

Title: Stacking Induced Spontaneous Polarization in Rhombohedral MoS2

Speakers: Ziliang Ye

Collection: Quantum Matter Workshop

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Abstract: "The relatively weak van der Waals bond in 2D materials has ushered in a rich new era of stacking engineering. We recently found in rhombohedrally stacked MoS₂, a Berry phase contrast between layers can induce an asymmetric interlayer coupling and an out-of-plane spontaneous electrical polarization (1). The polarization direction can be switched via interlayer sliding, forming a new type of ferroelectricity. In addition, we demonstrated that such a polarization can lead to a spontaneous photovoltaic effect without any pn junctions (2). Compared to conventional PV effects, our device shows a similar quantum efficiency with an ultrafast speed and potentially a programmable polarity. The rhombohedrally stacked transition metal dichalcogenides therefore provide a new platform for studying spontaneous polarization at the atomic scale.

(1) Jing Liang, et al, arXiv:2209.06966 (2022).

(2) Dongyang Yang, et al, Nature Photonics, 16, 469-474 (2022)."

Stacking Induced Spontaneous Polarization in Rhombohedral MoS₂



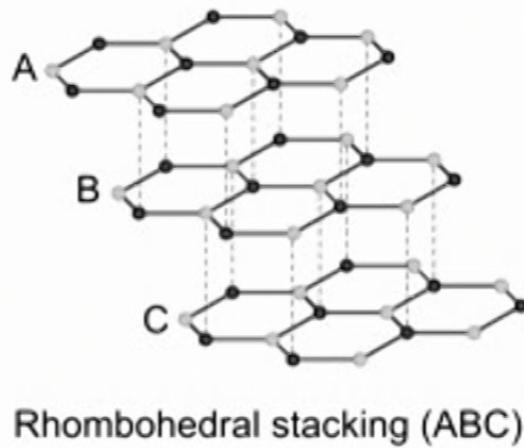
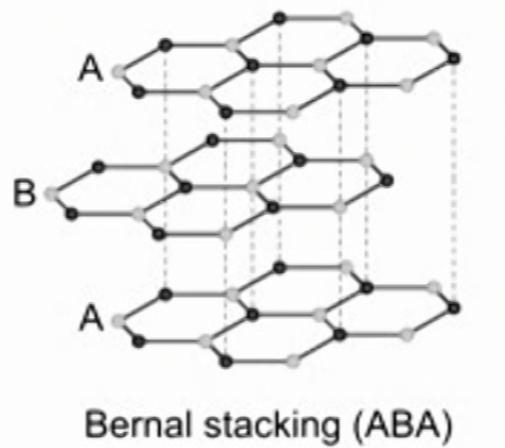
Quantum Matter Workshop

Perimeter Institute, Nov. 2022

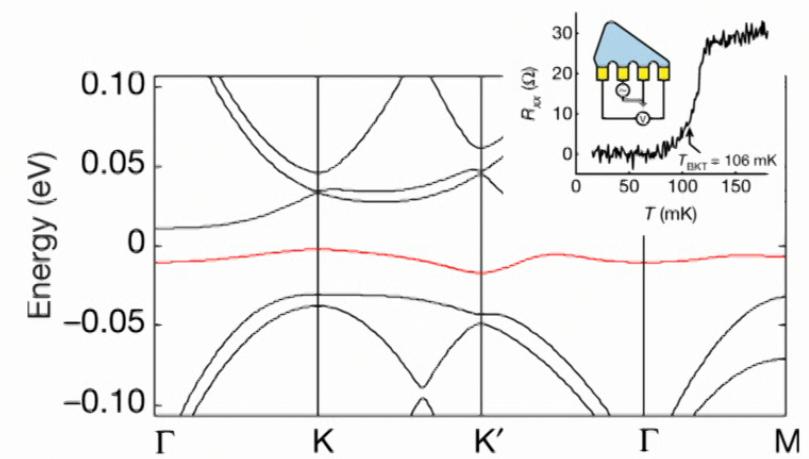
Ziliang Ye

**UNIVERSITY OF BRITISH COLUMBIA
DEPARTMENT OF PHYSICS AND ASTRONOMY
QUANTUM MATTER INSTITUTE**

Unconventional superconductivity in rhombohedral graphite



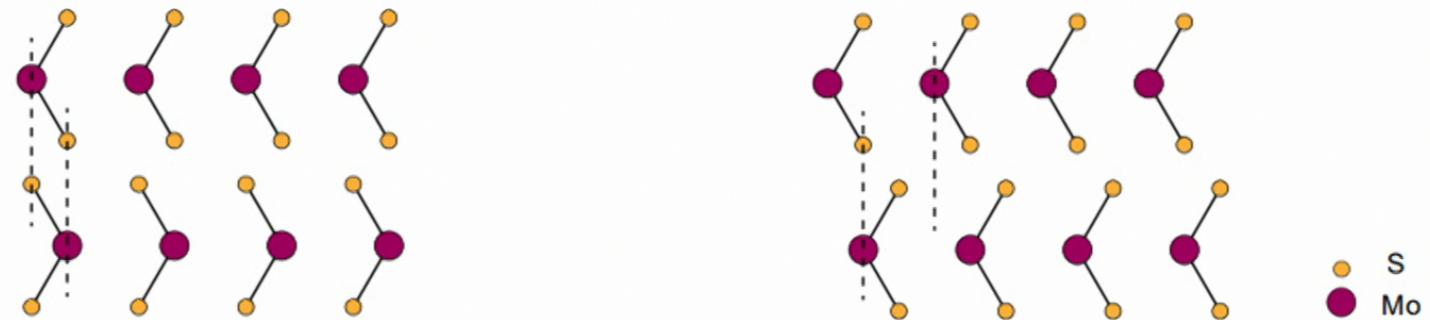
Rhombohedral graphite



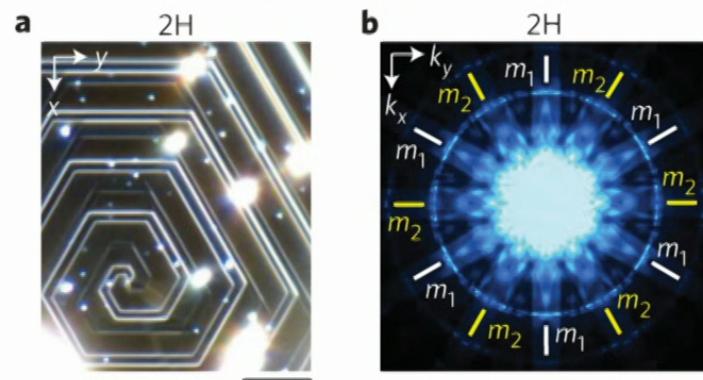
Superconductivity in ABC trilayer graphene

A. Young group, Nature 2021
F. Wang group, Nature 2019, 2020

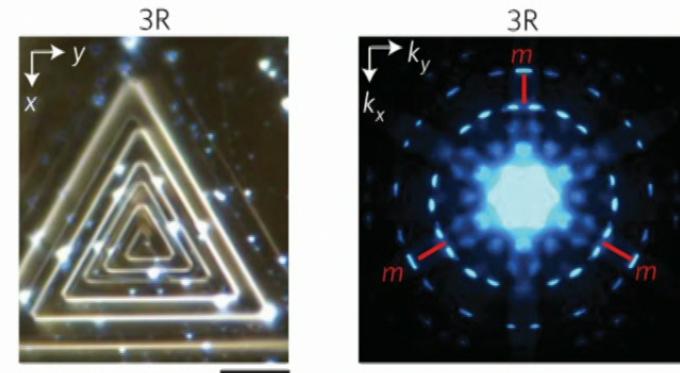
Rhombohedral MoS₂



hexagonal stacking

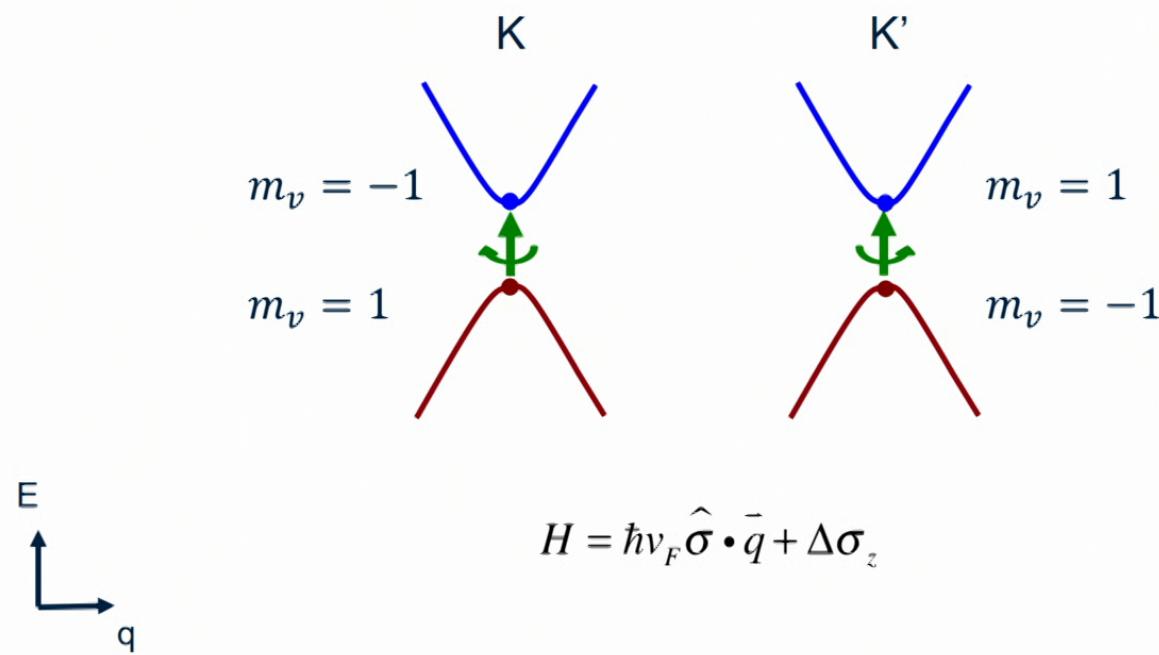


rhombohedral stacking



Iwasa group, Nature Nano. 2014 4
J. Wildervanck, 1970

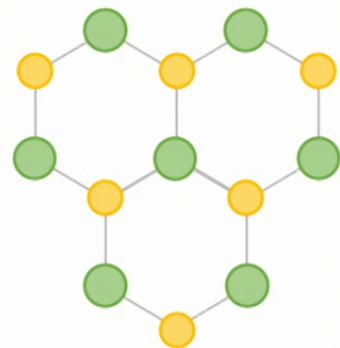
Valley selection rule



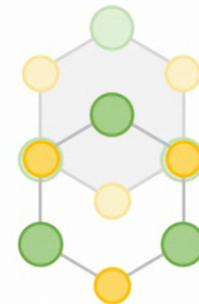
Y. Yafet, Solid State Phys. Vol 14, 1963
W. Yao, D. Xiao & Q. Niu, PRB, 2008 5

