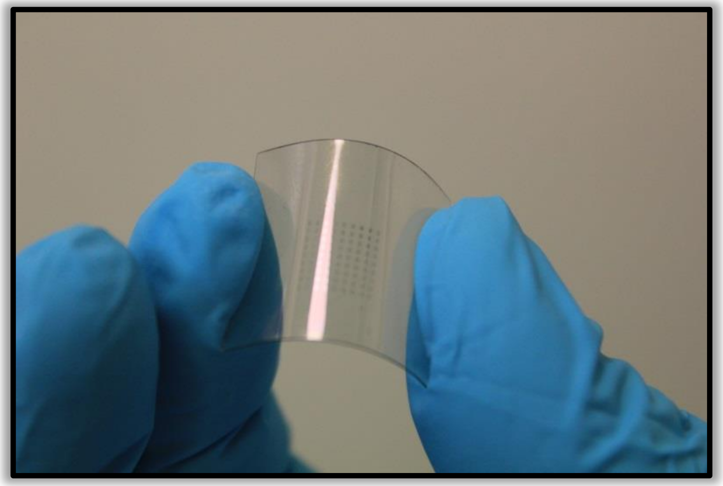
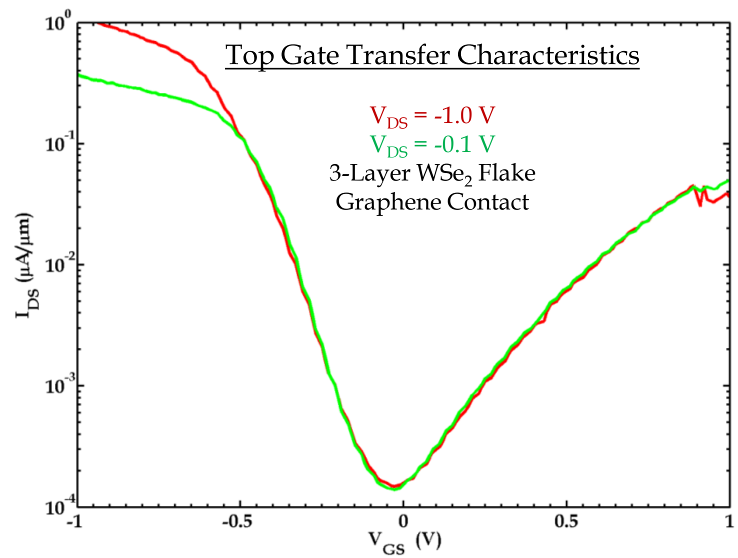
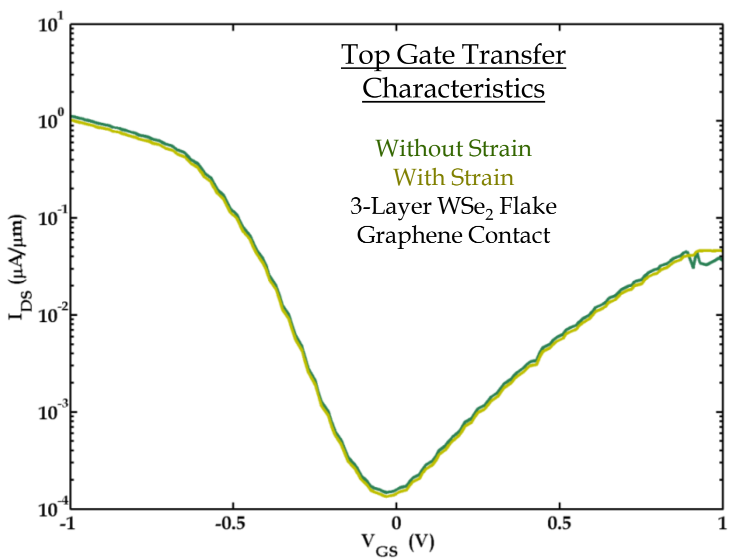
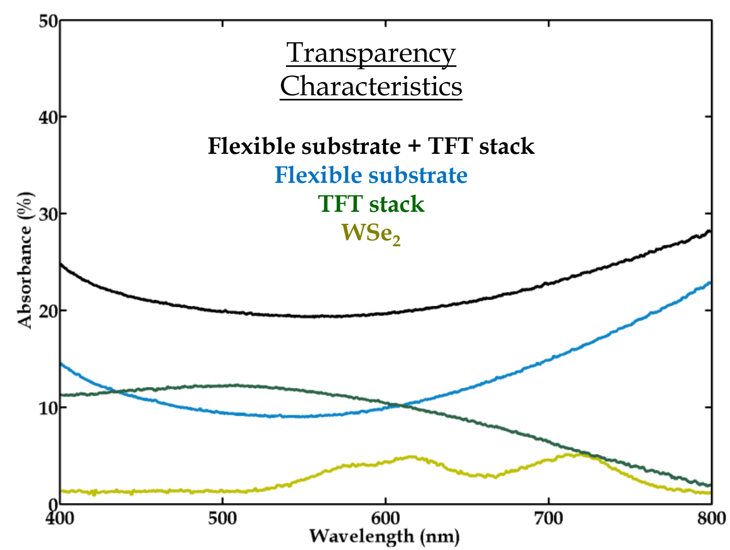


