Title: Stacking Induced Spontaneous Polarization in Rhombohedral MoS2

Speakers: Ziliang Ye

Collection: Quantum Matter Workshop

Date: November 14, 2022 - 10:15 AM

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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 MoS_2

Quantum Matter Workshop

Perimeter Institute, Nov. 2022

Ziliang Ye

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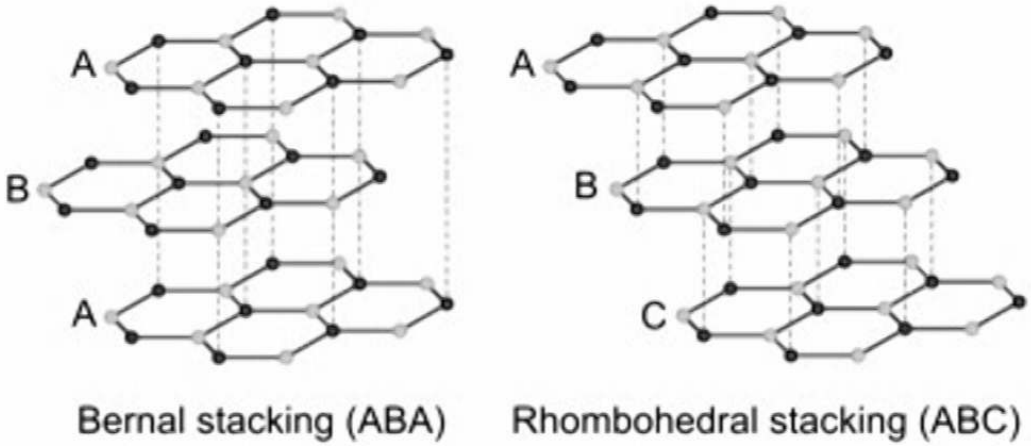
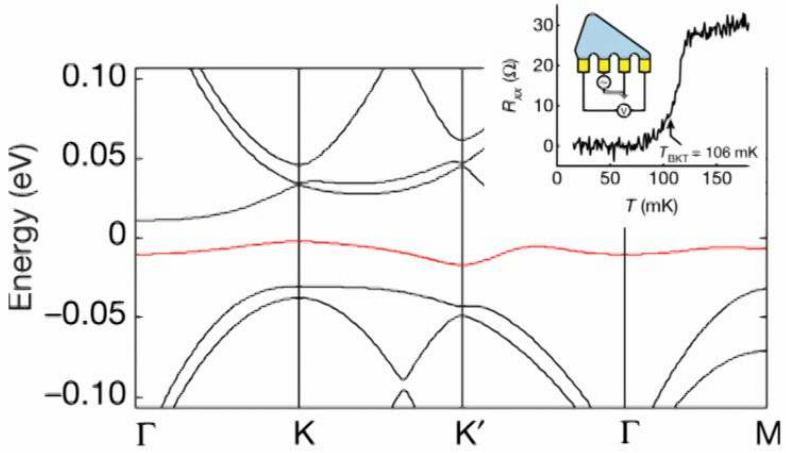
DEPARTMENT OF PHYSICS AND ASTRONOMY
QUANTUM MATTER INSTITUTE

Unconventional superconductivity in rhombohedral graphite



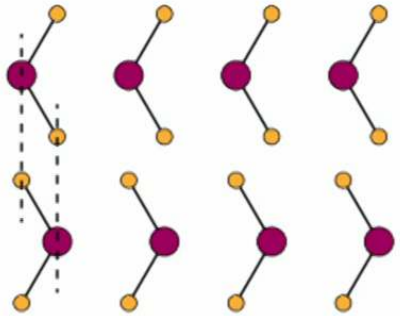
Rhombohedral graphite

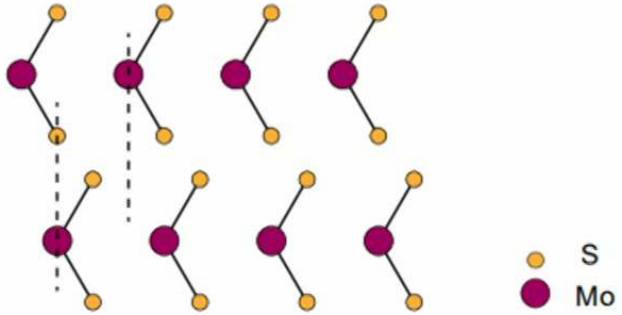


Superconductivity in ABC trilayer graphene

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

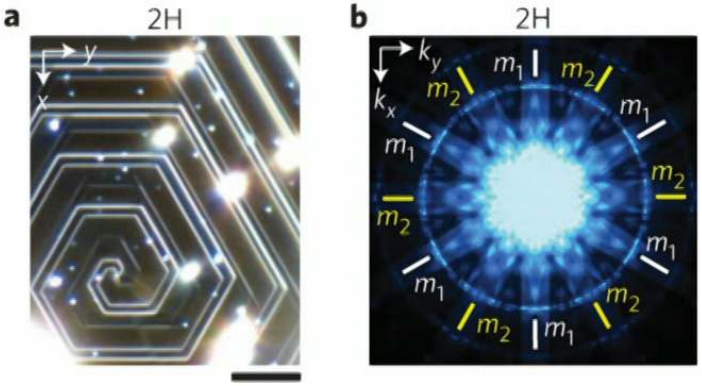
Rhombohedral MoS_2

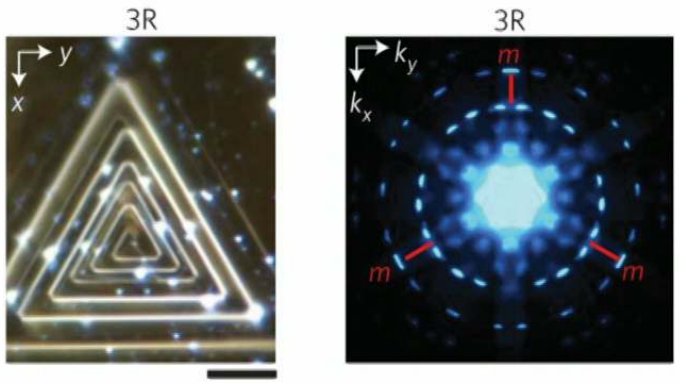




hexagonal stacking

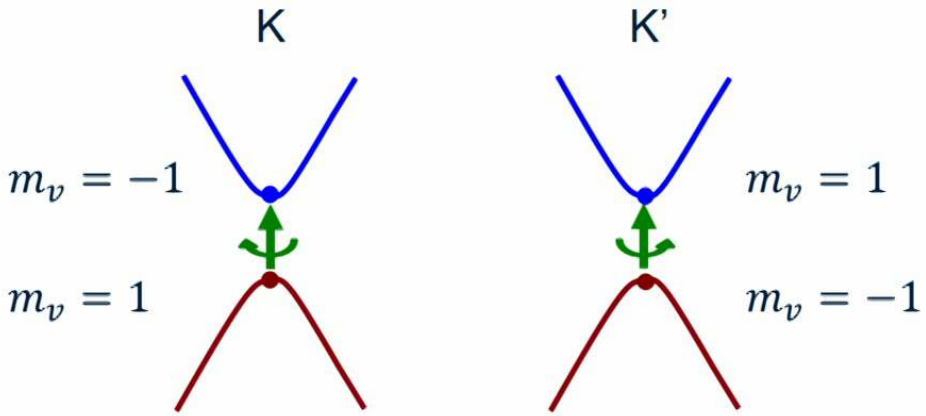
rhombohedral stacking





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

Valley selection rule

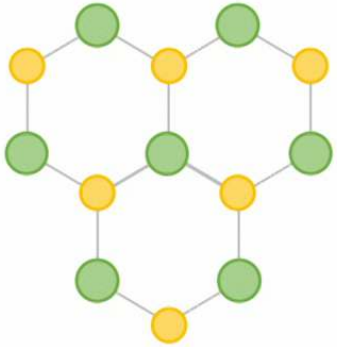


$$H = \hbar v_F \hat{\sigma} \cdot \vec{q} + \Delta \sigma_z$$

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

Layer dependent Berry phase winding

Top



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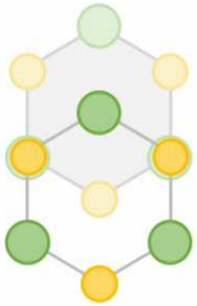
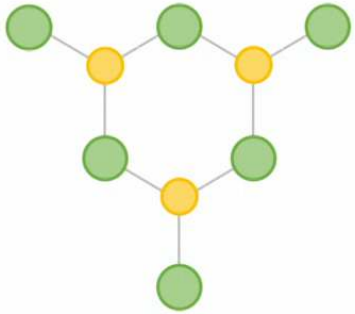
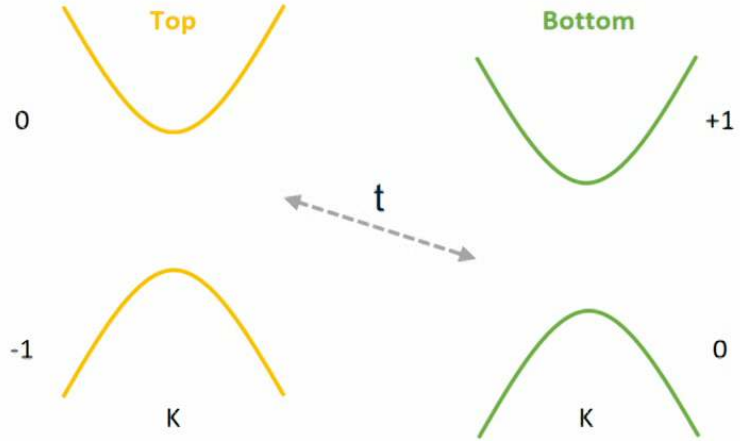
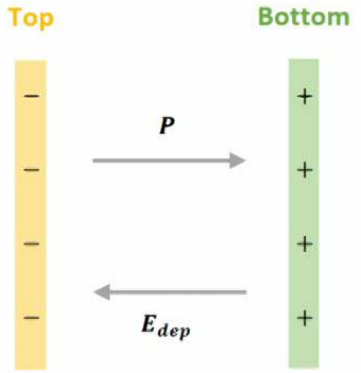


