Nanoscale Quantum Materials

2018 Quantum Science Summer School (NSF/DOE/AFSOR)

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Overview

- Why Nanoscale Materials
  - Emergent properties (band engineering, surface properties)
  - Examples (quantum dots, carbon nanotubes, mechanical properties)
- Synthesis of Nanowires
  - Various growth methods
  - Vapor-liquid-solid growth
  - Doping / surface passivation
- Synthesis of 2D Materials
  - Chemical vapor deposition
  - Precursors / additives

Overview

- Case Study of Nanowires: Si Nanowires
  - Thermal transport modulation
  - Si nanowire batteries
- Case study of topological nanomaterials
  - Bi_2Se_3 topological insulator nanoribbons
  - SnTe Topological crystalline insulator nanowires
- Case study of 2D materials for energy
  - MoS_2 for hydrogen evolution reaction (HER)
  - Phase transition via intercalation and consequences for HER

Topological Materials: Pick Your Favorite!

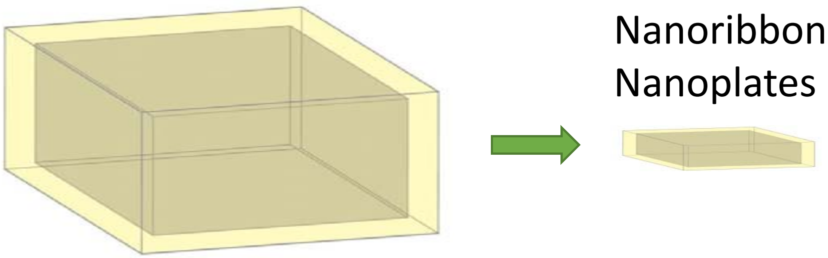
http://www.issp.ac.ru/lpcbc/DANDP/Bi-Ch.html

Explosion of Topological Materials

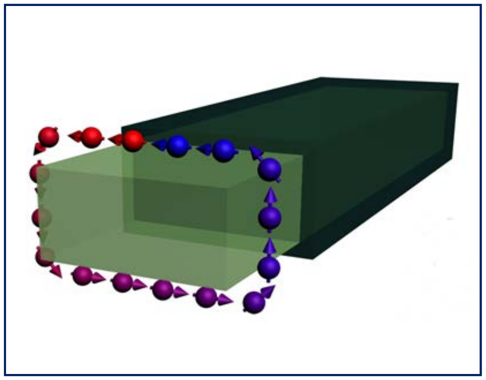
2007: CdTe/HgTe/CdTe quantum wells to show topological edge states (Science, Molenkamp)
2009: $Bi_{1-x}Sb_x$ alloy (Science, Princeton)
2009: Bi_2Se_3, Bi_2Te_3, Sb_2Te_3 Topological Insulators (Nature Phys, Nature, Science, Stanford)
2010: Half Heusler compounds: LnPtSb, LnPtBi, LnPdBi, (Nat. Mater, Max Planck)
2011: SnTe Topological Crystalline Insulators (Nat. Phys, Experimental Verification 2012, MIT)
2011: Weyl Semimetals (PRL, Experimental Verification 2015 Science): WTe_2, TaAs, …
2014: Monolayer transition metal dichalcogenides (2014 Science theory): 1T'-MoS_2, …

Nanostructure Approach to Study Topological Insulators

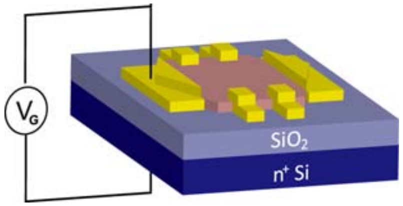
Increase Surface-to-Volume Ratio

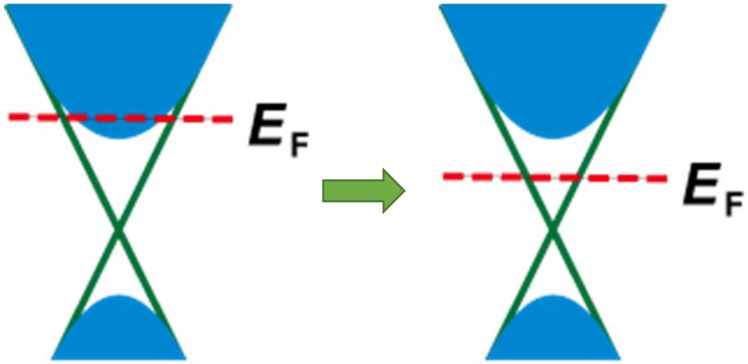


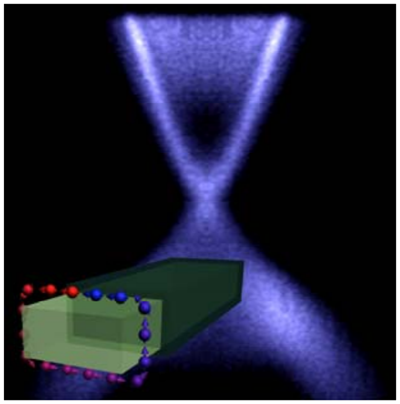
Nanoribbons,
Nanoplates



Manipulate Fermi Energy by Gating



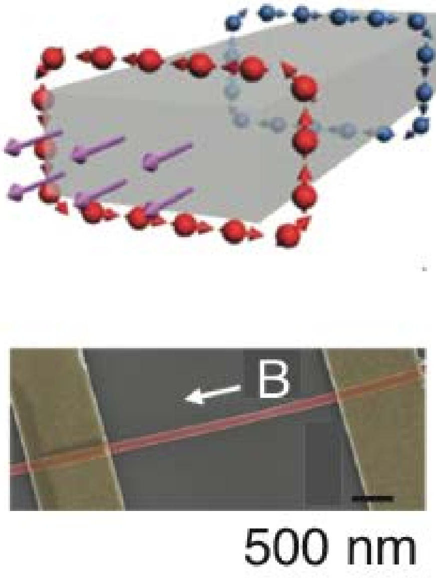


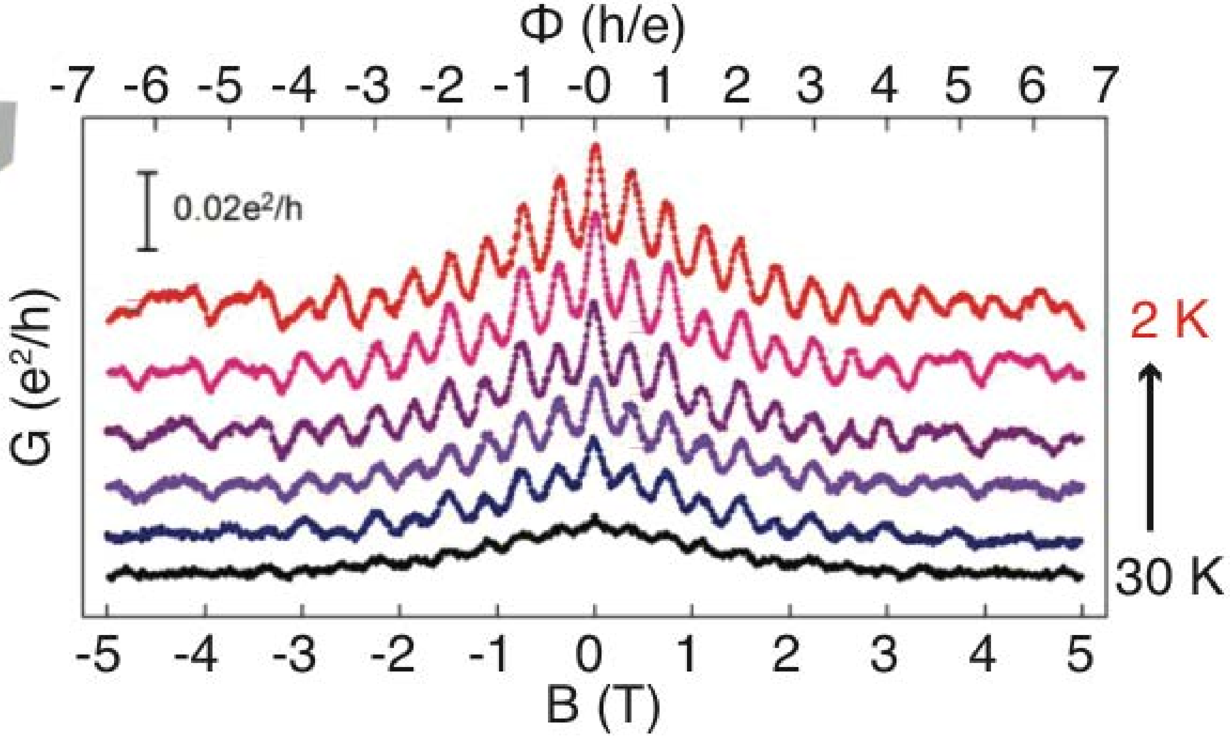


Nature Nanotech. 6, 705 (2011); Nano Lett. 14 2815 (2014)

1D Nanowire Interferometer

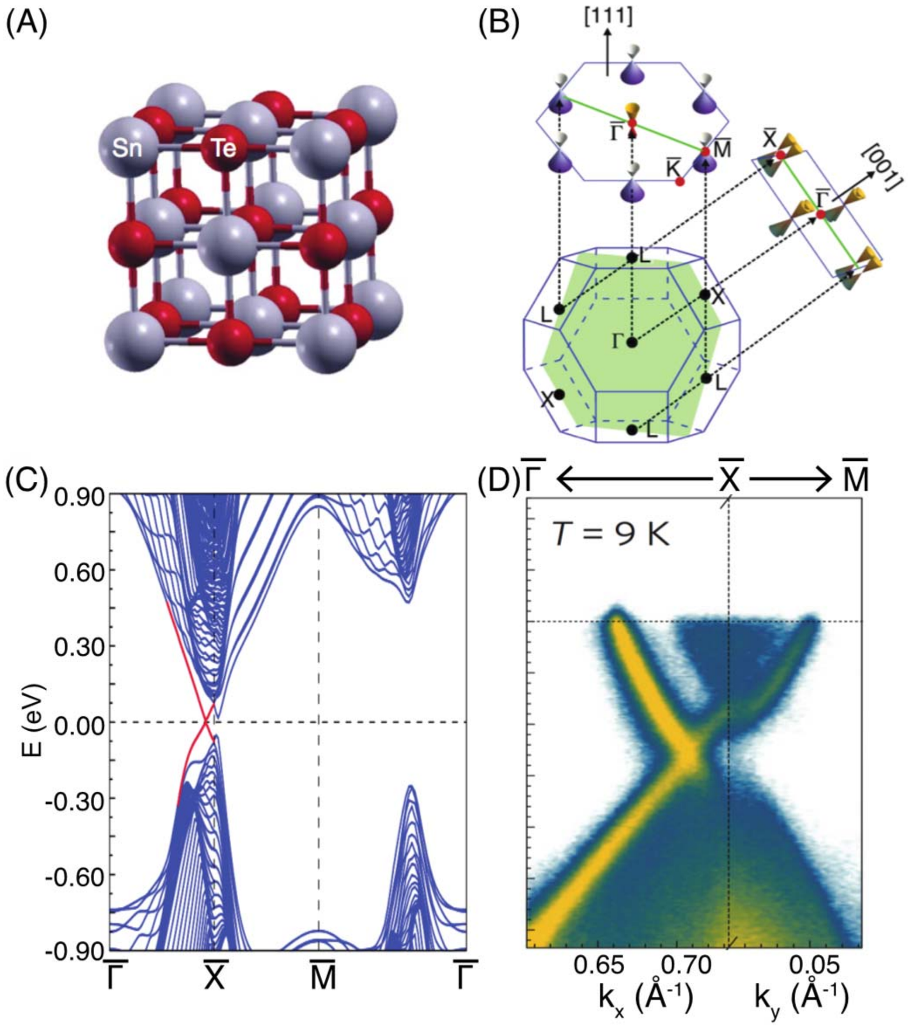
Aharonov Bohm oscillations in Bi_2Se_3 nanoribbons





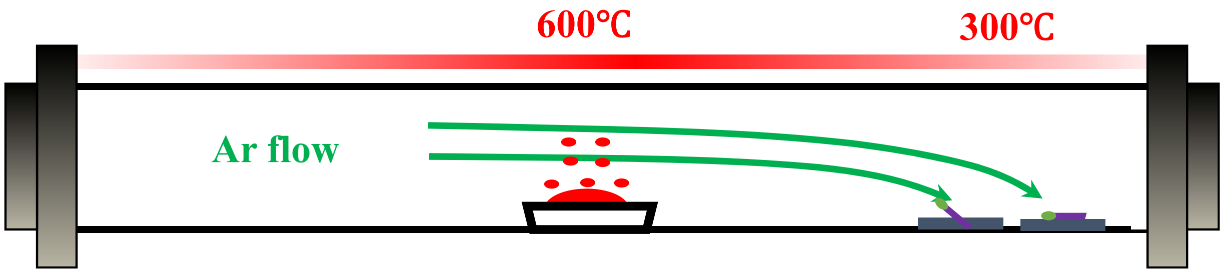
Nano Lett. 14, 2815 (2014)

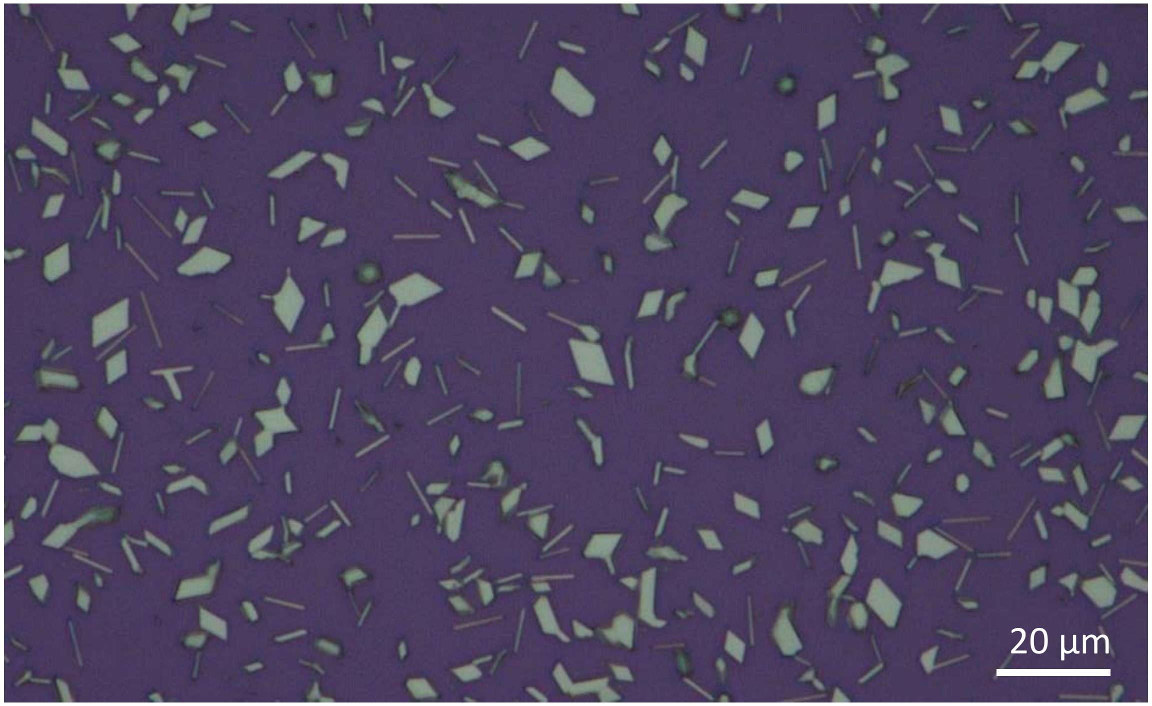
SnTe: Topological Crystalline Insulator



References:
Nat. Commun. 3:982 (2012)
Nat. Mater. 11, 1023 (2012)

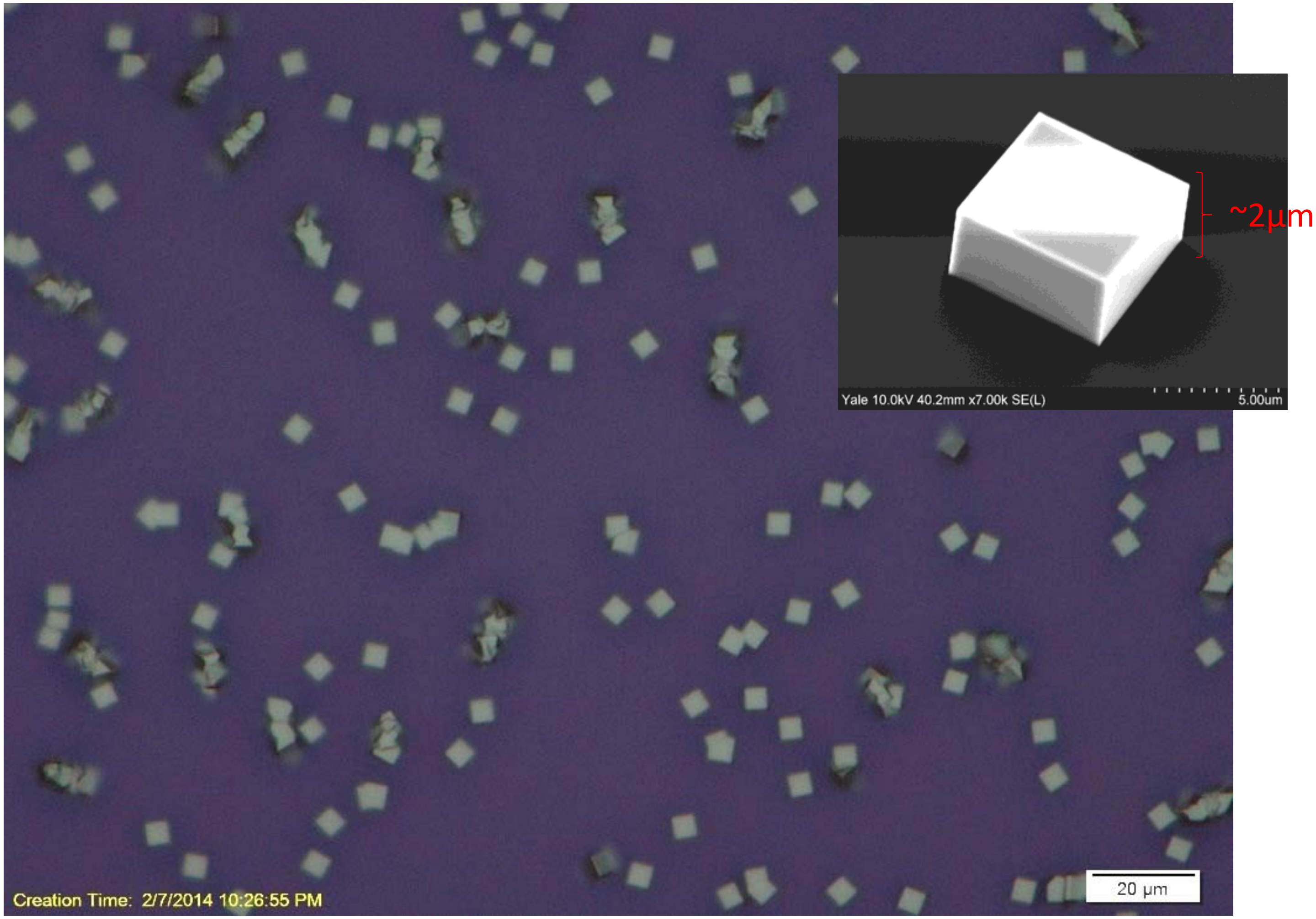
SnTe Nanostructure Growth



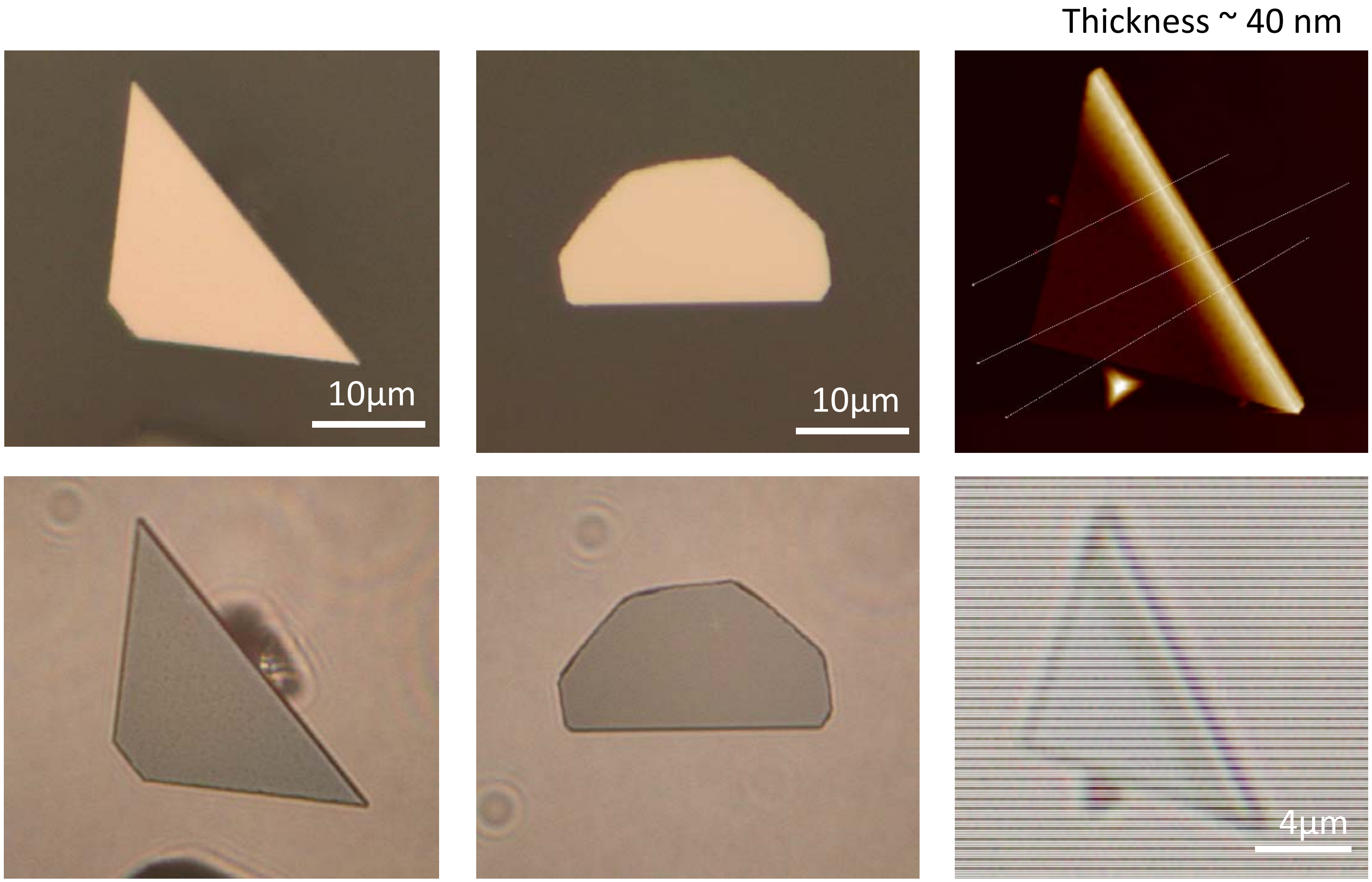


Nano Lett. 14 p.4183 (2014)

SnTe Nanoblocks on SiO_2 without Au Catalyst



Substrate Effects: SnTe grown on Mica



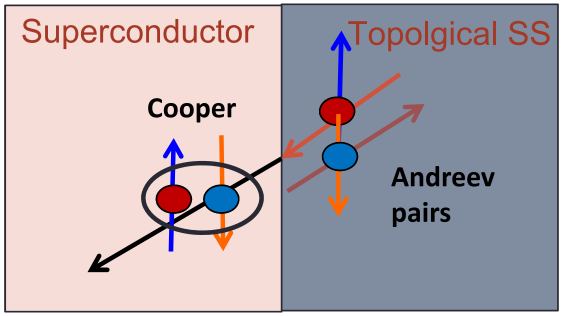
Topological Superconductors (TSCs)

Topological surface states + Superconductor correlations

⇓

Potential base system for a quantum information processor

Approach 1: Proximity-induced superconductivity
(Contacting TIs to superconducting metals to induce superconductivity to SS)

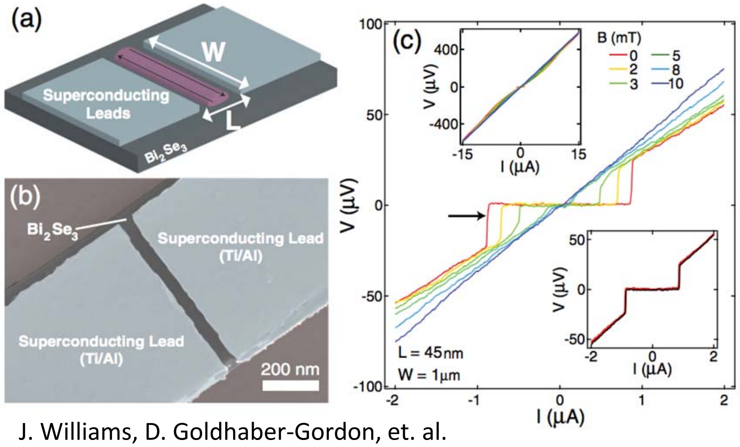


Superconducting proximity effect via Andreev refelction

Approach 2: Directly synthesize a bulk TSC

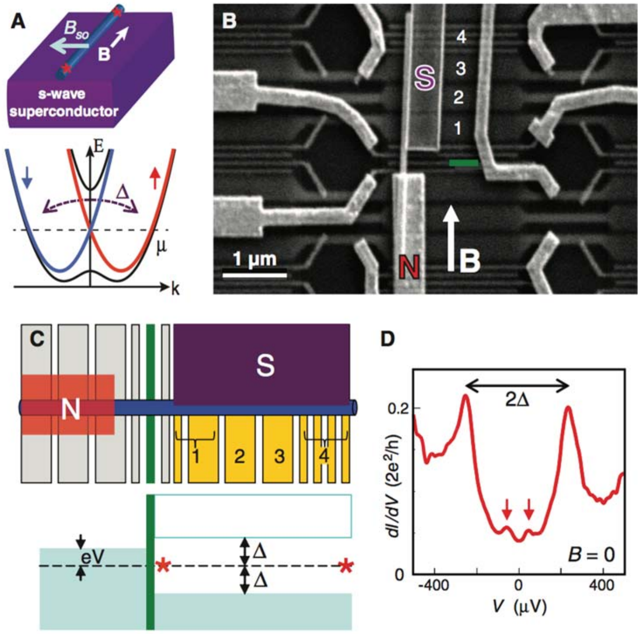
Examples based on Approach 1

TI - SC Josephson junctions



J. Williams, D. Goldhaber-Gordon, et. al.
PRL 109, 056803 (2012)

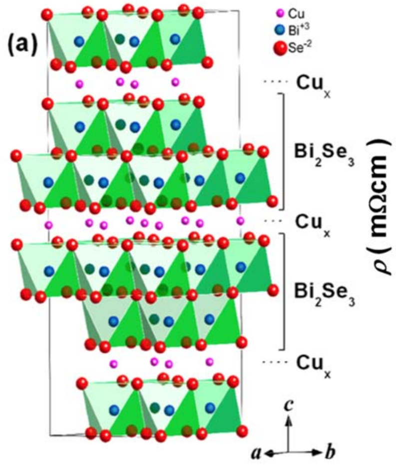
Semiconducting NW + SC contacts

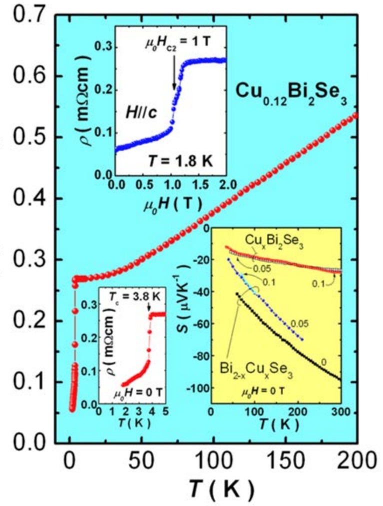


Kouwenhoven et. al., Science 336 p.1003 (2012)
Yazdani et. al., Science 346, p.6209 (2014)
Markus et. al., Nat. Nanotech 10, p.232 (2015)