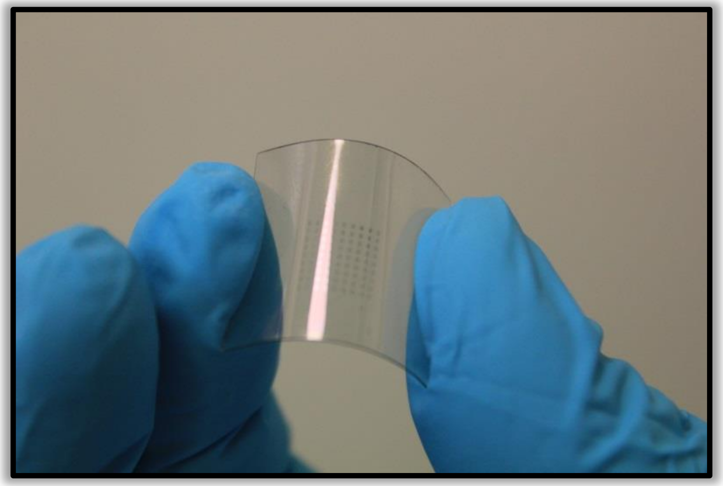


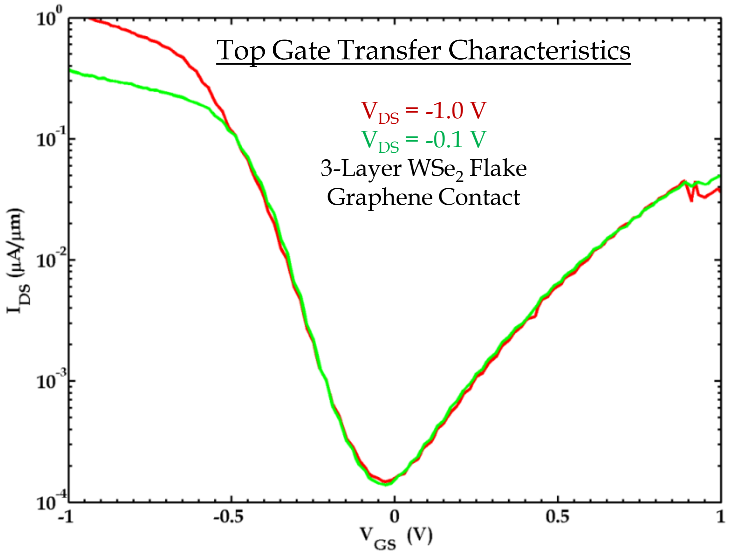




Flexible Transparent Transistor

Center for Nanoscale Materials

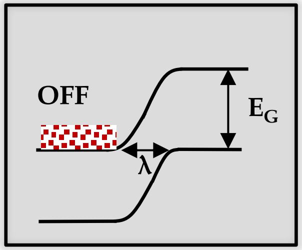


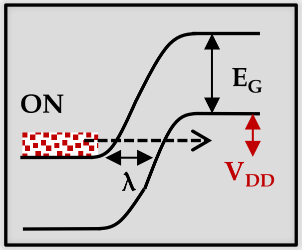


Saptarshi Das , et al., **“**All 2D, High Mobility, Flexible and Transparent Thin Film Transistor**”, submitted**, **2014**

