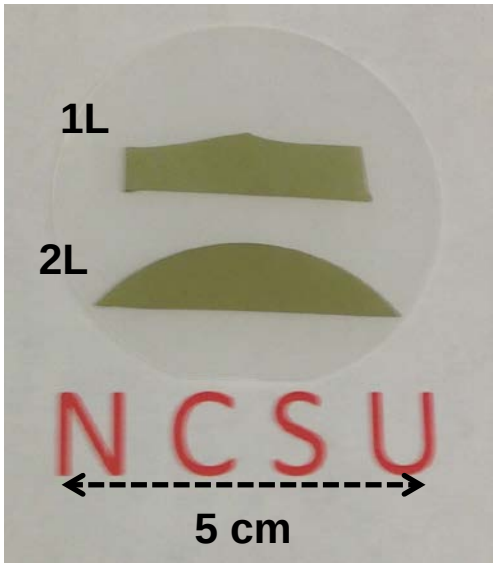
NC STATE UNIVERSITY

2D Transtion Metal Dichalcogenide (TMDC) Materials : Synthesis, Properties, and Applications



Linyou Cao
Department of Materials Science and Engineering, North Carolina State University

Oct. 3, 2015 CCDM Tutorial

Outline

I. Introduction of 2D TMDC materials

I. Synthesis and transfer of 2D TMDC materials

- Synthesis
- Transfer

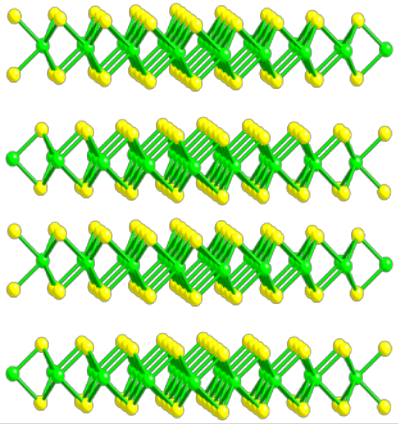
II. Fundamental Properties

- Raman
- Catalytic
- Electrical
- Optical

I. Introduction of 2D TMDC Materials

Transition Metal Dichalcogenide (TMDC) Materials: Compositions

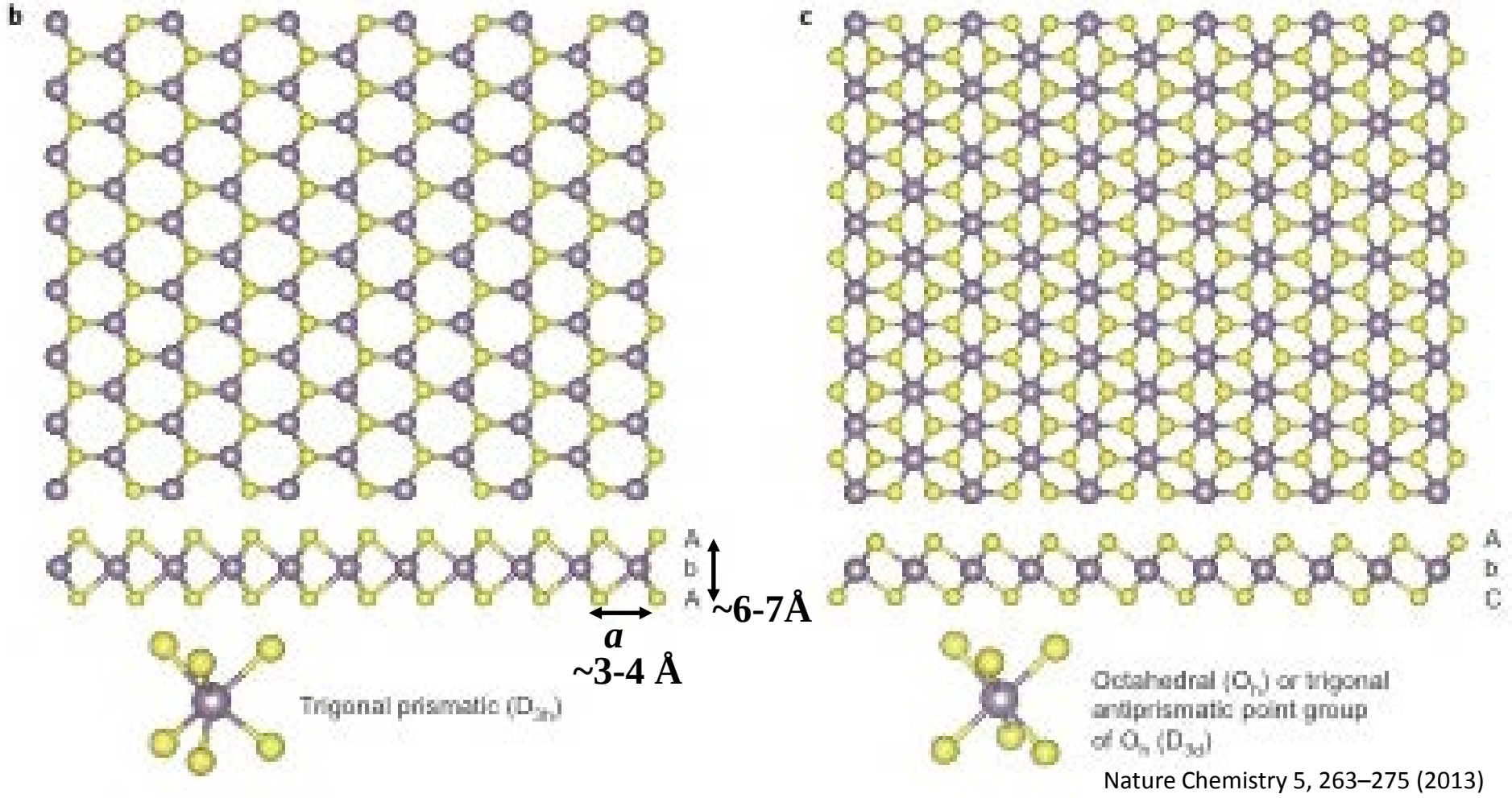
MX_2
M = Transition metal
X = Chalcogen



H																He
Li	Be											B	C	N	O	F	Ne
Na	Mg	3	4	5	6	7	8	9	10	11	12	Al	Si	P	**S**	Cl	Ar
K	Ca	Sc	**Ti**	**V**	Cr	Mn	Fe	**Co**	**Ni**	Cu	Zn	Ga	Ge	As	**Se**	Br	Kr
Rb	Sr	Y	**Zr**	**Nb**	**Mo**	**Tc**	Ru	**Rh**	**Pd**	Ag	Cd	In	Sn	Sb	**Te**	I	Xe
Cs	Ba	La - Lu	**Hf**	**Ta**	**W**	**Re**	Os	**Ir**	**Pt**	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac - Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo

Nature Chemistry 5, 263–275 (2013)

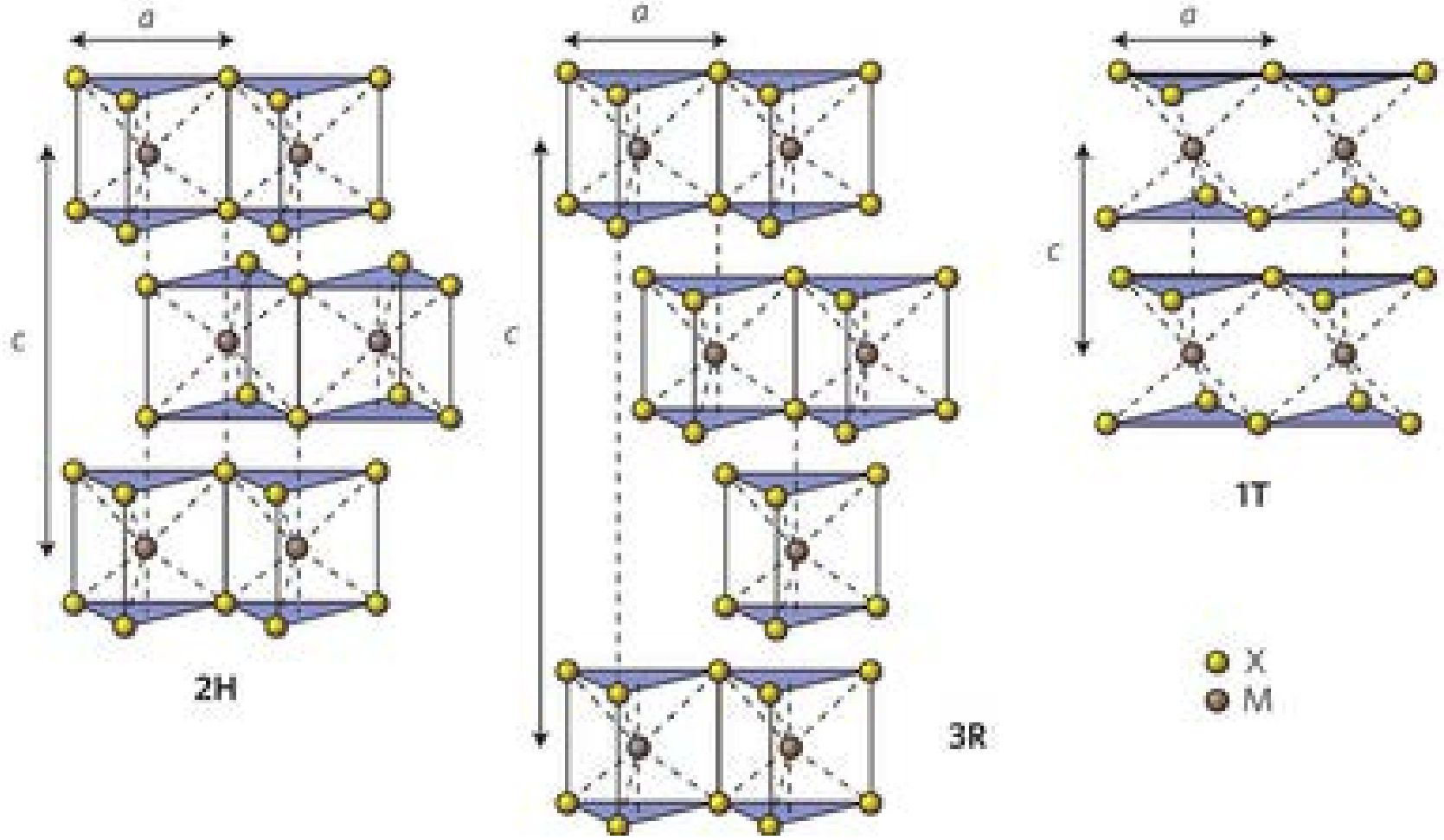
TMDC Materials: Crystal Structures



Nature Chemistry 5, 263–275 (2013)

Two polymorphs in monolayer : trigonal prismatic (1H) and octahedral (1T).

TMDC Materials: Crystal Structures

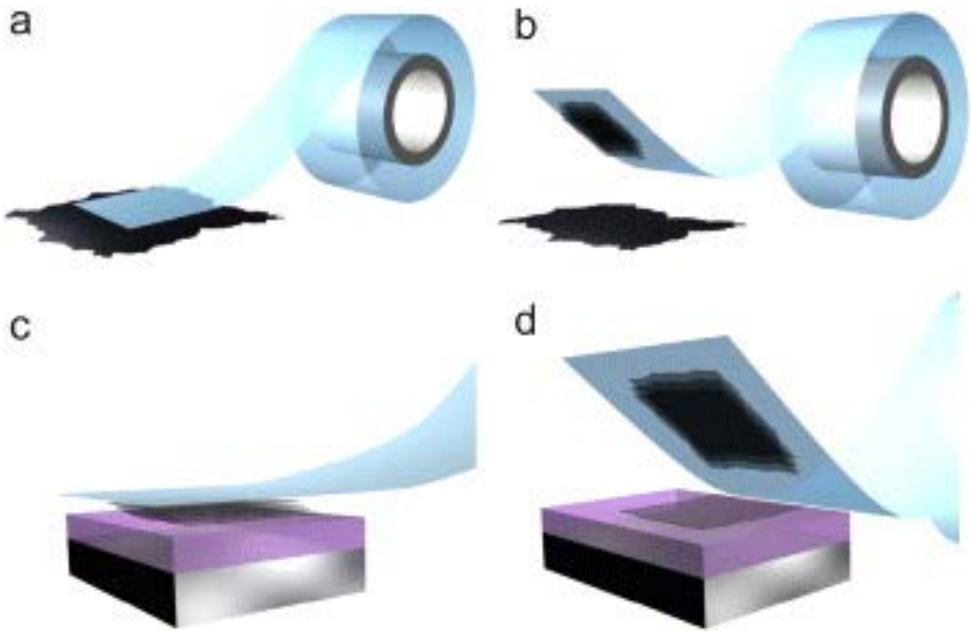


Bulk TMDCs exhibit a wide variety of polymorphs and stacking polytypes

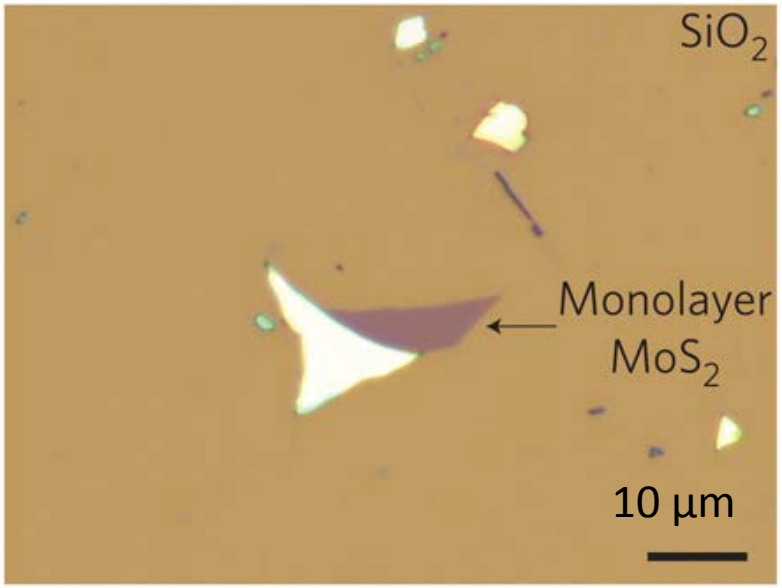
II. Synthesis and Transfer of 2D TMDC Materials/Heterostructres

II.1 Synthesis

Mechanical Exfoliation



Credit: K S Novoselov and A H Castro Neto

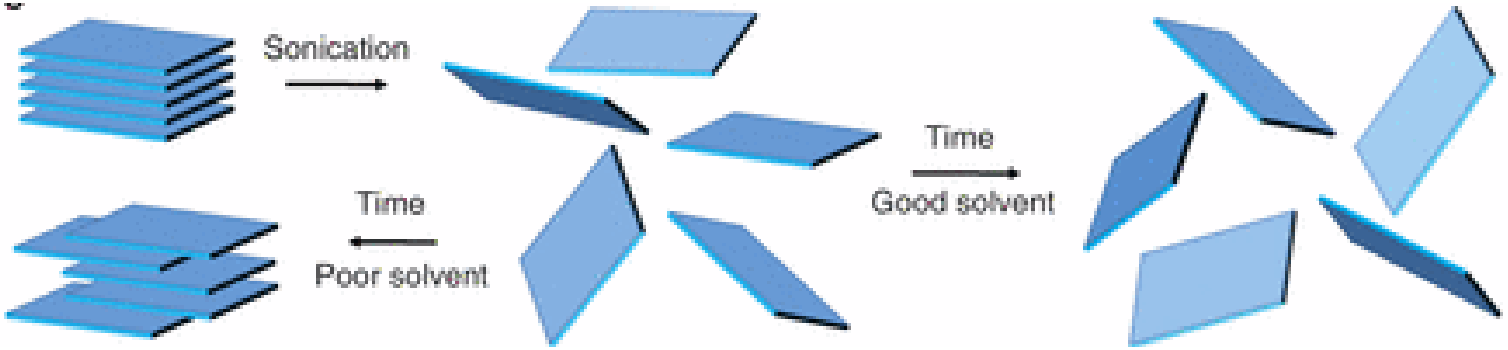


Nature Nanotechnology 6, 147–150 (2011)

- Low yield, not scalable
- Limited control in layer number
- Low uniformity (mixed layer numbers)
- Small size

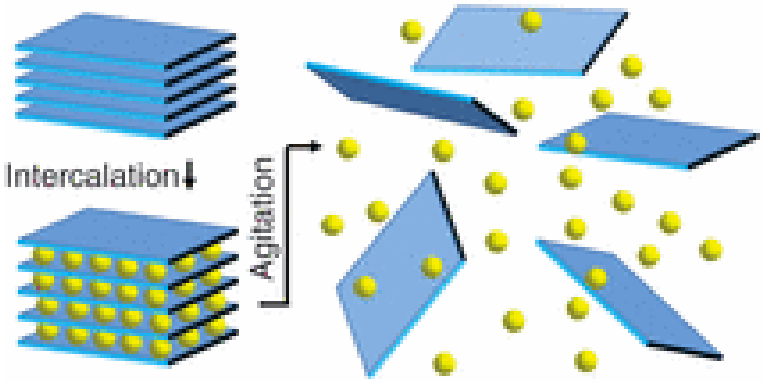
Liquid Exfoliation

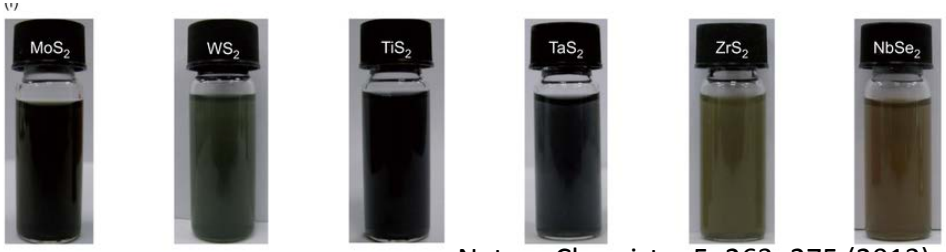
Sonication-assisted exfoliation (both monoalyer and fewlayers)



Key: good solvent (its surface energy is similar to that of the layered material, dimethylformamide or N-methyl-pyrrolidone), surface surfactant or polymer

Ion intercalation - assisted exfoliation





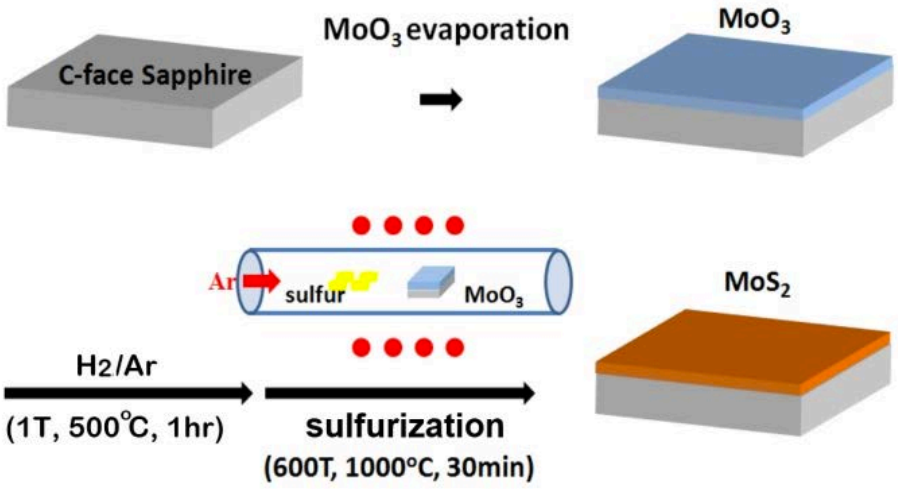
Nature Chemistry 5, 263–275 (2013)

Intercalants such as n-butyllithium in hexane (exclusively monolayers)

- Surface contamination
- Structure distortion or damage

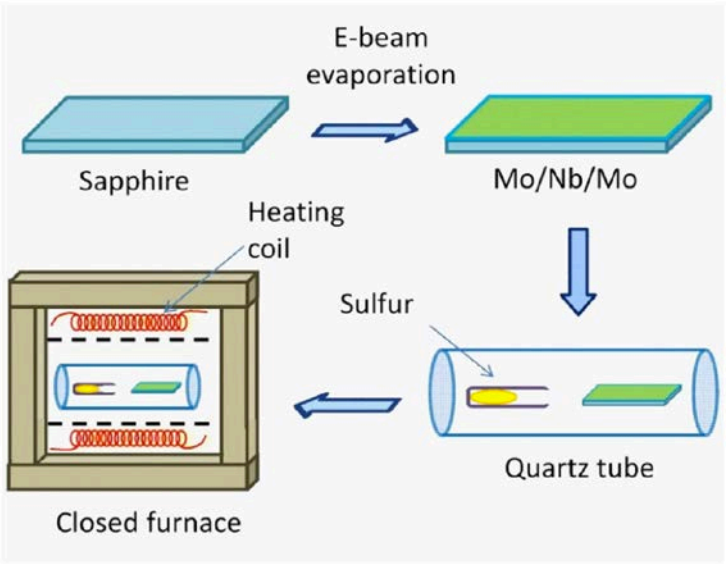
Sulfurization of Pre-deposited Precursors

Oxide precursor: MoO_3 or WO_3



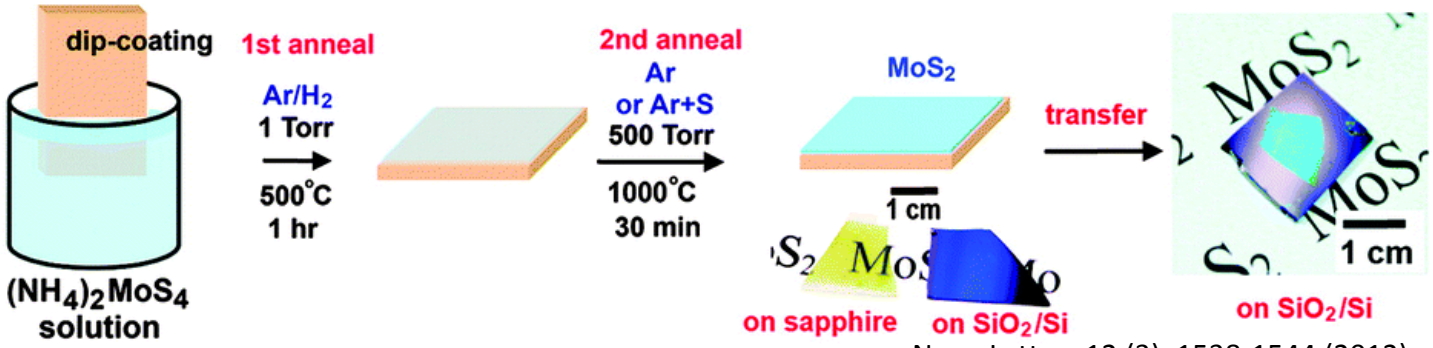
Nanoscale 4, 6637-6641 (2012)

Metal precursor: Mo or W



Applied Physics Letters, 102, 252108 (2013)

Thiosalt

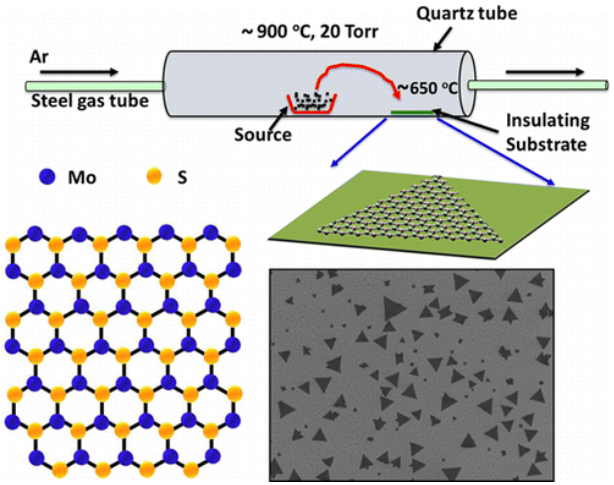


Nano Letters 12 (3), 1538-1544 (2012)

Uniformity & Control of layer number?

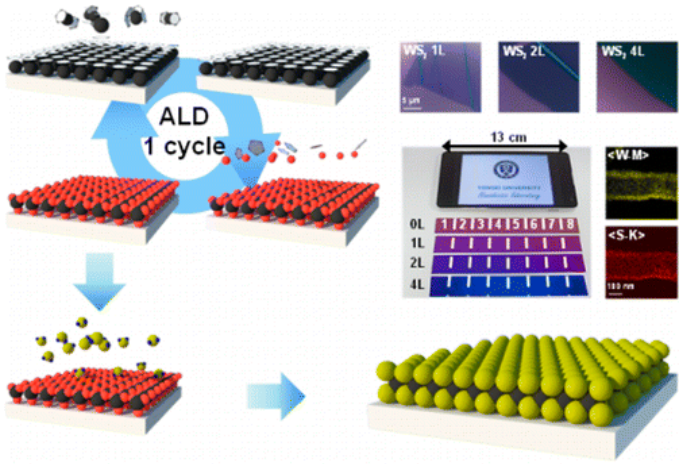
PVD, ALD, and MBE Growth

Physical vapor deposition

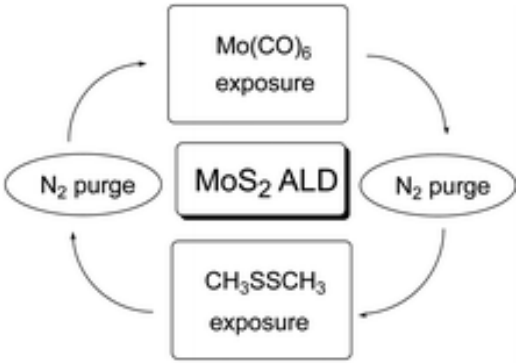


ACS Nano, 2013, 7 (3), pp 2768–2772

Atomic layer deposition

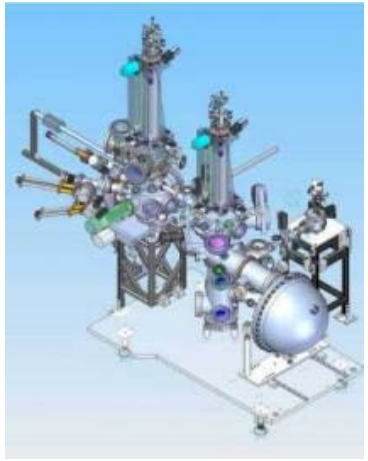


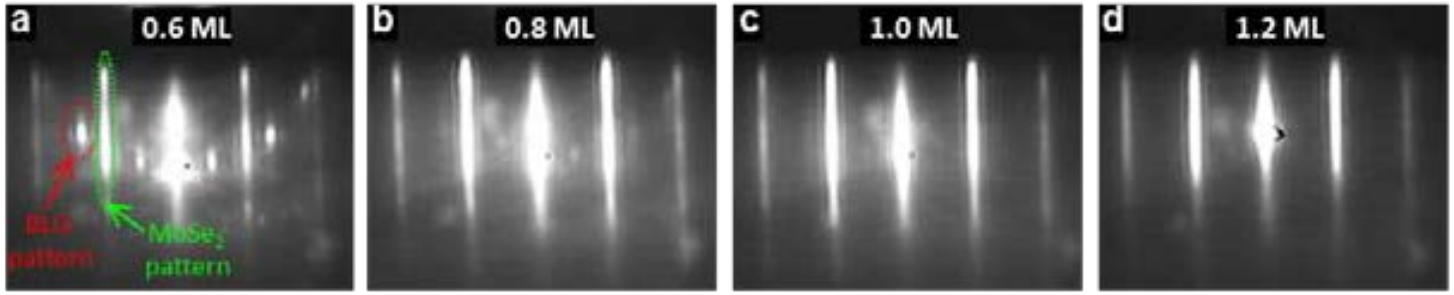
ACS Nano, 2013, 7 (12), pp 11333–11340



Nanoscale, 2014,6, 14453-14458

Molecular beam epitaxy (only MoSe2 reported to date)

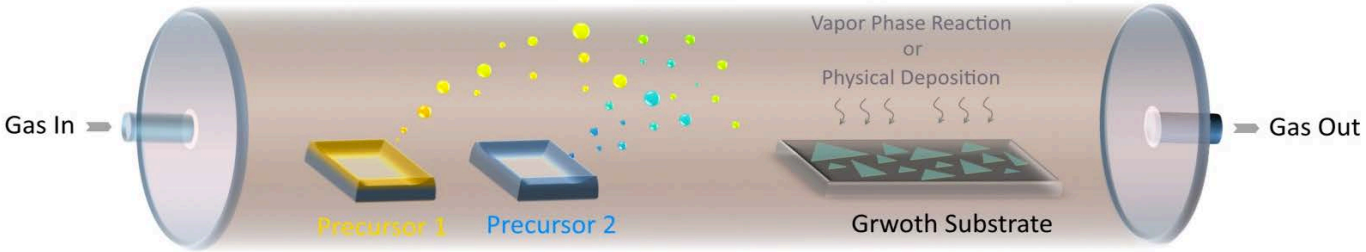




Nature Nanotechnology 9, 111–115 (2014)

Cost, Uniformity & Control of layer number?

