

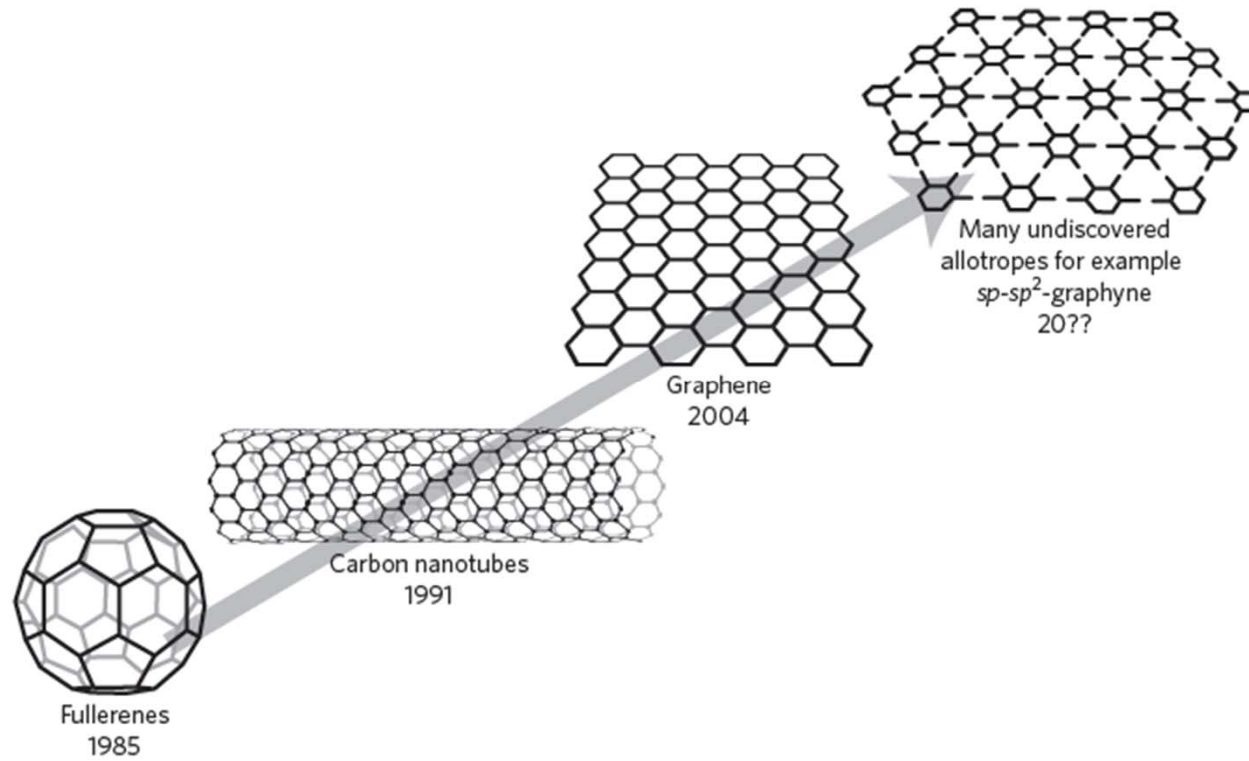
“凝聚态物理-北京大学论坛”  
Forum on condensed matter physics at PKU  
2014

# 为什么是 $\text{MoS}_2$ ?

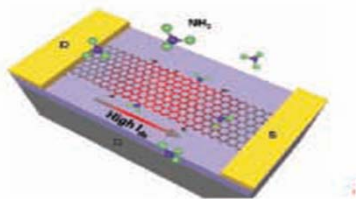
报告人 吕劲

北京大学物理学院  
人工微结构与介观物理国家重点实验室  
量子物质科学协同创新中心  
2014 年10月30日

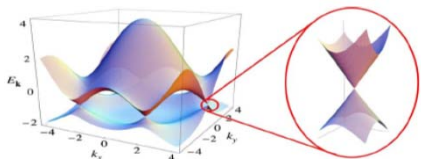
# 纳米材料按照维度的发展



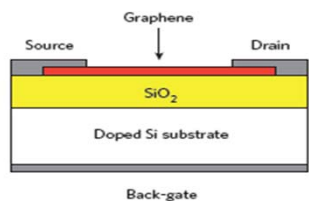
与三维块材，零维的团簇，一维的纳米线和管，二维材料是人认识最少的维度材料



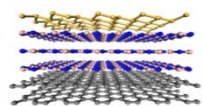
最大的表面积，高的探测效率



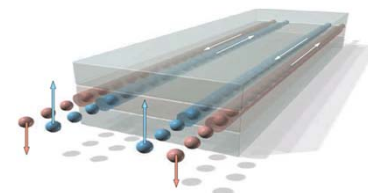
狄拉克锥 非常高的载流子迁移率快速装置



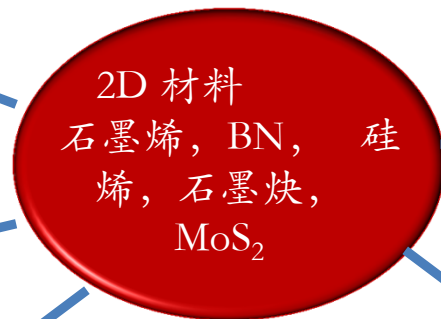
做场效应管 短沟道效应受抑制



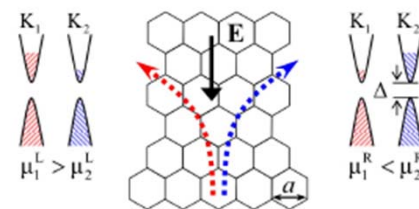
用堆积造出新的结构



2D的拓扑绝缘体  
可以有量子自旋  
霍尔效应  
反常量子霍尔效应



Valley Hall effect



平面结构易于  
加工成需要的平板电路

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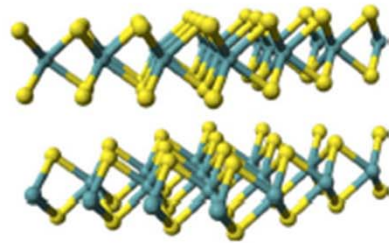
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# 1 电子结构

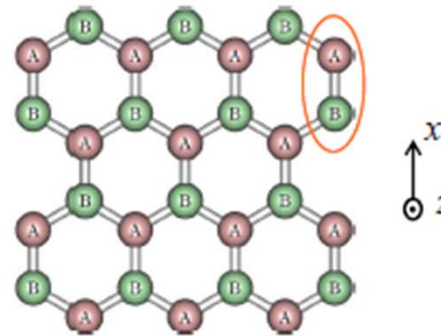
## 2D transition metal dichalcogenides

$\text{MX}_2$    $M = \text{Mo, W}$   $X = \text{S, Se}$

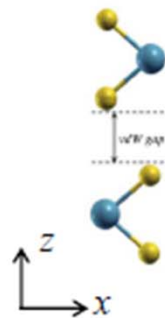


Layered structure suitable for extracting monolayer by mechanical exfoliation

Top view



**Bulk or even-layers**



Indirect bandgap

with inversion symmetry

Even-odd oscillation of SHG  
Zeng, et al. Sci Rep 13''



**Monolayer**

Direct bandgap

without inversion symmetry

Splendiani et al., NL 10''  
Mak et al., PRL 10''



## 层数依赖

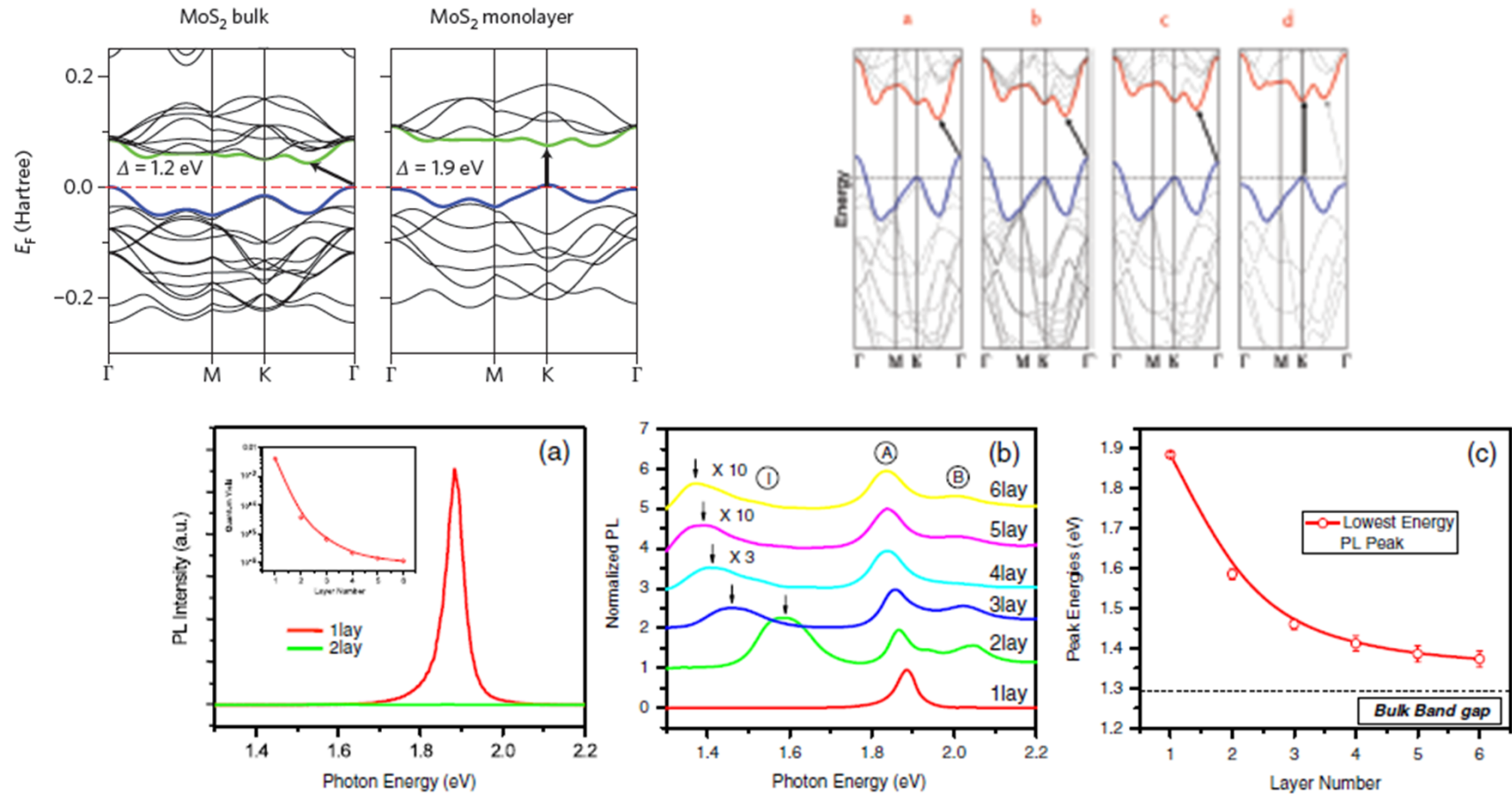
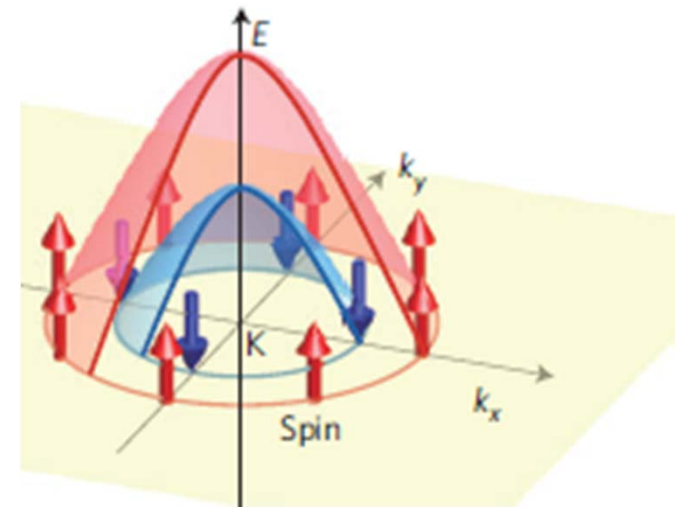
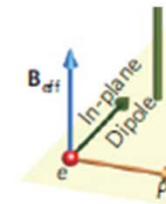
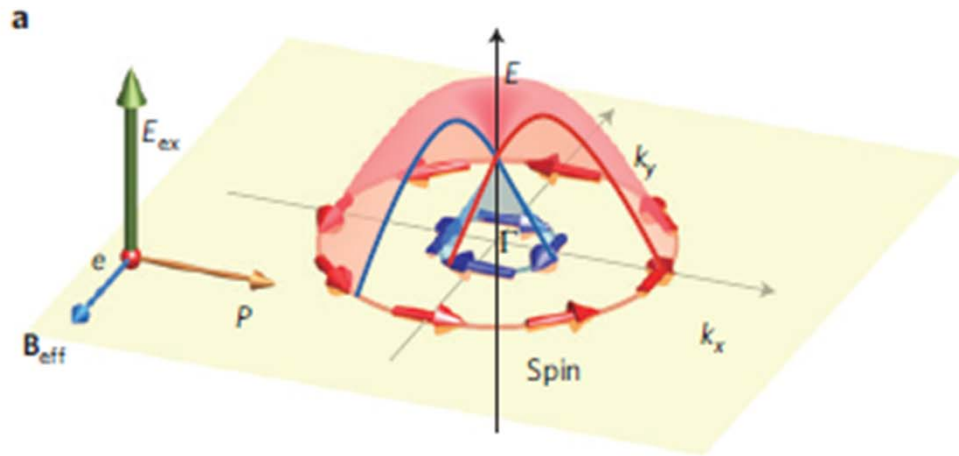


FIG. 3 (color online). (a) PL spectra for mono- and bilayer MoS<sub>2</sub> samples in the photon energy range from 1.3 to 2.2 eV. Inset: PL QY of thin layers for  $N = 1-6$ . (b) Normalized PL spectra by the intensity of peak A of thin layers of MoS<sub>2</sub> for  $N = 1-6$ . Feature I for  $N = 4-6$  is magnified and the spectra are displaced for clarity. (c) Band-gap energy of thin layers of MoS<sub>2</sub>, inferred from the energy of the PL feature I for  $N = 2-6$  and from the energy of the PL peak A for  $N = 1$ . The dashed line represents the (indirect) band-gap energy of bulk MoS<sub>2</sub>.

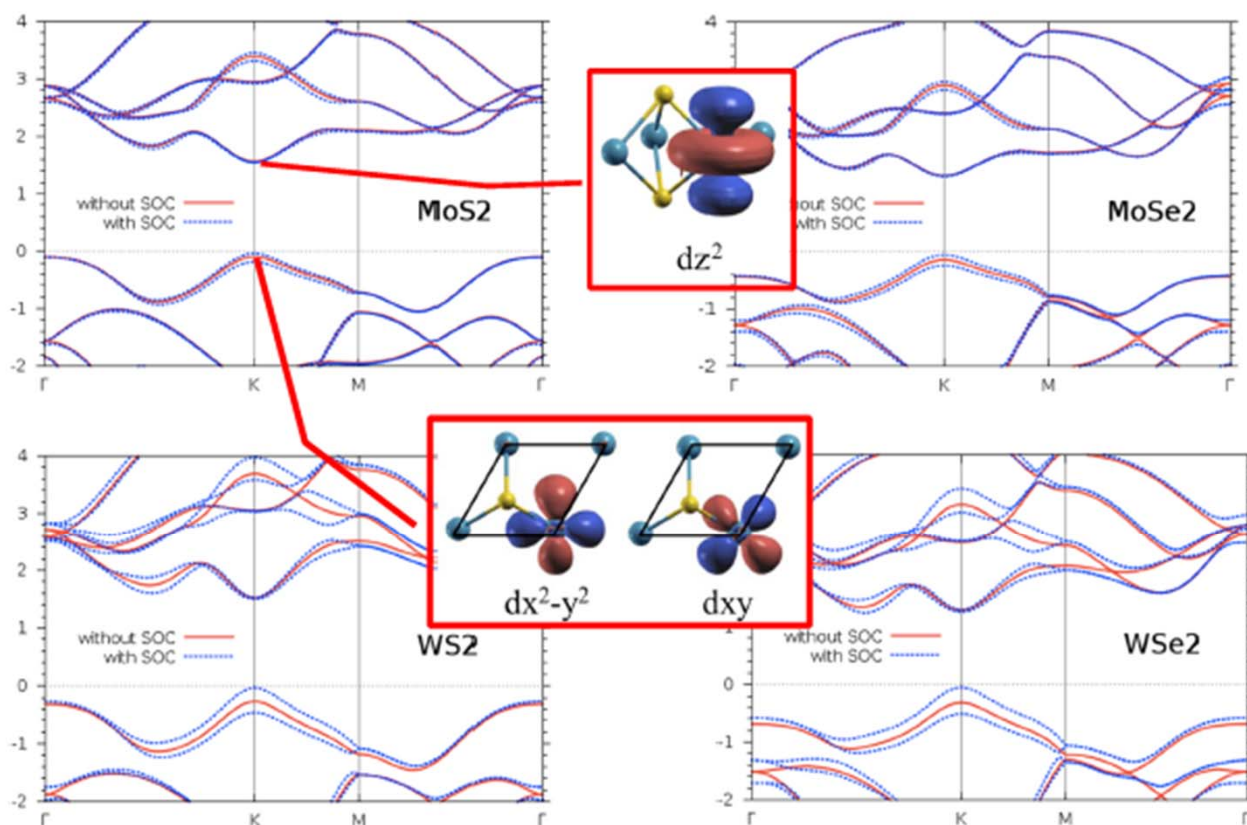
# 强烈的自旋轨道耦合

$$H_{SO} = \frac{g\mu_B}{2c^2} (\mathbf{v} \times \mathbf{E}) \cdot \sigma,$$

$$\mathbf{B} = (\mathbf{v} \times \mathbf{E})/c^2.$$

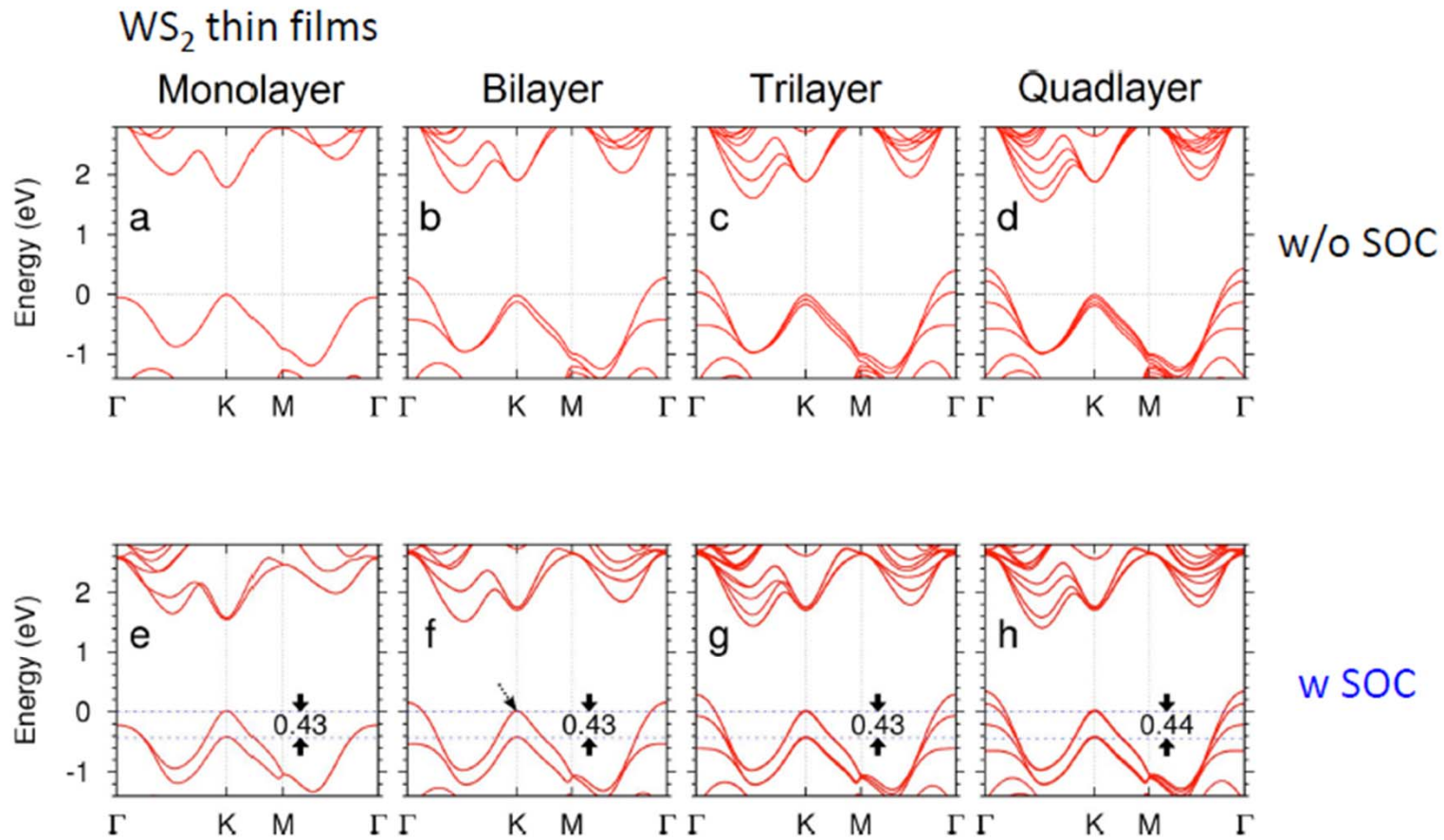


# Monolayer group VIB TMDCs





# 自旋轨道耦合的层数依赖的能带



Zeng, Liu, et al. Scientific Reports 3, 168 (2013)

## DFT

$$\left[ -\frac{\nabla^2}{2} + V_{ion} + V_{Hartree} + V_{xc}[\rho(\mathbf{r})] \right] \psi_{nk} = E_{nk} \psi_{nk}$$

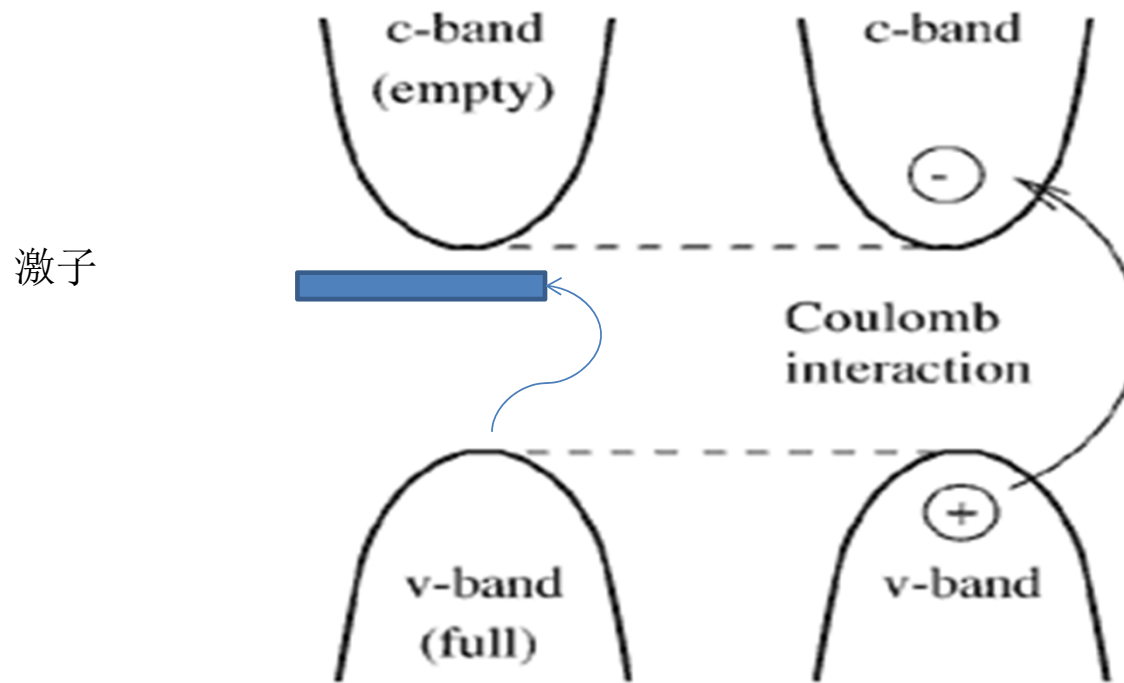
LDA 单做电子近似，与实验值比起，通常低估能隙 30-50%，  
考虑多体效应可以有效修正