Tunneling FET

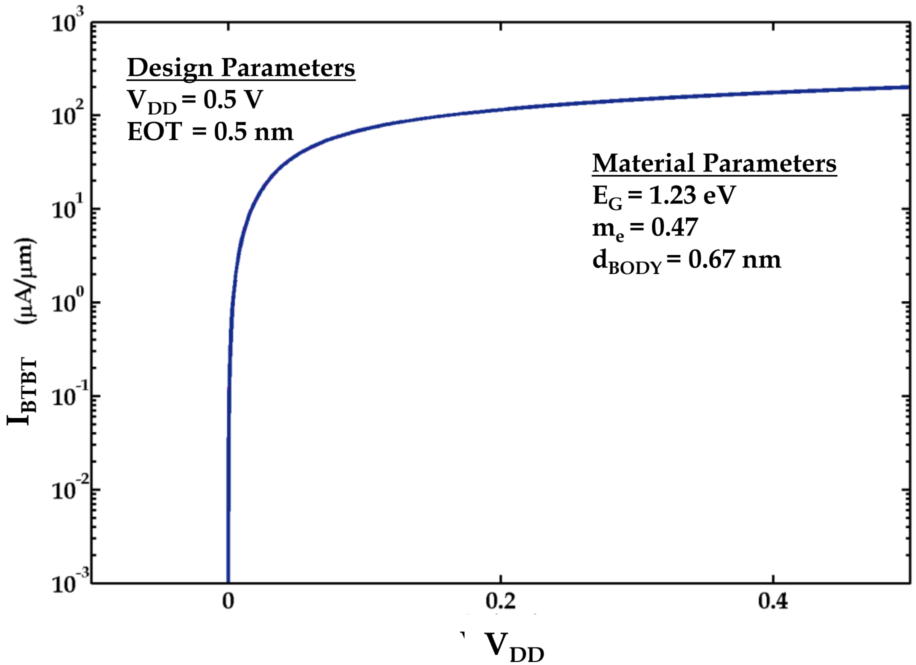
Band to Band Tunneling



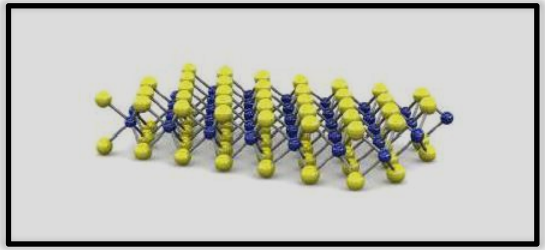


$$I_{ON} \propto T_{WKB} = exp(-\frac{4}{3\hbar}\sqrt{2m_eE_G}\lambda)$$

$$T_{WKB} = \exp(-\frac{4}{3\hbar}\sqrt{2m_eE_Gd_{OX}\mathbf{d_{BODY}}})$$

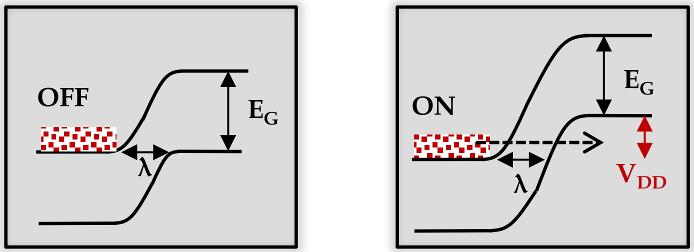


TMDs



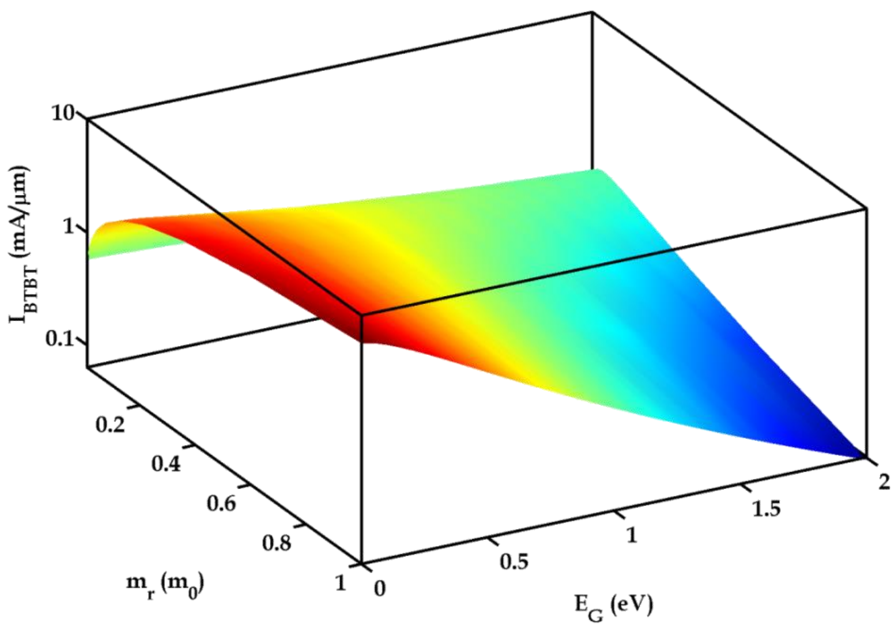
Important Parameters for Tunneling

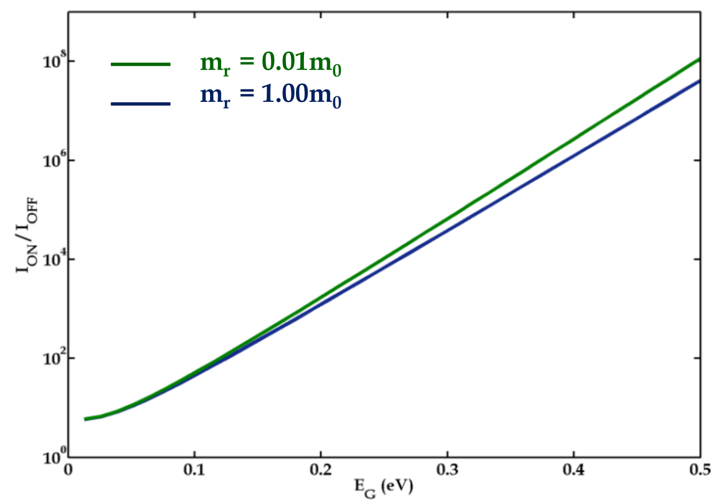
Band to Band Tunneling



$$I_{ON} \propto T_{WKB} = exp(-\frac{4}{3\hbar}\sqrt{2m_eE_G\lambda})$$

$$T_{WKB} = \exp(-\frac{4}{3\hbar}\sqrt{2\mathbf{m_e}\mathbf{E_G}d_{OX}d_{BODY}})$$



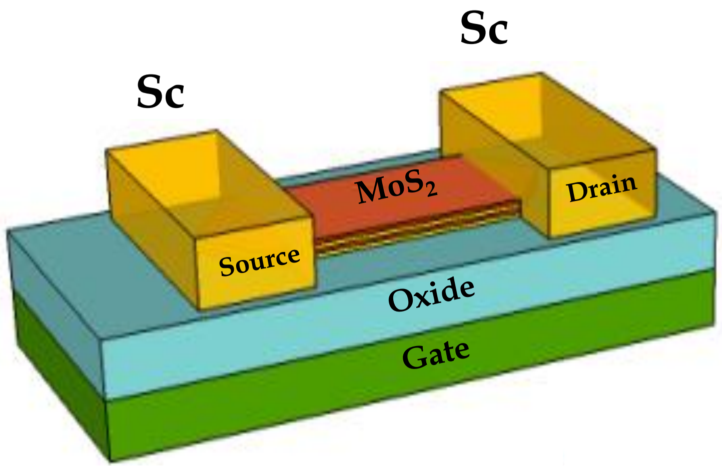


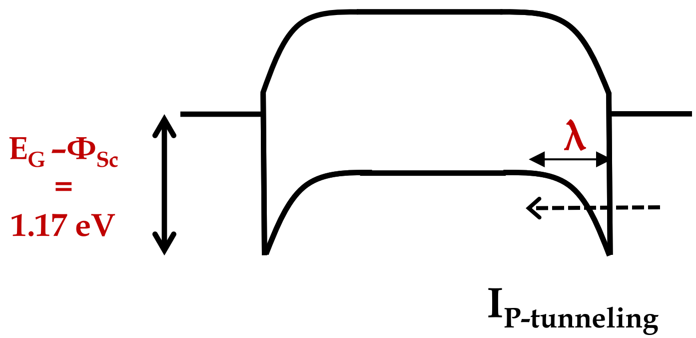
TMDs for TFETs

Mono-layer Dichalcogenide	E_G (eV)	m_n (m_0)	m_p (m_0)	I_{BTBT} (mA/µm)
MoS_2	1.79	0.46	0.56	0.16
$MoSe_2$	1.49	0.55	0.64	0.18
$MoTe_2$	1.13	0.55	0.67	0.27
WS_2	1.96	0.30	0.41	0.18
WSe_2	1.61	0.34	0.44	0.20
WTe_2	0.71	0.31	0.41	0.67

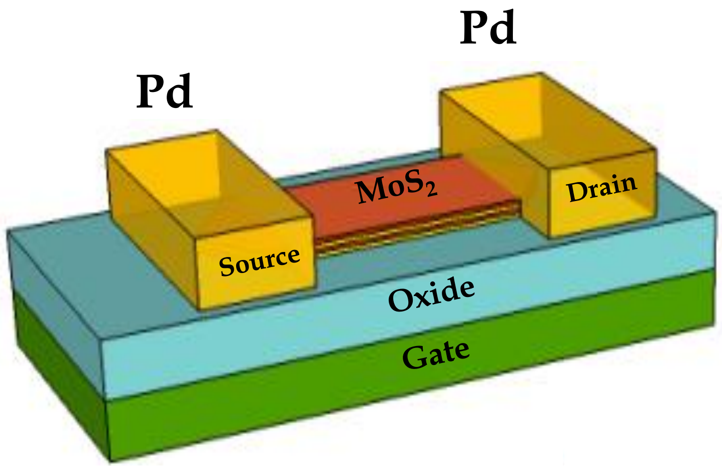
Saptarshi Das, et al., " Towards Low Power Electronics: Tunneling Phenomena in Dichalcogenides", **ACS Nano, 2014.**