Chemical Vapor Deposition: Oxide Precursor



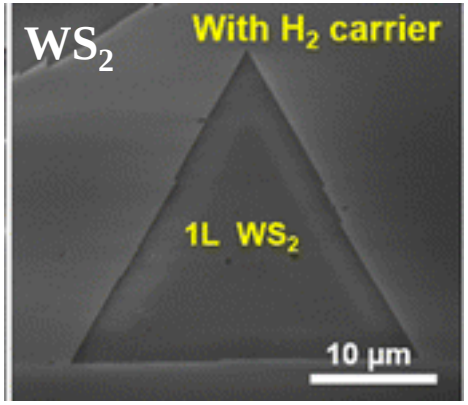
Credit: Lain-Jong Li

Precursor 1: S or Se

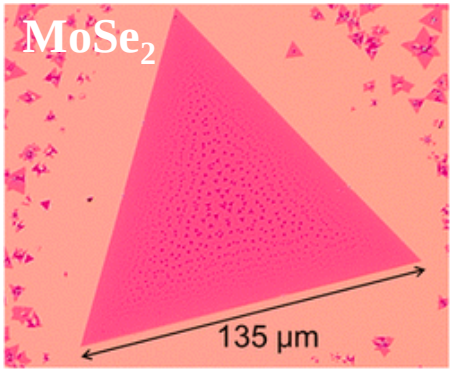
Precursor 2: MoO3 or WO3

Nat. Mater. 12, 554, **2013**

Nat. Mater. 12, 754, **2013**

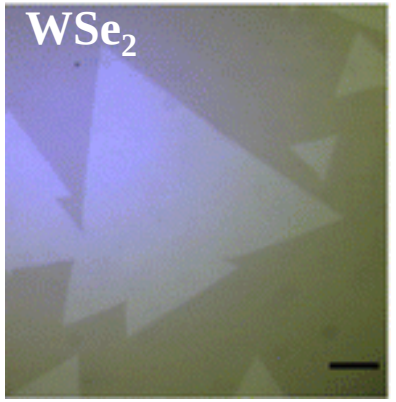


ACS Nano, 2013, 7 (10), 8963–8971



ACS Nano, 2014, 8 (5), 5125–5131

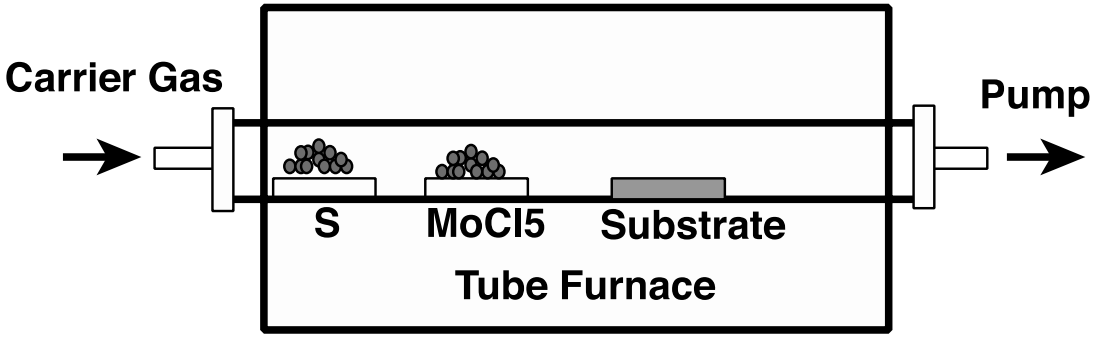
ACS Nano, 2014, 8 (8), 8582–8590



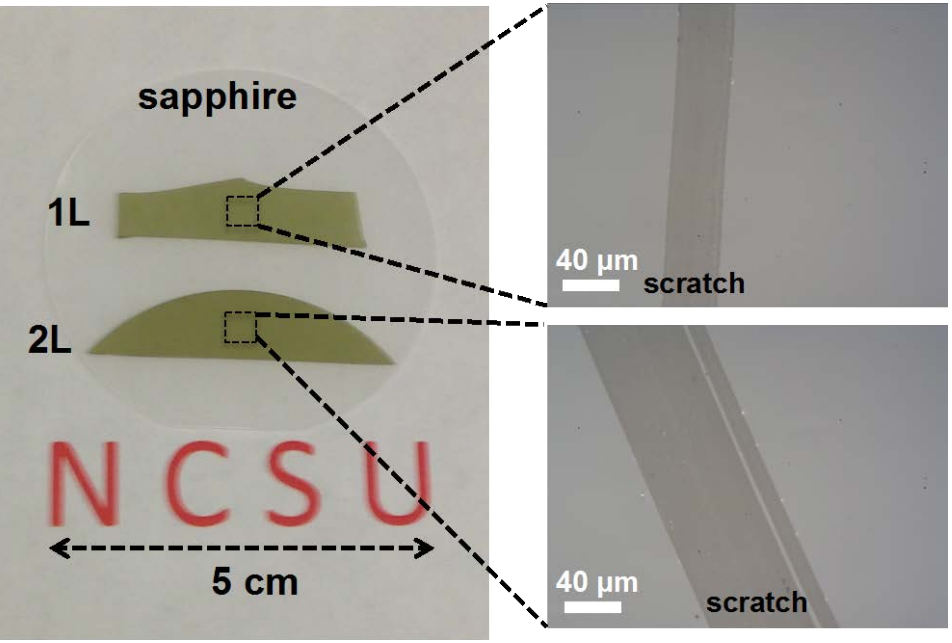
ACS Nano, 2014, 8 (1), 923–930

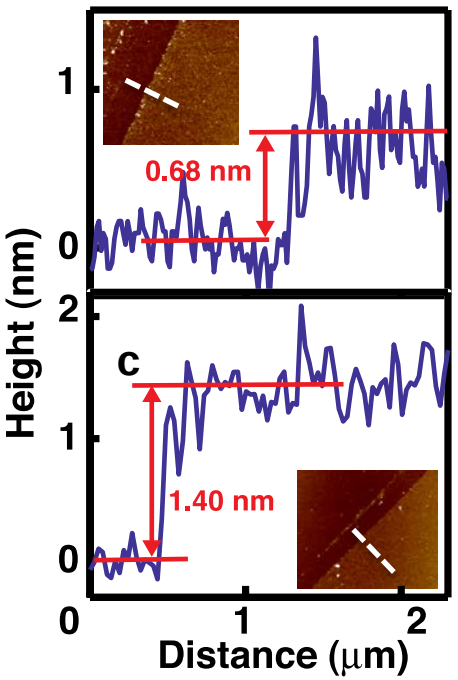
Large size & Control of layer number?

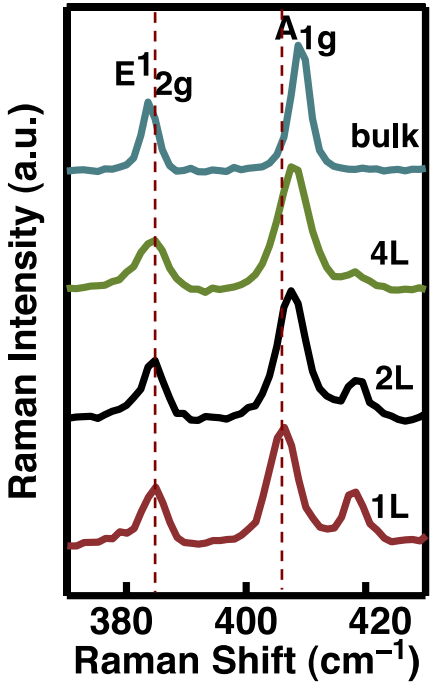
Self-limiting CVD Growth



Conditions:
- 850 °C
- 1-2 Torr
- 1-20 mg MoCl5
- 1 g sulfur
- Carrier gas: Ar



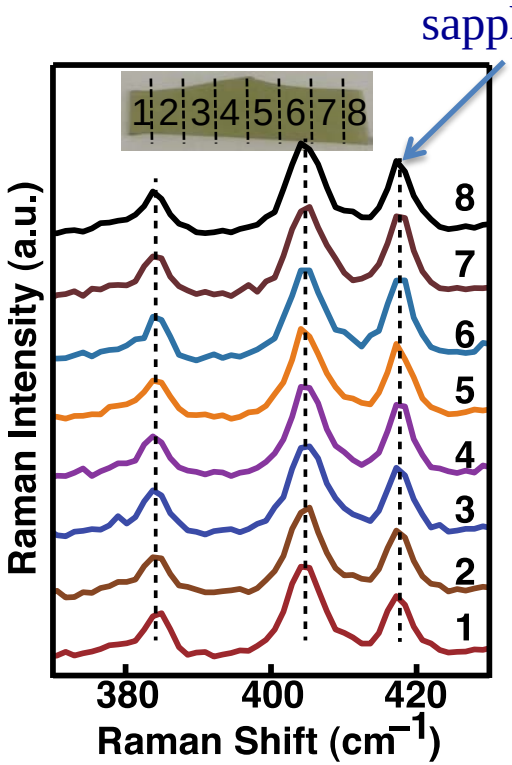




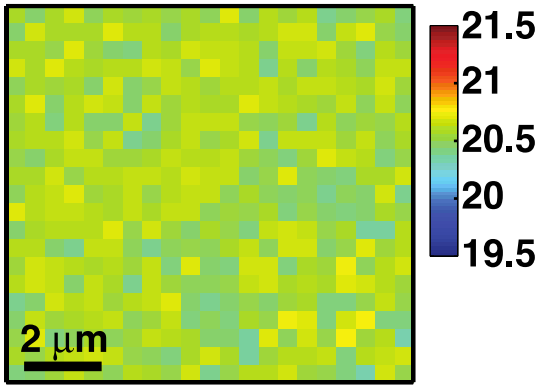
Growth of large-area, uniform monolayer and fewlayer MoS2.

Yifei Yu et al. *Sci. Rep.* 3, 1866, **2013**

Remarkable Uniformity



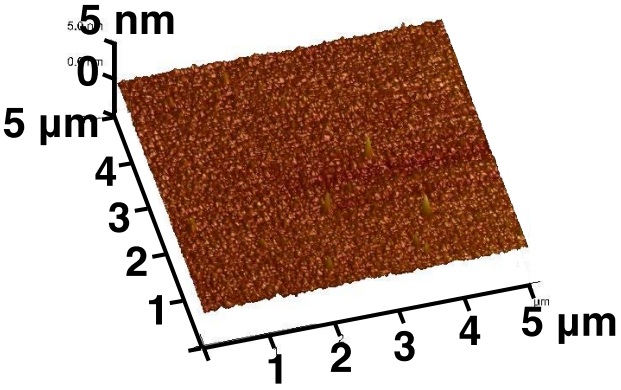
Raman mapping

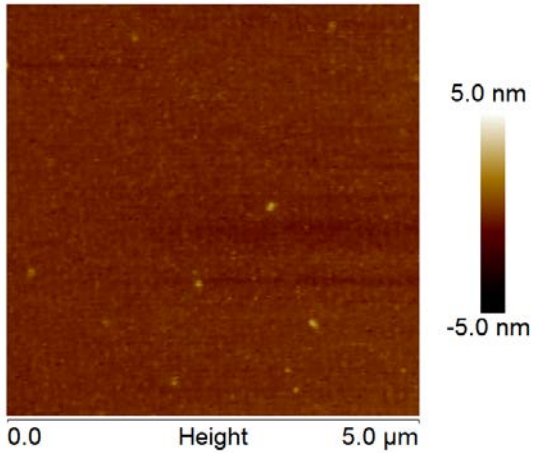


The frequency difference
Is in the range of 20.3 - 20.7 cm^{-1}

The frequencies of the A_{1g} and E^1_{2g} peaks remain constant cross the entire film!

Roughness < 0.2 nm



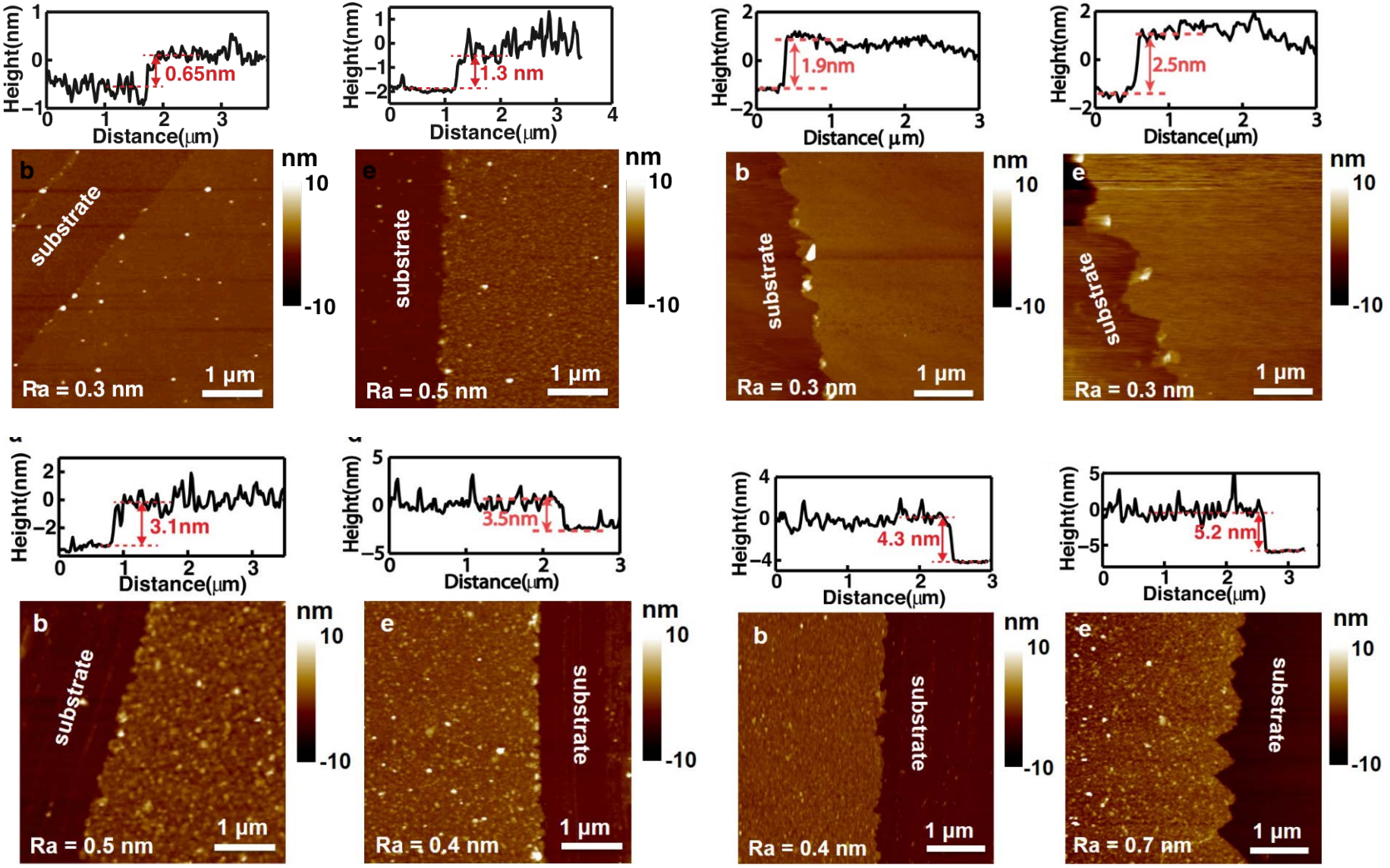


No void, step, edge!

The synthesized MoS2 film shows remarkable uniformity.

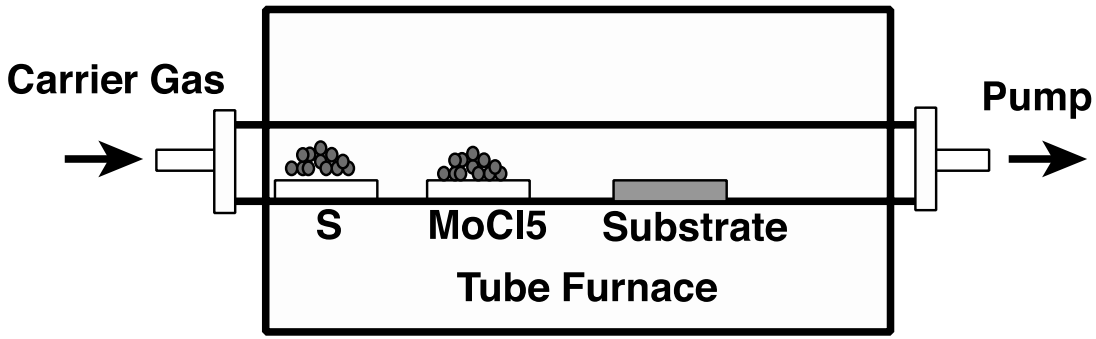
Yifei Yu et al. *Sci. Rep.* 3, 1866, **2013**

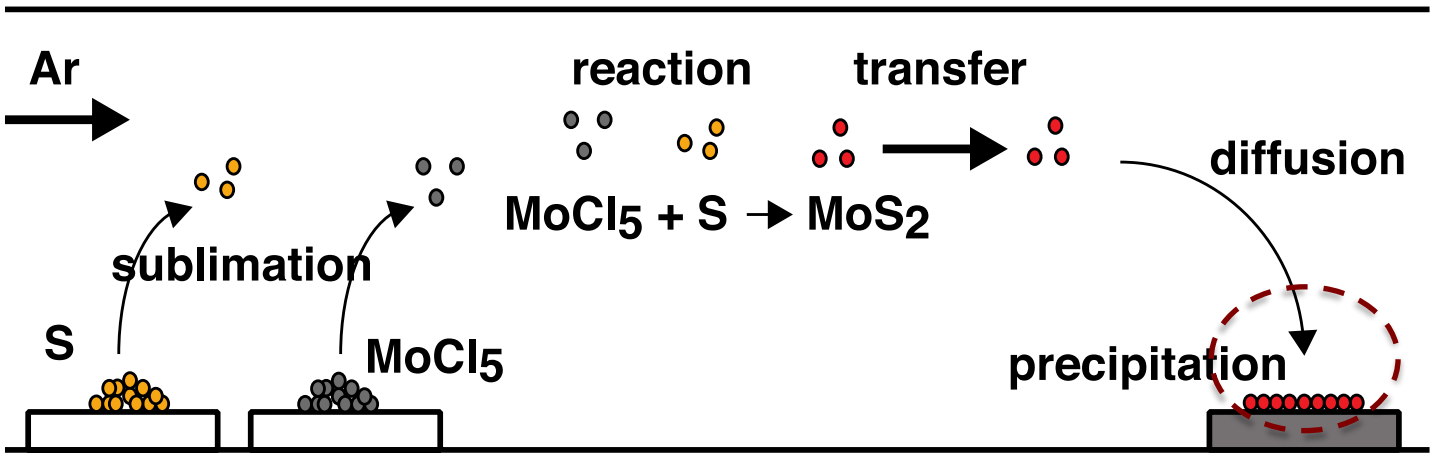
Precise Control of Layer Number



Key of Self-limiting Growth

Synthetic Setup





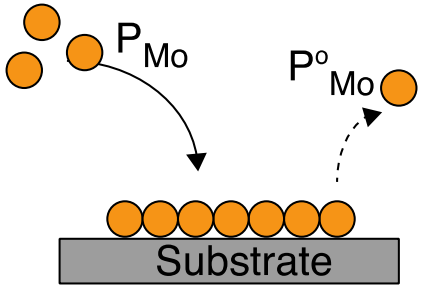
The rate-determining step is the precipitation reaction:

MoS_2 (g) ➔ MoS_2 (s)

Yifei Yu et al. *Sci. Rep.* 3, 1866, **2013**

Key of Self-limiting Growth

MoS_2 (g) ➔ MoS_2 (s)

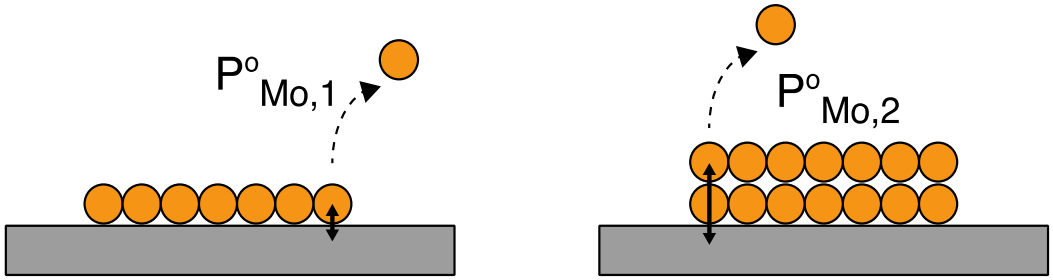


Two pressures dictate the precipitation:

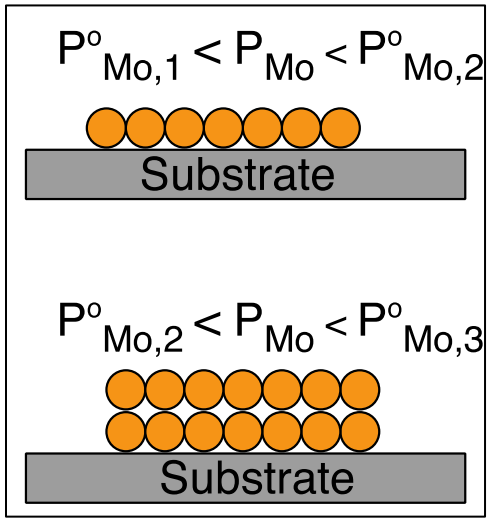
1. partial pressure of the gaseous MoS_2, P_{Mo}
2. vapor pressure of the MoS_2 film. P^o_{Mo}

To drive the precipitation, $P_{Mo} > P^o_{Mo}$

The balance between the partial pressure and the vapor pressure provides the self-limiting growth mechanism.



Layer dependent vapor pressure of the film due to interaction with the substrate.

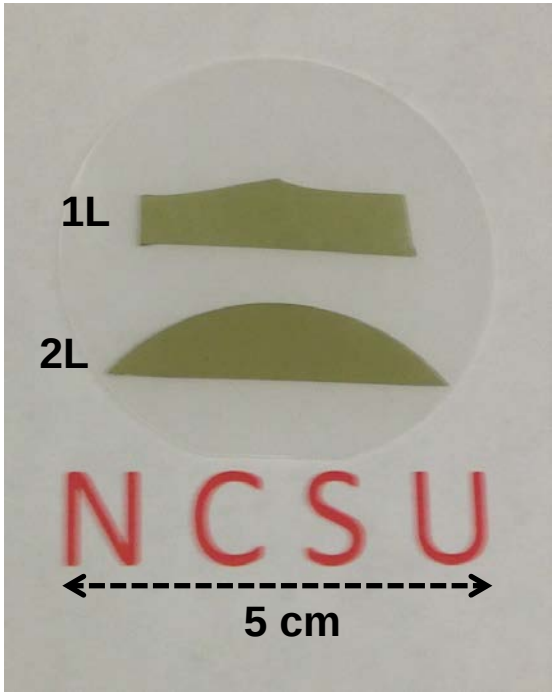


Yifei Yu et al. *Sci. Rep.* 3, 1866, **2013**

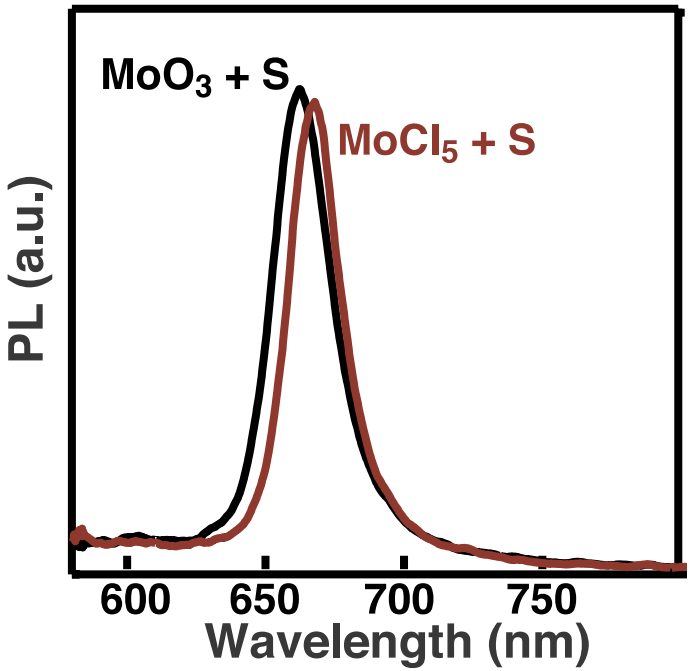
Key Advantages of Self-limiting CVD Growth

Self-limiting CVD

MoCl5 +S

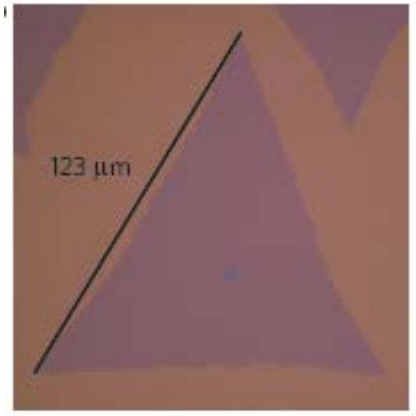


Comparable Quality

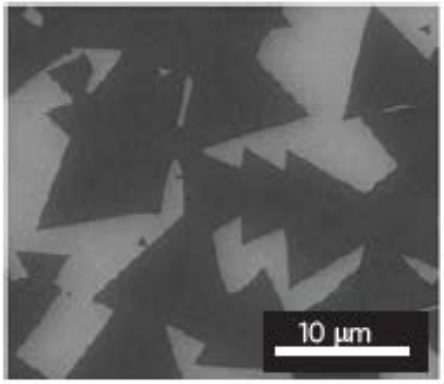


Other CVD Method

MoO3 +S



Nat. Mater. 12, 554, **2013**



Nat. Mater. 12, 754, **2013**

Key advantage of the self-limiting CVD approach :

- Much larger size (5 cm vs mm)
- Control of layer numbers

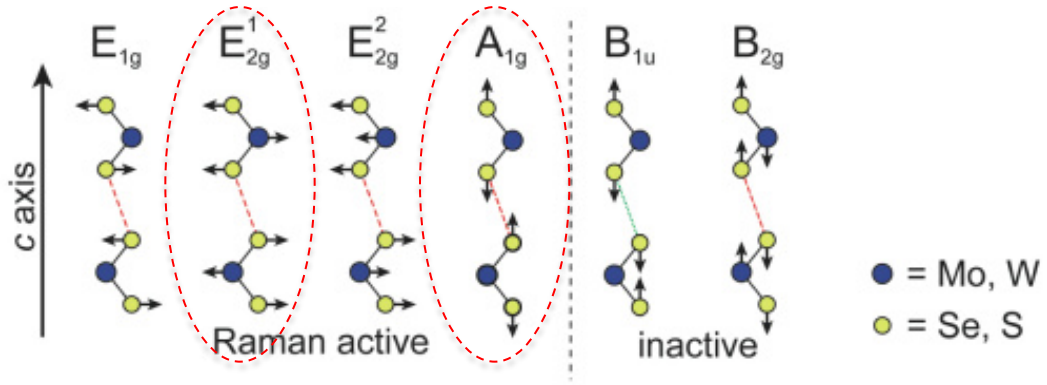
Yifei Yu et al. *Sci. Rep.* 3, 1866, **2013**

II. Fundamental Properties

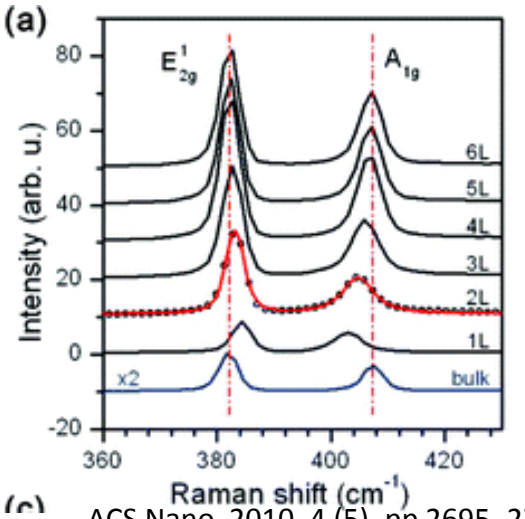
III.1 Raman

Raman vs. Layer Number

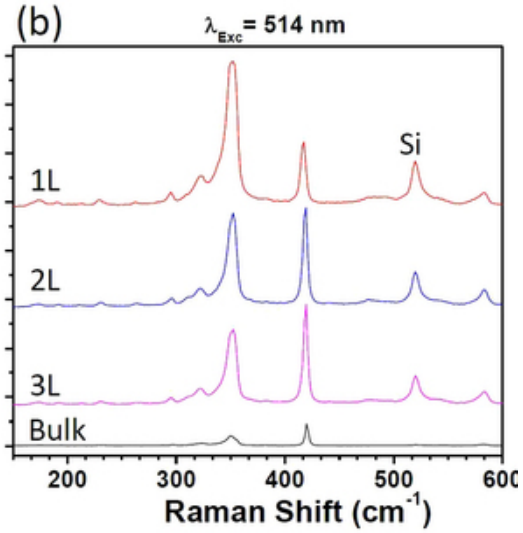
Two most important modes



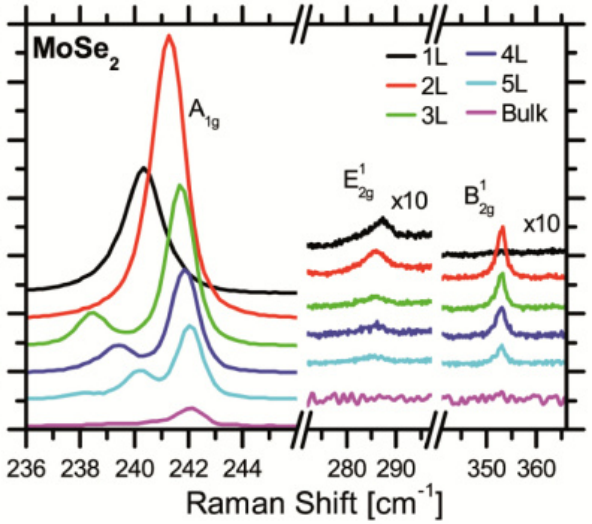
Optics Express, Vol. 21, Issue 4, pp. 4908-4916 (2013)

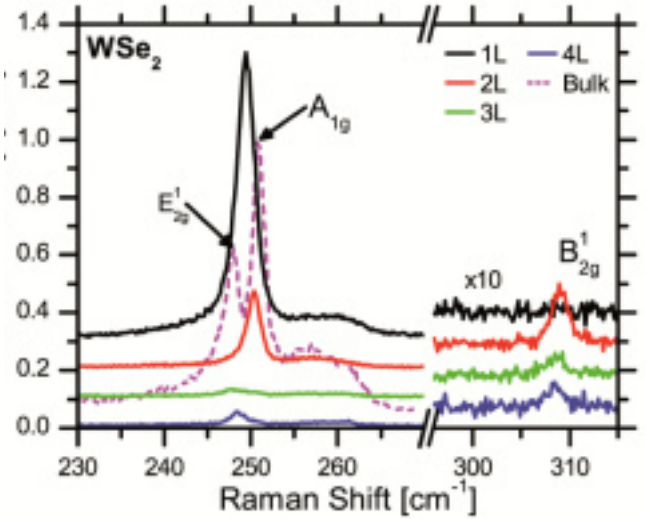


ACS Nano, 2010, 4 (5), pp 2695–2700



Scientific Reports 3, Article number: 1755



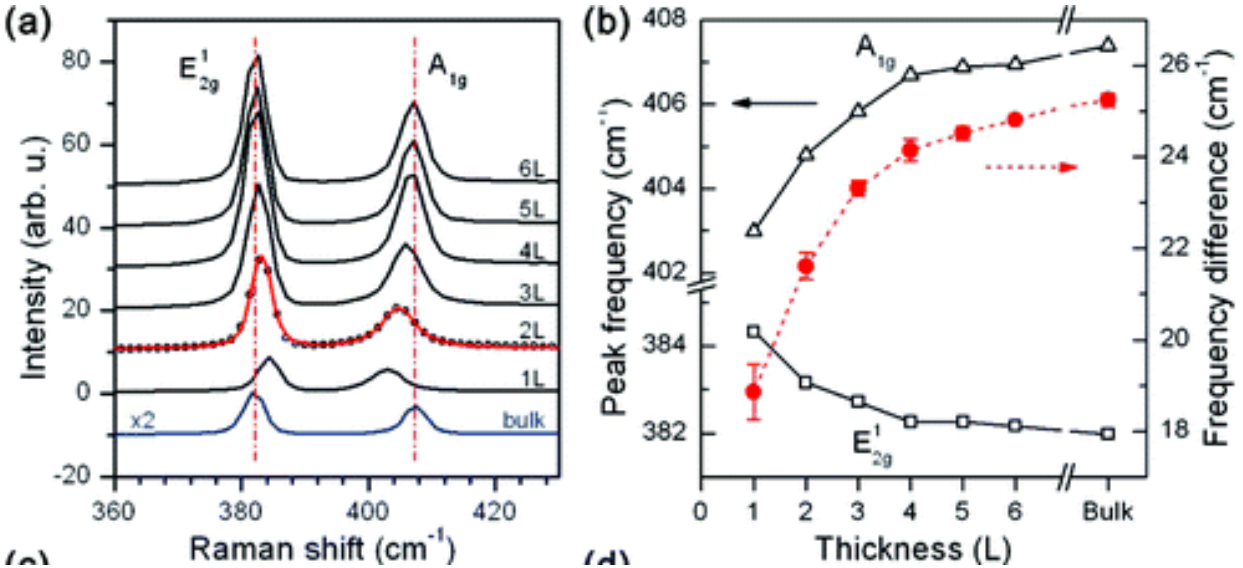


Optics Express, Vol. 21, Issue 4, pp. 4908-4916 (2013)

Raman intensity and peak position depend on the layer number.