Layer dependent Berry phase winding

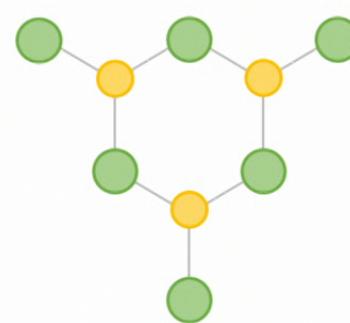
Top



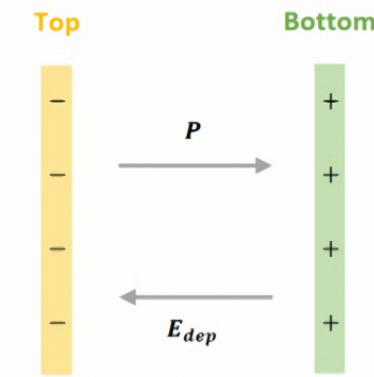
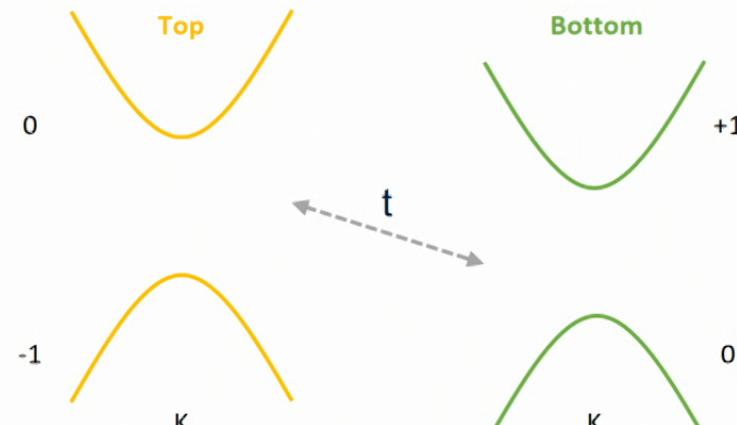
BA



Bottom

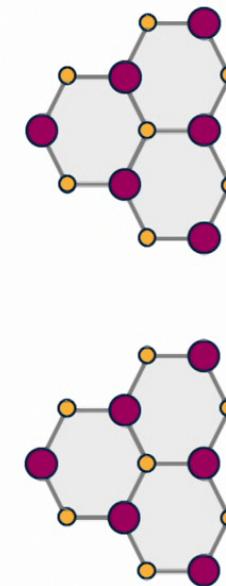
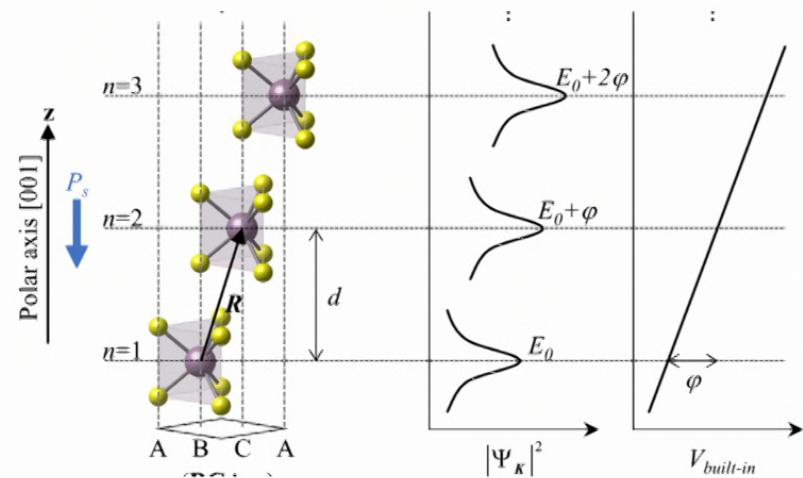


Asymmetric interlayer coupling and spontaneous polarization



$$\text{Interlayer potential } \phi_0 = \frac{P}{\epsilon_0 \epsilon_m} d_0$$

First-principle calculations

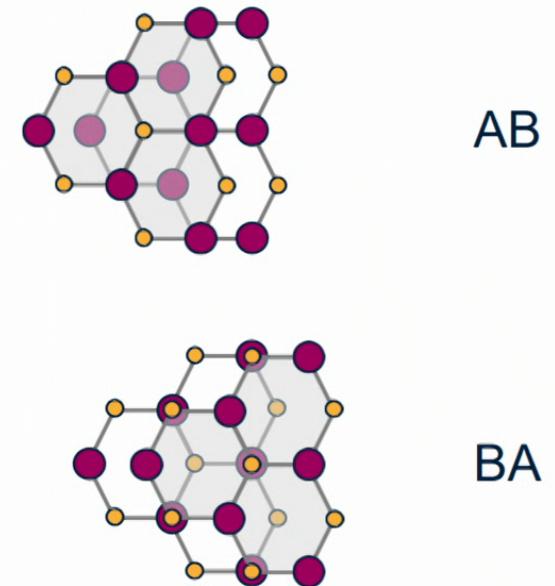
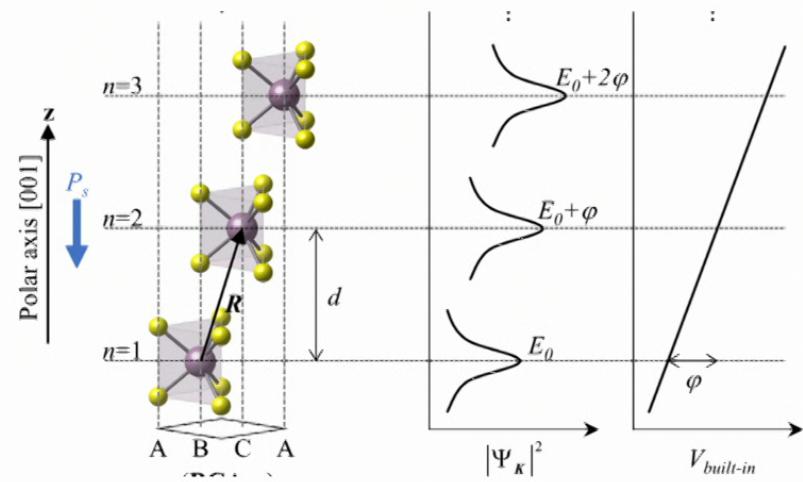