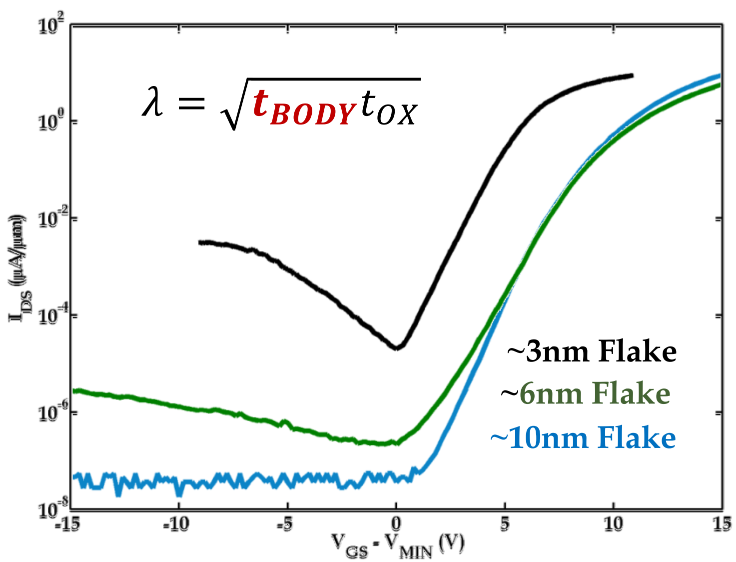
Schottky Barrier Tunneling : MoS_2

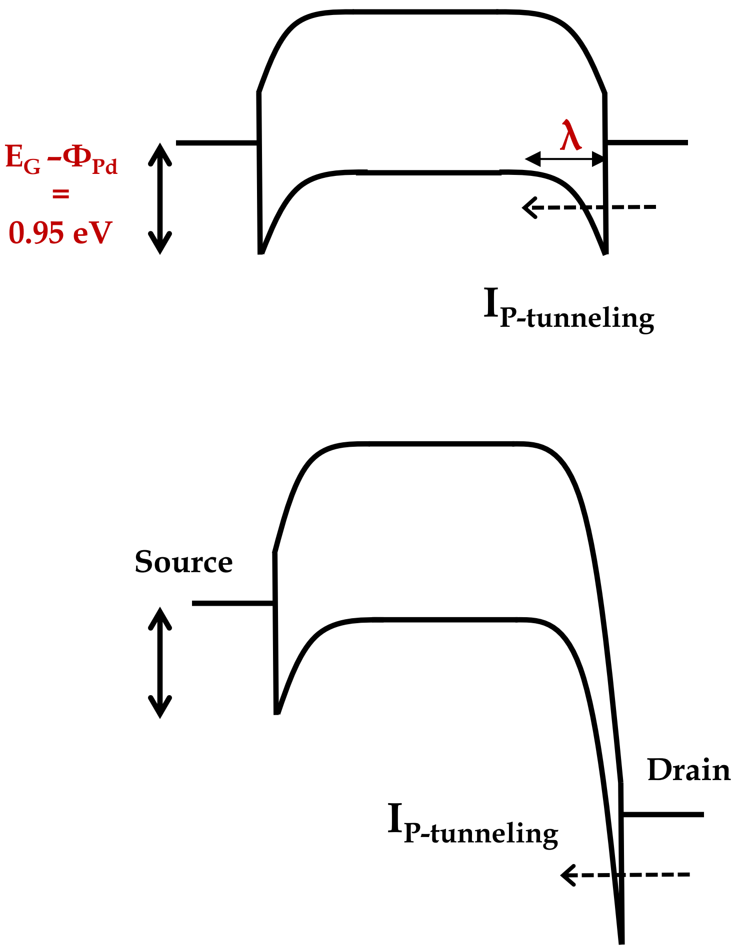




Schottky Barrier Tunneling : MoS_2







Schottky Barrier Tunneling : MoS_2

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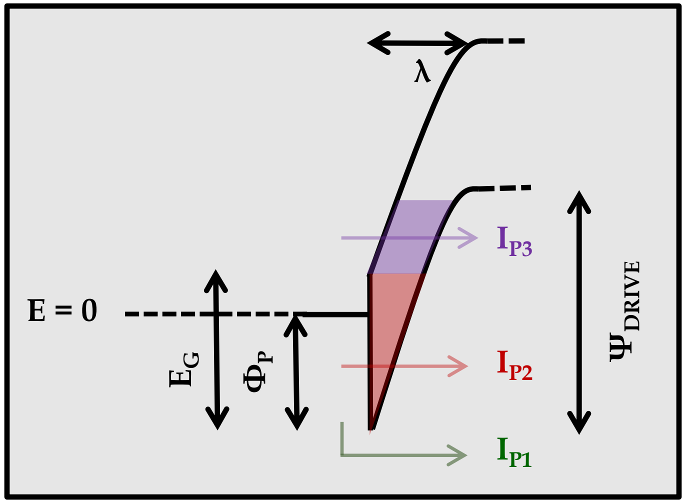
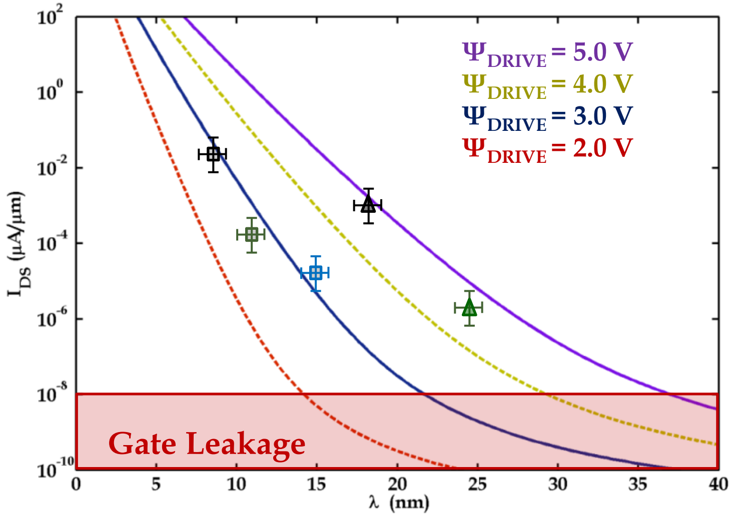
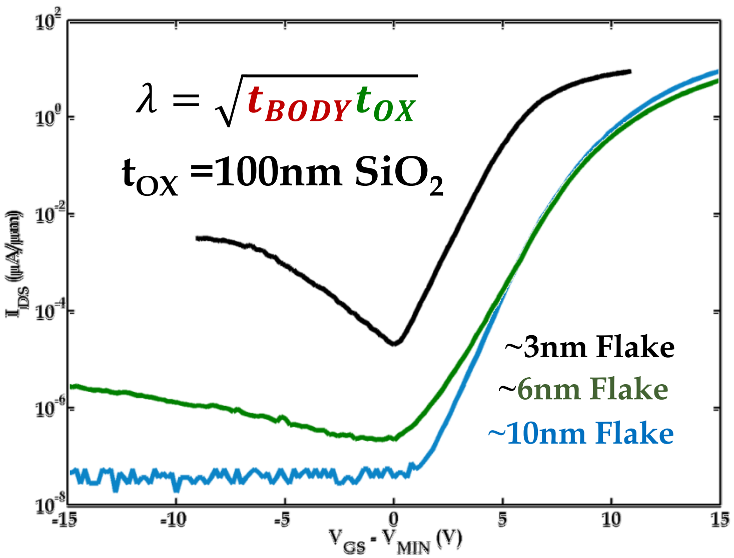
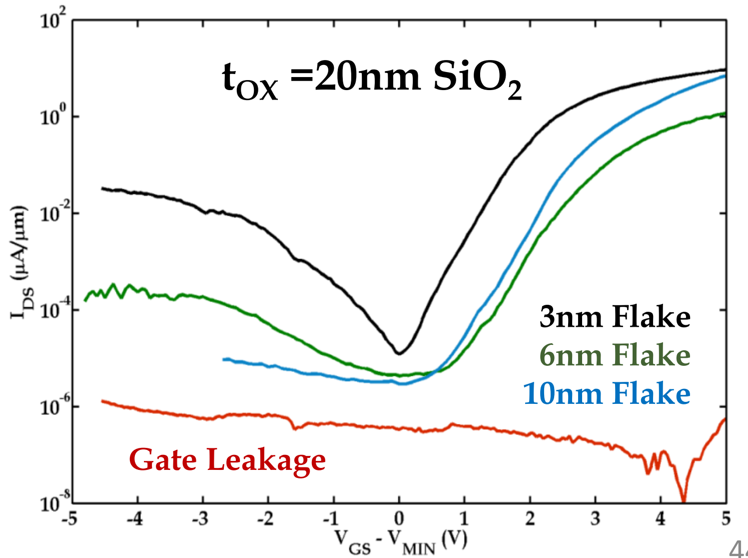
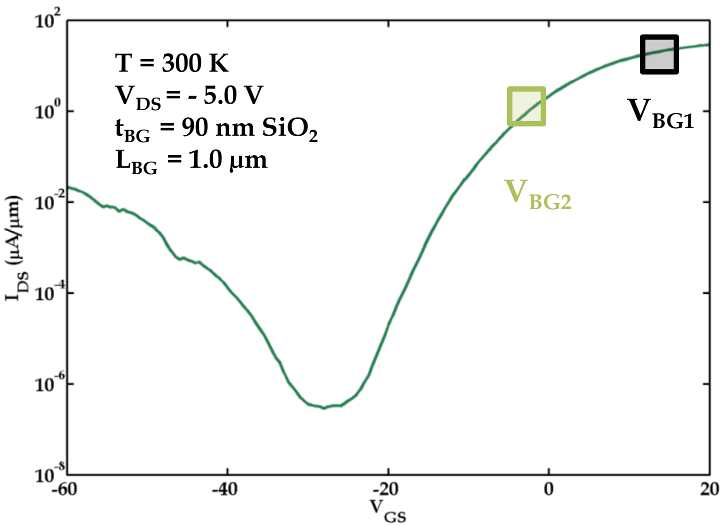