低维系统 电子较少，屏蔽减弱，电子间库仑作用增强，多体效应更加明显  
能带修正更大

GW----- 准粒子方法 (G 格林函数, W屏蔽作用)

$$\left[ -\frac{\nabla^2}{2} + V_{ion} + V_{Hartree} + \Sigma(E_{nk}) \right] \psi_{nk} = E_{nk} \psi_{nk}$$
$$\Sigma = iGW$$

(G 格林函数, W屏蔽作用)



光吸收图解

低维系统 → 电子-空穴作用变强

→ 激子效应增强（激子能量更加低于导带底部）

光学吸收性质由激子决定！

# 多体效应

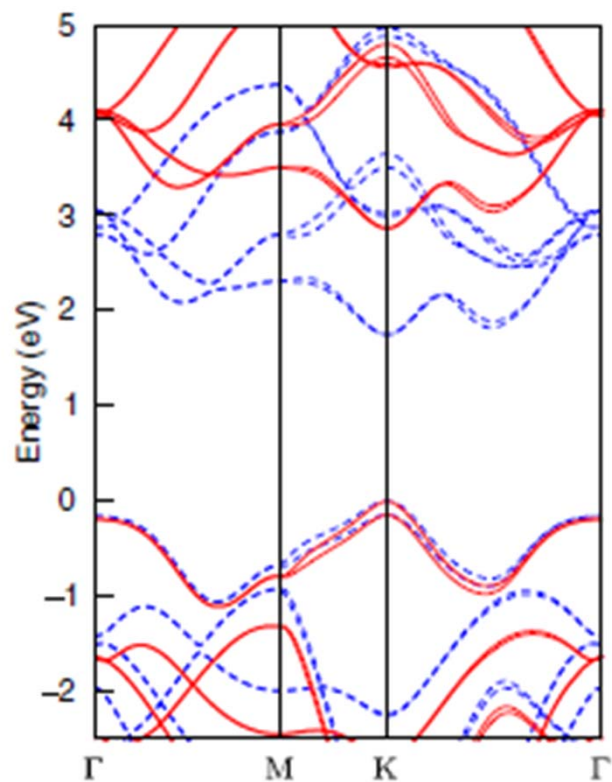


FIG. 1 (color online). Left: LDA (dashed blue curve) and GW (solid red curve) band structure of monolayer MoS<sub>2</sub>. Top right:

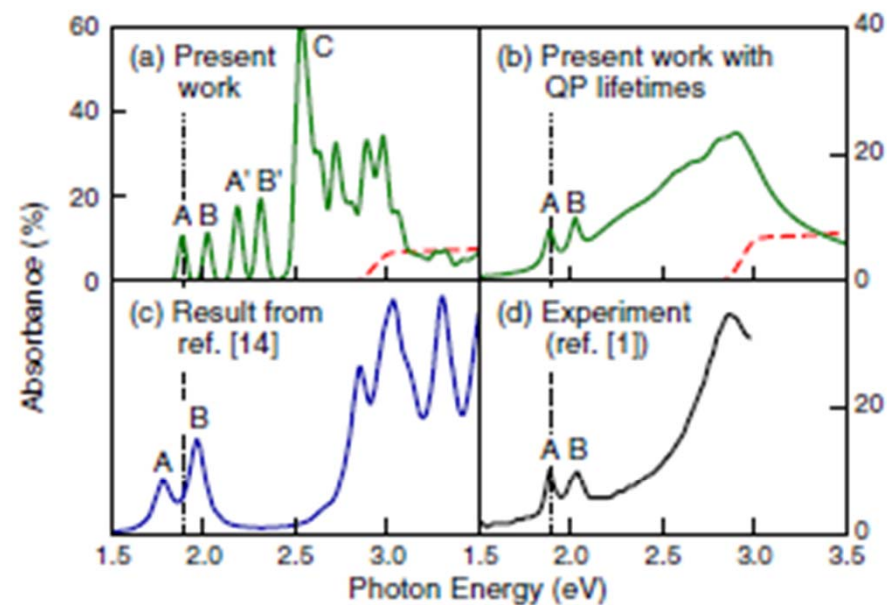
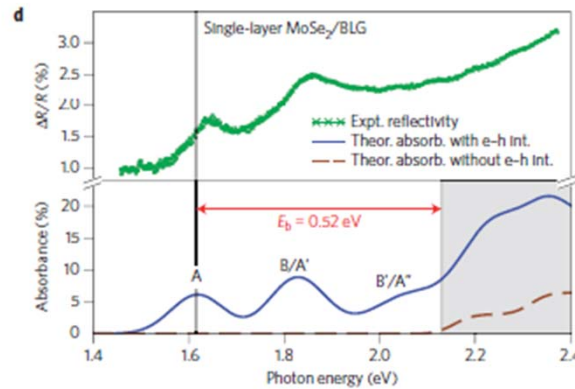
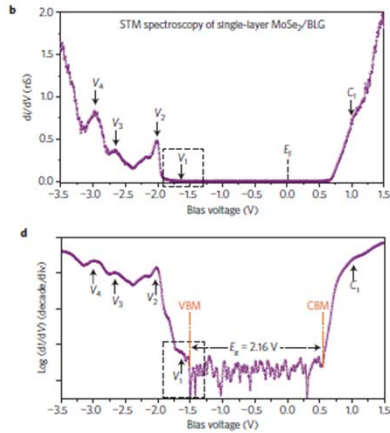


FIG. 2 (color online). (a) Absorption spectra of MoS<sub>2</sub> without (dashed red curve) and with (solid green curve) electron-hole interactions using a constant broadening of 20 meV. (b) Same calculated data as in Fig. 2(a), but using an *ab initio* broadening based on the electron-phonon interactions [27,28]. (c) Previous  $G_0W_0$  calculation (in arbitrary units). Note that the region between 2.2 and 2.8 eV is completely flat. (d) Experimental absorbance [1].

# 多体效应

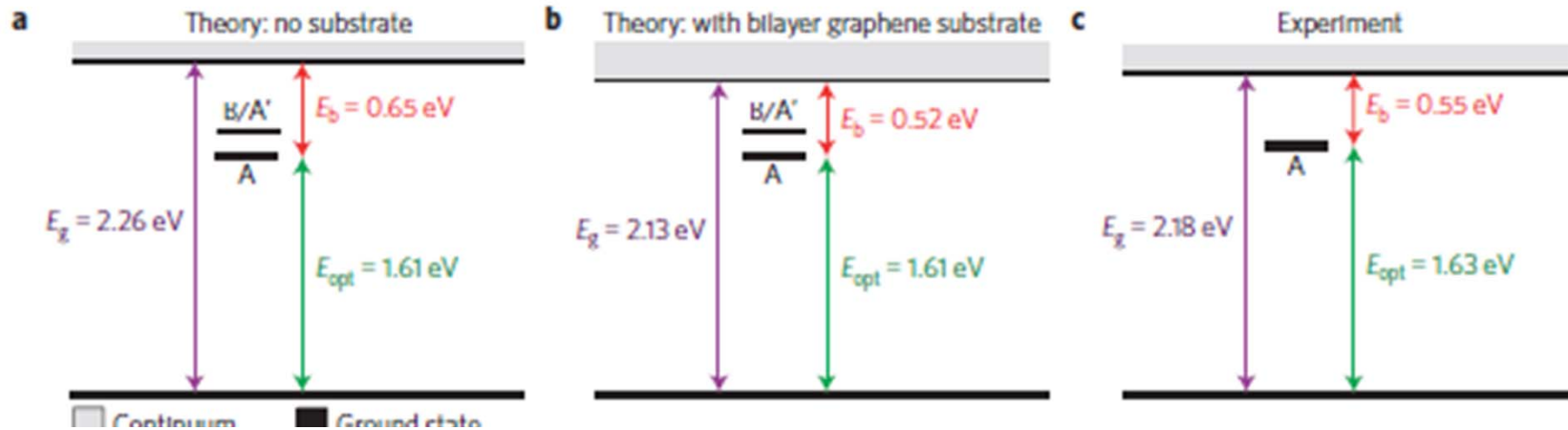
## Giant bandgap renormalization and excitonic effects in a monolayer transition metal dichalcogenide semiconductor

Miguel M. Ugeda<sup>1\*</sup>, Aaron J. Bradley<sup>1\*</sup>, Su-Fei Shi<sup>1\*</sup>, Felipe H. da Jornada<sup>1,2</sup>, Yi Zhang<sup>3,4</sup>, Diana Y. Qiu<sup>1,2</sup>, Wei Ruan<sup>1,5</sup>, Sung-Kwan Mo<sup>6</sup>, Zahid Hussain<sup>7</sup>, Zhi-Xun Shen<sup>4,6</sup>, Feng Wang<sup>1,2,7</sup>, Steven G. Louie<sup>1,2</sup> and Michael F. Crommie<sup>1,2,7\*</sup>



问题:1 其他材料 MoS<sub>2</sub>?  
WSe<sub>2</sub>? 激子效应。

2 衬底的效应?



# Valley index of Bloch electron

---

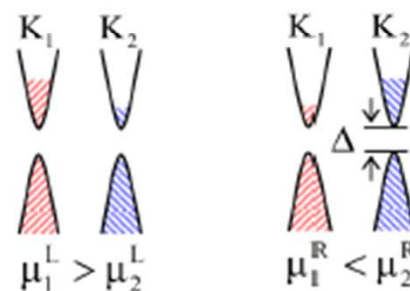
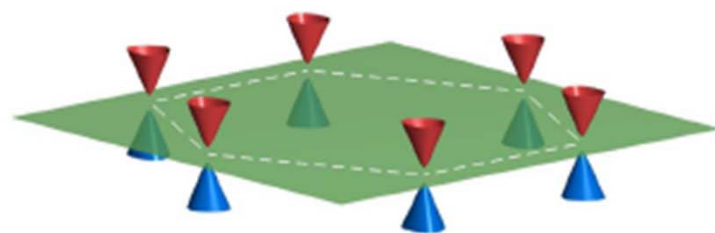
- ♦ Valley index of Bloch electron

Degenerate energy extrema of Bloch bands in momentum space

In atomically thin 2D crystals: graphene, BN, MoS<sub>2</sub> etc.

- ♦ Long lifetime of valley polarization expected

Intervalley scattering suppressed by large k-space separation



Valley polarization

## Valley vs spin for information processing

---

Associated physical phenomena \ Index of Bloch electron	Spin	Valley	
Magnetic moment	✓	✓	} Xiao, WY & Niu, PRL 07"
Hall effect	✓	✓	
Optical selection rule	✓	✓	WY, Xiao & Niu, PRR 08" $\Omega(k) =$

- Valley physics from inversion symmetry breaking
- Valley can be manipulated in ways similar to spin
- Key quantities: Berry curvature & orbital magnetic moment

Hall effect

$$\Omega(k) = \nabla_k \times \langle u(k) | i \nabla_k | u(k) \rangle$$

## Valley contrasting properties by ISB

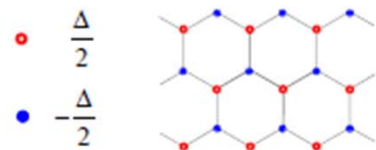
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Time-reversal symmetry	$\Omega(k) = -\Omega(-k)$	$m(k) = -m(-k)$
Space-inversion symmetry	$\Omega(k) = \Omega(-k)$	$m(k) = m(-k)$
Both symmetries	$\Omega(k) = 0$	$m(k) = 0$

### ♦ Valley contrasting properties

- Opposite  $\Omega$  &  $m$  for a time reversal pair of valleys
- Necessary condition: inversion symmetry breaking (ISB)

### ♦ Example: graphene with staggered sublattice potential



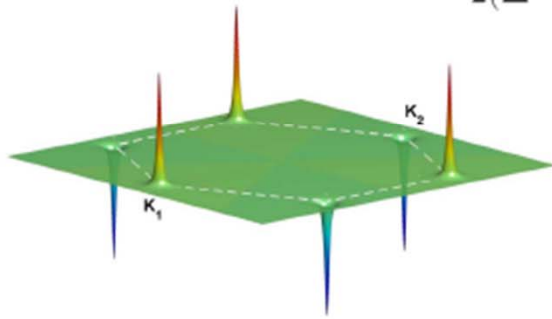
Massive Dirac fermion:

$$\hat{H} = at(k_x \hat{\sigma}_x + k_y \hat{\sigma}_y) + \frac{\Delta}{2} \hat{\sigma}_z$$

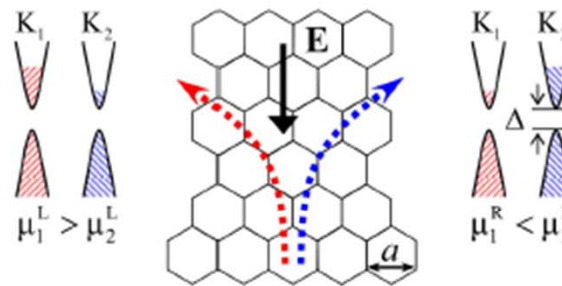


# Valley contrasting Berry curvature

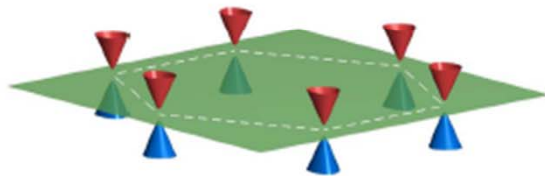
Berry curvature  $\Omega(\mathbf{q}) = \tau_z \frac{3\Delta t^2}{2(\Delta^2 + 3q^2 a^2 t^2)^{3/2}}$   $\tau_z = 1 (-1)$  at valley K (-K)



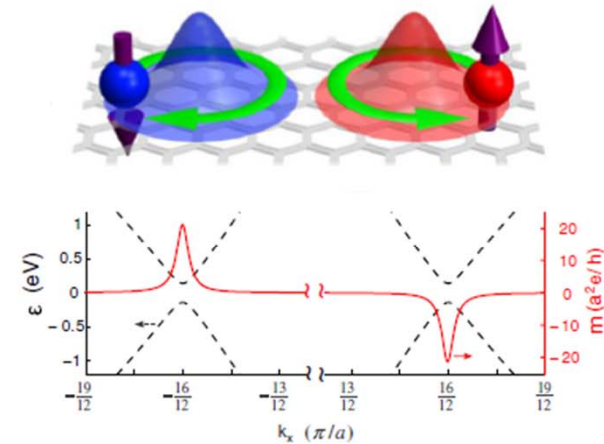
## Valley Hall effect



## Gapped energy dispersion



gapped Dirac cones

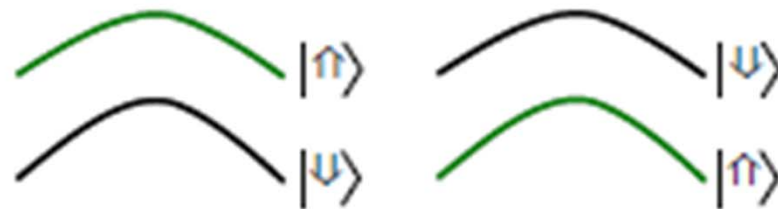
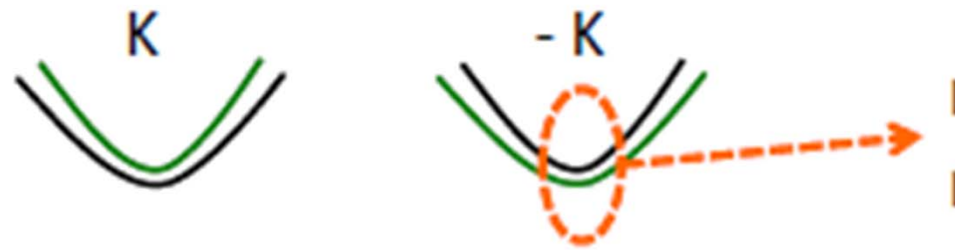


Xiao, WY & Niu, PRL 99, 236809 (2007)

谷磁矩

# Spin-valley coupled massive Dirac fermions

$WX_2$



# 2 FET

**摩尔定律**：集成电路上可容纳的晶体管数目，约每隔18个月便会增加一倍。

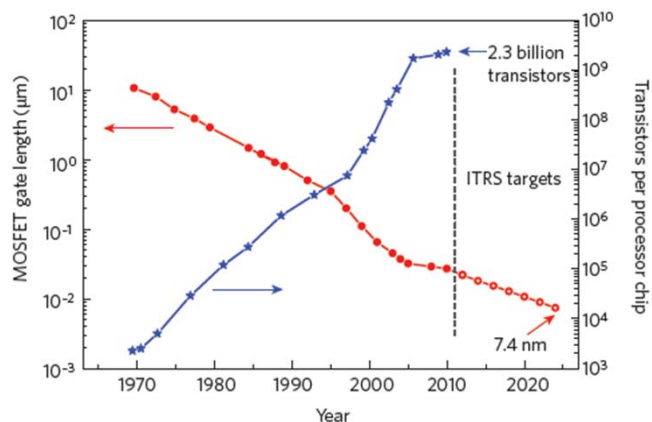


Figure 1 | Trends in digital electronics. Evolution of MOSFET gate length

**挑战**：目前的计算机晶体管尺寸已经缩短到20 nm。下一个十年晶体管的沟道长度要小于10个纳米。但块材硅做沟道的晶体管在10纳米以下的尺度由于显著的短沟道效应实际已经不能可靠工作了。

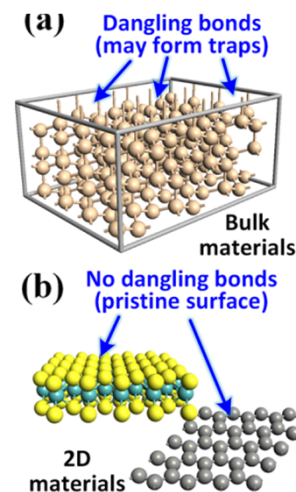
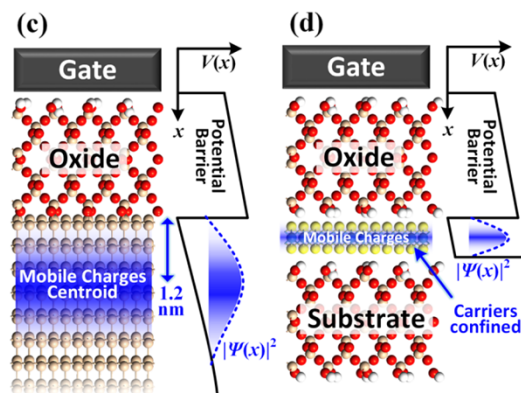
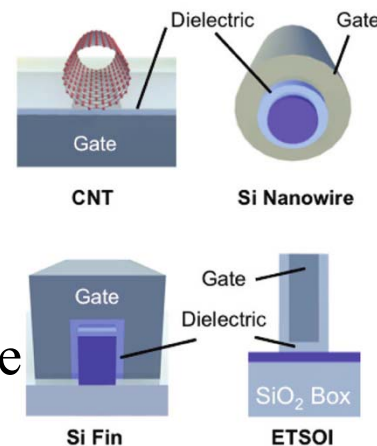
可能的解决方案

1 可以改进硅的结构，

2 低维材料

1D nanotube

2D材料

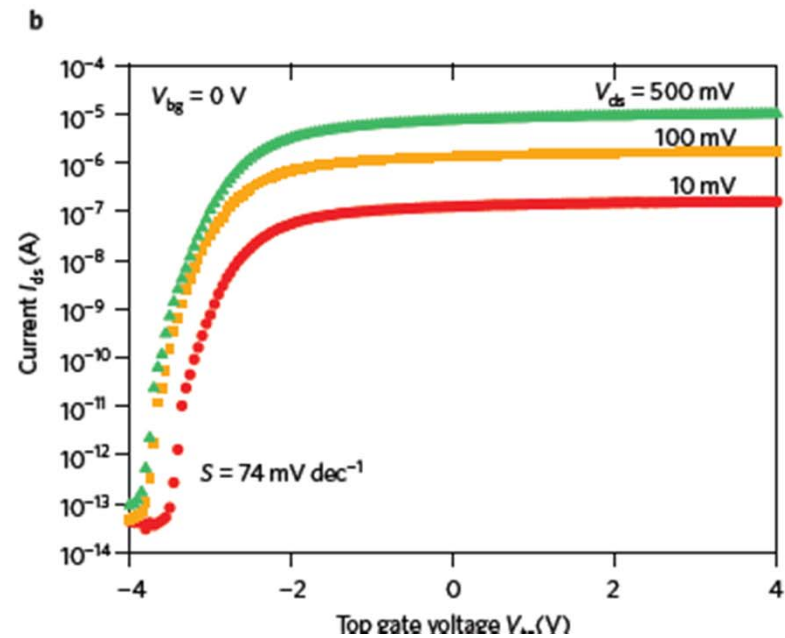
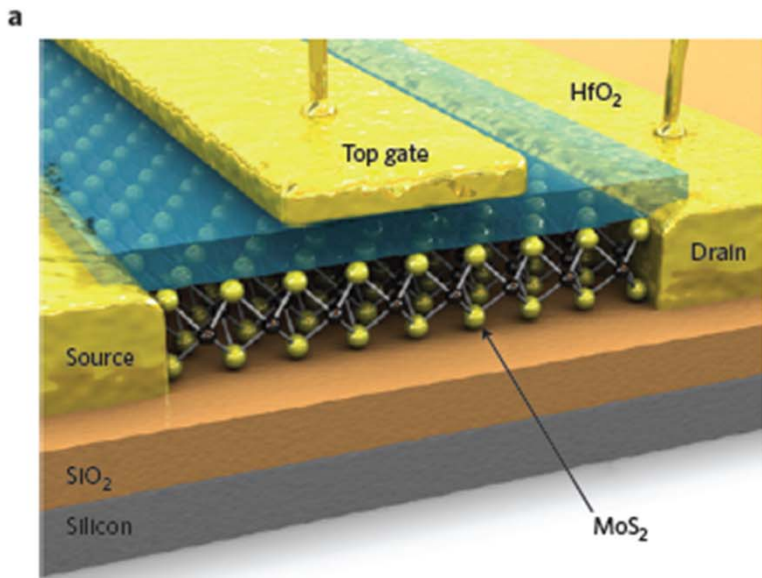


优势：门可控性好，削弱短沟道效应

无侧向的悬挂键，没有界面陷阱

Single-layer MoS<sub>2</sub> transistors

B. Radisavljević, A. Radenović, J. Brivio, V. Giacometti and A. Kis\*



电子器件 光电器件 谷电子学 自旋电子学

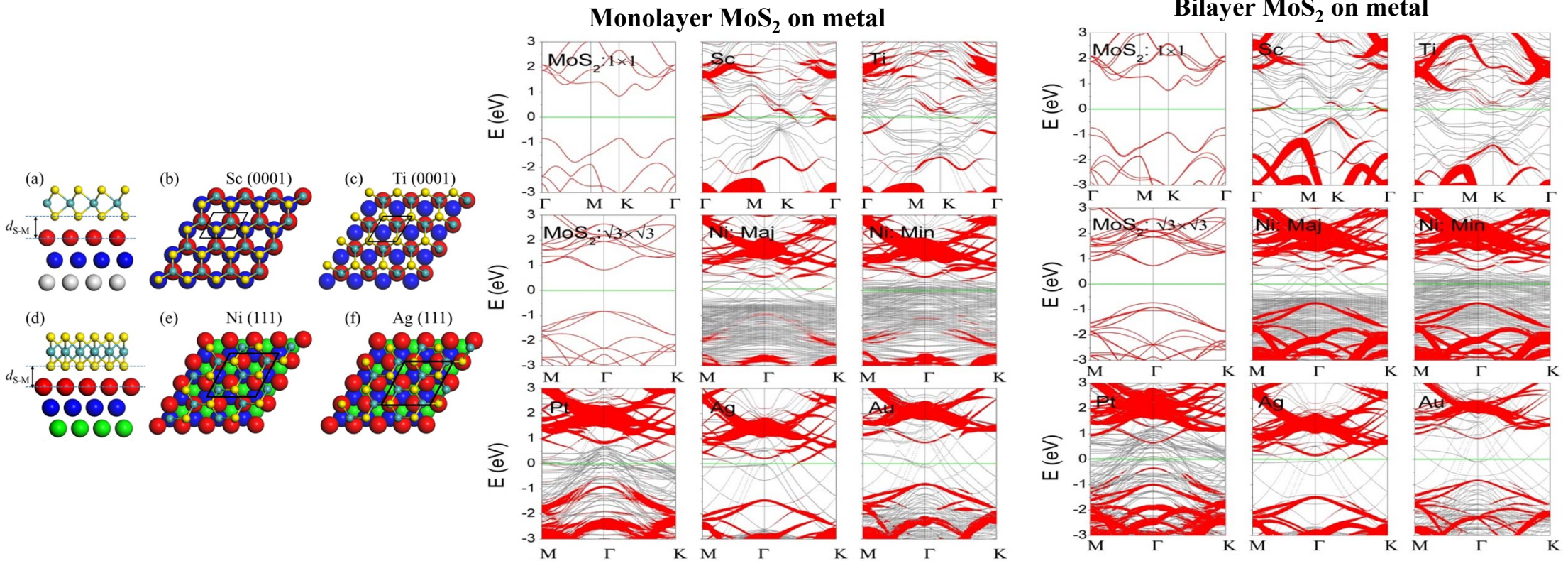
载流子迁移率：  
200 cm<sup>2</sup>/V·s  
沟道 L = 50 nm