J. Park, et al, J. Phys. Condens. Matter 31, 315502 (2019)

Y. Wang, et al, PRB 95, 115429 (2017)

L. Li, et al, ACS Nano 11, 6382 (2017)

First-principle calculations

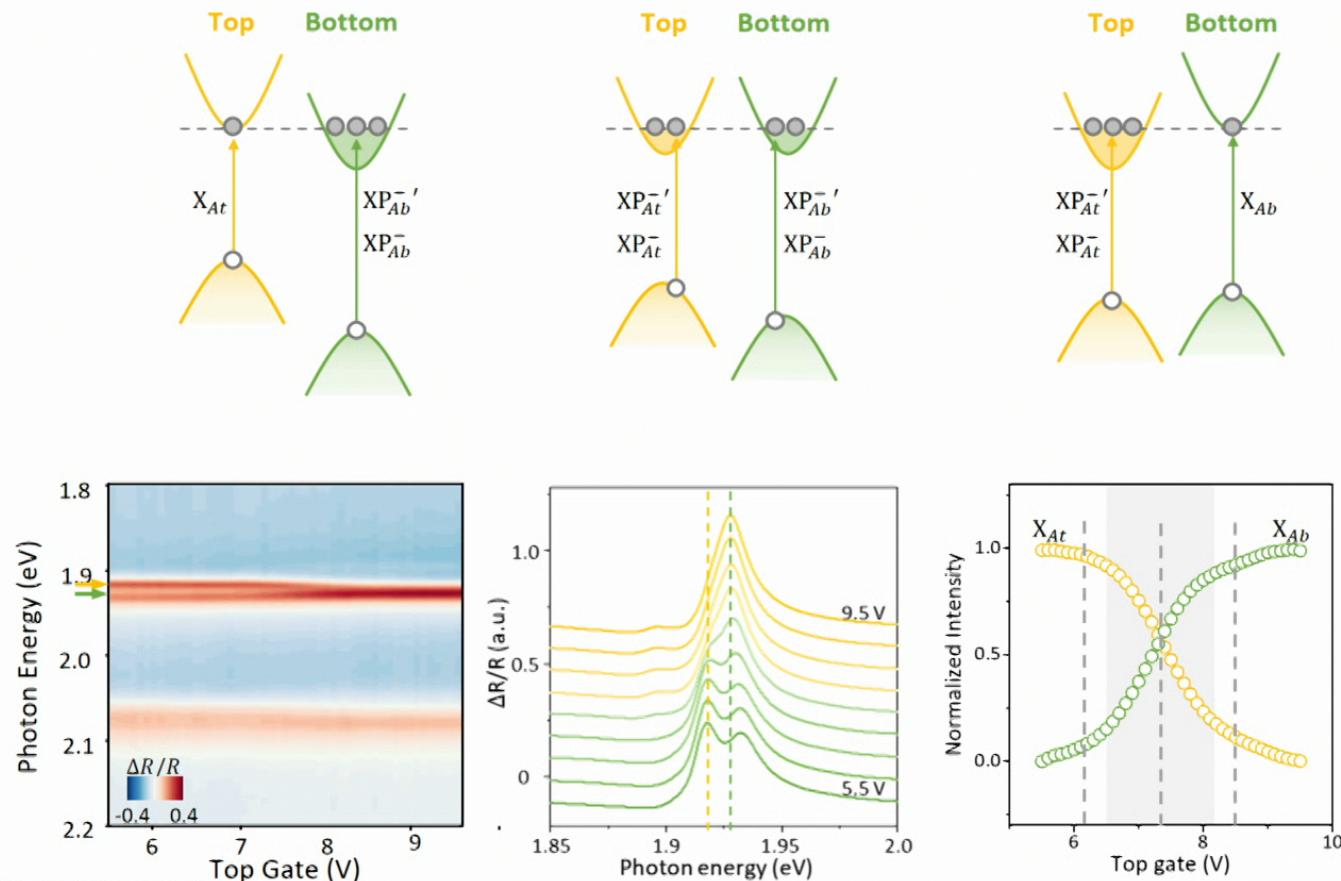


J. Park, et al, J. Phys. Condens. Matter 31, 315502 (2019)

Y. Wang, et al, PRB 95, 115429 (2017)

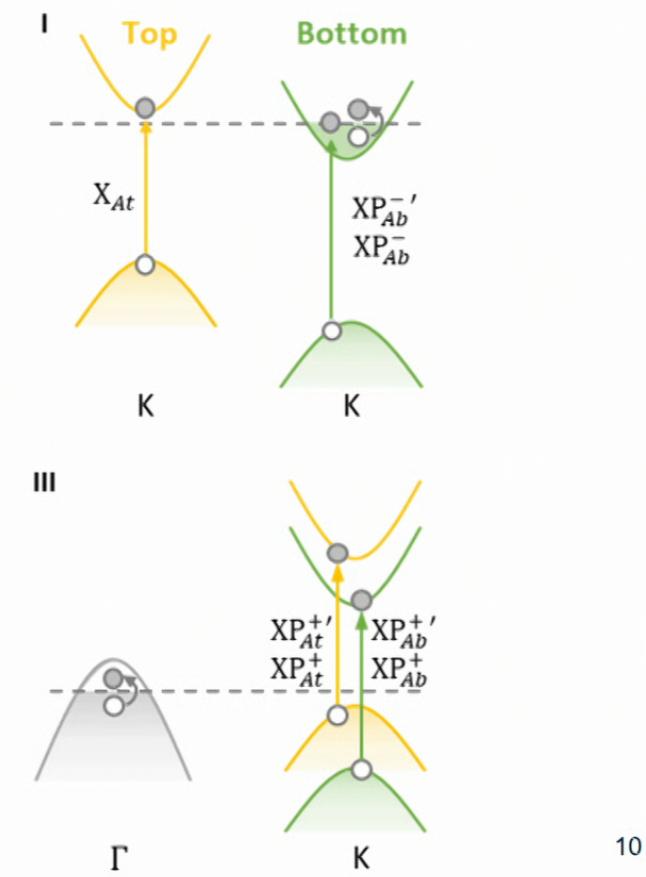
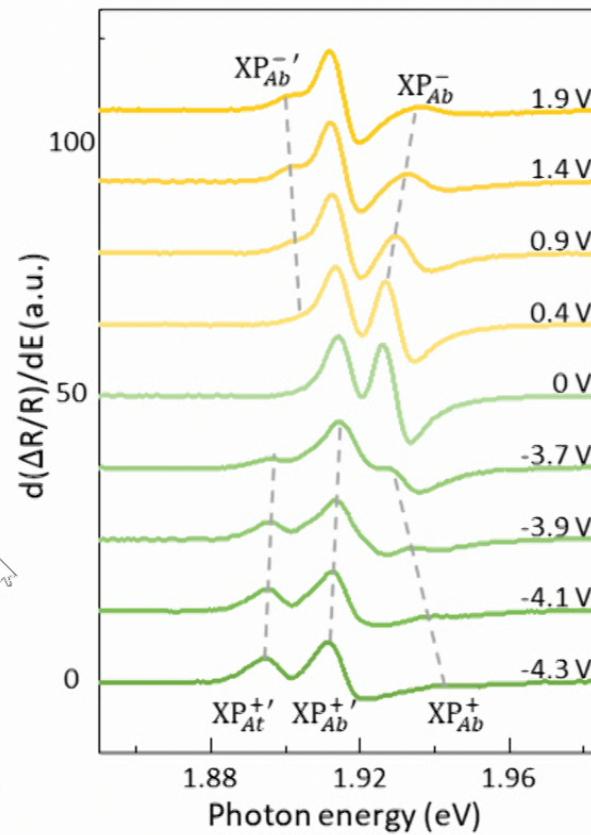
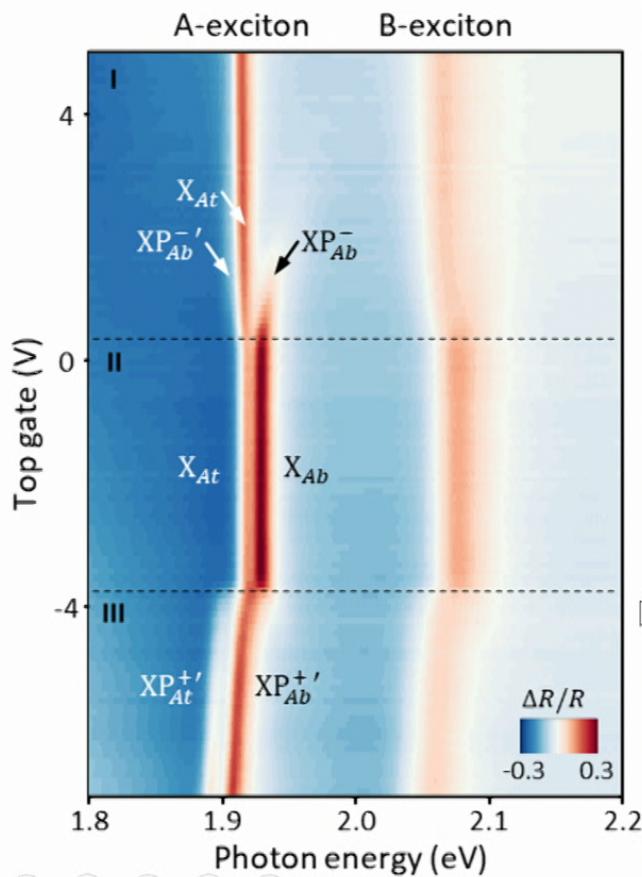
L. Li, et al, ACS Nano 11, 6382 (2017)

Optically probing the interlayer potential and asymmetric coupling

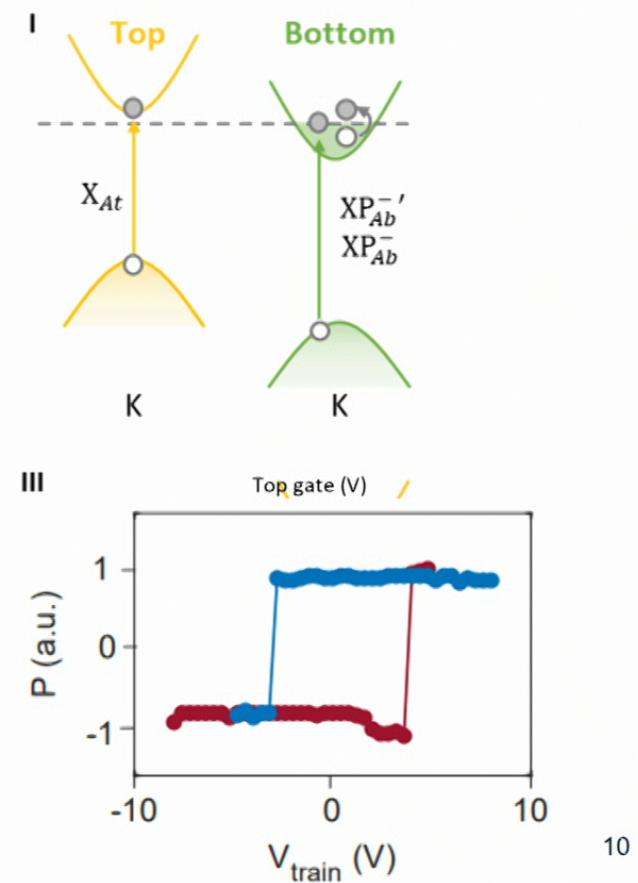
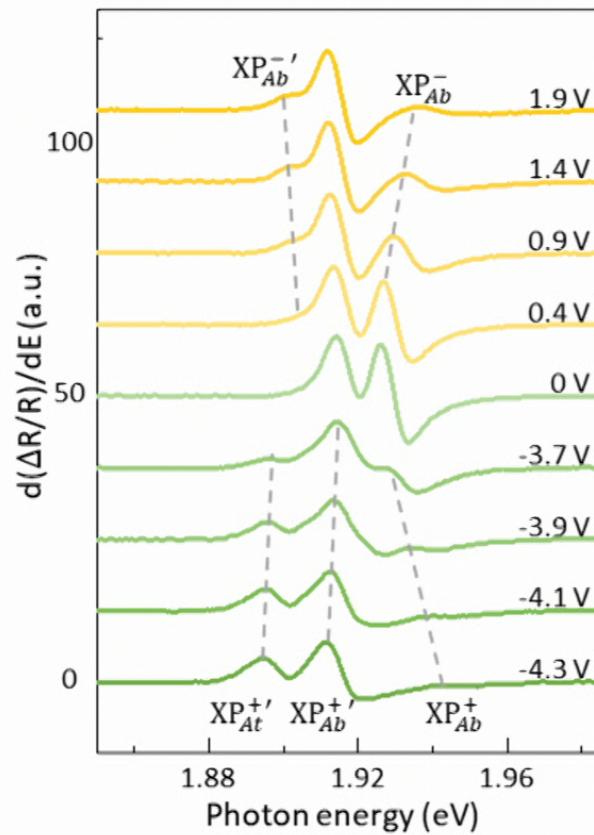
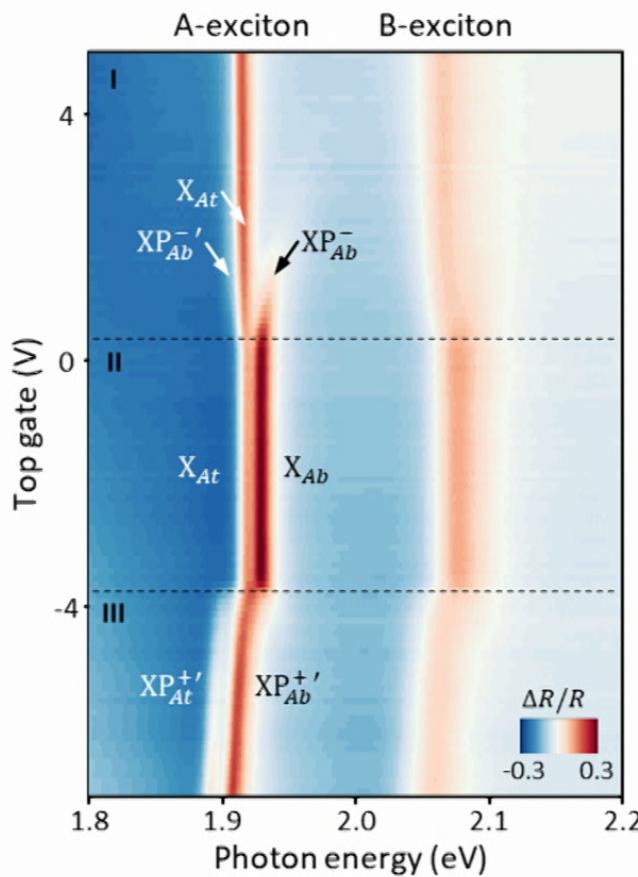


