Moire superlattice in van der Waals interface: Experimental opportunities and challenges

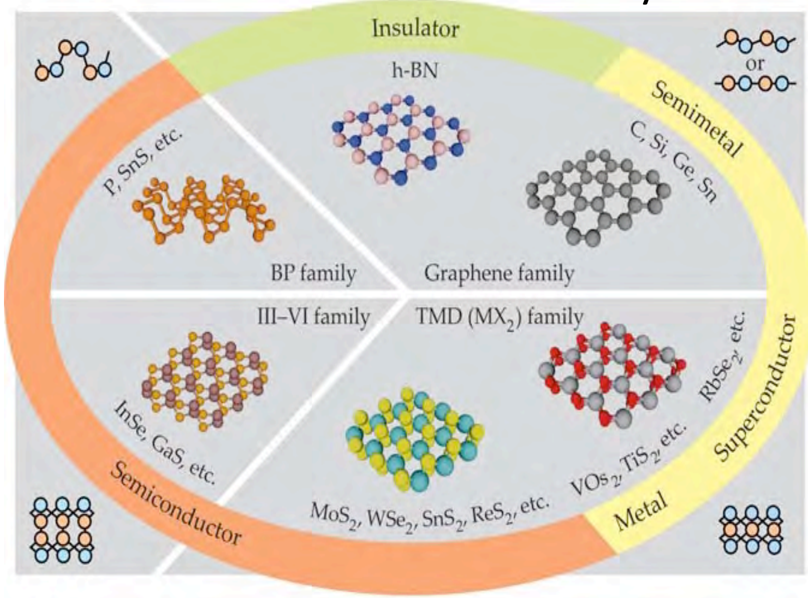
Philip Kim

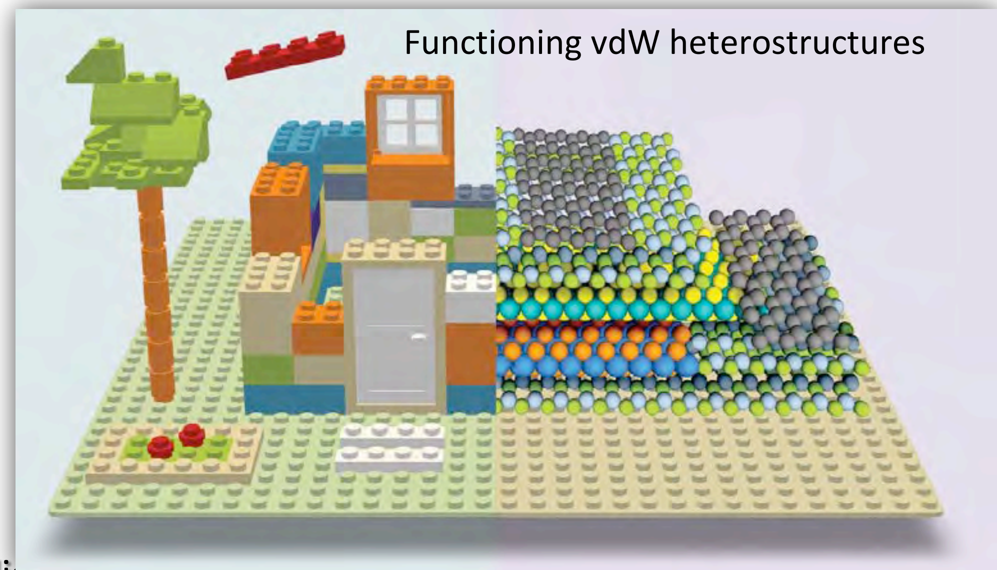
Department of Physics, Harvard University

Assembling van der Waals Materials

2D van der Waals Materials Family

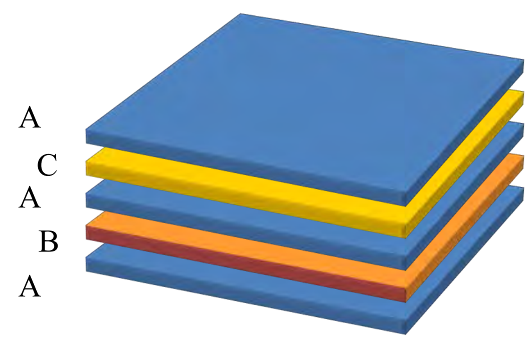
Ajayan, Kim and Banerjee, Physics Today (2016)