Approach 2: Make TIs Superconducting

Cu-intercalated Bi_2Se_3



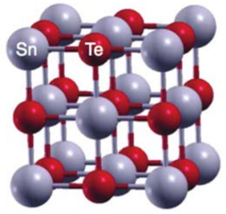


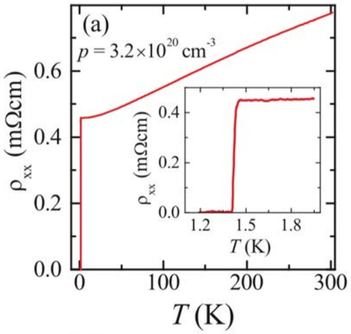
Intercalation: Sr, Tl, …

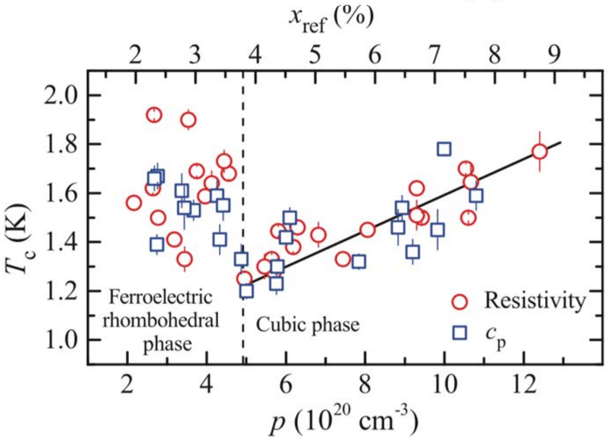
PRB 104, 057001 (2010), PRL 107, 217001 (2011)
JACS 137, 10512 (2015), …

JACS (2012), Nano Lett (2013), Nat. Commun. (2014)

In-doped SnTe

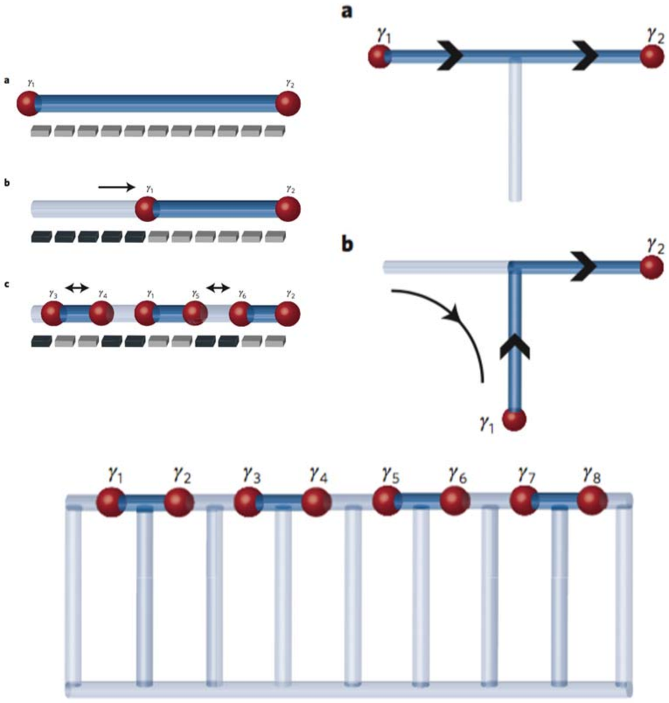


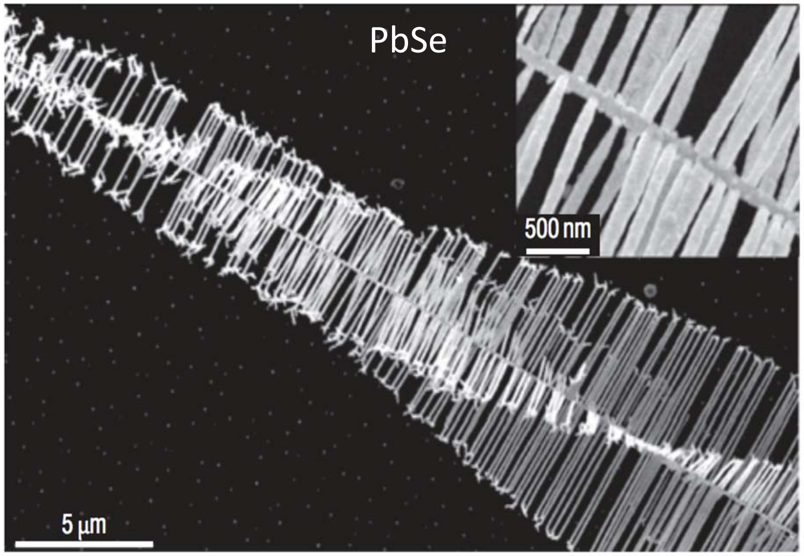




PRB 88, 140502 (2013), PRL 109, 217004 (2012),
PRL 110, 206804 (2013), PRB 93, 024520 (2016), …

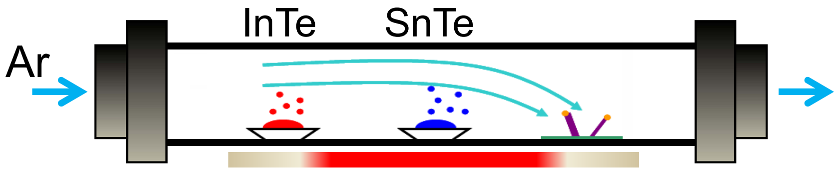
Quantum Processing in 1D Wire Networks



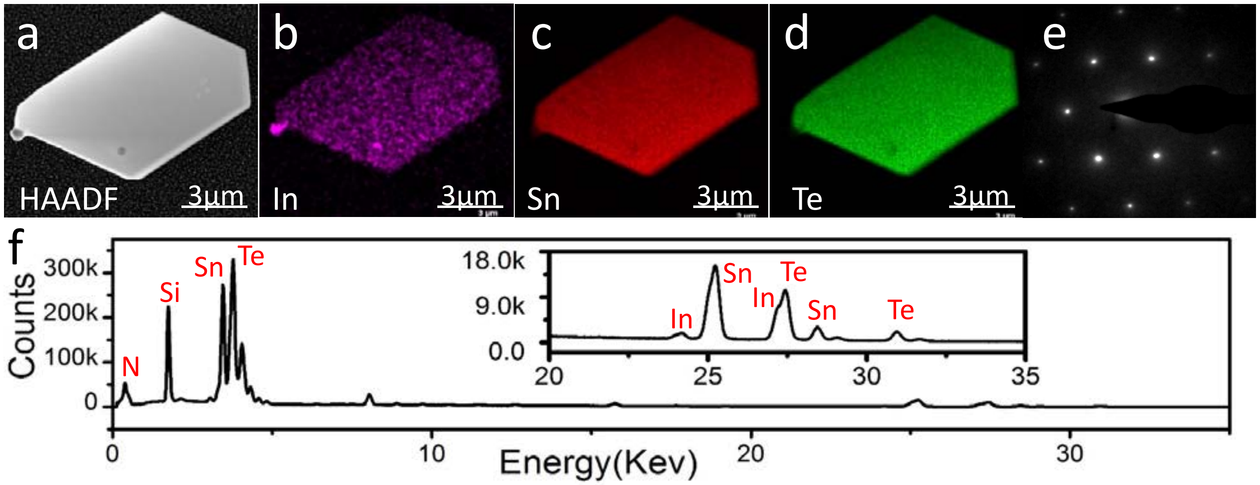


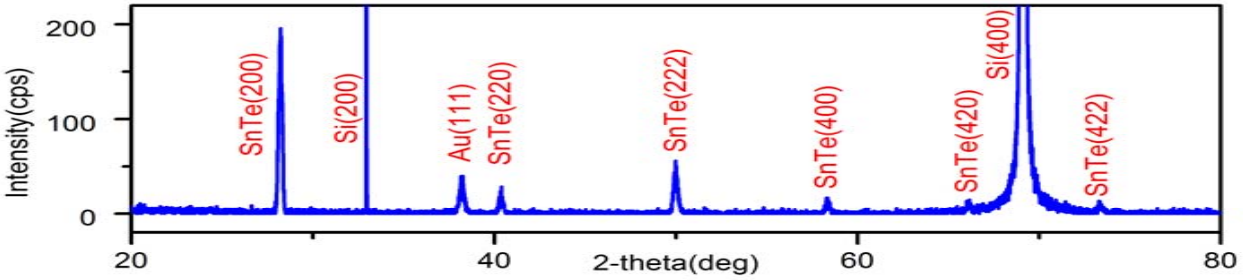
J. Alicea, P. A. Fisher, et. al, Nature Physics 7, 412 (2011)
J. Zhu, Y. Cui, et. al. , Nature Nanotech 3, 477 (2008)

In doping into SnTe Nanoplates

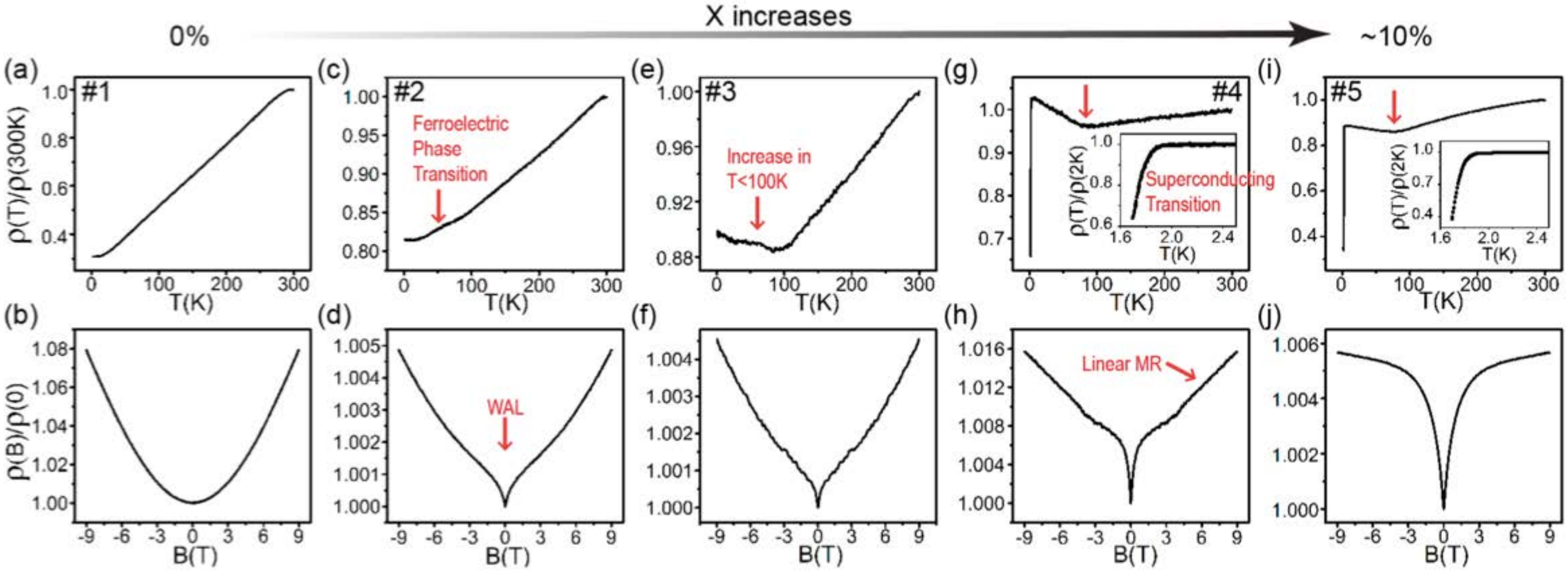


(111) In-doped SnTe Nanoplate



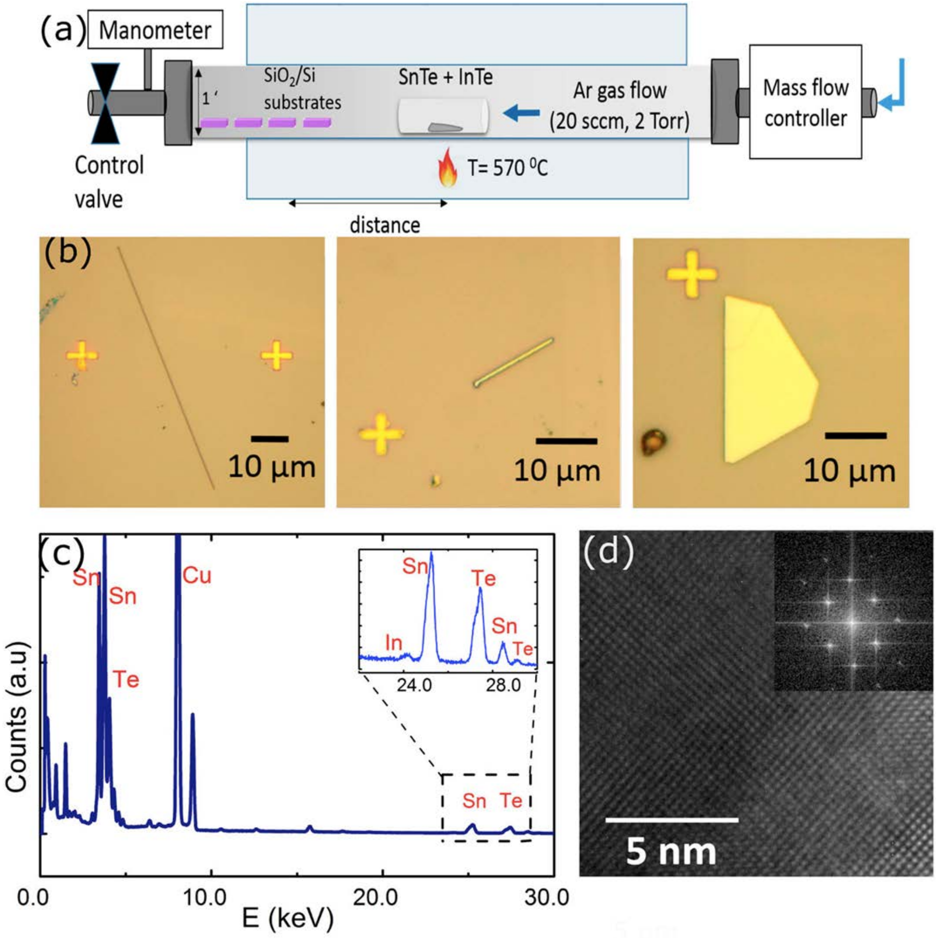


Transport Properties in $In_xSn_{1-x}Te$



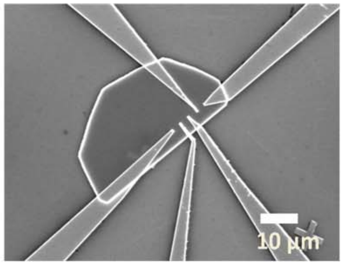
Nano Lett. 15 p.3827 – 3832 (2015)

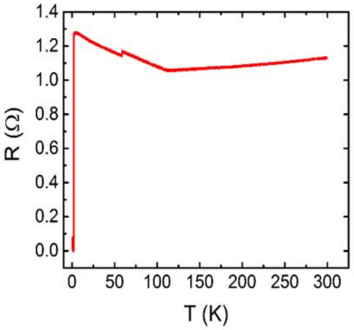
In-doped SnTe Nanowires

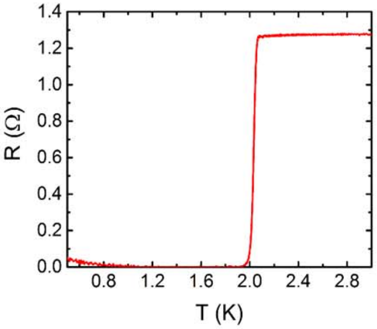


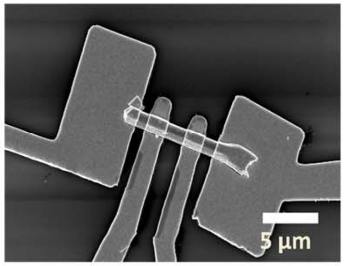
APL Materials 5, 076110 (2017)

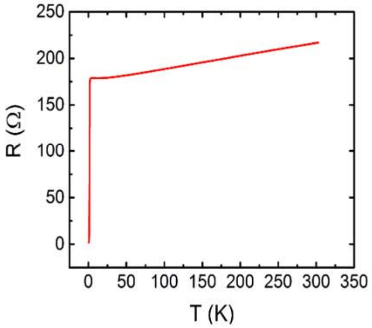
Morphology-dependent Superconducting Behavior

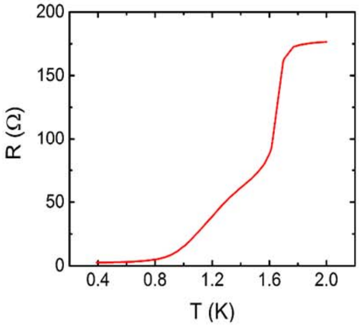


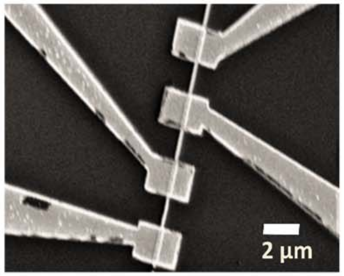


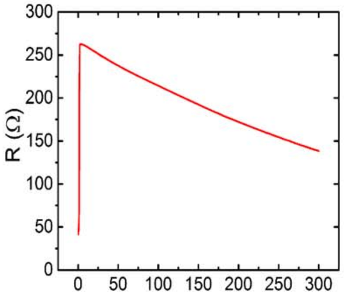


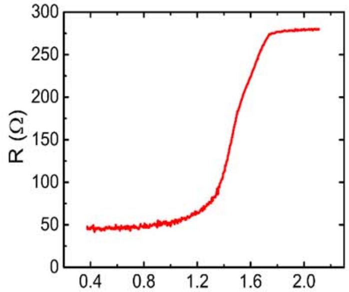








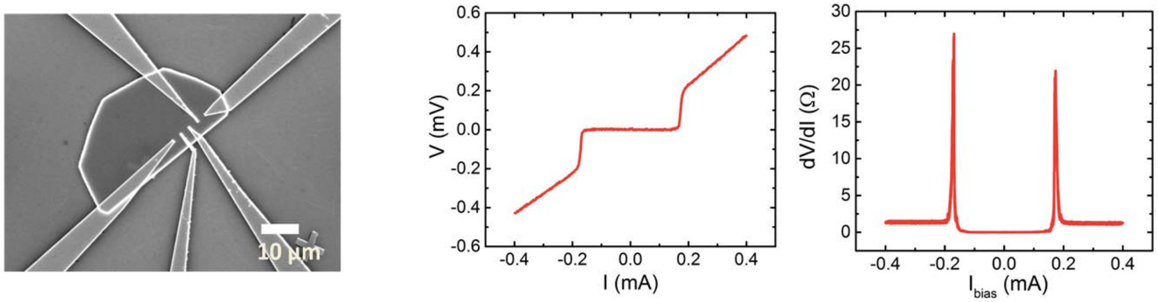




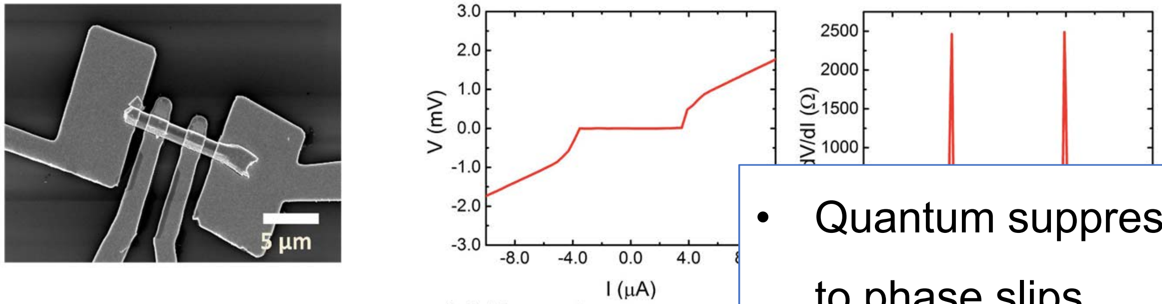
APL Materials 5, 076110 (2017)

Morphology-dependent Superconducting Behavior

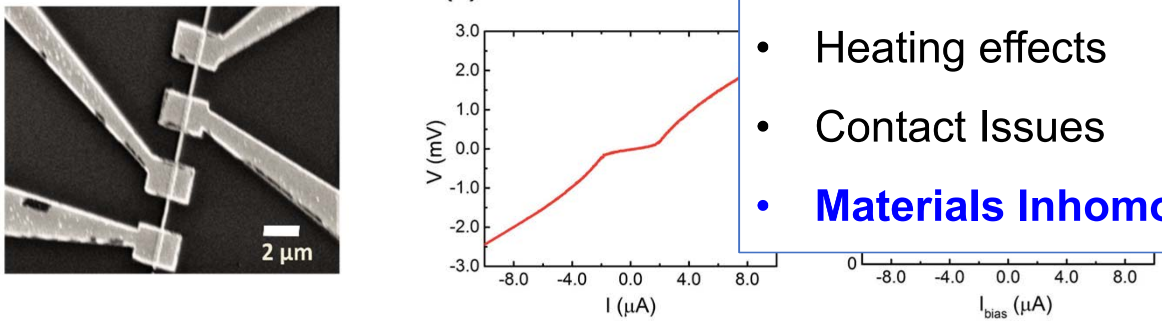
(a) Nanoplate



(b) Nanoribbon

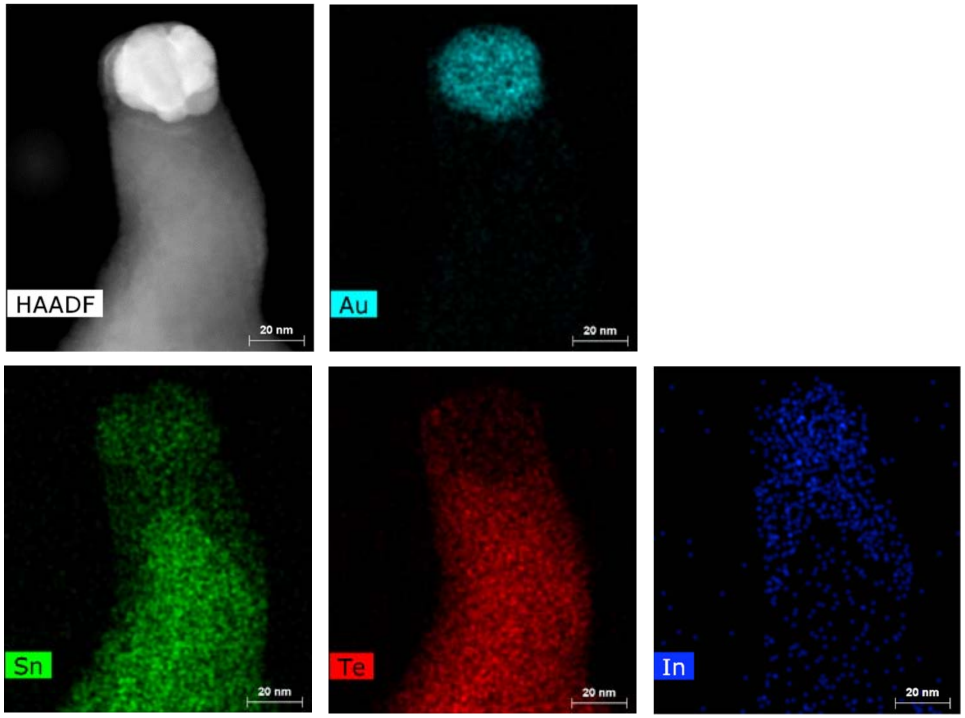


(c) Nanowire

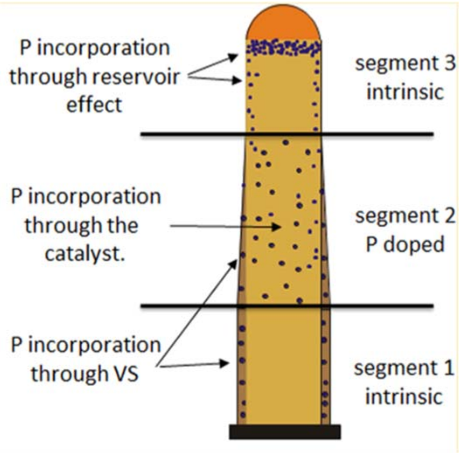


- Quantum suppression due to phase slips
- Heating effects
- Contact Issues
- **Materials Inhomogeneity**

Material Inhomogeneity: In Doping



P-doped Si Nanowires



Nano Lett. 13, 2598 (2013)

Overview

- Why Nanoscale Materials
  - Emergent properties (band engineering, surface properties)
  - Examples (quantum dots, carbon nanotubes, mechanical properties)
- Synthesis of Nanowires
  - Various growth methods
  - Vapor-liquid-solid growth
  - Doping / surface passivation
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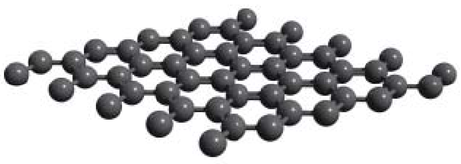
Why 2D Materials?