问题：1 MoS<sub>2</sub>-金属界面不是很清楚！  
DFT肖特基势垒理论和实验对不上  
Ti-单层：DFT欧姆 ↔ 实验很大SBH

20

2 亚10nm FET能否很好工作？

# Interfacial band structure



- The band structure of MoS<sub>2</sub> is identifiable clearly for MoS<sub>2</sub> on Au surface
- is slightly destroyed by Pt and Ag surfaces
- destroyed seriously by Sc, Ti, and Ni surfaces,
-

# 新方案

1. 区分两种界面 肖特基势垒

2. MoS<sub>2</sub>的能隙1.8 (DFT) -2.8 eV (GW)  
能带做GW修正

单层: 大的 SBH NO Ohmic contact

双层: Sc Ohmic, Ti small SBH **71 meV**

单层: MoS<sub>2</sub>-Ti: larger SBH

双层 MoS<sub>2</sub>-Ti: with SBH ~ **65 meV**

at low temperature

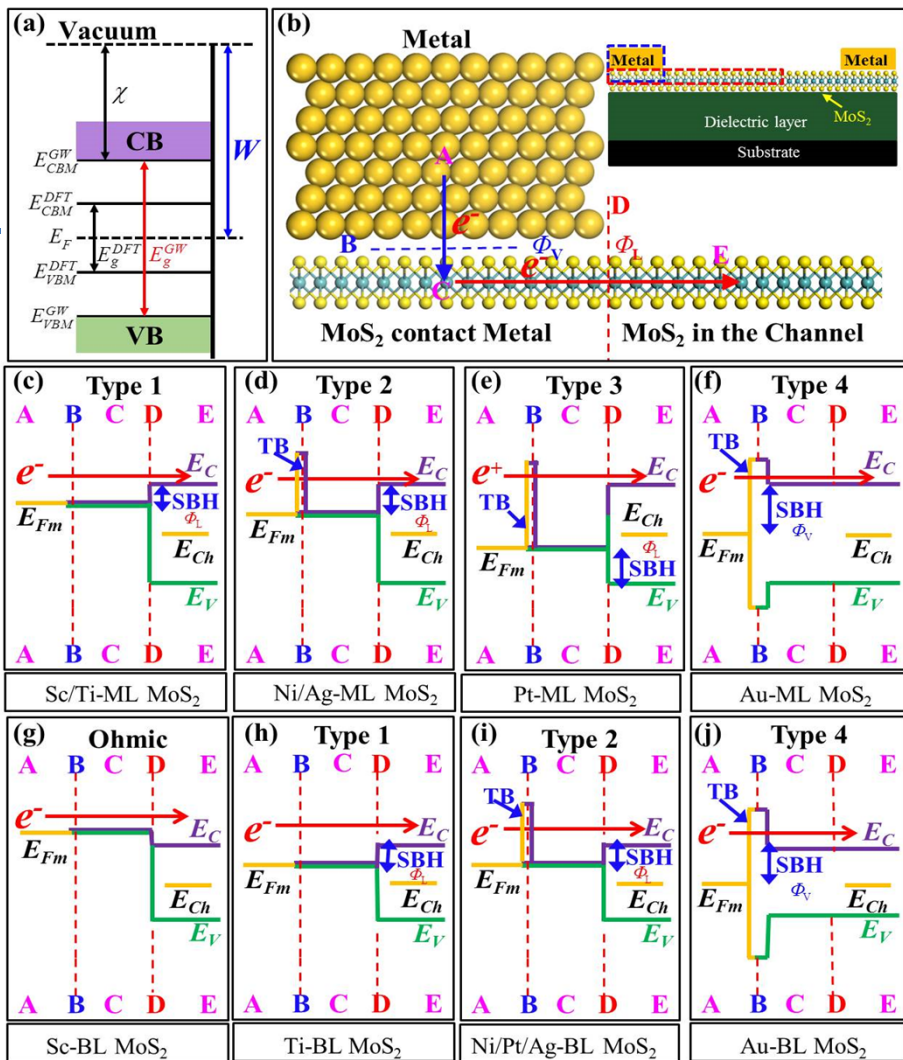
(*Appl. Phys. Lett.* **2012**, *100*, 123104.)

这套计算肖特基势垒方案是普适的。

$E_f$

单层

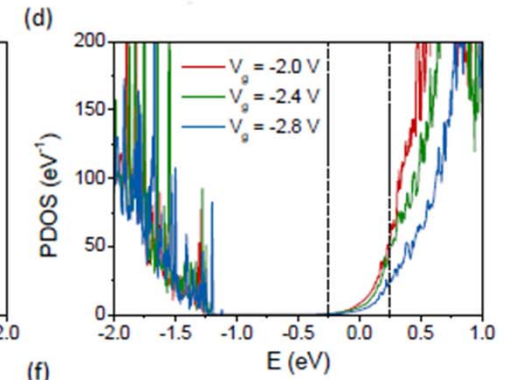
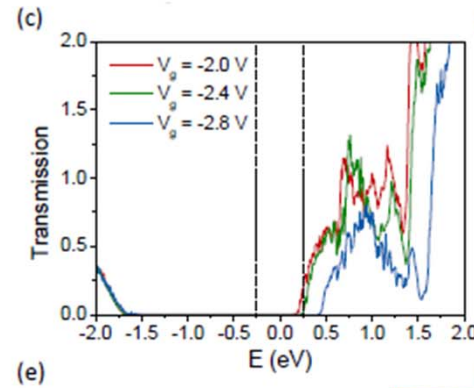
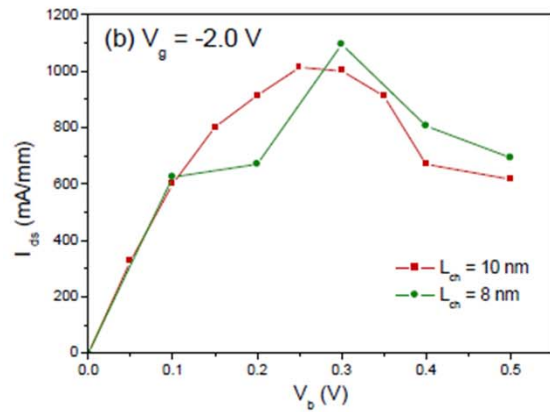
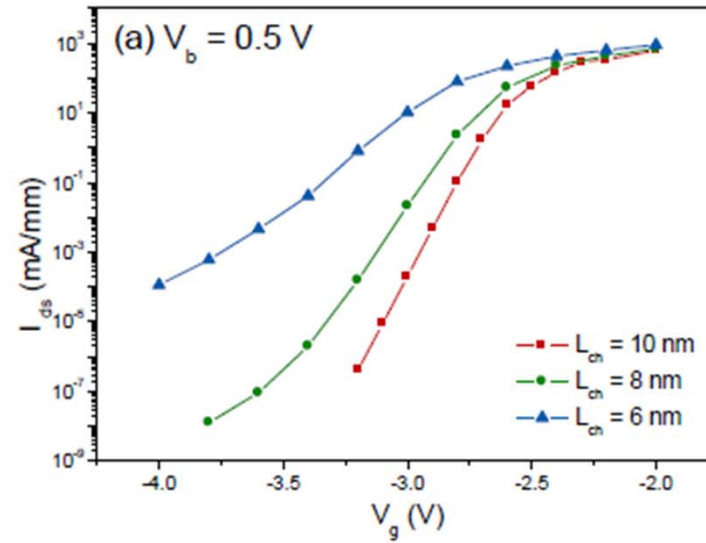
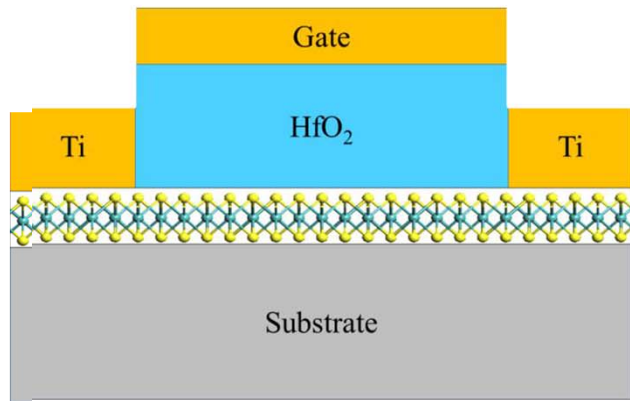
双层



理论

实验

# 10nm MoS<sub>2</sub> FET



与其他FET对比（相同的供应电压）

Category	$L_{ch}$ (nm)	$I_{on}$ (mA/mm)	$I_{on}/I_{off}$	SS (mV/dec)
MoS <sub>2</sub> FET	10	1030	$1.0 \times 10^4$	62
CNT	9	630	$1.0 \times 10^4$	94
Si nanowire	10	300	$1.0 \times 10^4$	89
Si Fin	10	138	$1.0 \times 10^3$	125
UTSOI	8	41	$1.0 \times 10^4$	83

与国际半导体路线图（ITRS）2018年的要求对比

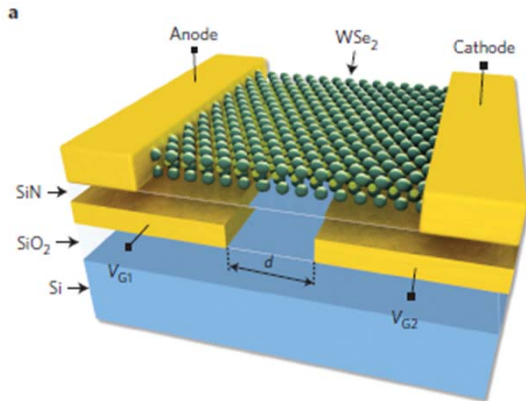
FET	$L_{ch}$ (nm)	$I_{on}$ ( $\mu$ A/ $\mu$ m)	$I_{on}/I_{off}$
MoS <sub>2</sub> FET	10	2929	$2.9 \times 10^4$
ITRS HP transistor 2018	10.2	1610	$1.6 \times 10^4$



# 3 光电器件

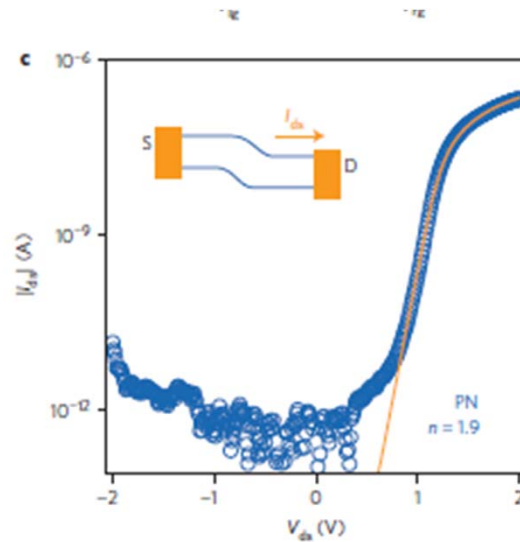
## Electrically tunable excitonic light-emitting diodes based on monolayer WSe<sub>2</sub> p-n junctions

Jason S. Ross<sup>1</sup>, Philip Klement<sup>2,3</sup>, Aaron M. Jones<sup>3</sup>, Nirmal J. Ghimire<sup>4,5</sup>, Jiaqiang Yan<sup>5,6</sup>, D. G. Mandrus<sup>4,5,6</sup>, Takashi Taniguchi<sup>7</sup>, Kenji Watanabe<sup>7</sup>, Kenji Kitamura<sup>7</sup>, Wang Yao<sup>8</sup>, David H. Cobden<sup>2</sup> and Xiaodong Xu<sup>1,2,\*</sup>

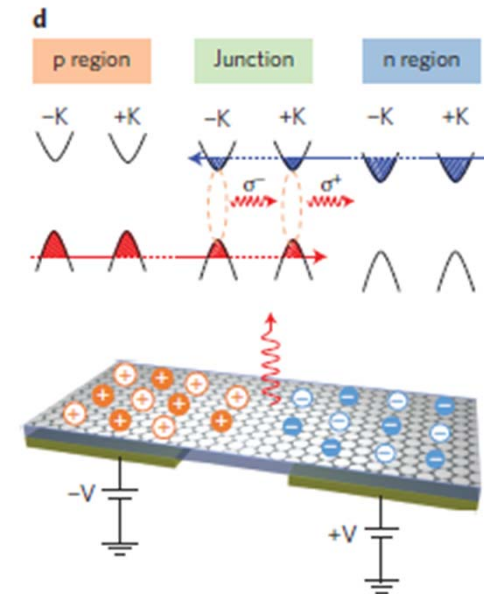


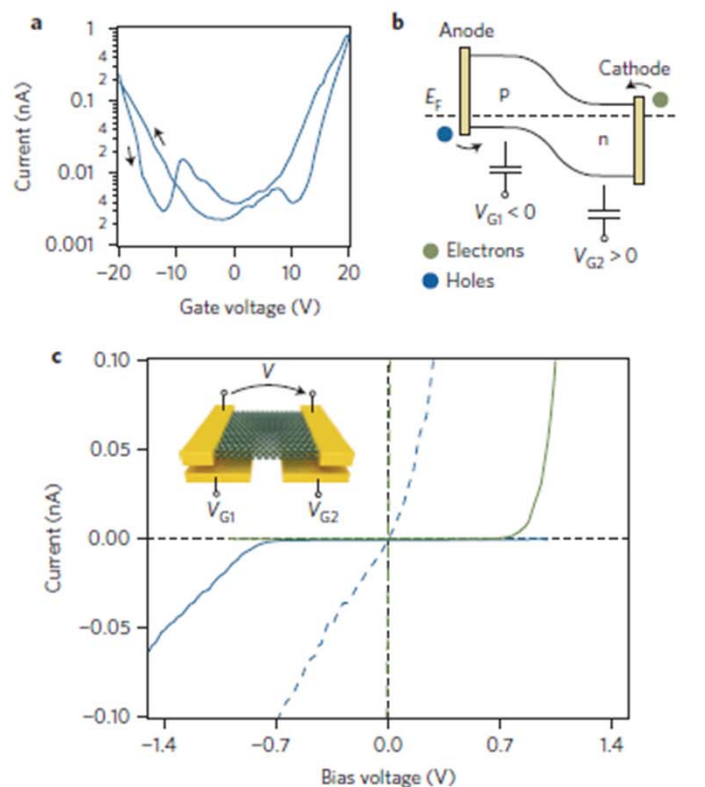
## Solar-energy conversion and light emission in an atomic monolayer p-n diode

Andreas Pospischil, Marco M. Furchi and Thomas Mueller\*

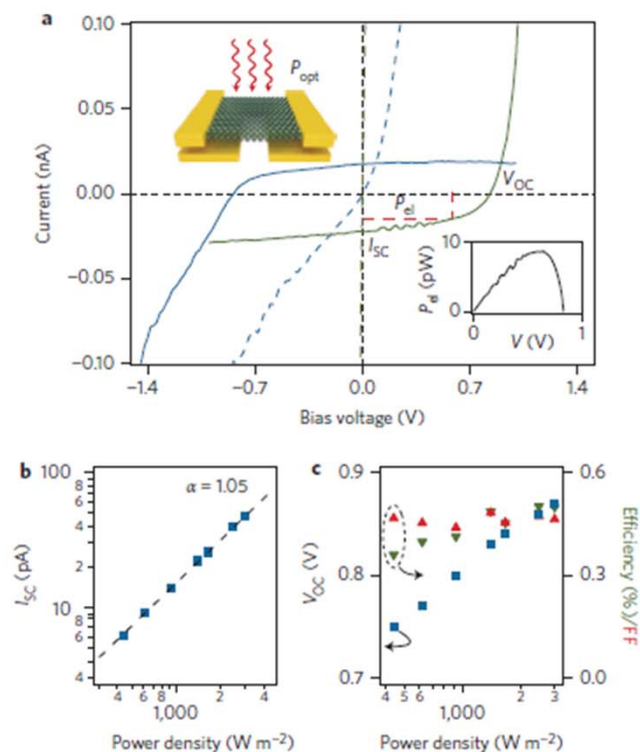


## Optoelectronic devices based on electrically tunable p-n diodes in a monolayer dichalcogenide

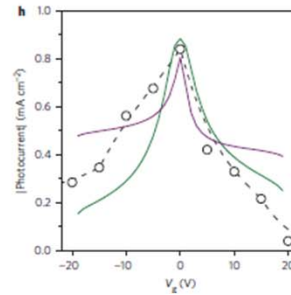
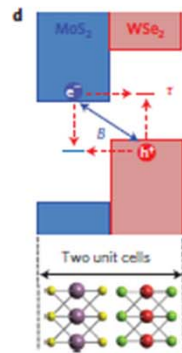
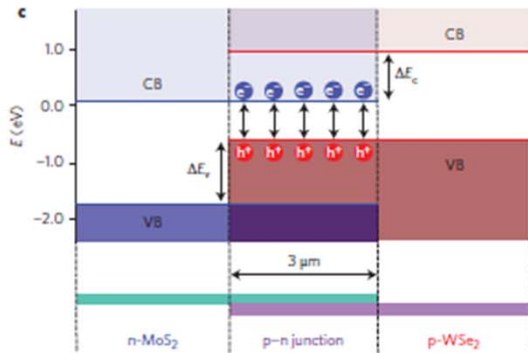
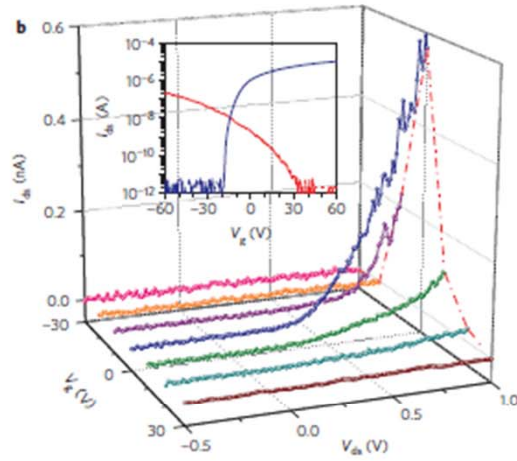
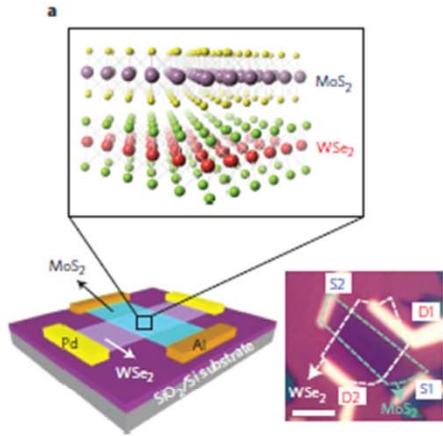




**Figure 2 | Electrical characterization.** **a**, Gate characteristic of the device (0.2 V bias voltage). Both electrons ( $V_{G1} = V_{G2} > 10$  V) and holes ( $V_{G1} = V_{G2} < -10$  V) can be injected into the channel. The curve was obtained by scanning the gate voltage from  $-20$  V to  $20$  V and back. **b**, Band diagram when operating as a p-n junction diode. Asymmetric contact metallization allows more efficient electron (green) and hole (blue) injection. **c**,  $I$ - $V$  characteristics of the device in the dark for biasing conditions as shown in the inset: p-n (solid green line;  $V_{G1} = -40$  V,  $V_{G2} = 40$  V), n-p (solid blue line;  $V_{G1} = 40$  V,  $V_{G2} = -40$  V), n-n (dashed green line;  $V_{G1} = V_{G2} = 40$  V), p-p (dashed blue line;  $V_{G1} = V_{G2} = -40$  V).



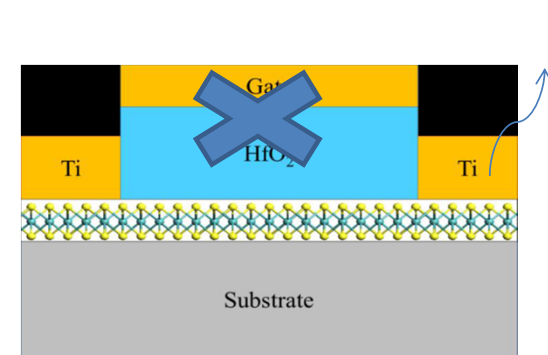
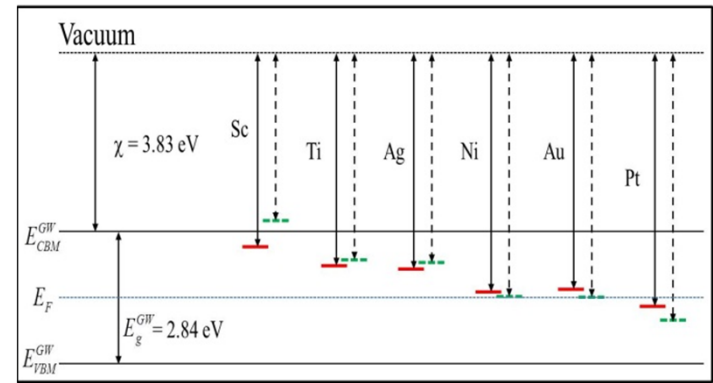
**Figure 3 | Device operation as solar cell and photodiode.** **a**,  $I$ - $V$  characteristics of the device under optical illumination with  $1,400 \text{ W m}^{-2}$ . The biasing conditions are the same as in Fig. 2c: p-n (solid green line;  $V_{G1} = -40$  V,  $V_{G2} = 40$  V), n-p (solid blue line;  $V_{G1} = 40$  V,  $V_{G2} = -40$  V), n-n (dashed green line;  $V_{G1} = V_{G2} = 40$  V), p-p (dashed blue line;  $V_{G1} = V_{G2} = -40$  V). When operated as a diode (solid lines), electrical power ( $P_{ei}$ ) can be extracted. Top inset: Schematic of experiment. Lower inset:  $P_{ei}$  versus voltage under incident illumination of  $1,400 \text{ W m}^{-2}$ . Maximum power conversion efficiency is obtained for  $V = 0.64$  V and  $I = 14$  pA. The red dashed rectangle in the main panel shows the corresponding power area. **b**, Short-circuit current  $I_{sc}$ . Symbols, measurements; dashed line, fit of power law. **c**, Open-circuit voltage  $V_{OC}$  (blue symbols), fill factor FF (red symbols) and power conversion efficiency  $\eta_{PV}$  (green symbols). All parameters are plotted versus incident light intensity.