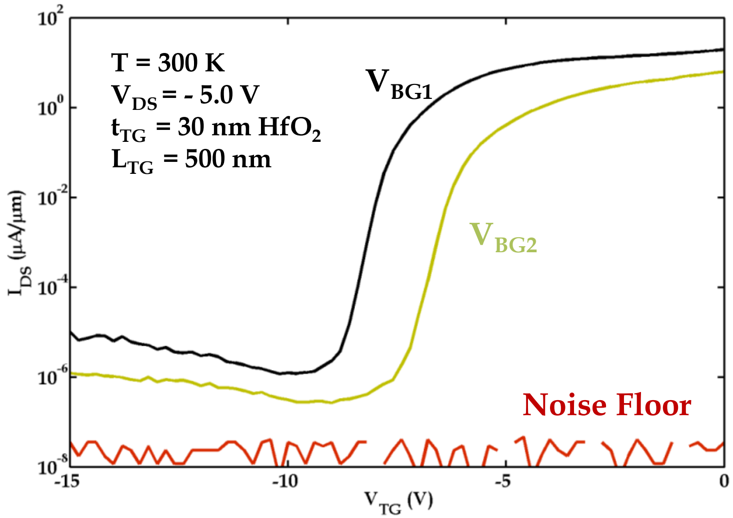


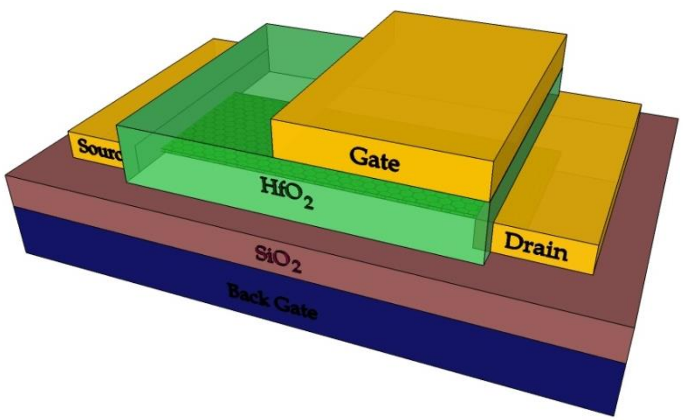


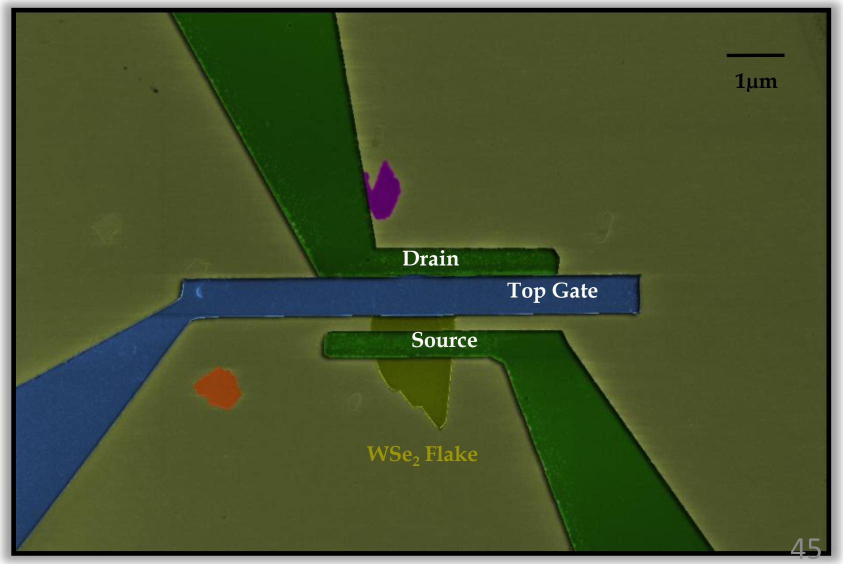


Band to Band Tunneling: WSe_2









Band to Band Tunneling: WSe_2

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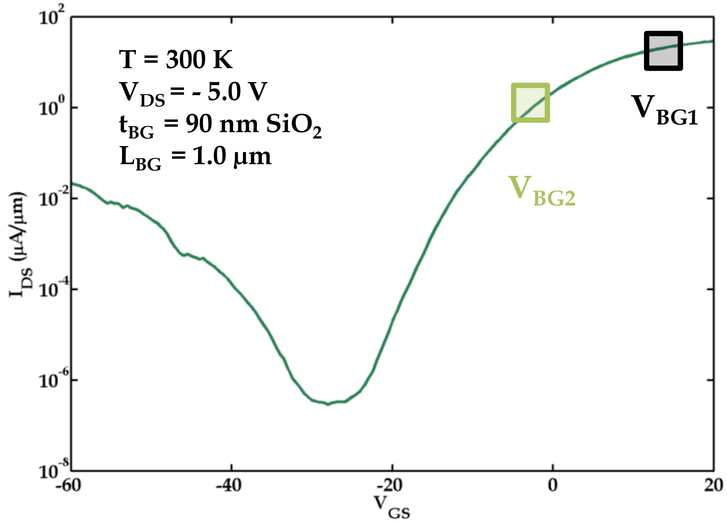