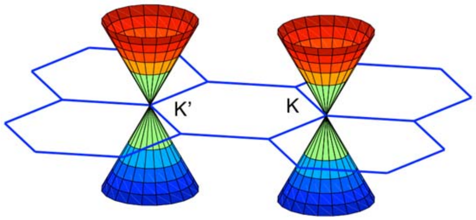
- New Physics
  - Dirac band dispersion in Graphene
- New Materials
  - Graphene, Silicene, …
- Ultimate thickness in 2D technology
  - Bandgap engineering via thickness
  - Flexible, transparent electronics
  - 2D materials can potentially be integrated into existing CMOS technology

2D Materials Are Interesting

Graphene

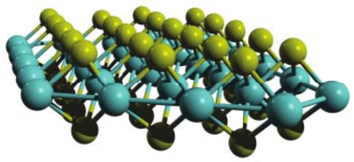


Dirac Physics

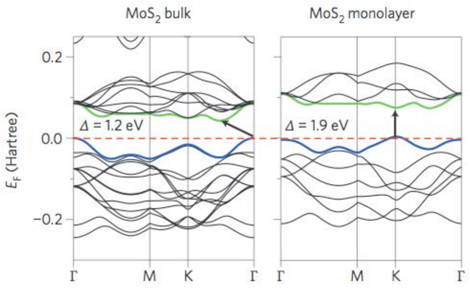


- Transparent electrodes
- Conducting layer for energy applications

MoS$_2$



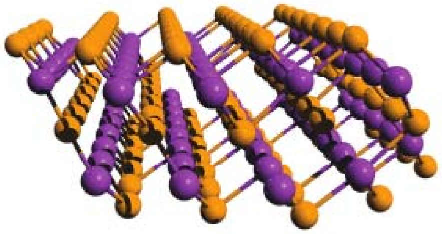
Indirect → Direct Semiconductor



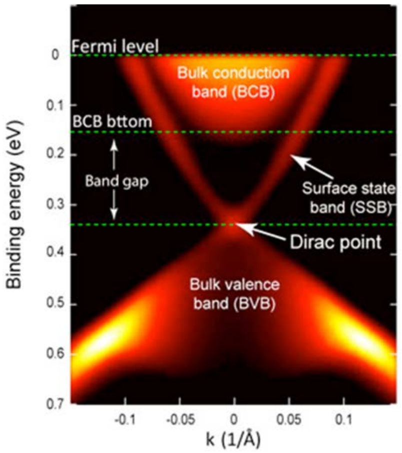
PRB 83, 245213 (2011)

- Field-effect transistor
- Hydrogen evolution reaction catalyst

Bi$_2$Se$_3$



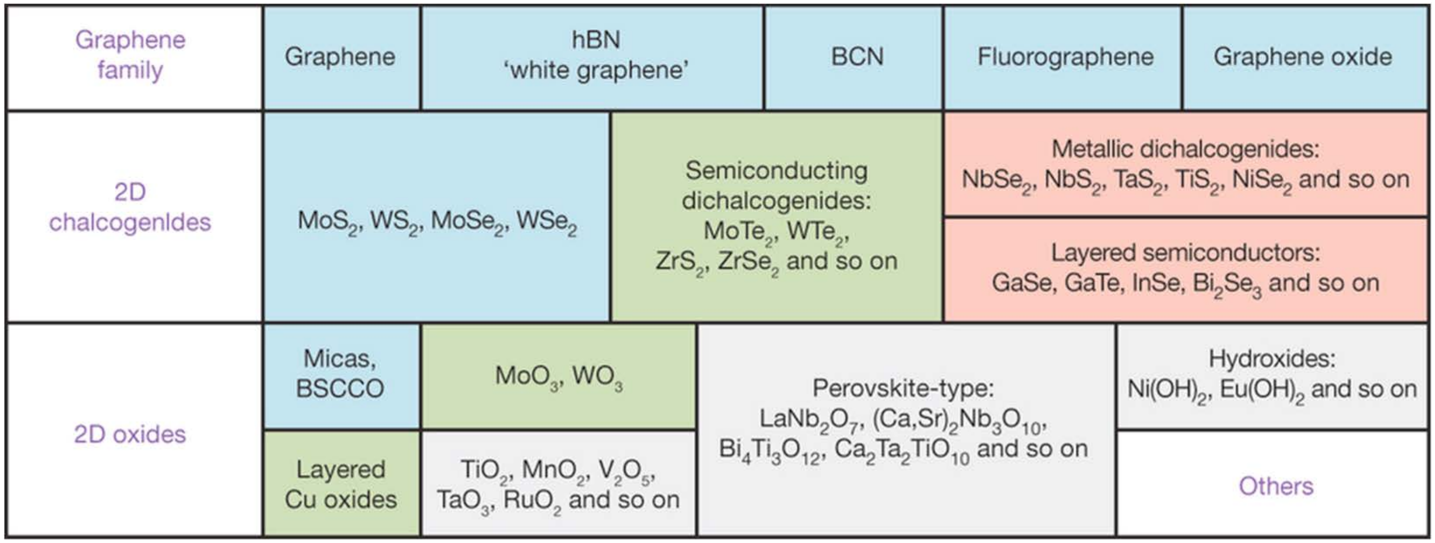
Topological Insulator



Science 329, 659 (2010)

2D Materials Choice

Topological Insulators: Bi_2Se_3, Bi_2Te_3, …

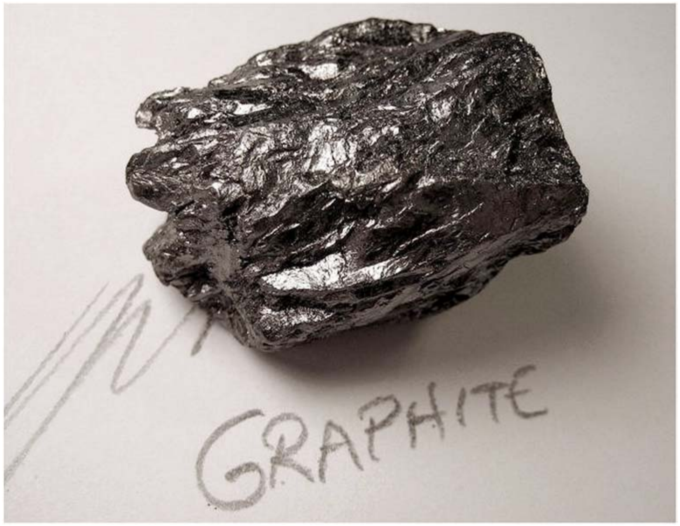


Graphene family	Graphene hBN ‘white graphene’ BCN Fluorographene Graphene oxide
2D chalcogenides	MoS_2, WS_2, $MoSe_2$, WSe_2 Semiconducting dichalcogenides: $MoTe_2$, WTe_2, ZrS_2, $ZrSe_2$ and so on Metallic dichalcogenides: $NbSe_2$, NbS_2, TaS_2, TiS_2, $NiSe_2$ and so on Layered semiconductors: GaSe, GaTe, InSe, Bi_2Se_3 and so on
2D oxides	Micas, BSCCO MoO_3, WO_3 Layered Cu oxides TiO_2, MnO_2, V_2O_5, TaO_3, RuO_2 and so on Perovskite-type: $LaNb_2O_7$, $(Ca,Sr)_2Nb_3O_{10}$, $Bi_4Ti_3O_{12}$, $Ca_2Ta_2TiO_{10}$ and so on Hydroxides: $Ni(OH)_2$, $Eu(OH)_2$ and so on Others

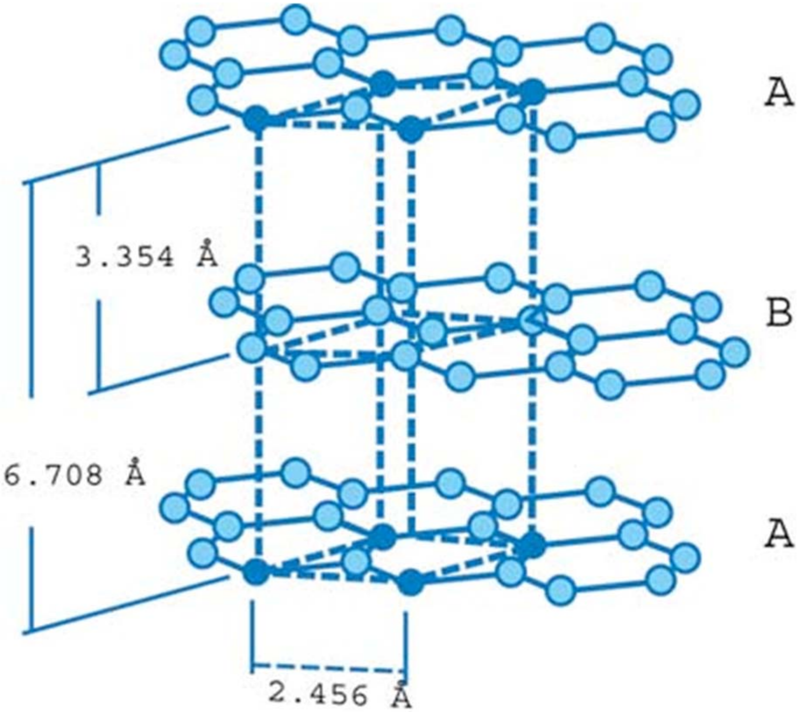
Geim & Grigorieva,
Nature 499, 419–425 (25 July 2013)

Top Down Approach: From Graphite

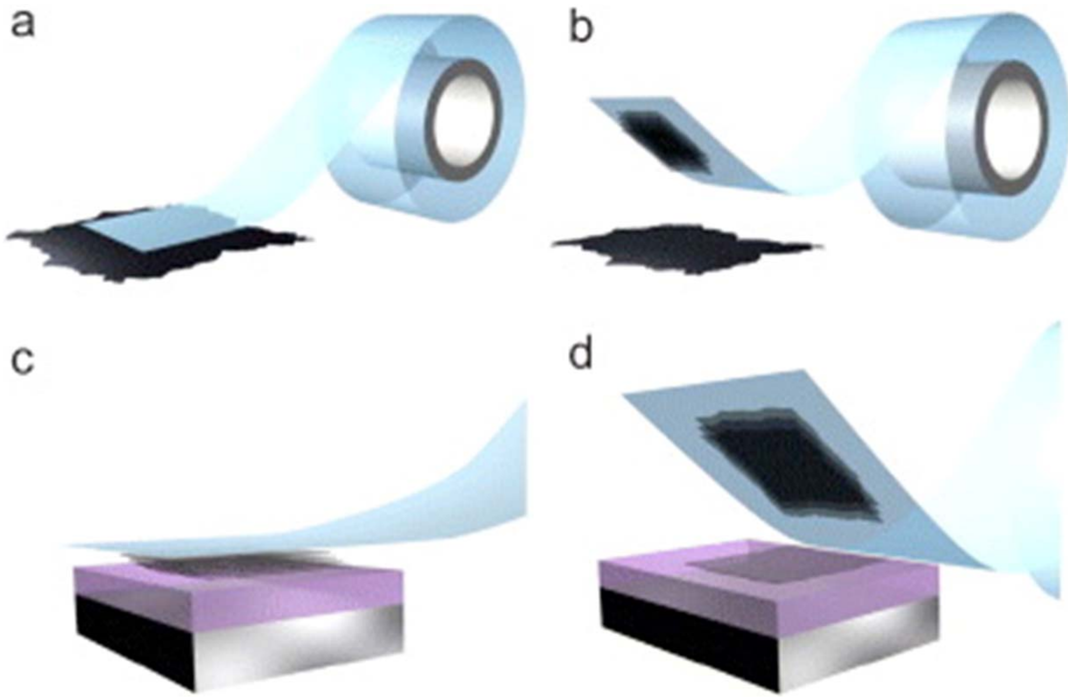
Graphite: Layered Crystal Structure



- Mechanical Exfoliation
- Chemical Exfoliation
- Direct Growth
    - CVD, Evaporation of SiC



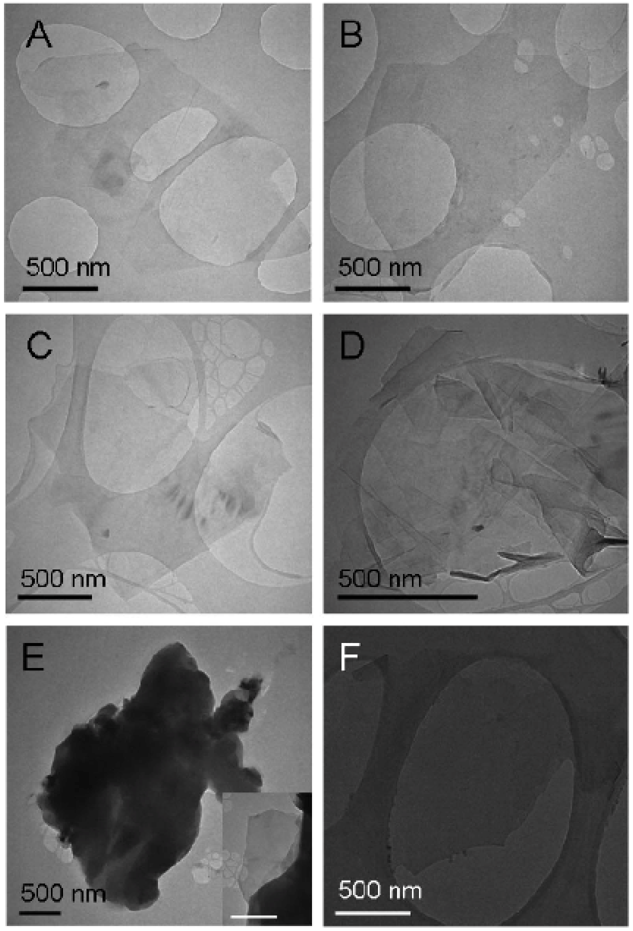
Mechanical Exfoliation



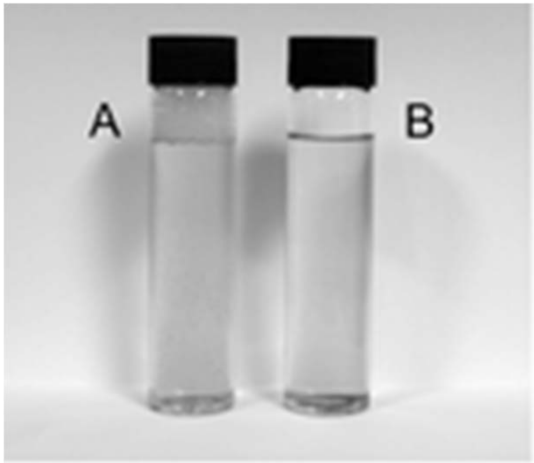
Physica Scripta **2012**, 014006

http://www.youtube.com/watch?v=waO020l25sU

Chemical Exfoliation of Graphite

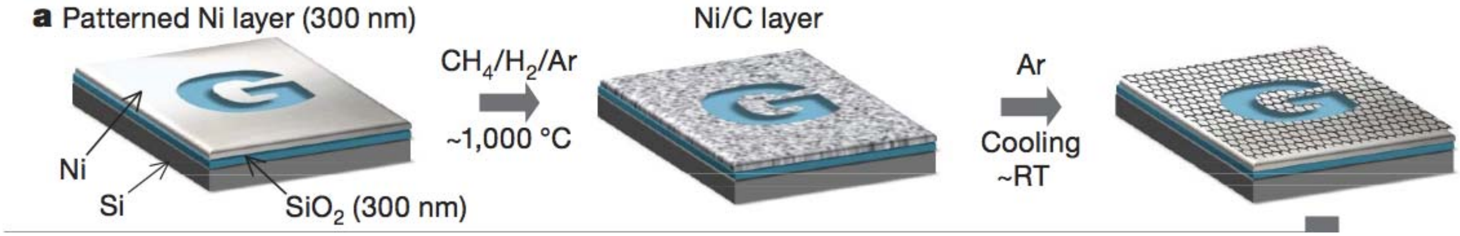


Surfactant-Water Solution

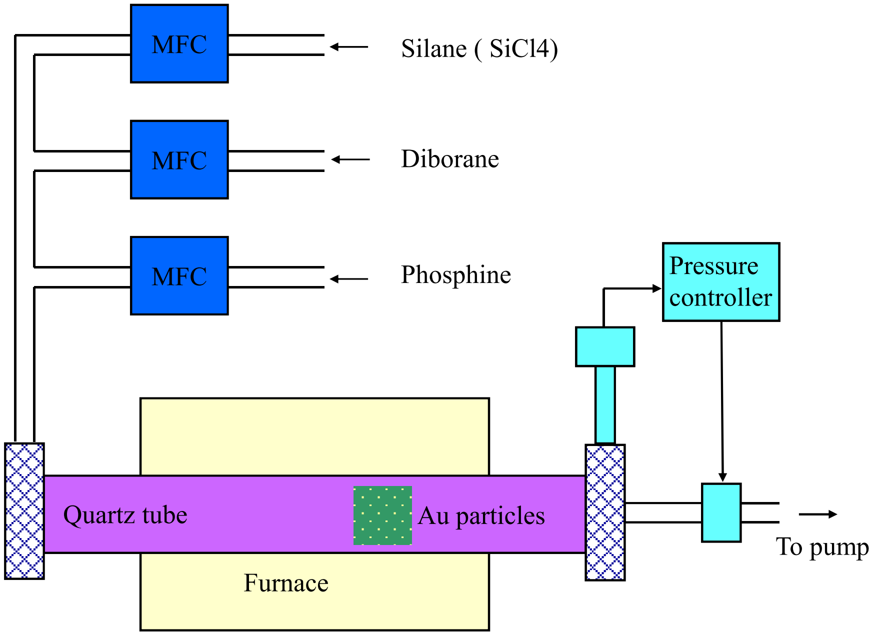


JACS 131, p.3611 (2009)

CVD Growth of Graphene

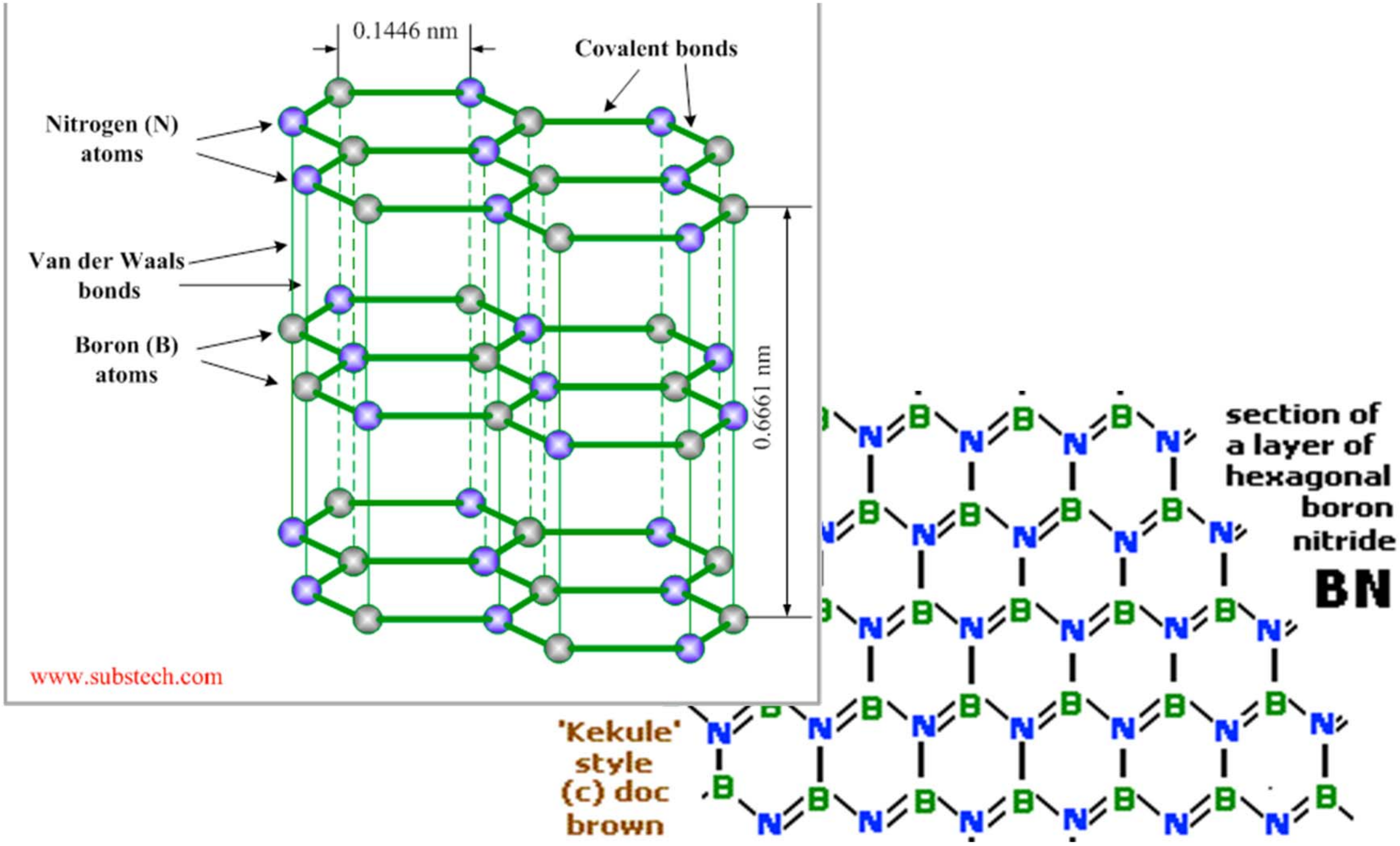


Nature 457, p.706 (2009)

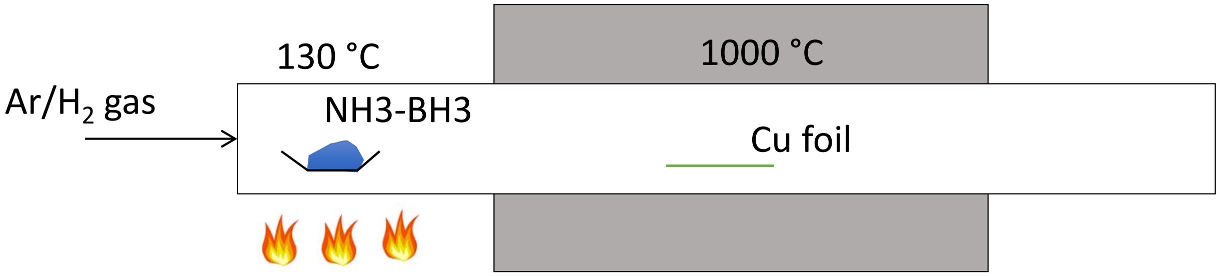


- Cu
- Pt
- Ni
- …

Hexagonal Boron Nitride



CVD of Boron Nitride

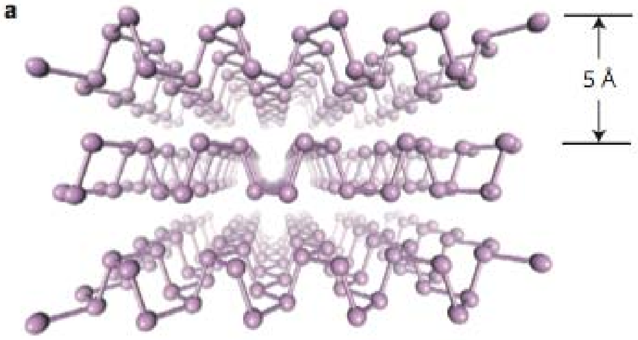


- tube furnace with a fused quartz processing tube.
- A copper foil with 25 µm thickness was used as substrate.

1) The Cu foil was quick washed by nitric acid and deionized water.
2) It was placed in the center of a furnace, annealed at 600 °C for 20 min in Ar/H2 (15 vol % H2, 85 vol % argon) flow with 500 sccm.
3) The furnace was gradually heated up to 1000 °C in 40 min.
4) Ammonia borane (NH3−BH3) was sublimated at 120−130 °C by using a heating belt and then carried into the reaction region by Ar/H2 gas glow.
5) During the growth process, Ar/H2 flow was kept as 200 sccm. The typical growth time is 30−60 min.
6) After growth, the furnace was cooled down to room temperature quickly.

Nano Letters 10, p.3209 (2010)

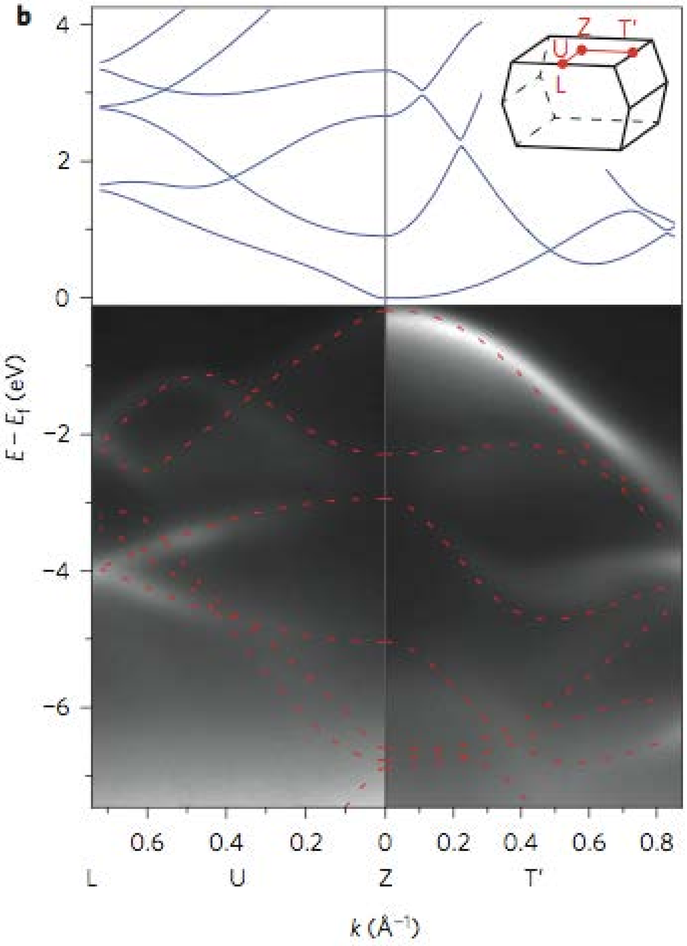
2D, Layered Black Phosphorus



Two atomic sheets of Phosphorus atoms make a sheet.