# Atomically thin p-n junctions with van der Waals heterointerfaces

Chul-Ho Lee<sup>1,2,3</sup>, Gwan-Hyoung Lee<sup>4</sup>, Arend M. van der Zande<sup>5</sup>, Wenchao Chen<sup>6</sup>, Yilei Li<sup>1</sup>, Minyong Han<sup>7</sup>, Xu Cui<sup>8</sup>, Ghidewon Arefe<sup>8</sup>, Colin Nuckolls<sup>2</sup>, Tony F. Heinz<sup>1,9</sup>, Jing Guo<sup>6</sup>, James Hone<sup>8</sup> and Philip Kim<sup>1\*</sup>

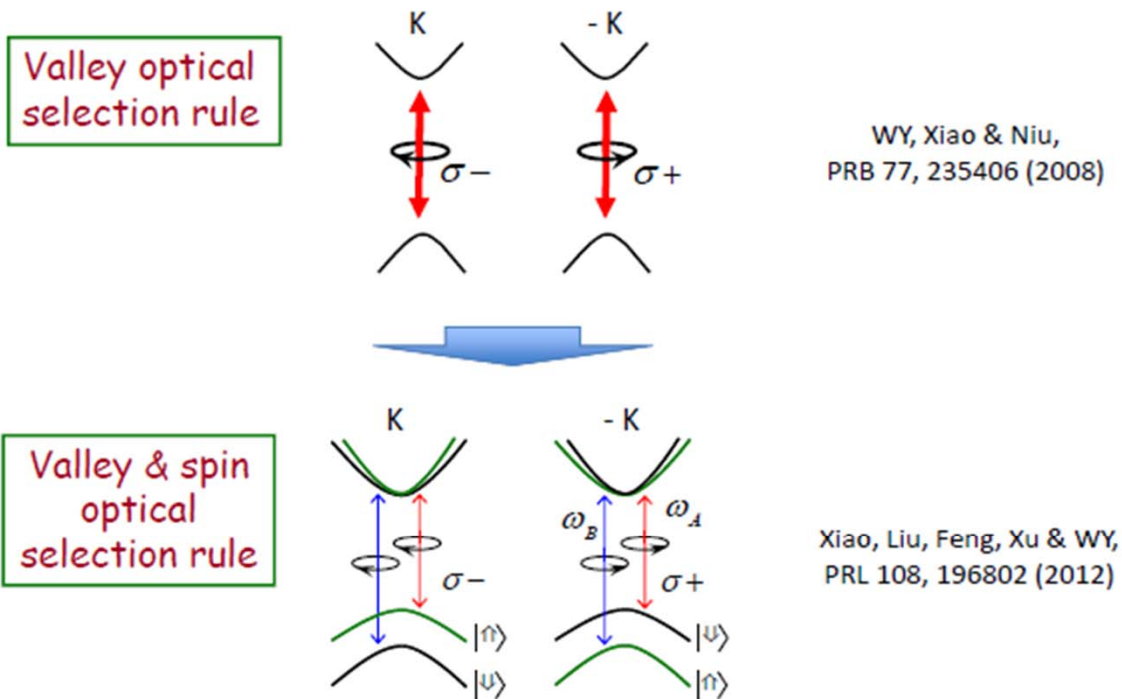
问题: 1 同质MX2 不用门 能否实现p-n 结?



2. 实现TFET (隧穿场效应管) ?

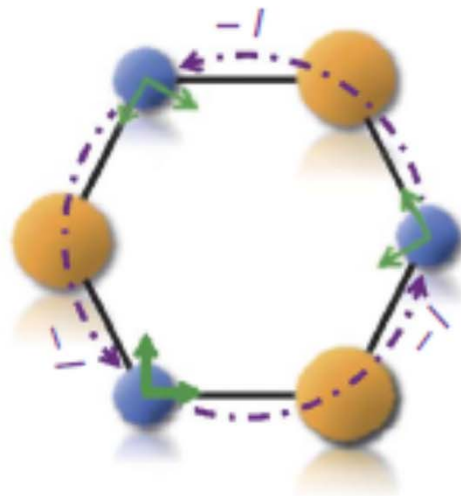
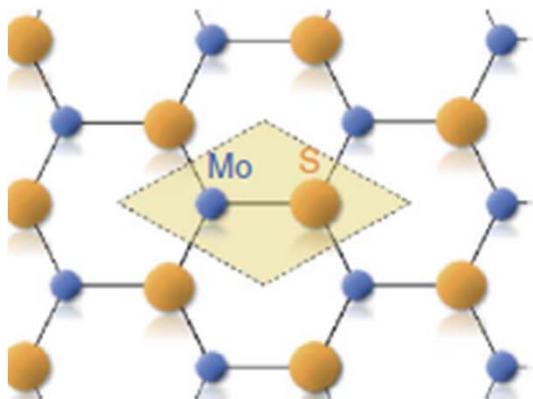
# 4 谷电子学自旋电子学器件

## Spin dependent optical selection rule



Selective excitation of valley & spin controlled by light polarization & freq

光学选择性的起源



$$w_l(\mathbf{r}) = e^{il\phi} f(\theta, r),$$

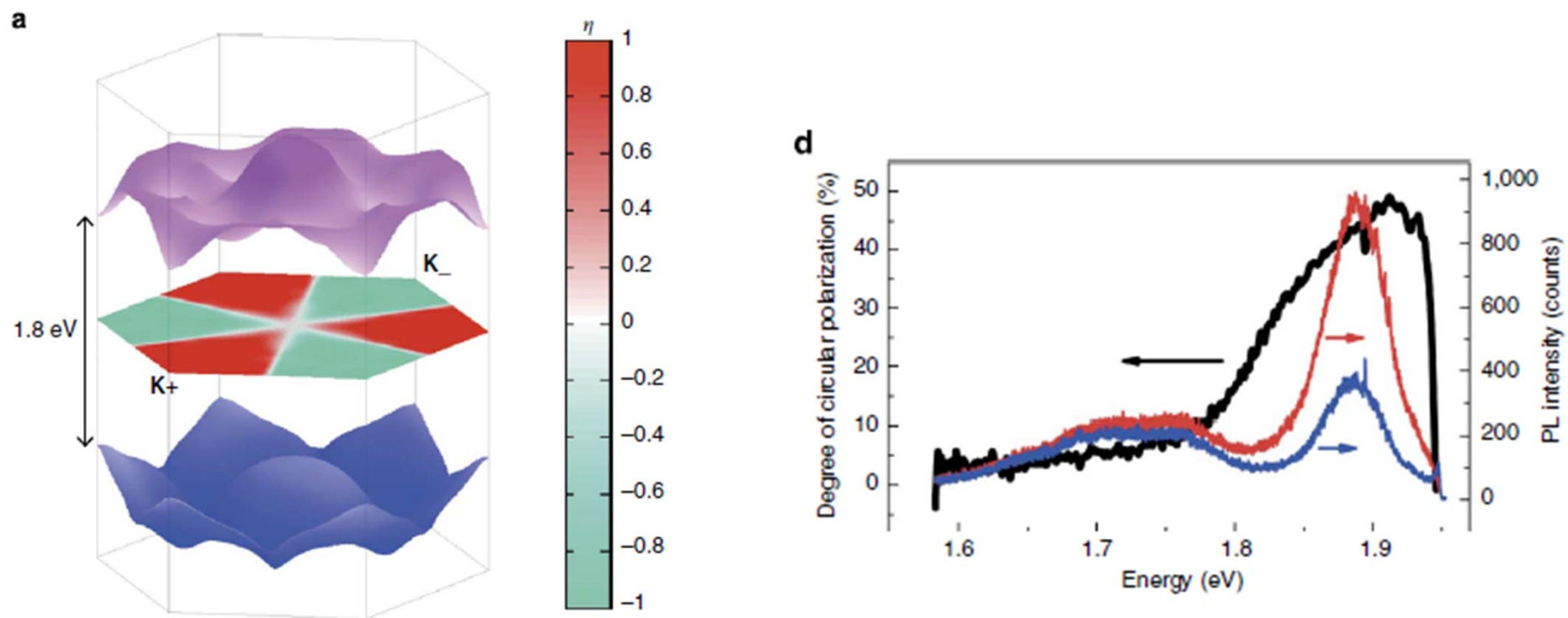
$$\hat{C}_3 |v(\mathbf{K}_\pm)\rangle = |v(\mathbf{K}_\pm)\rangle,$$

$$|\phi_c\rangle = |d_z\rangle, \quad |\phi_v^\tau\rangle = \frac{1}{\sqrt{2}}(|d_{x^2-y^2}\rangle + i\tau|d_{xy}\rangle),$$

$$\hat{C}_3 |c(\mathbf{K}_\pm)\rangle = e^{\mp i2\pi/3} |c(\mathbf{K}_\pm)\rangle,$$

Now the chiral optical selectivity of the valleys can be deduced. The bottom of the conduction bands at the valleys, dominated by the  $l=0$   $d$ -states on Mo, bears an overall azimuthal quantum number  $m_\pm = \pm 1$ , at  $\mathbf{K}_\pm$ . At the top of the valence bands,  $m_\pm = 0$ . Then for an optical transition at  $\mathbf{K}_\pm$ , the angular momentum selection rule indicates that  $\Delta m_\pm = \pm 1$ , corresponding to the absorption of left- and right-handed photons. Therefore, our den-

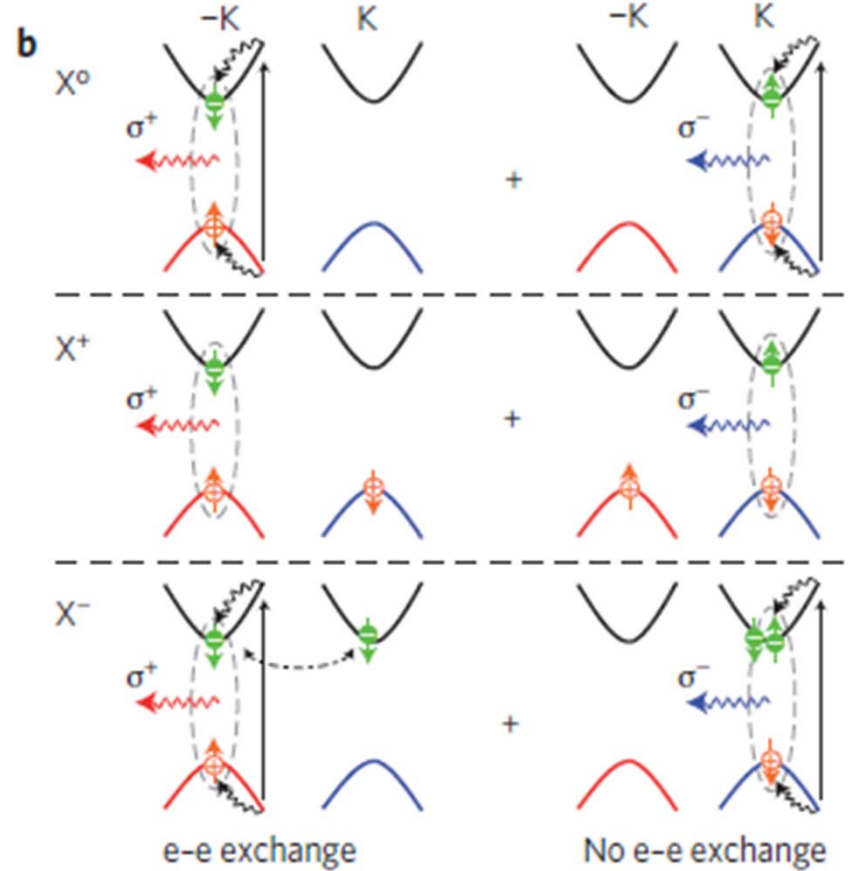
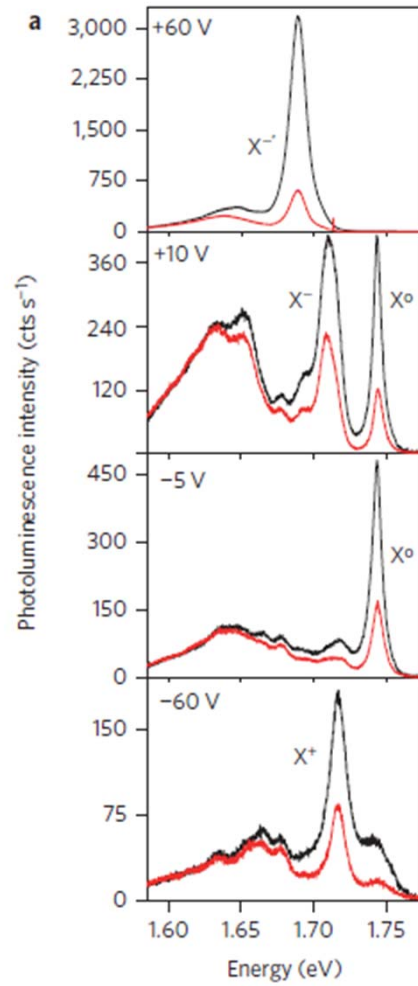
# MoS<sub>2</sub> 的在整个布里渊区的旋光选择性 以及实验的观测



# 门压对发光谱的控制

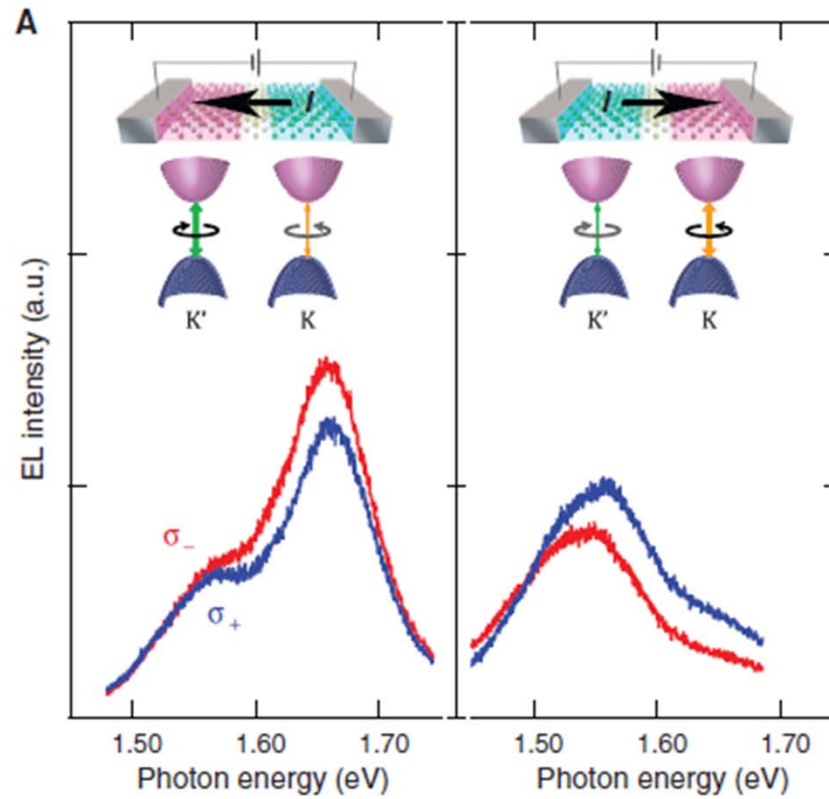
## Optical generation of excitonic valley coherence in monolayer $\text{WSe}_2$

Aaron M. Jones<sup>1</sup>, Hongyi Yu<sup>2</sup>, Nirmal J. Ghimire<sup>3,4</sup>, Sanfeng Wu<sup>1</sup>, Grant Aivazian<sup>1</sup>, Jason S. Ross<sup>5</sup>, Bo Zhao<sup>1</sup>, Jiaqiang Yan<sup>4,6</sup>, David G. Mandrus<sup>3,4,6</sup>, Di Xiao<sup>7</sup>, Wang Yao<sup>2\*</sup> and Xiaodong Xu<sup>1,5\*</sup>





**Electrically Switchable Chiral Light-Emitting Transistor**  
Y. J. Zhang *et al.*  
*Science* 344, 725 (2014);  
DOI: 10.1126/science.1251329



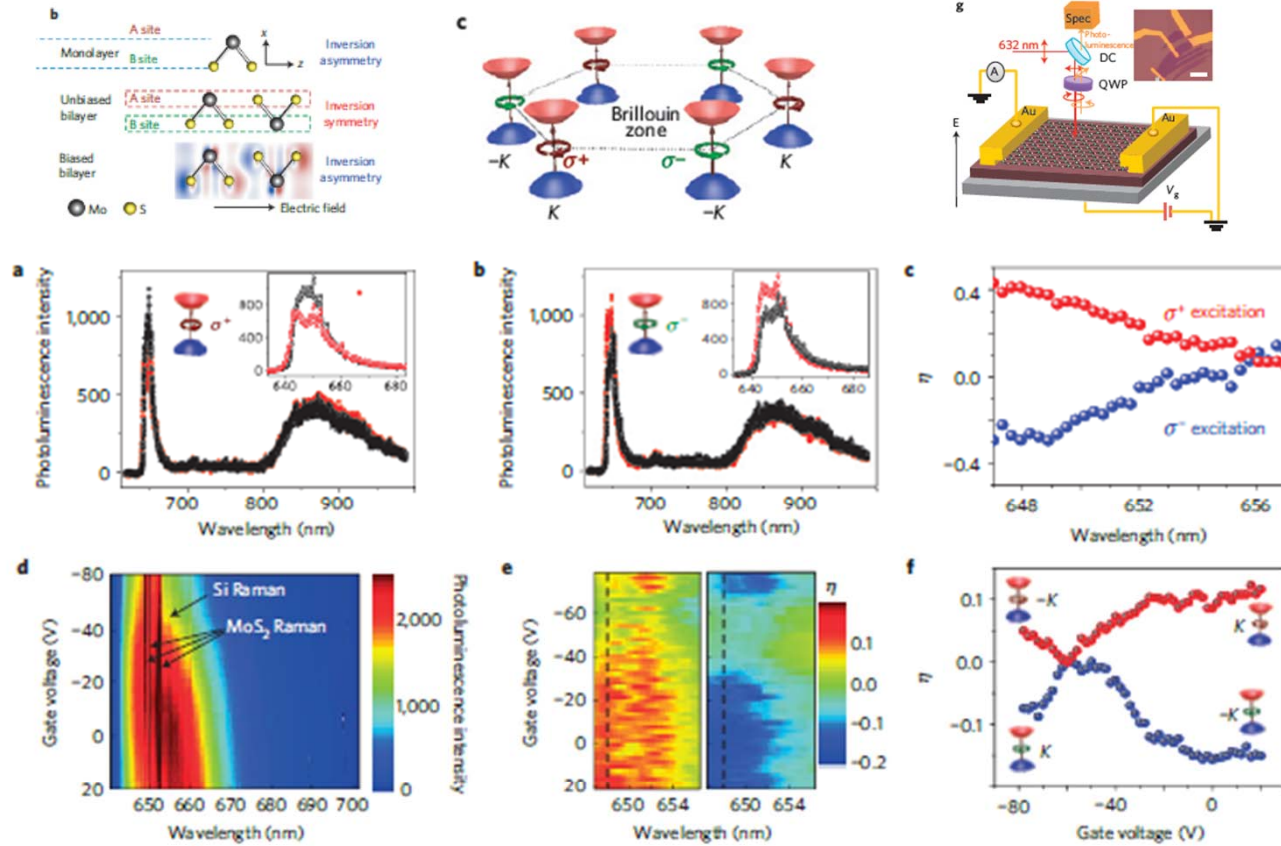
偏压方向改变， 璇光性也改变



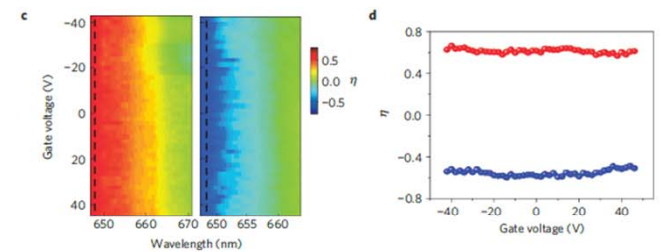
# 双层MoS<sub>2</sub> 的谷极化

## Electrical tuning of valley magnetic moment through symmetry control in bilayer MoS<sub>2</sub>

Sanfeng Wu<sup>1</sup>, Jason S. Ross<sup>2</sup>, Gui-Bin Liu<sup>3</sup>, Grant Aivazian<sup>1</sup>, Aaron Jones<sup>1</sup>, Zaiyao Fei<sup>1</sup>, Wenguang Zhu<sup>4,5,6</sup>, Di Xiao<sup>5,7</sup>, Wang Yao<sup>3</sup>, David Cobden<sup>1</sup> and Xiaodong Xu<sup>1,2\*</sup>

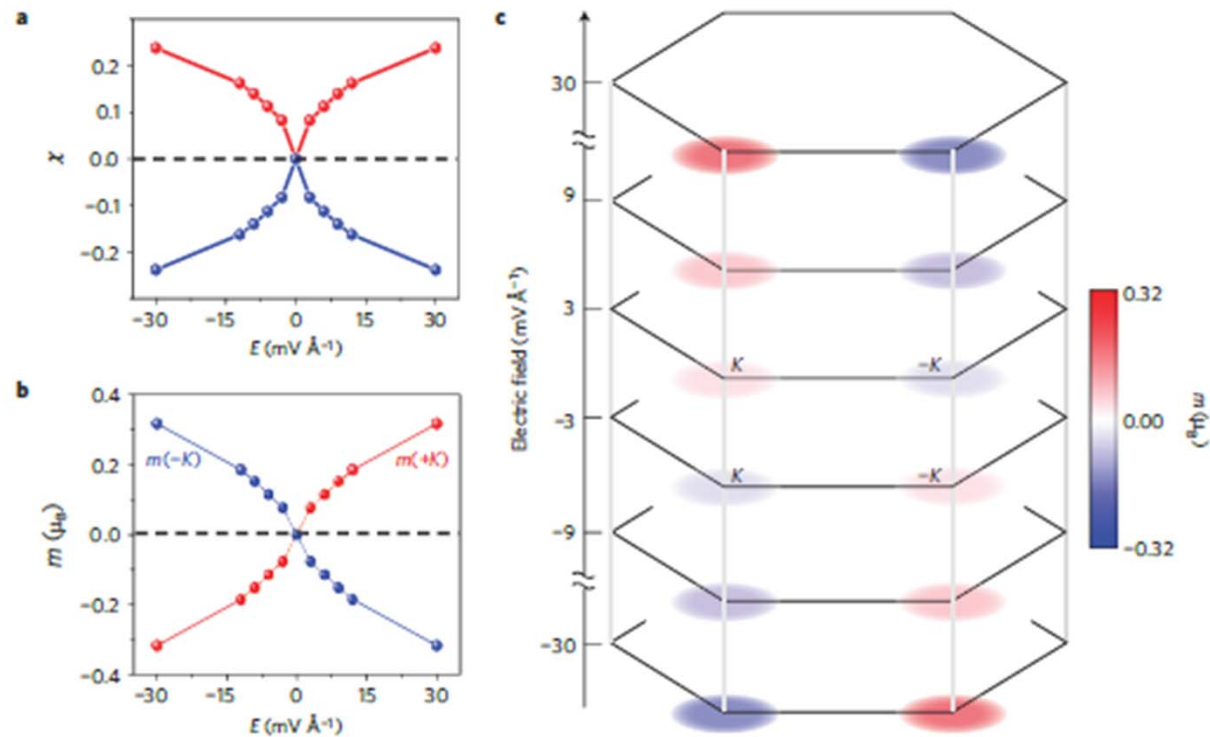


**Figure 2 | Electrical control of valley magnetic moment in bilayer MoS<sub>2</sub> FETs.** **a, b**, Polarization-resolved photoluminescence excited by  $\sigma^+$  (**a**) and  $\sigma^-$  (**b**) light at  $V_g = 0$ . Insets: zoomed-in photoluminescence spectra around 650 nm. Black (red):  $P(\sigma^+)$  ( $P(\sigma^-)$ ) signals. **c**, Degree of photoluminescence polarization as a function of wavelength. Red (blue):  $\sigma^+$  ( $\sigma^-$ ) excitation. **d**, Photoluminescence intensity map as a function of wavelength and gate voltage. **e**, Degree of photoluminescence polarization as a function of wavelength and gate voltage. The left (right) plot is obtained for  $\sigma^+$  ( $\sigma^-$ ) excitation. **f**, Degree of photoluminescence polarization as a function of gate voltage at 648 nm (line cuts along the dashed lines in **e**). Red (blue) dots denote  $\sigma^+$  ( $\sigma^-$ ) excitation.