J. Liang, et al, PRX, 12, 041005 2022

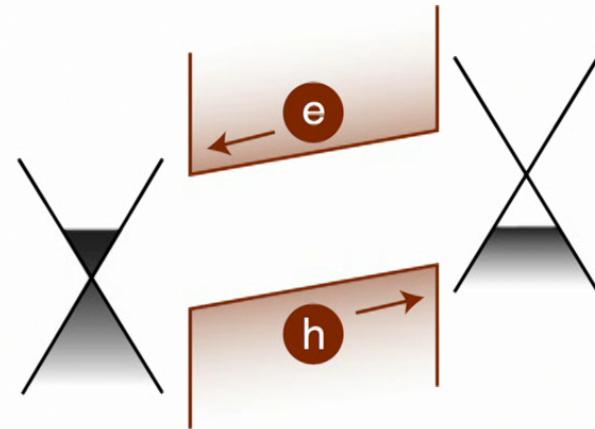
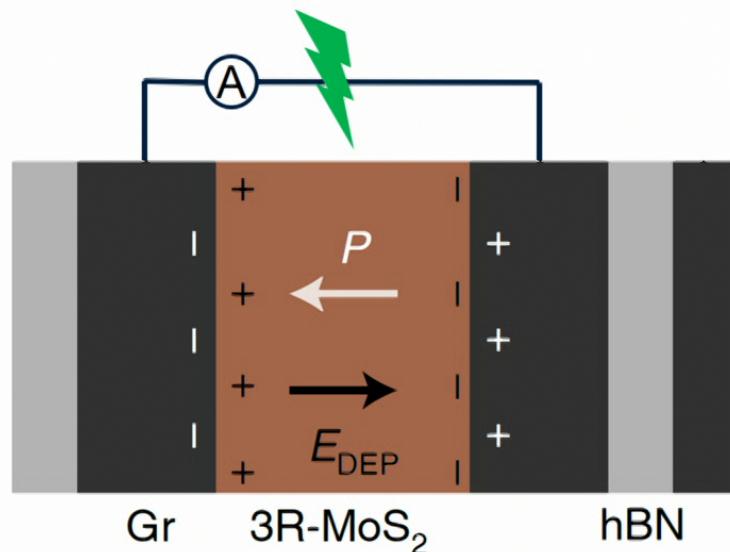
Doping dependence



Doping dependence



Photovoltaic Device

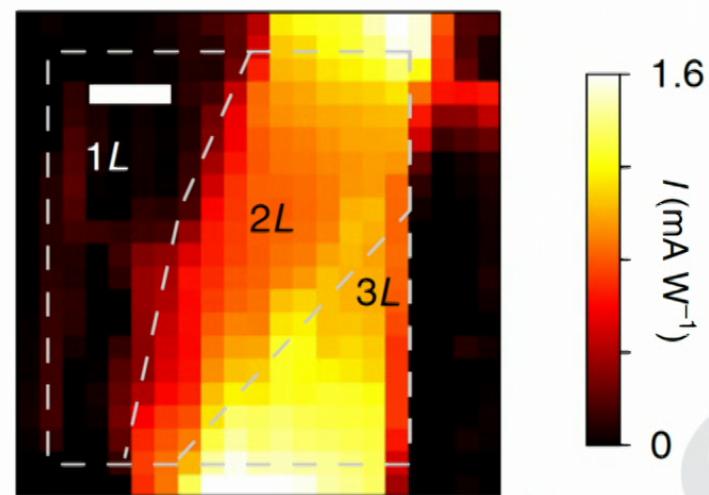
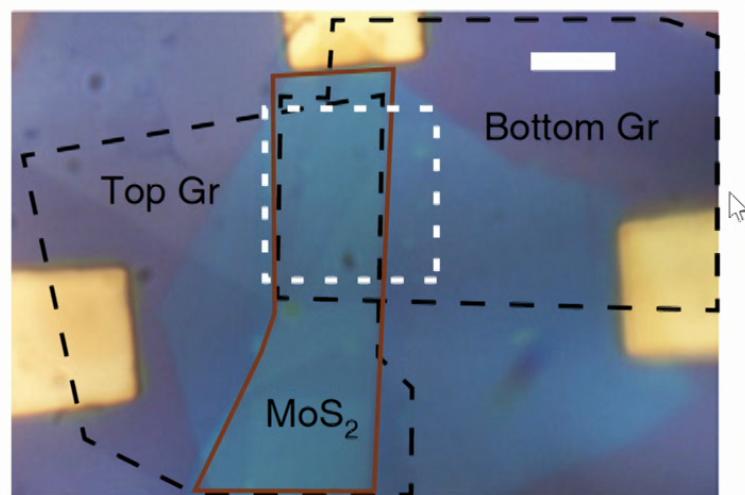


Graphene contacts can preserve 95% of the E_{dep}

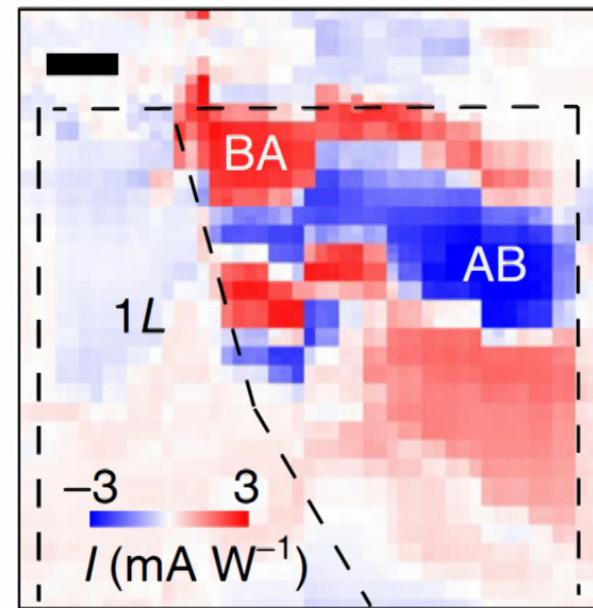
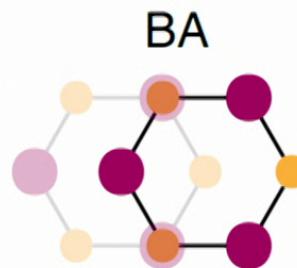
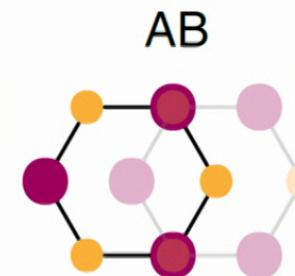
D. Yang, et al, Nat. Photonics, 16, 469 (2022)