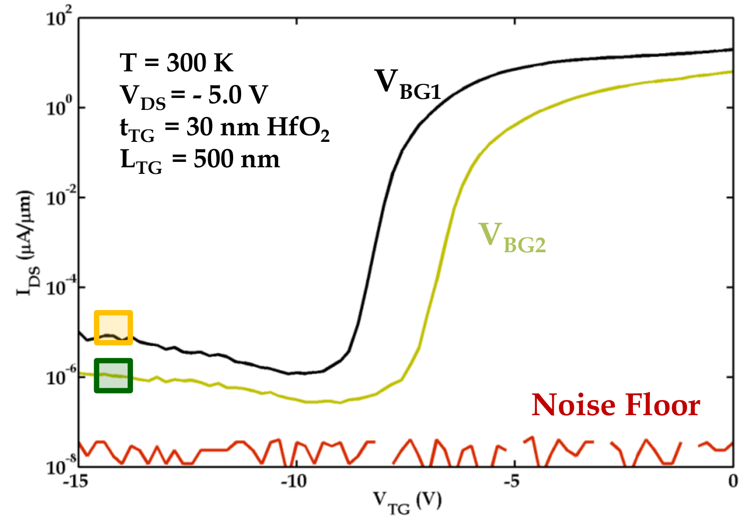

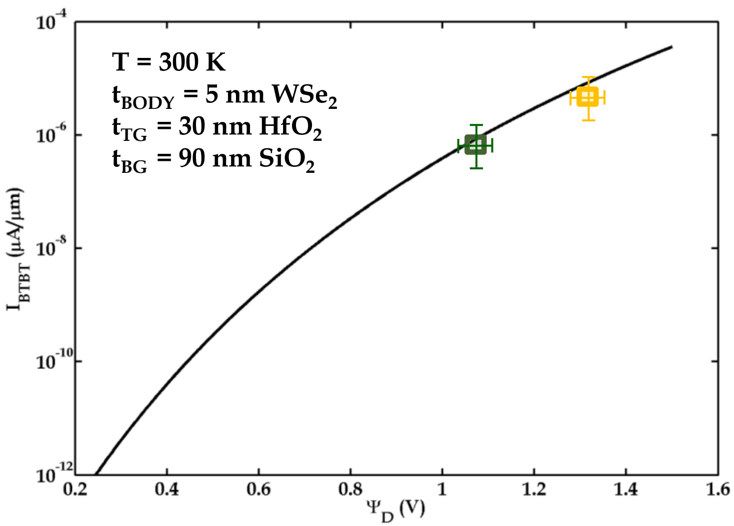

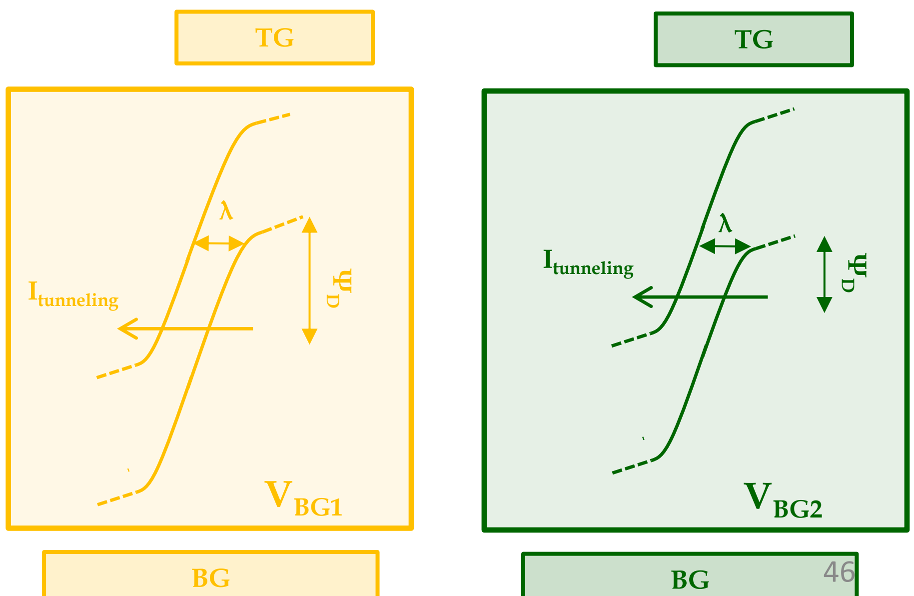

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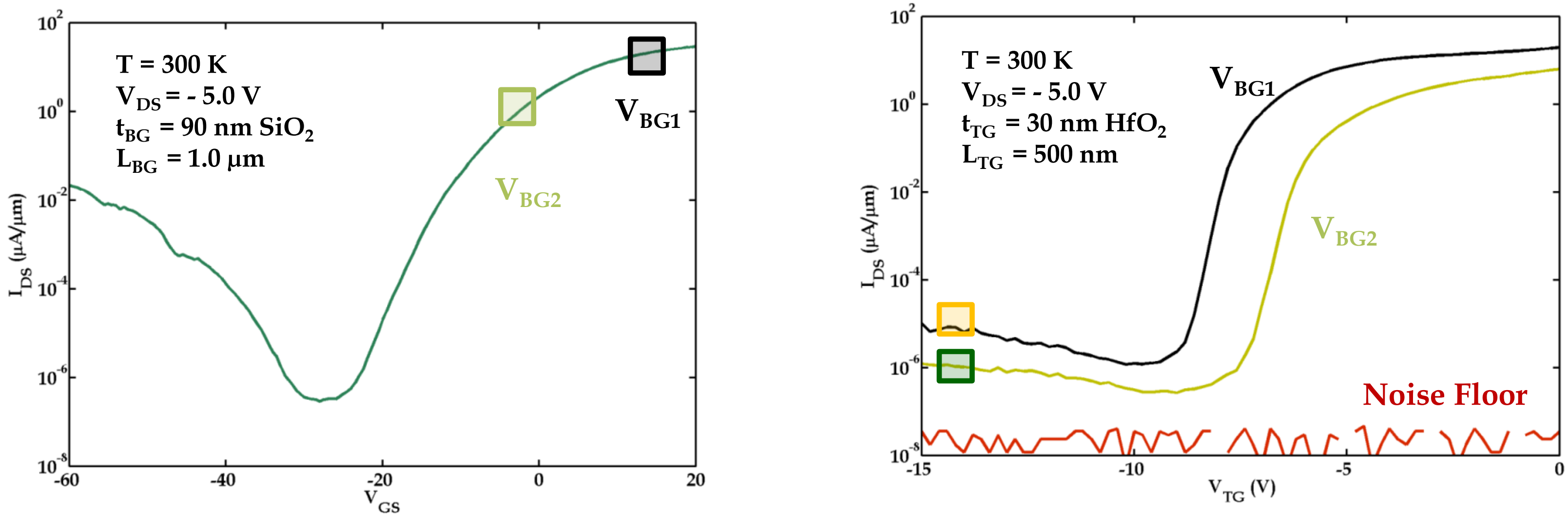
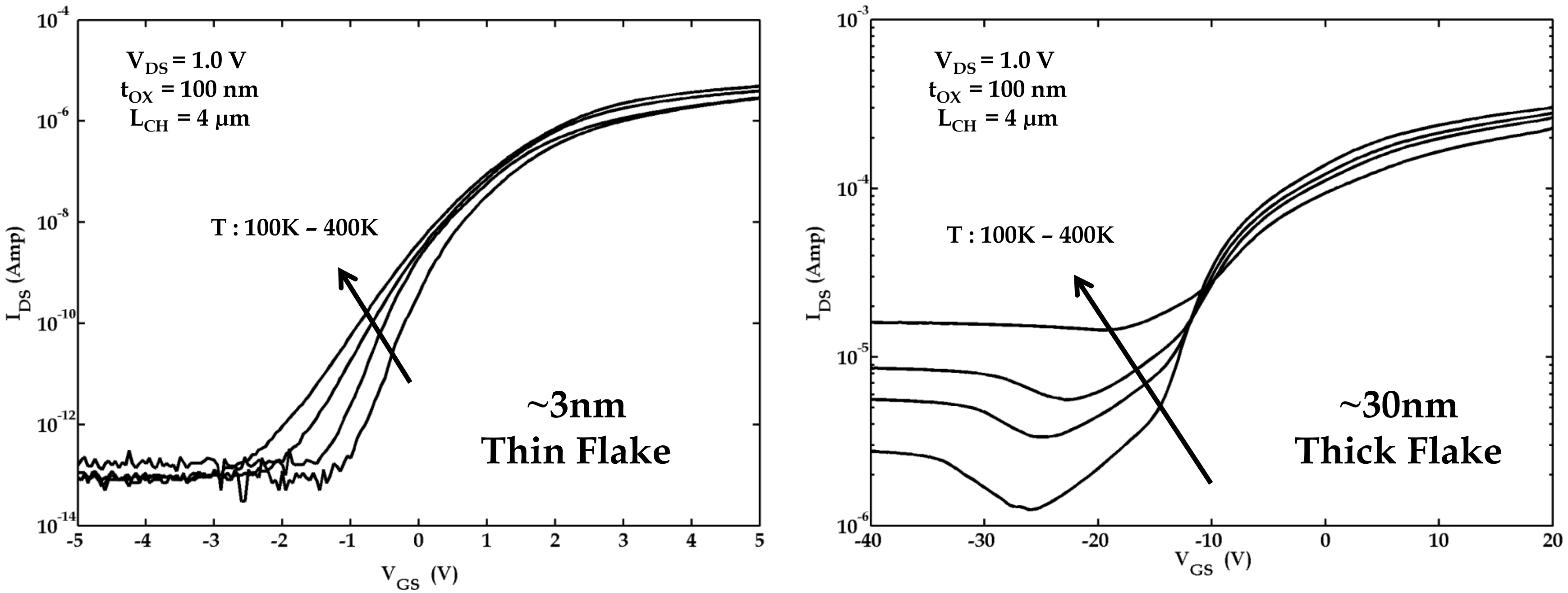