单层

$$\mathbf{m}_s(\mathbf{k}) = (\hbar \mu_B / 2m_e) \sum_{n \neq s} (|P_+^{ns}(\mathbf{k})|^2 - |P_-^{ns}(\mathbf{k})|^2) / (\epsilon_n(\mathbf{k}) - \epsilon_s(\mathbf{k})),$$

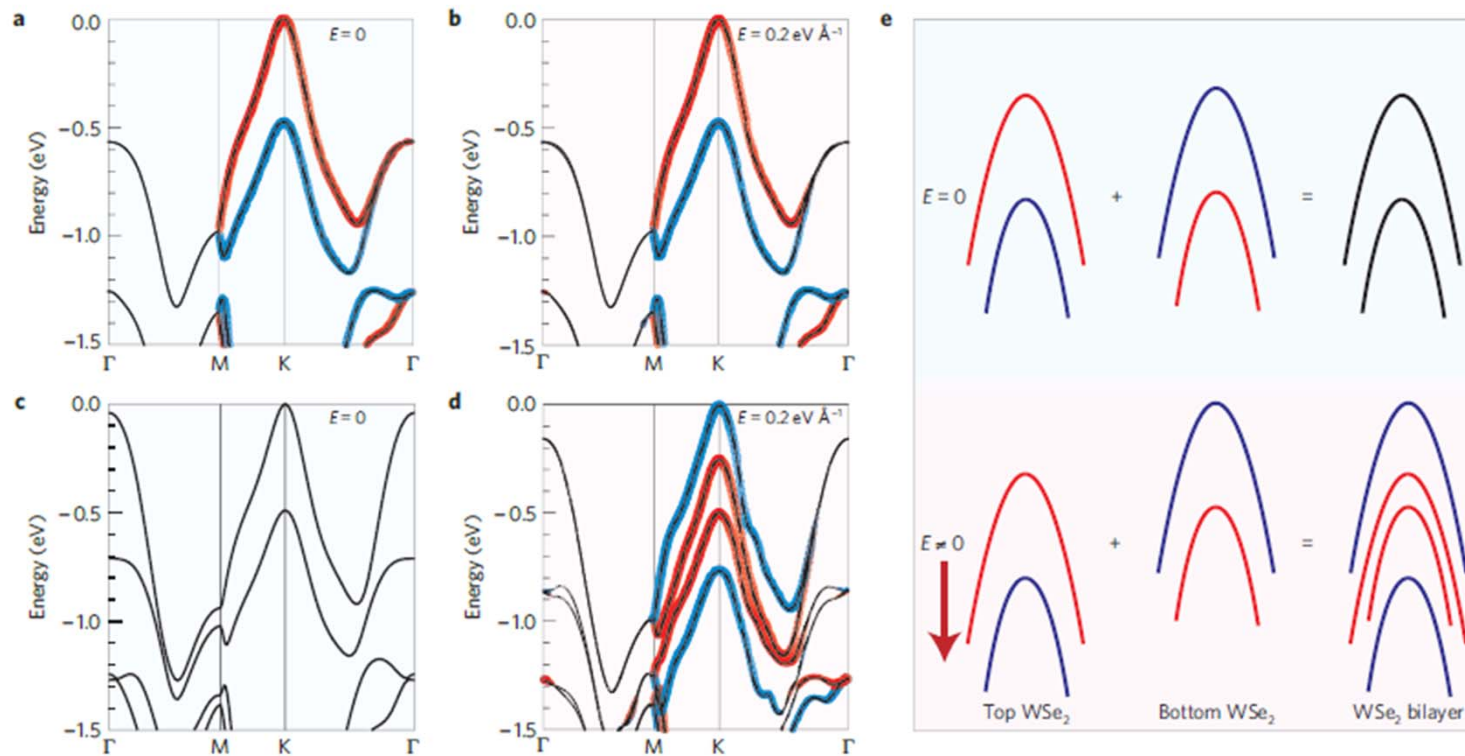


**Figure 4 | DFT calculation of magnetoelectric effect and associated circular dichroism.** **a**, Absorption circular dichroism  $\chi$  as a function of electric field. The positive (negative) value represents  $\sigma^+$  ( $\sigma^-$ ) excitation. **b**,  $m$  at  $\pm K$  as a function of electric field, which shows that  $m$  is an odd function of electric field. **c**, Colour map of  $m$  as a function of electric fields near  $\pm K$  points in the momentum space.

# 双层加电场 引起自旋劈裂

## Zeeman-type spin splitting controlled by an electric field

Hongtao Yuan<sup>1,2\*</sup>, Mohammad Saeed Bahramy<sup>1,3\*</sup>, Kazuhiro Morimoto<sup>1</sup>, Sanfeng Wu<sup>4</sup>, Kentaro Nomura<sup>3,5</sup>, Bohm-Jung Yang<sup>3</sup>, Hidekazu Shimotani<sup>1,6</sup>, Ryuji Suzuki<sup>1</sup>, Minglin Toh<sup>7</sup>, Christian Kloc<sup>7</sup>, Xiaodong Xu<sup>4,8</sup>, Ryotaro Arita<sup>1,3</sup>, Naoto Nagaosa<sup>1,3</sup> and Yoshihiro Iwasa<sup>1,3\*</sup>

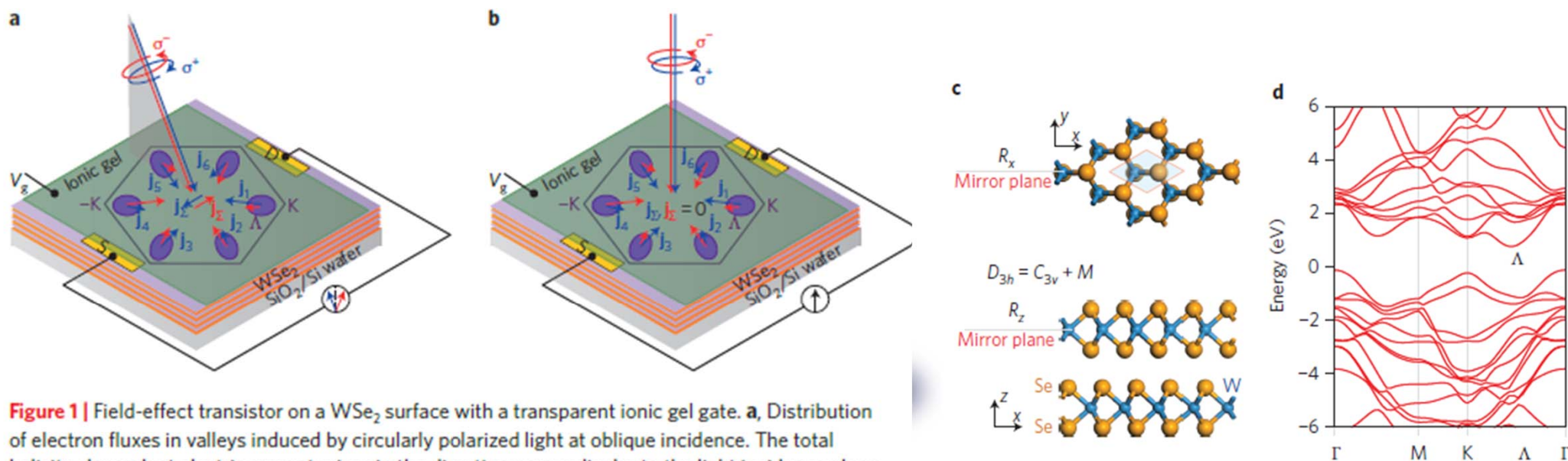


**Figure 5 | Origin of out-of-plane spin polarization in WSe<sub>2</sub> under the external electric field. a, b**, Electronic band structures of a monolayer of WSe<sub>2</sub> under the external electric field (E = 0 and E = 0.2 eV Å<sup>-1</sup>) at the high-symmetry points  $\Gamma$ , M, K, and  $\Gamma$ . **c, d**, Electronic band structures of a bilayer of WSe<sub>2</sub> under the external electric field (E = 0 and E = 0.2 eV Å<sup>-1</sup>) at the high-symmetry points  $\Gamma$ , M, K, and  $\Gamma$ . **e**, Zeeman-type spin splitting controlled by an electric field. The band structures of the top and bottom layers are combined to form the bilayer structure.

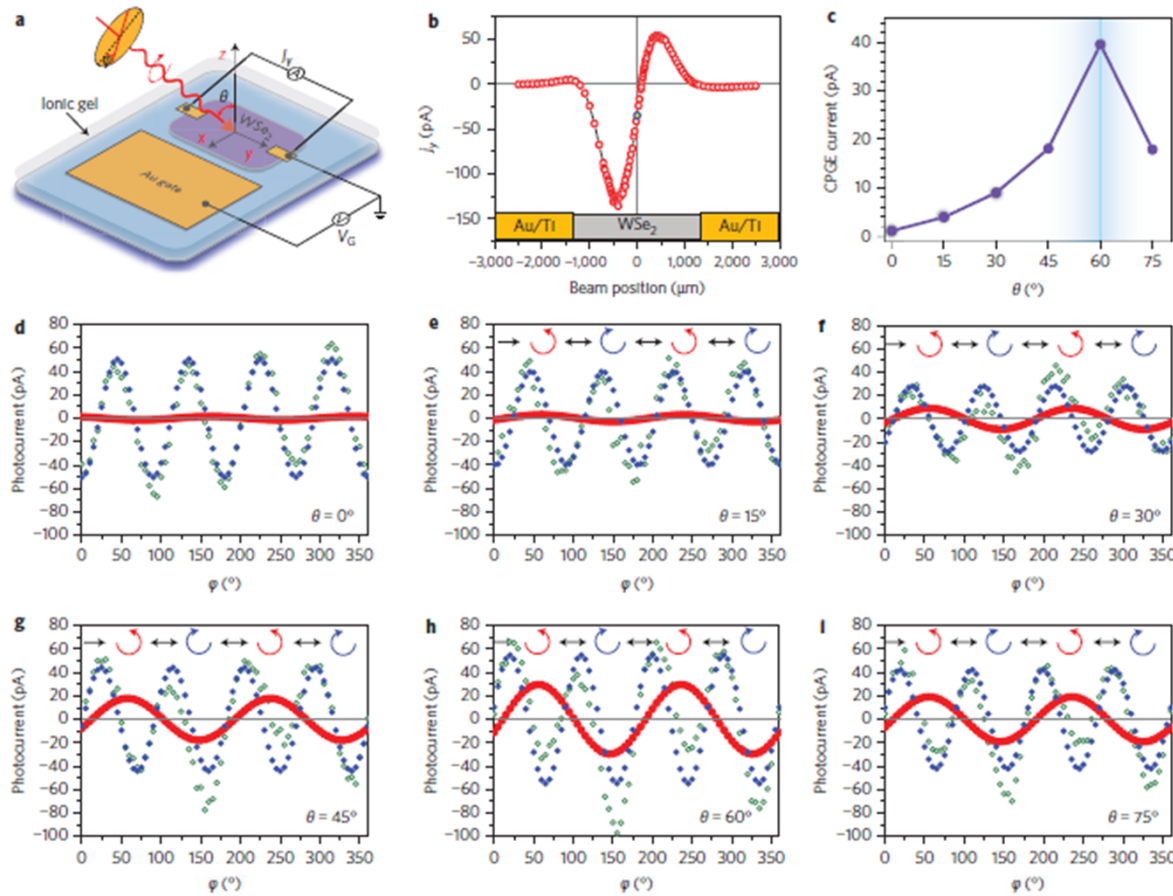
# 旋光伏特效应 (CPGE)

## Generation and electric control of spin-valley-coupled circular photogalvanic current in WSe<sub>2</sub>

Hongtao Yuan<sup>1,2</sup>, Xinqiang Wang<sup>3,4</sup>, Biao Lian<sup>1</sup>, Haijun Zhang<sup>1</sup>, Xianfa Fang<sup>3,4</sup>, Bo Shen<sup>3,4</sup>, Gang Xu<sup>1</sup>, Yong Xu<sup>1</sup>, Shou-Cheng Zhang<sup>1,2</sup>, Harold Y. Hwang<sup>1,2\*</sup> and Yi Cui<sup>1,2\*</sup>



**Figure 1** | Field-effect transistor on a WSe<sub>2</sub> surface with a transparent ionic gel gate. **a**, Distribution of electron fluxes in valleys induced by circularly polarized light at oblique incidence. The total helicity-dependent electric current arises in the direction perpendicular to the light incidence plane. **b**, Distribution of electron fluxes in valleys for normally incident circularly polarized light. Ellipsoids show electron valleys in the Brillouin zone, represented by the hexagonal shape. Points K and -K are shown. S, source; D, drain;  $V_g$ , gate voltage. Left-handed ( $\sigma^-$ ; red) or right-handed ( $\sigma^+$ ; blue) circularly polarized light induces different currents ( $J$  vectors) in the electron valleys. The total current in **a** is shown by the red and blue arrows labelled  $J_z$ .



**Figure 2 | Schematic diagram and incident angle-dependent CPGE measurement of ambipolar WSe<sub>2</sub> EDLTs.** **a.** Schematic structure of a typical WSe<sub>2</sub> EDLT with ionic gel gating. By applying a gate voltage  $V_G$  to the lateral Au gate electrode, ions in the gel are driven to the WSe<sub>2</sub> surface, forming a perpendicular electric field at the EDL interface. Even without an external bias, a relatively low carrier-density accumulation layer exists at the WSe<sub>2</sub> surface owing to the Fermi level realignment between the gel/WSe<sub>2</sub> interface. **b.** A position-dependent photocurrent from sweeping the laser spot across the two electrodes (yellow rectangles shown at the bottom) in the zero-biased WSe<sub>2</sub> EDLT device with a fixed polarization. **c.** CPGE photocurrent  $j_{CPGE}$  as a function of the incident angle,  $\theta$ , which shows a peak around  $\theta = 60^\circ$  (indicated by the blue line). **d-i.** Light polarization dependence of photocurrent  $j_y$  in a biased WSe<sub>2</sub> EDLT, measured at  $y = 0$  with different incident angles  $\theta$ . The open green circles are the measured  $j_y$  following the form  $j_y = C \sin 2\varphi + L \sin 4\varphi + A$ . The filled blue circles are the photocurrent that originates from the linear photogalvanic effect and obtained from the  $\pi/2$ -period oscillation term  $L \sin 4\varphi$  by fitting. The filled red dots are the CPGE photocurrent with a  $\pi$ -periodic current oscillation. Polarization of the incident light at each quarter-wave plate angle,  $\varphi$ , is given by the symbols shown in the inset of each figure.

$$j_y = C \sin 2\varphi + L \sin 4\varphi + A$$

$L \sin 4\varphi$  corresponding to the linear photogalvanic effect (LPGE).

$$j_{CPGE} = \eta \gamma I \sin \theta \sin 2\varphi,$$

$$j_{CPGE} = C \sin 2\varphi$$

# 谷霍尔效应 自旋霍尔效应

$$\sigma^{\text{int}} = (e^2/\hbar) \int [dk] f(k) \Omega(k)$$

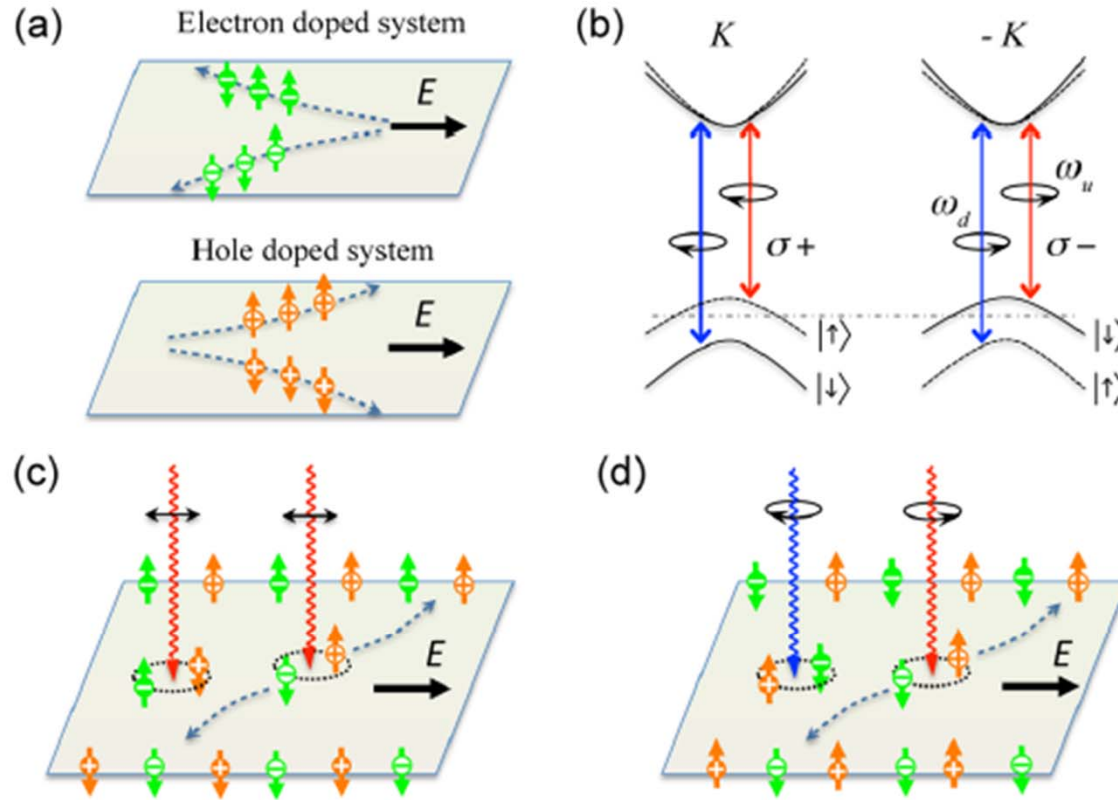
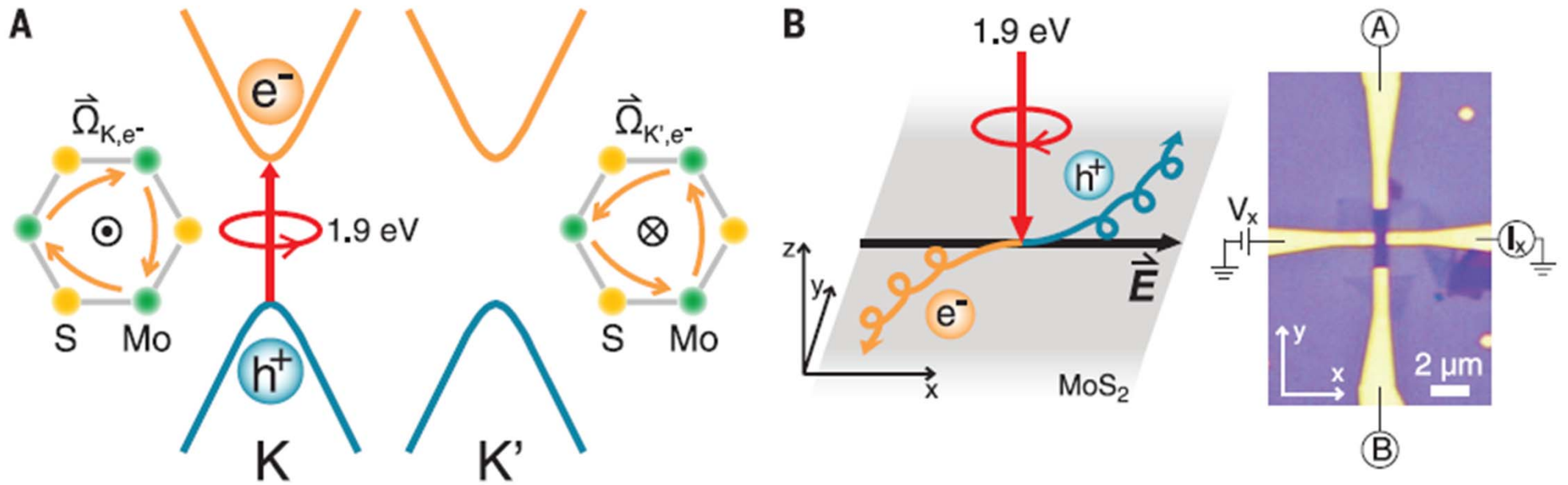
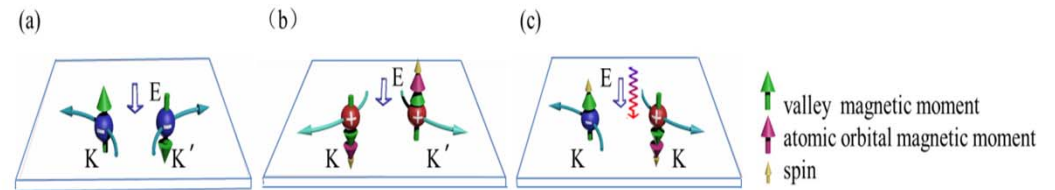
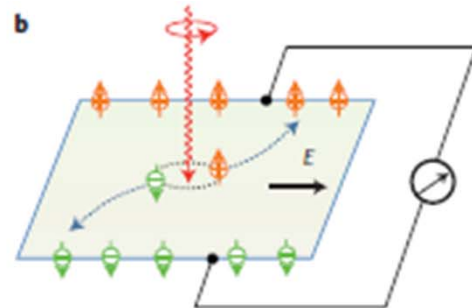
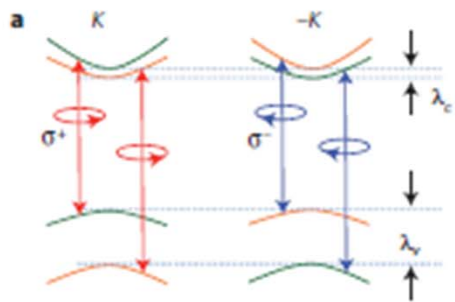
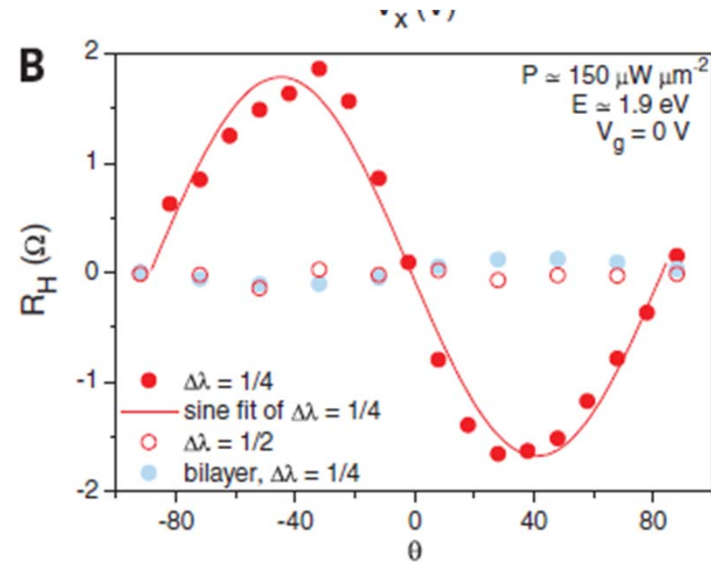
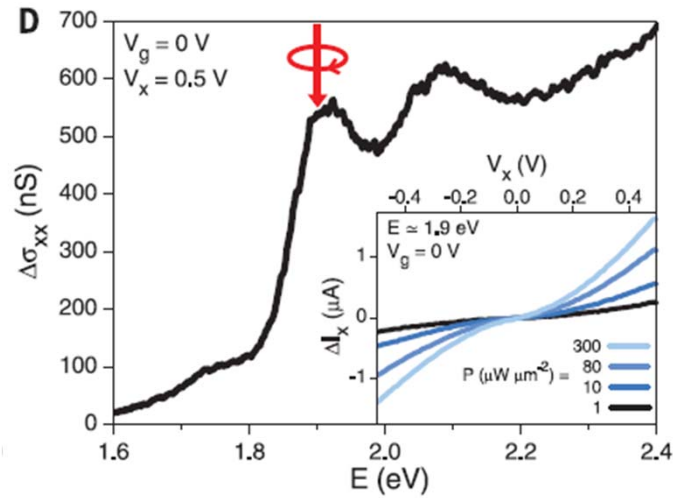


FIG. 2 (color online). Coupled spin and valley physics in monolayer group-VI dichalcogenides. The electrons and holes



The valley Hall effect in MoS<sub>2</sub> transistors  
K. F. Mak *et al.*  
*Science* 344, 1489 (2014);  
DOI: 10.1126/science.1250140





问题: 1 证明是自旋流

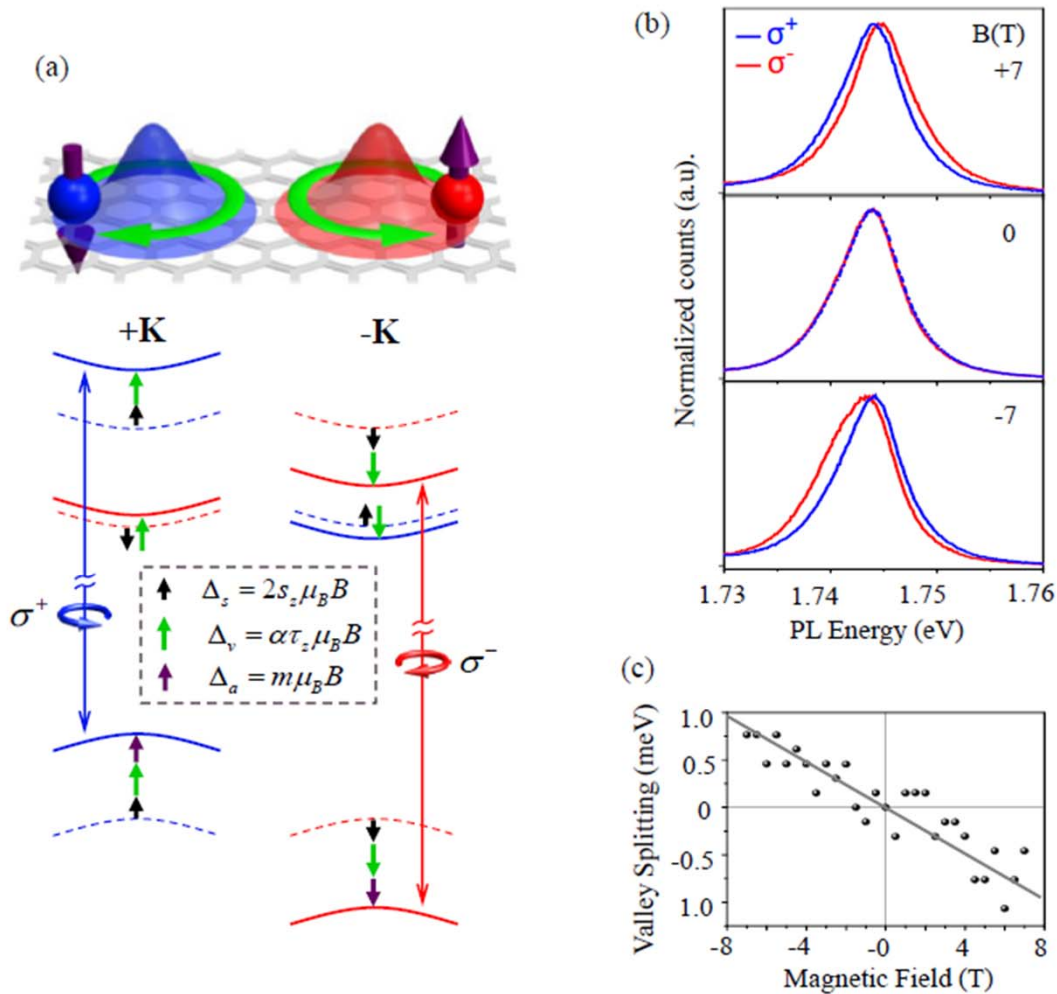
2 双层WS<sub>2</sub>加垂直电场 也应该观察谷霍尔效应

3 谷轨道磁矩霍尔效应?