Bottom



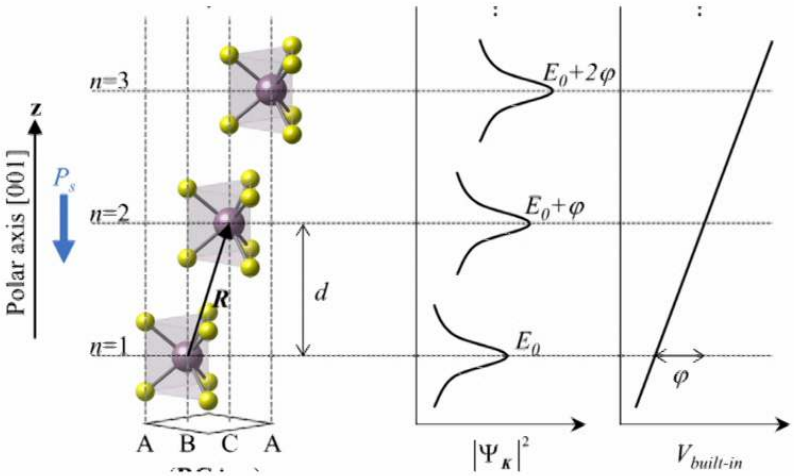
Asymmetric interlayer coupling and spontaneous polarization

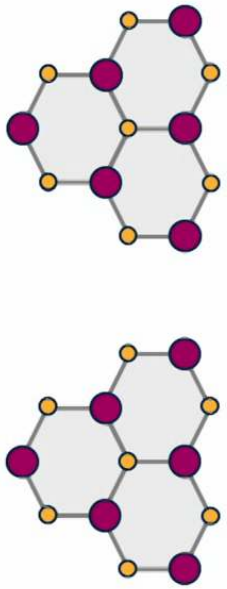




Interlayer potential $\phi_0 = \frac{P}{\varepsilon_0 \varepsilon_m} d_0$

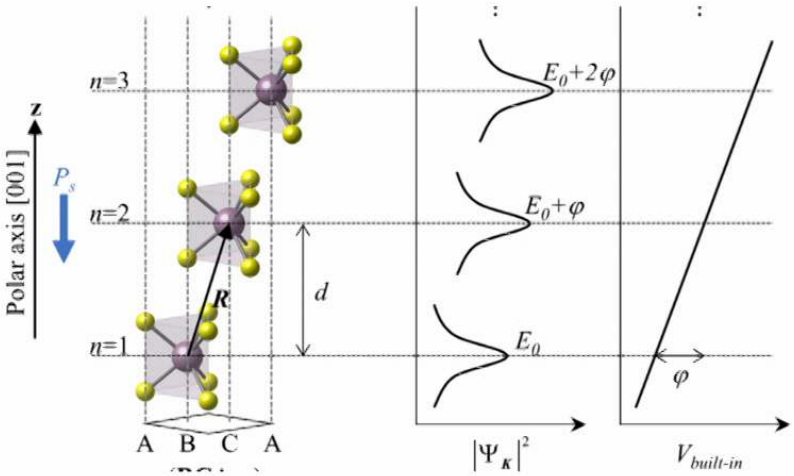
First-principle calculations

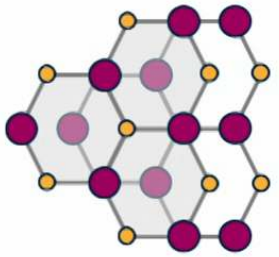




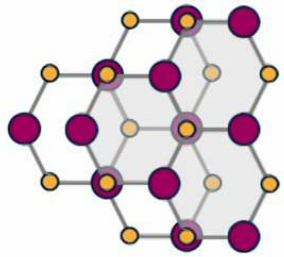
J. Park, et al, J. Phys. Condens. Matter 31, 315502 (2019)
Y. Wang, et al, PRB 95, 115429 (2017)
L. Li, et al, ACS Nano 11, 6382 (2017)