Unlike graphene, which is a metal (no intrinsic bandgap), BP has a bandgap.
In addition, mobility of BP is relatively high.
: ~ 1,000 cm^2/Vs

- Not as high as graphene
- But much higher than MoS_2 (~ 100 cm^2/Vs)



Nature Nanotechnology, 9 p.372 (2014)

CVD Growth of Black Phosphorus Thin Film

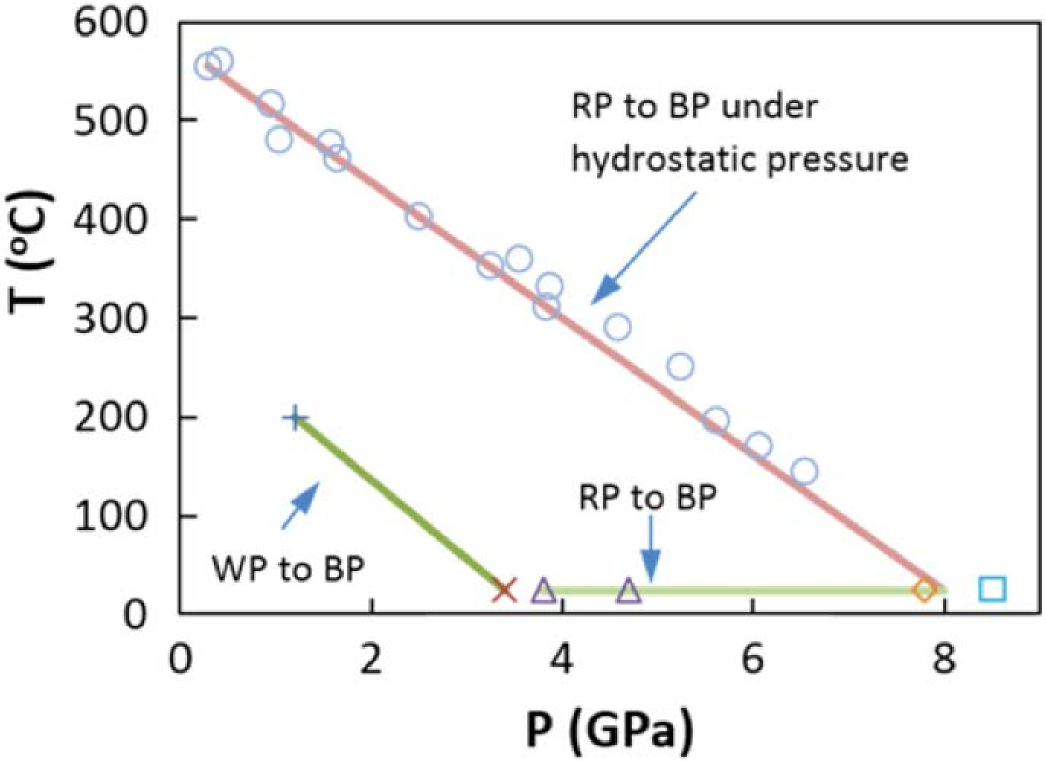
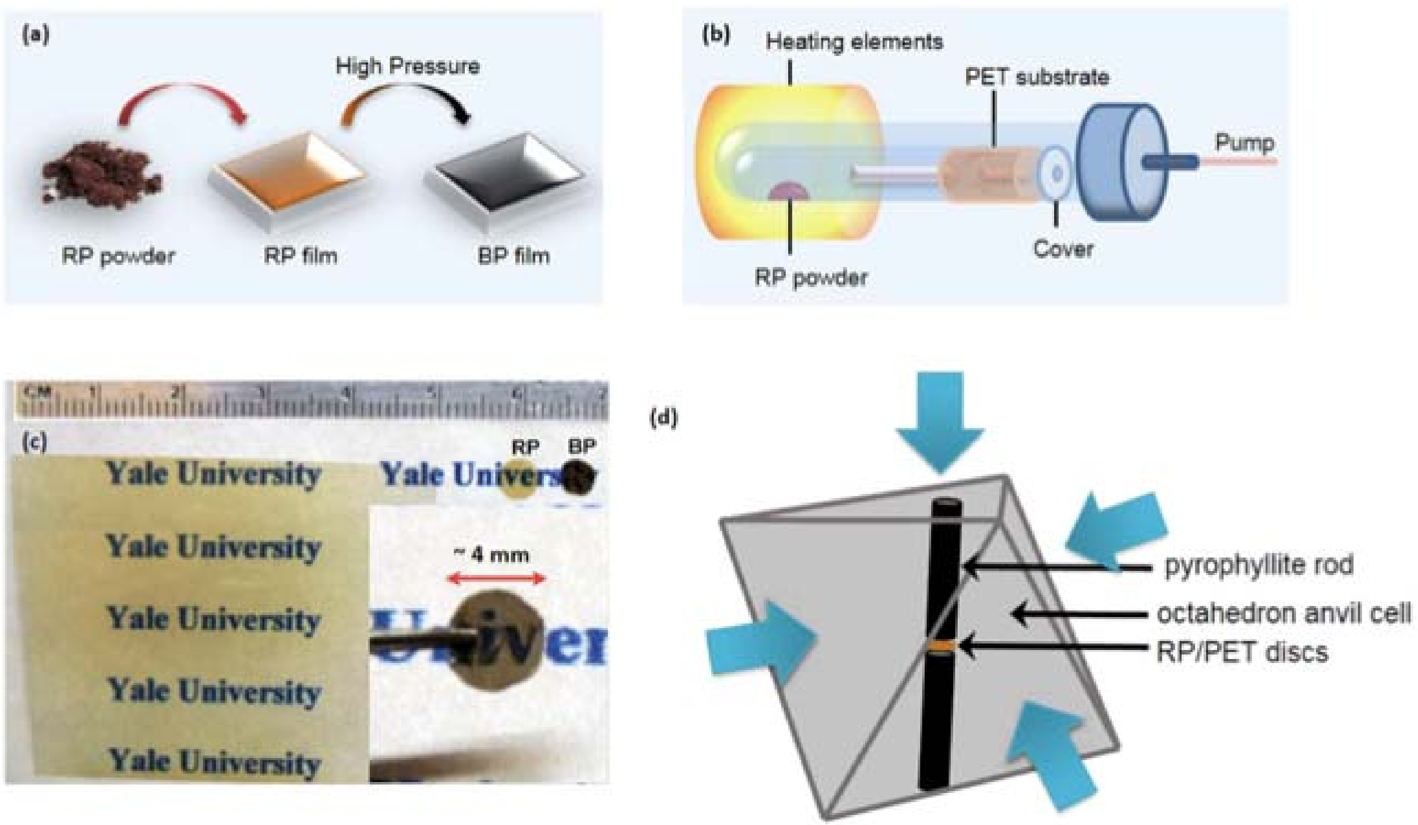


Figure 1. Criteria for the conversion of BP from WP or RP at various pressures and temperatures summarized from the literature: +[14], ×[15], △[18, 19], □[16], ◇[17], ○[20].

2D Mater. 2 (2015) 031002

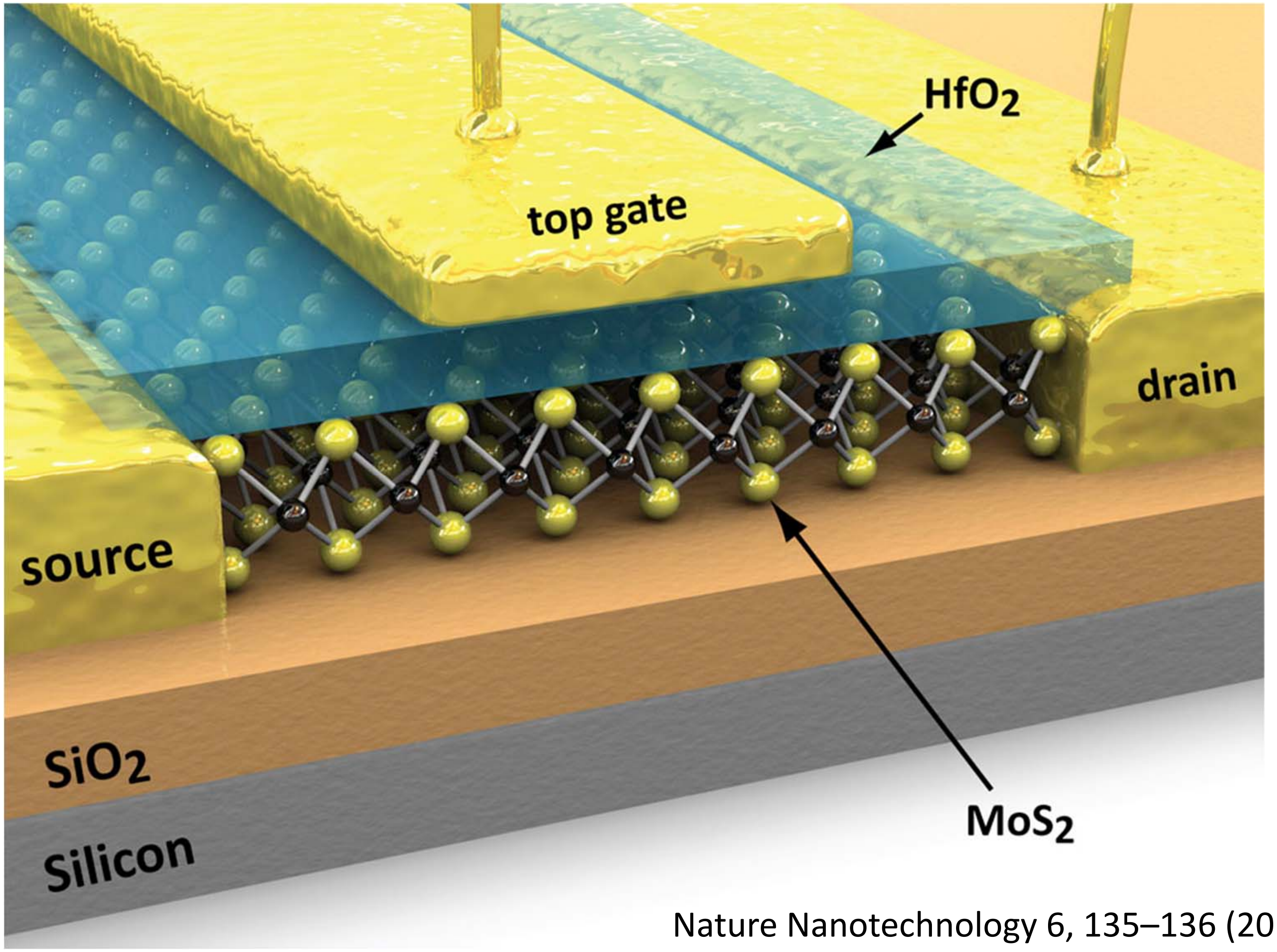
CVD Growth of Black Phosphorus Thin Film



B) Heat red phosphorus powder. At the colder zone, flexible PET (polyethylene terephthalate).
D) Pressurizing Diamond Anvil Cell
C) Large, converted Black Phosphorus Film

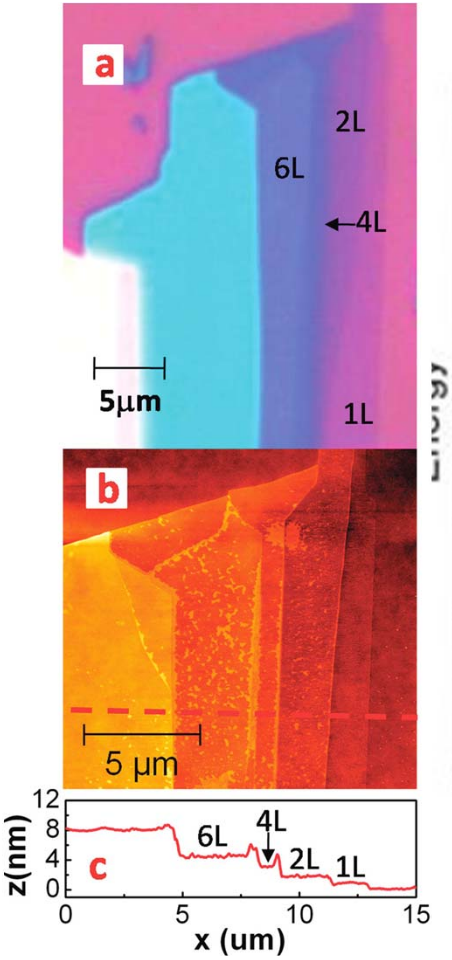
2D Mater. 2 (2015) 031002

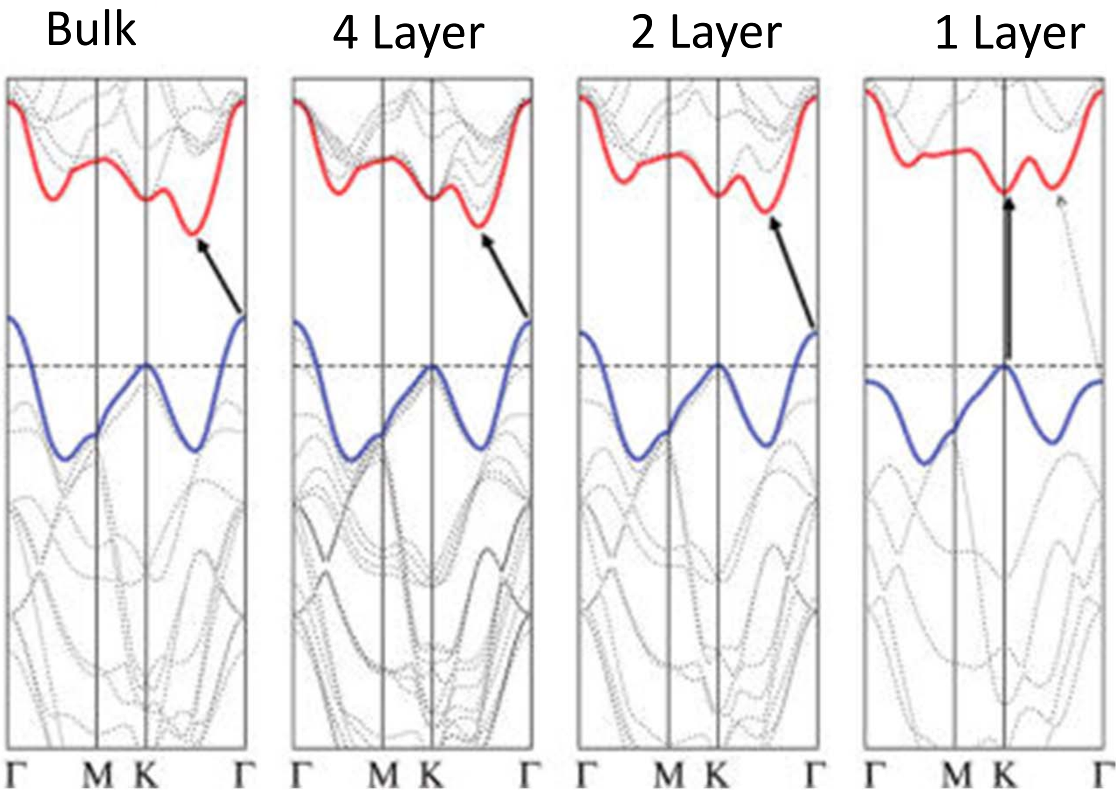
MoS_2



Nature Nanotechnology 6, 135–136 (2011)

MoS$_2$: Indirect to Direct Semiconductor




Bulk

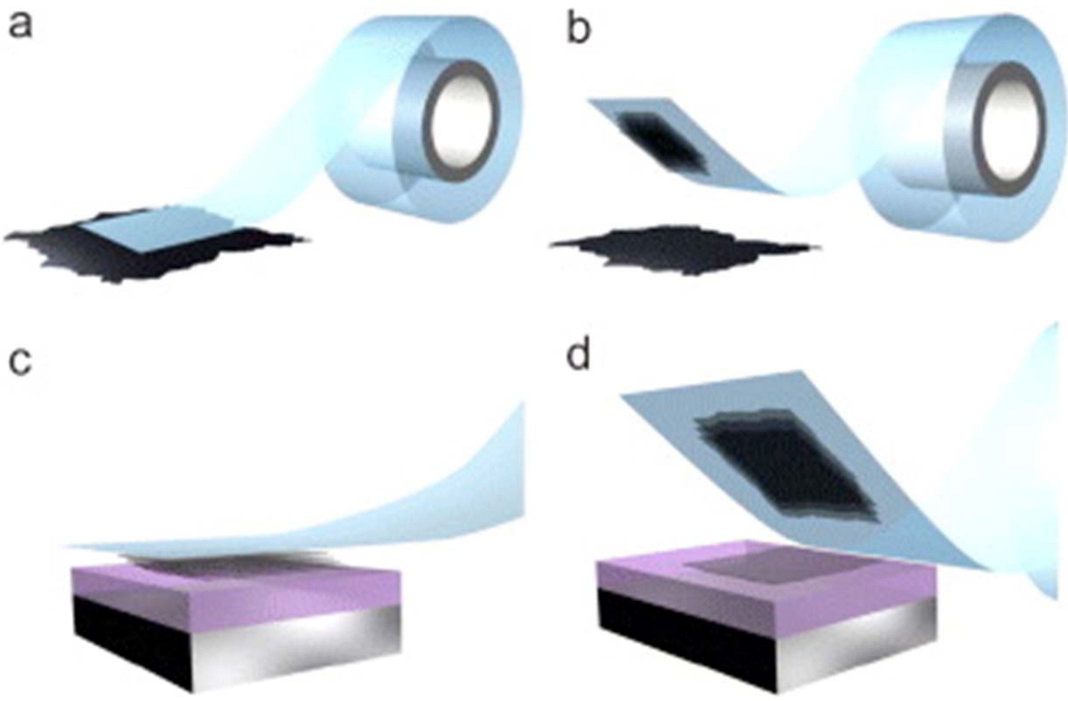
4 Layer

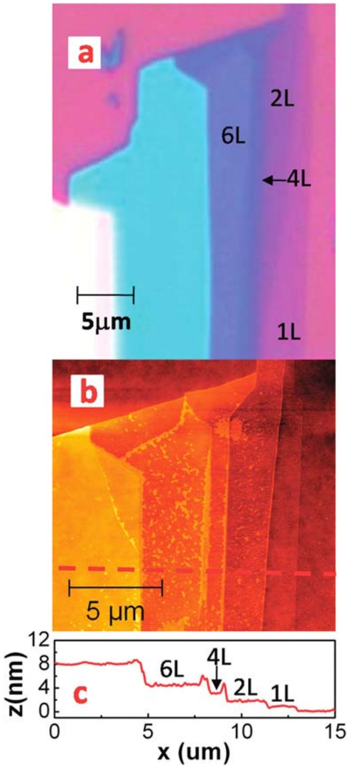
2 Layer

1 Layer

Nano Letters 10, p.1271 (2010)

Mechanical Exfoliation

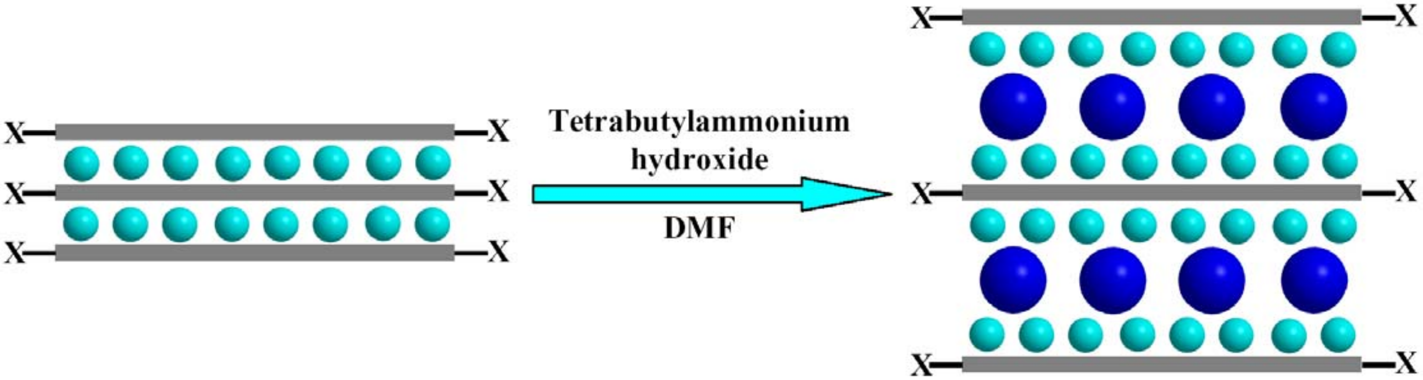




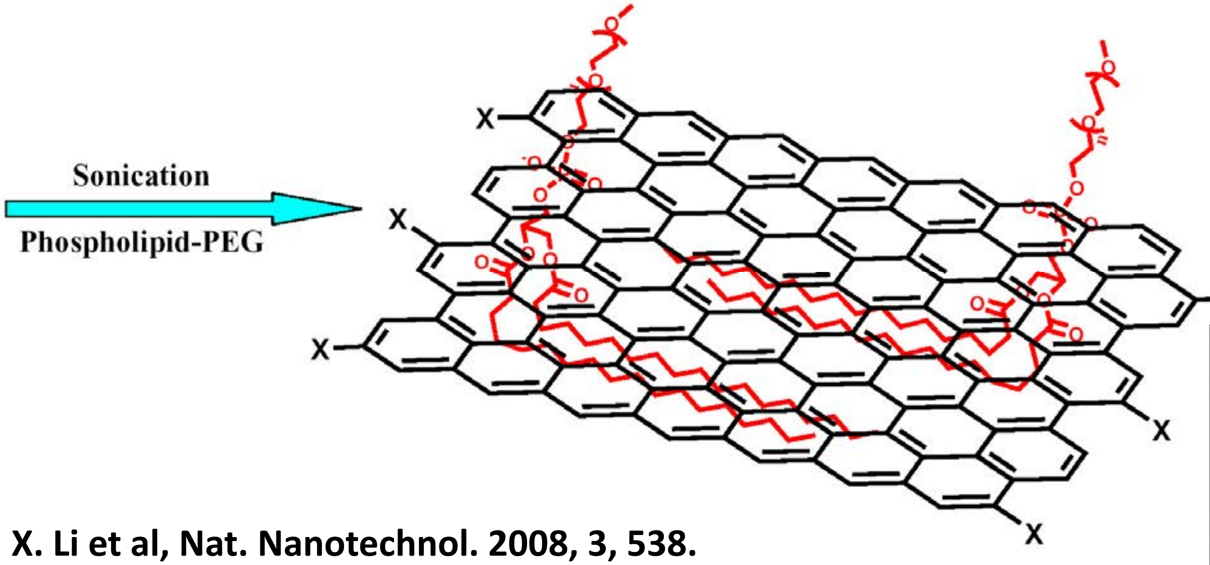
Physica Scripta **2012**, 014006

http://www.youtube.com/watch?v=waO020l25sU

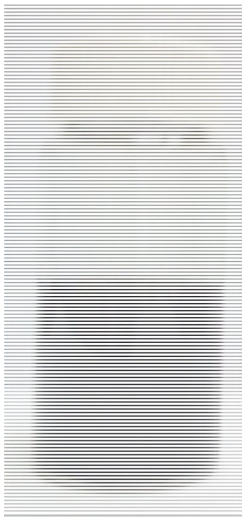
Chemical exfoliation


Tetrabutylammonium hydroxide

DMF


Sonication

Phospholipid-PEG

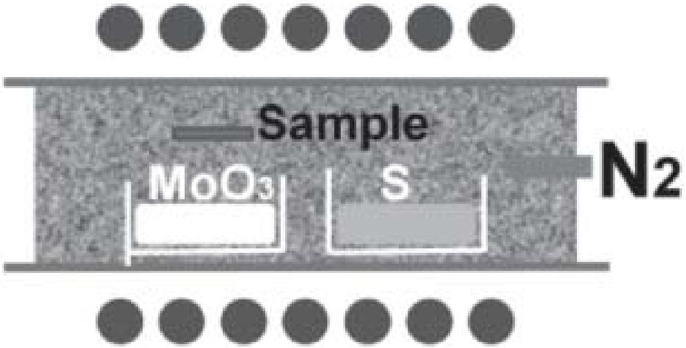


X. Li et al, Nat. Nanotechnol. 2008, 3, 538.

H. Wang et al, Nano Res. 2009, 2, 336.

H. Wang et al, JACS 2010, 132, 3270.

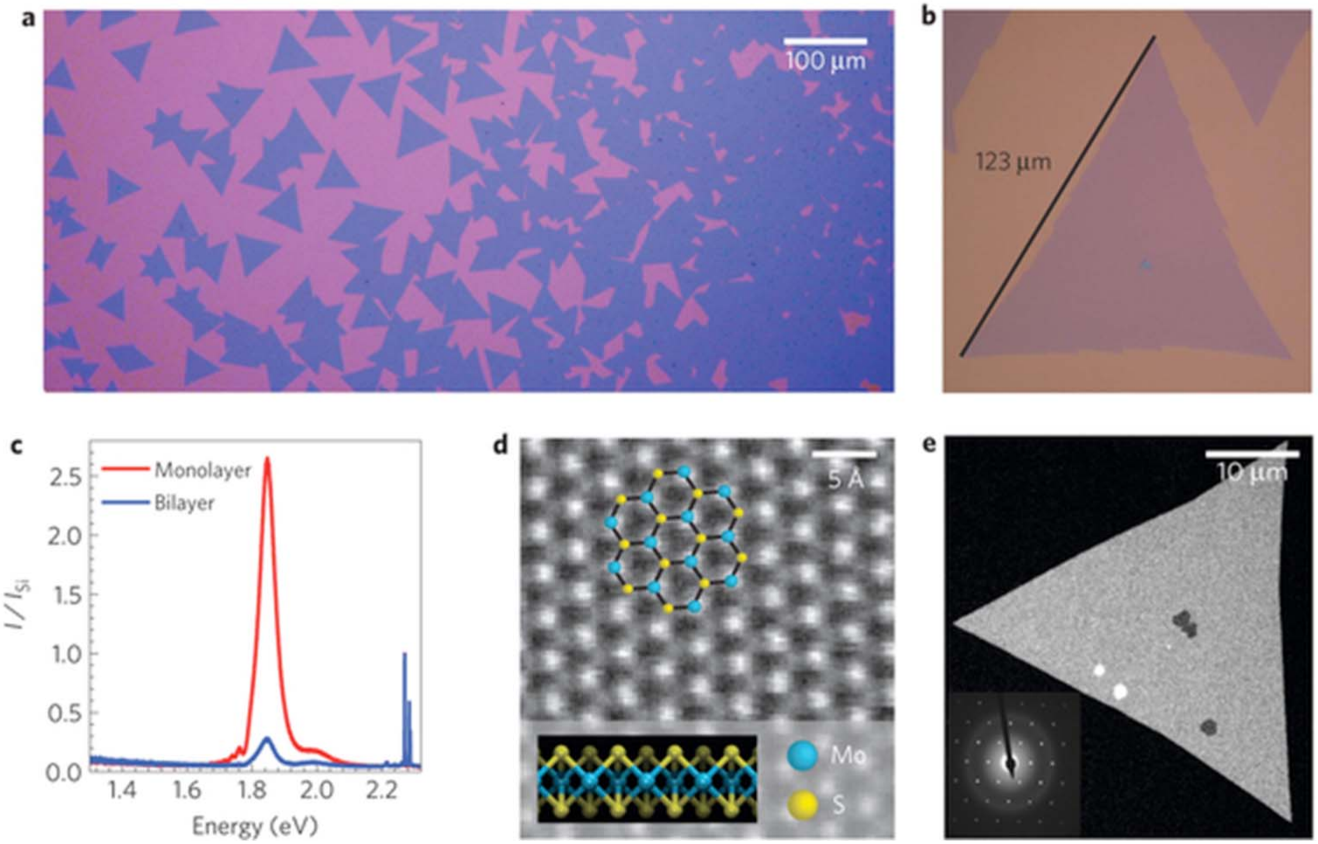
CVD Growth of MoS_2 Using MoO_3 powder



1) The MoO_3 powder was placed in a ceramic boat and the SiO_2/Si substrate was faced down and mounted on the top of boat.
2) A separate ceramic boat with sulfur powder was placed next to the MoO_3 powder.
3) During the synthesis of MoS_2 sheets, the reaction chamber was heated to 650 °C in a nitrogen environment.
4) At such a high temperature, MoO_3 powder was reduced by the sulfur vapor to form volatile suboxide MoO_{3-x}.
5) These suboxide compounds diffused to the substrate and further reacted with sulfur vapor to grow MoS_2 films.