Saptarshi Das, et al., " Towards Low Power Electronics: Tunneling Phenomena in Dichalcogenides", **ACS Nano, 2014.**

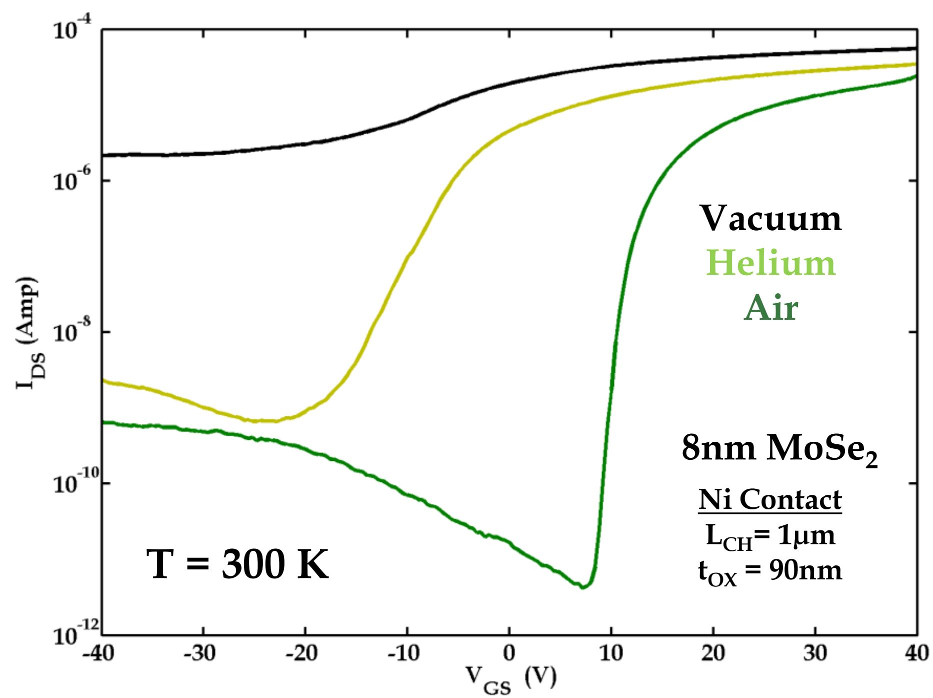
1. What is Unique about TMDs ?
2. Exploring Transistors based on TMDs
3. Tunneling Phenomenon in TMDs
4. **Extreme Sensitivity of TMDs to External Forces**