First-principle calculations





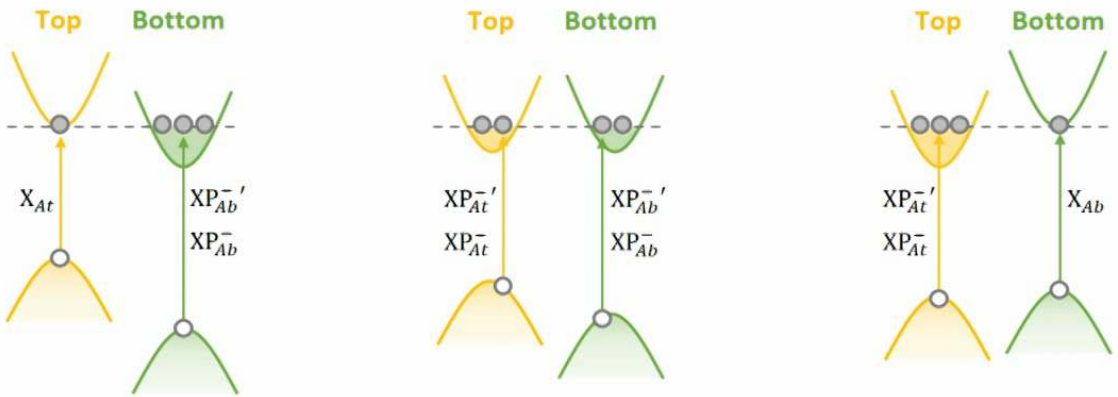
AB

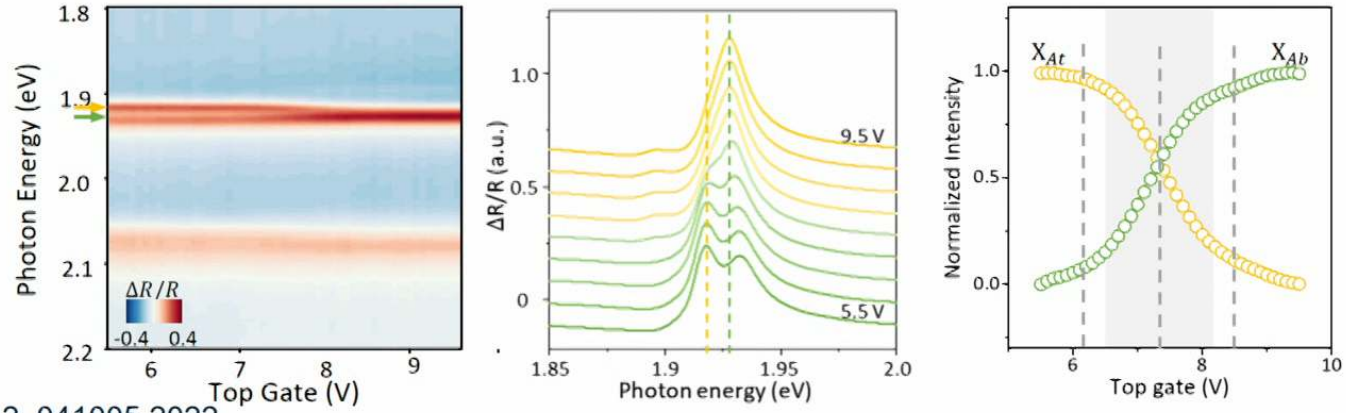


BA

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

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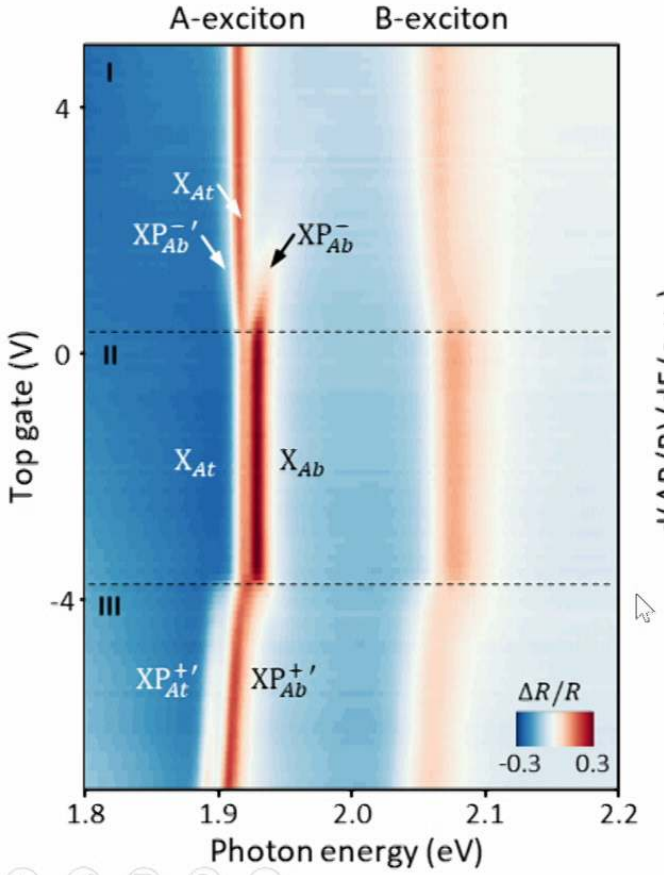
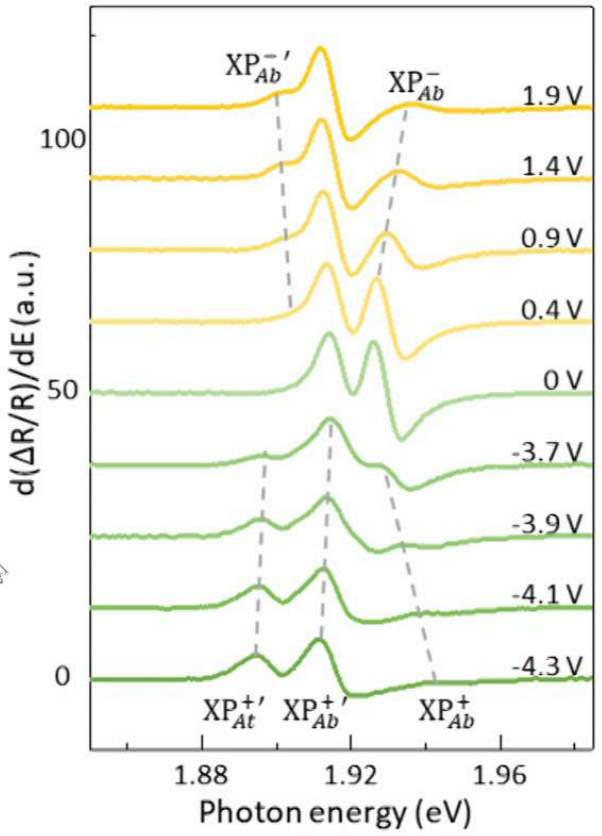
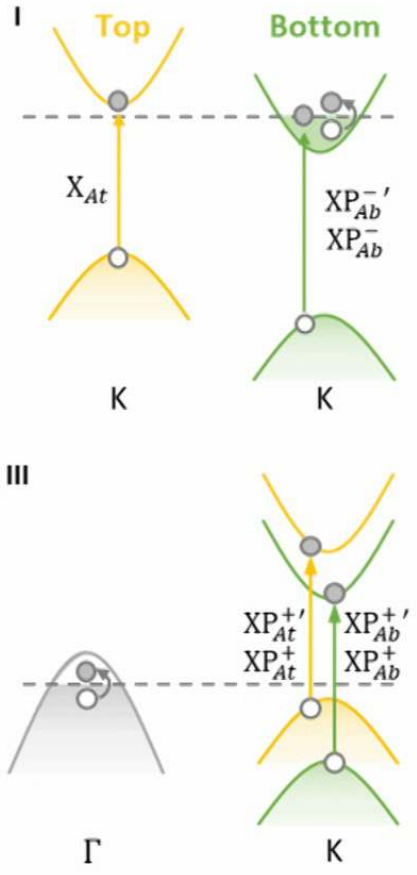
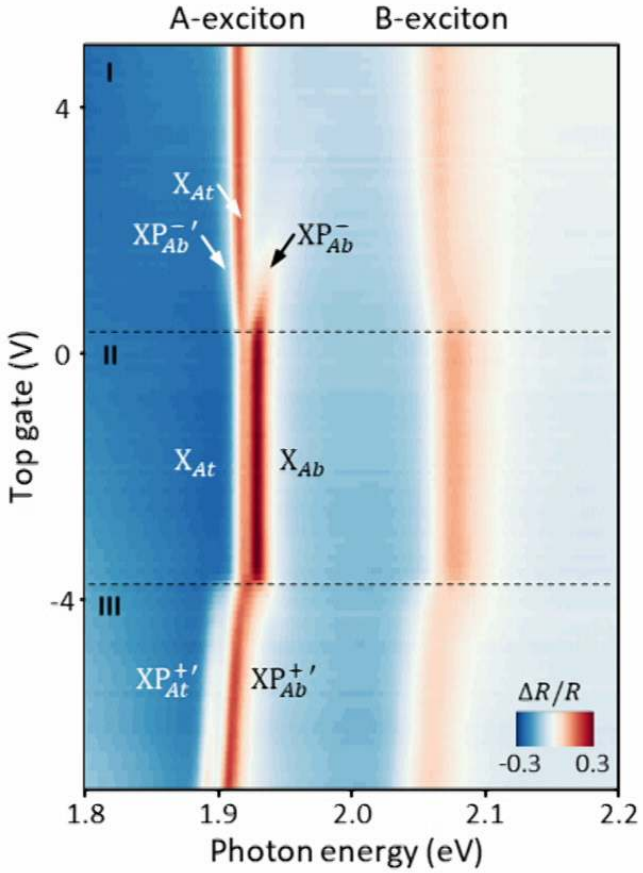
Doping dependence

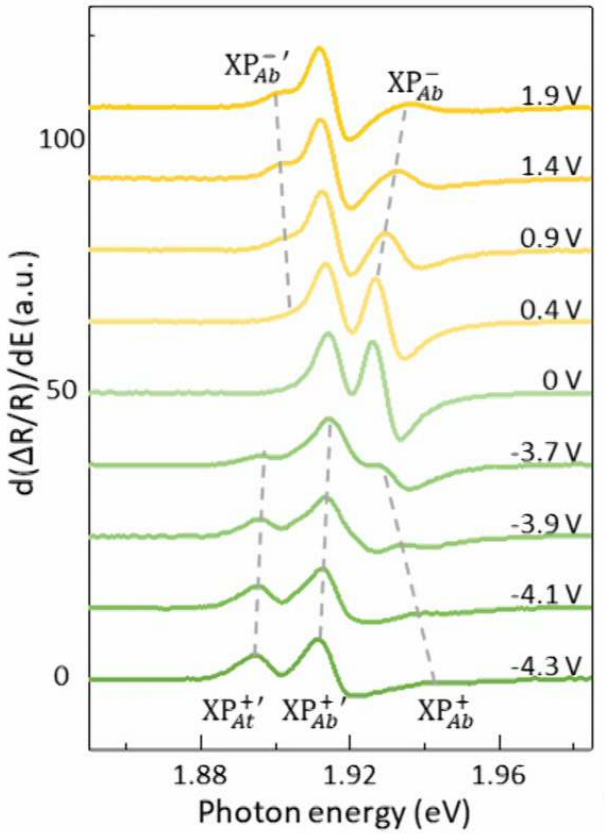


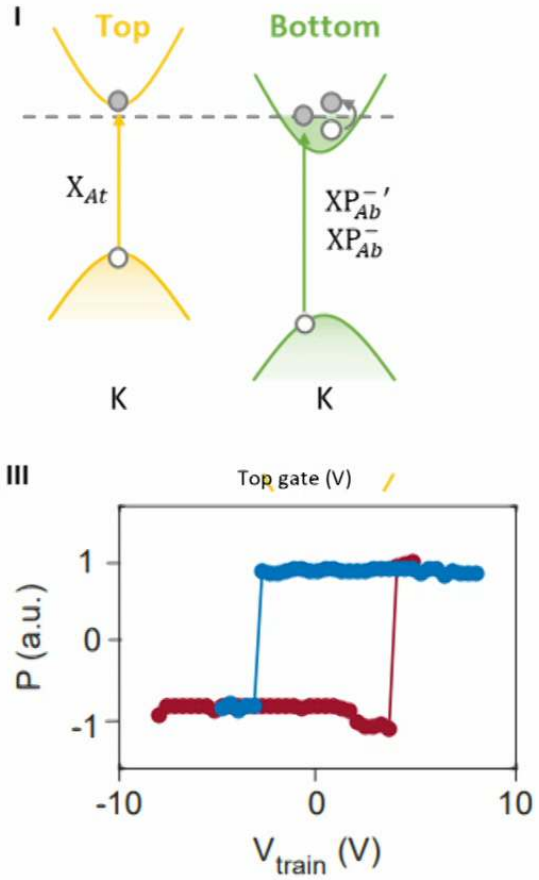




Doping dependence







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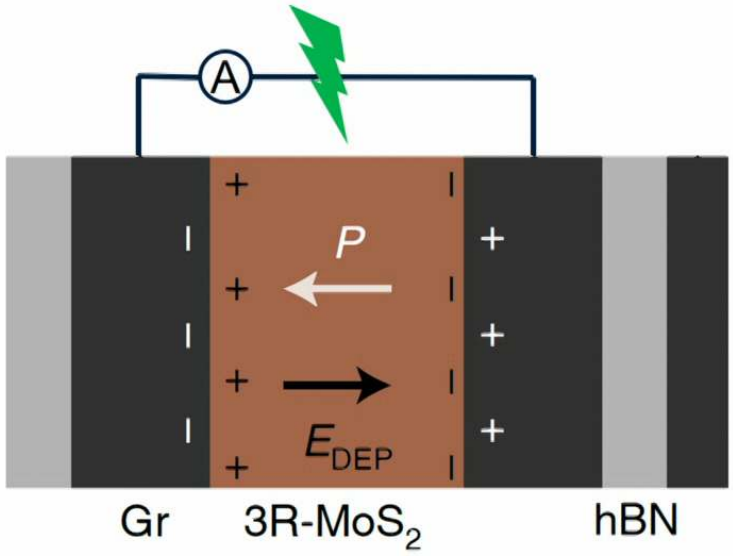
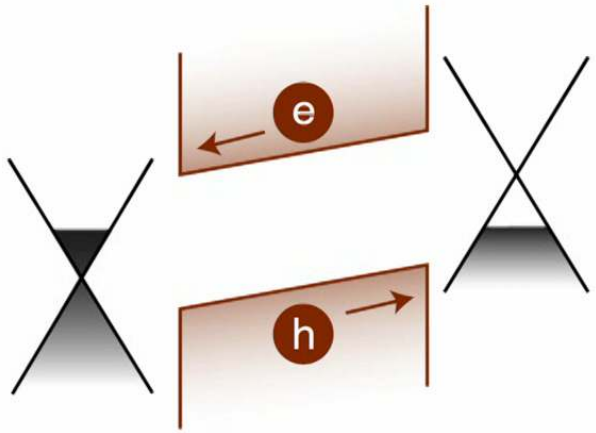
Photovoltaic Device