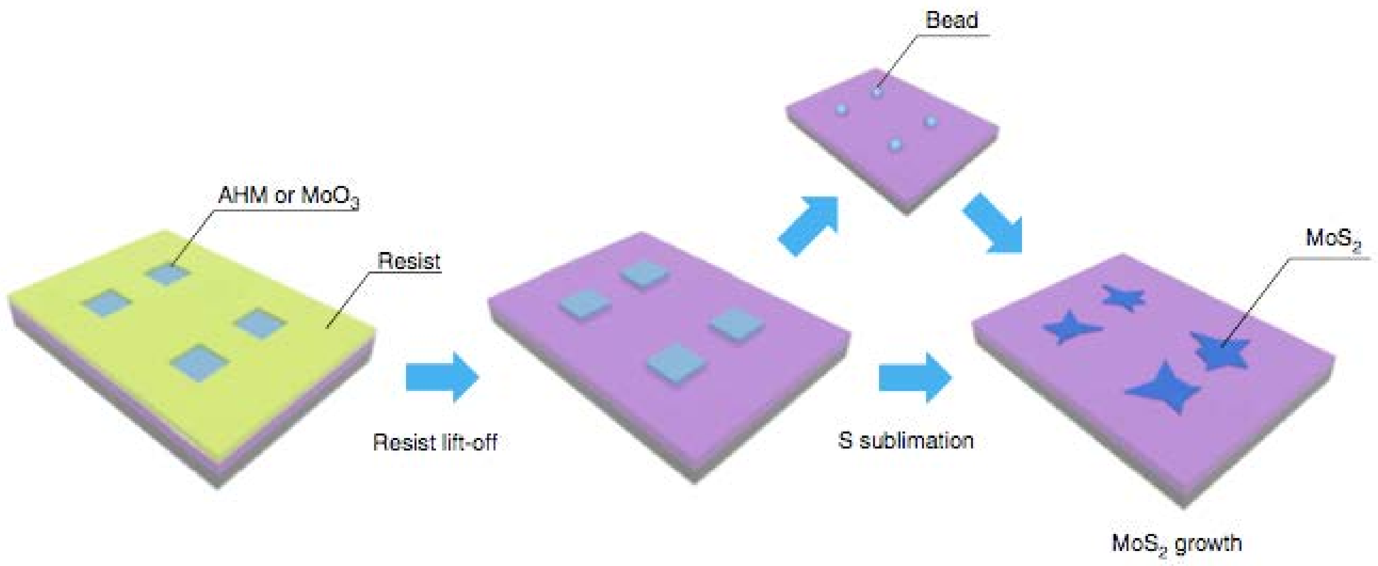
Adv. Mater. 24, p.2320 (2012)

MoS_2 using MoO_3 powder



Nat. Mater. 12, p.554 (2013)

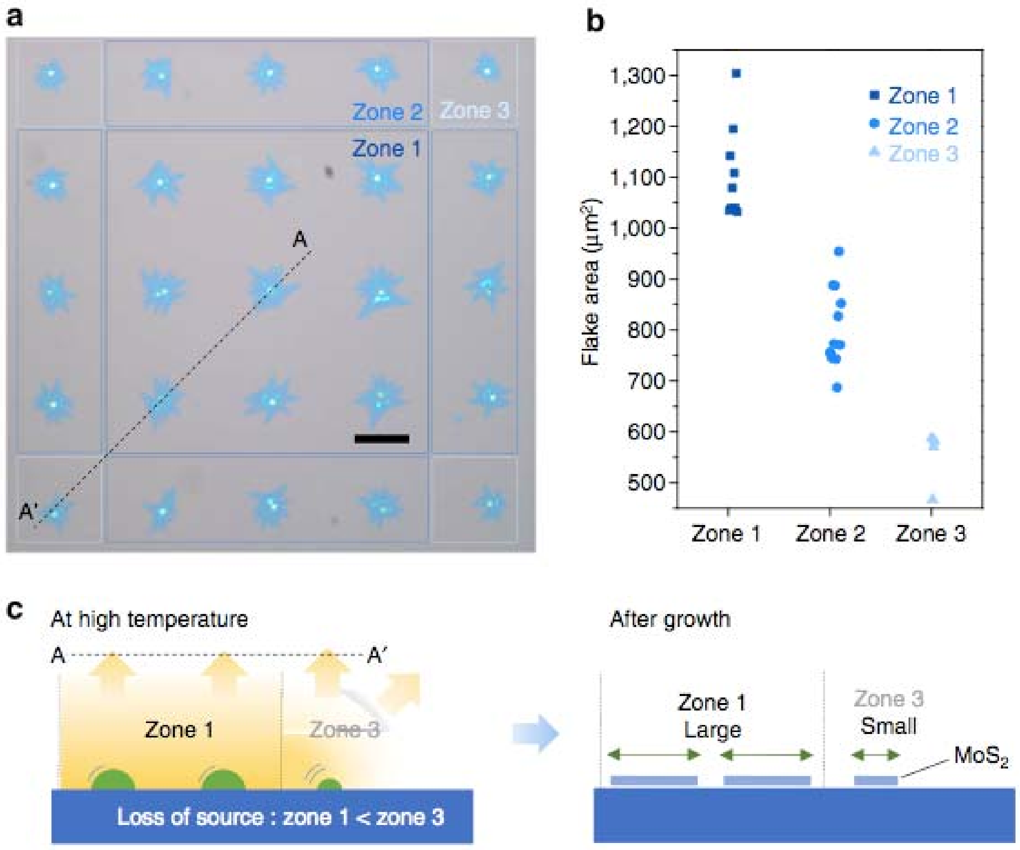
Growth of MoS_2 at Controlled Locations



1) Wells are locally created by conventional photolithography
2) Wells are filled with precursors (MoO_3 powder or Ammonium heptamolybdate ($(NH_4)_6Mo_7O_{24}*4H_2O$))
3) The photoresist is then removed
4) Sulrfurize the substrate (Evaporation of Sulfur powder)
5) Growth of MoS_2 at the specified well locations.

Nature Communications 6:6128 (2015)

Growth of MoS_2 at Controlled Locations

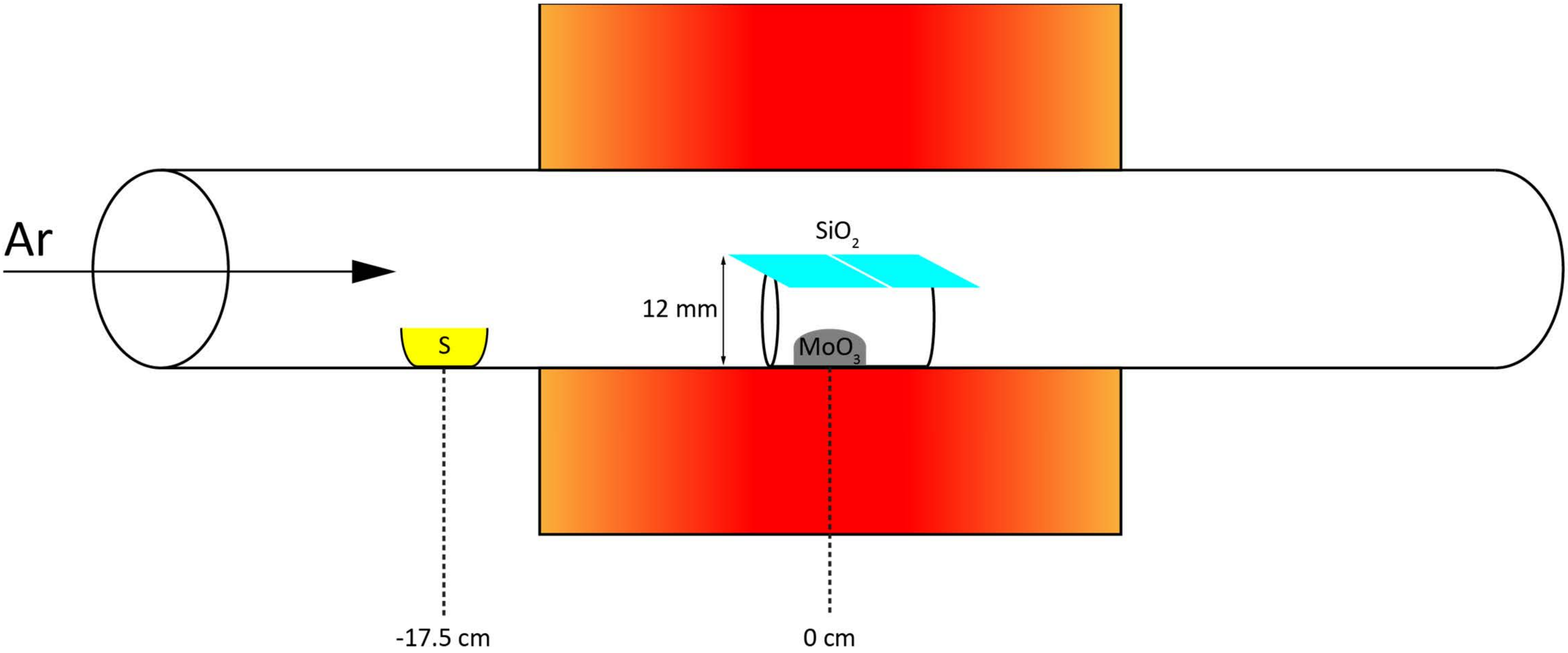


A,b) MoS_2 flake size depends on the temperature profile and the vapor pressure difference across the substrate.

: Larger flakes in the center of the substrate compared to the edge

Nature Communications 6:6128 (2015)

This CVD growth is sensitive to Mo:S vapor ratio



CVD Growth of MoS_2

- Sulfur must be present at a 3.5:1 stoichiometric ratio to Mo to fully sulfurize MoO_3 to MoS_2

- Loading S at a ratio >> 3.5:1 is necessary to ensure the reaction goes to completion because the intermediates are stable

$$2MoO_3 + S \rightleftharpoons 2MoO_2 + SO_2$$

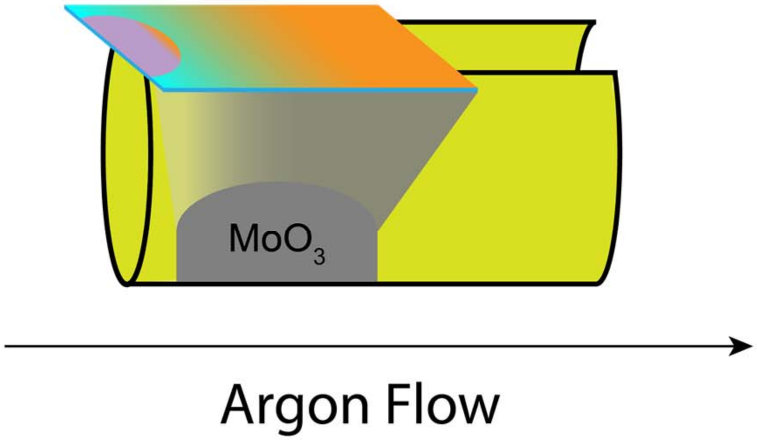
$$2MoO_2 + 5S \rightleftharpoons 2MoOS_2 + SO_2$$

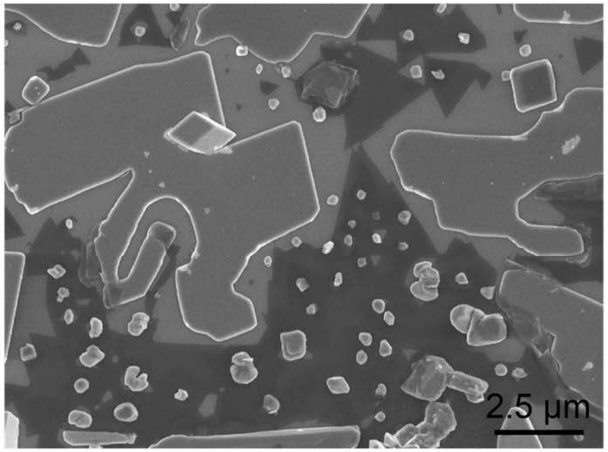
$$2MoOS_2 + S \rightleftharpoons 2MoS_2 + SO_2$$

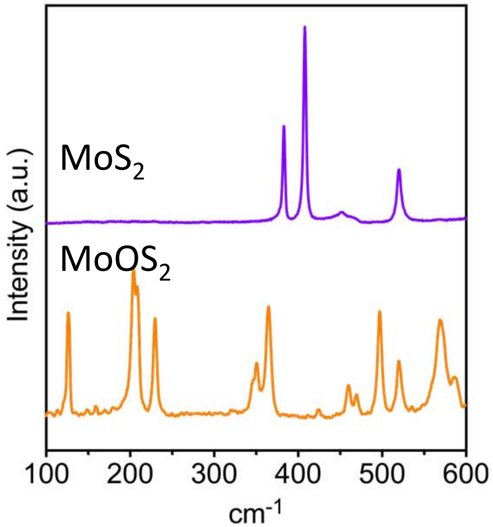
$$2MoO_3 + 7S \rightleftharpoons 2MoS_2 + 3SO_2$$

T. Weber, *et al.*, *J. Phys. Chem.* 100, 1996.
X. Li, *et al.* S. *Chem.-A Eur. J.* 9, 2003.
S. Najmaei, *et al*. *Nat. Mater.* 12, 2013.

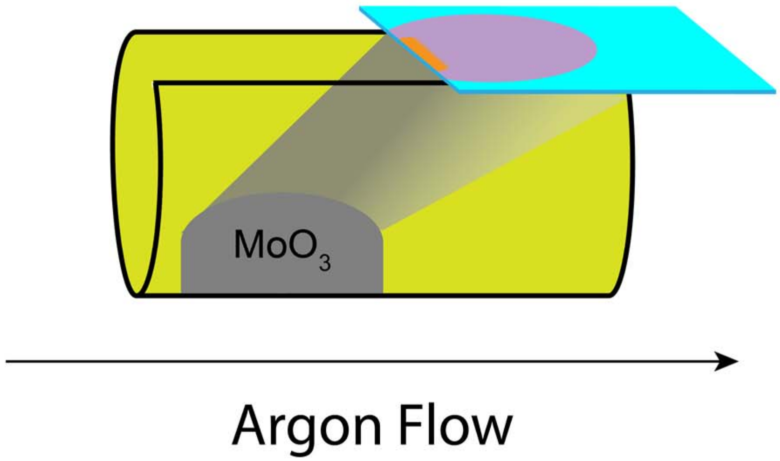
CVD Growth of MoS_2: Locally Increased S:Mo Ratio

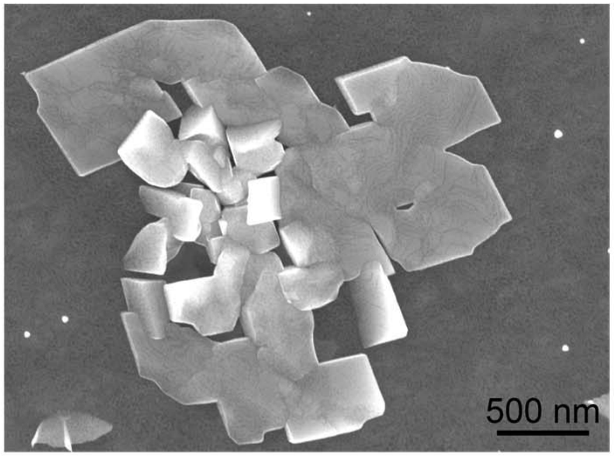


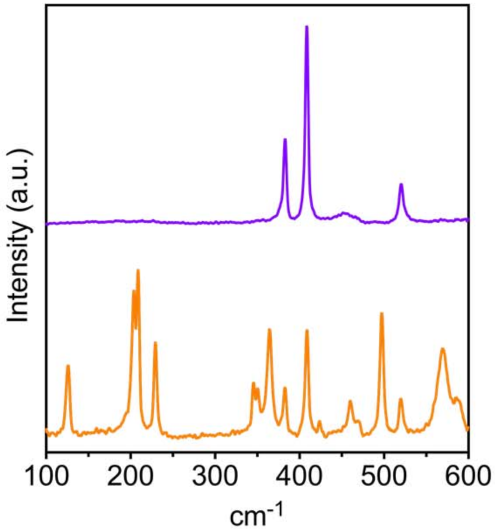




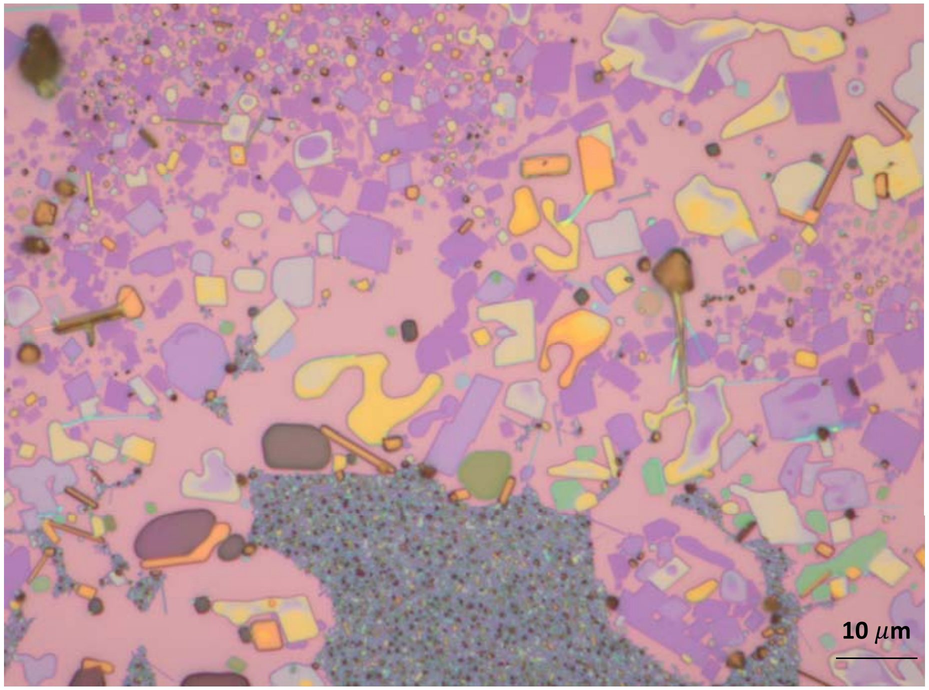
CVD Growth of MoS_2: Locally Decreased S:Mo Ratio



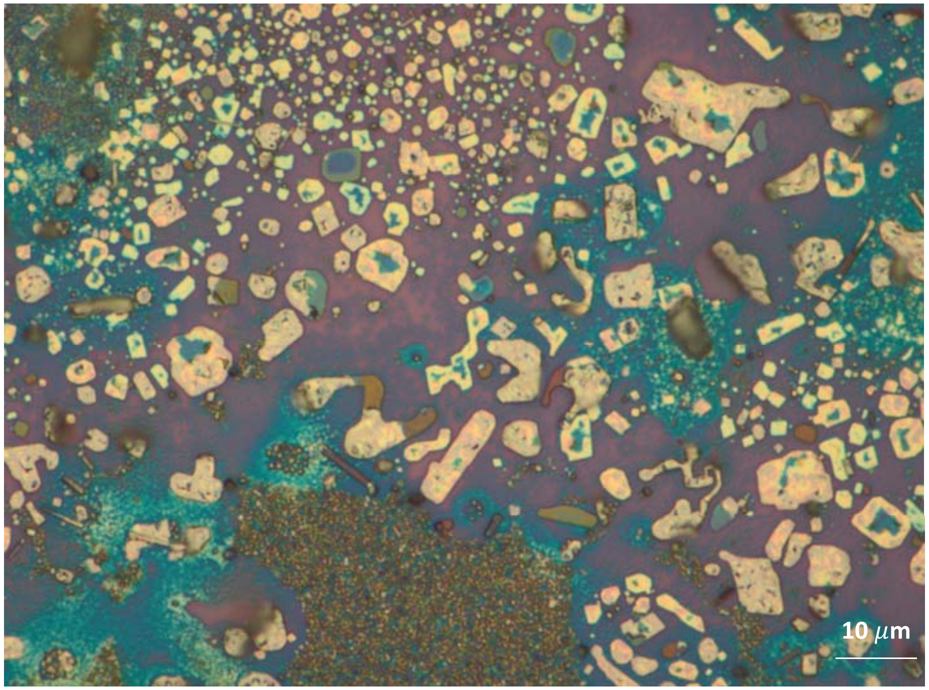




Sulfurization of $MoOS_2$



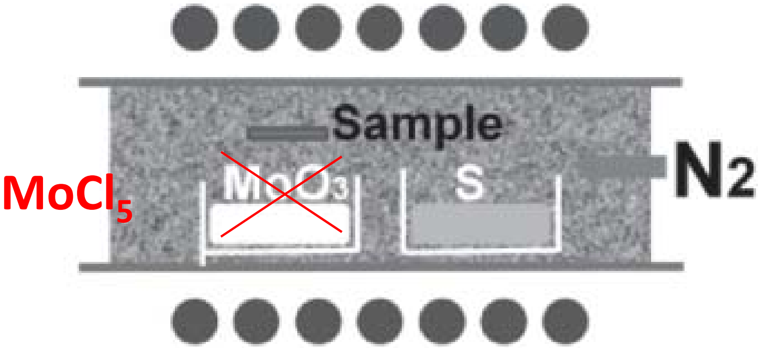
$MoOS_2$ Crystals



MoS_2 Crystals After Sulfurization

Sulfurization of $MoOS_2$

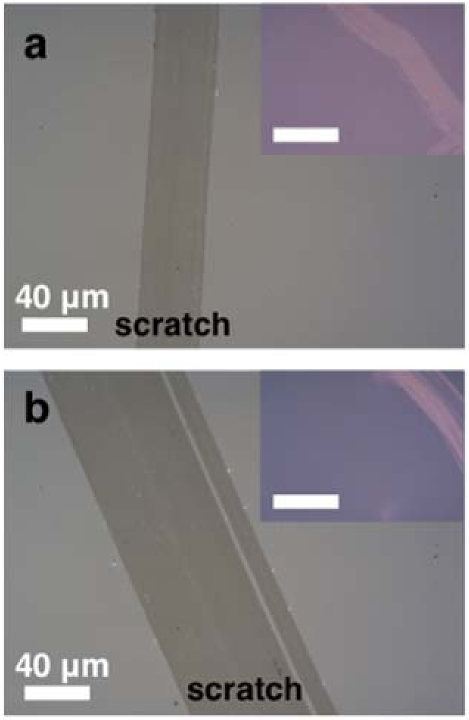
CVD Growth of MoS_2 Using $MoCl_5$ powder

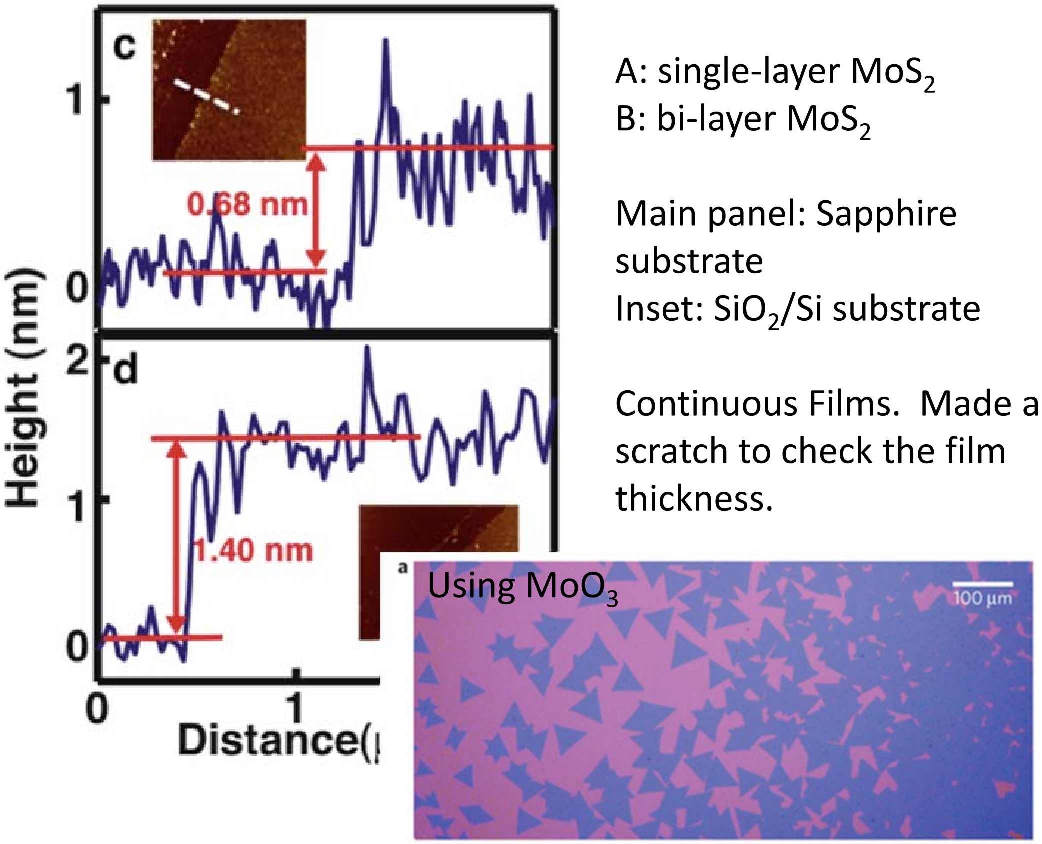


- $MoCl_5$ and S powders were heated to 800 C .
- Various substrates were successful in growing MoS_2
  - SiO_2, Sapphire (Al_2O_3), Graphite
- Large-area, continuous MoS_2 film
- The # of layers of MoS_2 could be controlled by tuning the $MoCl_5$ amount, which controls the partial pressure of dissociated Mo vapor.