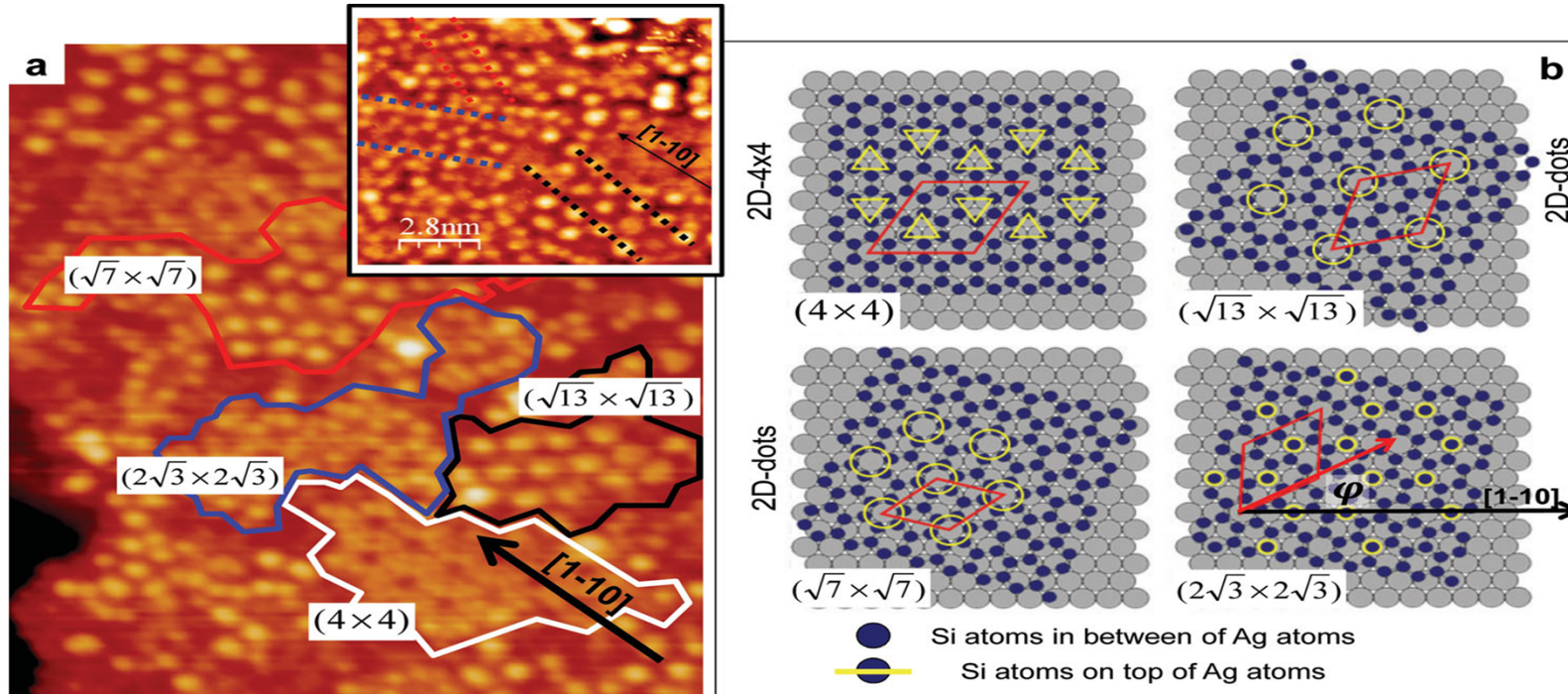
# Title: Magnetic Control of Valley Pseudospin in Monolayer WSe<sub>2</sub>

Authors: G. Aivazian<sup>1</sup>, Zhirui Gong<sup>2</sup>, Aaron M. Jones<sup>1</sup>, Rui-Lin Chu<sup>3</sup>, J. Yan<sup>4,5</sup>, D. G. Mandrus<sup>4,5,6</sup>, Chuanwei Zhang<sup>3</sup>, David Cobden<sup>1</sup>, Wang Yao<sup>2\*</sup>, X. Xu<sup>1,7\*</sup>



# 5 其他2D 材料 硅烯

## Silicene on metals

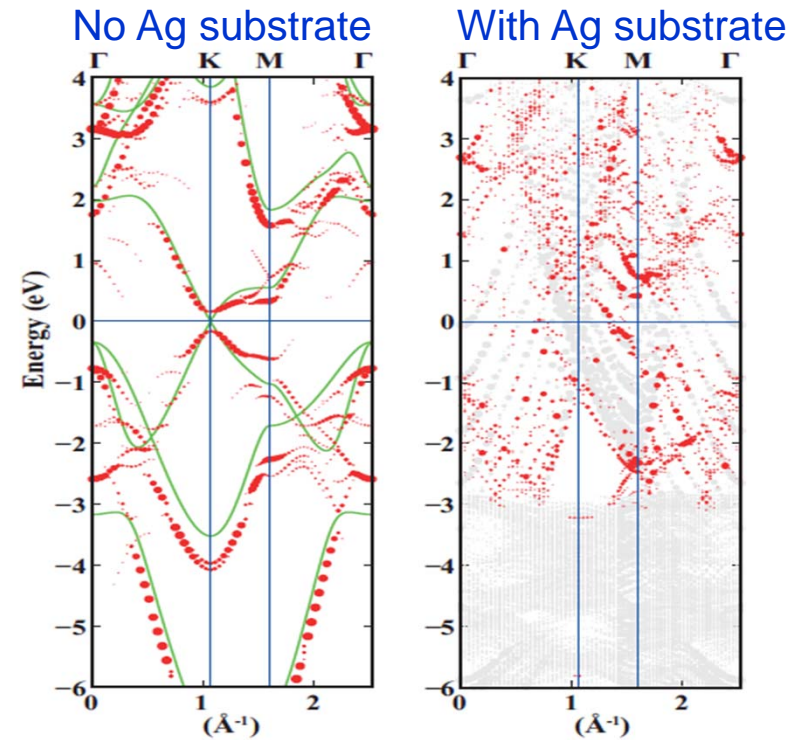
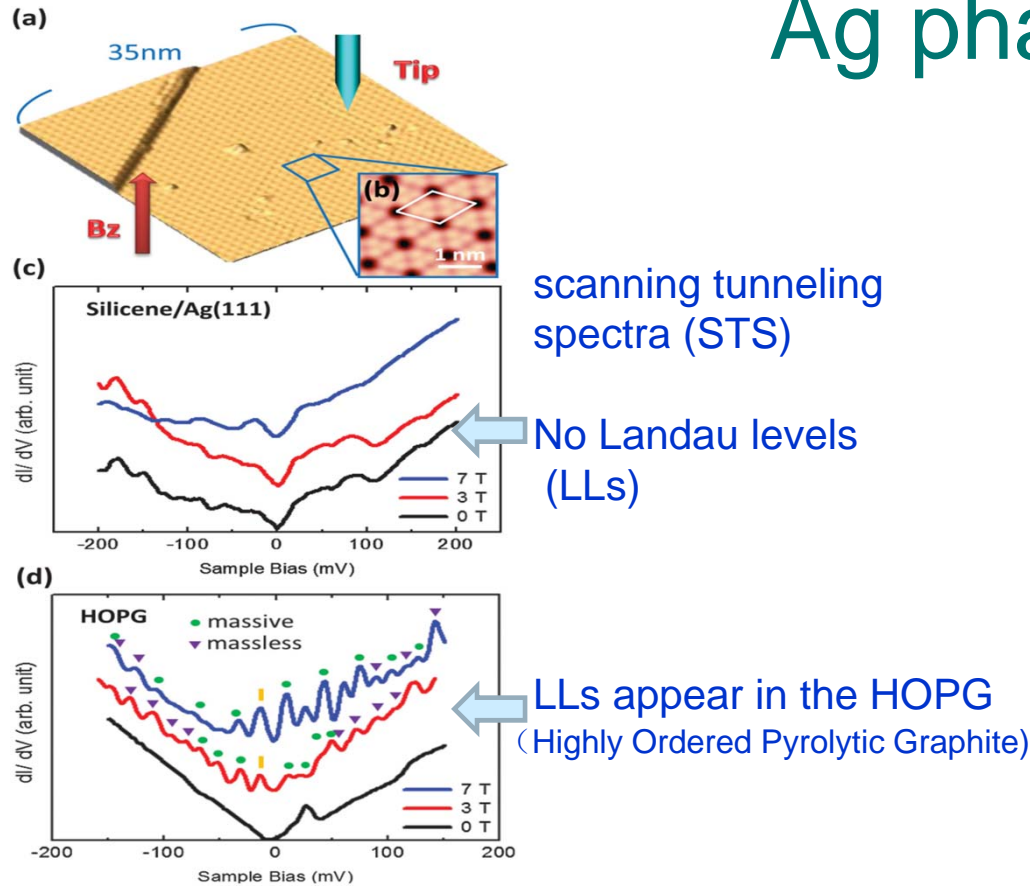


Ag index

(a) STM characterization of multi-oriented silicene domains on Ag(111)  
 (b) Sequence of ball models

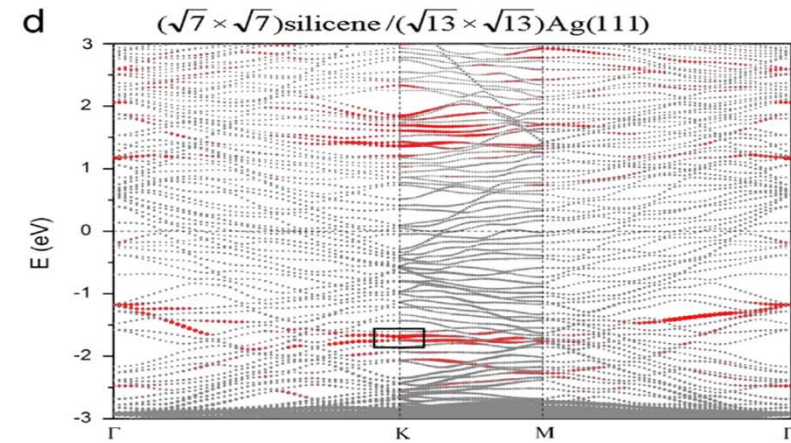
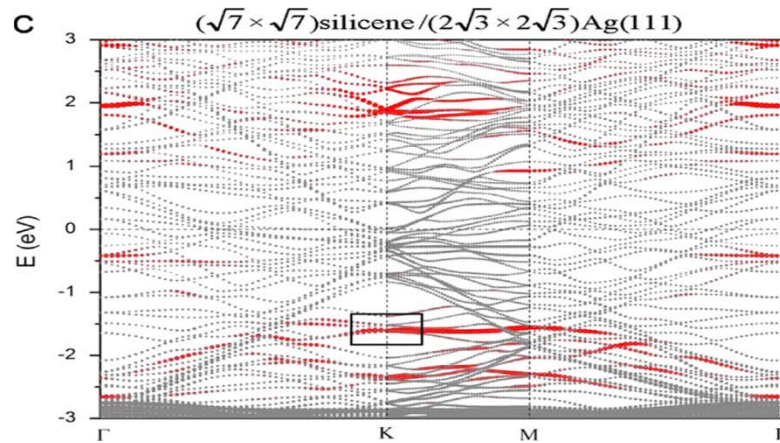
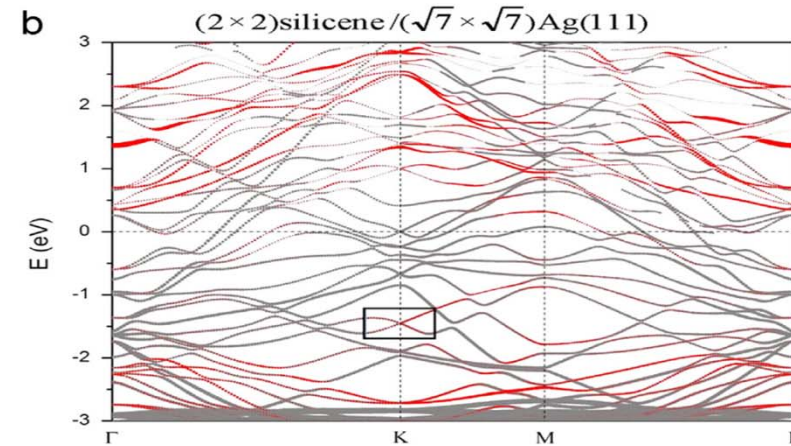
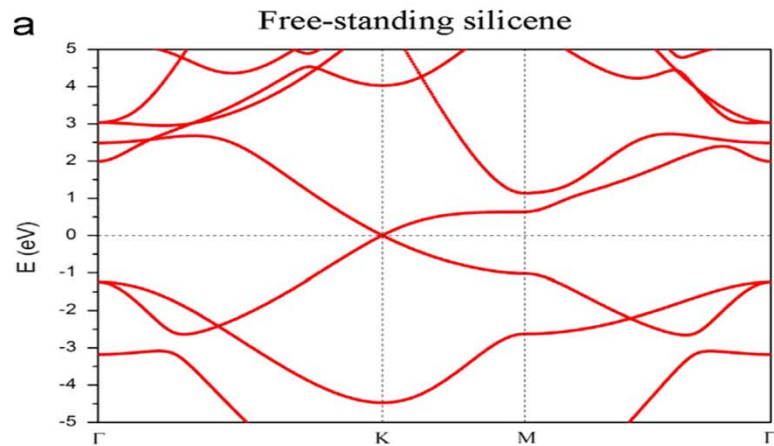
*Adv. Mater.* **24**, 5088-5093 (2012)  
*Phys. Rev. Lett.* **108**, 155501 (2012)  
*Phys. Rev. Lett.* **107**, 076802 (2011)

# Absence of Dirac cone: $(3 \times 3)$ silicene on $(4 \times 4)$ Ag phase



Red color: Si orbitals

# Absence of Dirac cone: other phases



Red line: Silicon component

## Absence of Dirac cone on $\text{ZrB}_2$ and $\text{MoS}_2$ substrates

Fig. 3: Silicene on  $\text{ZrB}_2$ .  
Phys. Rev. Lett., 108, 245501 (2012).

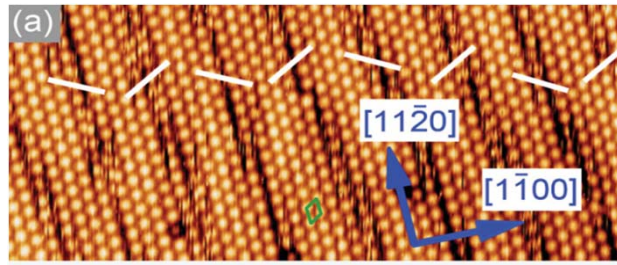
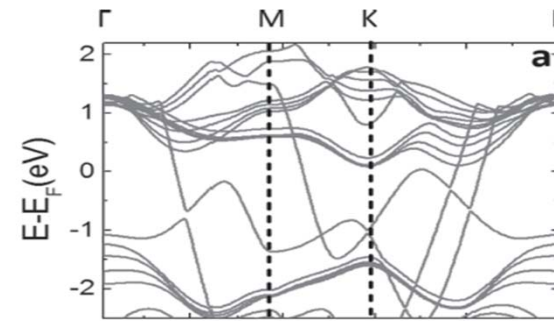
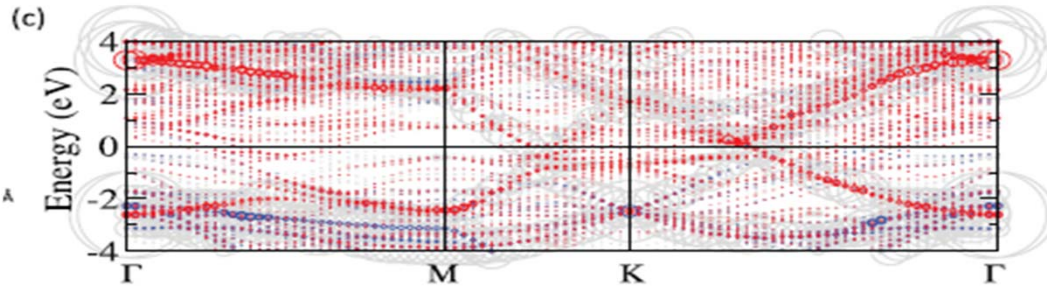


Fig. 4: Silicene on  $\text{MoS}_2$ .  
Adv. Mater., 26, 2096-2101 (2014).

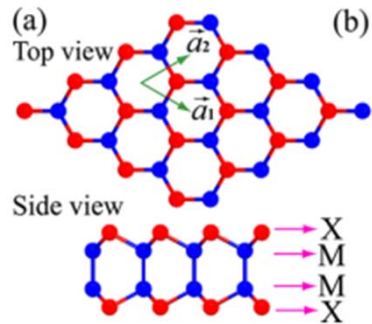


Dirac cone of silicene can be kept on graphene, BN et al  
Unsuitable as growth substrate

Question : Is there growth substrate that does not  
destroy the Dirac cone of silicene?

---

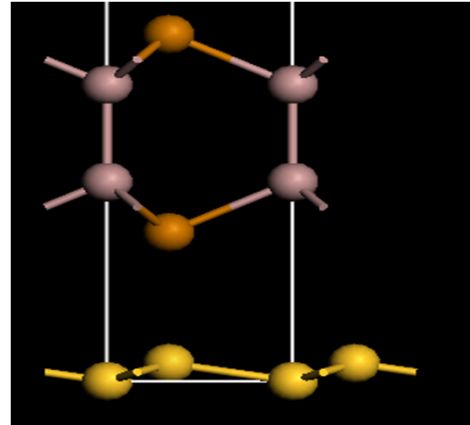
## Ideal novel substrates for silicene growth — Group III MonoChalcogenide (G3MC)



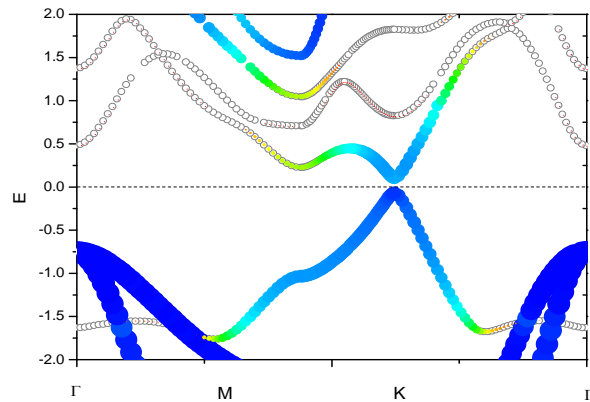
2D G3MC

Lattice constant: 3.6~4.3 Å

Silicene: 3.8~3.9 Å



configuration of silicene on G3MC (GaSe)



Band structure of silicene on GaSe. The color indicates the projection of Si atoms.

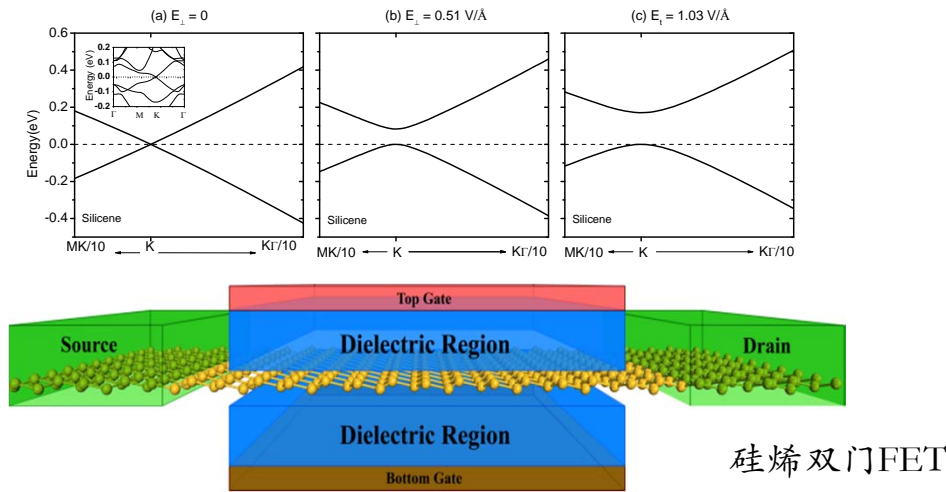
Table 1 Bandgap of silicene on several G3MCs. \* indicates indirect bandgap.