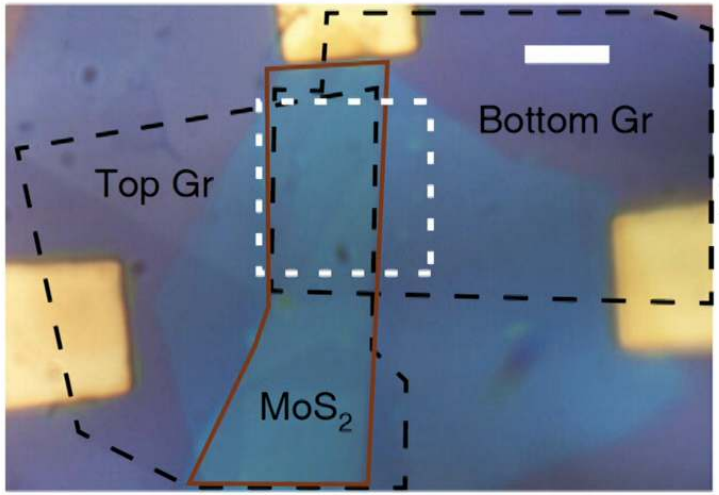


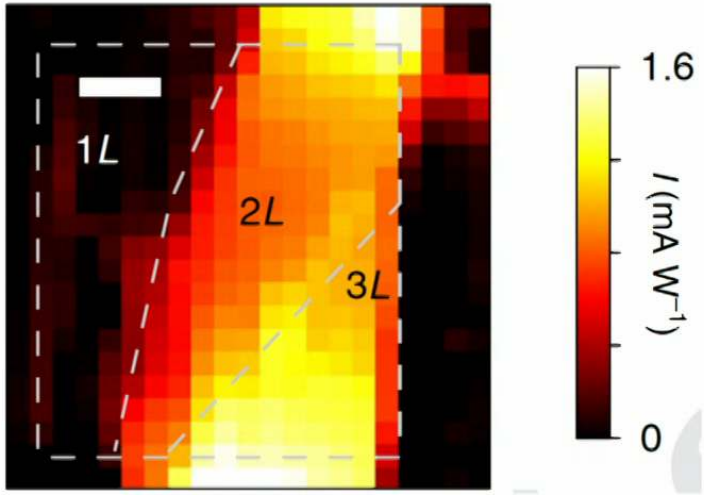


Graphene contacts can preserve 95% of the E_{dep}

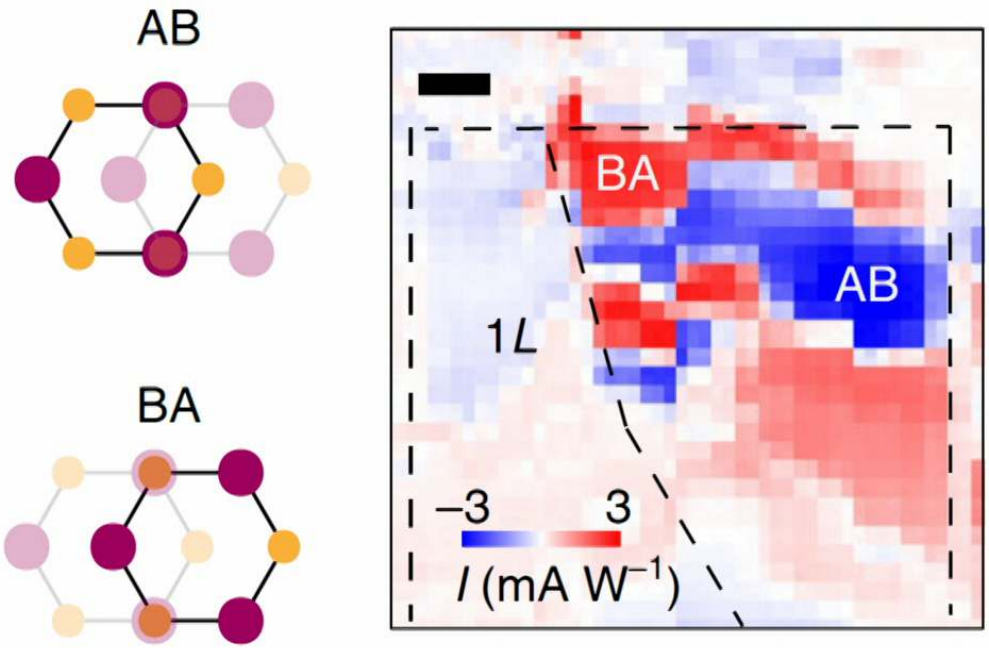
D. Yang, et al, Nat. Photonics, 16, 469 (2022)