Scientific Report, 3:1866 (2013)

CVD Growth of MoS_2 Using $MoCl_5$ powder





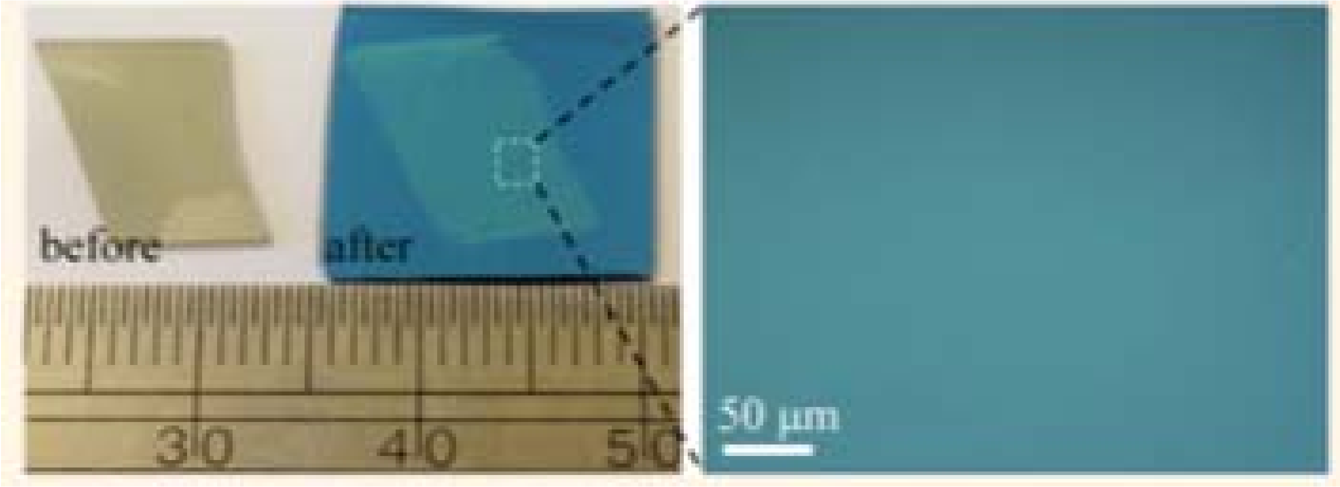
A: single-layer MoS_2
B: bi-layer MoS_2

Main panel: Sapphire substrate
Inset: SiO_2/Si substrate

Continuous Films. Made a scratch to check the film thickness.

Scientific Report, 3:1866 (2013)

Transfer of Cm-scale MoS_2 onto Arbitrary Substrates



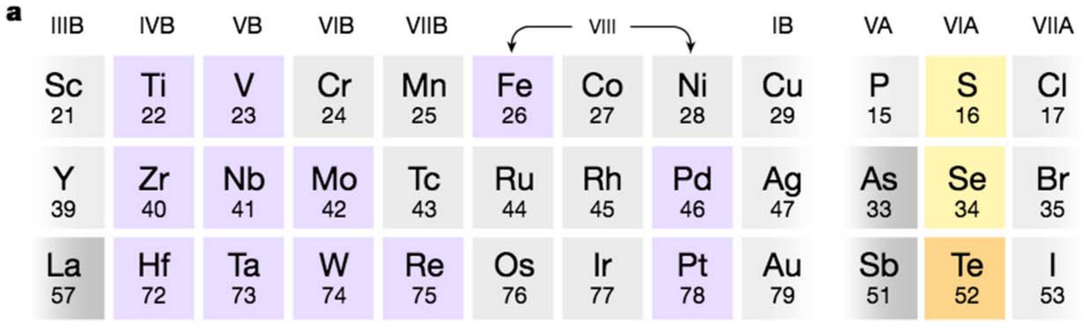
Large-area, single-layer MoS_2 film being transferred from growth substrates to other substrates
- Necessary if growth substrates are not compatible with device substrates

ACS Nano 8, p.11522 (2014)

A library of atomically thin metal chalcogenides

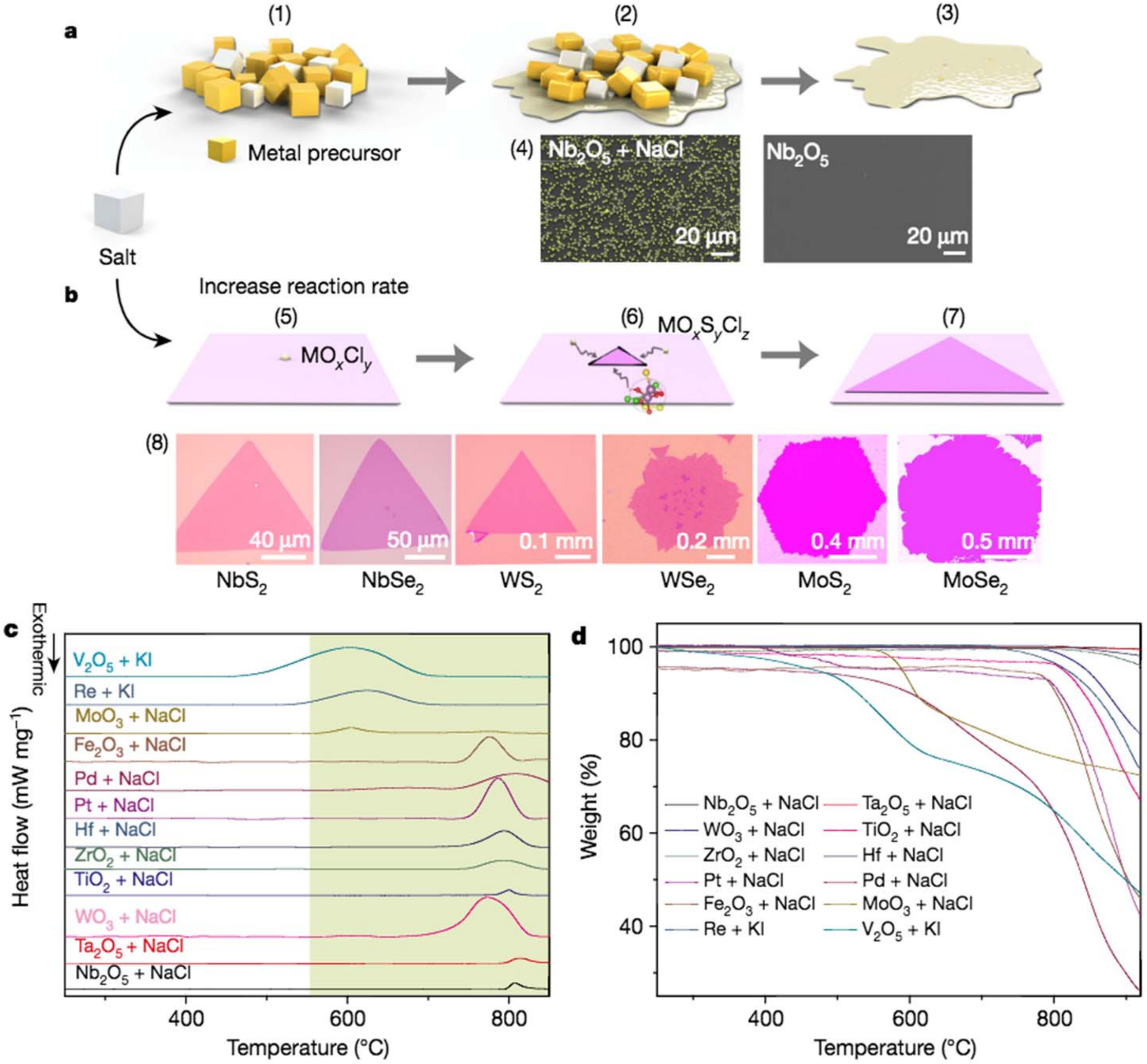
Jiadong Zhou[1,15], Junhao Lin[2,15]*, Xiangwei Huang[3], Yao Zhou[4], Yu Chen[5], Juan Xia[5], Hong Wang[1], Yu Xie[6], Huimei Yu[7], Jincheng Lei[6], Di Wu[8,9], Fucai Liu[1], Qundong Fu[1], Qingsheng Zeng[1], Chuang-Han Hsu[8,9], Changli Yang[3,10], Li Lu[3,10], Ting Yu[5], Zexiang Shen[5], Hsin Lin[8,9,11], Boris I. Yakobson[6], Qian Liu[4], Kazu Suenaga[2], Guangtong Liu[3]* & Zheng Liu[1,12,13,14]*

a



IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	VA	VIA	VIIA
Sc 21	Ti 22	V 23	Cr 24	Mn 25	Fe 26	Co 27	Ni 28	Cu 29	P 15	S 16	Cl 17
Y 39	Zr 40	Nb 41	Mo 42	Tc 43	Ru 44	Rh 45	Pd 46	Ag 47	As 33	Se 34	Br 35
La 57	Hf 72	Ta 73	W 74	Re 75	Os 76	Ir 77	Pt 78	Au 79	Sb 51	Te 52	I 53

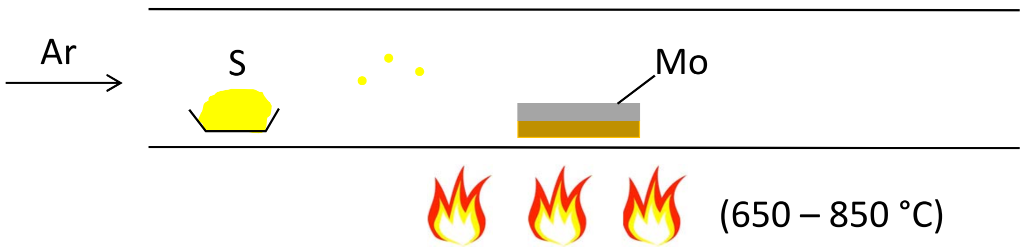
Nature 556, 355 (2018)

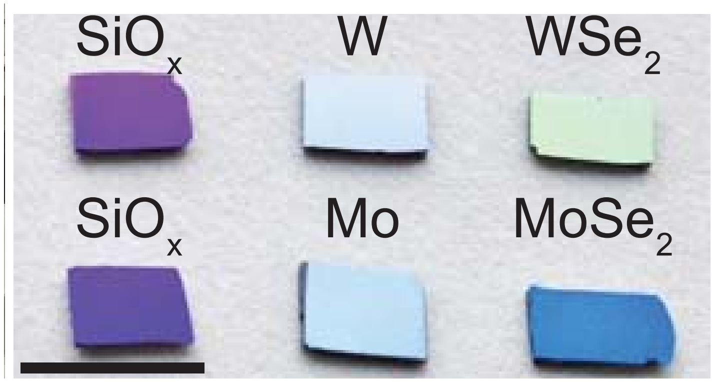

a
(1)
(2)
(3)
Metal precursor
Salt
(4) Nb$_2$O$_5$ + NaCl
20 µm
Nb$_2$O$_5$
20 µm
b
Increase reaction rate
(5) MO$_x$Cl$_y$
(6) MO$_x$S$_y$Cl$_z$
(7)
(8)
40 µm
50 µm
0.1 mm
0.2 mm
0.4 mm
0.5 mm
NbS$_2$
NbSe$_2$
WS$_2$
WSe$_2$
MoS$_2$
MoSe$_2$
c
Exothermic
Heat flow (mW mg^{-1})
V$_2$O$_5$ + KI
Re + KI
MoO$_3$ + NaCl
Fe$_2$O$_3$ + NaCl
Pd + NaCl
Pt + NaCl
Hf + NaCl
ZrO$_2$ + NaCl
TiO$_2$ + NaCl
WO$_3$ + NaCl
Ta$_2$O$_5$ + NaCl
Nb$_2$O$_5$ + NaCl
400
600
800
Temperature (°C)
d
Weight (%)
100
80
60
40
Nb$_2$O$_5$ + NaCl
Ta$_2$O$_5$ + NaCl
WO$_3$ + NaCl
TiO$_2$ + NaCl
ZrO$_2$ + NaCl
Hf + NaCl
Pt + NaCl
Pd + NaCl
Fe$_2$O$_3$ + NaCl
MoO$_3$ + NaCl
Re + KI
V$_2$O$_5$ + KI
400
600
800
Temperature (°C)

Synthesis of Vertically-Aligned MoS_2 Film

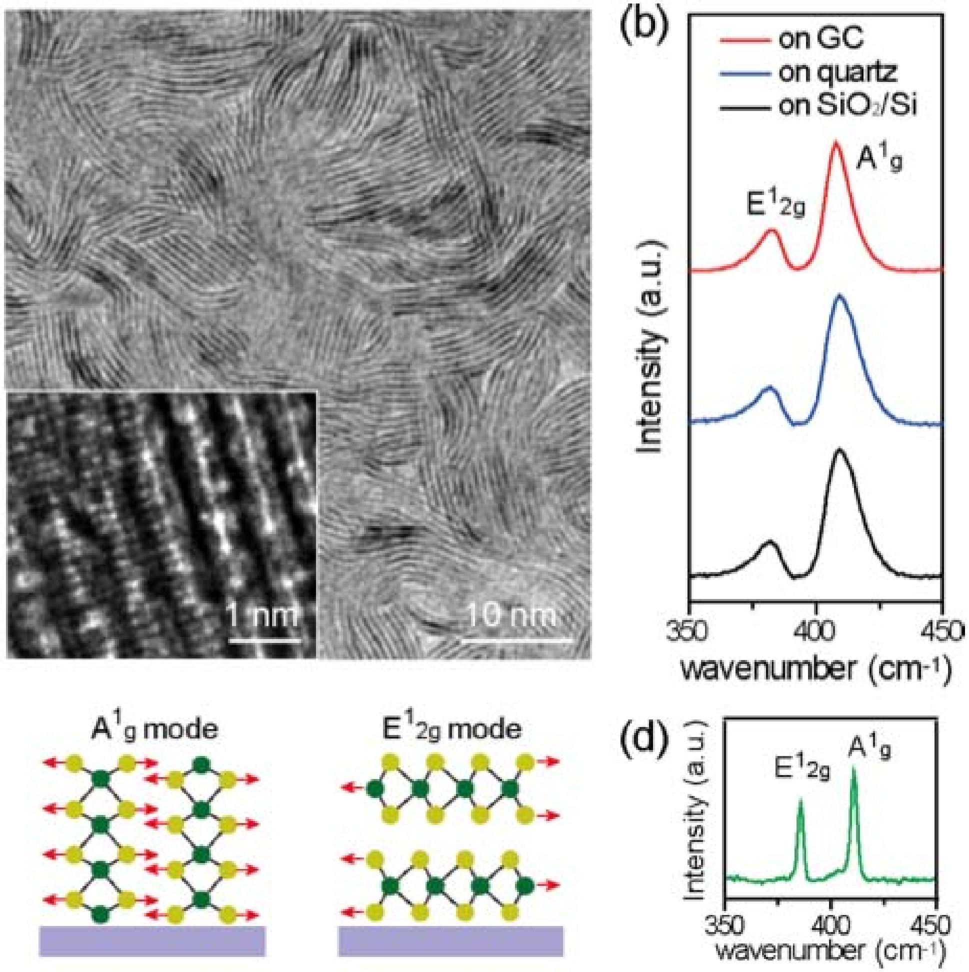
Growth:

Sulfurization of Mo/SiO_2 & W/SiO_2 substrates



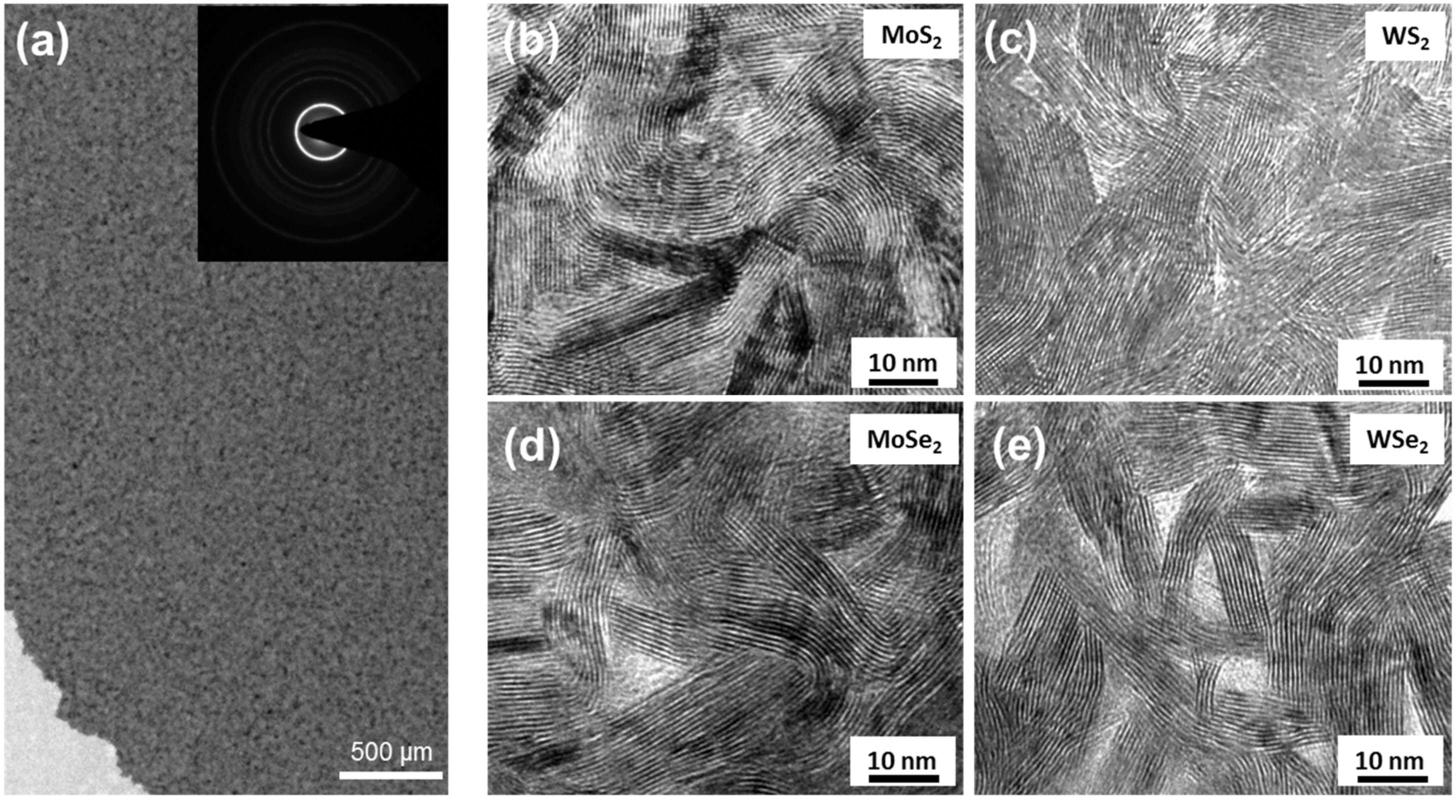


Synthesis of Vertically-Aligned MoS_2 Film



Nano Lett. 13, p.1341 (2013)

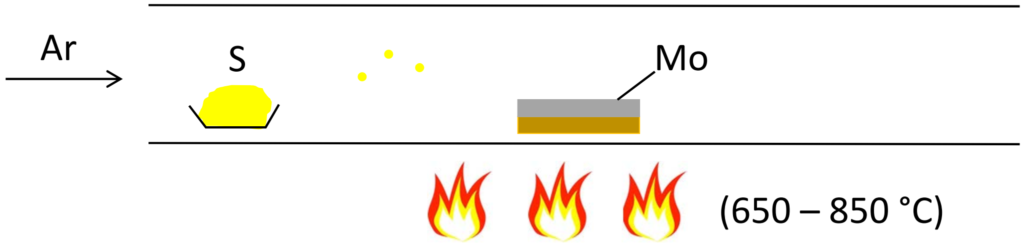
Large-Area, Densely-Packed Films

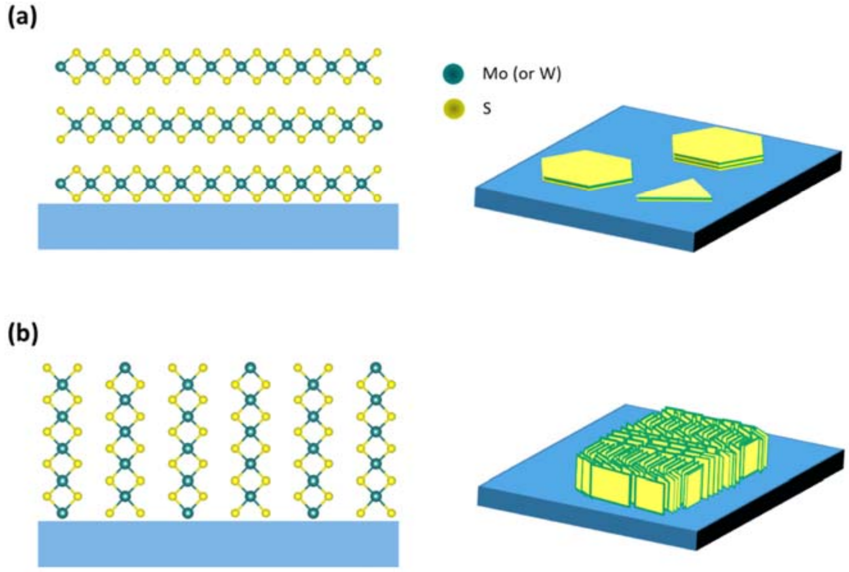


Vertical to Horizontal Growth of MoS_2

Why do we grow MoS_2 vertically even though growth conditions are similar?

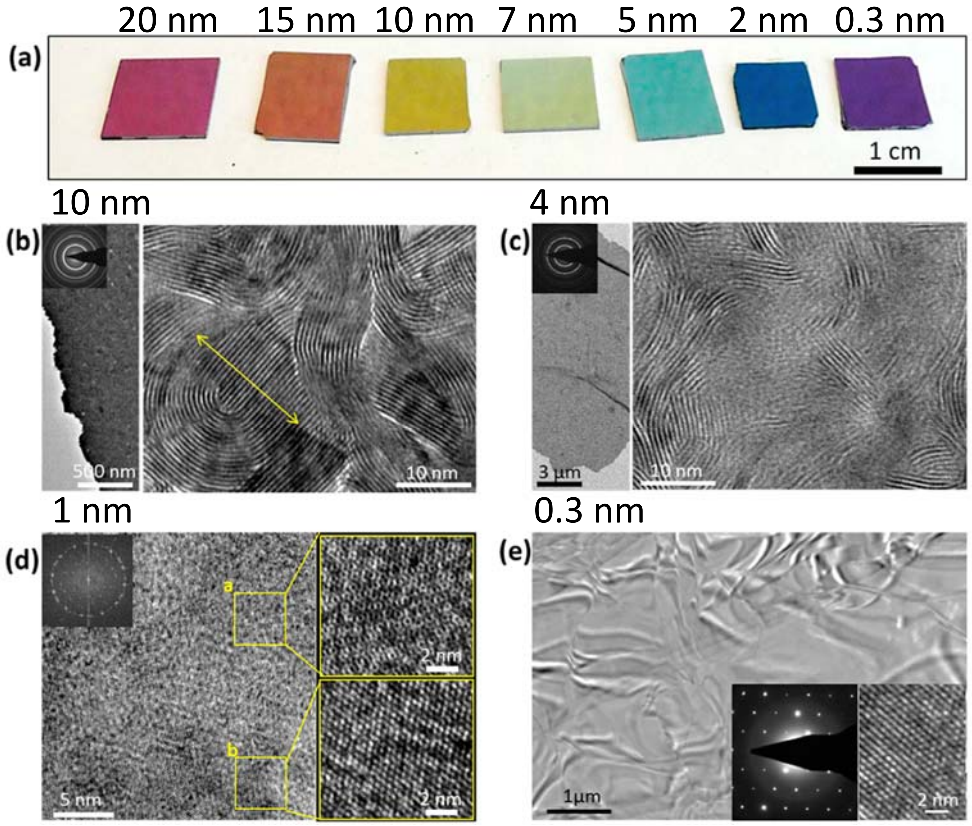
Growth: Sulfurization of Mo/SiO_2 substrates



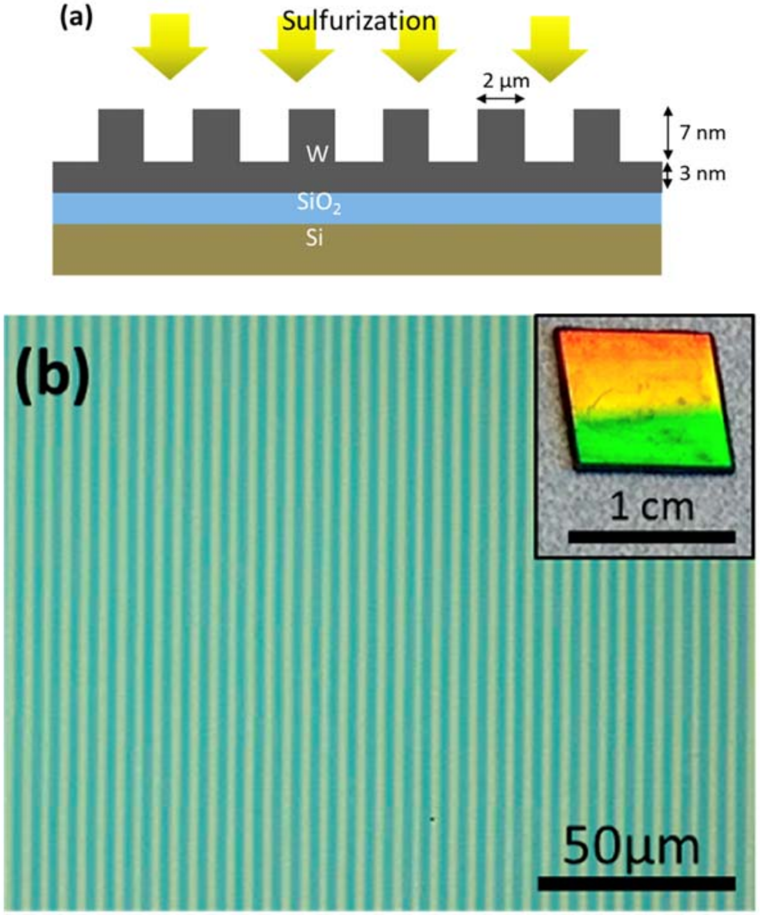


Nano Lett. 14, 6842 (2014)