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Photocurrent map

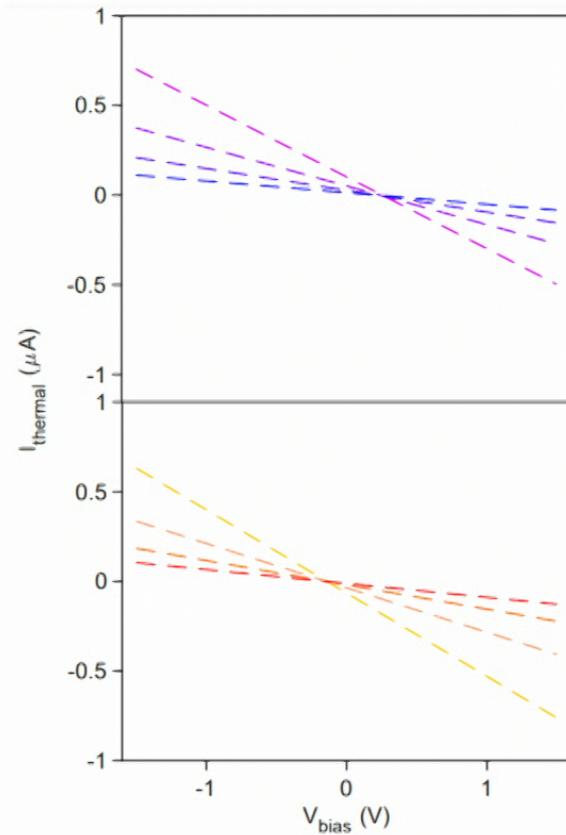
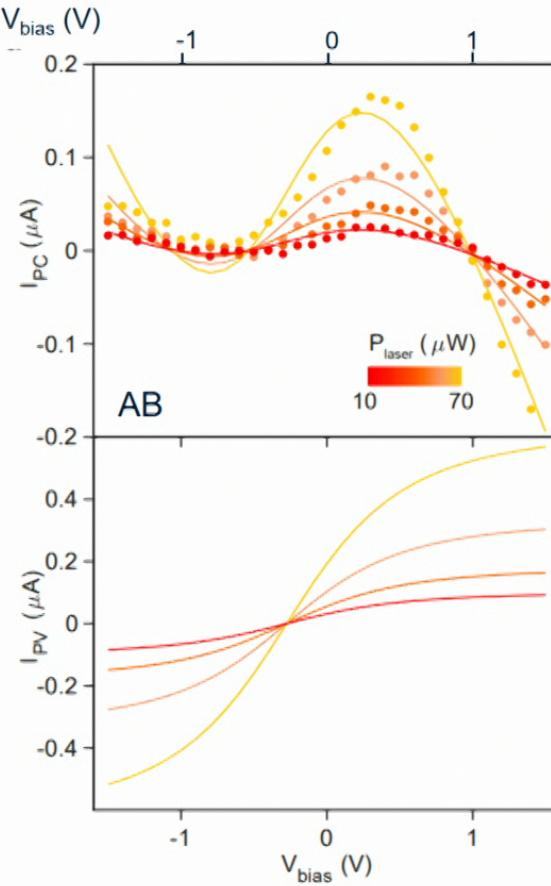
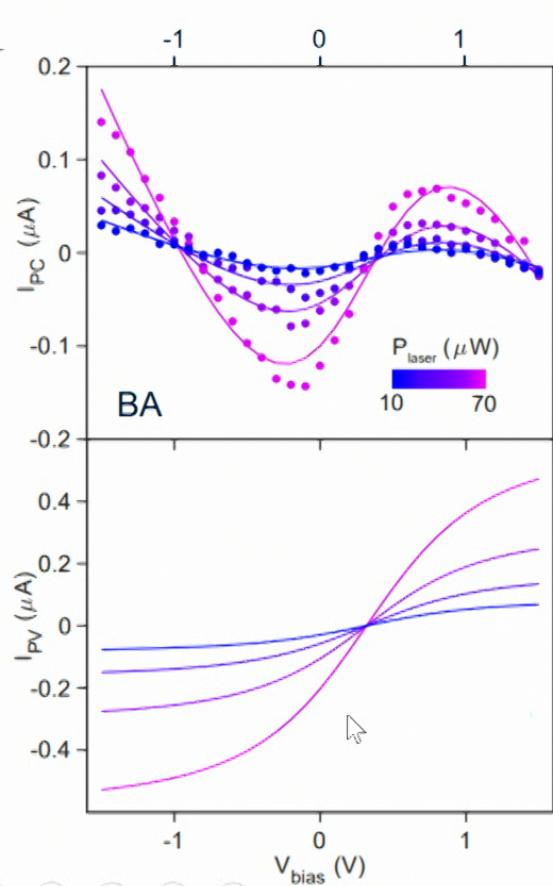


Mixed domain

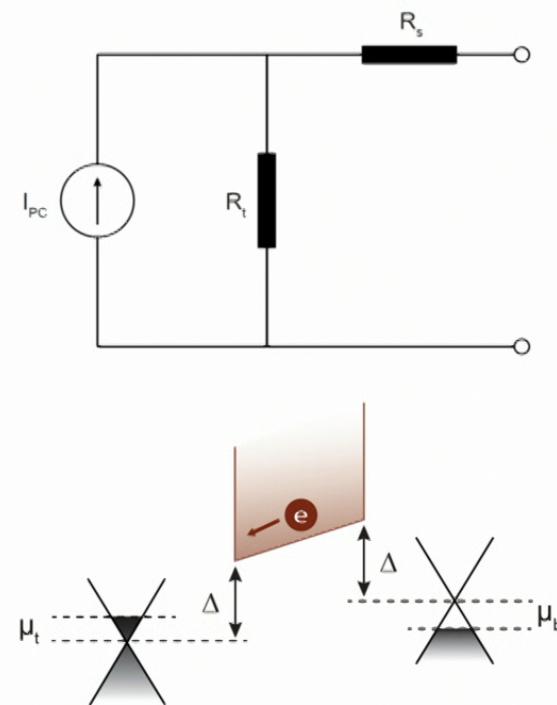


Thermal contributions

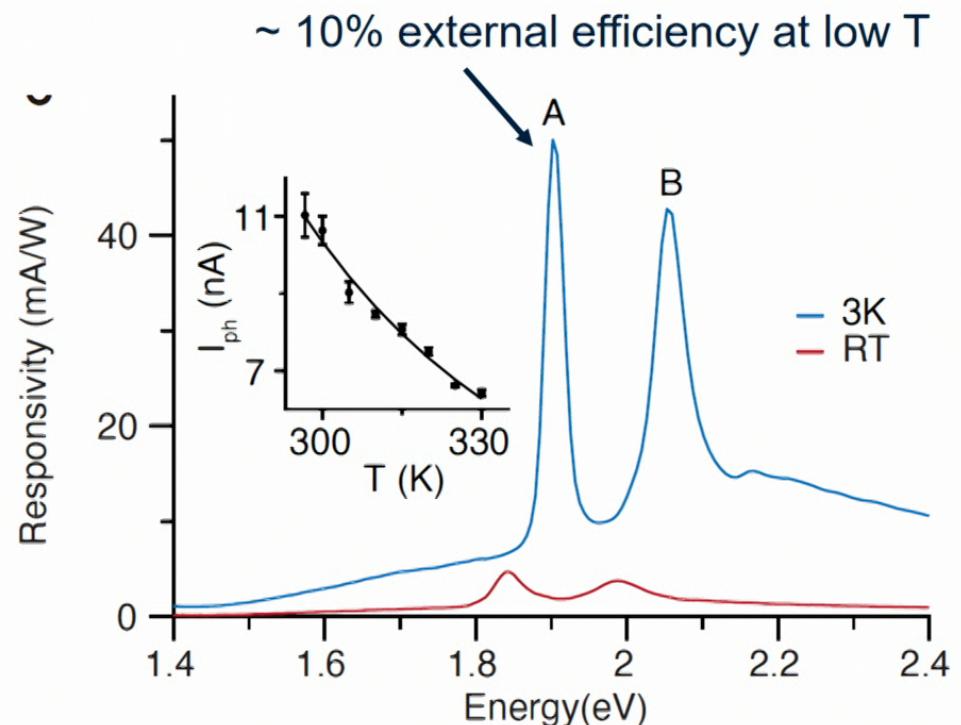
$$I_{PC} = I_{PV} + I_{bolo} + I_{PTE}$$



Shunt resistance model



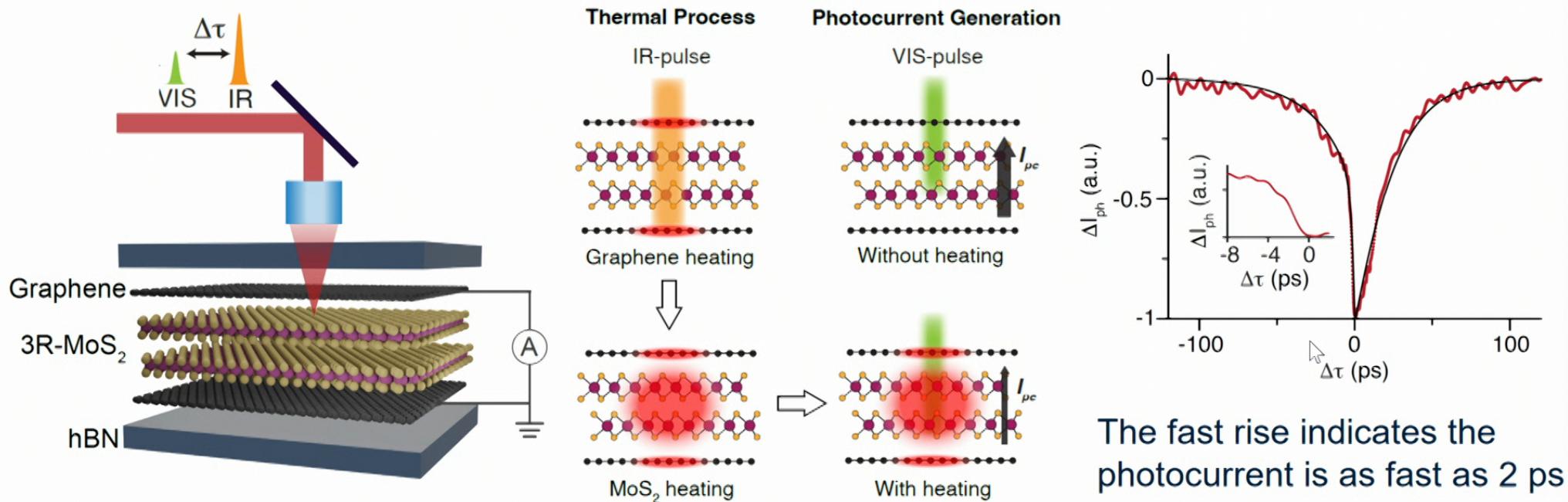
$$\sigma = 4A \frac{e^2}{h} \frac{1}{\pi^2(hv_f)^4} \int_{\Delta}^{+\infty} (E + \mu_t)(E + \mu_b) \frac{1}{k_B T} \exp\left(-\frac{E}{k_B T}\right) dE$$