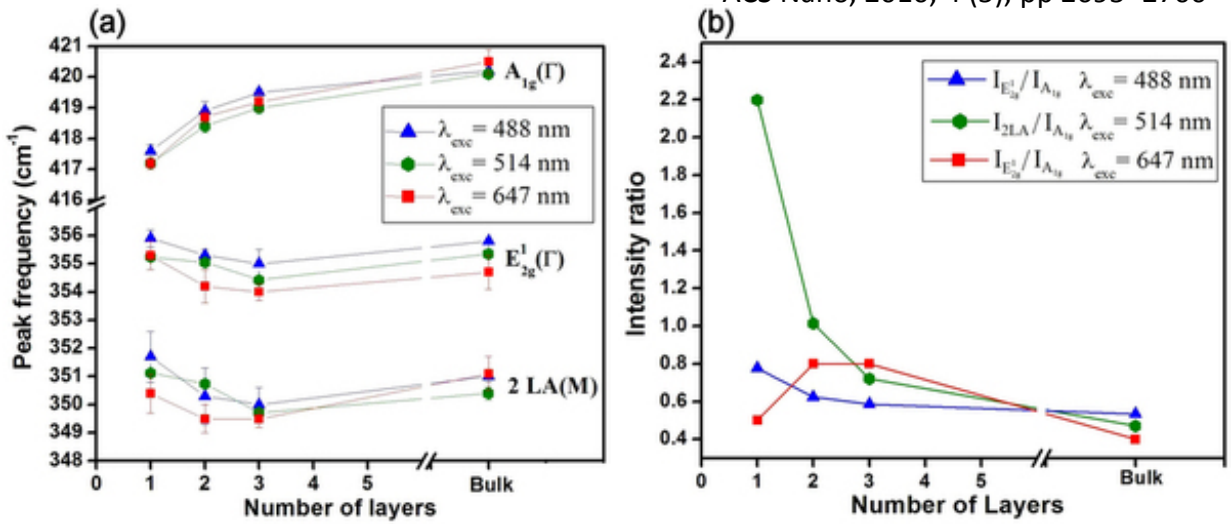
Raman vs. Layer Number

MoS2



ACS Nano, 2010, 4 (5), pp 2695–2700

WS2



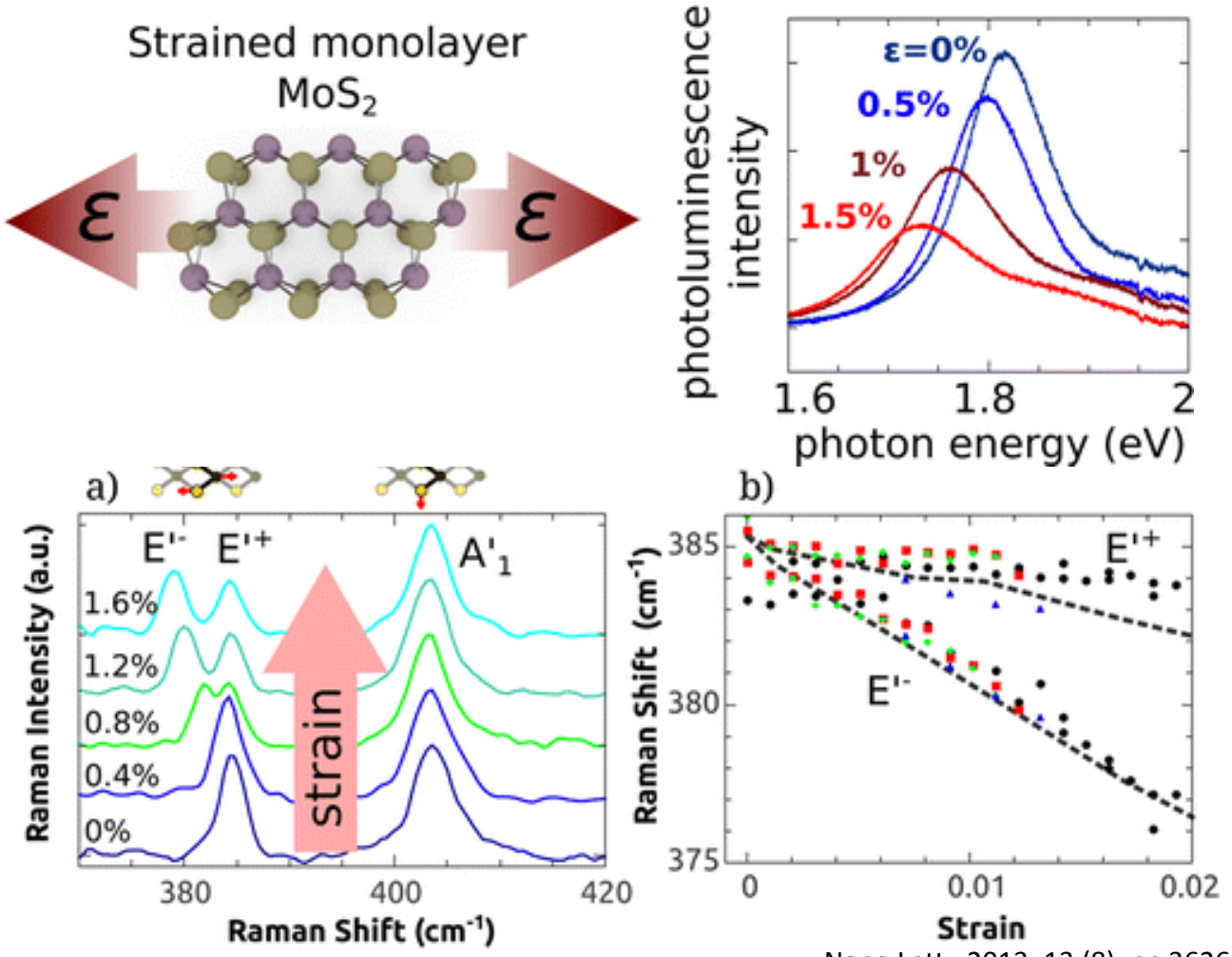
Scientific Reports 3, Article number: 1755

Raman can serve as a credible tool to indentify the layer number.

Raman vs. Strain

E′–:
4.5 ± 0.3 cm–1/% strain 1L
4.6 ± 0.4 cm–1/% strain 2L

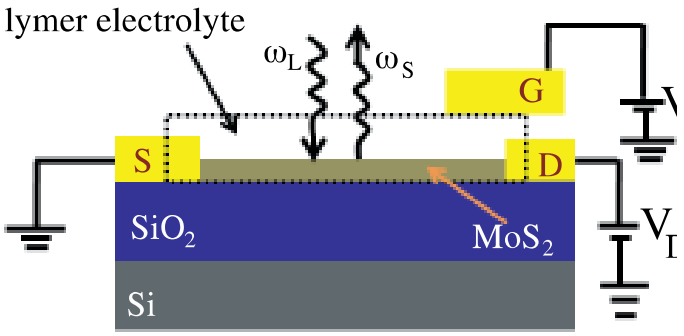
E′+:
1.0 ± 1 cm–1/% strain 1L
1.0 ± 0.9 cm–1/% strain 2L

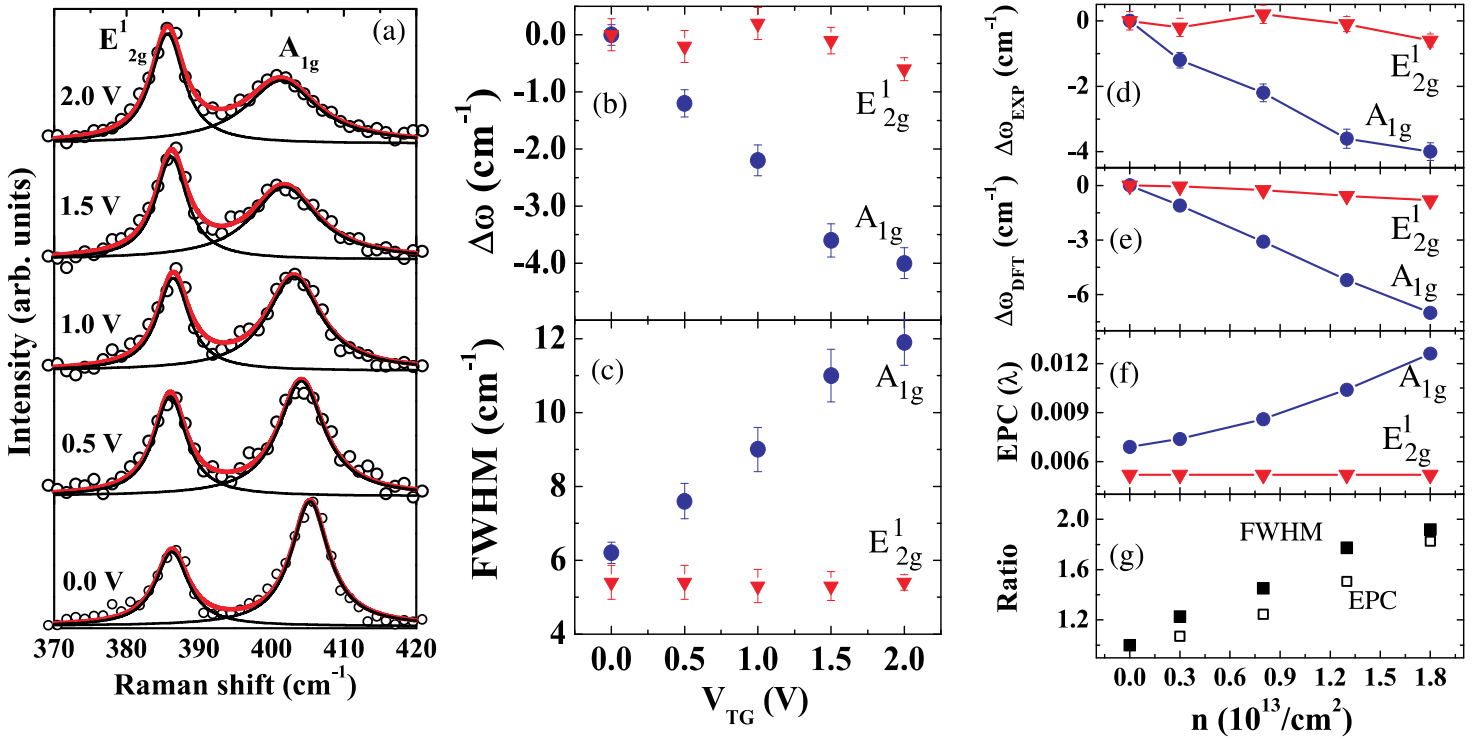


Nano Lett., 2013, 13 (8), pp 3626–3

- **the A_{1g} peak shows no measurable shift in position**
- **the degenerate E′ peak splits into two subpeaks**

Raman vs. Carrier Concentration

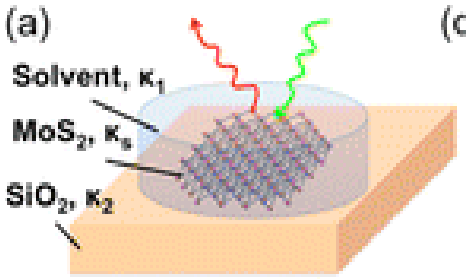


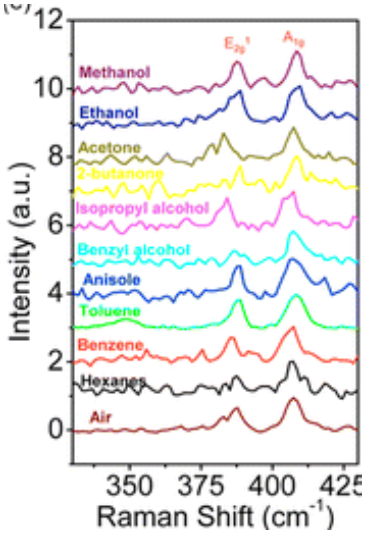


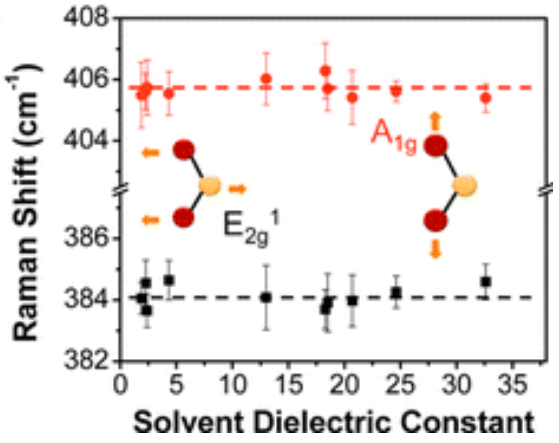
Phys. Rev. B 85, 161403(R), 2012

A_{1g} strongly depends on the carrier concentration.

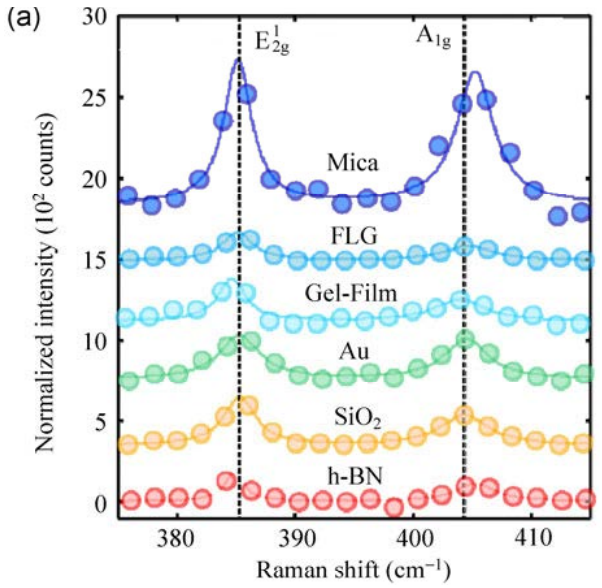
Raman vs. Substrate/Dielectric Screening

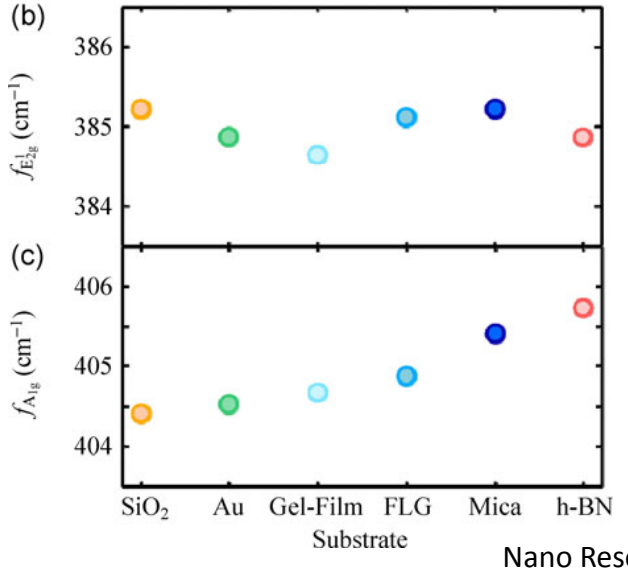






Nano Lett., 2014, 14 (10), pp 5569–5576





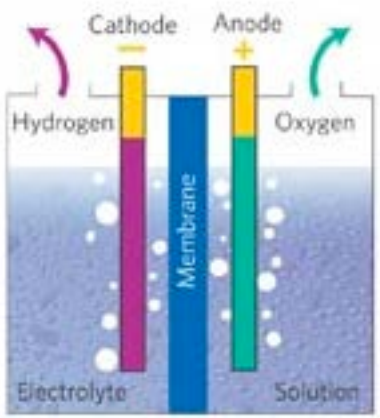
Nano Research 2014, 7(4): 561–571

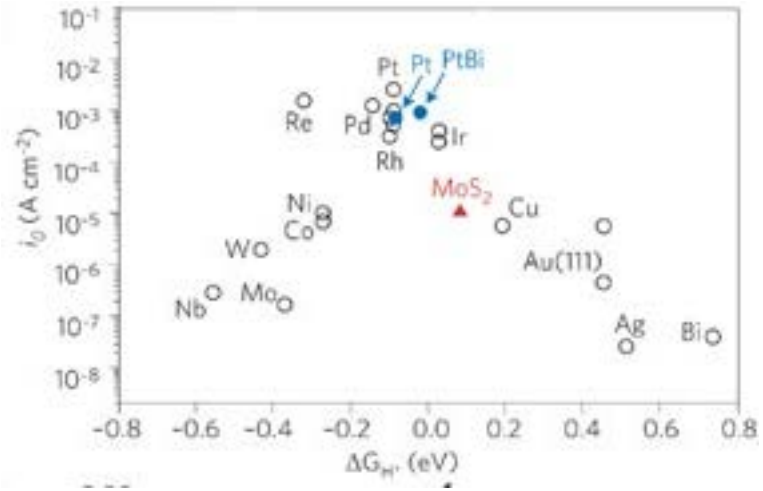
- **No obvious dependence on the dielectric environment, but substantial dependence on the substrate (doping, strain).**

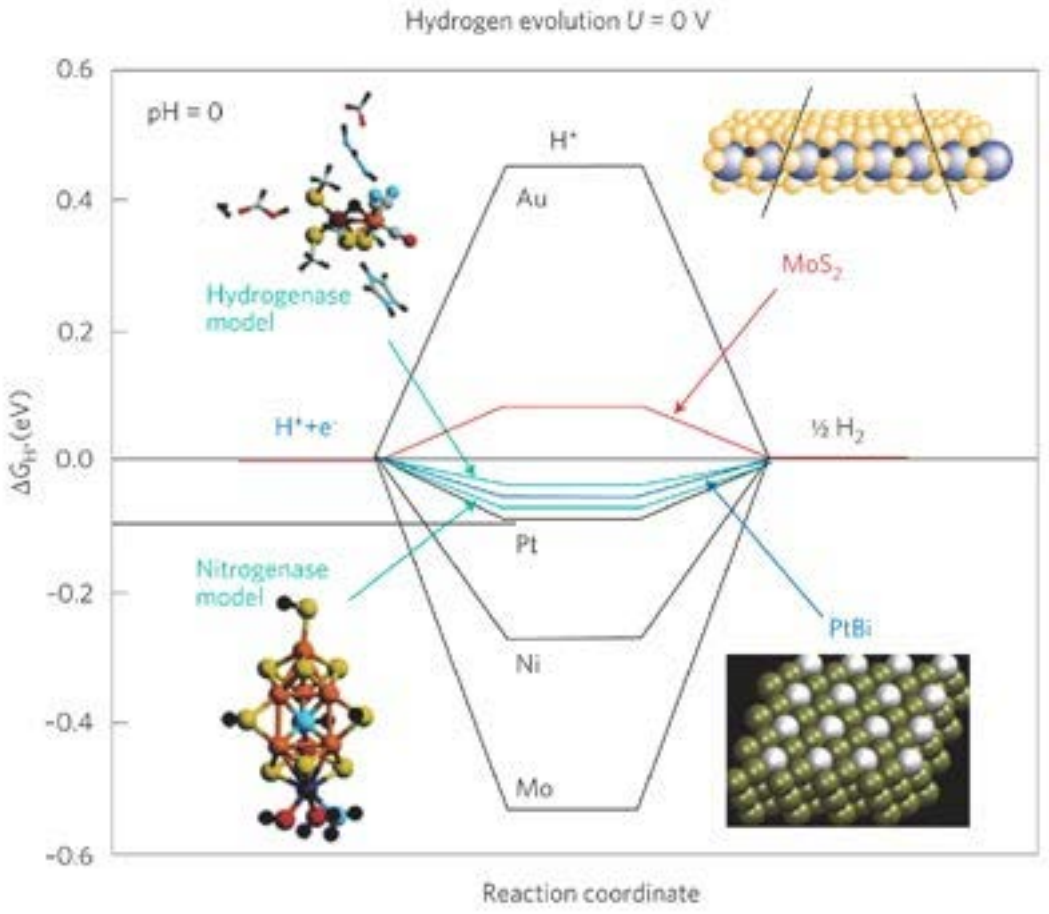
III. Fundamental Properties

III.2 Catalytic Properties

MX2 (M= Mo, W, X= S, Se): HER Catalyst





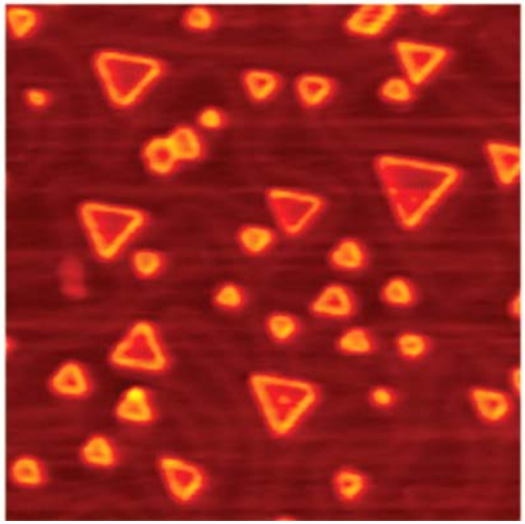


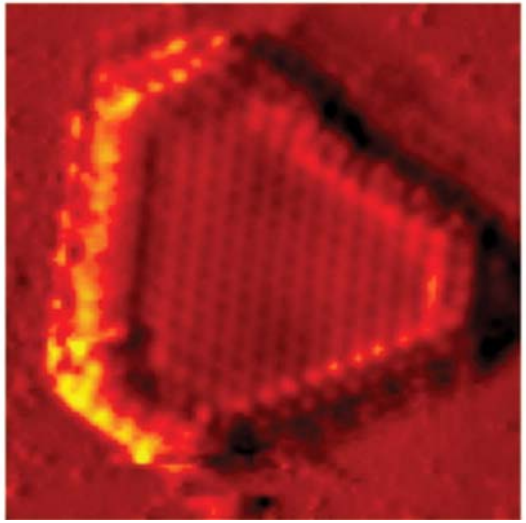
Nature Chemistry 1, 37 - 46 (2009)

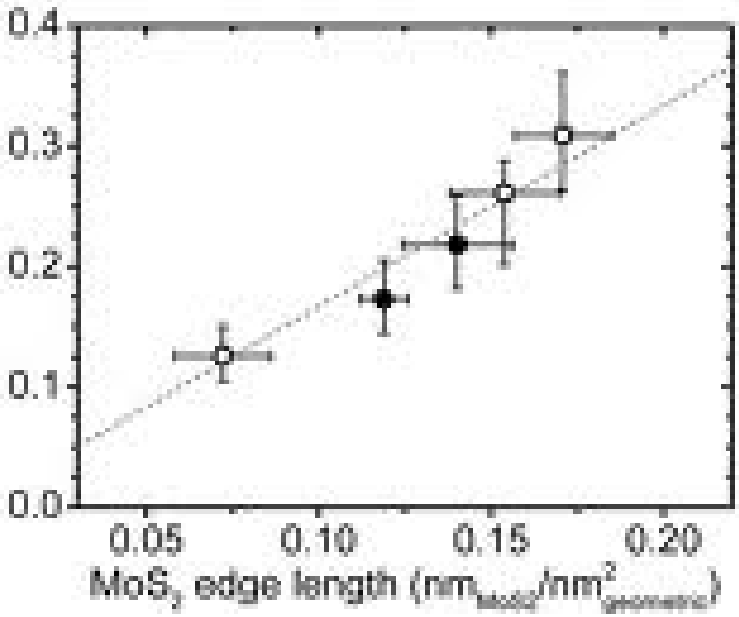
MX2 (M= Mo, W, X= S, Se) are predicted as good catalysts for the hydrogen evolution reaction (HER)

Current Theory: Edge Sites Matter.

MoS2



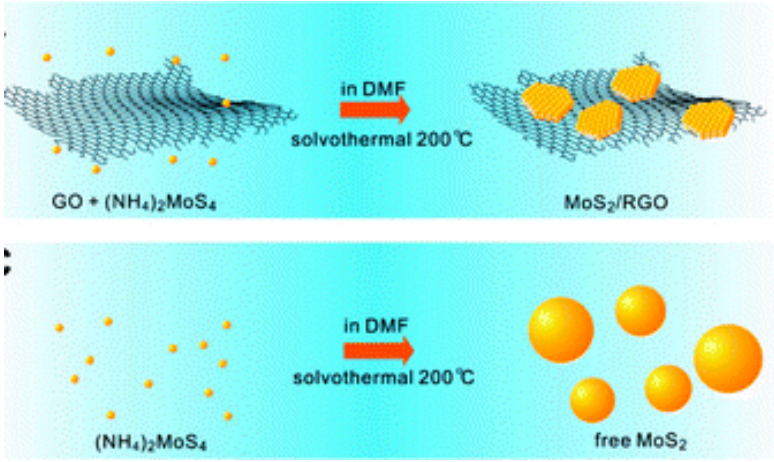


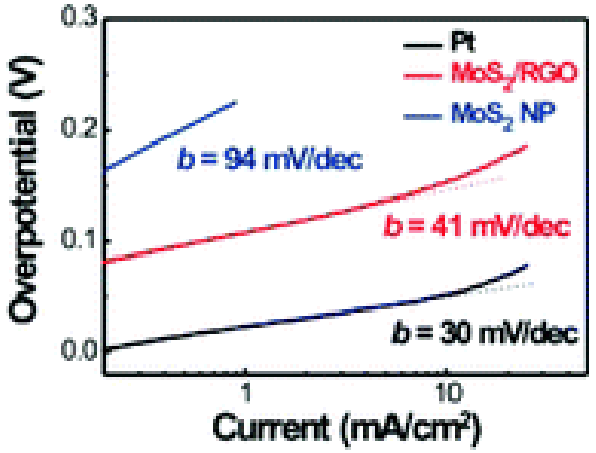


Science 6 July 2007:
vol. 317 no. 5834 100-102

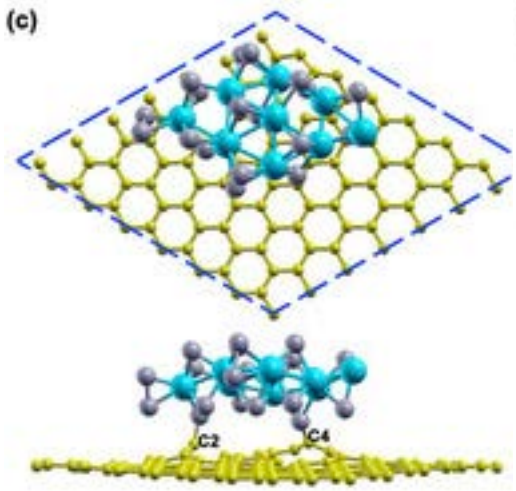
Conventional wisdom: **exchange current density is proportional to the number of edge sites.**

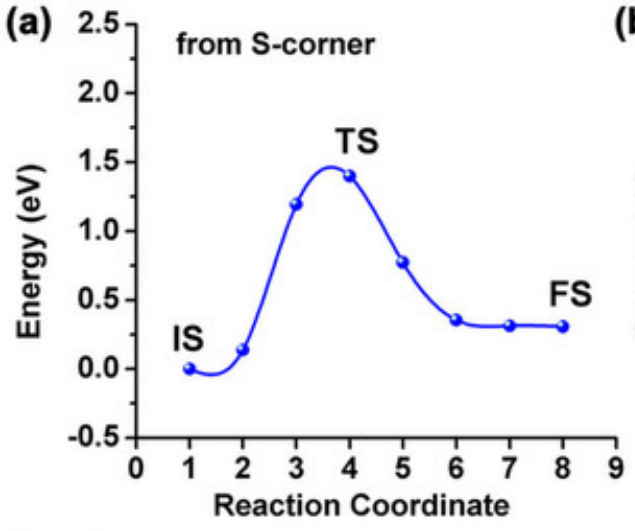
Recent Studies: Coupling with Graphene

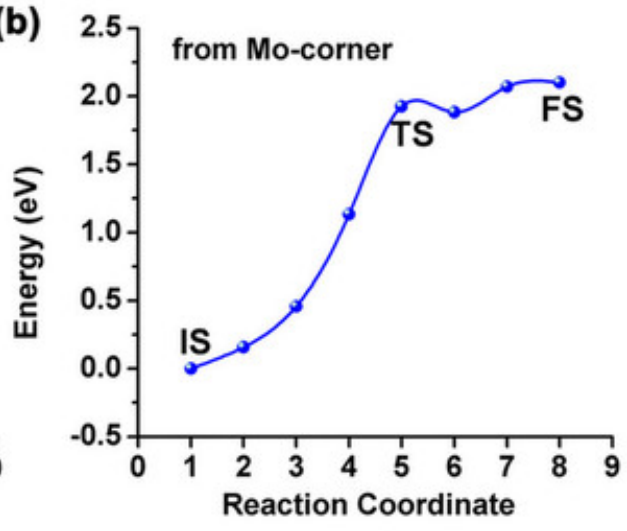




J. Am. Chem. Soc., 2011, 133 (19), pp 7296–7299



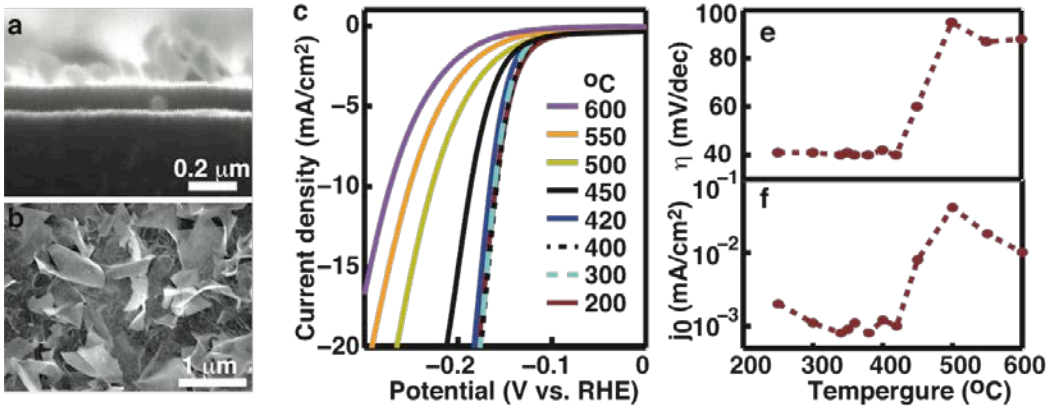




Scientific Reports 4, Article number: 6256

The electronic coupling with graphene is helpful.