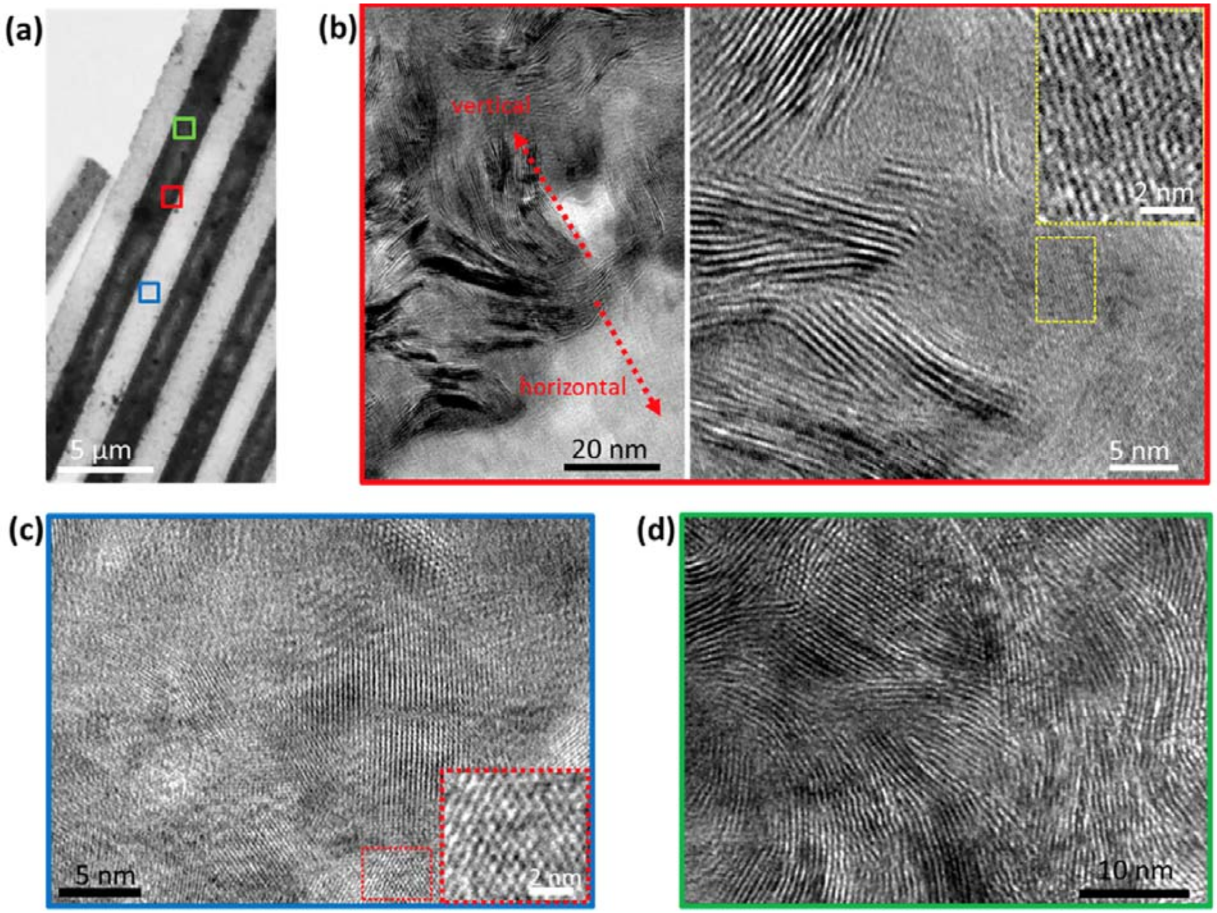
Mo Film Thickness-Dependent MoS_2 Growth



W Film Thickness-Dependent WS_2 Growth

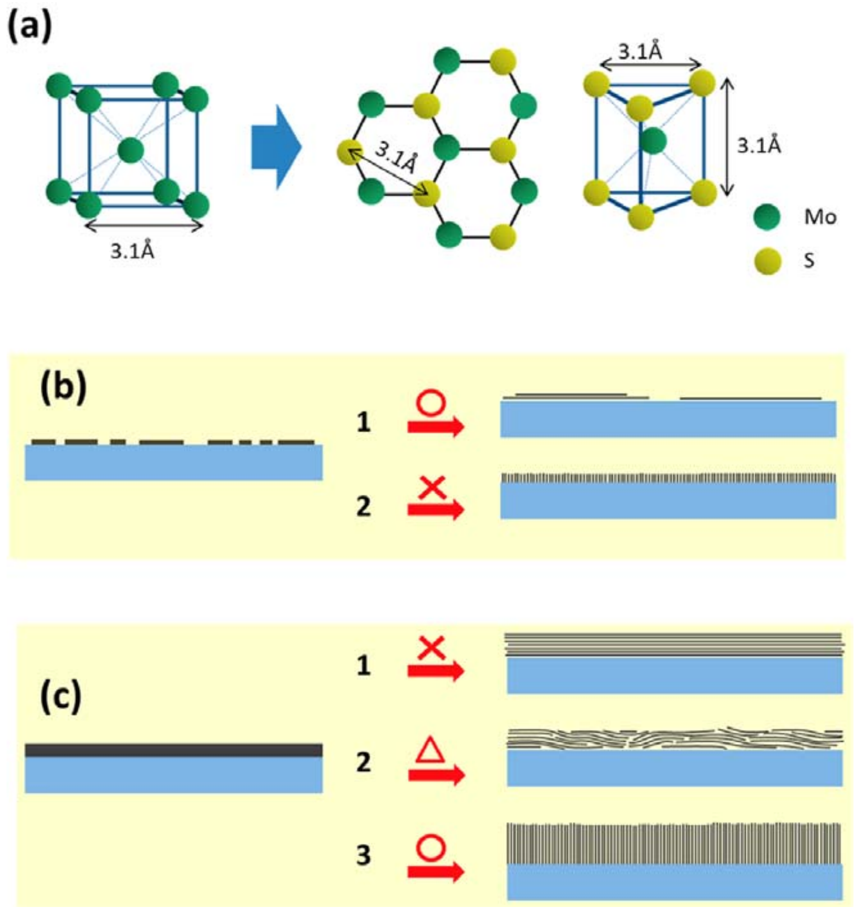


Vertical and Horizontal WS_2 Films



Nano Lett. 14, 6842 (2014)

Volume Expansion and Strain Effects



Overview

- Why Nanoscale Materials
  - Emergent properties (band engineering, surface properties)
  - Examples (quantum dots, carbon nanotubes, mechanical properties)
- Synthesis of Nanowires
  - Various growth methods
  - Vapor-liquid-solid growth
  - Doping / surface passivation
- Synthesis of 2D Materials
  - Chemical vapor deposition
  - Precursors / additives

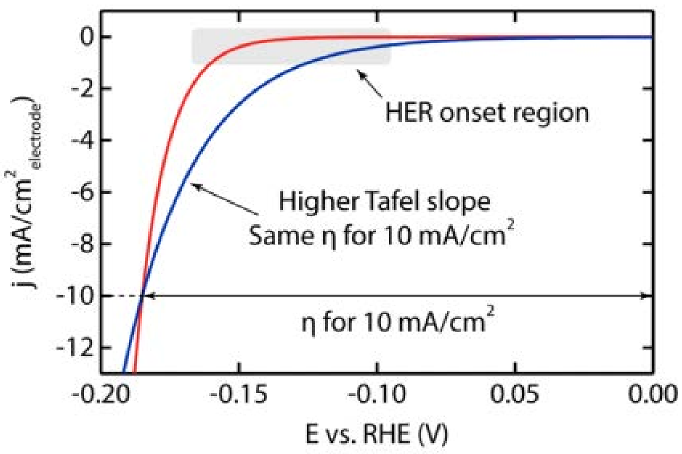
Overview

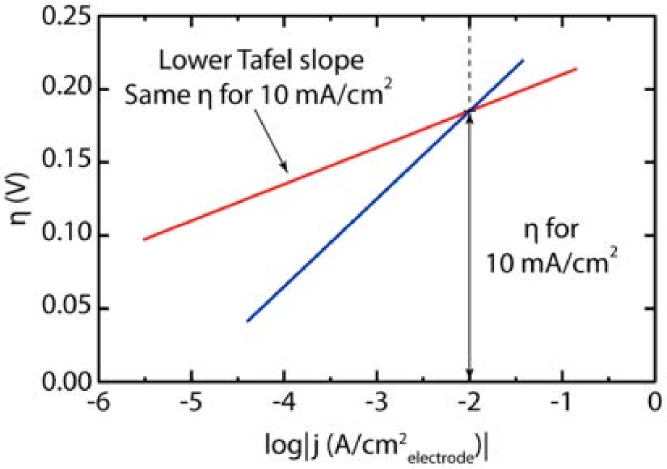
- Case Study of Nanowires: Si Nanowires
  - Thermal transport modulation
  - Si nanowire batteries
- Case study of topological nanomaterials
  - Bi_2Se_3 topological insulator nanoribbons
  - SnTe Topological crystalline insulator nanowires
- Case study of 2D materials for energy
  - MoS_2 for hydrogen evolution reaction (HER)
  - Phase transition via intercalation and consequences for HER

Hydrogen Evolution Reaction (HER)

Water Splitting: $H_2O \rightarrow H_2 + 1/2O_2$

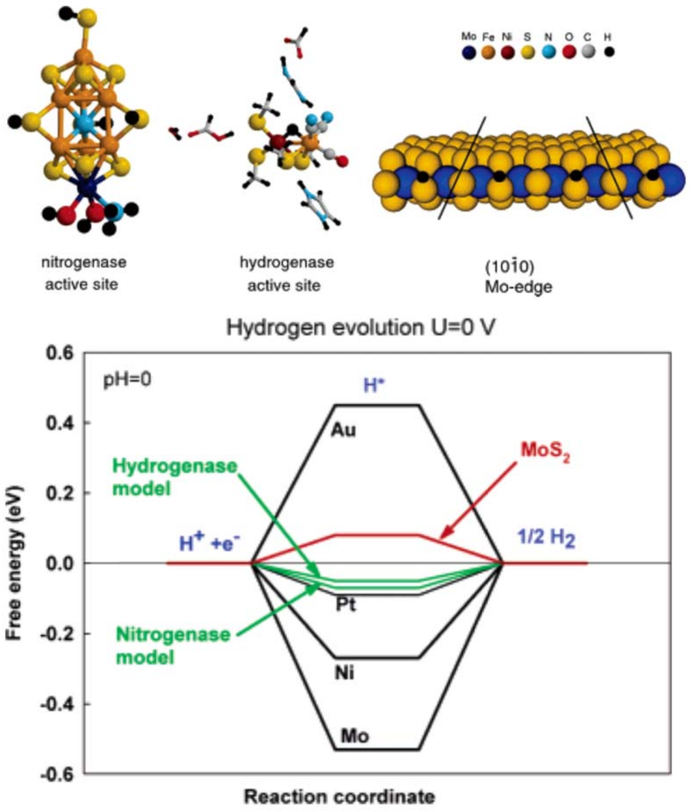
Hydrogen Evolution Reaction (HER): $2H^+ + 2e^- \rightarrow H_2$
Oxygen Evolution Reaction (OER): $H_2O \rightarrow 1/2O_2 + 2H^+ + 2e^-$



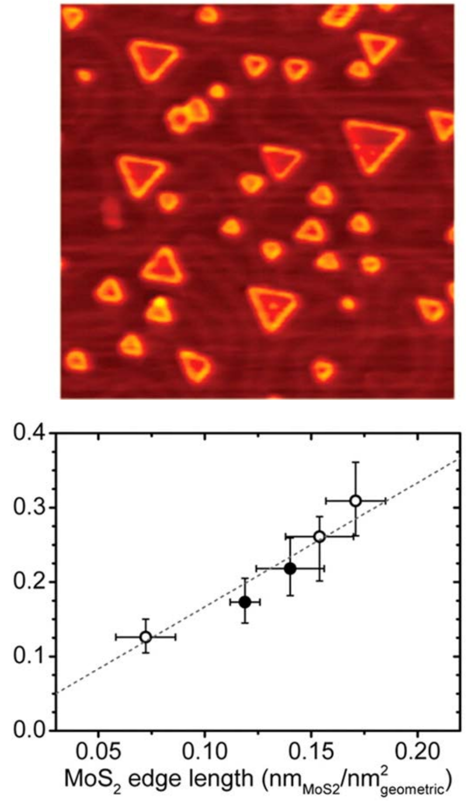


Low overpotential, low Tafel slope

MoS_2 as a Promising HER Catalyst

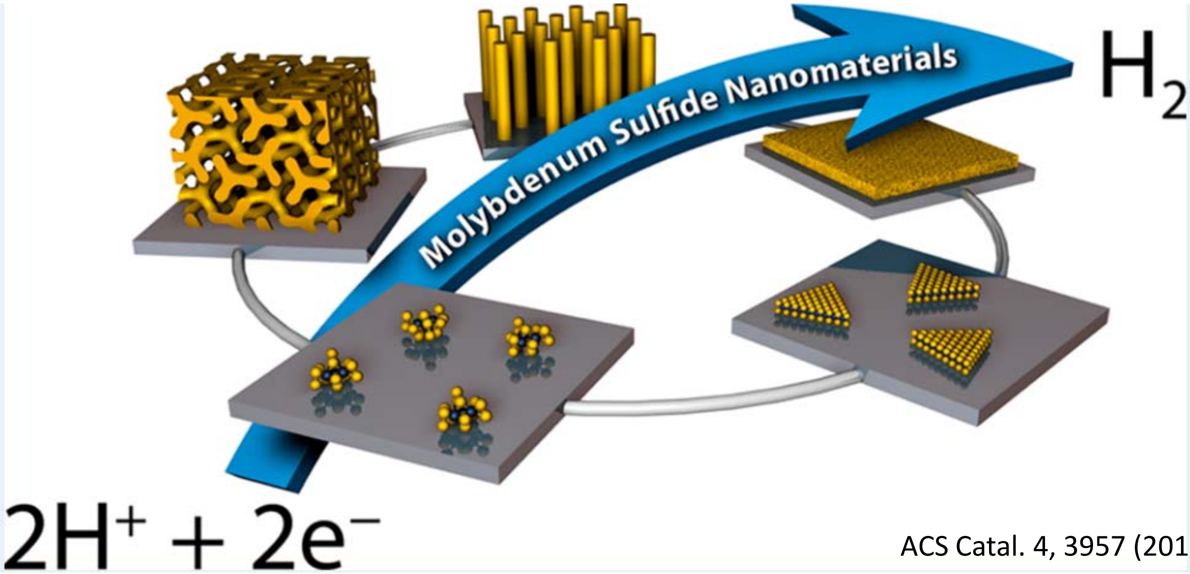


JACS 127, p.5308 (2005)



Science 317, 100 (2007)

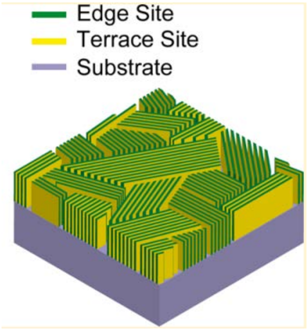
Catalyzing the HER with MoS_2 Nanomaterials



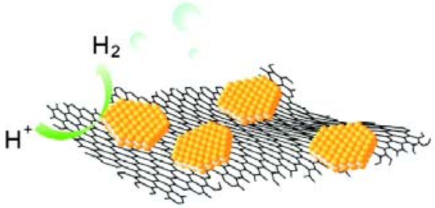
ACS Catal. 4, 3957 (2014)

Progress in MoS_2 as HER catalyst

1. Increase S edge sites
2. Better transfer to current collector
3. Improve electrical properties
4. ΔG_H tuning to lower energy barrier



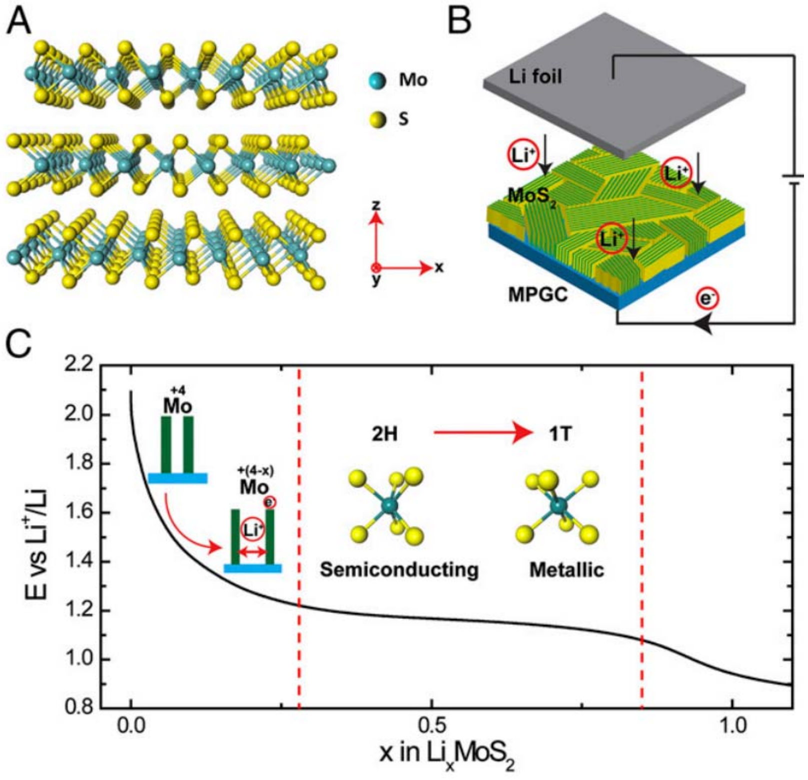
Nano Lett. 13, 1341 (2013)

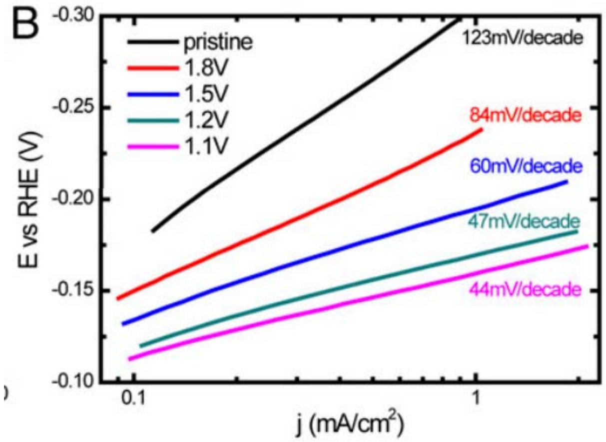


JACS 133, 7296 (2011)

Improve Electronic Property

Phase transition from semiconducting 2H → metallic 1T : Lower Tafel slope

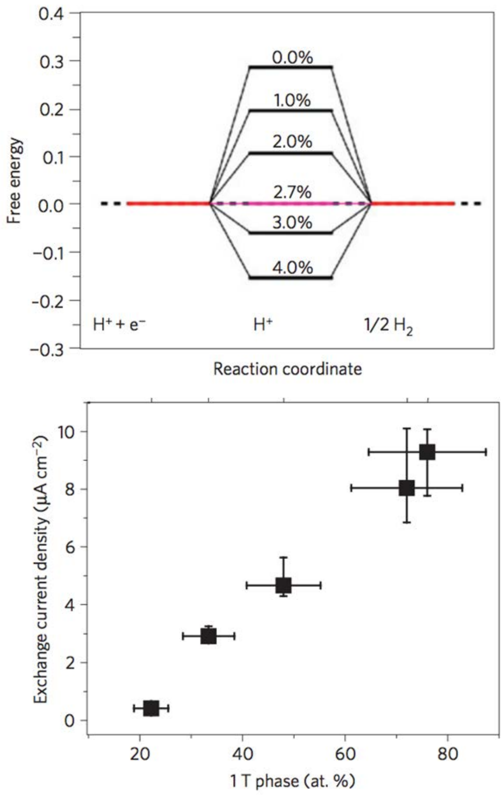




PNAS 110, 19701 (2013)

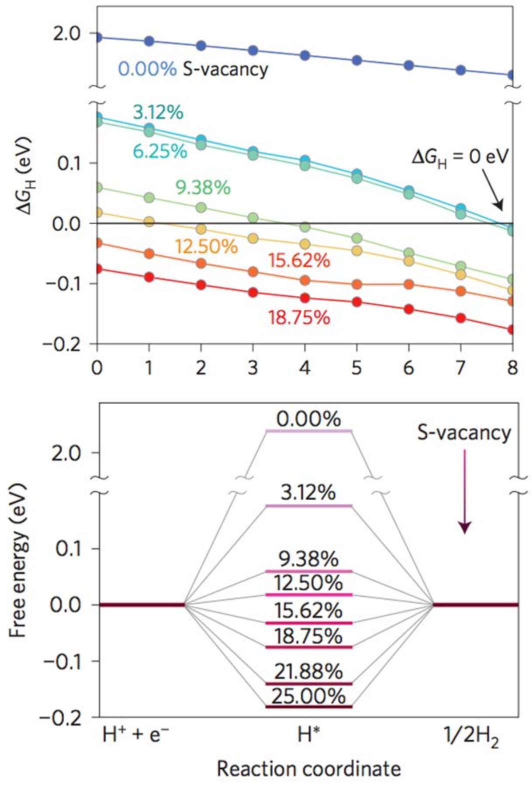
Tuning ΔG_H to improve HER

WS_2: Strain engineering by 1T’
2H → 1T’ by Li^+ exfoliation



Nat. Mater. 12, p.850 (2013)

MoS_2: Strain engineering by S vacancies
Basal plane activation



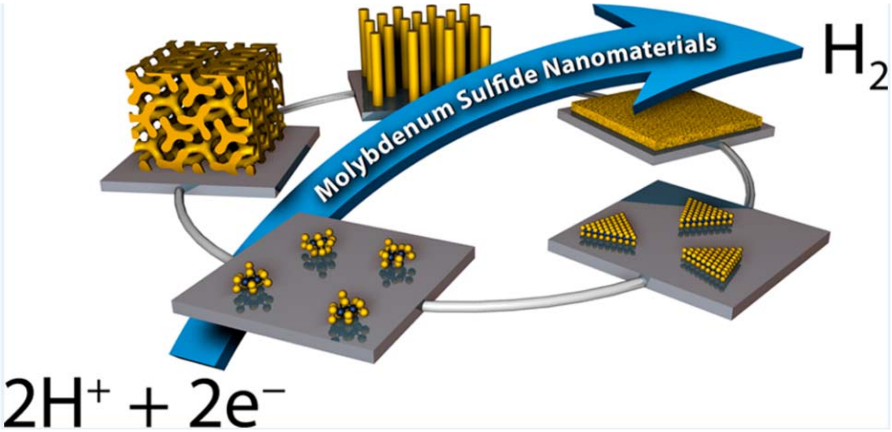
Nat. Mater. 15, p.48 (2016)

Interconnected HER Parameters

Progress in MoS_2 as HER catalyst

1. Increase S edge sites
2. Better transfer to current collector
3. Improve electrical properties 2H → 1T', but also changes ΔG_H
4. ΔG_H tuning to lower energy barrier Effects of S vacancies on conductivity?

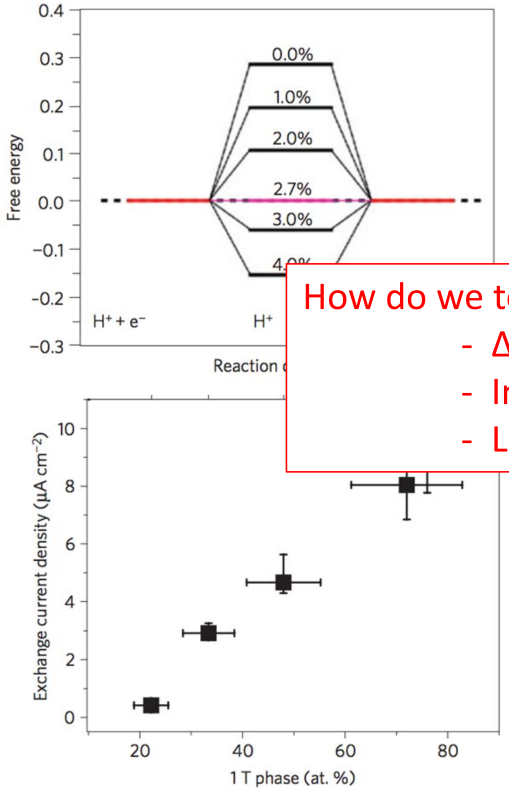
HER parameters: ΔG_H, σ, $\Phi_{interface}$. What's most important?



What is the role of interface?