Temperature



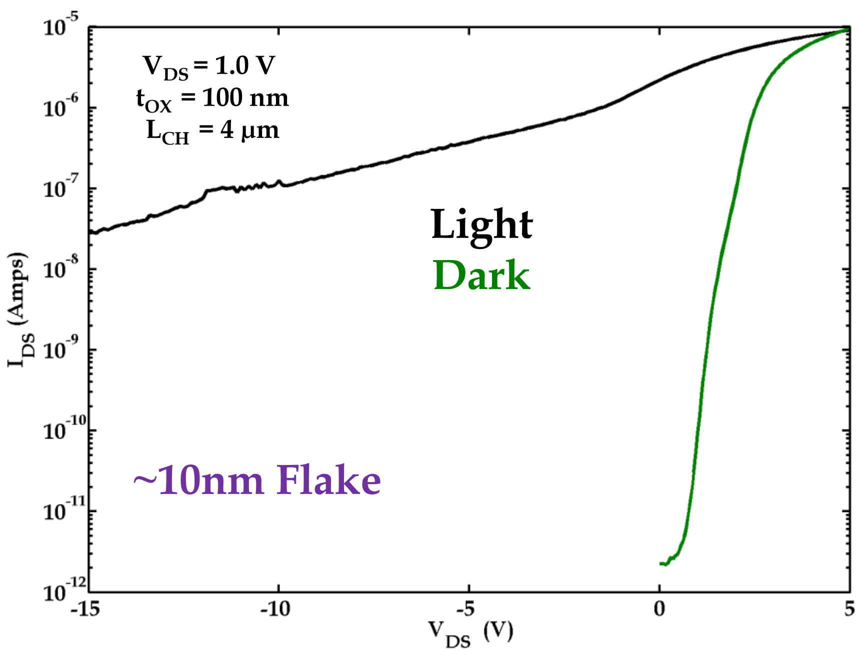
Thicker Flakes are extremely sensitive to Temperature Change

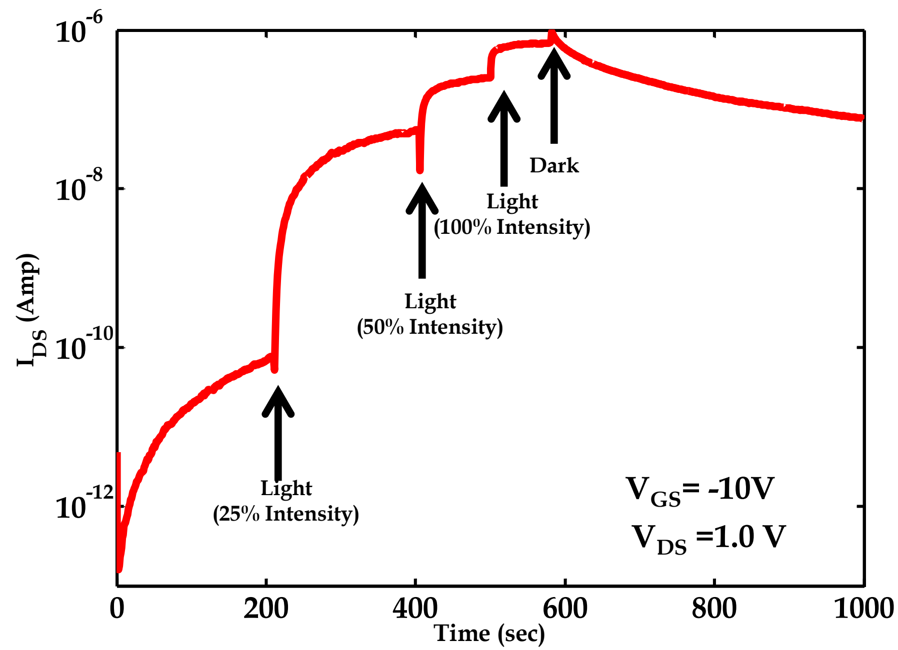
Gas Environment



Extremely sensitive to Environment

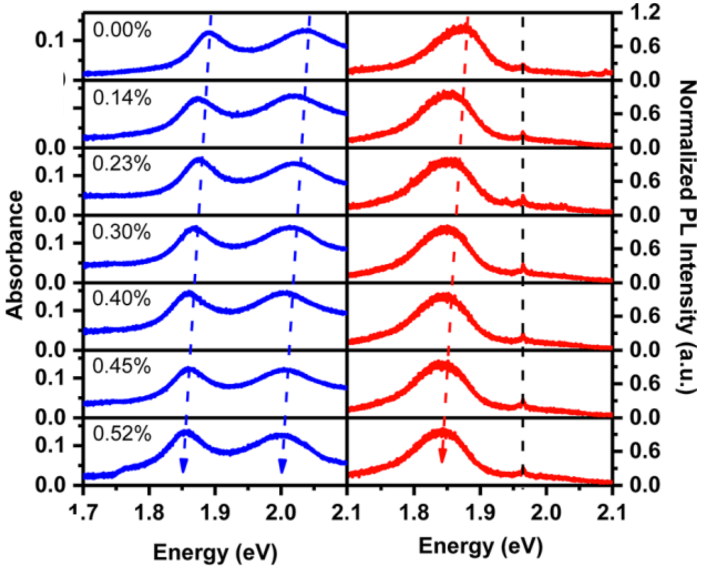
Light

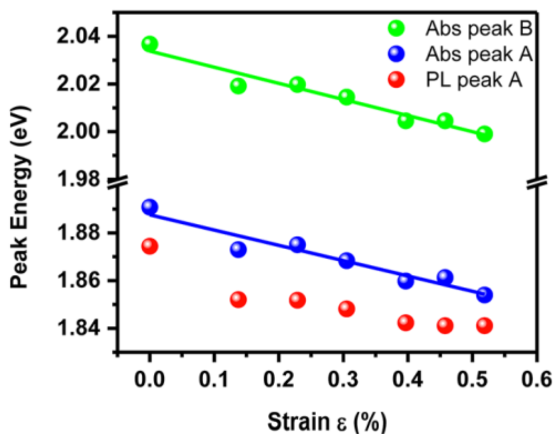




Extremely sensitive to Light

Strain





Band gap Engineering through Strain

Strain Induced Metal Insulator Transition

Conclusion

1. What is Unique about TMDs ?

- ✓ Natural 2D System.
- ✓ Exfoliation gives easy access to pristine quality of the material.
- ✓ For the first time Semiconductors with d-orbital electronics.

2. Exploring Transistors based on TMDs

- ✓ How to make good quality Contact
- ✓ How to optimize layer thickness
- ✓ Scalability beyond 10nm CMOS node
- ✓ Where does the Current flow in layered systems
- ✓ Flexible Electronics

3. Tunneling Phenomenon in TMDs

- ✓ Schottky Barrier Tunneling in MoS_2
- ✓ Band to Band Tunneling in WSe_2
- ✓ Projection for TFETs based on TMDs

4. Extreme Sensitivity of TMDs to External Forces

- ✓ Temperature, Pressure, Light and Strain changes electronic transport in TMDs

Acknowledgement

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LEAST LOW ENERGY SYSTEMS TECHNOLOGY

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Thank You