J. Wu, et al, accepted by Science Advances

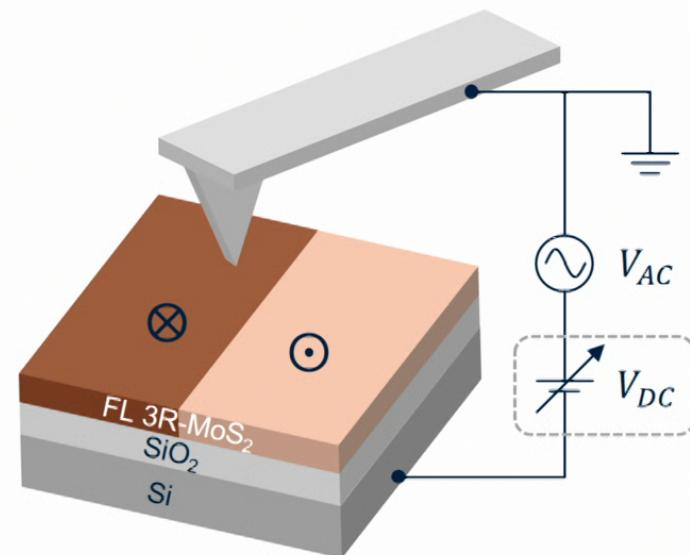
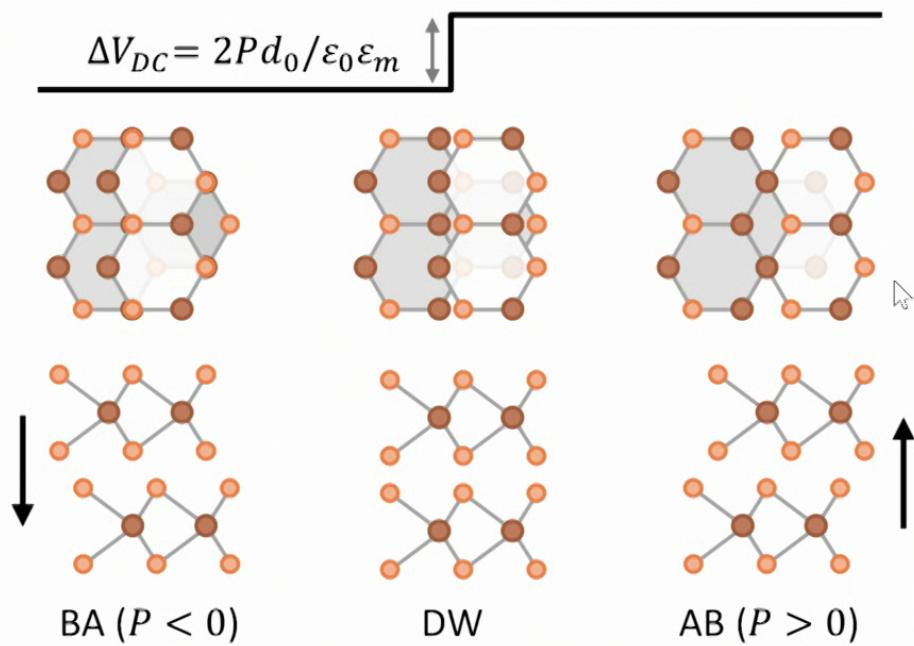
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Ultrafast photoresponse



The fast rise indicates the photocurrent is as fast as 2 ps

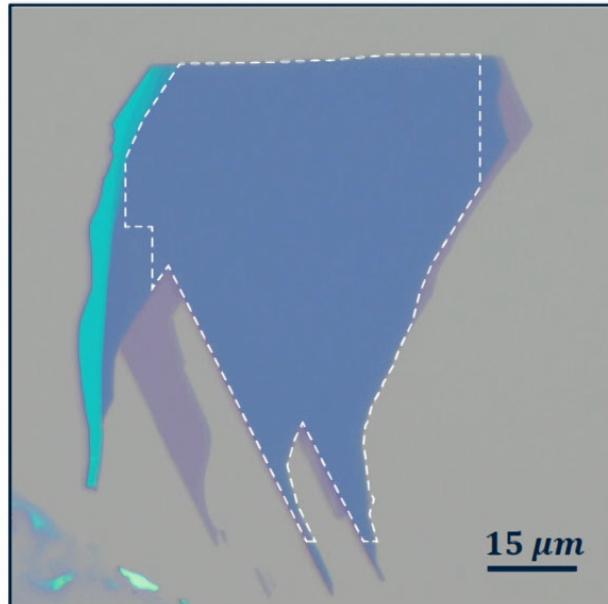
Probing the stacking order with scanning probe microscopy



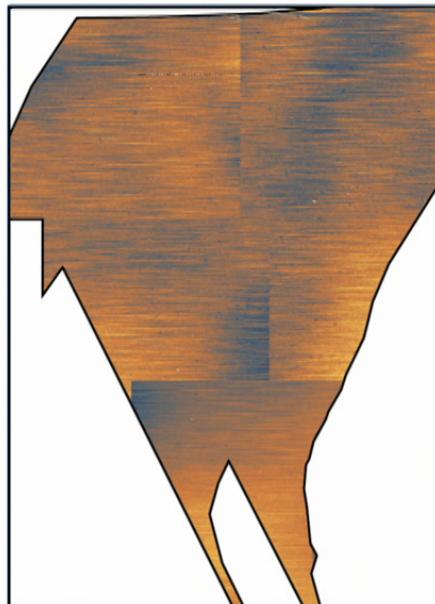
**Electrostatic Force Microscopy (EFM)/
Kelvin Probe Force Microscopy (KPFM)**

Domains in a trilayer sample

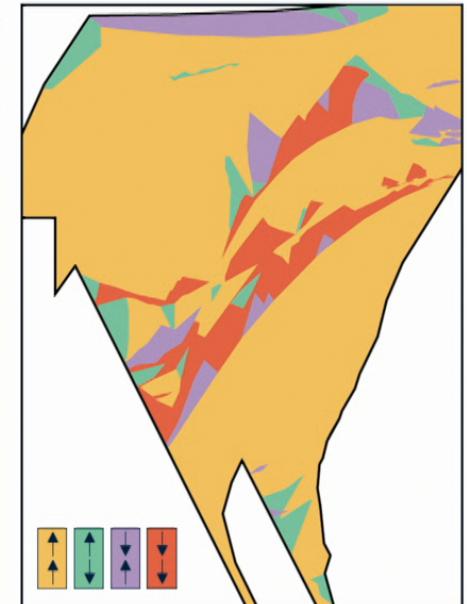
Optical image



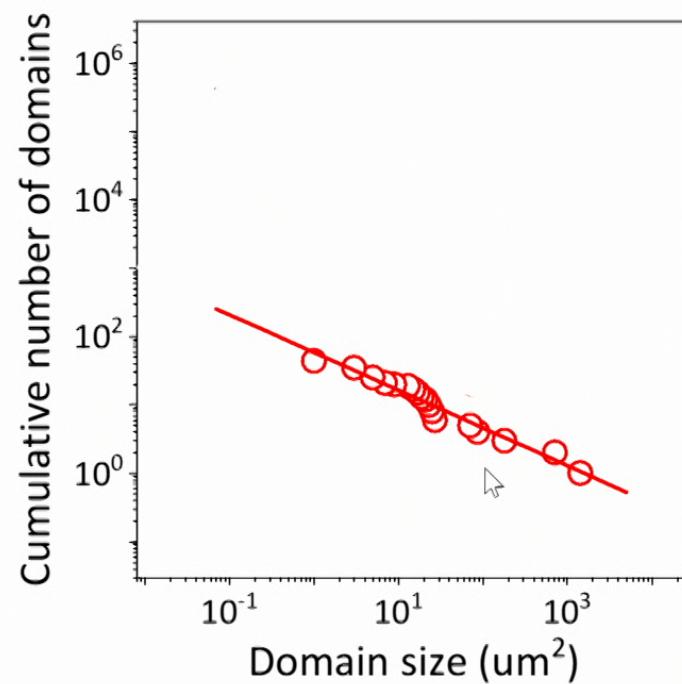
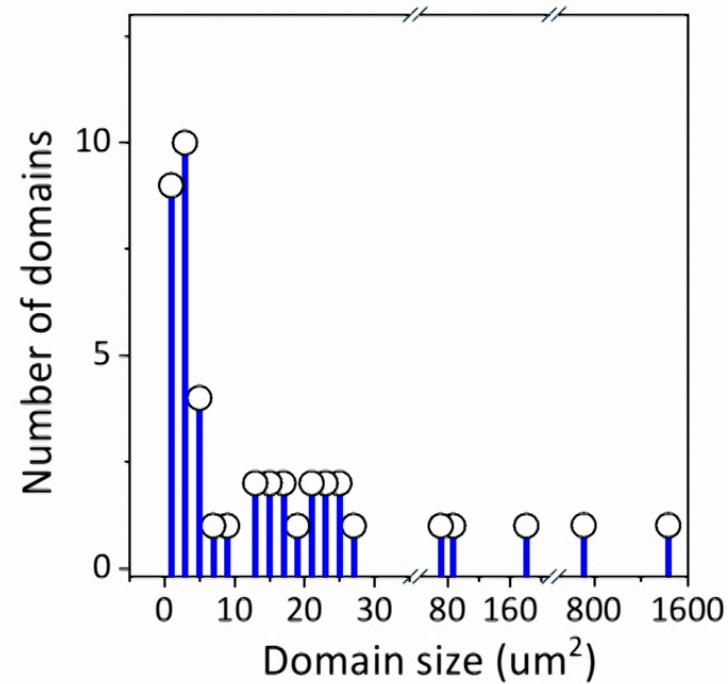
Topography