Photocurrent map

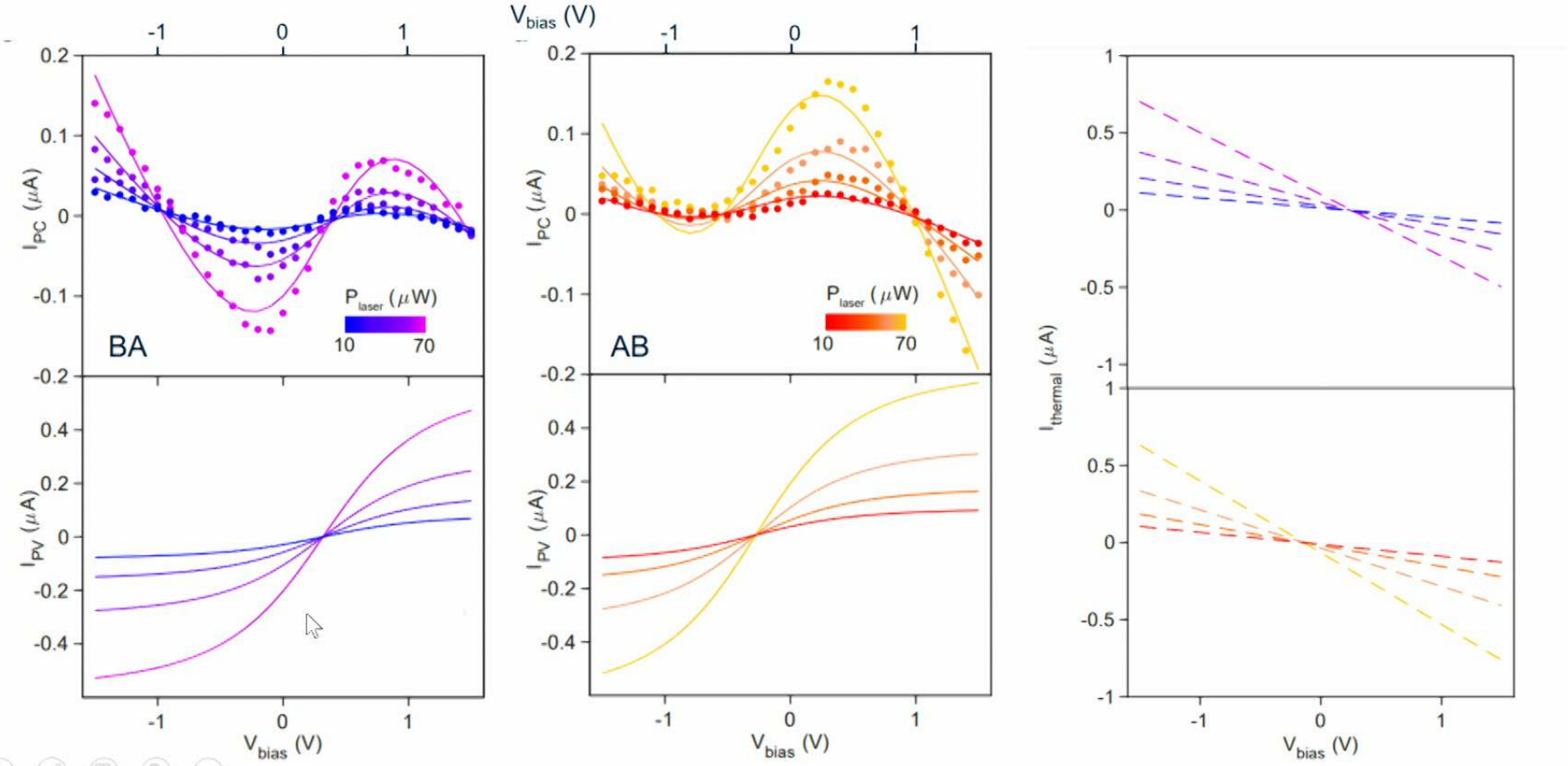




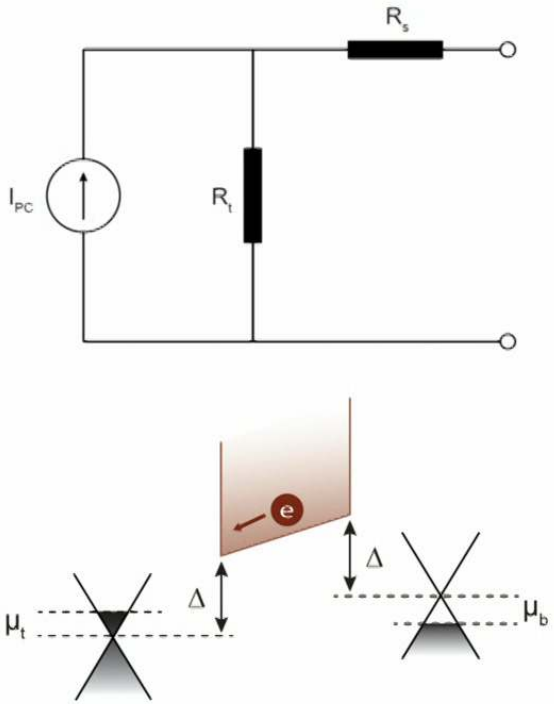
Mixed domain



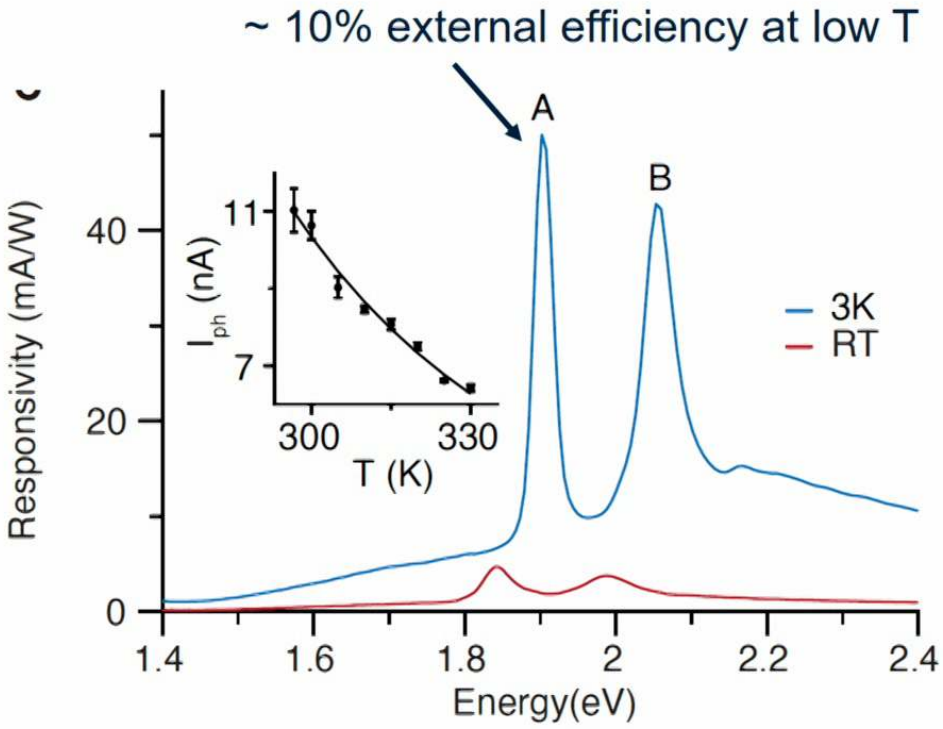
Thermal contributions $I_{PC} = I_{PV} + I_{bolo} + I_{PTE}$



Shunt resistance model

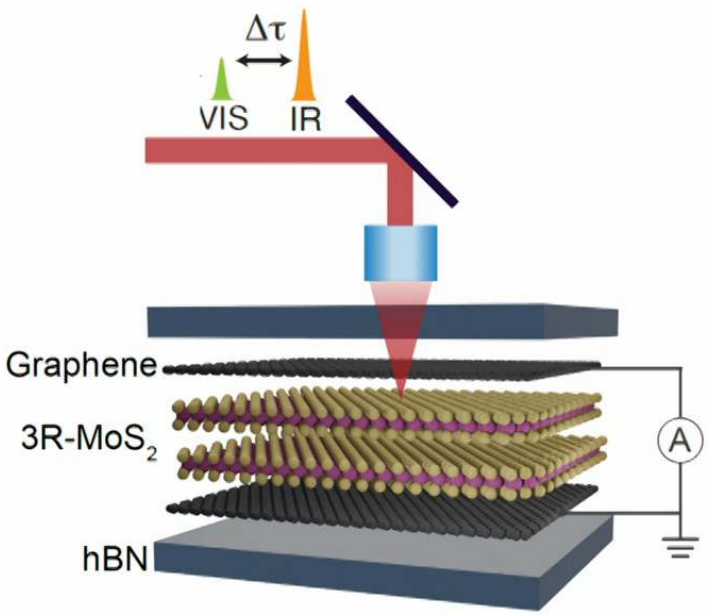


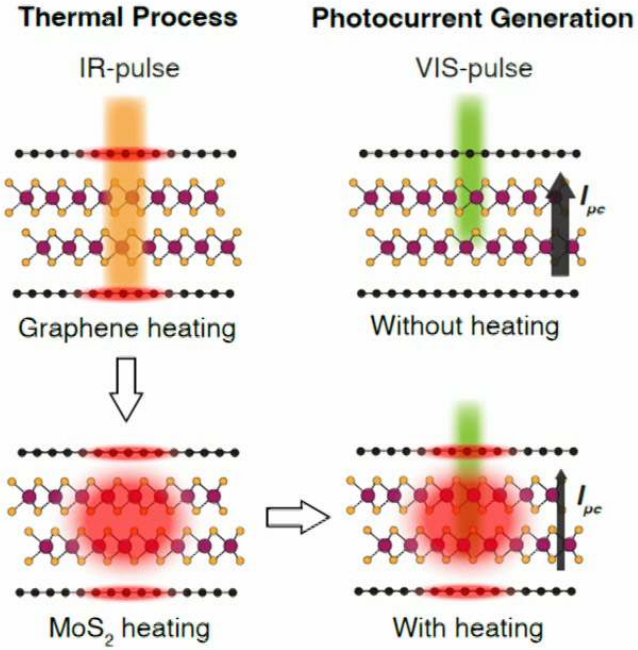
$$\sigma = 4A\frac{e^2}{h}\frac{1}{\pi^2(hv_f)^4}\int_{\Delta}^{+\infty}(E+\mu_t)(E+\mu_b)\frac{1}{k_BT}\exp(-\frac{E}{k_BT})dE$$