Recent Studies: Composition and Crystallinity



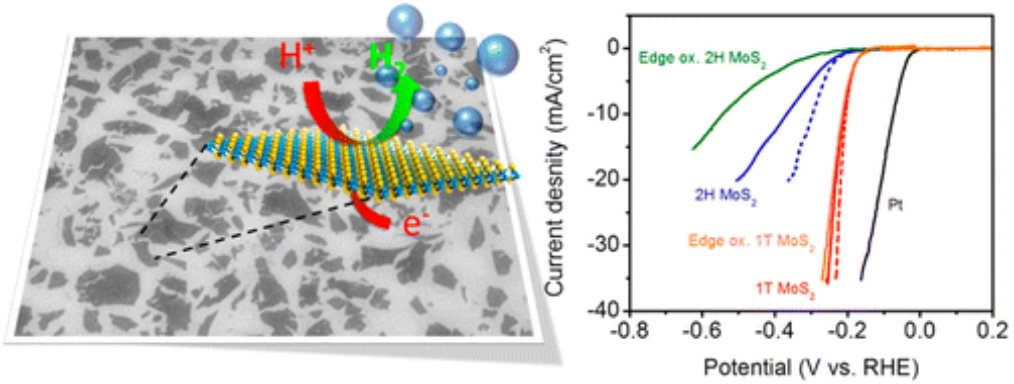
	Compositio n	Structure	Tafel slope (mV/dec)	J_0 (μA/ cm²)	Capacita nce (mF/ cm²)	TOF (10^{-3} s^{-1})
200°C - 380°C	MoS_3	amorphous	39	~1-2	10-20	0.01-0.03
400°C	MoS_3 (70%) MoS_2 (30%)	amorphous nanocrystalline	42	1.2	10	0.027
420°C	MoS_3 (40%) MoS_2(60%)	amorphous nanocrystalline	40	1.0	12	0.012
450°C	MoS_2	polycrystalline	50-60	8	8	0.14
500°C - 600°C	MoS_2	single crystalline	80-90	10-40	0.5-1.5	2.5-3.5

ACS Catal., 2015, 5 (1), pp 448–455

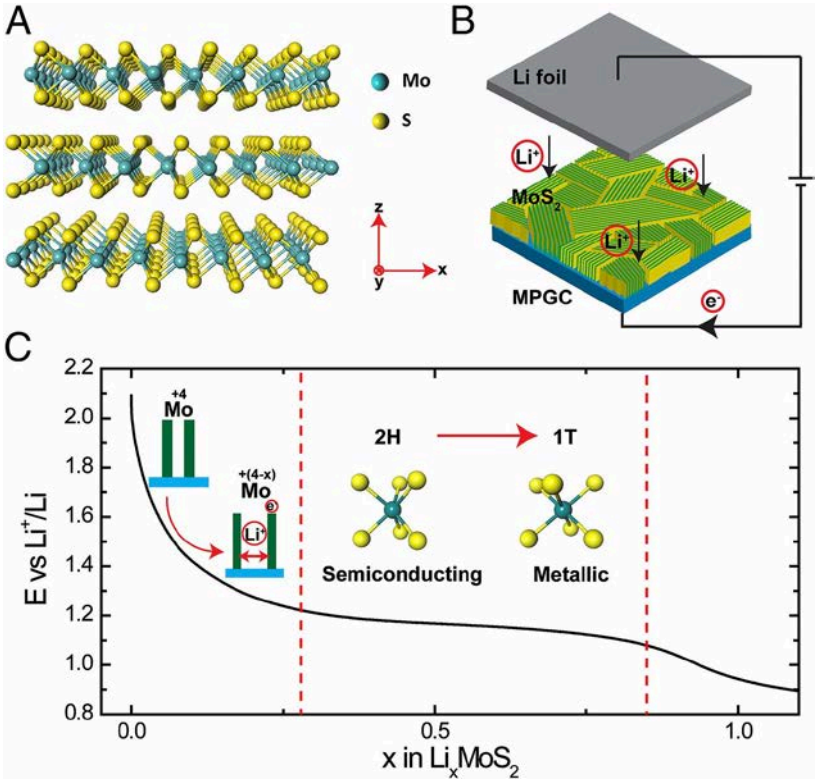
1. The stoichiometric ratio of Mo: S does not matter much.
2. The crystallinity may affect the Tafel Slope and TOF in opposite ways
   Low crystallinity: 40 mV/dec and low TOF
   Highly crystalline : 80-90 mV/dec and high TOF

Does Edge Sites Really Matter?

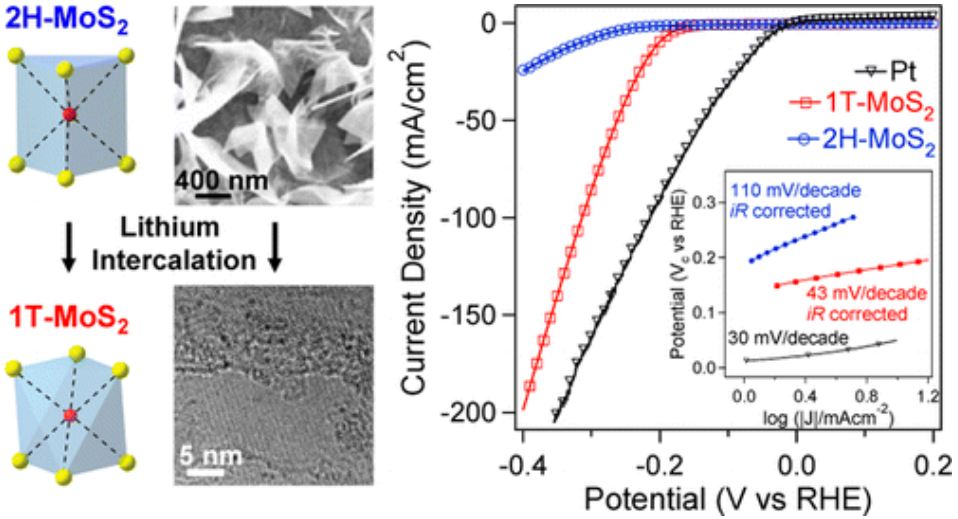
Recent Studies: Not Just Edge Sites



Nano Lett., 2013, 13 (12), pp 6222–6227



PNAS, 2013, vol. 110, 19701–19706

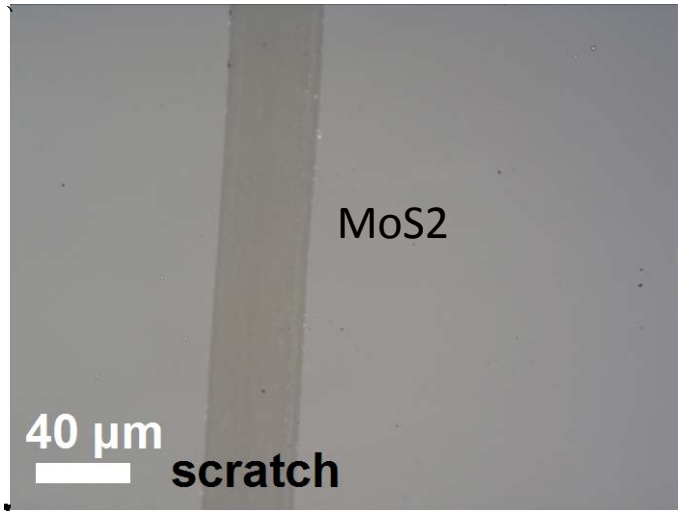


J. Am. Chem. Soc., 2013, 135 (28), pp 10274–10277

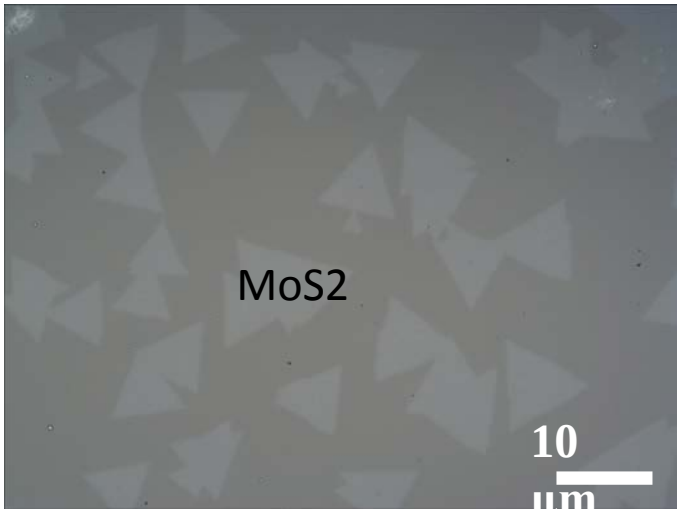
1T-MoS2 is better than 2H-MoS2 in terms of catalyzing the HER.

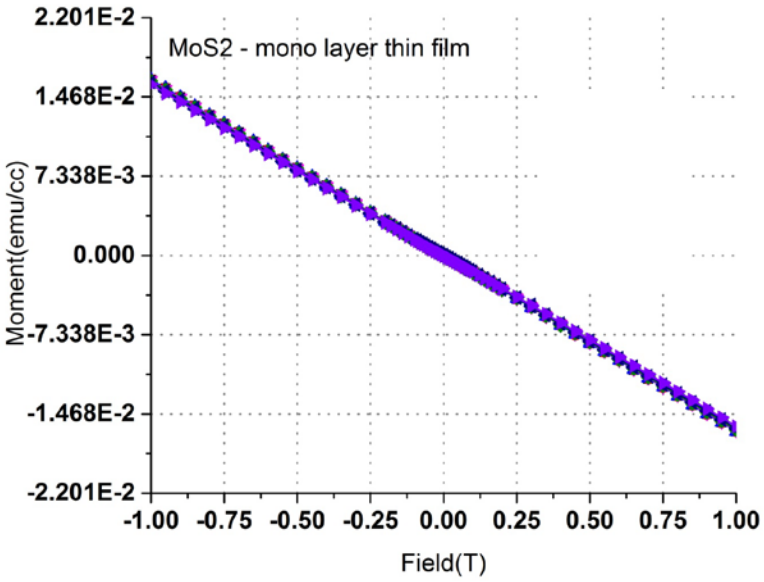
Does The Edge Sites Really Matter?

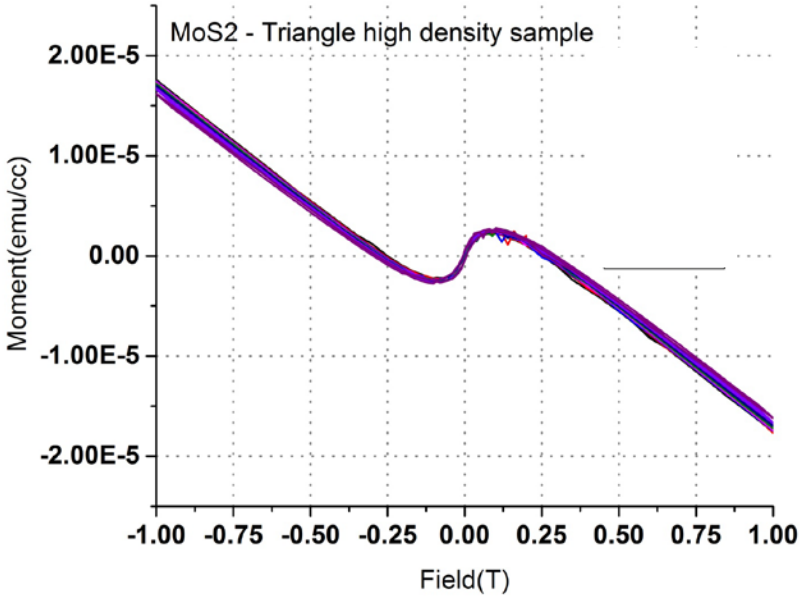
Continuous Film



Discontinuous MoS2 Flakes





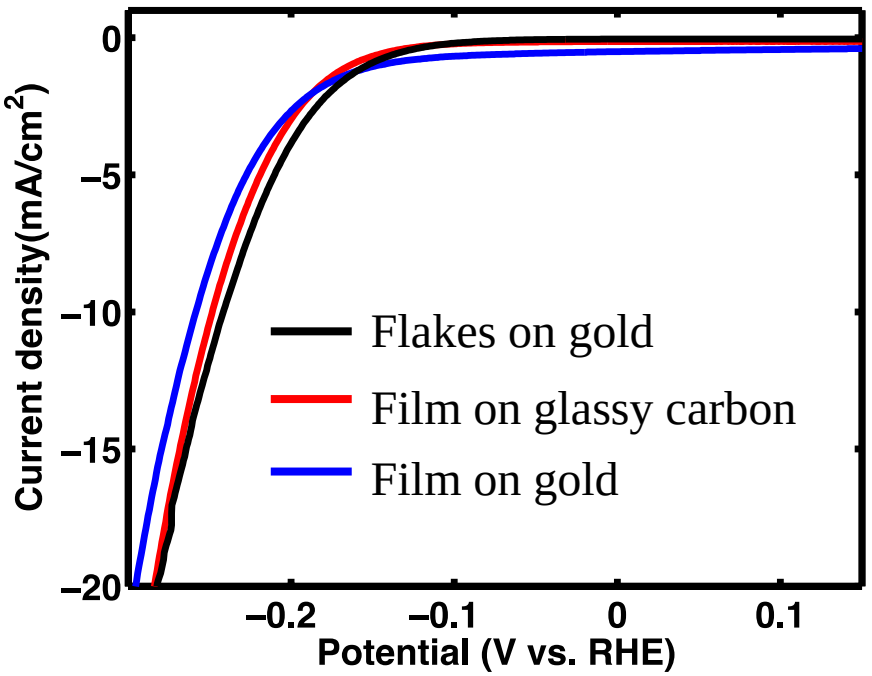


Magnetic measurements indicate No substantial edge sites in the film

Unpublished Results

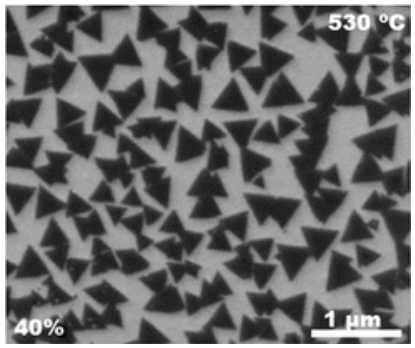
Does The Edge Sites Really Matter?

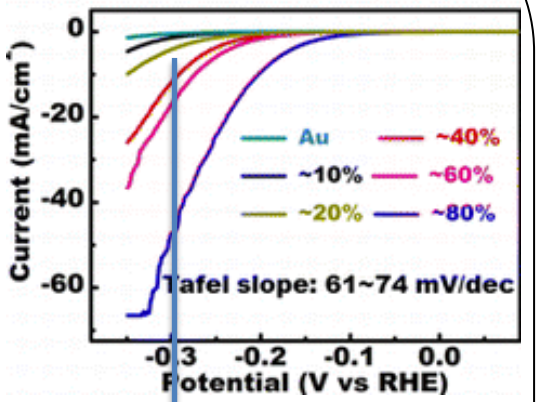
Exchange current density: 25-40 μA/cm2
Tafel slope: 75mV/dec



Submitted

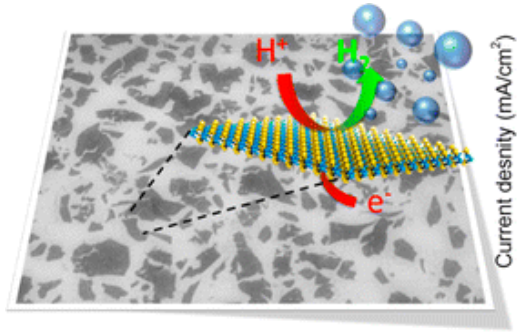
36.8μA/cm2 and 61-74 mV/dec

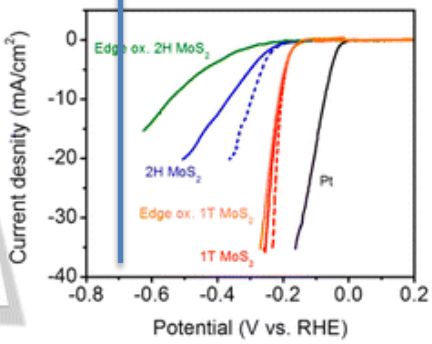




ACS Nano, 2014, 8 (10), pp 10196–10204

?? μA/cm2 and 75-85 mV/dec



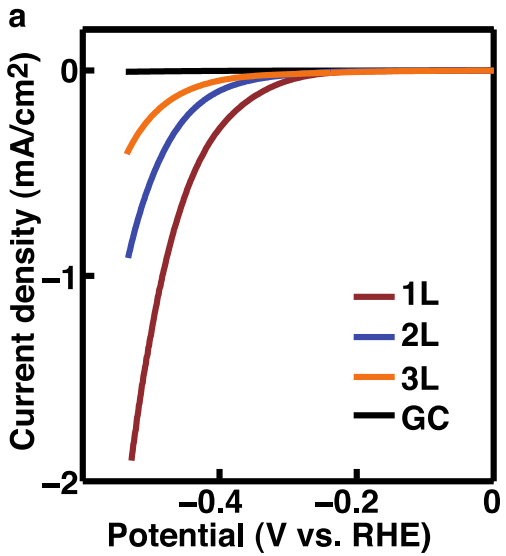


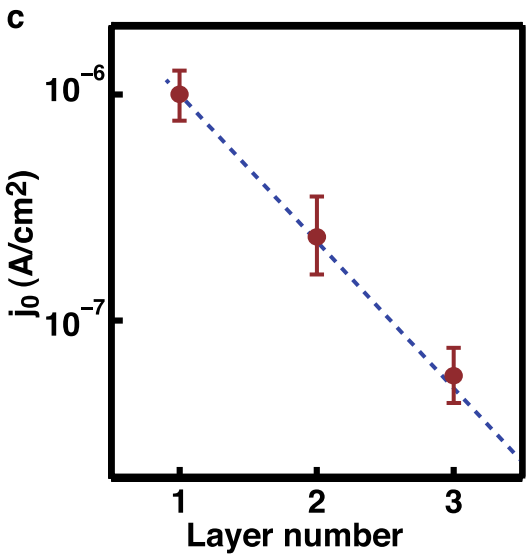
Nano Lett., 2013, 13 (12), pp 6222–6227

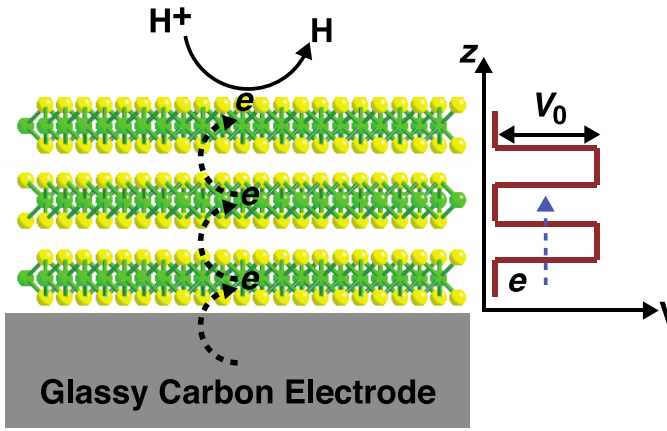
No substantial difference in the exchange current density at the edge site and basal plane of MoS2

Unpublished Results

Recent Studies: Layer Dependence Electrocatalysis



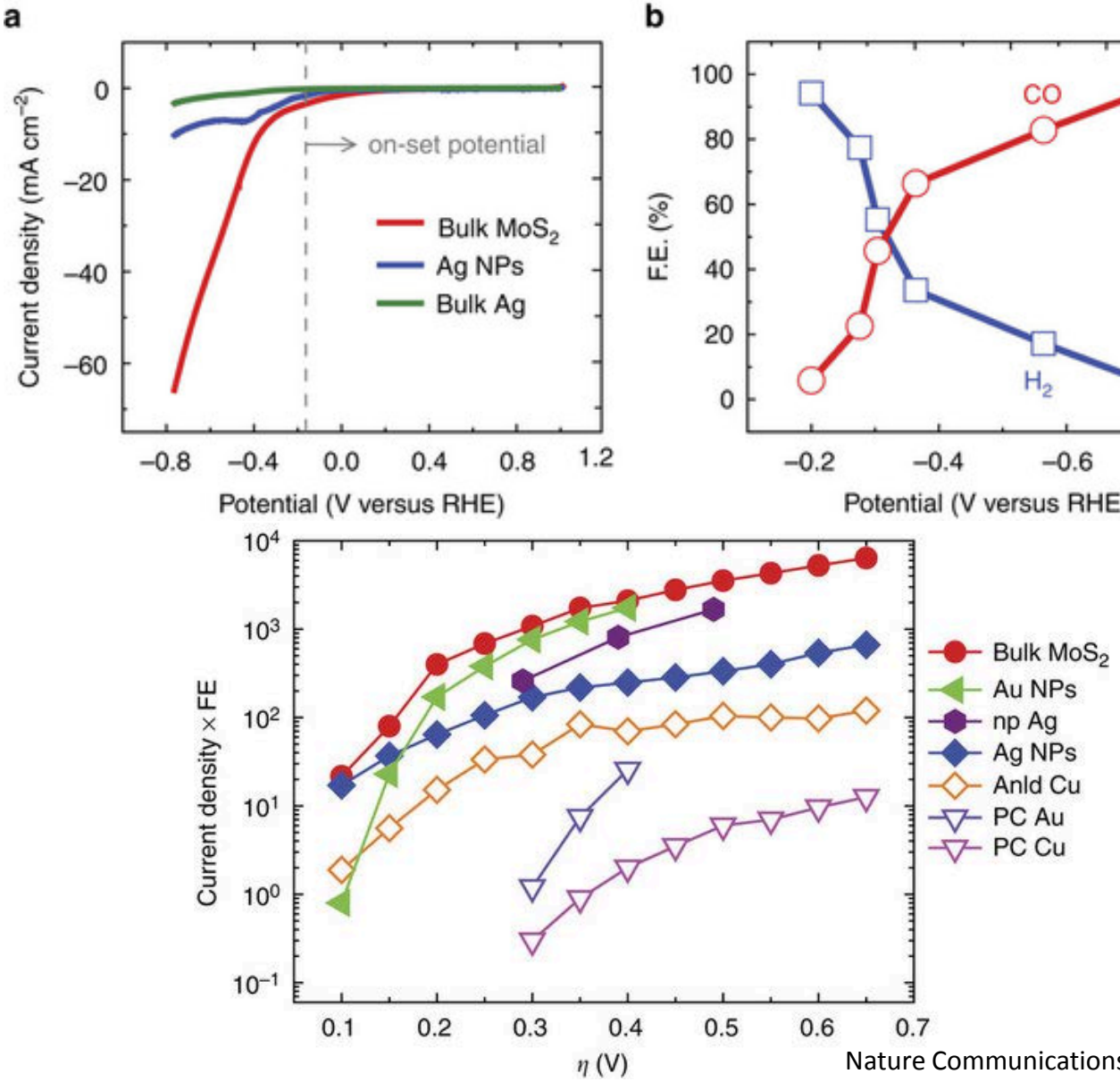




Nano Lett., 2014, 14 (2), pp 553–558

Efficiency of electron hopping plays a important role

MoS2: Catalyst for Carbon Dioxide Reduction



Nature Communications 5, Article number: 4470

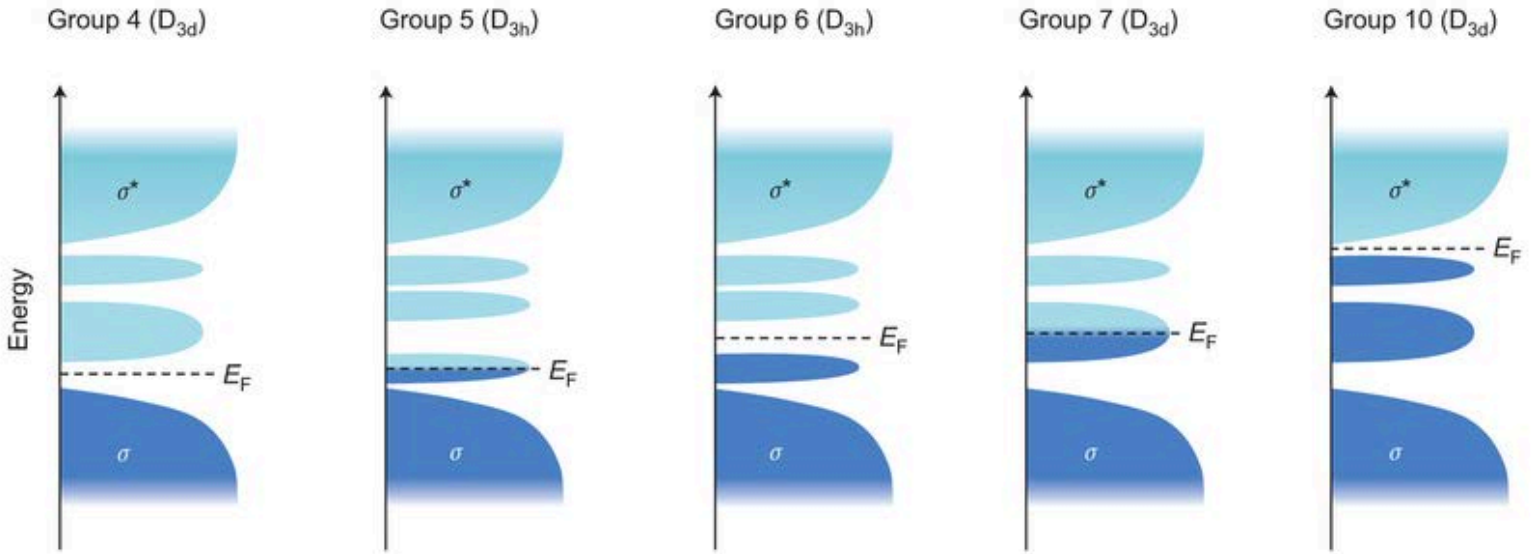
MoS2 is a promising catalyst for the reduction o fcarbon dioxide

III. Fundamental Properties

III.3 Electronic Structures/Properties

III.3.1 Band Structures

Electronic character of TMDCs: d-Orbital filling



Nature Chemistry 5, 263–275 (2013)

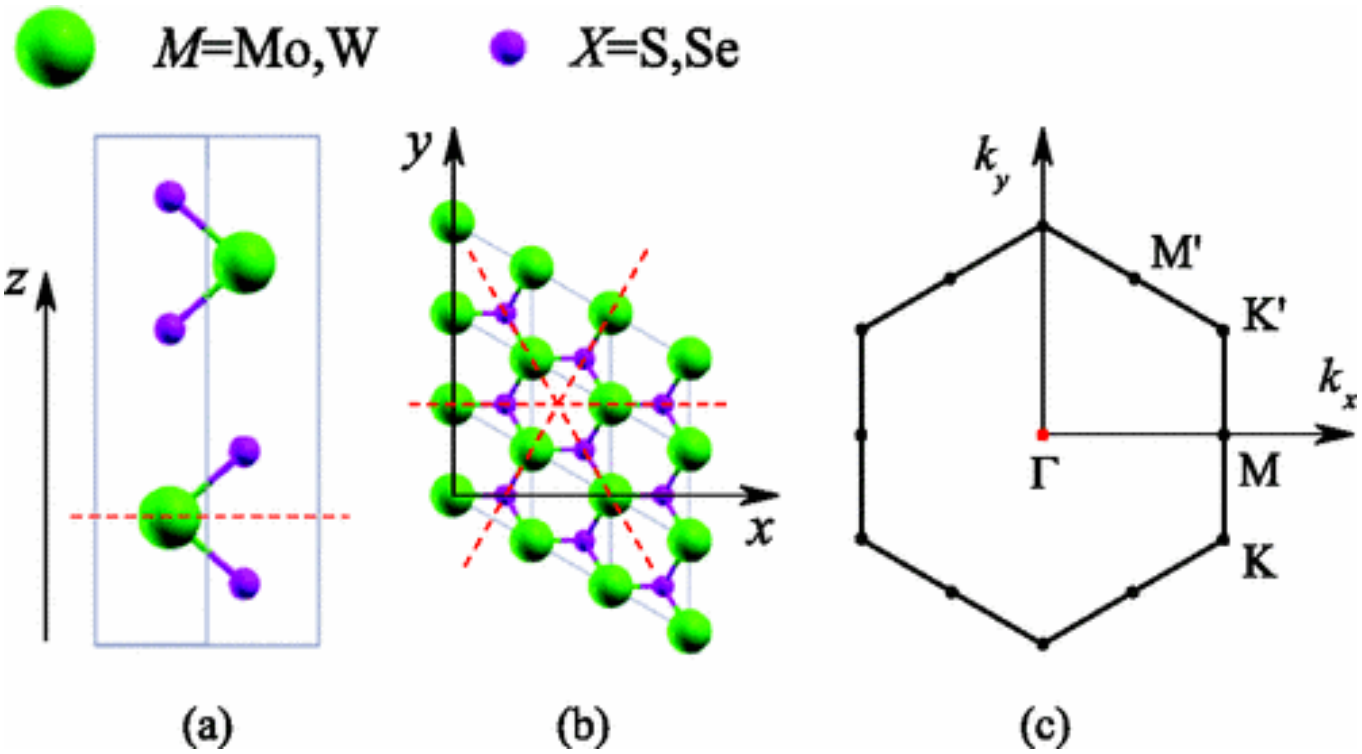
Table 1 | Electronic character of different layered TMDs[15].