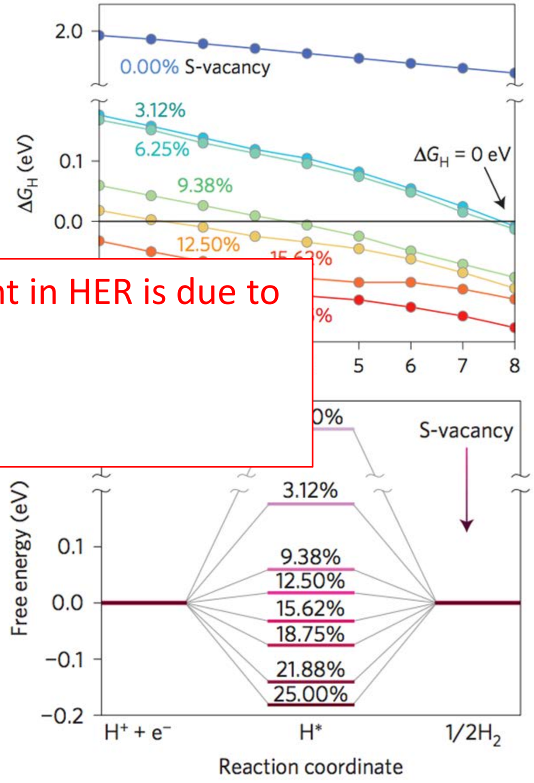
Tuning ΔG_H to improve HER

WS_2: Strain engineering by 1T’
2H → 1T’ by Li+ exfoliation



Nat. Mater. 12, p.850 (2013)

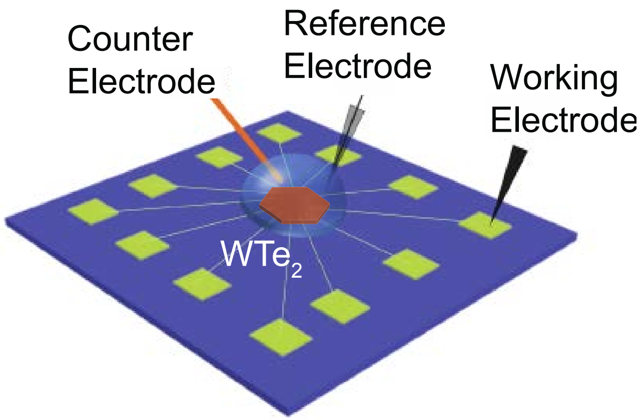
MoS_2: Strain engineering by S vacancies
Basal plane activation



Nat. Mater. 15, p.48 (2016)

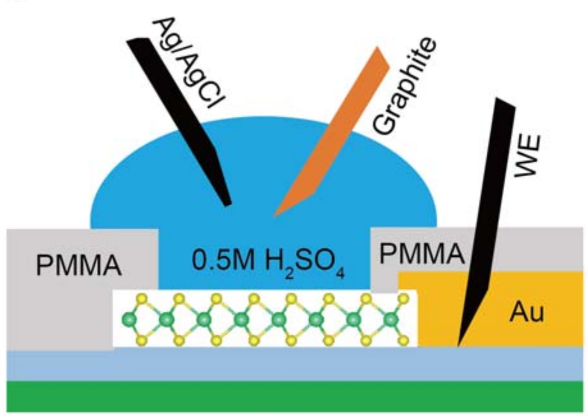
How do we tell if improvement in HER is due to
- ΔG_H tuning
- Improving σ
- Lowering Φ_{SC}

Nanodevices as Micro-reactors for HER

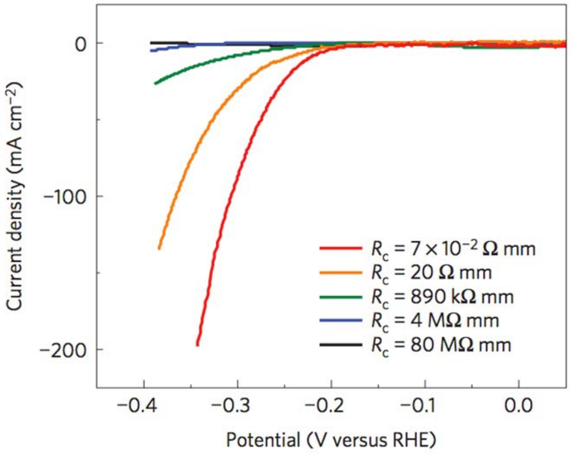


We accurately control and measure

- Types and densities of active sites (ΔG_H)
- Electron transport within catalyst (σ)
- Electron transfer at interface (Φ_{SC})

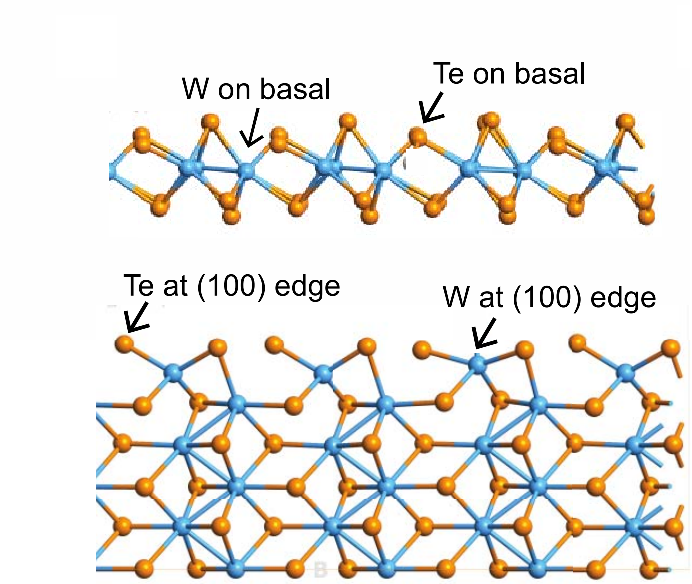


Basal plane MoS$_2$ with R$_c$ tuning

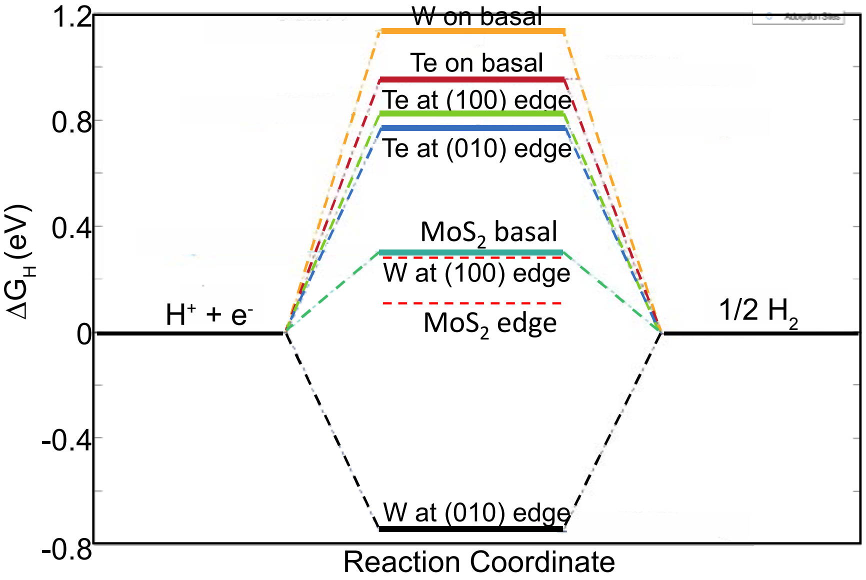


Nat. Mater. 15, p.1003 (2016)

MoS_2 and WTe_2: Contrasting Model Systems

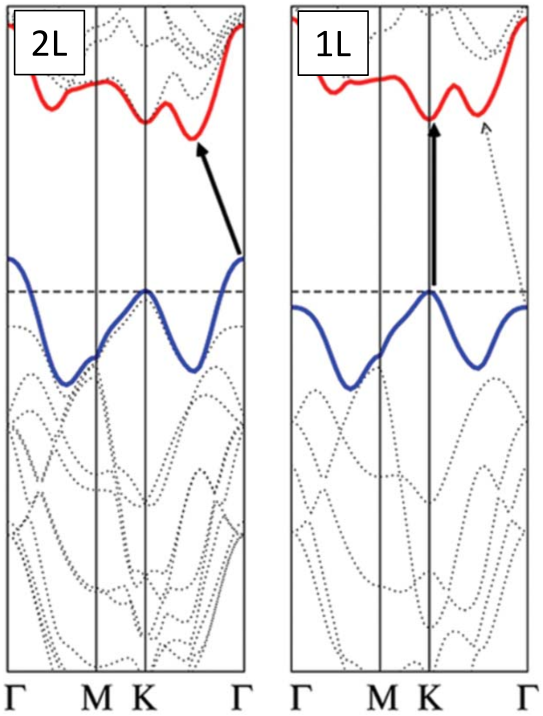


Moyses Araujo from Uppsala University



MoS_2 and WTe_2: Contrasting Model Systems

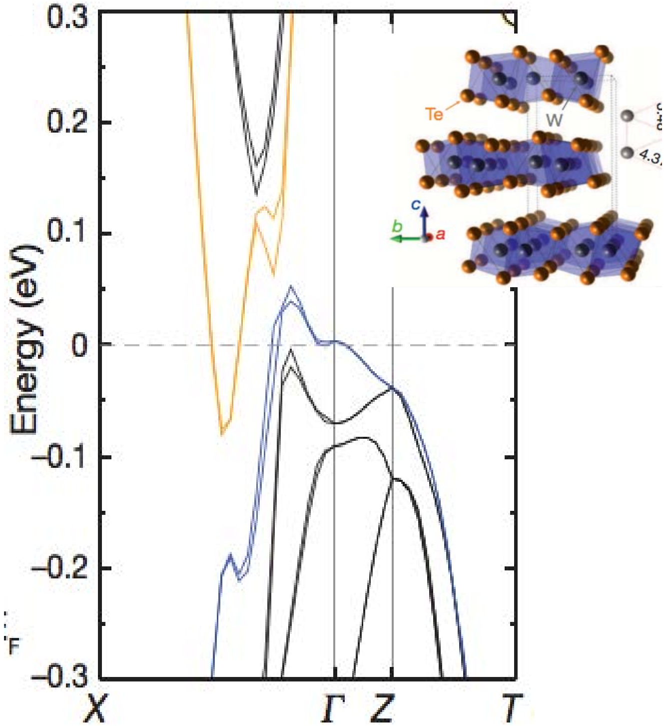
Semiconducting MoS_2 (2H)



Nano Lett. 10, 1271 (2010)

Mobility (μ) ~ 100 cm^2/Vs

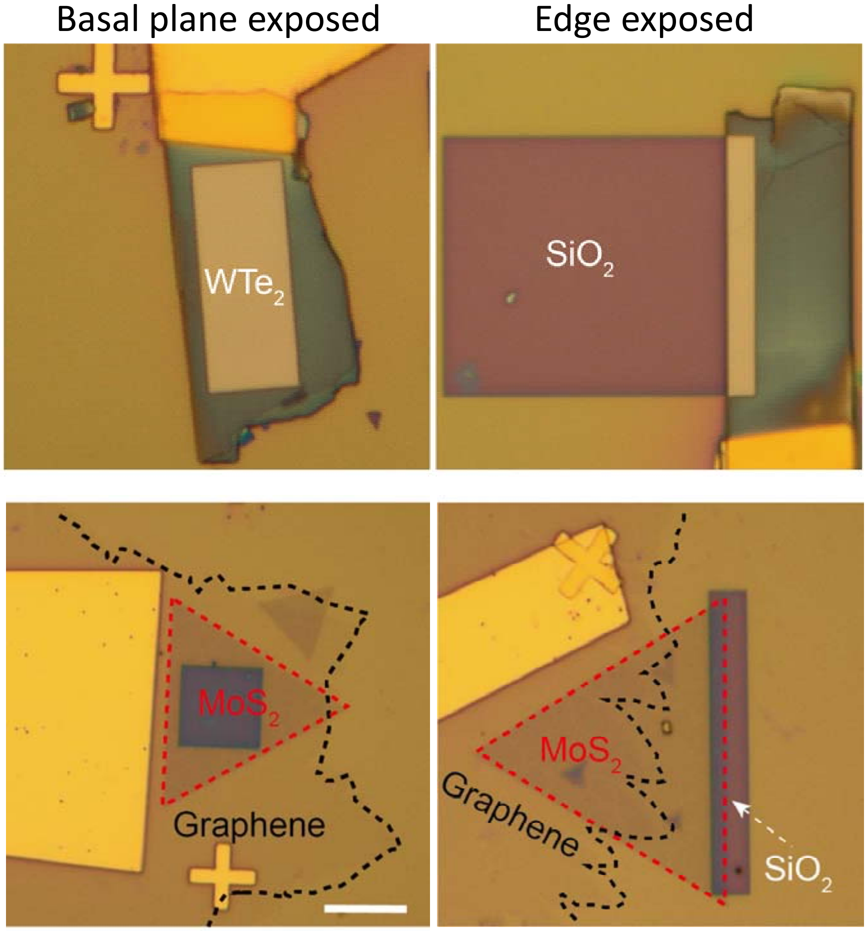
Semimetallic WTe_2 (T_d)



Nature 514, 205 (2014)

Mobility (μ) ~ 10,000 cm^2/Vs

Nanodevice HER Micr-reactor

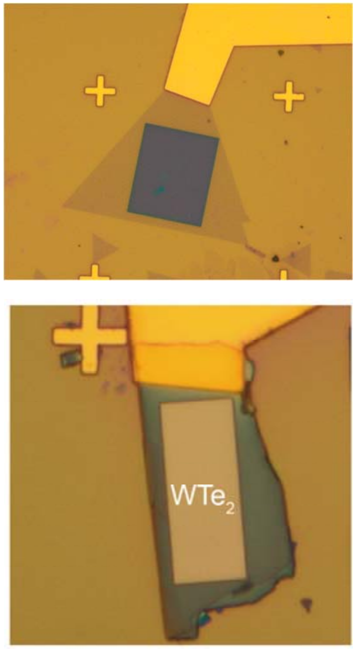


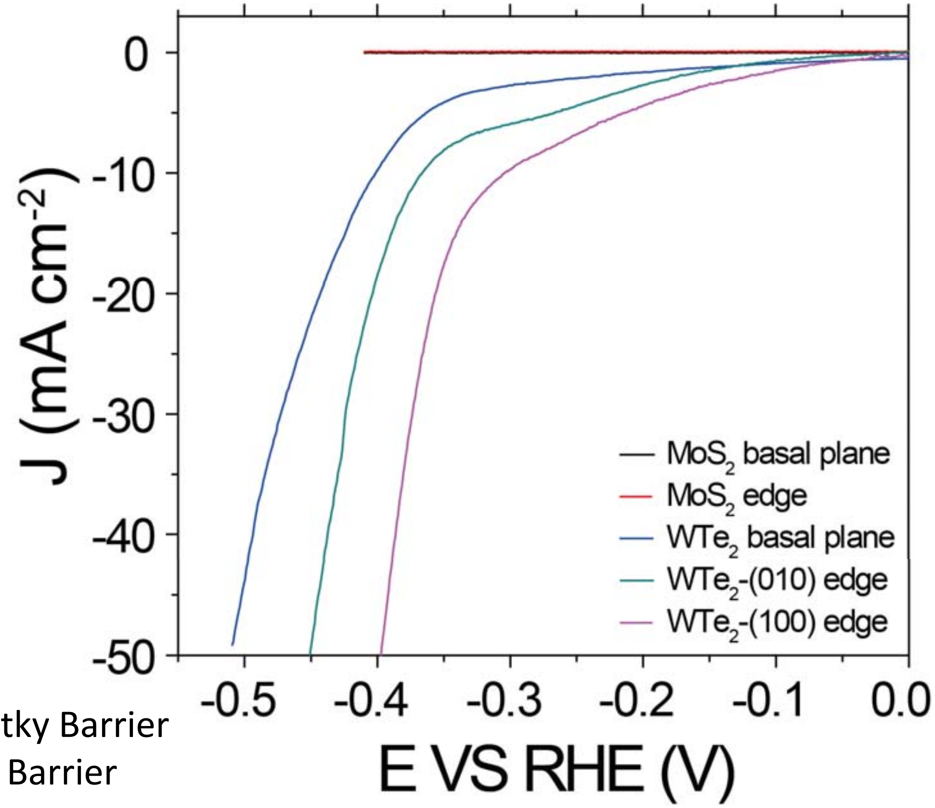
Basal plane exposed

Edge exposed

Modulating Schottky Barrier (Φ_{SC})

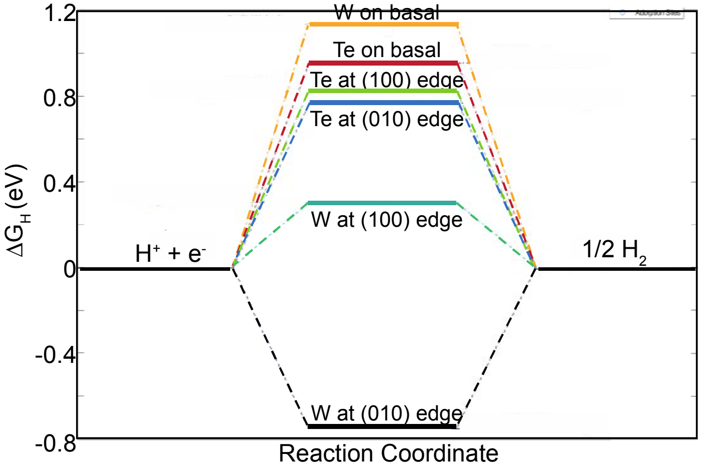
Using Au as electrodes

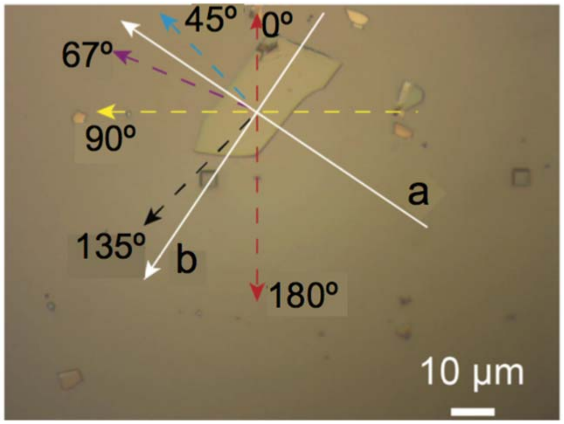




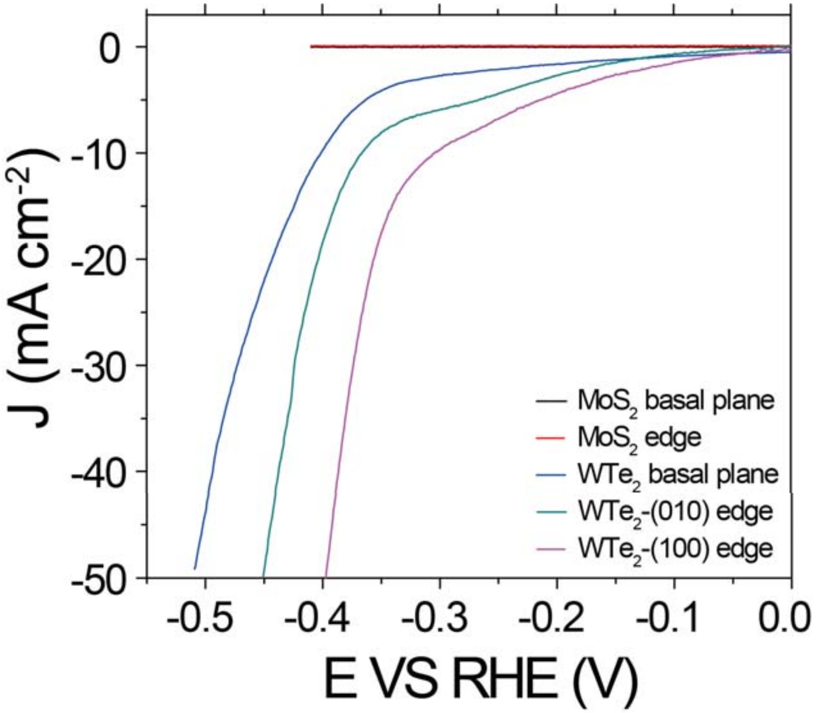
MoS_2/Au : Large Schottky Barrier
WTe^2/Au: No Schottky Barrier

ΔG_H effect in WTe_2

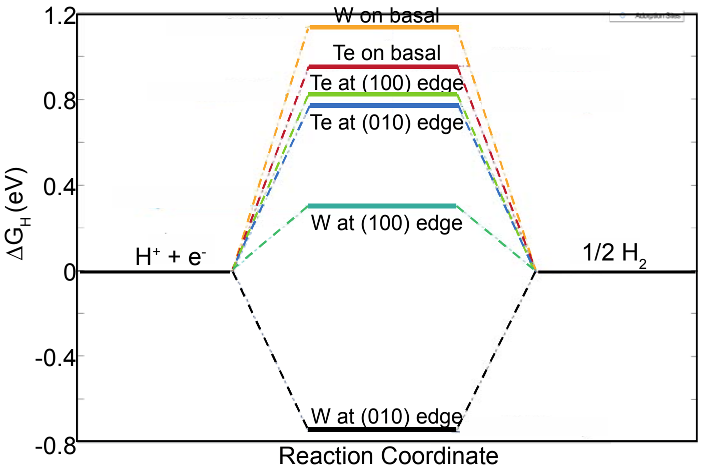


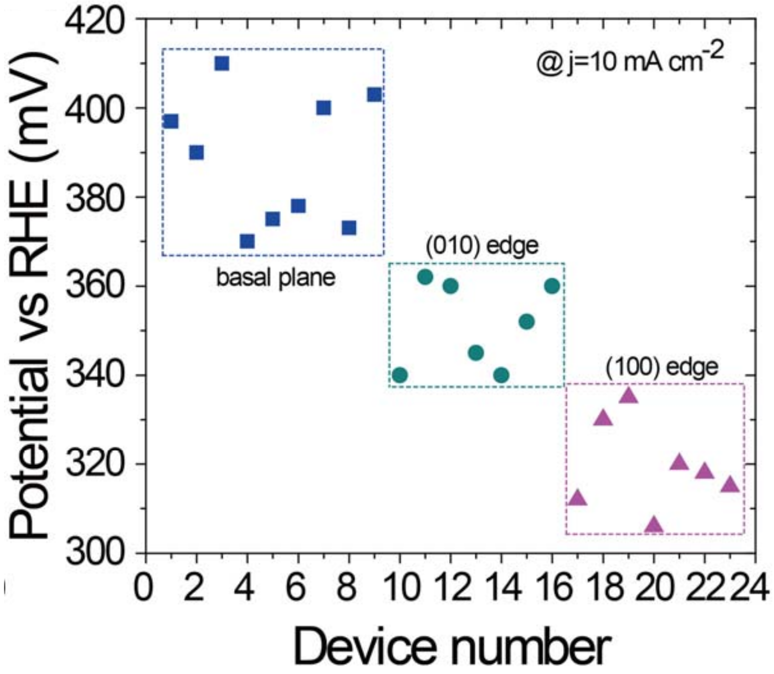


With F. Xia group



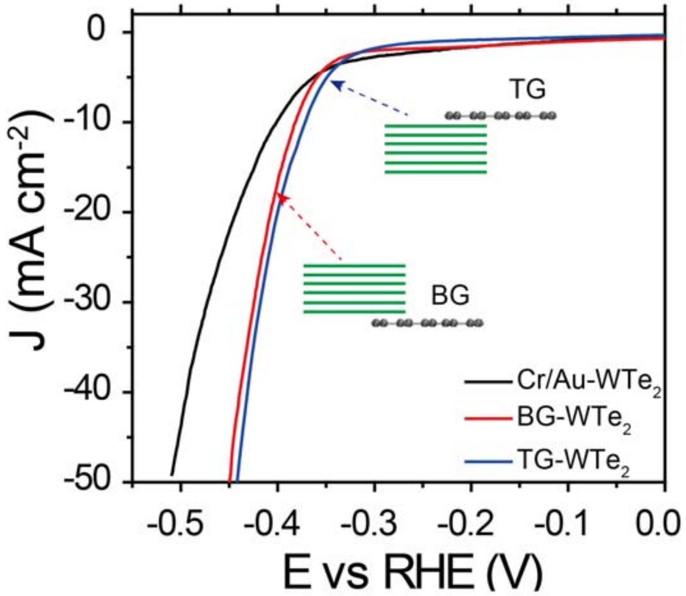
ΔG_H effect in WTe_2

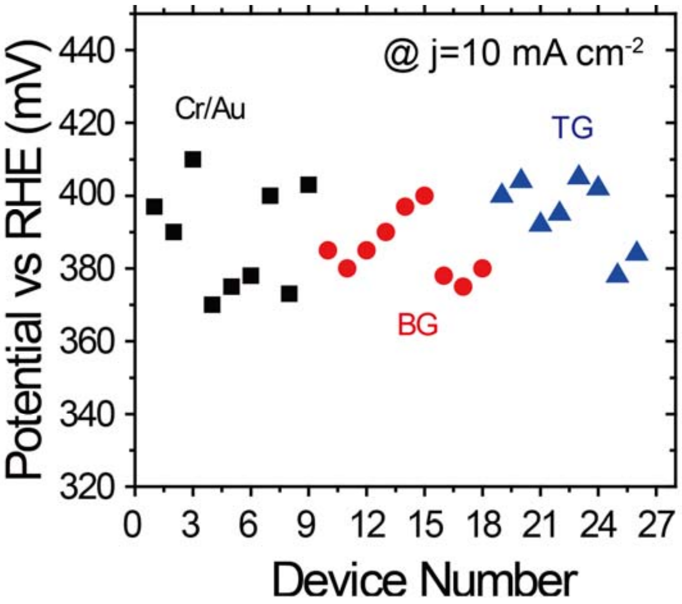




Electron Transport Within Catalyst (σ)

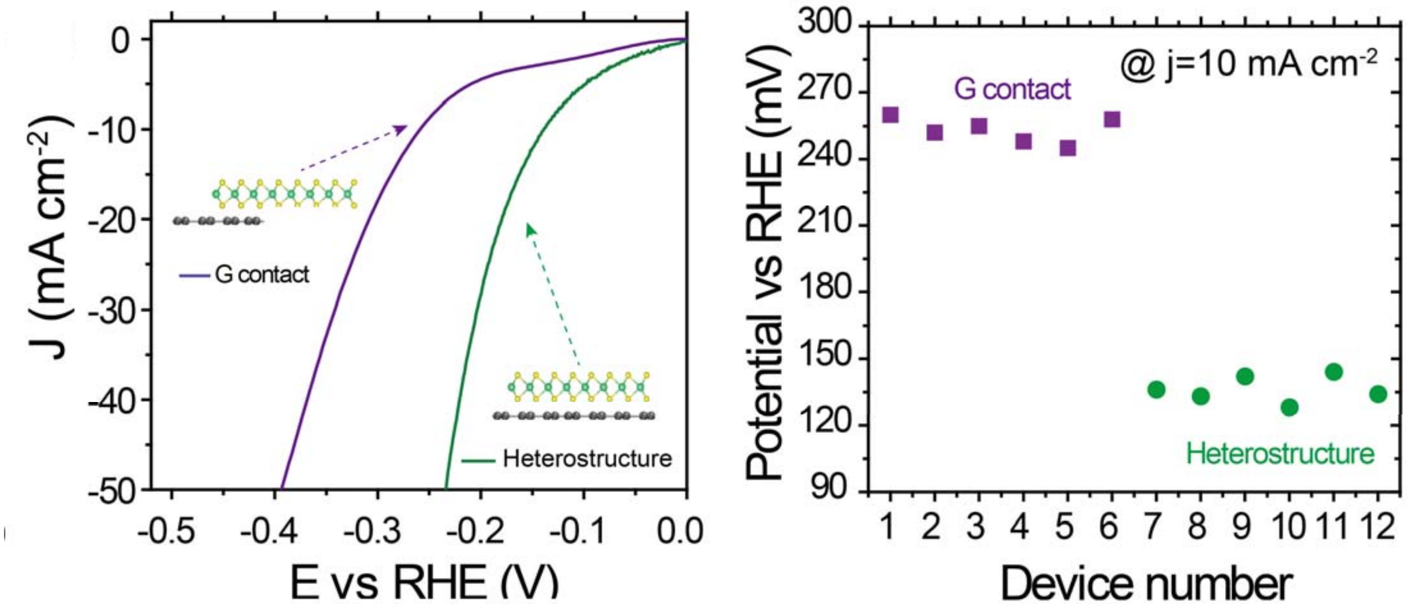
WTe_2: Semimetallic, high electron mobility





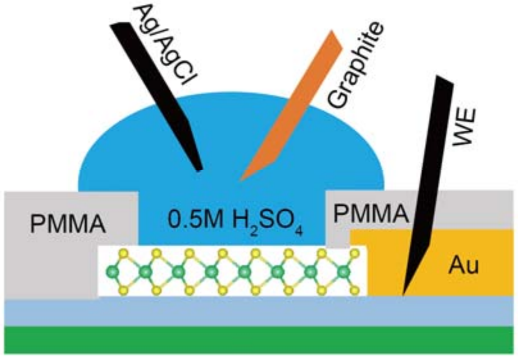
Electron Transport Within Catalyst (σ)

MoS_2: Semiconducting, low electron mobility

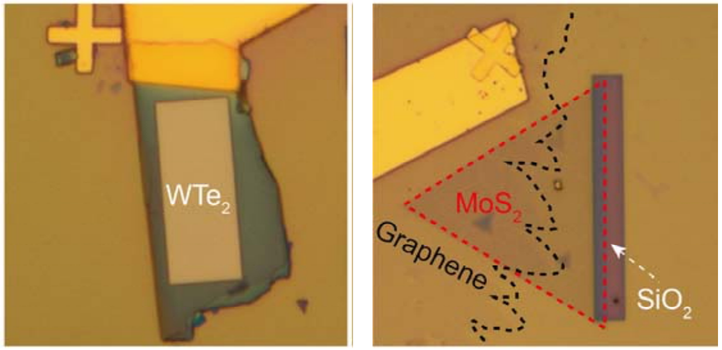


Nanodevice to Unravel HER

- Electrocatlytic reactions are complex
- For HER, ΔG_H, σ, and Φ_{SC} are interdepedent



- Types and densities of active sites (ΔG_H)
- Electron transport within catalyst (σ)
- Electron transfer at interface (Φ_{SC})



HER of 2D TMDCs

- Interface barrier as a bottleneck
- Electron transport important
- ΔG_H dependent activity