G3MC	Gap of silicene $E_g$ (eV)
GaS*	0.034
GaSe	0.14
GaTe	0.18
InSe	0.14

# 硅烯FET

硅烯具有极高的载流子迁移率  $1 \times 10^4 \text{ cm}^2/\text{V}\cdot\text{s}$ , 能隙0

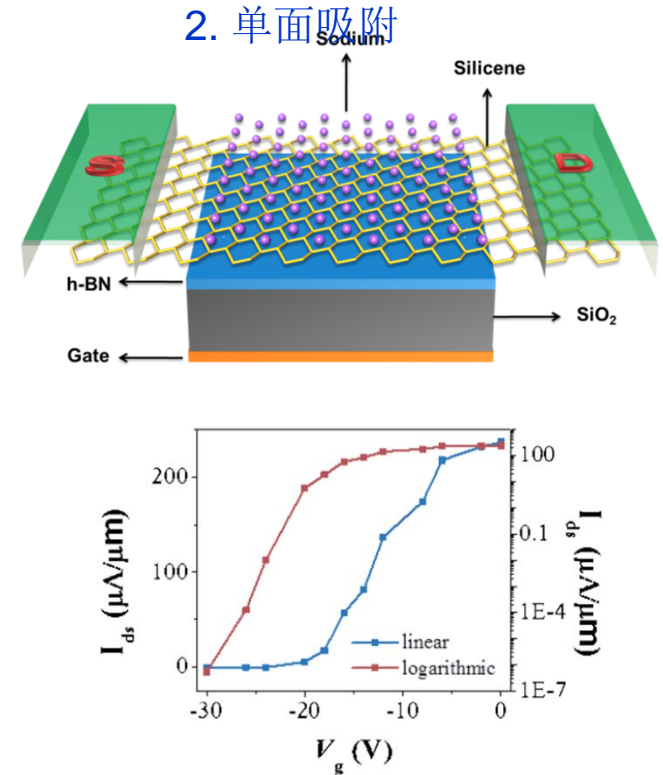
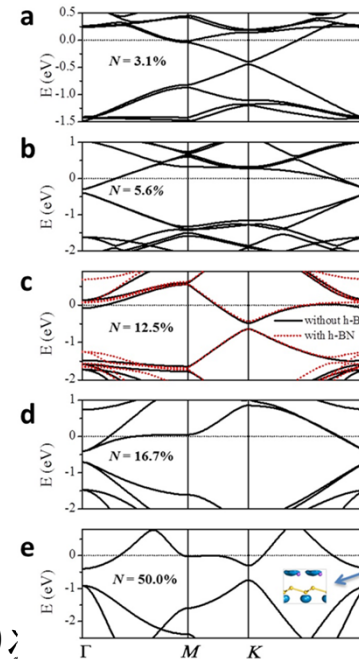
## 1. 垂直电场



这是国际上最先意识到硅烯具有电场可调能隙  
倪泽远 吕劲 Nano Lett 12, 113 (2012), 被引200;  
12/1099

主要缺点: 实验最大电场下能隙太小 0.1 eV  
双门

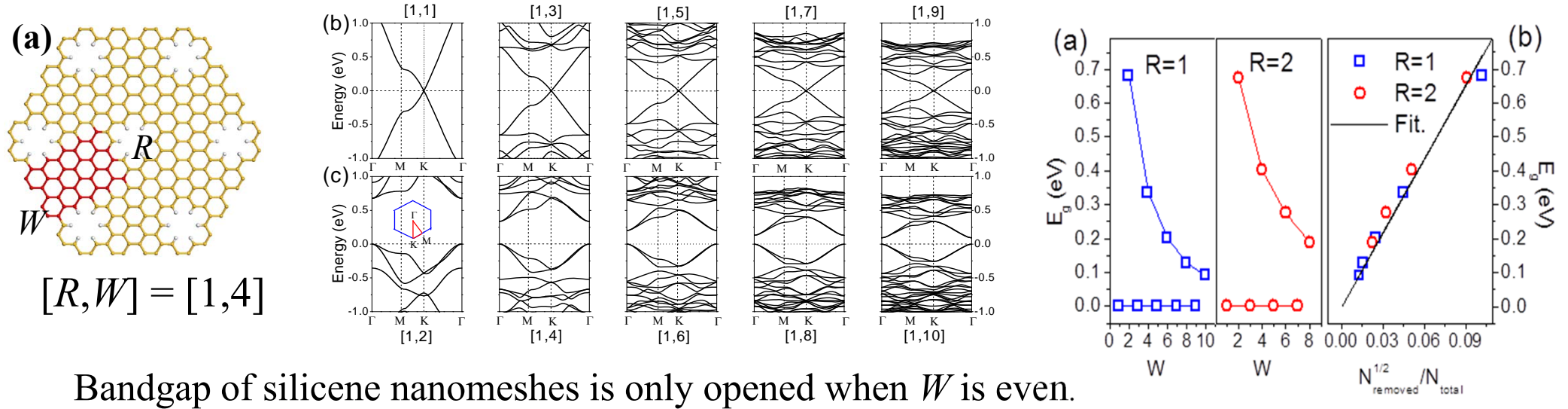
## 2. 单面吸附



问题: 供应电压太大, 功耗太大

屈贺 吕劲 Scientific Reports 2: 853 (2012)

## Silicene Nanomesh



Bandgap of silicene nanomeshes is only opened when  $W$  is even.

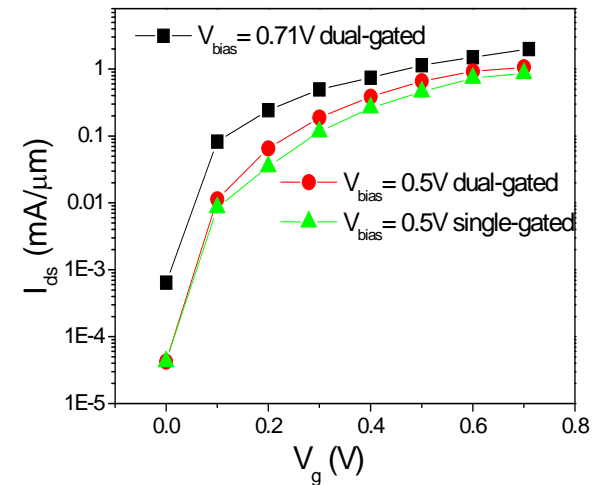
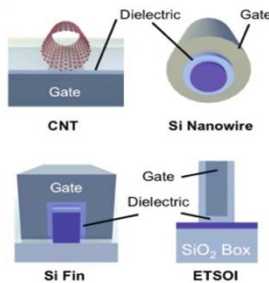




Table Comparison of Performance Metrics Between Sub-10nm Silicene Nanomesh (SNM), Advance Si, carbon nanotube (CNT) Transistors under  $V_{bias}=0.5V$  and  $V_{gate}=0.5V$ .

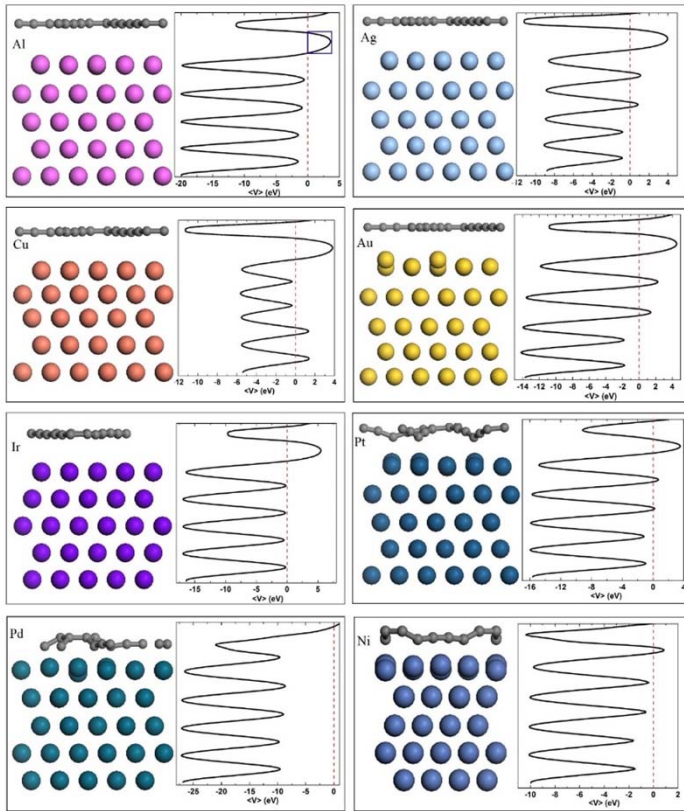
Channel	$L_{ch}$ (nm)	$I_{on}(\mu A/\mu m)$	$I_{on}/I_{off}$	Subthreshold swing $SS$ (mV/dec)
SNM dual-gated	7.8	607	$1.6 \times 10^4$	72
Si nanowire	10	300	$1.0 \times 10^4$	89 ( $V_{bias}=1.0V$ )
Si Fin	10	138	$1.0 \times 10^3$	125 ( $V_{bias}=1.2 V$ )
ETSOI	8	41	$1.0 \times 10^4$	83 ( $V_{bias}=1.2 V$ )
CNT	9	630	$1.0 \times 10^4$	94



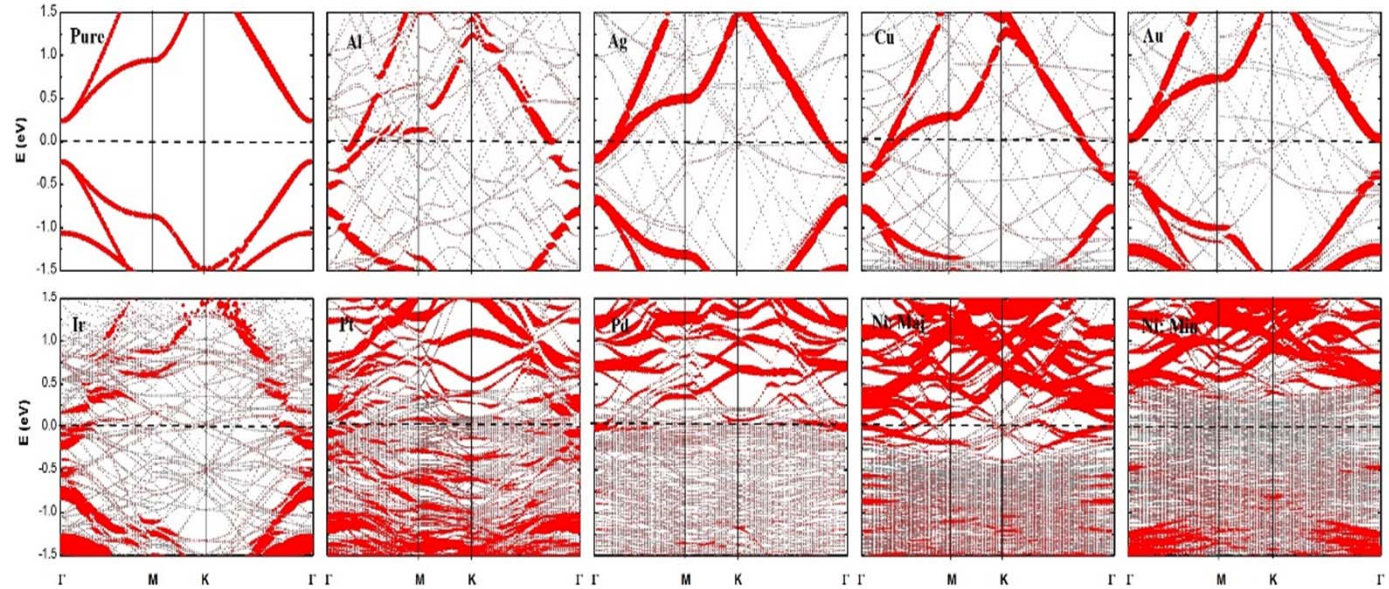
Scientific Reports, in revision

### 3 石墨炔

研究动机： 石墨炔有高的载流子迁移率( $1 \times 10^5 \text{ cm}^2/\text{V}\cdot\text{s}$ )  
和合适的能隙(0.5 eV (DFT) 1.1 eV (GW))

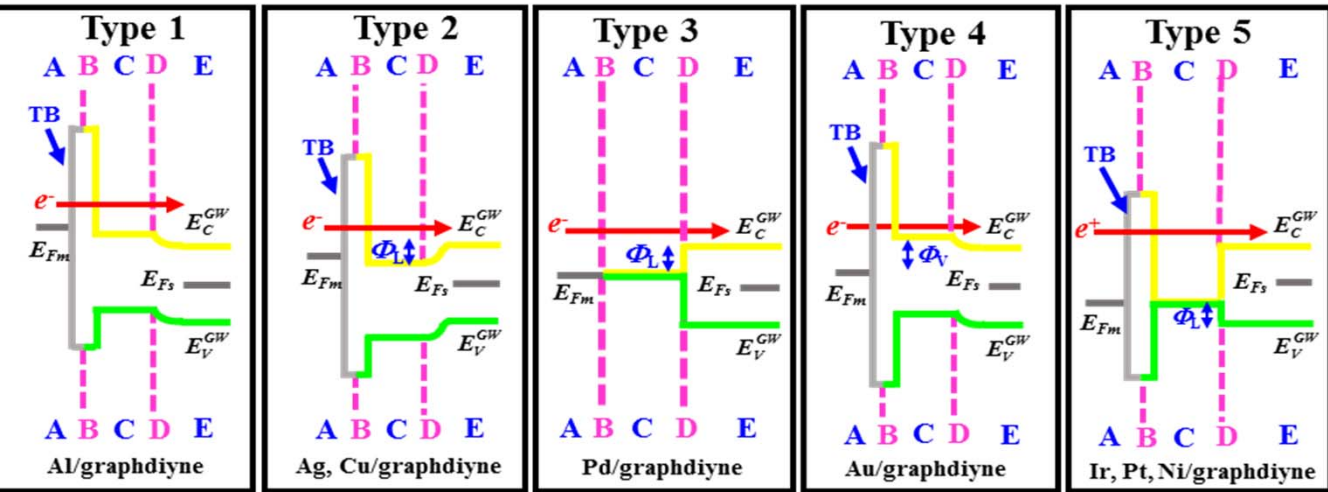
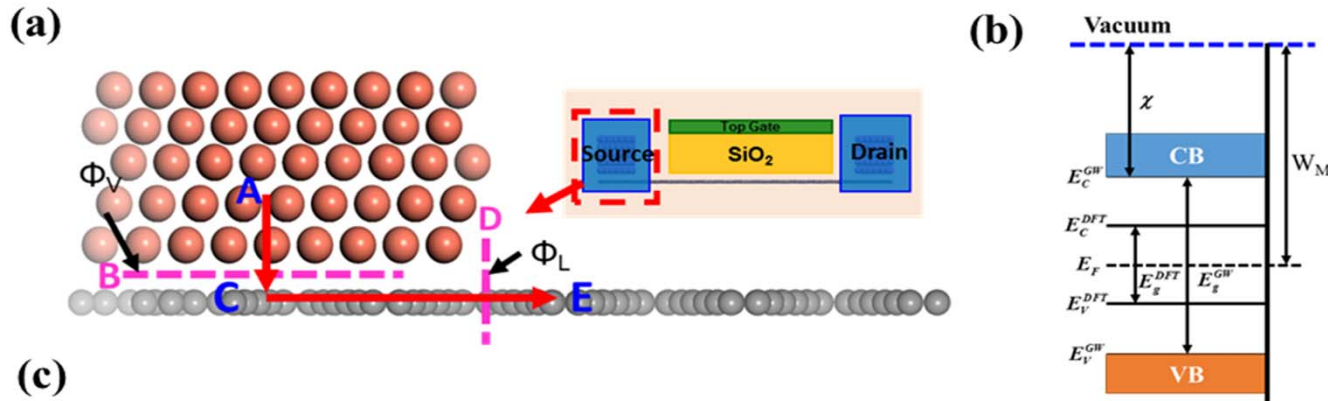


界面结构



石墨炔与金属接触的能带图

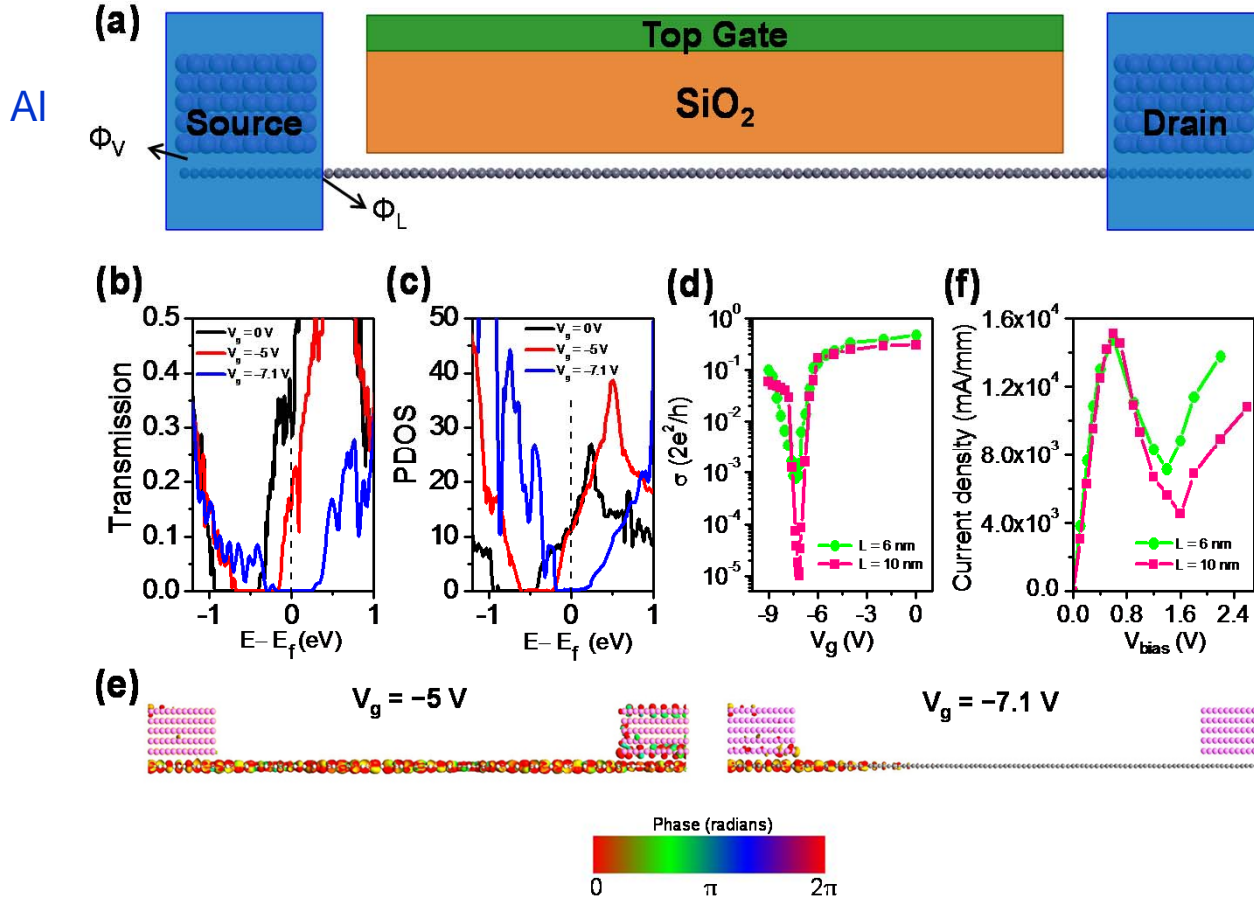
# 石墨炔FET 界面



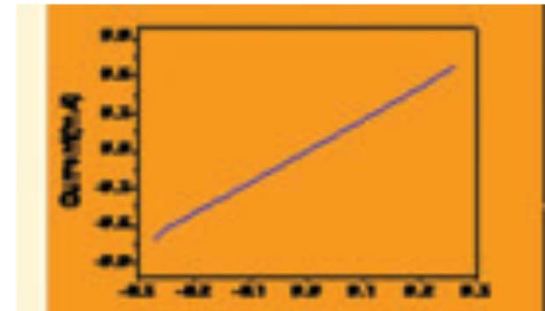
1 Al 欧姆接触 Ag, Cu 准欧姆  
其他金属有大的肖特基势垒。

2 Al Ag Cu Pd Au n-type  
Ir, Pt, Ni P-type

# 石墨炔FET



实验



Al, Cu 石墨炔欧姆接触!

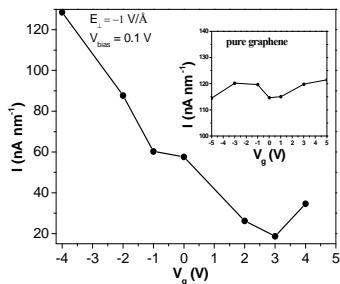
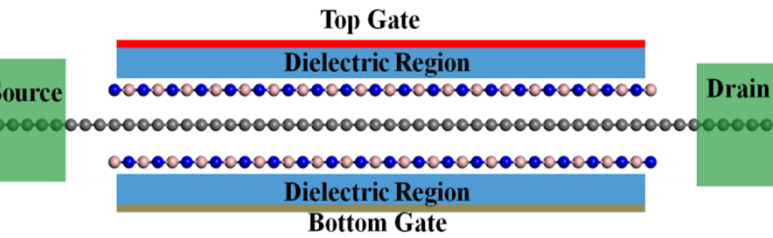
李玉良等 Chem. Commun., 2010, 46, 3256

This device exhibits an on-off ratio up to  $10^4$  and a sub-threshold swing of 117 mV/dec in a 10 nm channel length. 潘圆圆 王洋洋 吕劲

# 4 石墨烯

室温载流子迁移率:  $1.5 \times 10^4$  (SiO<sub>2</sub>做衬底) —  $2 \times 10^5$  cm<sup>2</sup>/V·s (悬浮)

## 1 石墨烯三明治

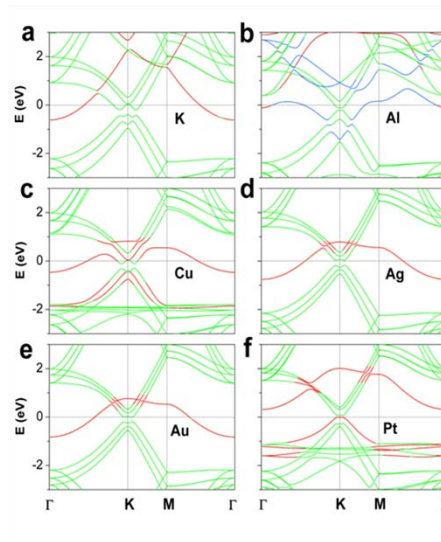
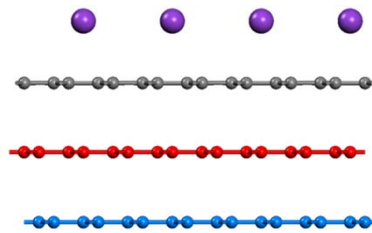


屈贺 吕劲等 被引60次

NPG Asia Materials (2012) 4, e6; doi:10.1038/am.2012.10  
© Nature Japan K.K. All rights reserved 1884-4057/12  
www.nature.com/am

问题: 能隙不超过0.4 eV

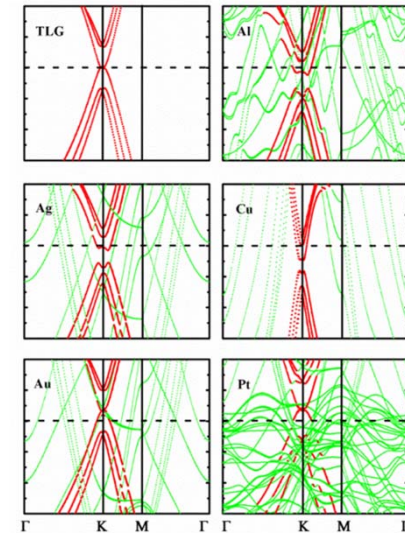
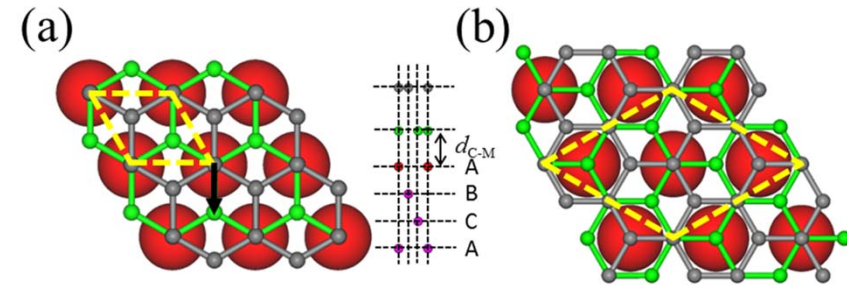
## 2 原子单面吸附



屈贺 吕劲等

Scientific Reports 3, 1794 (2013)