Group	M	X	Properties
4	Ti, Hf, Zr	S, Se, Te	Semiconducting (E_g = 0.2–2 eV). Diamagnetic.
5	V, Nb, Ta	S, Se, Te	Narrow band metals (ρ ~ 10^{-4} Ω cm) or semimetals. Superconducting. Charge density wave (CDW). Paramagnetic, antiferromagnetic, or diamagnetic.
6	Mo, W	S, Se, Te	Sulfides and selenides are semiconducting (E_g ~ 1 eV). Tellurides are semimetallic (ρ ~ 10^{-3} Ω cm). Diamagnetic.
7	Tc, Re	S, Se, Te	Small-gap semiconductors. Diamagnetic.
10	Pd, Pt	S, Se, Te	Sulfides and selenides are semiconducting (E_g = 0.4 eV) and diamagnetic. Tellurides are metallic and paramagnetic. $PdTe_2$ is superconducting.

ρ, in-plane electrical resistivity.

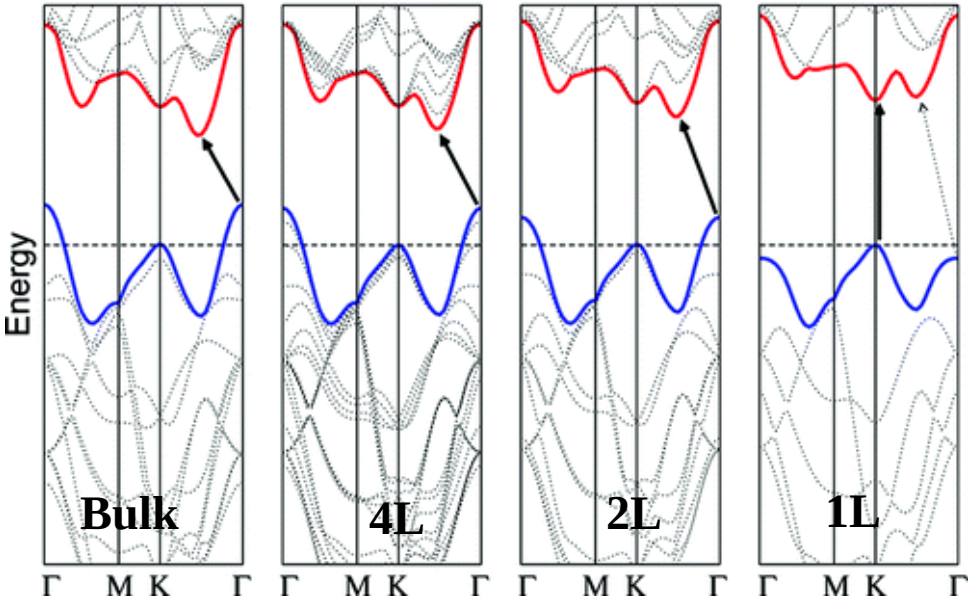
- The non-bonding *d* bands between the bonding (σ) and antibonding (σ*) bands are very important.
- The diverse electronic properties arise from the progressive filling of the non-bonding d bands
- The effect of chalcogen atoms on the electronic structure is minor compared with that of the metal atoms

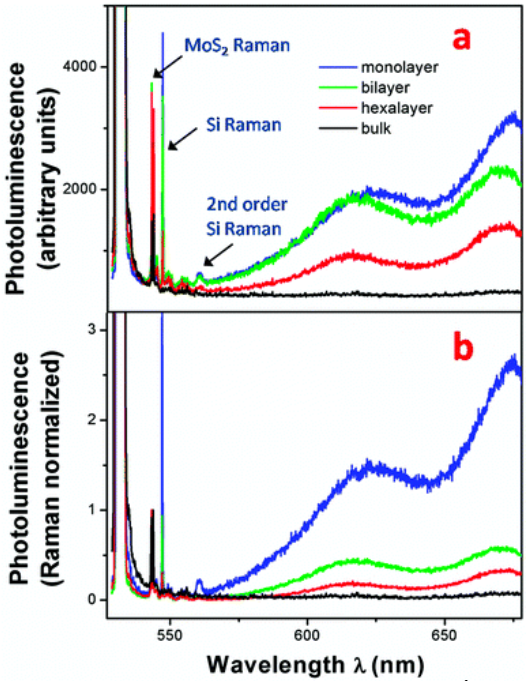
Hexagonal Brillouin Zone of TMDCs (MoS2)



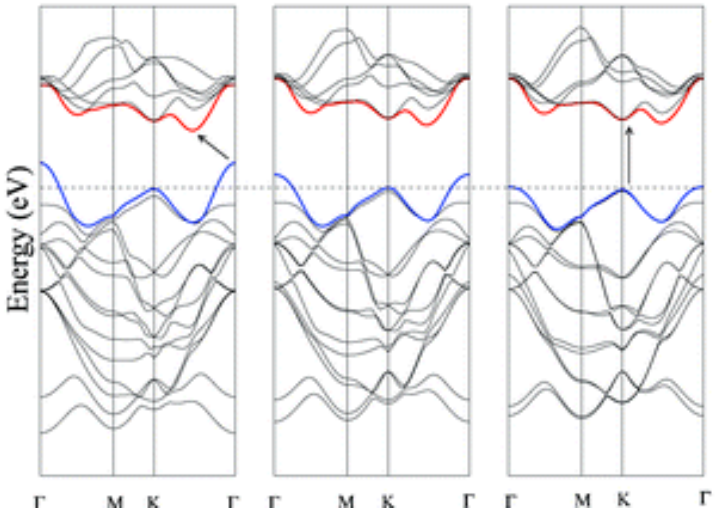
Phys. Rev. B 84, 153402

Evolution of Band Structure: Indirect to Direct

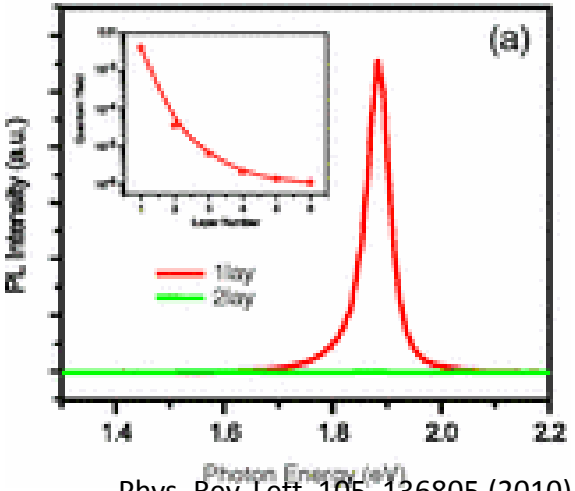




Nano Lett. 10, 1271 (2010)



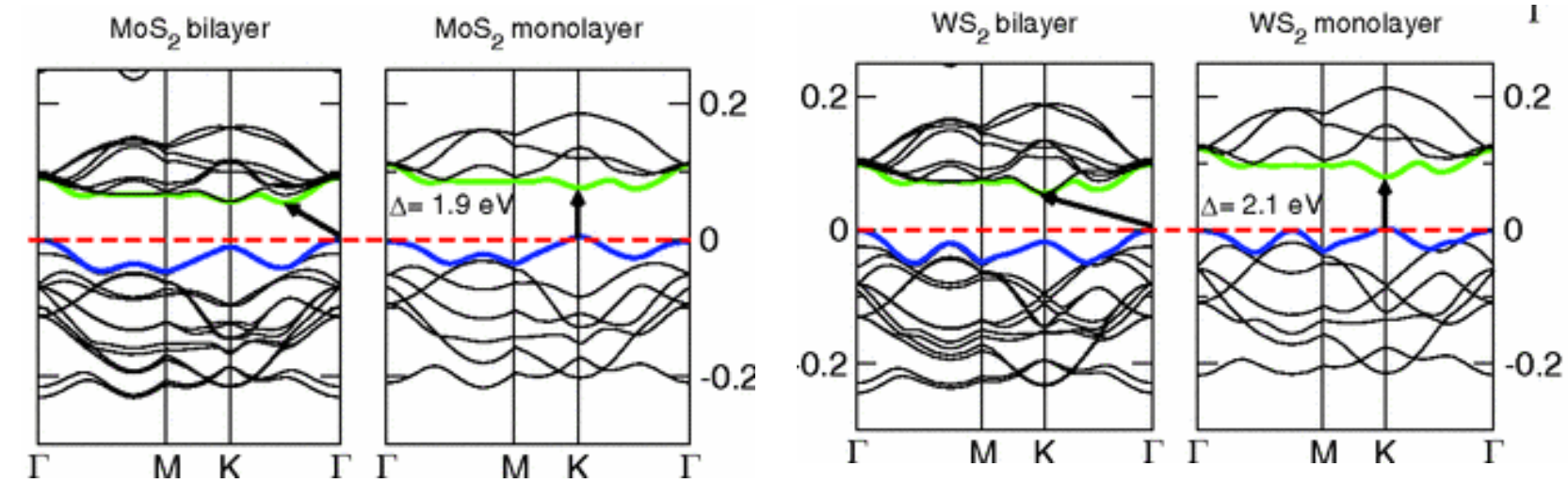
J. Phys. Chem. C, 2007, 111 (44), pp 16192–16196

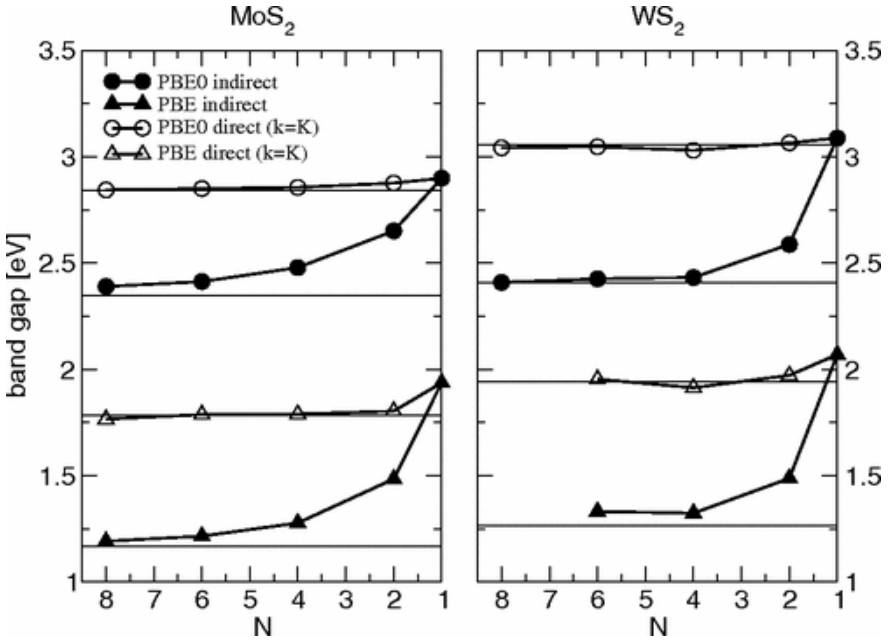


Phys. Rev. Lett. 105, 136805 (2010)

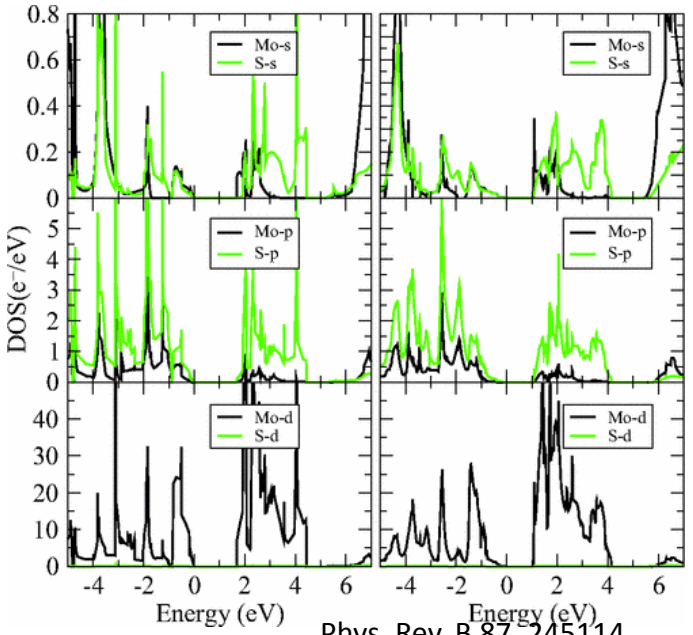
An indirect to direct bandgap transition at monolayer MoS2

Evolution of Band Structure: Indirect to Direct





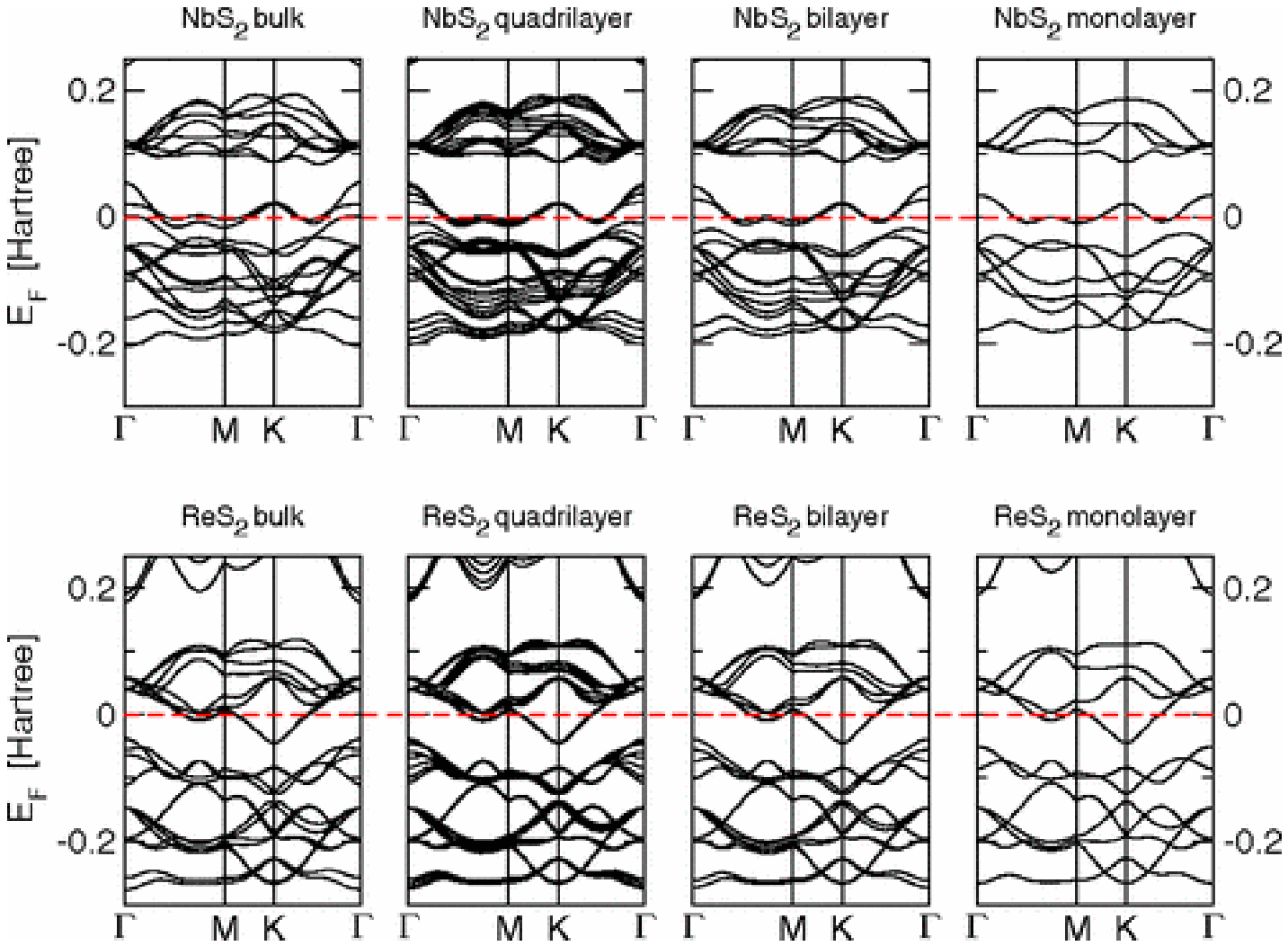
Phys. Rev. B 83, 245213



Phys. Rev. B 87, 245114

The d-electron orbitals dominate the valence and conduction bands

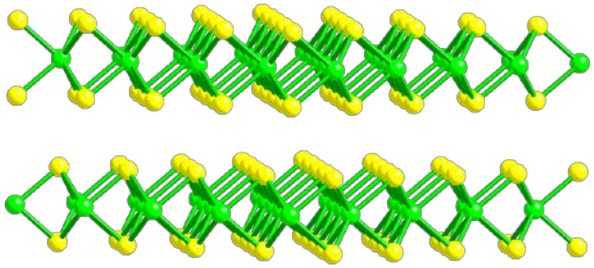
The Crossover of Indirect to Direct Not Universal



Phys. Rev. B 83, 245213

NbS2 and ReS2 are metallic because the $4dz_2$ orbital is half-filled. No layer dependence crossover.

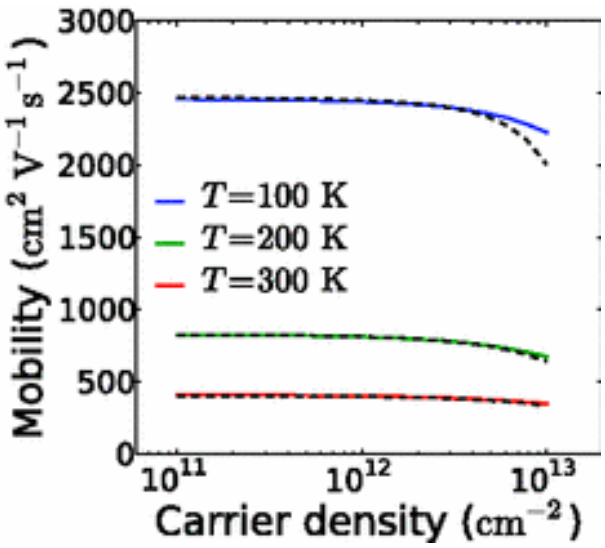
Key Points

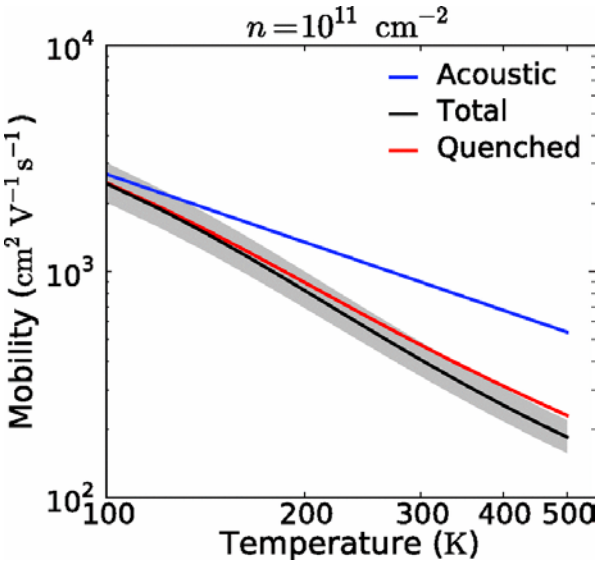


- Mo *4d* and S *3p* atomic orbitals play a decisive role in the band structure
- The energy levels dominated by the S *p*-orbitals is subject to the influence of interlayer interactions, while those mainly consisting of Mo *d*-orbitals not
- The valence band edge at *Γ* point involves the contribution from S *3p* orbitals, while the band edges at *K* point are mainly made of Mo *4d* orbitals

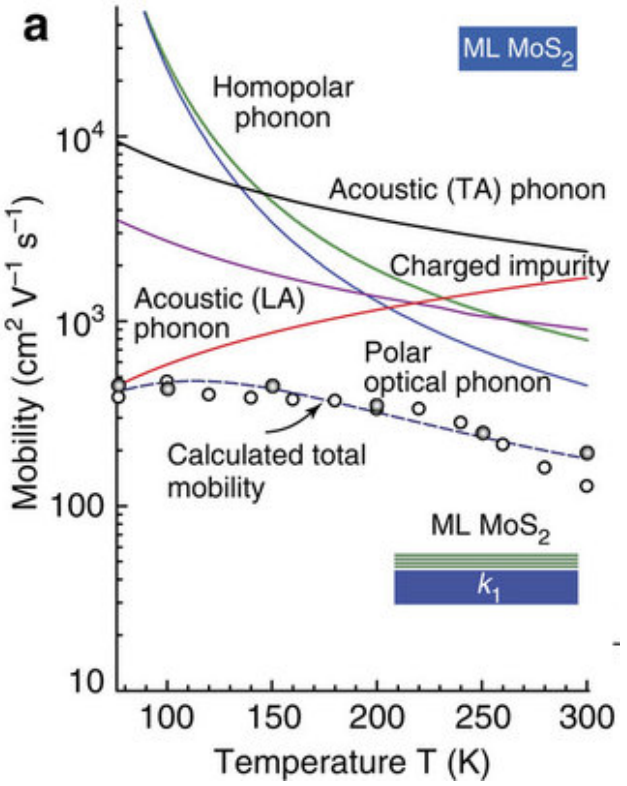
III.3.2 Mobility

Phonon-limited Charge Mobility in MoS2





Phys. Rev. B 85, 115317



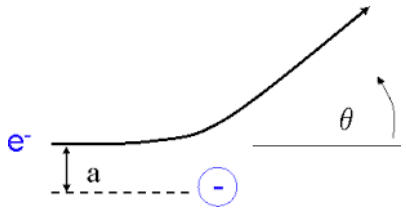
Nature Communications 3, 1011

The room-temperature mobility is dominated by optical phonon scattering.

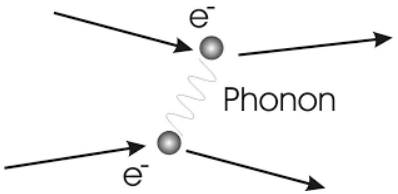
200 ~40 $cm^2V^{-1}s^{-1}$

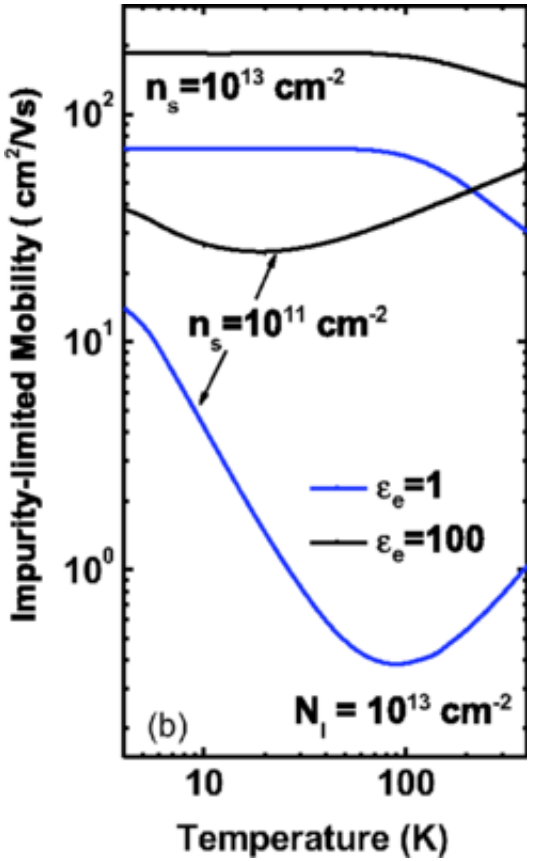
Charge Mobility of in MoS2: Substrate Effect

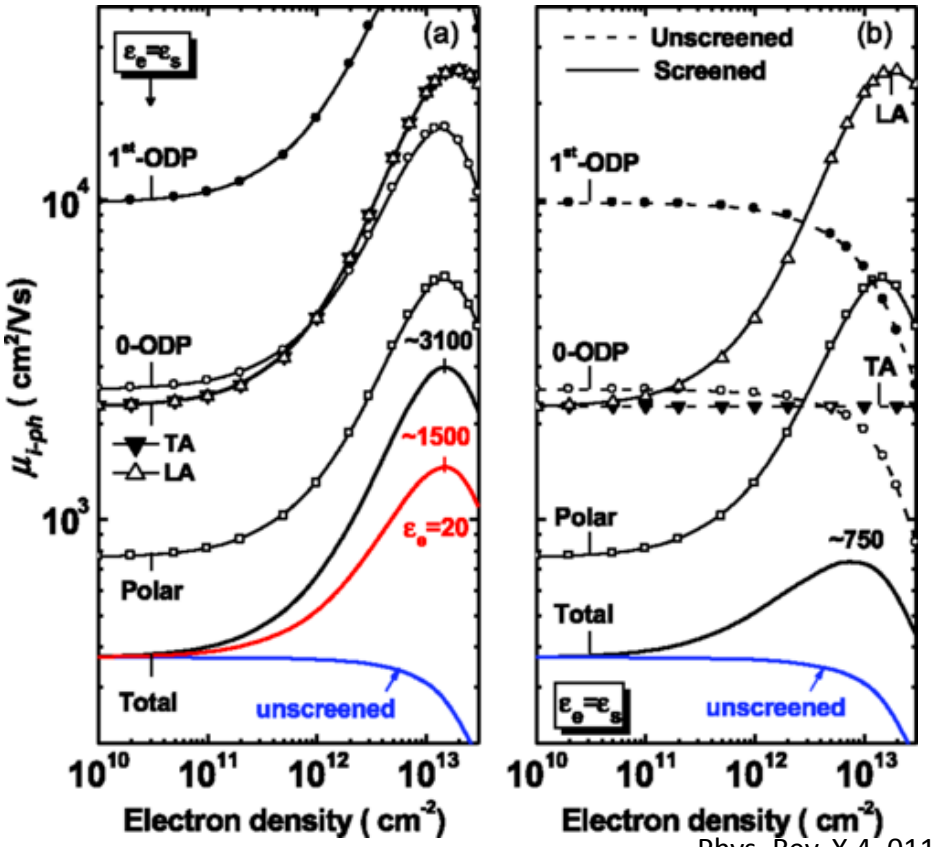
Charge impurity scattering



Phonon scattering





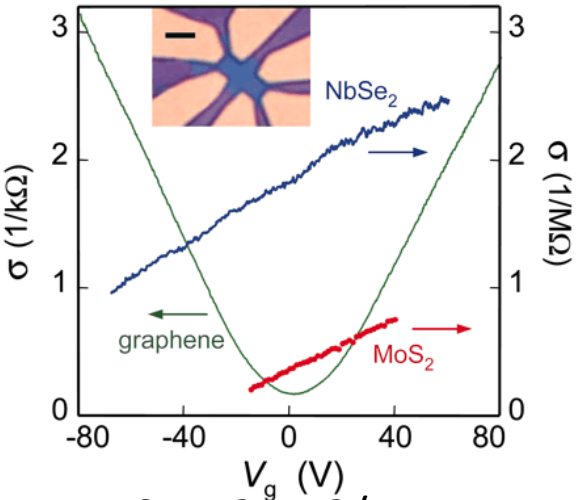


Phys. Rev. X 4, 011043

The ionized impurity scattering and remote phonon scattering are the major factors limiting the mobility