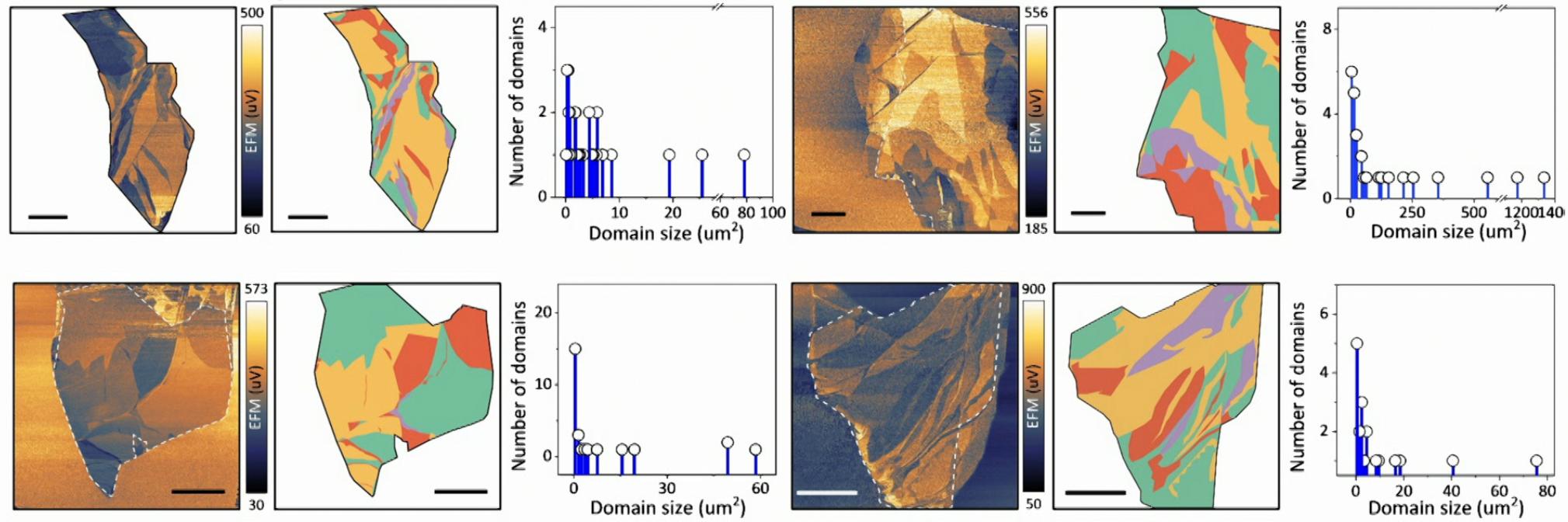
EFM



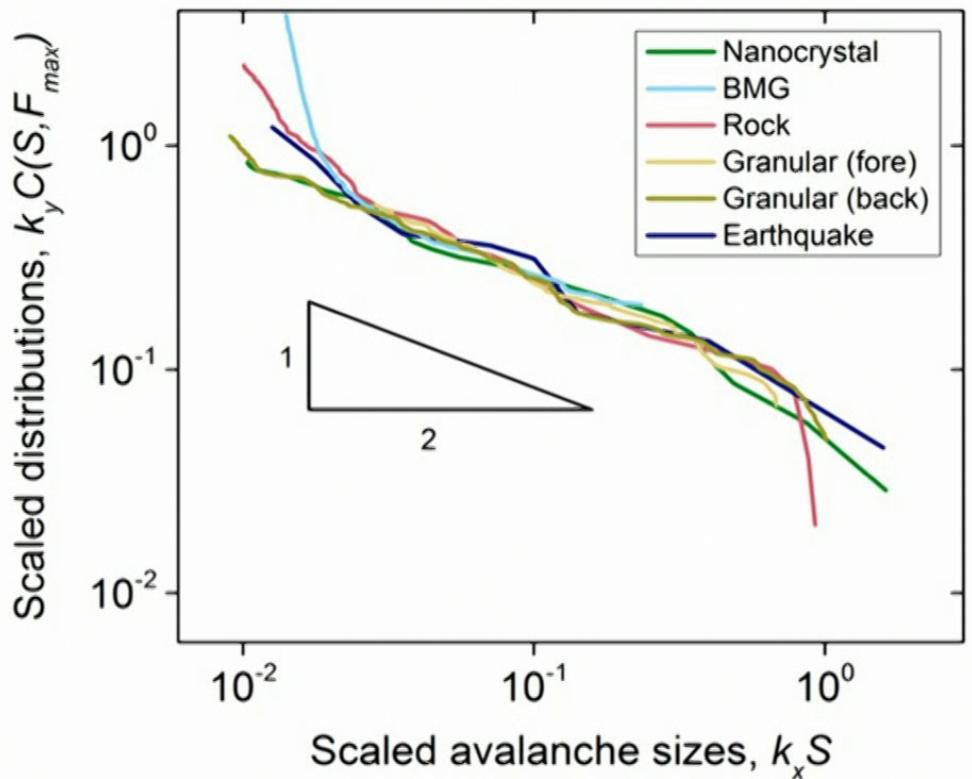
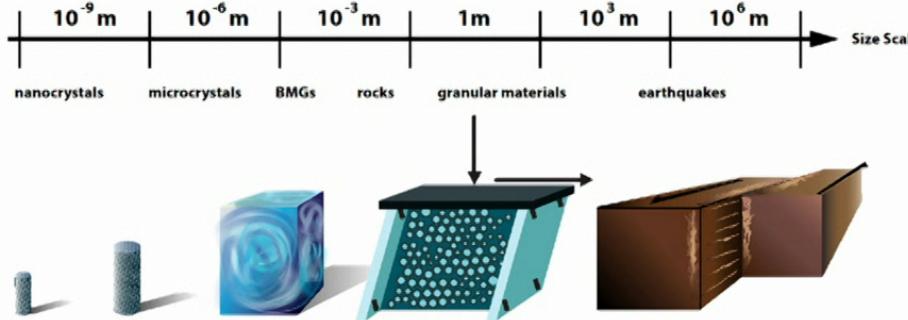
Domain size distribution



More data

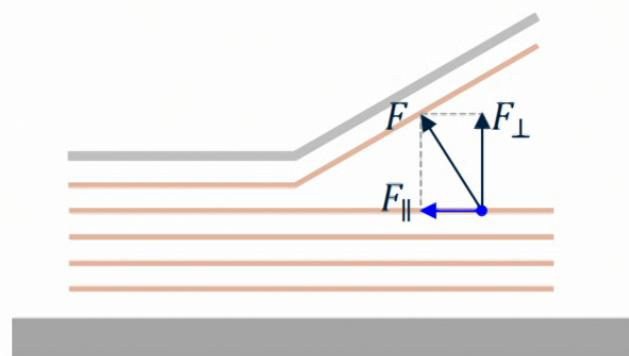


Universal slip size distribution under shear strain

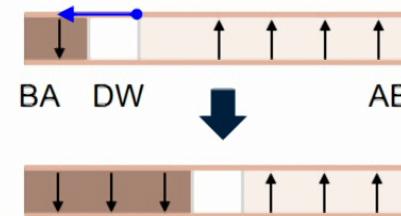


"Universal Quake Statistics: From Compressed Nanocrystals to Earthquakes" J. Uhl... K. Dahmen, Sci. Rep. 2015 21

Sliding induced by shear strain



Shear strain during exfoliation

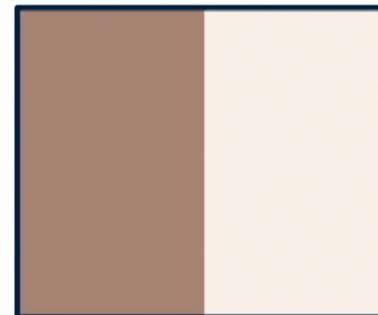
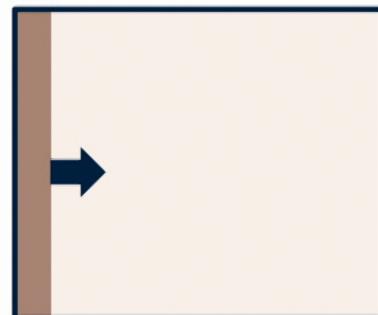


Domain wall movement

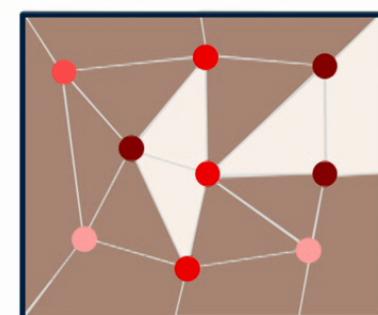
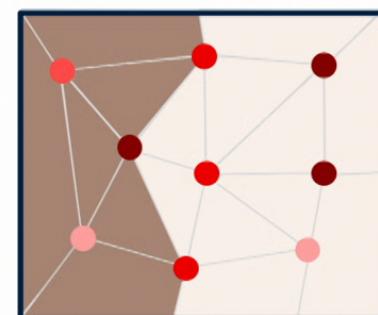
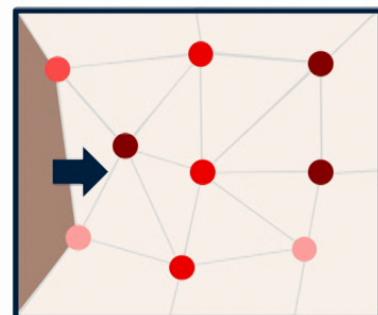
Sliding avalanche

  Polarization direction

Without
pinning
centers



With
pinning
centers

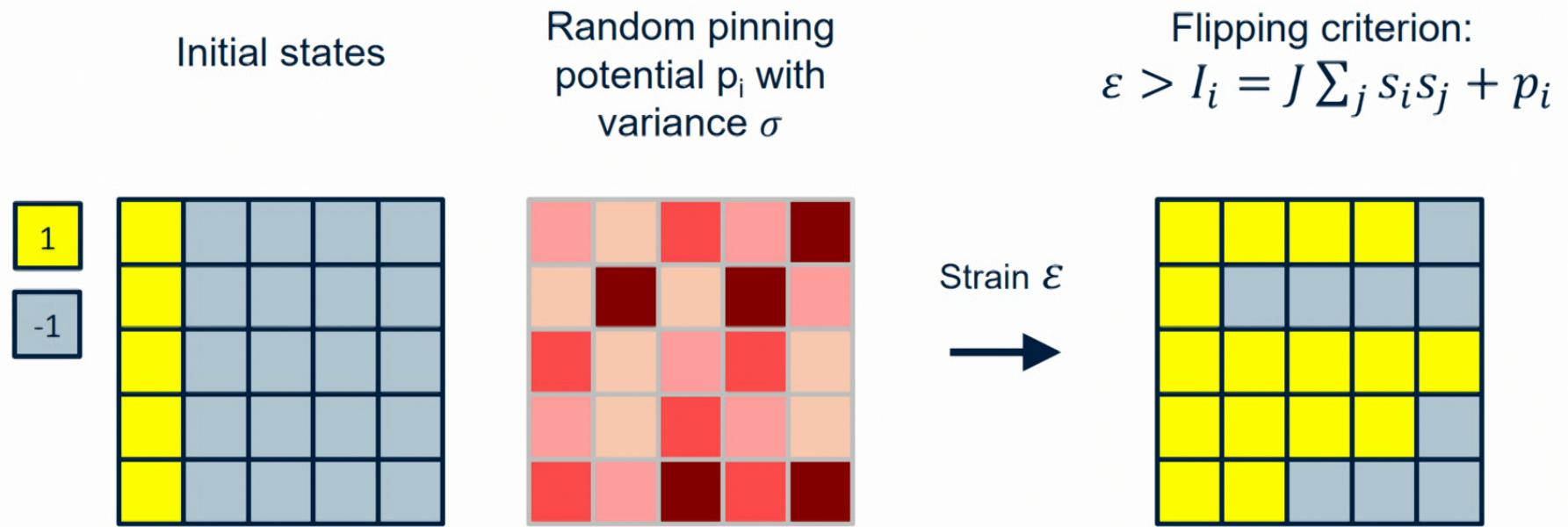


- The inhomogeneous pinning sites causes some domains to remain unflipped after the sliding avalanche passes.