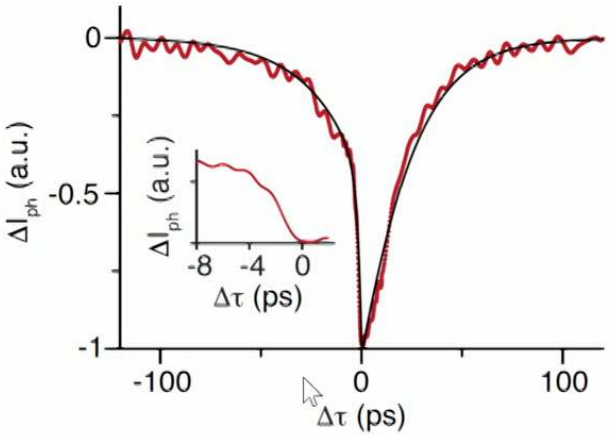


J. Wu, et al, accepted by Science Advances

Ultrafast photoresponse



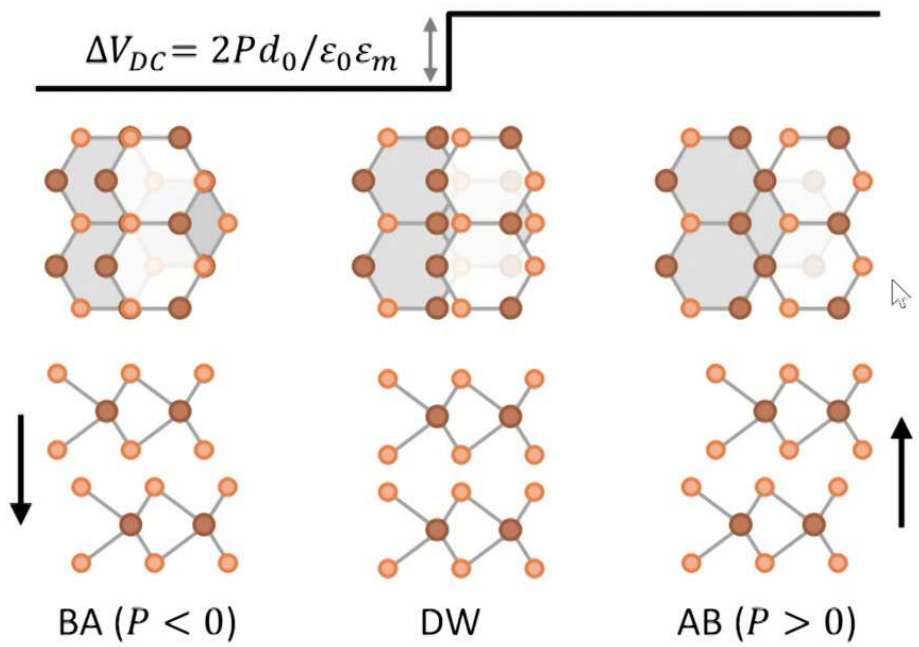


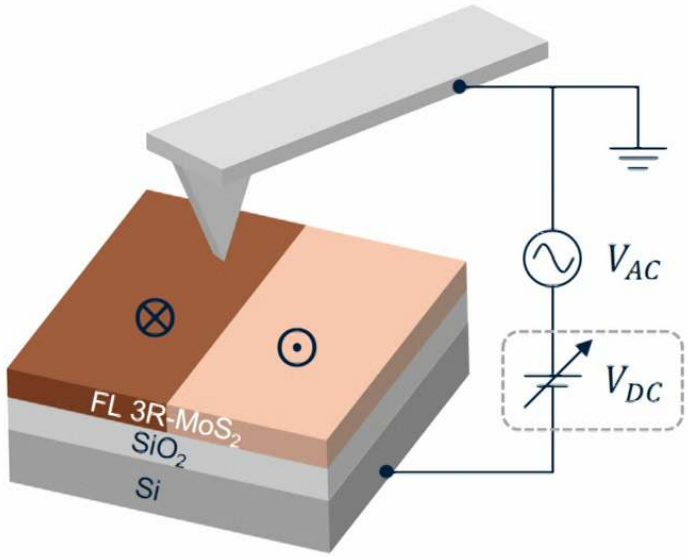


The fast rise indicates the photocurrent is as fast as 2 ps

J. Wu, et al, accepted by Science Advances

Probing the stacking order with scanning probe microscopy





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

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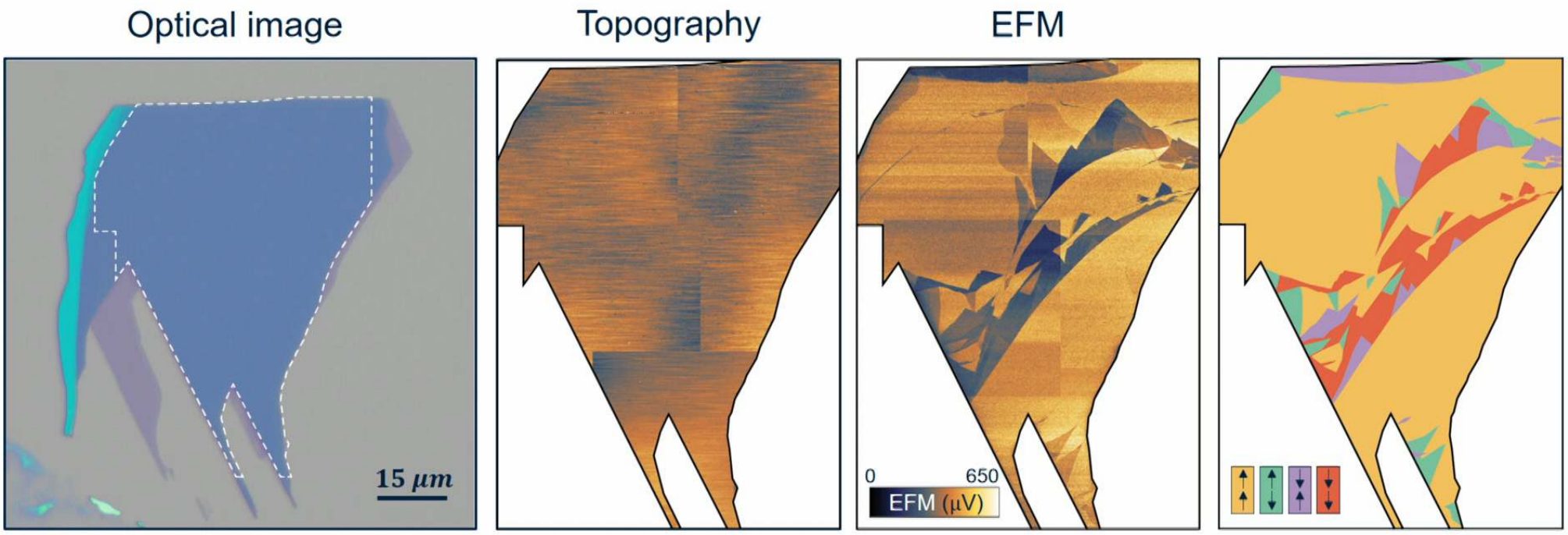
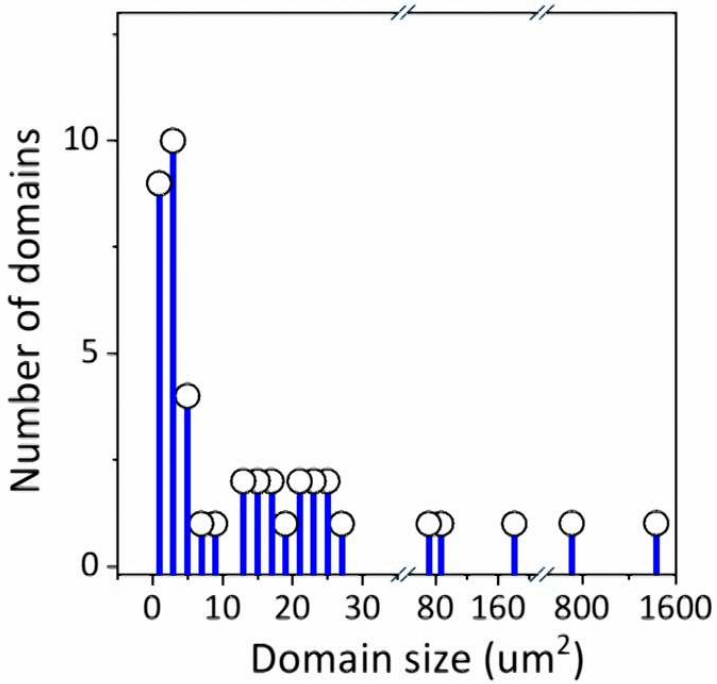
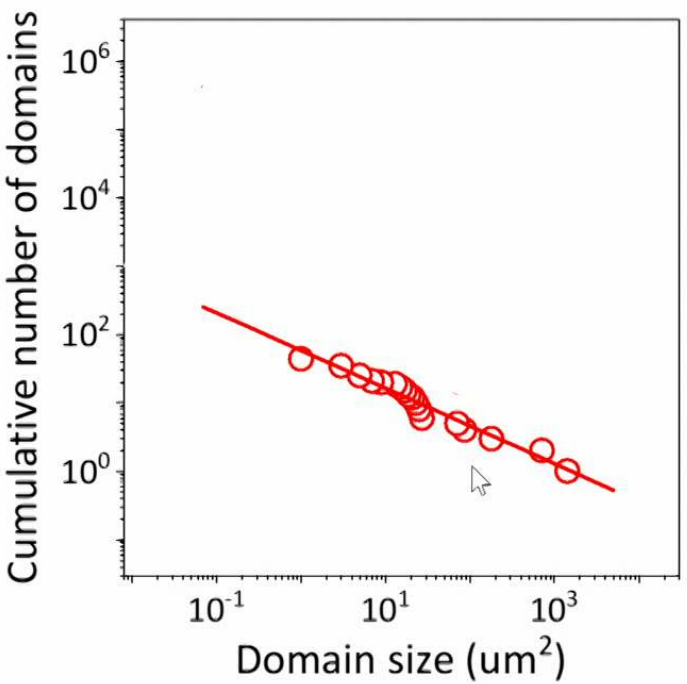
Domains in a trilayer sample