Charge Mobility in MoS2: Experiments

A wide variation in the measured results

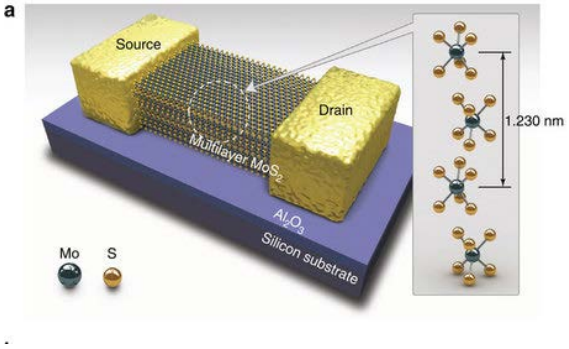


0.5 - 3 cm2/V

Proc. Natl. Acad. Sci. U. S. A. 102, 10451–10453

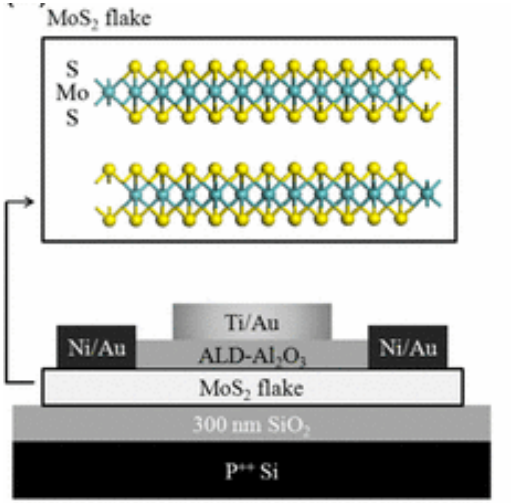
200 cm2 V−1 s−1,

Nature Nanotechnology 6, 147–150 (2011)



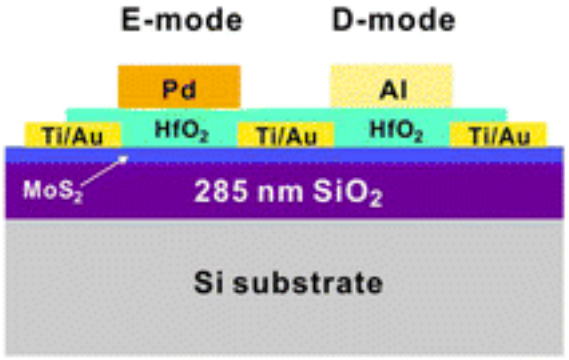
>100 cm2 V−1 s−1)

Nature Communications 3, 1011



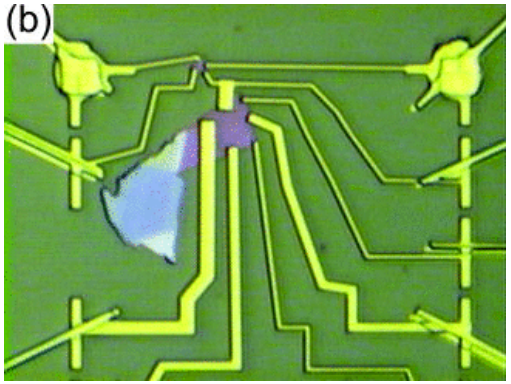
517 cm2/V·s

IEEE Electron Dev. Lett. 33, 546–548 (2012)



300 cm2 V−1 s−1

Nano Lett., 2012, 12 (9), pp 4674–4680

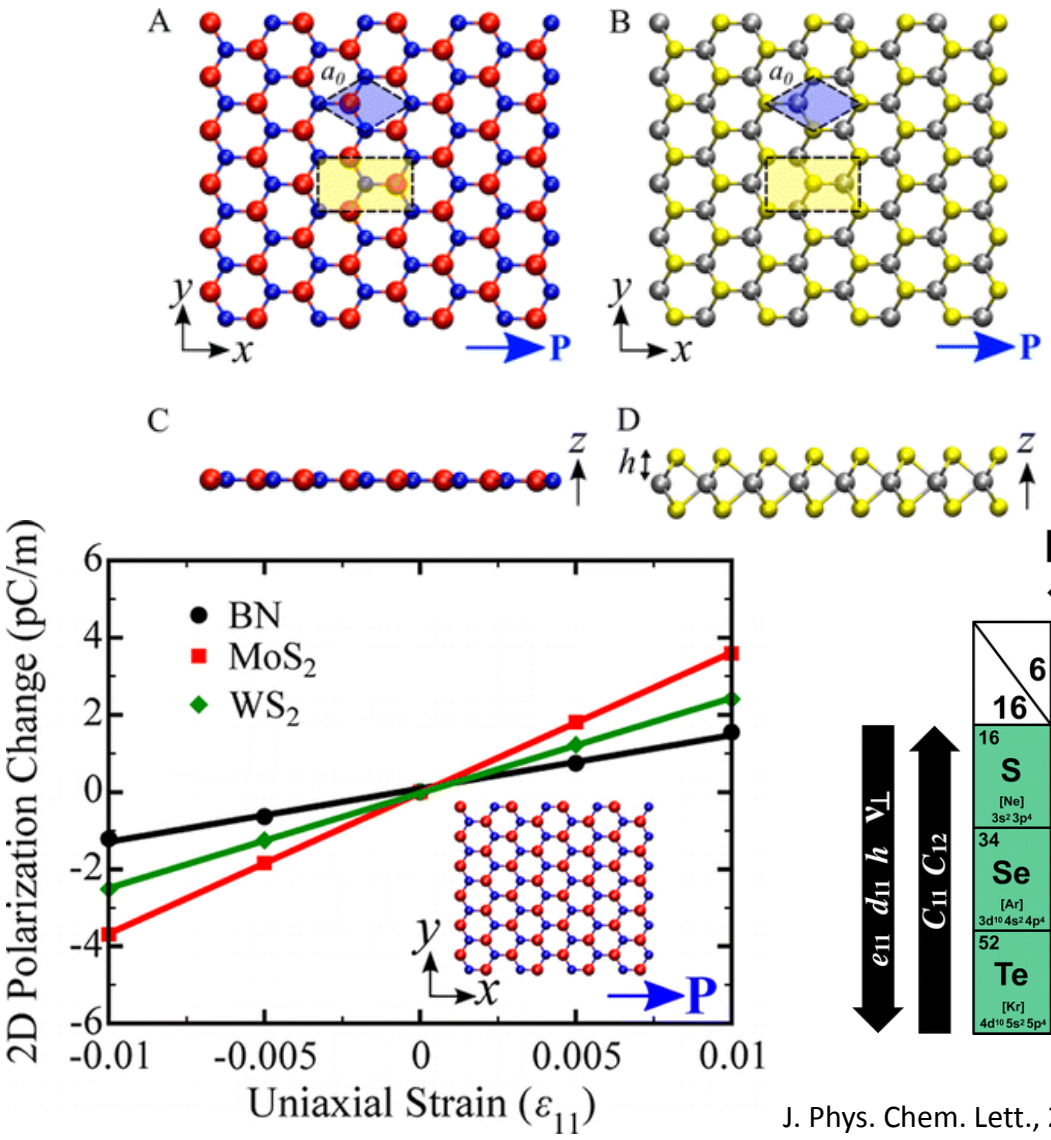


~ 10 cm2 V−1 s−1

J. Appl. Phys. 101, 014507 (2007)

III.3.3 Piezoelectricity

Piezoelectricity in 2D TMDC Materials: Theory



C_{11} $\nu_\perp$

e_{11} d_{11} C_{12}

e_{11} d_{11} h $\nu_\perp$

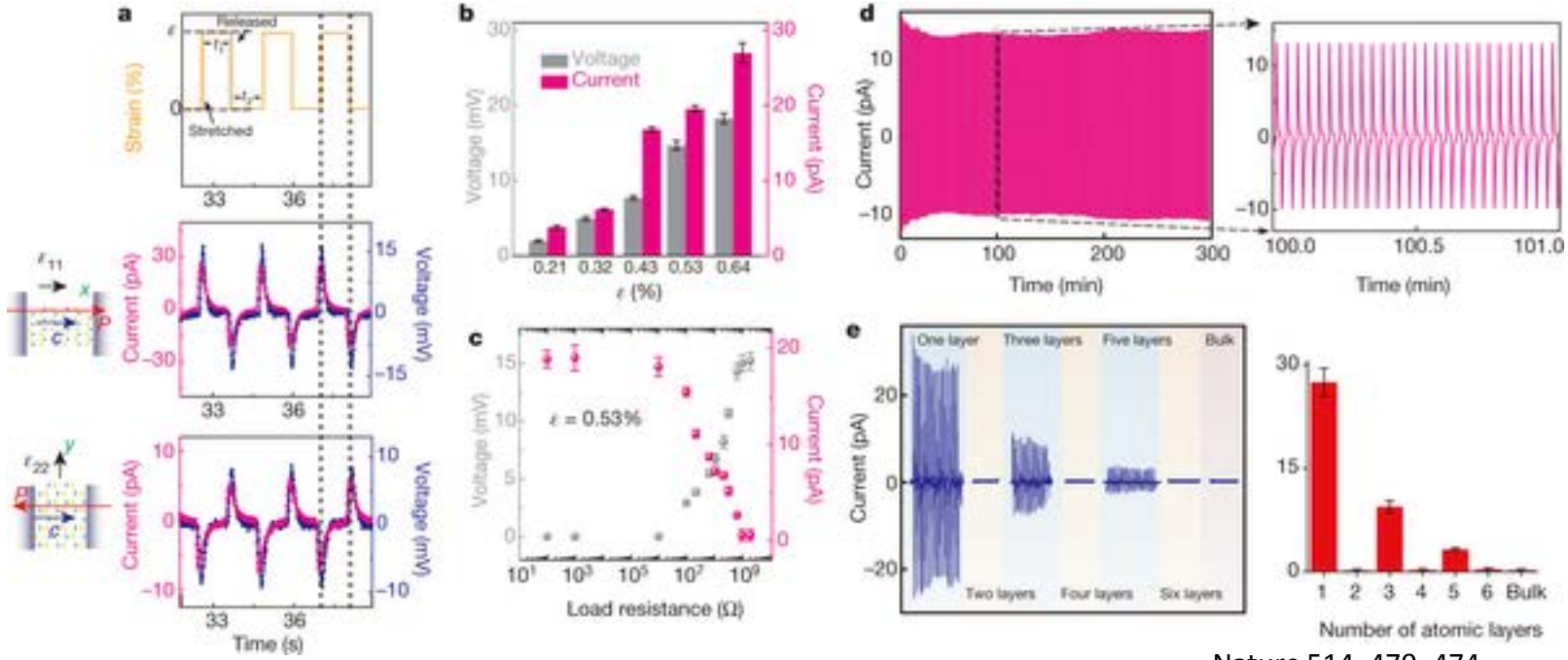
C_{11} C_{12}

16 \ 6	42 Mo [Kr] $4d^5 5s$	74 W [Xe] $4f^{14} 4d^5 5s$
16 S [Ne] $3s^2 3p^4$	3.73	2.19
34 Se [Ar] $3d^{10} 4s^2 4p^4$	4.72	2.79
52 Te [Kr] $4d^{10} 5s^2 5p^4$	9.13	4.60

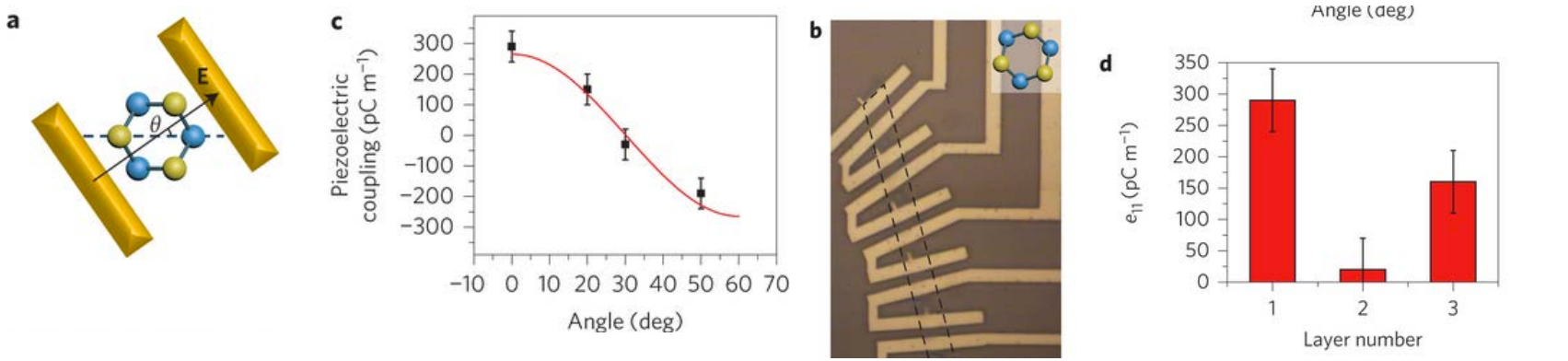
J. Phys. Chem. Lett., 2012, 3 (19), pp 2871–2876

Monolayer TMDC materials are piezoelectric

Piezoelectricity in MoS2: Experiments



Nature 514, 470–474

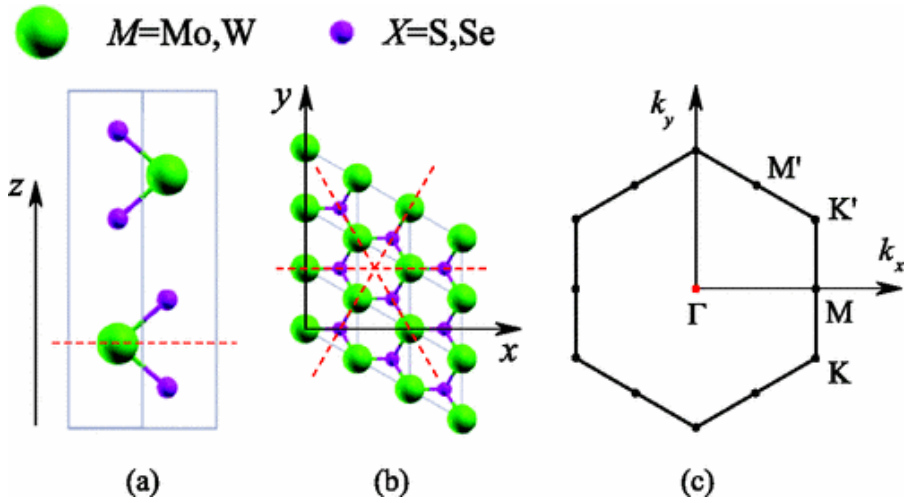


Nature Nanotechnology 10, 151–155 (2015)

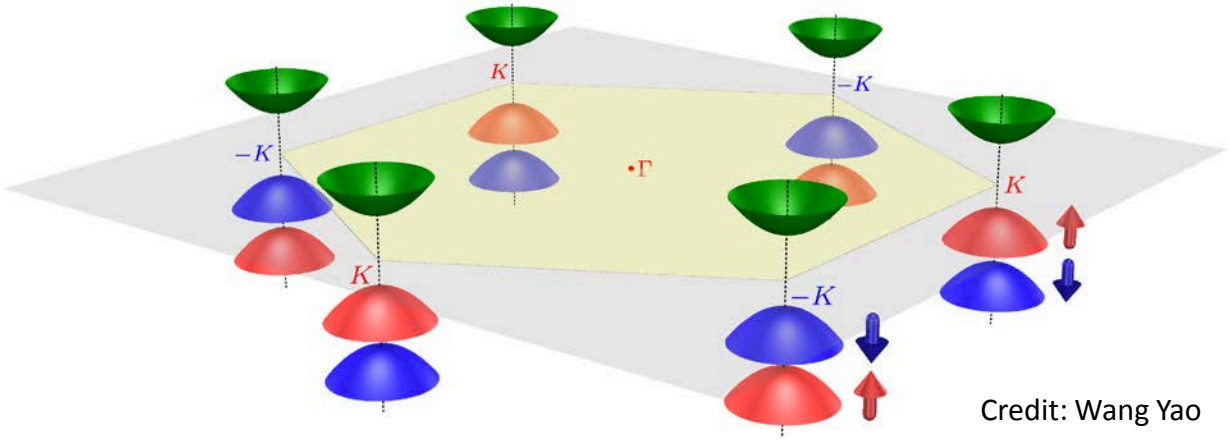
Depend on if the layer number is odd or even.

III.3.4 Spin-Valley Coupling

Coupled Valley-Spin of TMDCs (MoS2)



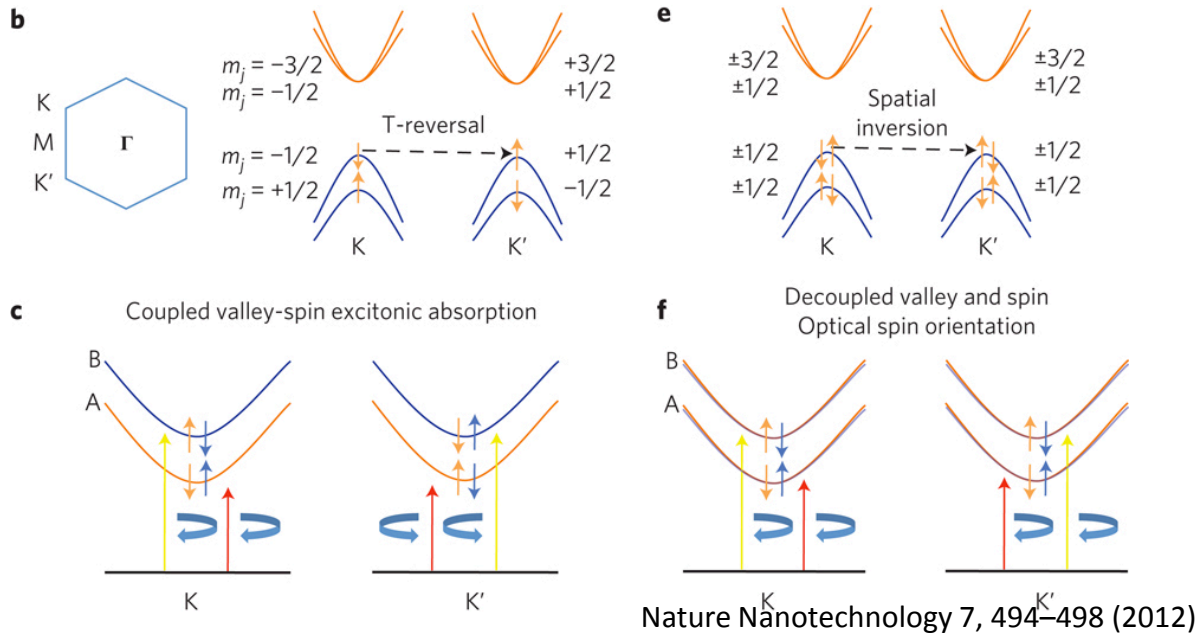
Phys. Rev. B 84, 153402



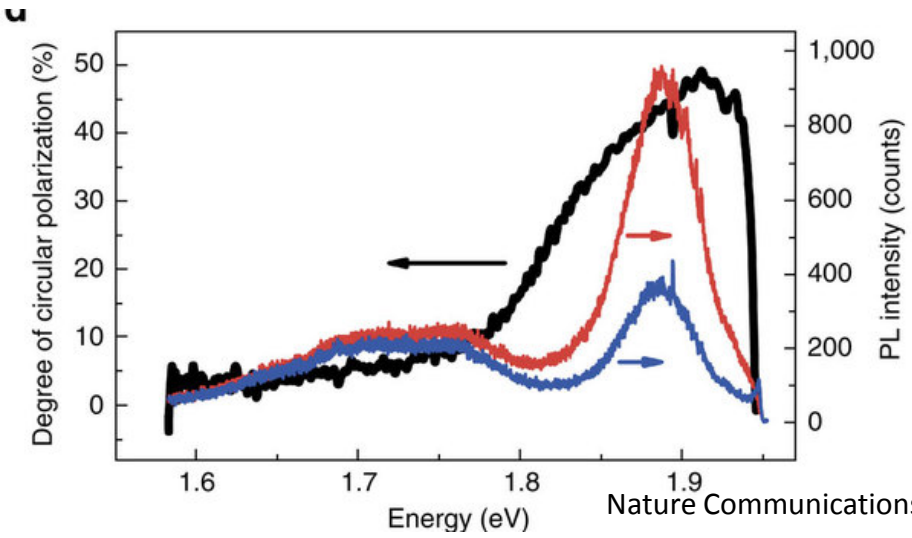
Credit: Wang Yao

- At the K and K′ valleys, the band edges are mainly of molybdenum d-orbital
- spin–orbit interactions split the valence bands by ~160 meV in monolayer
- The valley and spin of the valence bands are inherently coupled in monolayers

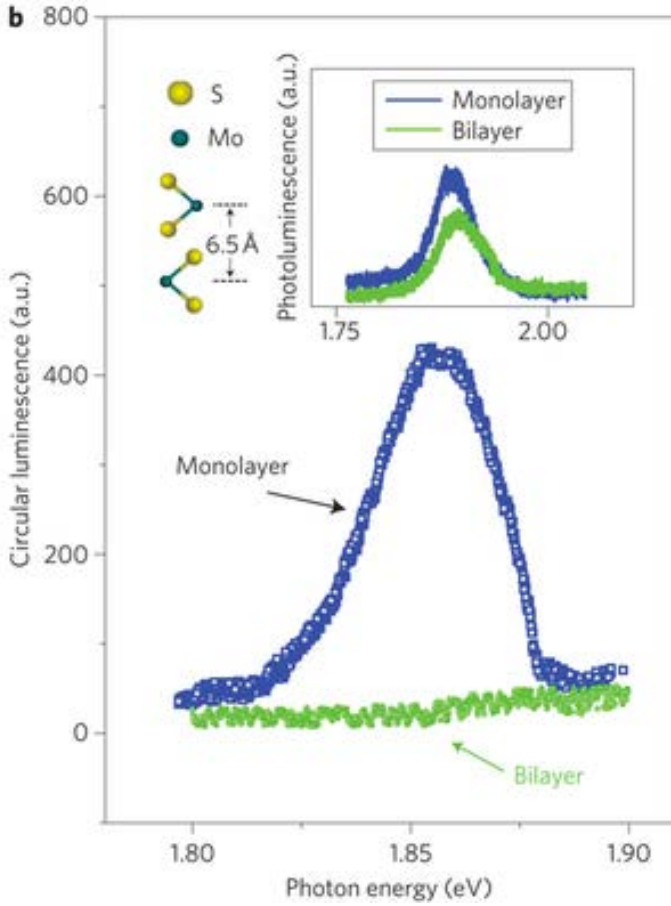
Valley-Spin Polarized Luminescence in Monolayer



Nature Nanotechnology 7, 494–498 (2012)



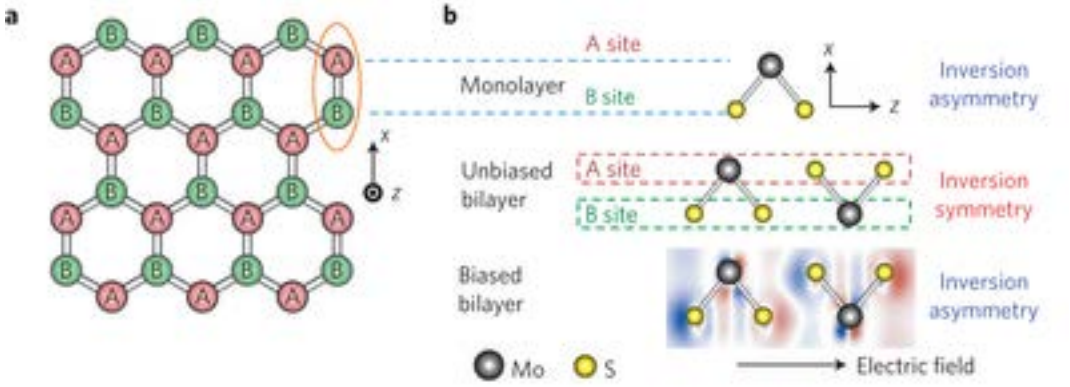
Nature Communications 3, Article number: 887

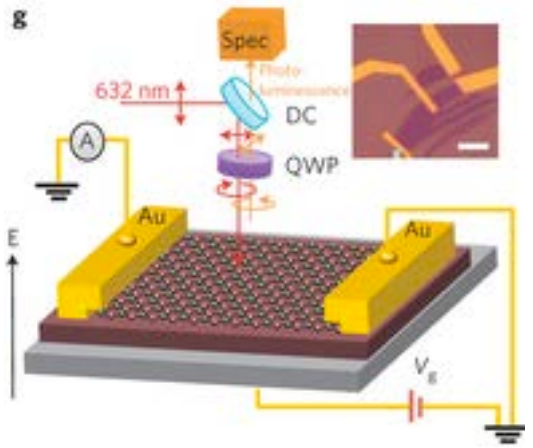


Nature Nanotechnology 7, 491–493 (2012)

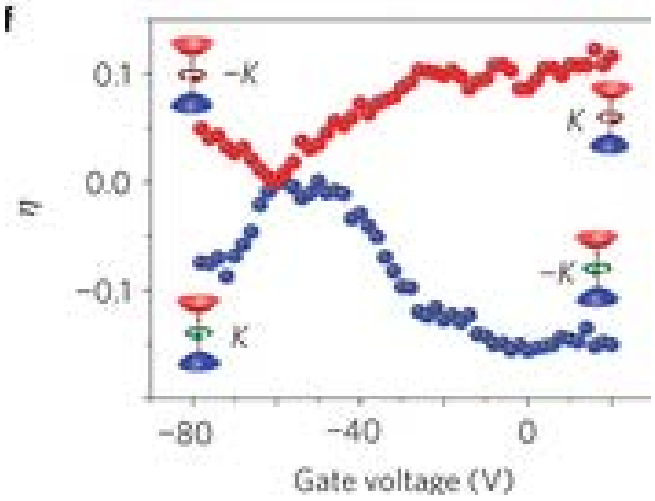
Left circularly polarized (σ−) and right circularly polarized (σ+) at the K and K′ valleys

Electrically Tuned Valley-Spin Polarization

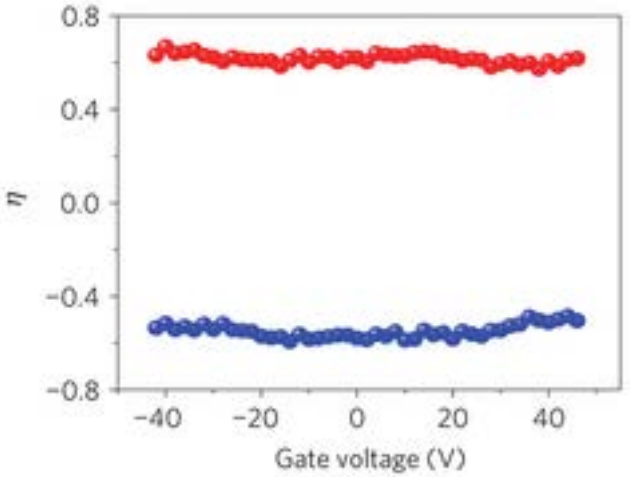




2L MoS2



1L MoS2



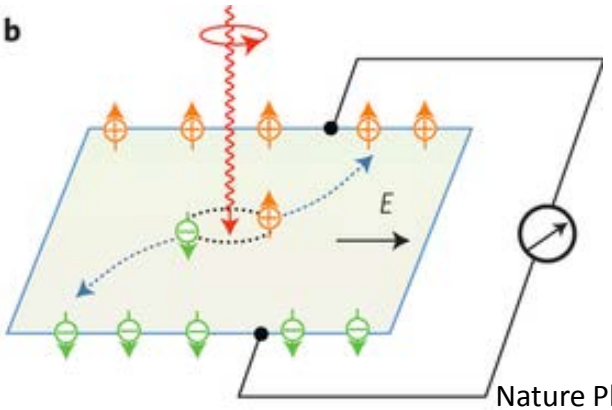
Nature Physics 9, 149–153 (2013)

$\eta = (P(\sigma+) - P(\sigma-))/(P(\sigma+) + P(\sigma-))$.

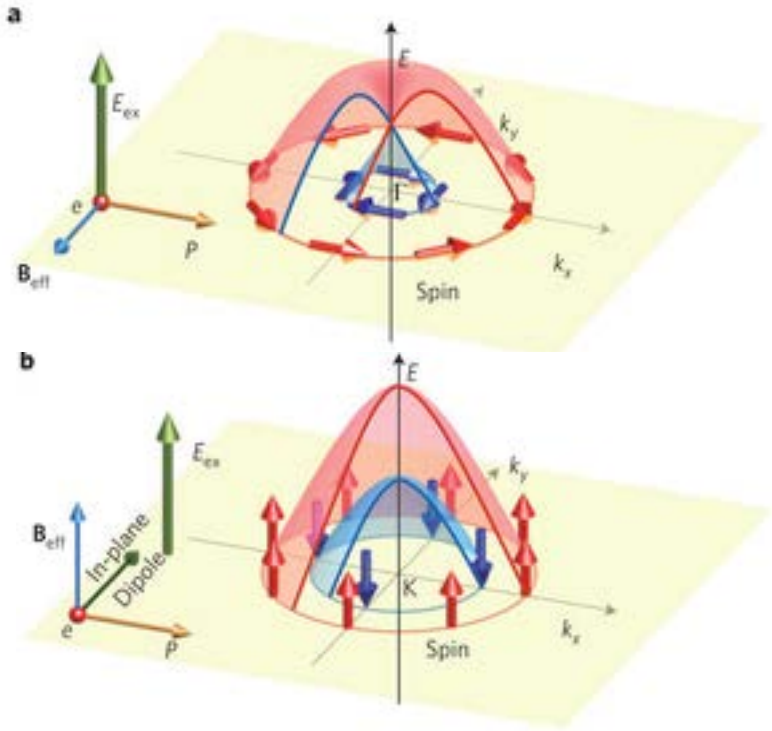
Optical helicity can be continuously tuned from −15% to 15% as a function of gate voltage in 2L MoS2, but is gate independent in monolayer MoS2

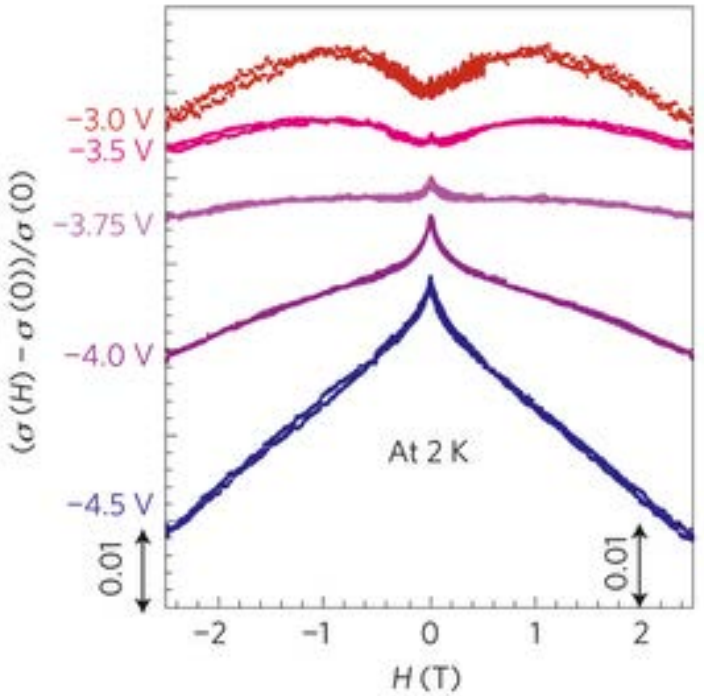
Valley-Hall Effect and Zeeman-Type Splitting

Valley Hall effect.