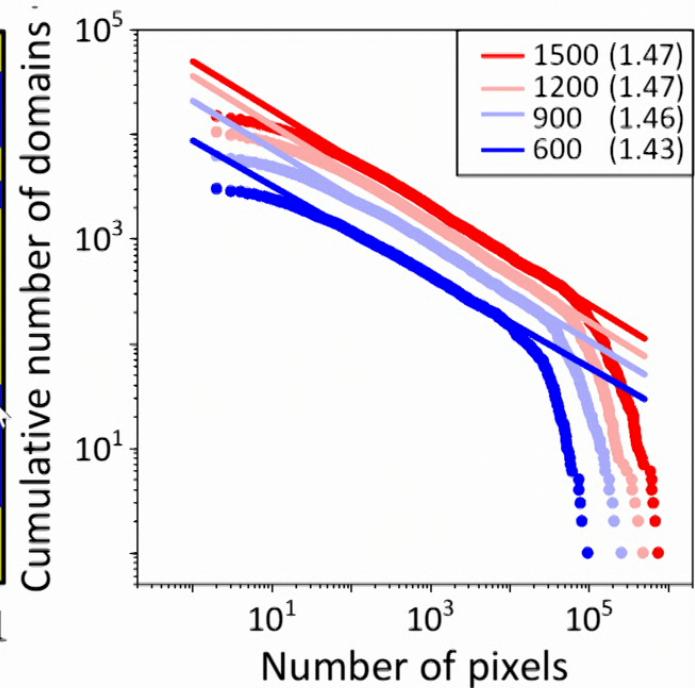
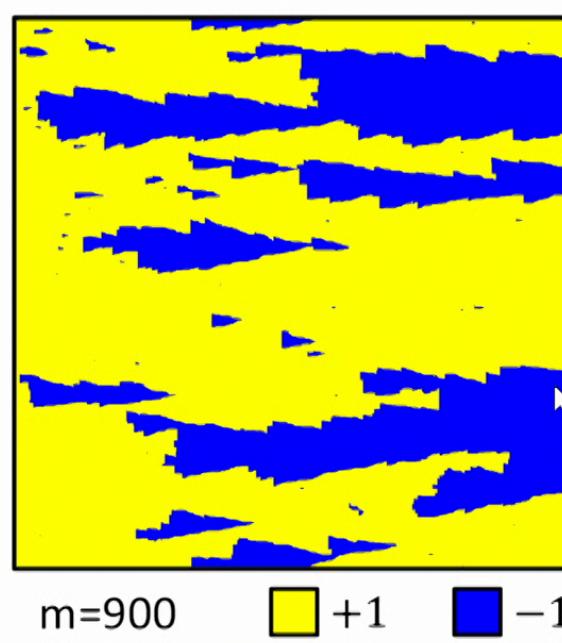
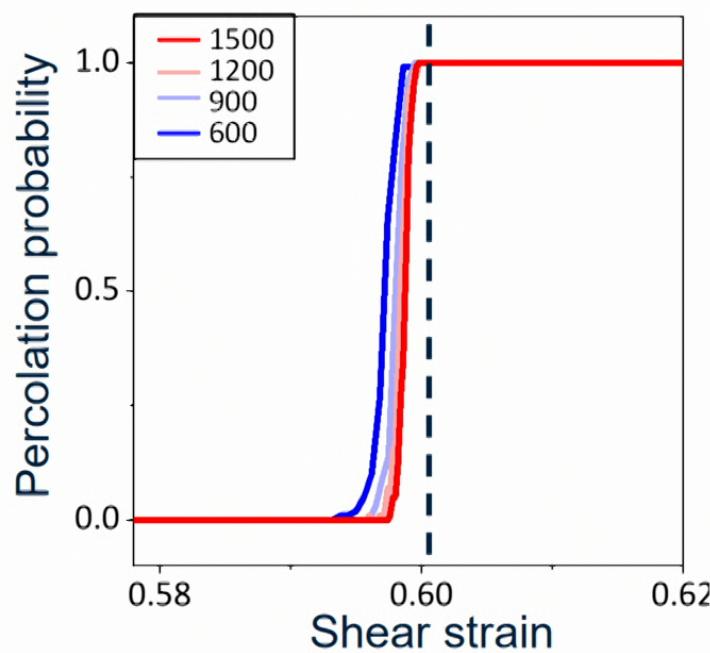
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Daniel Fisher, Phys. Rep. 1998

Numerical simulation based on random field Ising model

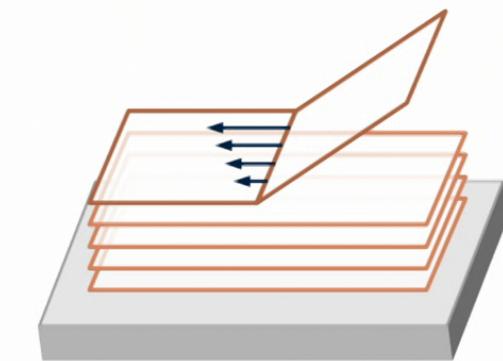


Percolation behavior

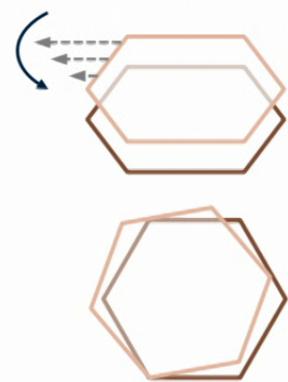


The critical field is slightly dependent on σ/J and simulation size.

Interlayer twist

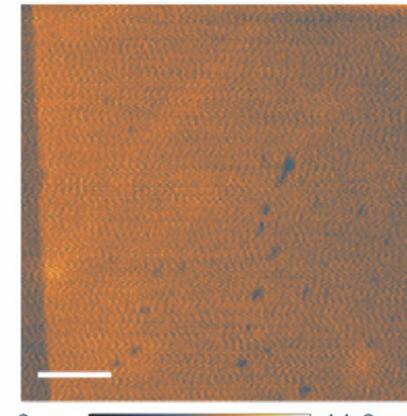


Inhomogeneous shear force

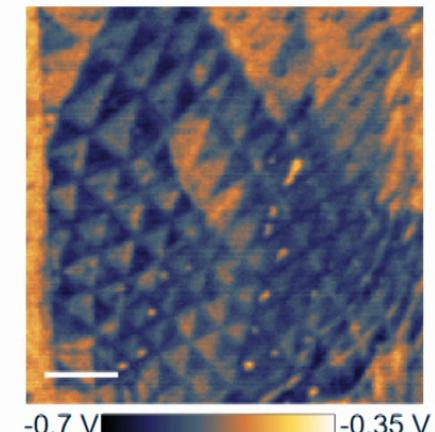


Interlayer twist

Topography

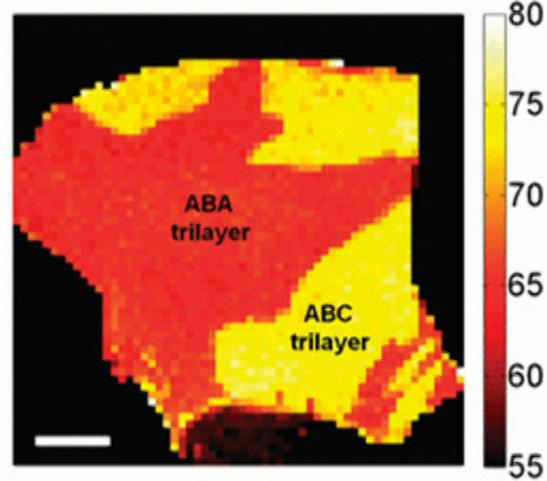


KPFM



Discussion

- A nonequilibrium critical phenomenon at the atomic thin limit.
- The stacking order of 2D materials can be changed by shear strain.

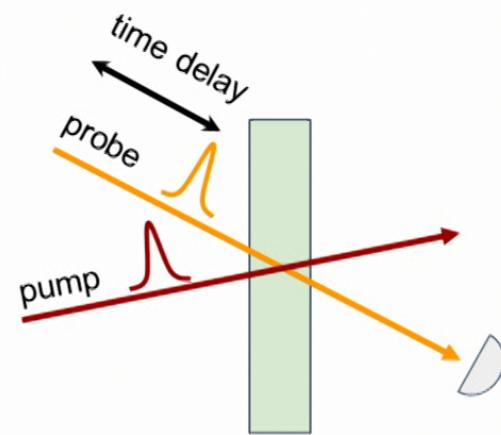


The characteristics of the stacking domains based on an analysis of 56 samples were found to be similar to those for trilayer graphene. In particular, the ratio of the area of ABAB to ABCA stacking was 85:15. The similarity of the domains in tetralayer and trilayer graphene confirms the common origin of the different stacking sequences, namely, the stacking order of the kish graphite, which remains unchanged during the exfoliation process.

C. Lui, ... T. Heinz, Nano Lett. 2010

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Optically probing superconductivity



Pump: 900 nm; Probe 800 nm

Summary

- 3R MoS₂ has a spontaneous polarization induced by an asymmetric interlayer coupling
- It leads to an ultrafast photovoltaic effect with a high quantum efficiency
- A power law distribution is observed in the polarization domain size which is visualized by EFM/KPFM
- We attribute the power law distribution to an avalanche of interlayer sliding during exfoliation in the presence of a network of pinning centers.

Acknowledgment

Dongyang Yang, Jing Liang, Jingda Wu, Yunhuan Xiao, Jerry I. Dadap
Benjamin Zhou, Marcel Franz, Joerg Rottler
Yoshihiro Iwasa, Toshiya Ideue, (UTokyo) Kenji Watanabe, Takashi Taniguchi (NIMS)



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