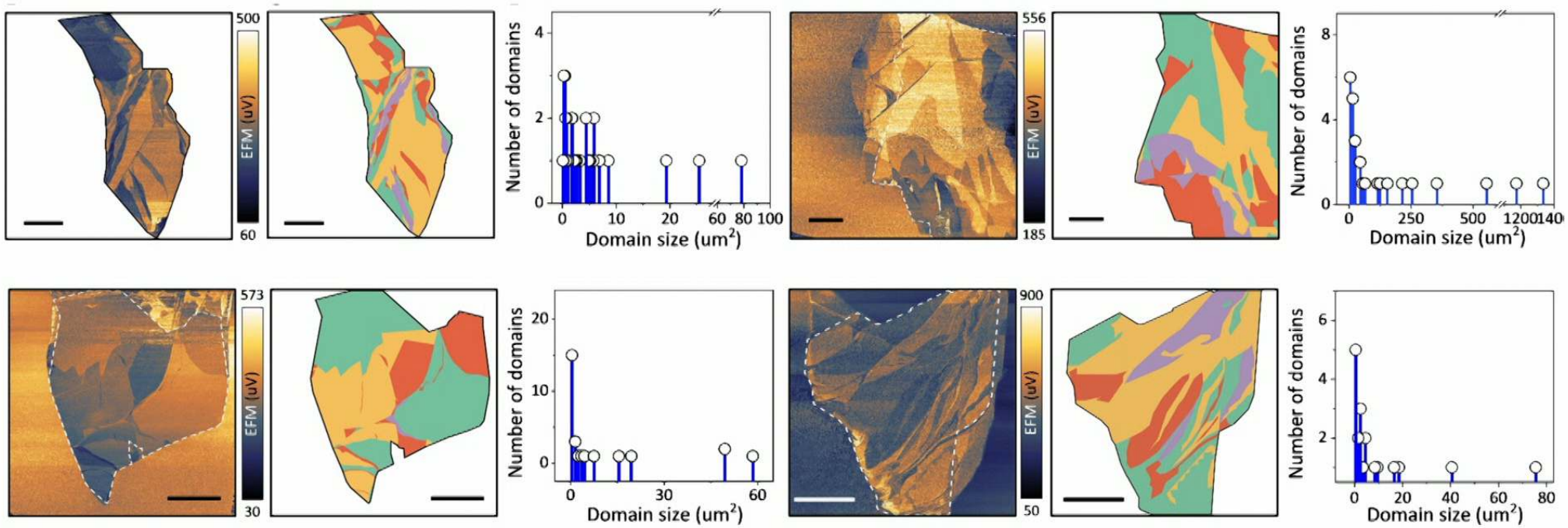


Domain size distribution

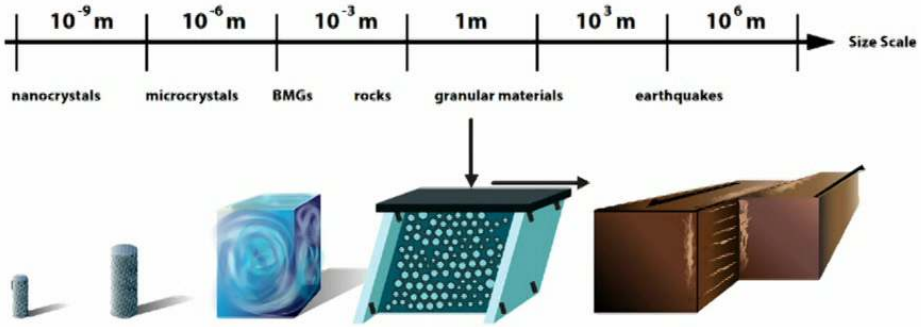


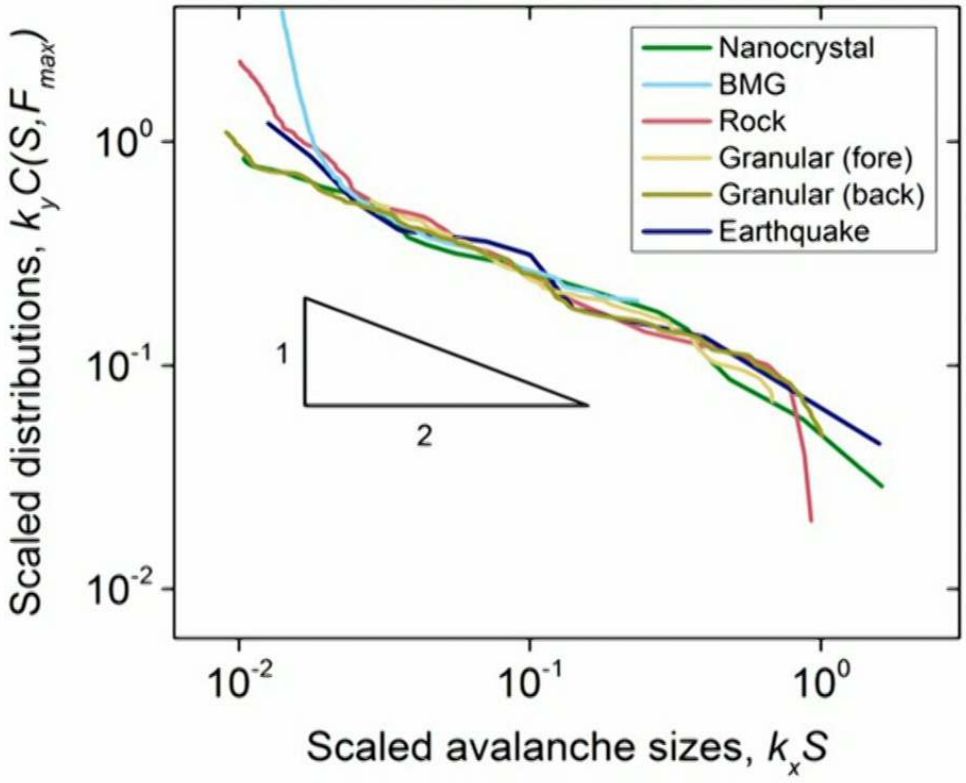


More data


500
EFM (uV)
60
Number of domains
Domain size (um²)
556
185
573
30
900
50

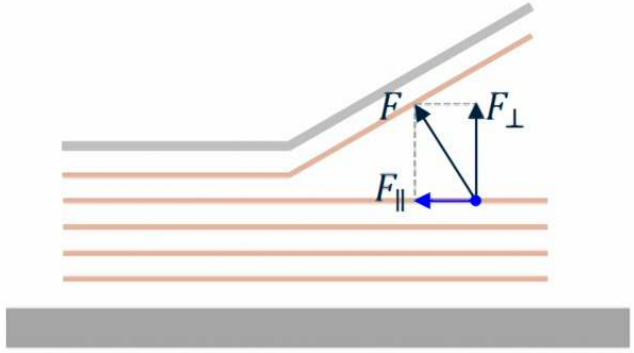
Universal slip size distribution under shear strain



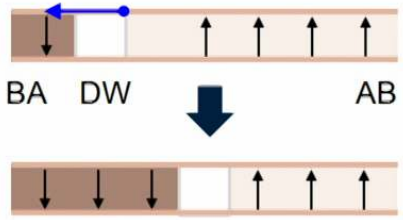


"Universal Quake Statistics: From Compressed Nanocrystals to Earthquakes" J. Uhl… K. Dahmen, Sci. Rep. 2015

Sliding induced by shear strain

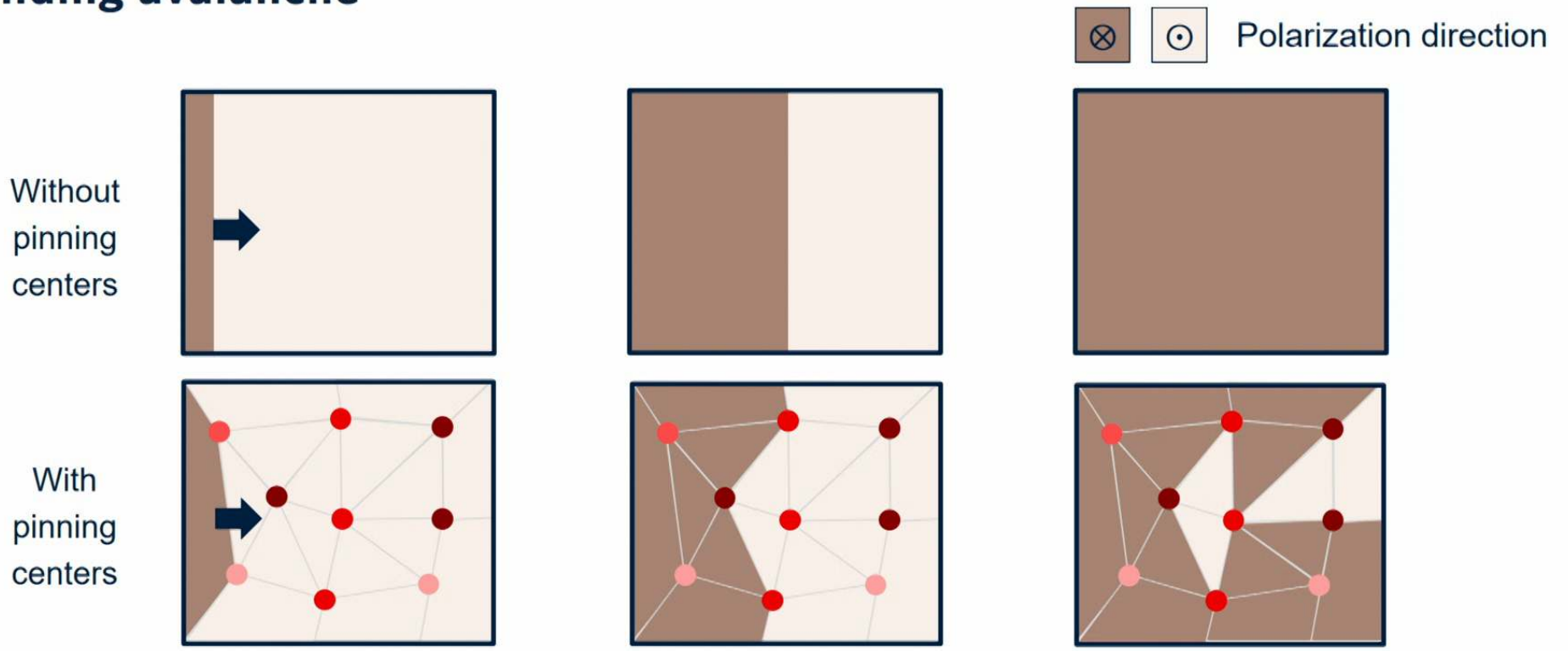


Shear strain during exfoliation



Domain wall movement

Sliding avalanche



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

Daniel Fisher, Phys. Rep. 1998

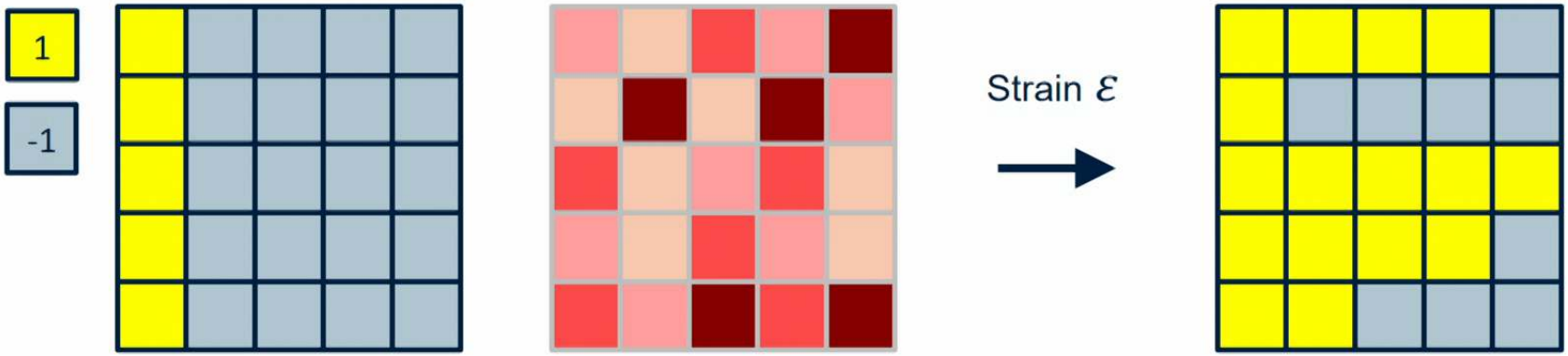
Numerical simulation based on random field Ising model