Nature Physics 10, 343–350 (2014)





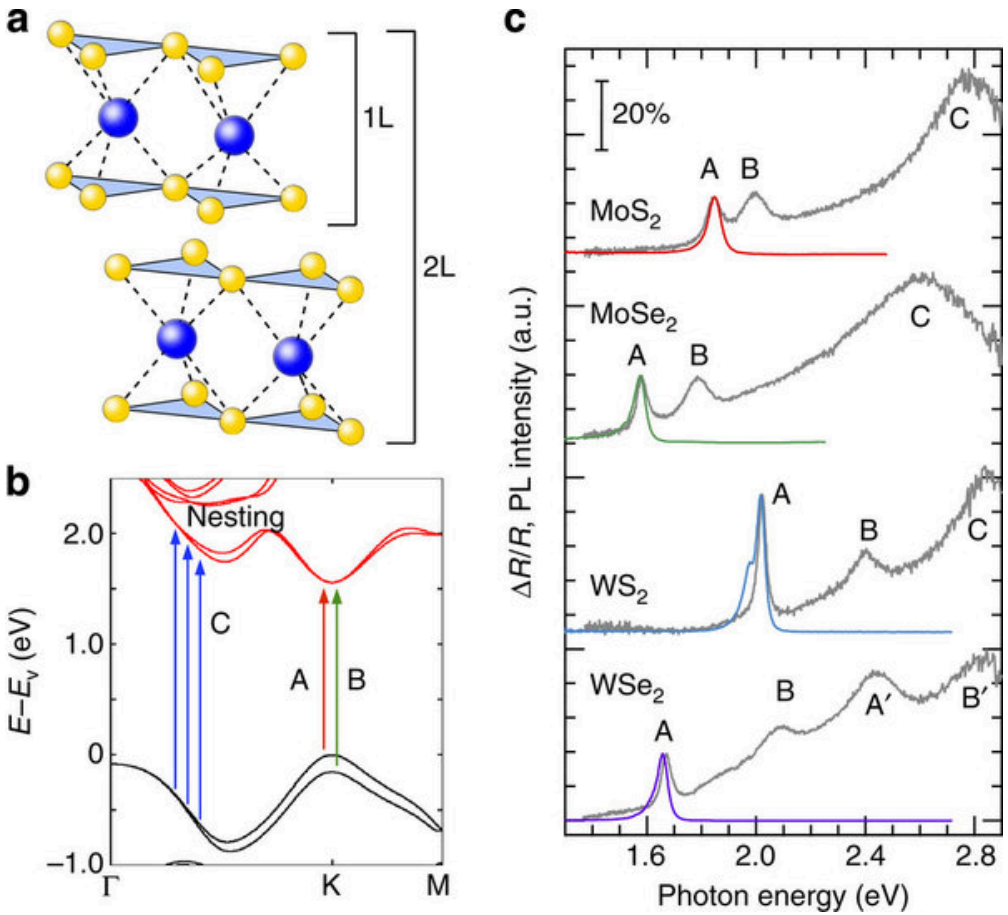
Nature Physics 9, 563–569 (2013)

III. Fundamental Properties

III.4 Optical Properties

III.4.1 Exciton, Binding Energy & Radius

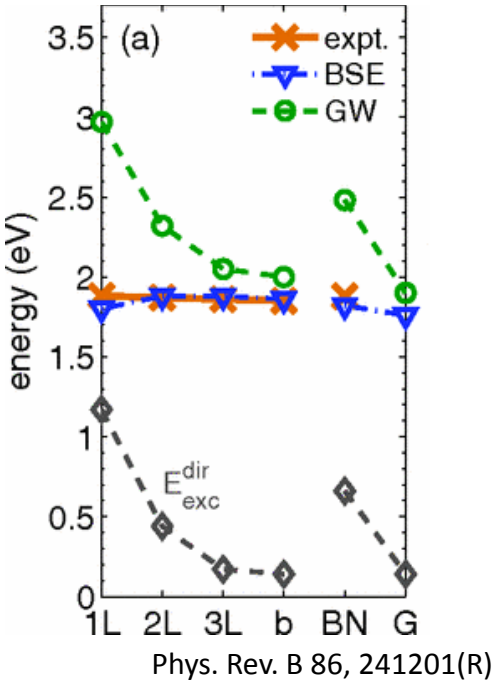
Excitonic States



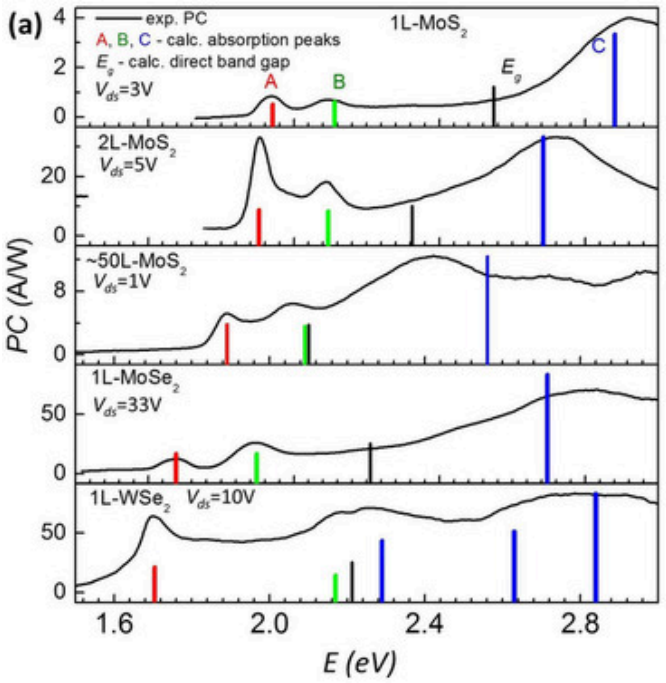
Nature Communications 5, 4543, (2014)

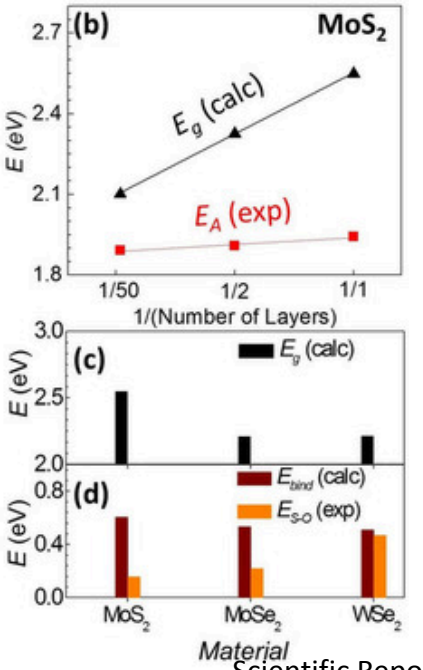
A and B from interband transtion of K/K' points, and C from transition in the Brillouin zone between Γ and Λ

Extraordinarily Strong Binding Energy



Phys. Rev. B 86, 241201(R)



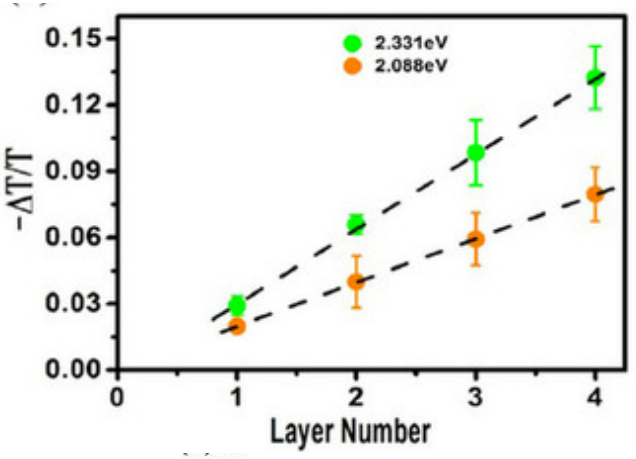


Scientific Reports 4, 6608, 2014

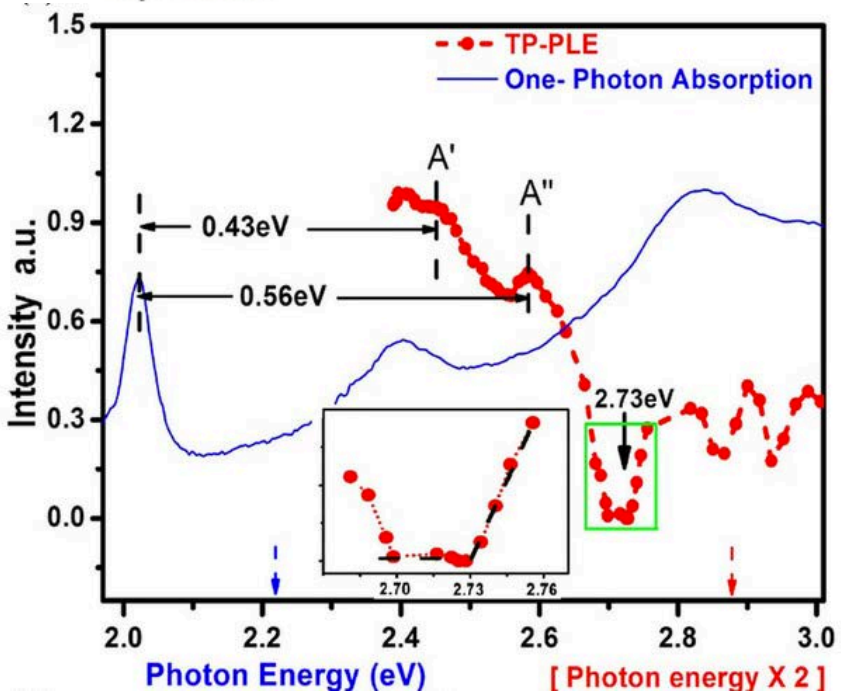
	Energy cutoffs	k point	E_g	E_g(optical)	Binding energy
Monolayer MoS_2 (3.160 Å)	400 and 200	6 × 6 × 1(SOC)	2.89	1.87	1.02
		6 × 6 × 1	2.99	1.96	1.03
		9×9×1	2.84	2.08	0.76
		12 × 12 × 1	2.78	2.16	0.62
		15 × 15 × 1	2.76	2.22	0.54
	600 and 300	12 × 12 × 1	2.80	2.17	0.63
Monolayer MoS_2 (3.190 Å)	600 and 300	12 × 12 × 1	2.66	2.04	0.62
Monolayer WS_2 (3.155 Å)	400 and 200	6 × 6 × 1(SOC)	3.02	1.97	1.05
		6 × 6 × 1	3.28	2.21	1.07
		9×9×1	3.12	2.34	0.78
		12 × 12 × 1	3.06	2.43	0.63
		15 × 15 × 1	3.05	2.51	0.54
	600 and 300	12 × 12 × 1	3.11	2.46	0.65
Monolayer WS_2 (3.190 Å)	600 and 300	12 × 12 × 1	2.92	2.28	0.64

The exciton binding energy in MoS2 monolayer is reported ~ 0.4-1.1 ev

Strong Binding Energy in WS2



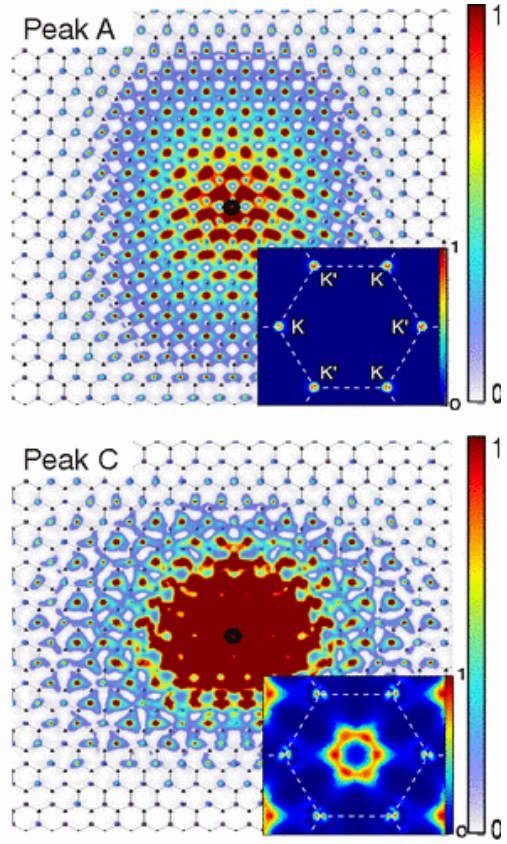
	1L(10K)	1L(300K)	2L(300K)	4L(300K)
A	2.123ev	2.020ev	1.987ev	1.981ev
B	2.505ev	2.403ev	2.366ev	2.380ev
C	2.884ev	2.825ev	2.737ev	2.702ev



Scientific Reports 5, 9218 (2015)

The exciton binding energy in WS2 monolayer is 0.71 ± 0.01 eV around K valley

Exciton Radius



Phys. Rev. Lett. 111, 216805

The exciton radius is estimated to be 0.5-2 nm

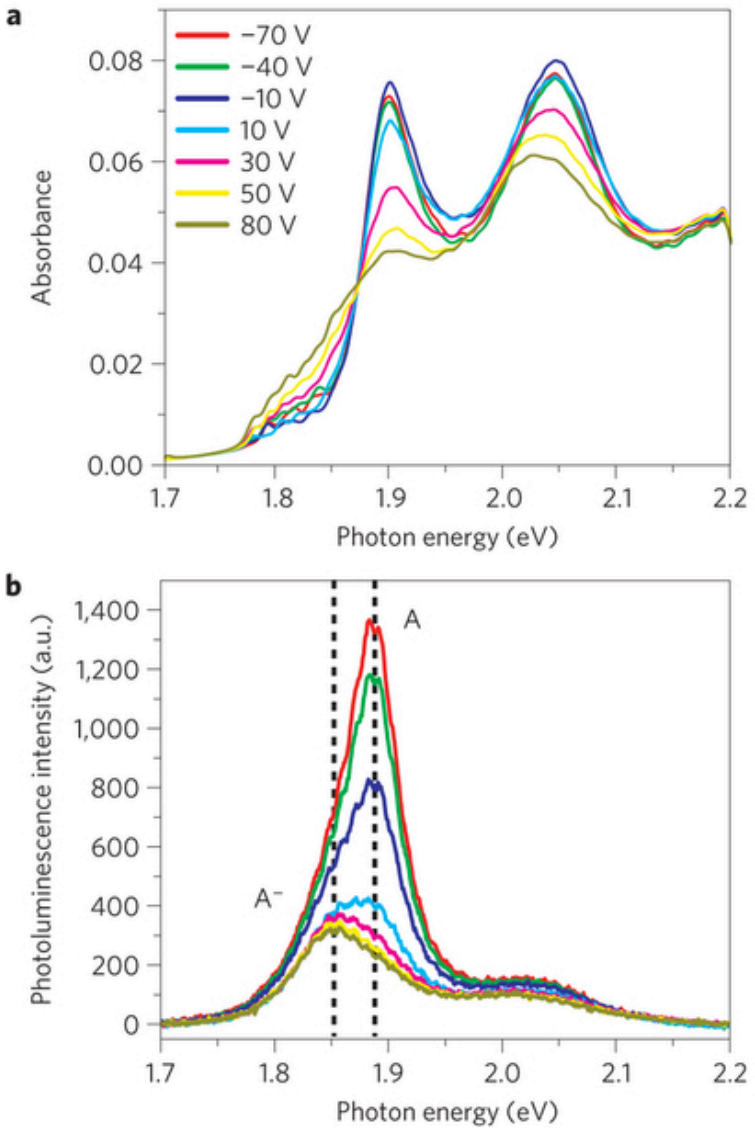
Comment

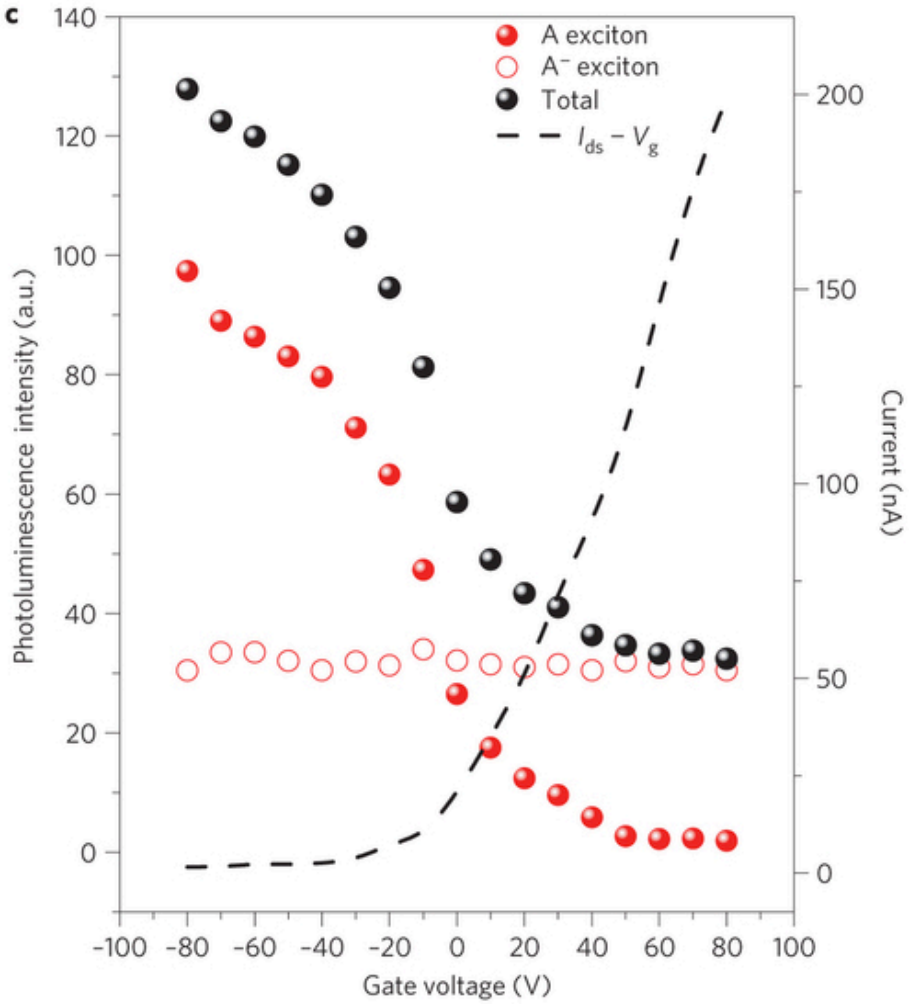
Most of the studies (binding energy, radius) focus on the A exciton

How these results could be applied to the B and C excitons is not clear.

III.4.2 Neutral and Charged Excitons

Neutral and Charged Exictons

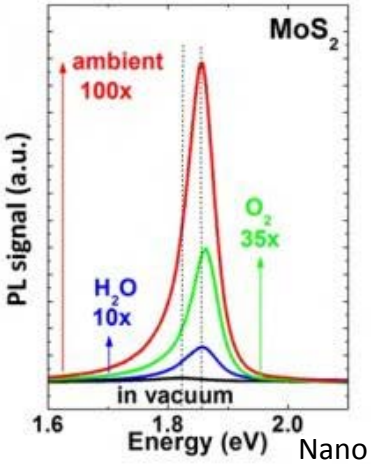


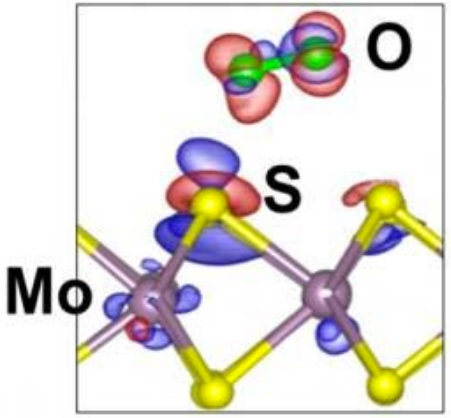


Nature Materials 12, 207–211 (2013)

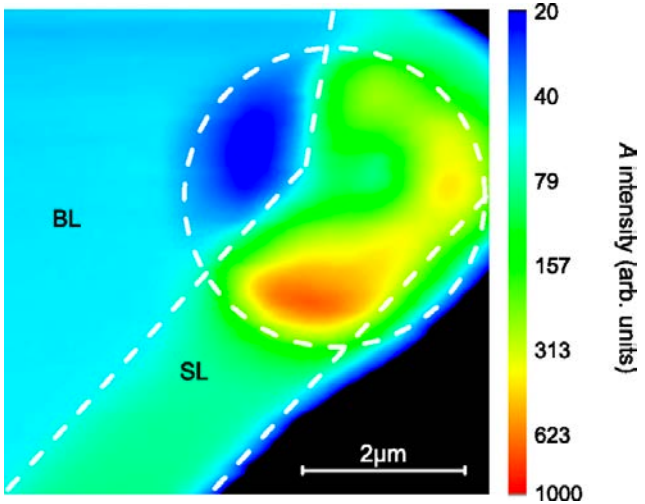
Tightly bound negative trions, a quasiparticle composed of two electrons and a hole with a binding energy estimated to be ~20meV

Neutral and Charged Exictons: Effects of Doping

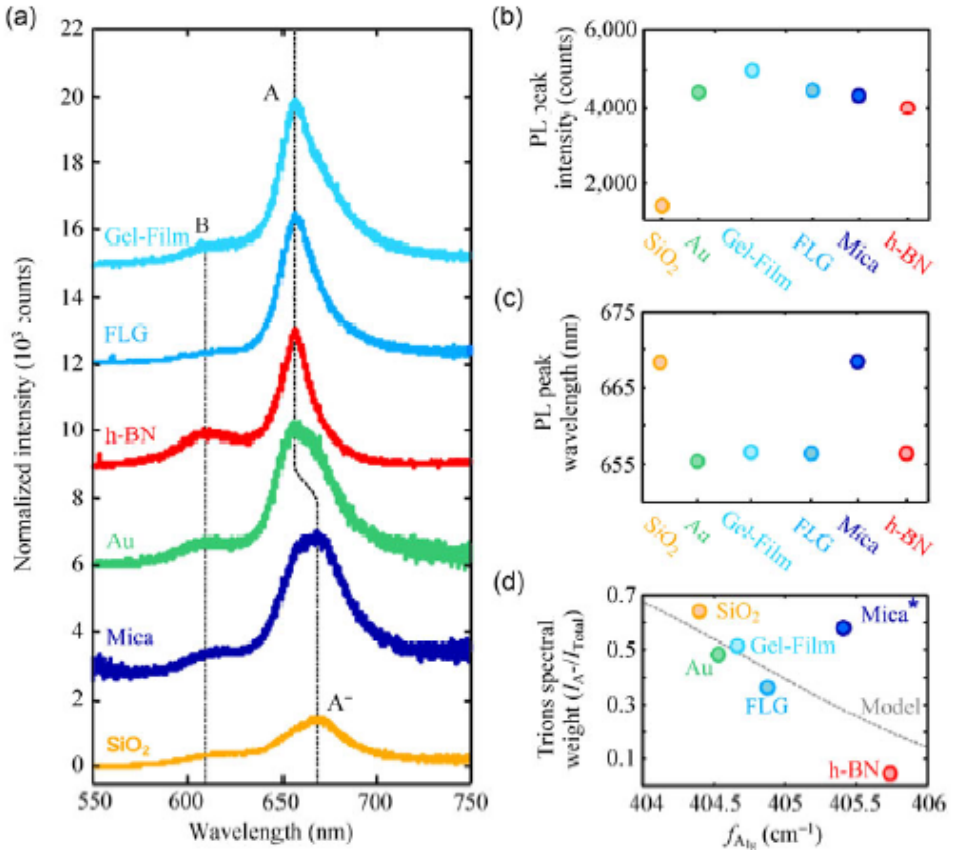




Nano Lett., 2013, 13 (6), pp 2831–2836



Phys. Rev. B 89, 125406

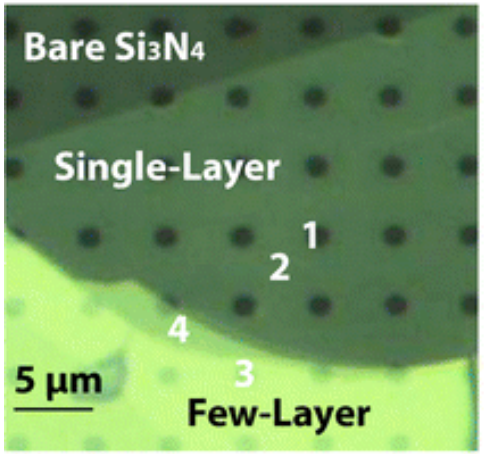


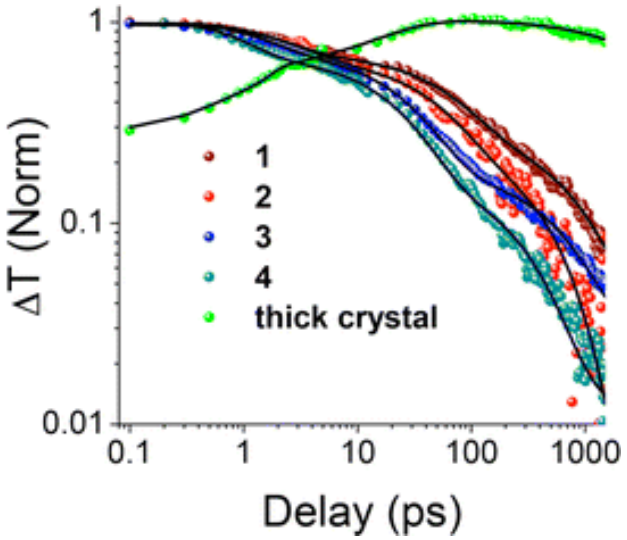
Nano Res. 2014, 7(4): 561–571

The PL intensity and position is subject to the effect of substrates and molecule adsorption, which may change doping level and the population of trions.