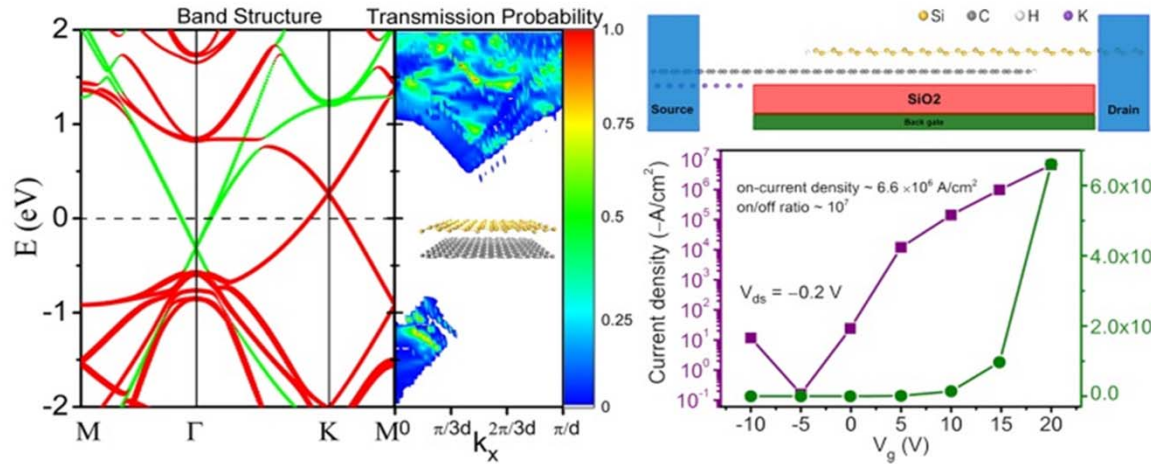
## 3 与金属接触



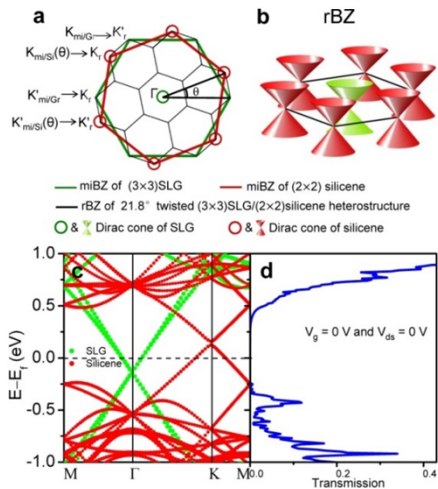
郑家新 王洋洋 吕劲

Scientific Reports 3, 2081 (2013);

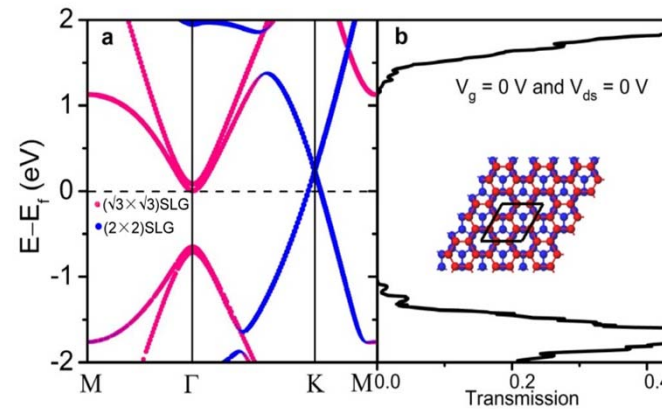
# 石墨烯与硅烯垂直结构FET



能隙 1.3 eV  
开关比  $10^7$



旋转不变能隙



全金属  
All-metallic FET

不需要打开能隙

旋转的石墨烯双层能隙存在

利用不同层的狄拉克锥

之间迁移禁止的特点<sup>E4</sup>

## Twist-controlled resonant tunnelling in graphene/boron nitride/graphene heterostructures

A. Mishchenko<sup>1</sup>, J. S. Tu<sup>2</sup>, Y. Cao<sup>2</sup>, R. V. Gorbachev<sup>2</sup>, J. R. Wallbank<sup>3</sup>, M. T. Greenaway<sup>4</sup>, V. E. Morozov<sup>1</sup>, S. V. Morozov<sup>2</sup>, M. J. Zhu<sup>1</sup>, S. L. Wong<sup>1</sup>, F. Withers<sup>1</sup>, C. R. Woods<sup>1</sup>, Y.-J. Kim<sup>2,6</sup>, K. Watanabe<sup>1</sup>, T. Taniguchi<sup>7</sup>, E. E. Vdovin<sup>1,5</sup>, O. Makarovsky<sup>4</sup>, T. M. Fromhold<sup>4</sup>, V. I. Fal'ko<sup>1</sup>, A. K. Geim<sup>1,2</sup>, L. Eaves<sup>1,4</sup> and K. S. Novoselov<sup>1\*</sup>

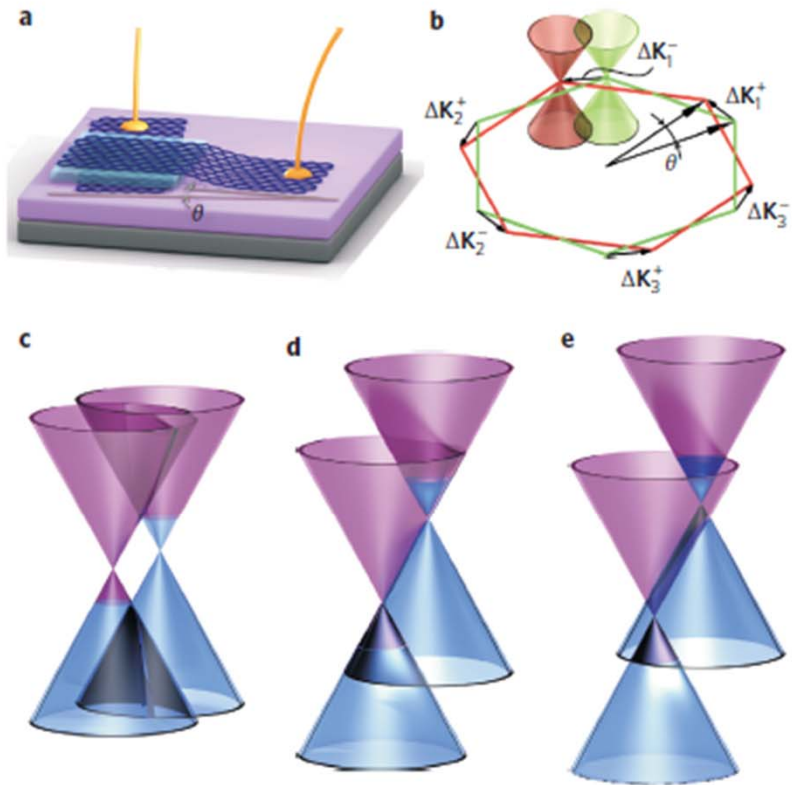
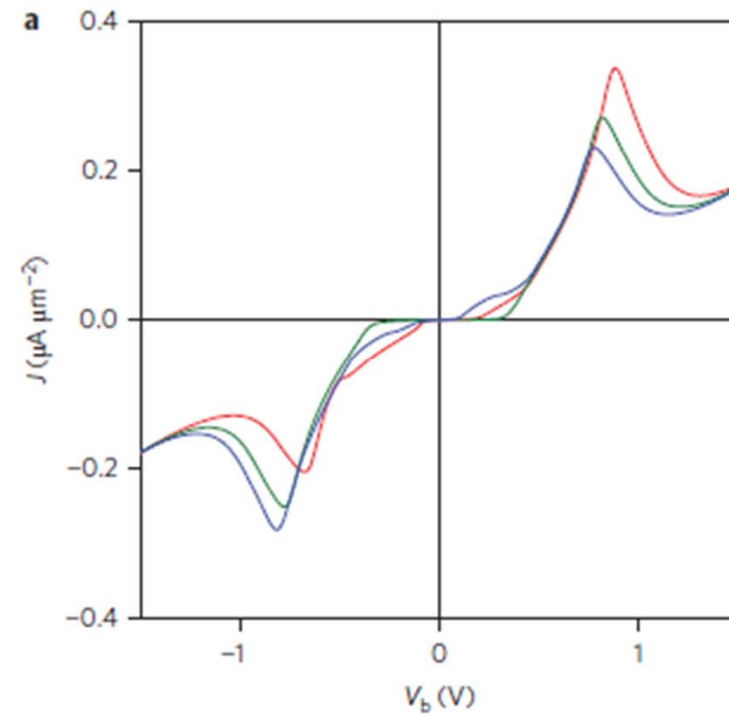
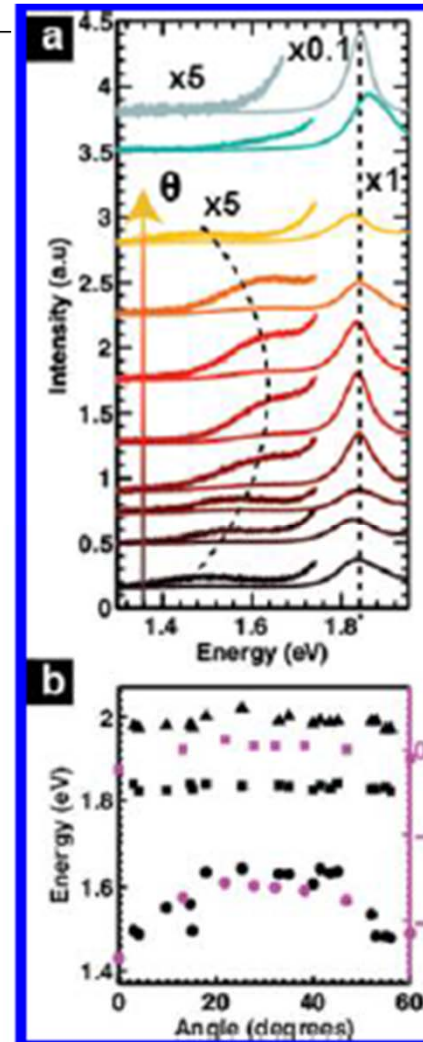
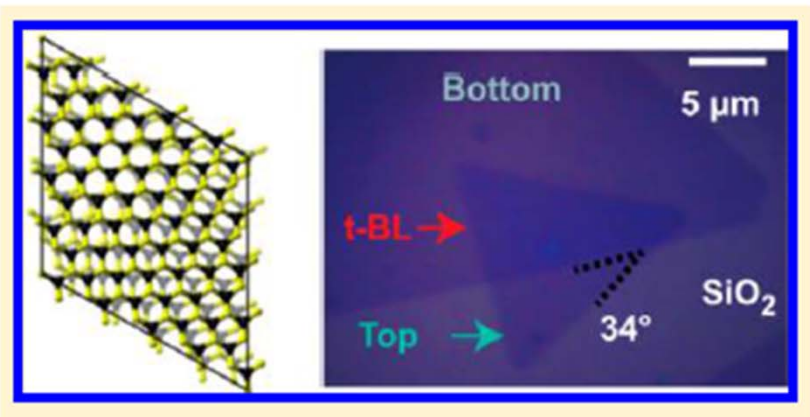


Figure 1 | Schematic representation of our device and its band structure.



### Tailoring the Electronic Structure in Bilayer Molybdenum Disulfide via Interlayer Twist

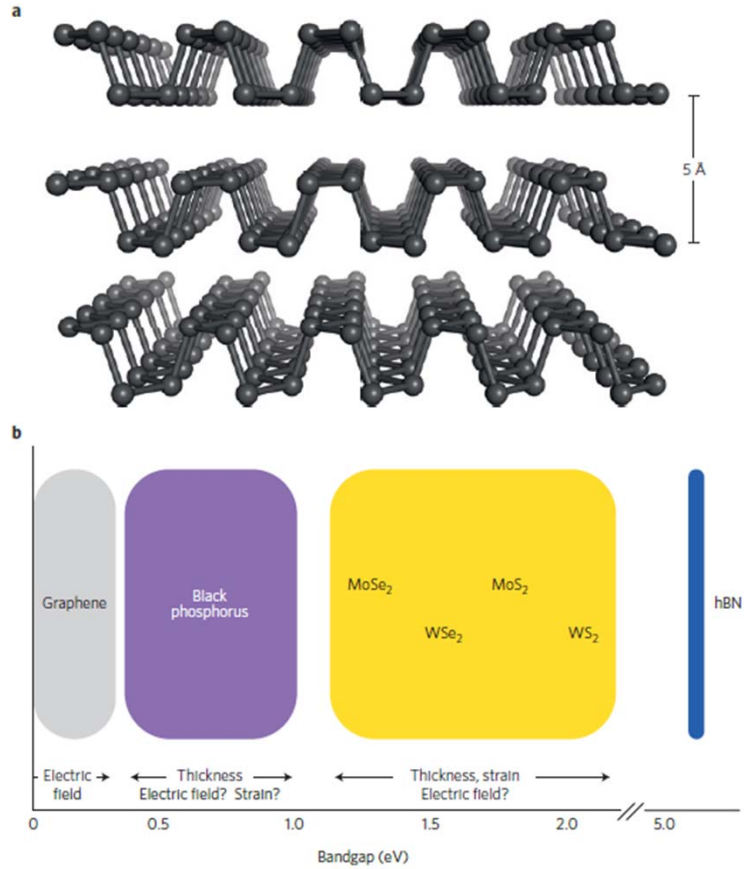
Arend M. van der Zande,<sup>†,‡,\*</sup> Jens Kunstmann,<sup>†,§</sup> Alexey Chernikov,<sup>||</sup> Daniel A. Chenet,<sup>‡</sup> YuMeng You,<sup>||</sup> XiaoXiao Zhang,<sup>||</sup> Pinshane Y. Huang,<sup>⊥</sup> Timothy C. Berkelbach,<sup>†,§</sup> Lei Wang,<sup>‡</sup> Fan Zhang,<sup>‡</sup> Mark S. Hybertsen,<sup>†,#</sup> David A. Muller,<sup>⊥,¶</sup> David R. Reichman,<sup>†,||</sup> Tony F. Heinz,<sup>†,||</sup> and James C. Hone,<sup>†,‡</sup>



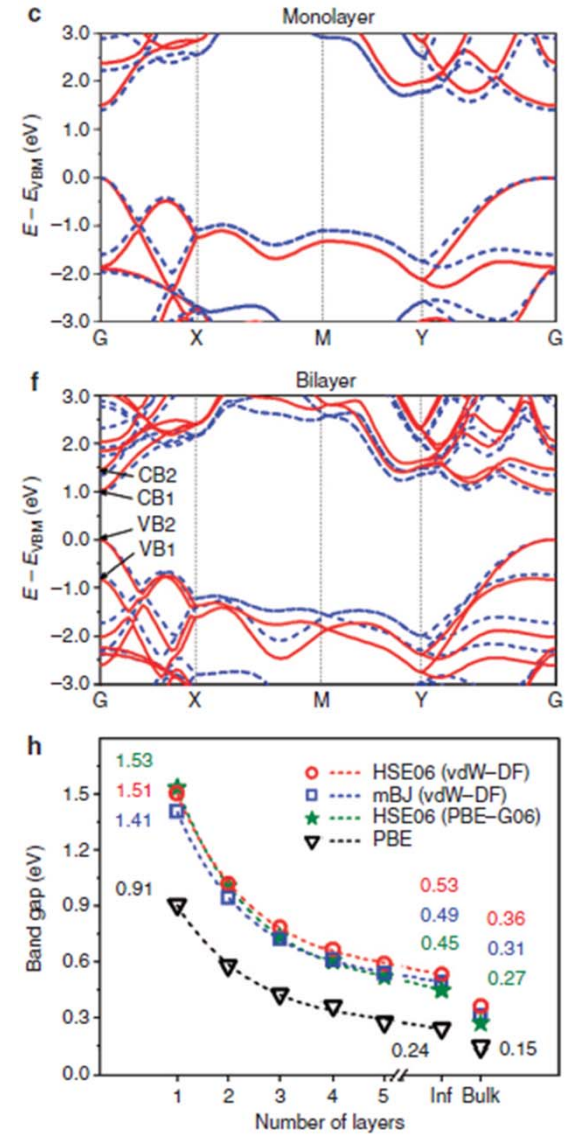
双层的MoS2 旋转后可以观察到圆偏振光的选择性

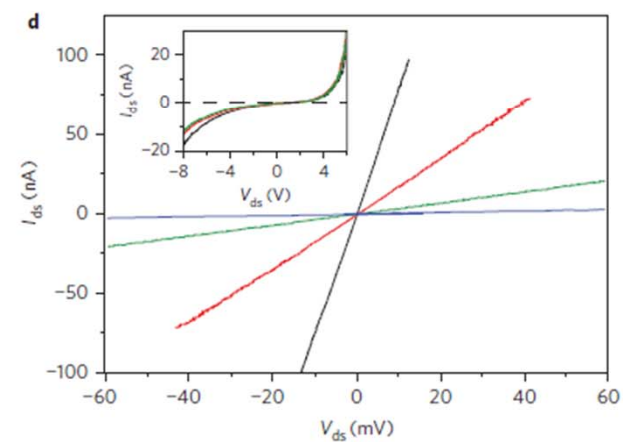
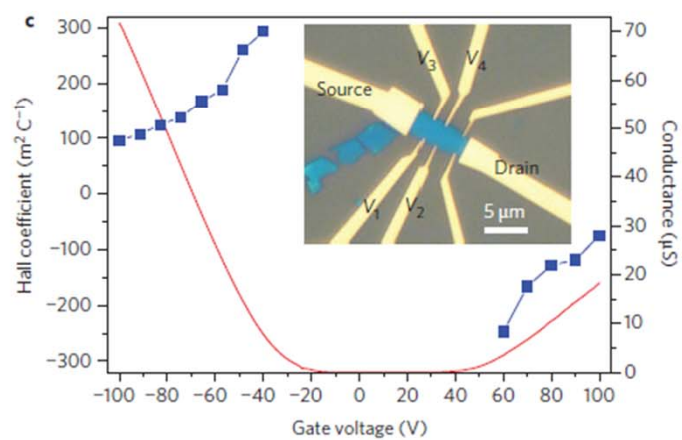
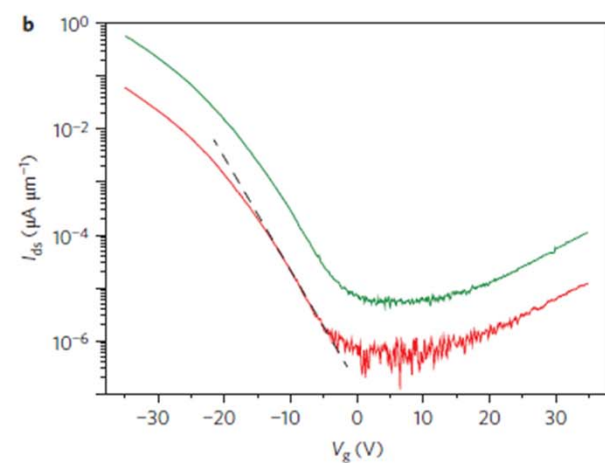
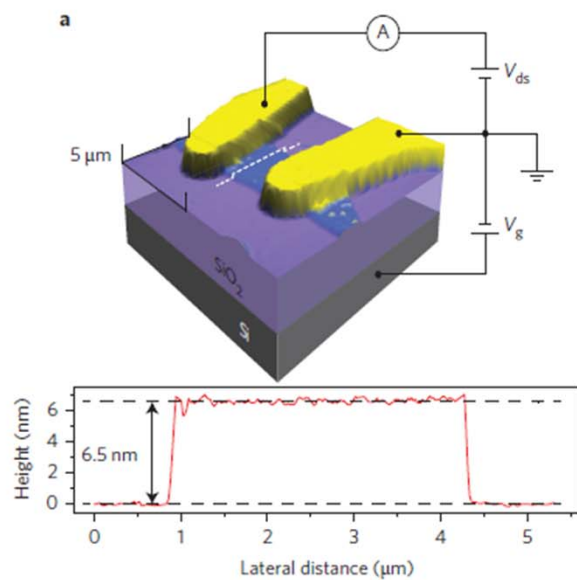


# 黑磷



**Figure 1** | Black phosphorus structure and bandgaps of layered materials. **a**, The layered and anisotropic crystal structure of elemental black phosphorus. **b**, Bandgap energies of several layered materials used for nanoelectronics. The range of values for each material can be achieved through a variety of means. For example, it is expected that variations in an applied perpendicular electric field, film thickness or strain could modify the bandgap value. hBN, hexagonal boron nitride.



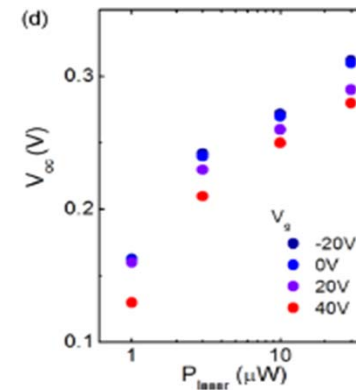
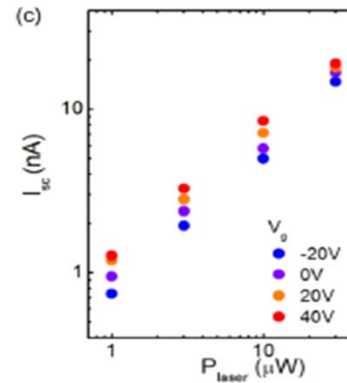
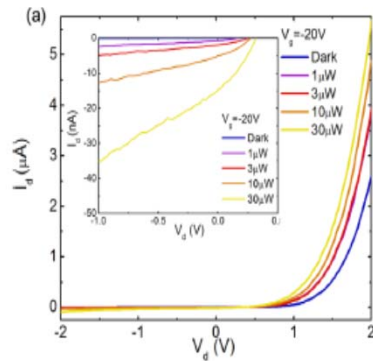
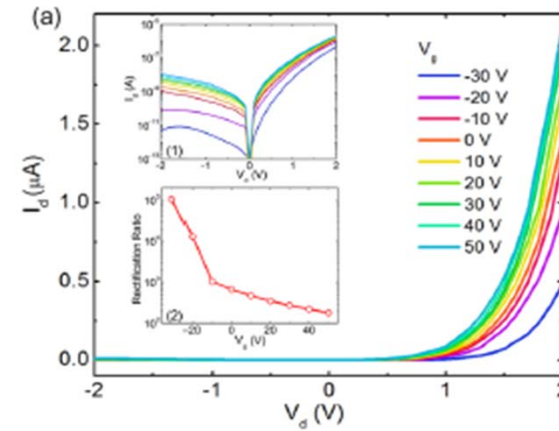
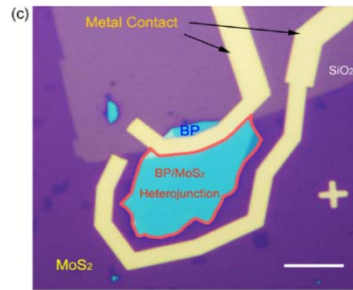
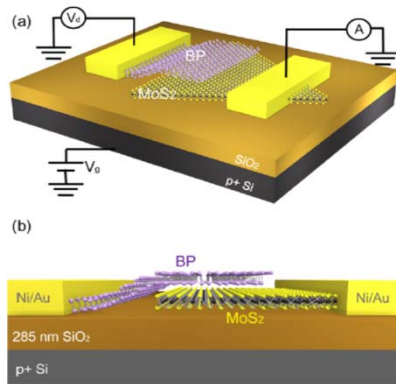


## Black phosphorus field-effect transistors

Likai Li<sup>1</sup>, Yijun Yu<sup>1</sup>, Guo Jun Ye<sup>2</sup>, Qingqin Ge<sup>1</sup>, Xuedong Ou<sup>1</sup>, Hua Wu<sup>1</sup>, Donglai Feng<sup>1</sup>, Xian Hui Chen<sup>2\*</sup> and Yuanbo Zhang<sup>1\*</sup>

# Black Phosphorus-Monolayer MoS<sub>2</sub> van der Waals Heterojunction p-n Diode<sup>1</sup>

1. Deng, Y. *et al.* *ACS Nano* **8**, 8292–8299 (2014).



- 可能发展:
- 1 门的控制p-n 结
  - 2 同质的材料

$I_{sc}$  as a function of laser power under different back gate voltage. (d)  $V_{oc}$  as a function of laser power under different back gate voltage. Increasing the back gate voltage increases  $I_{sc}$  but reduces  $V_{oc}$ .

## 总结

- 1 多体效应可期待在更多的MX<sub>2</sub>上观测。衬底的影响值得进一步研究。
- 2 MoS<sub>2</sub>还可以满足ITRS 10 nm 器件的要求。可以继续缩小FET。
- 3 光电器件可以进一步简化。努力实现TFET.
- 4 谷电子学-自旋电子学耦合在一起，显示了丰富的物理。  
双层MoS<sub>2</sub> 的谷霍尔效应应该在加垂直电场时候可以实现。
- 5 自旋流尚待测观。谷轨道磁矩流和霍尔效应也应存在。
- 6 层间旋转会带来新的调控。

# 致谢

基金委 科技部 教育部

合作者： 史俊杰， 杨金波， 俞大鹏， 李巨（MIT）， 杨李（华盛顿）

Ph. D candidates:



宋志刚



王洋洋

钟红霞 潘峰



屈贺如歌



倪泽远 Ni Zeyuan



潘圆圆