Initial states

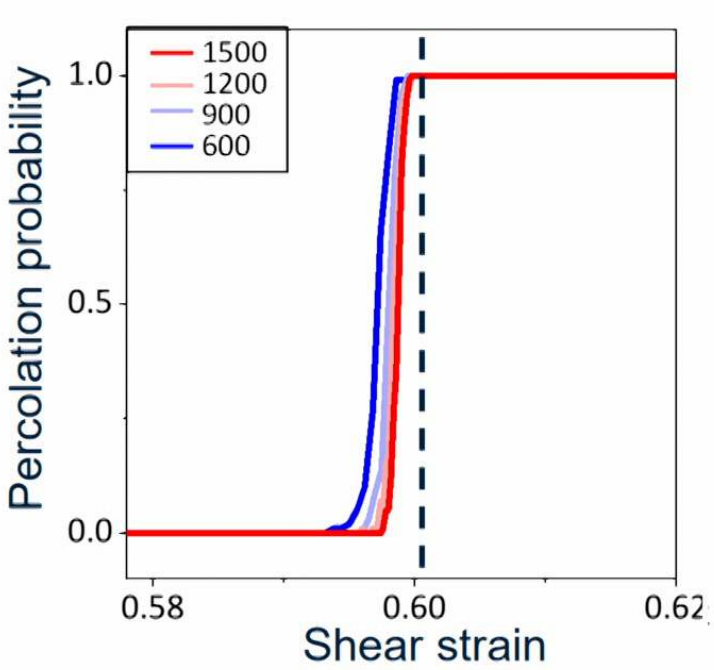
Random pinning potential p_i with variance σ

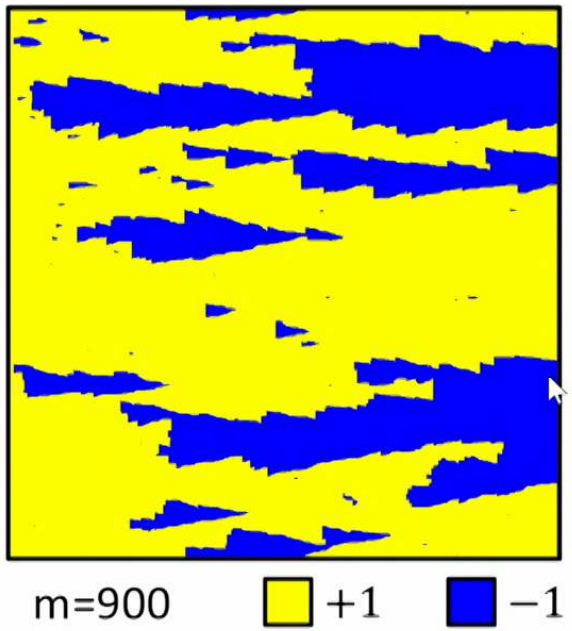
Flipping criterion:

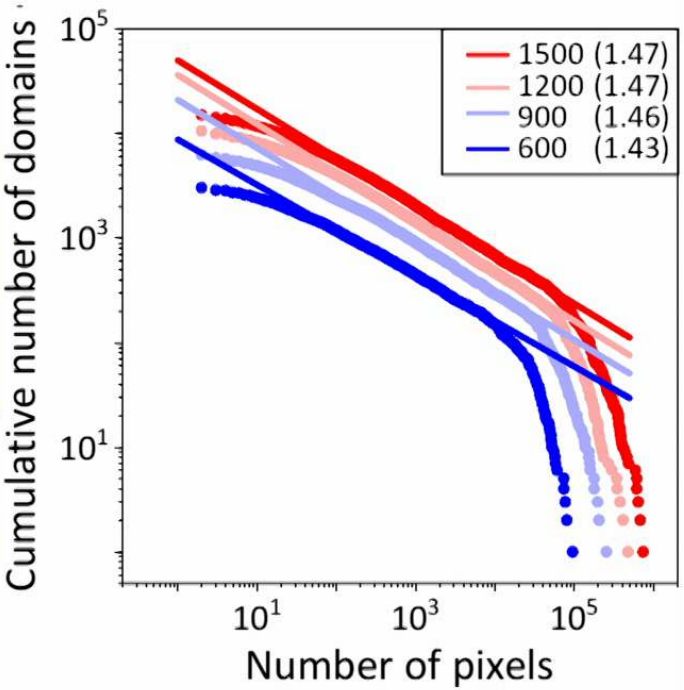
$$\varepsilon > I_i = J \sum_j s_i s_j + p_i$$



Percolation behavior

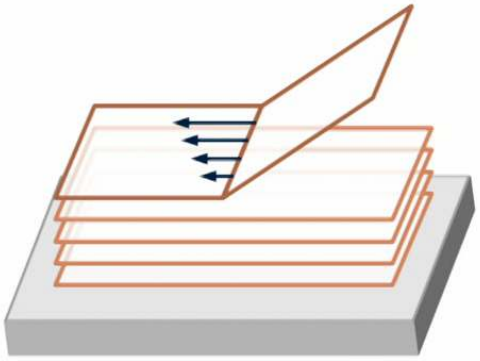




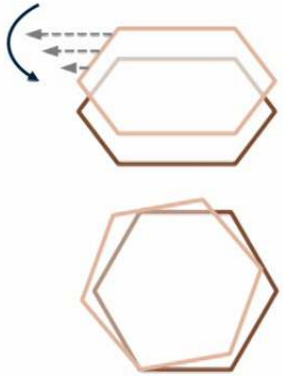


The critical field is slightly dependent on σ/J and simulation size.

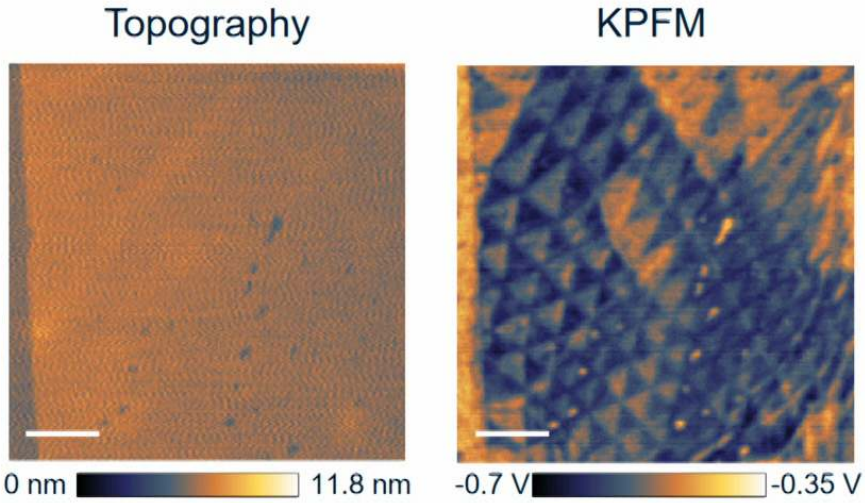
Interlayer twist



Inhomogeneous shear force

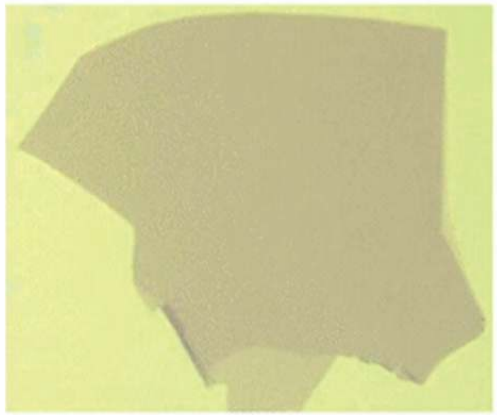


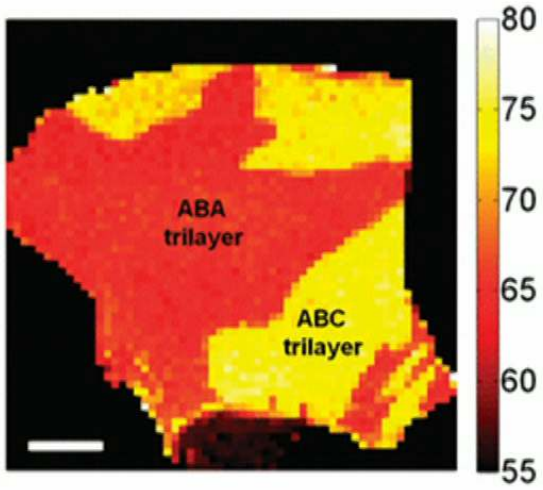
Interlayer twist



Discussion

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

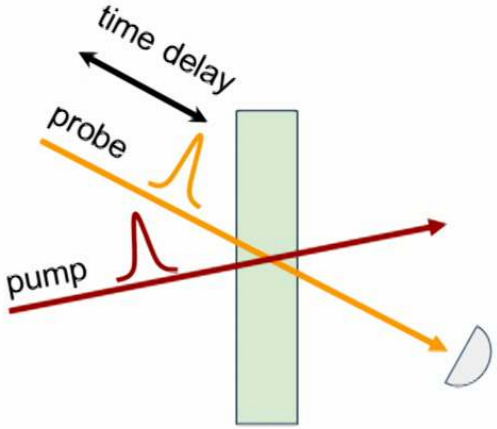




The characteristics of the stacking domains based on an analysis of 56 samples were found to be similar to those for trilayer graphene. In particular, the ratio of the area of ABAB to ABCA stacking was 85:15. The similarity of the domains in tetralayer and trilayer graphene confirms the common origin 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

Optically probing superconductivity



Pump: 900 nm; Probe 800 nm

Summary

- 3R MoS_2 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.

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