III.4.4 Exciton Dynamics and Manipulation

Exicton Dynamics



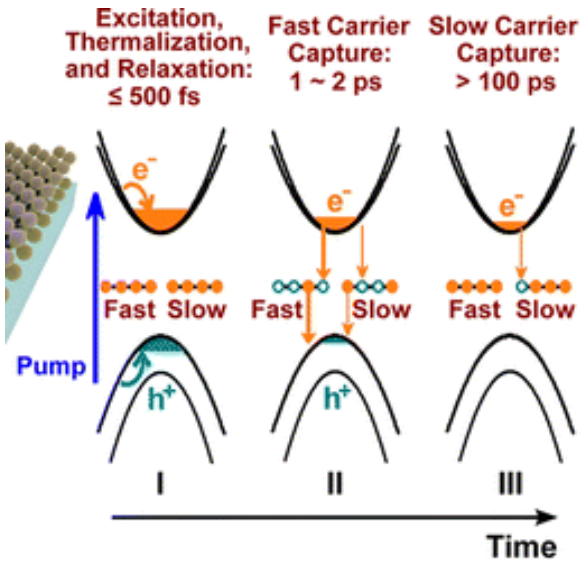


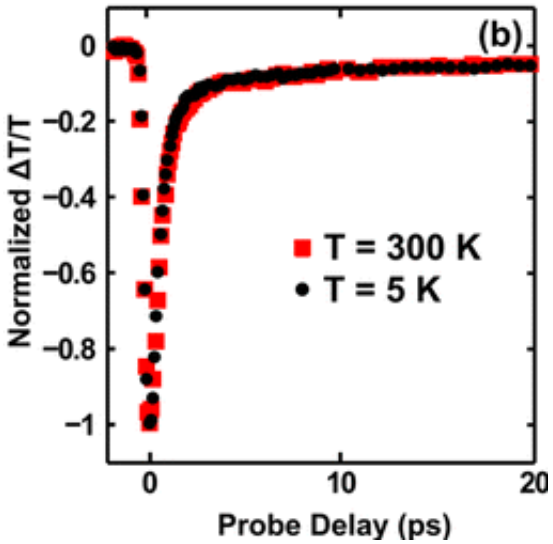
	τ_1 (ps)	τ_2 (ps)	τ_3 (ps)
1 (suspended monolayer)	2.6 ± 0.1 (39%)	74 ± 3 (39%)	850 ± 48 (22%)
2 (supported monolayer)	3.3 ± 0.2 (40%)	55 ± 3 (38%)	469 ± 26 (22%)
3 (suspended few-layer)	2.1 ± 0.1 (40%)	34 ± 1 (47%)	708 ± 55 (13%)
4 (supported few-layer)	1.2 ± 0.1 (47%)	29 ± 2 (41%)	344 ± 28 (12%)
thick crystal	1.8 ± 0.6 (19%) (rise)	20 ± 2 (81%) (rise)	2626 ± 192 (100%) (decay)

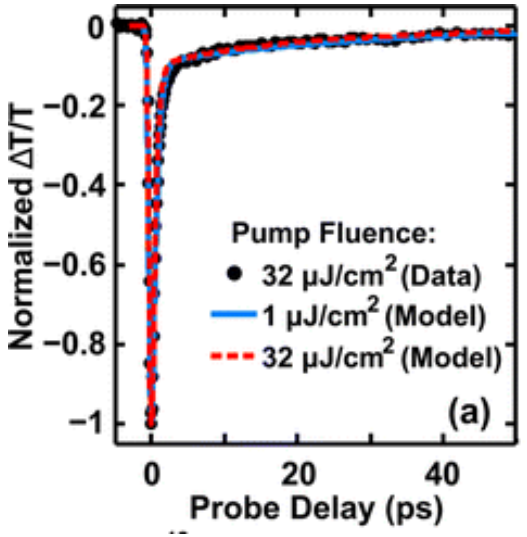
ACS Nano, 2013, 7 (2), pp 1072–1080

- **Nonradiative relaxation dominate**
- **Fast trapping of excitons by surface trap states**

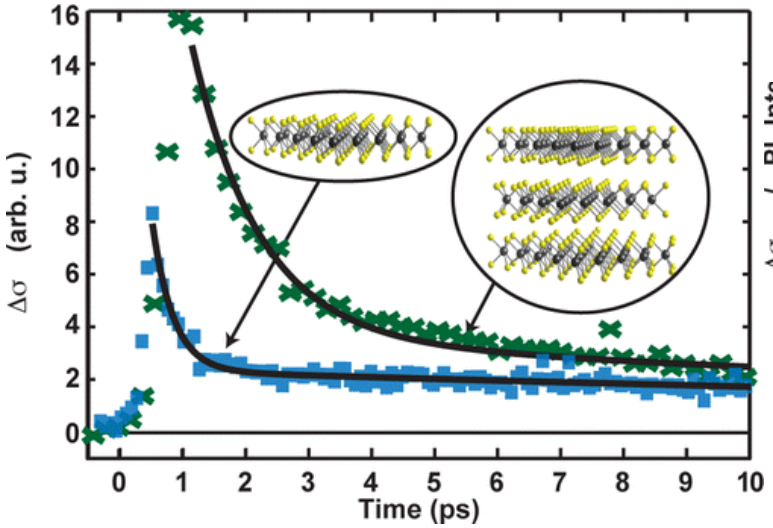
Exicton Dynamics

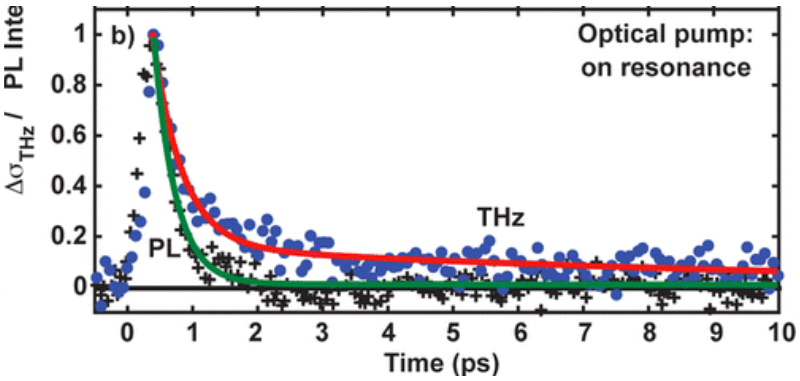






Nano Lett., 2015, 15 (1), pp 339–345

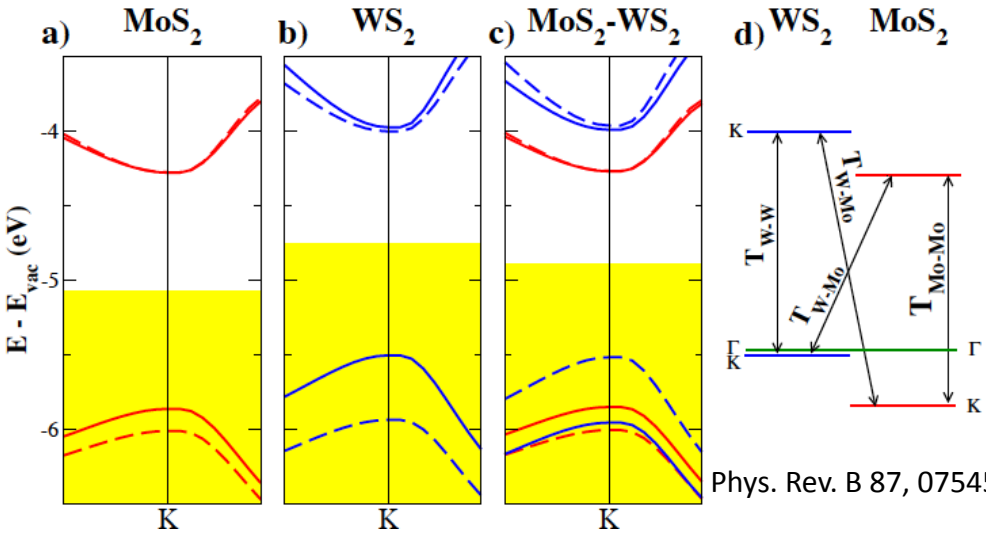




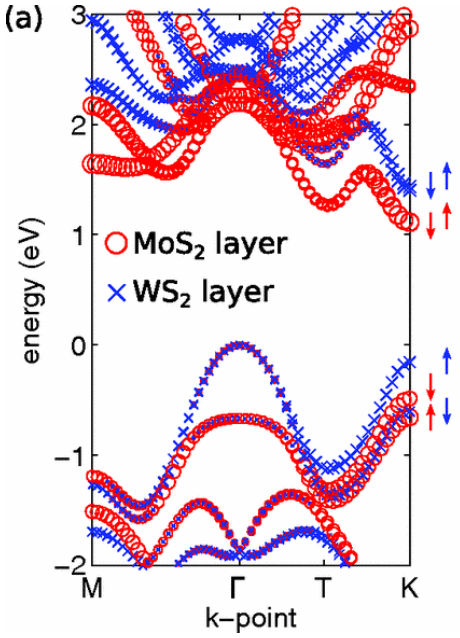
ACS Nano, 2014, 8 (11), pp 11147–11153

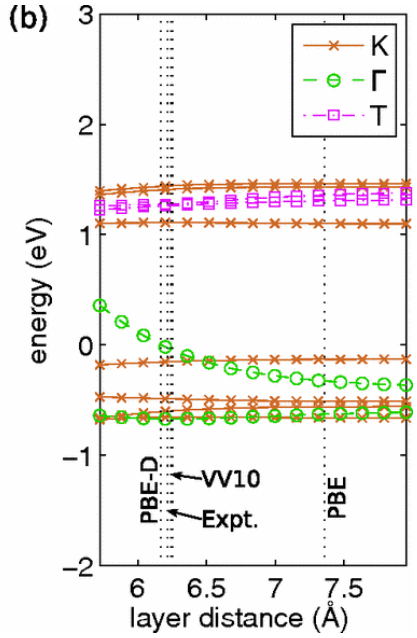
Defect-Assisted Electron–Hole Recombination

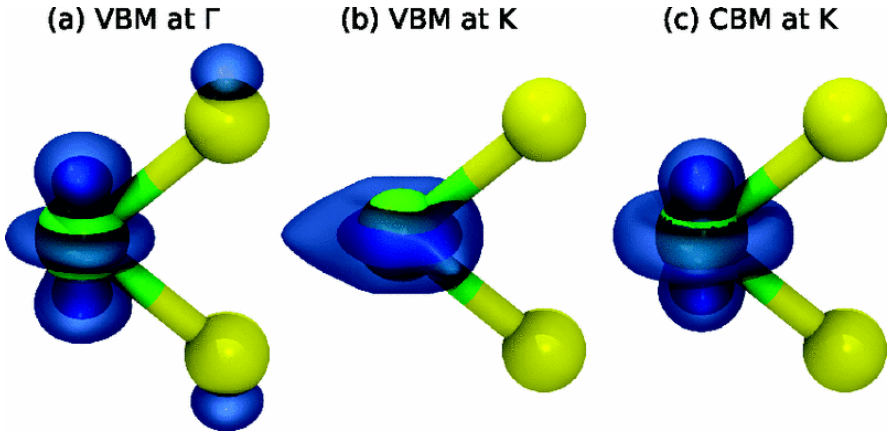
Band Structures in MoS2/WS2 Heterostructures



Phys. Rev. B 87, 075451 (2013)

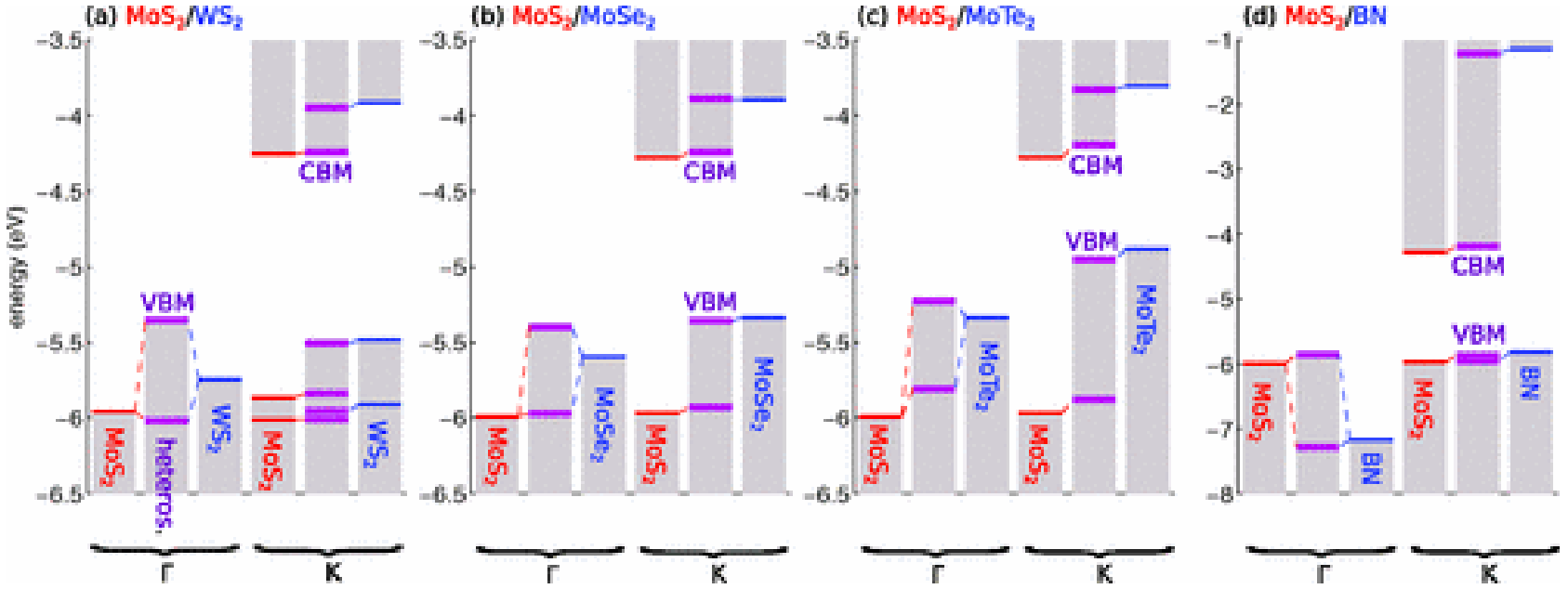






Phys. Rev. B 88, 085318

Band Structures in Other Heterostructures



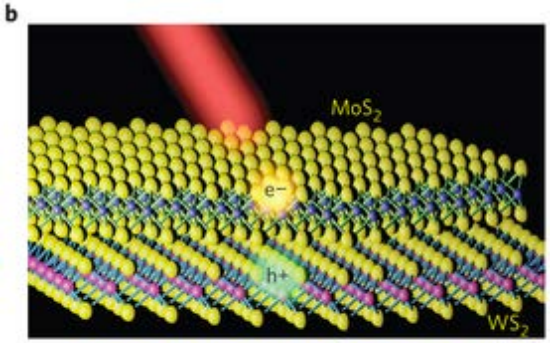
Phys. Rev. B 88, 085318

Table 1 | Direct and indirect (in parenthesis) band gaps in eV of hybrids of semiconducting transition metal dichalcogenides (STMD). Systems with a dominant direct band gap at the K point in the Brillouin zone have an asterisk. Cases with "+" show an indirect fundamental band gap Γ-K, and "&" corresponds to a dominant indirect gap K-I

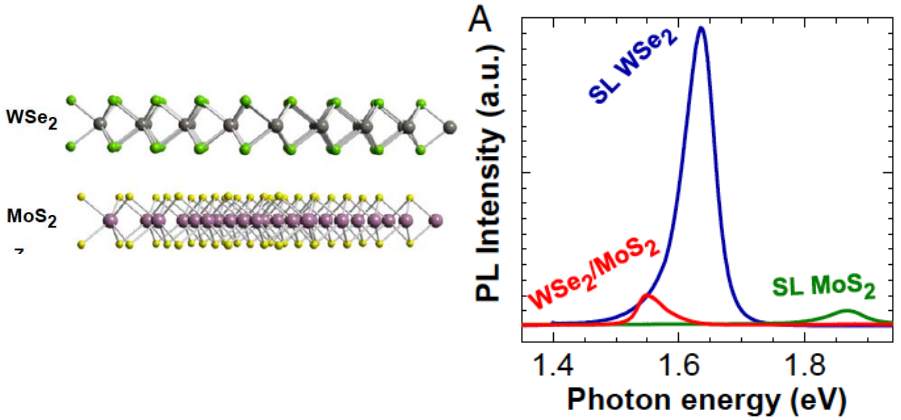
Hybrid-Structure	Bilayer-Stacking A	Bilayer-Stacking B	Crystal- stacking A	Crystal- stacking B
WS_2-MoS_2 Type 1	1.695(1.586 Γ-I)	1.708(1.190 Γ-I)	1.669(1.284 Γ-I)	1.664 (0.764 Γ-I)
WS_2-WSe_2 Type 2	1.007(1.725 Γ-I)*	1.068(1.314 Γ-I)*	1.007(1.406 Γ-I)*	1.037 (0.883 Γ-I)
MoS_2-WSe_2Type 2	0.790(1.525 Γ-I)*	0.891(1.147 Γ-I)*	0.802(1.245 Γ-I)*	0.883 (0.736 Γ-I)
WS_2-$MoSe_2$Type 3	1.154(1.594 Γ-I)*	1.180(1.052 Γ-K)+	1.157(1.316 Γ-I)*	1.155 (0.790 Γ-I)
MoS_2-$MoSe_2$Type 3	0.945(1.560 Γ-I)*	1.013(0.899 Γ-K)+	0.949(1.260 Γ-I)*	0.998 (0.699 Γ-I)
WSe_2-$MoSe_2$Type 4	1.443(1.330 K-I)&	1.471(1.116 Γ-I)	1.444(1.215 K-I)&	1.418 (0.761 Γ-I)

Scientific Reports 3, Article number: 1549, 2013

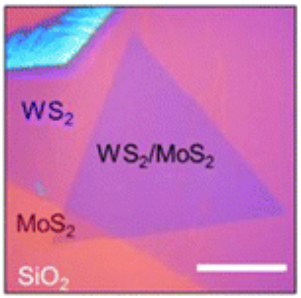
Exicton Dynamics in Heterostructures

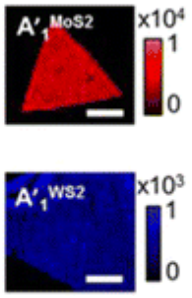


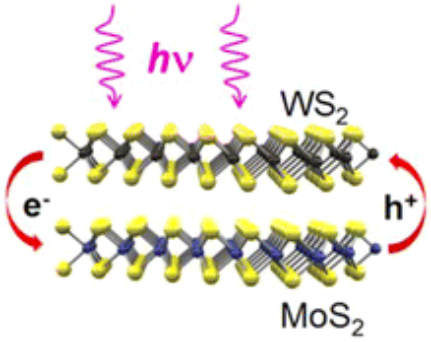
Nature Nanotechnology 9, 682–686 (2014)



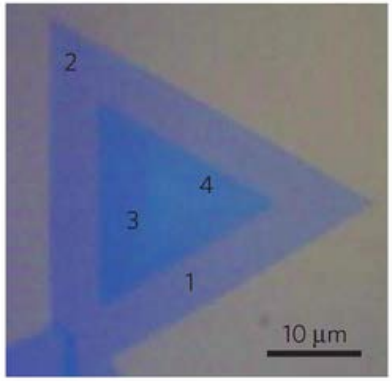
| PNAS | | vol. 111 | 6198–6202 , 2014

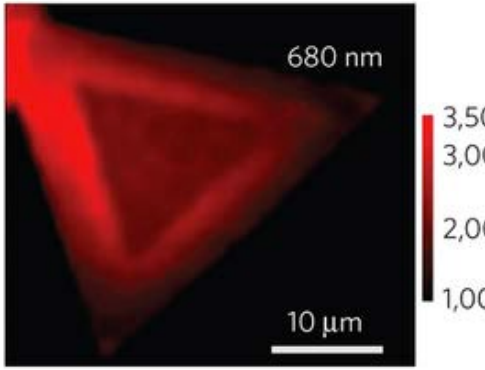




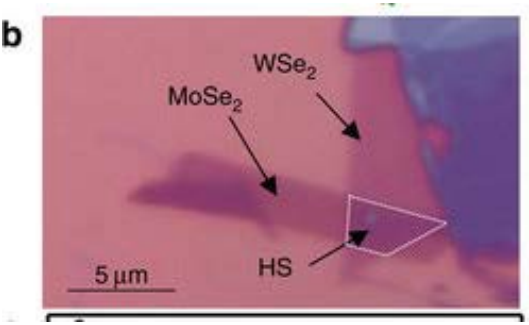


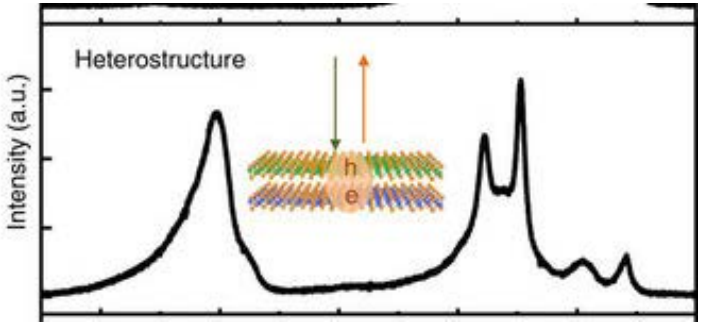
Nano Lett., 2014, 14 (6), pp 3185–3190





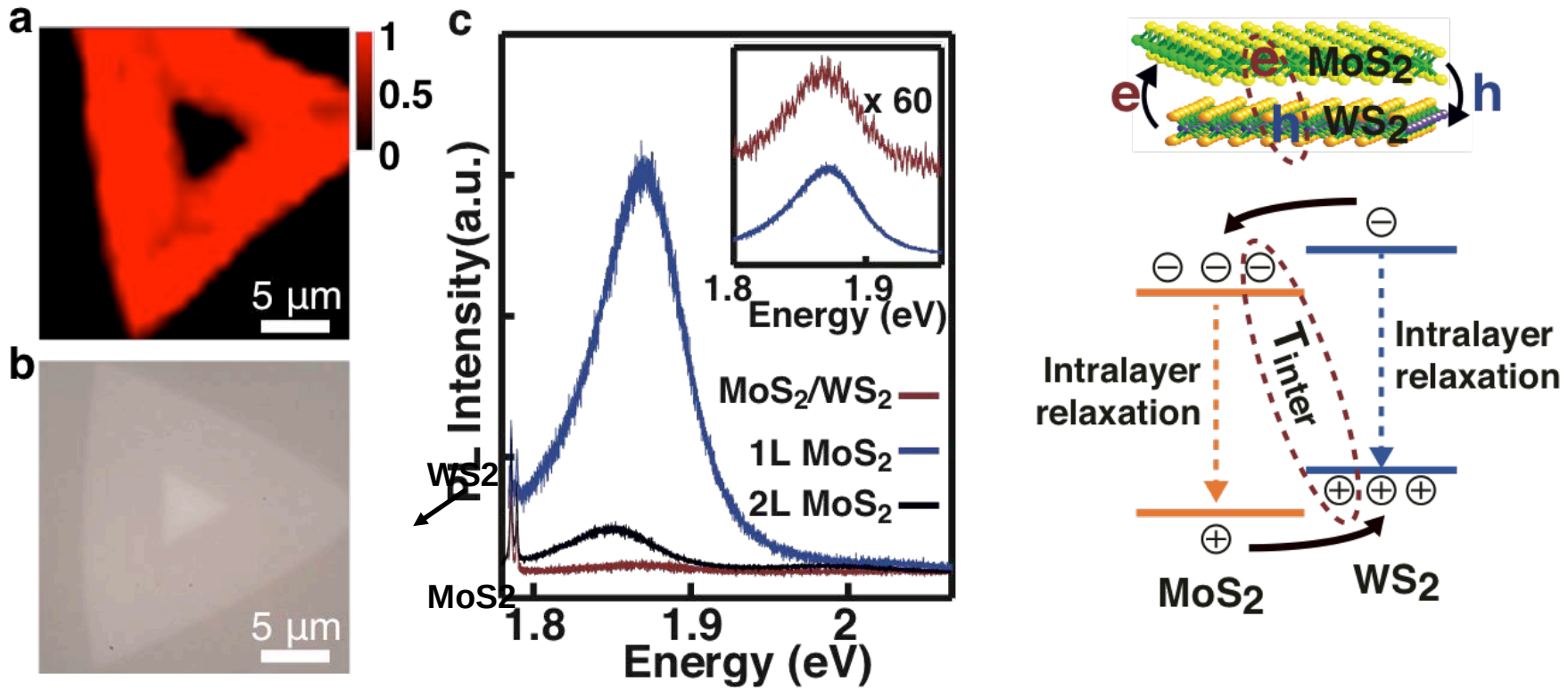
Nature Materials 13, 1135–1142 (2014)





Nature Communications 6, Article number: 6242

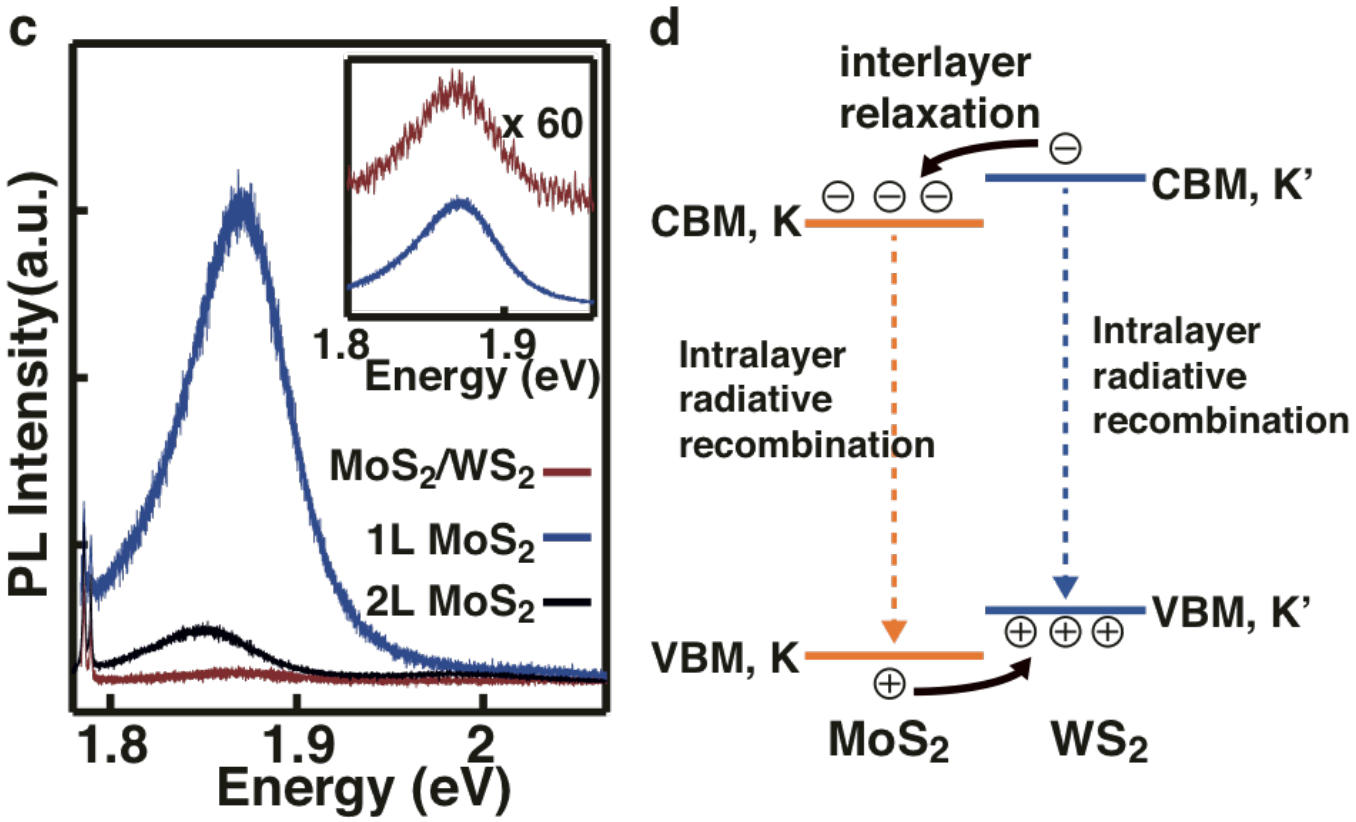
Equally Efficient Interlayer Charge Transfer in Epitaxial and Non-epitaxial MoS2/WS2 Heterostructures



The PL in MoS2/WS2 is two orders of magnitude less!

Yifei Yu et al. *Nano Lett*, DOI: 10.1021/nl5038177, **2014**

Efficient Interlayer Exciton Relaxation

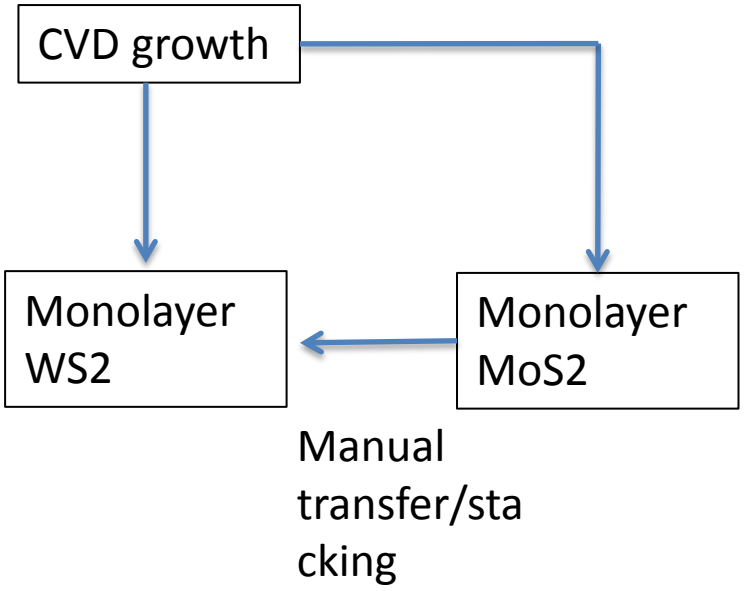


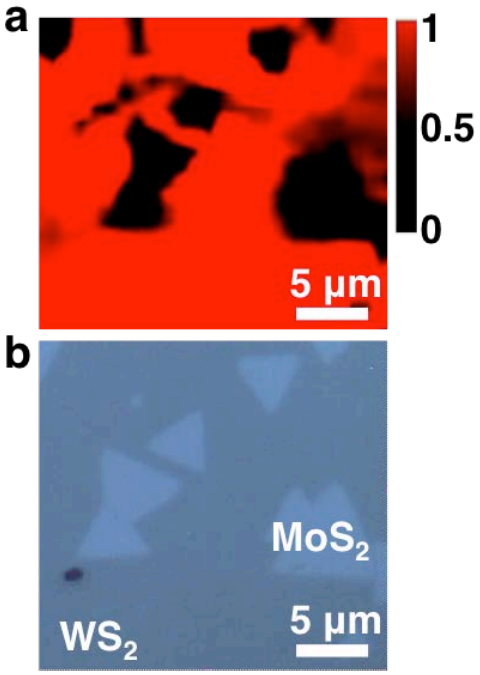
- The radiative lifetime of excitons in MoS2 is around 1-5 ps.
- The PL is supressed by 50 -100 times after the heterostructuring.

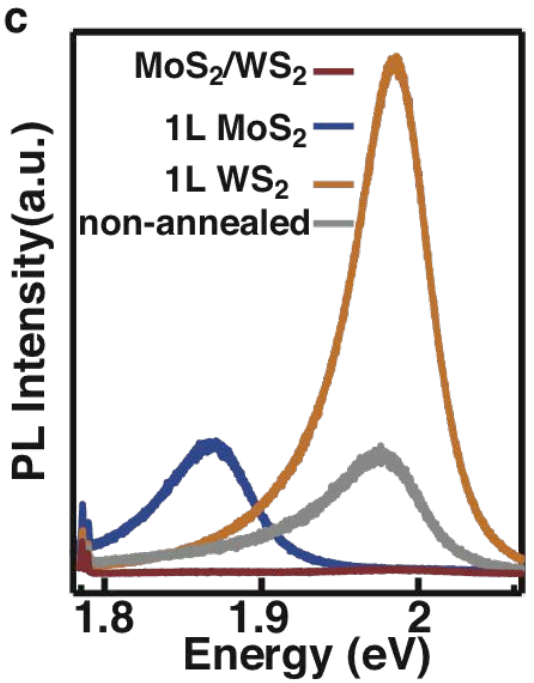
The interfacial charge transfer is in scale of 10-100 fs!

Yifei Yu et al. *Nano Lett*, DOI: 10.1021/nl5038177, **2014**

Equally Efficient Interlayer Charge Transfer in Epitaxial and Non-epitaxial MoS2/WS2 Heterostructures







Efficient interlayer relaxation in non-epitaxial heterostructures!

Yifei Yu et al. *Nano Lett*, DOI: 10.1021/nl5038177, **2014**

Disclaimer

This tutorial is not meant to be comprehensive. The instructor would like to apologize for missing any important papers/works and would appreciate it if the missing work could be brought to the instructor's attention at lcao2@ncsu.edu.

Thank You!