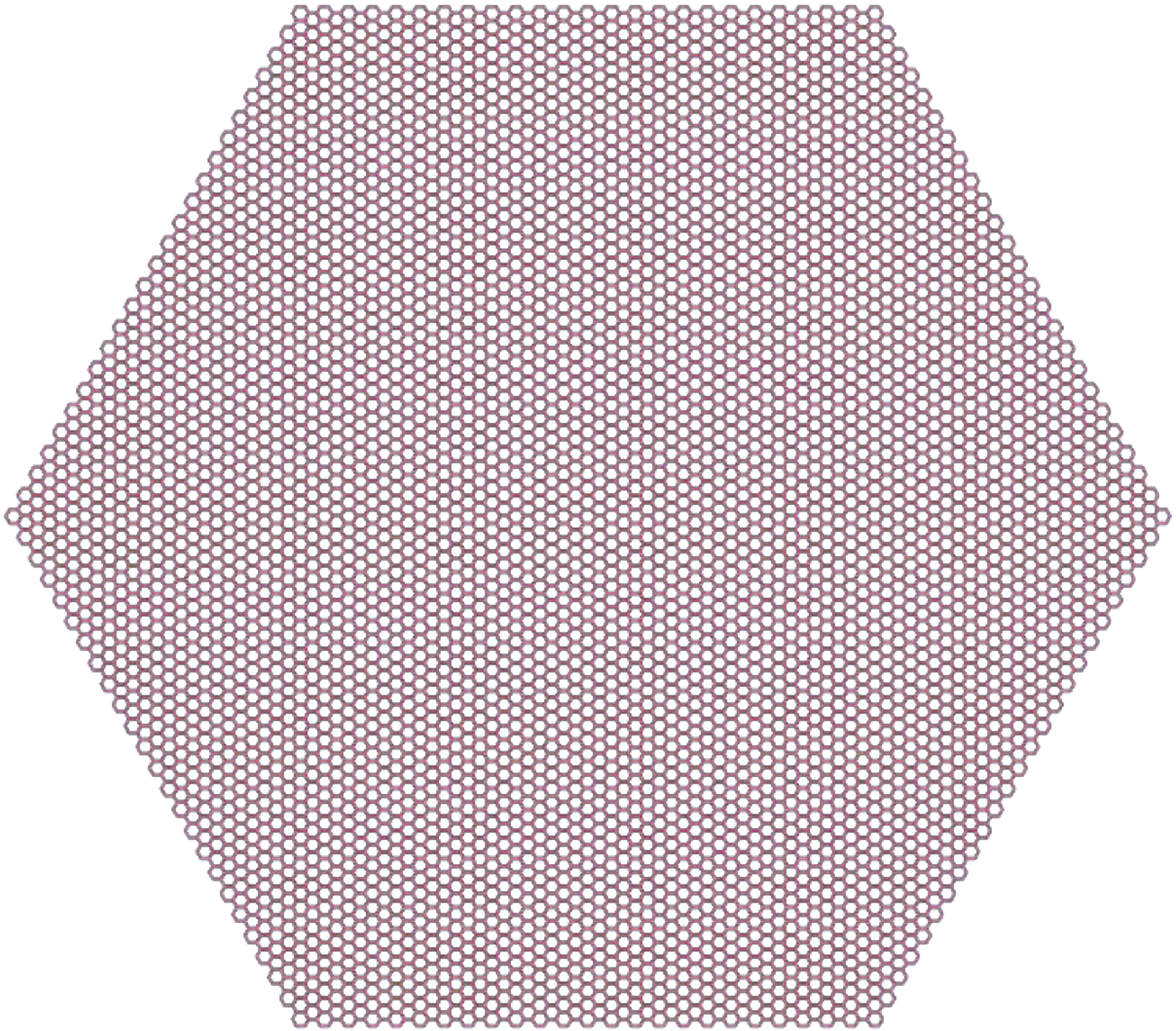


Experimentally popular vdW Materials (partial list)

- Semiconducting materials: WSe_2, $MoSe_2$, MoS_2, WS_2, BP…
- Complex-metallic compounds : $TaSe_2$, TaS_2, …
- Magnetic materials: Fe-TaS_2, $CrSiTe_3$, CrI_3…
- Superconducting: $NbSe_2$, $Bi_2Sr_2CaCu_2O_{8-x}$,…
- Topological Insulator/Wyle SM: Bi_2Se_3, $MoTe_2$



Moire Superlattice Engineering in van der Waals Interface

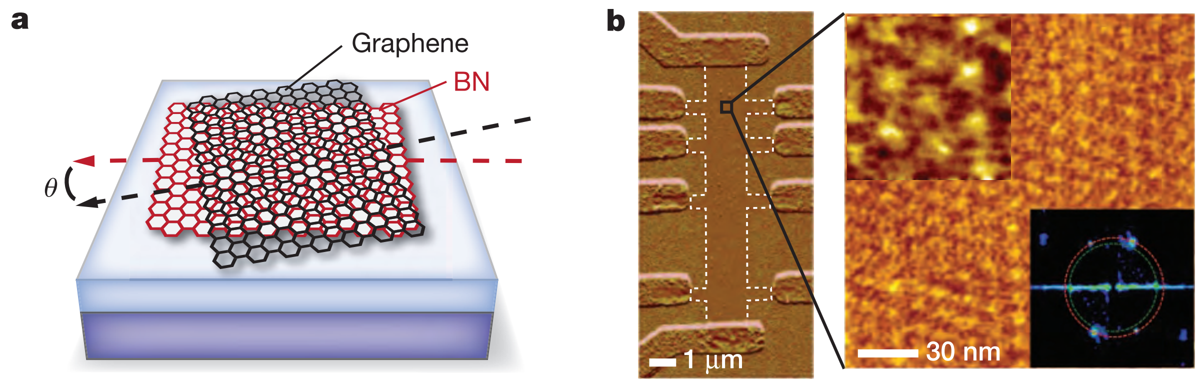


Twisted van der Waal interface of homo & hetero structure

Moire Superlattice Engineering in van der Waals Interface

Dean *et al*,, Nature (2013)

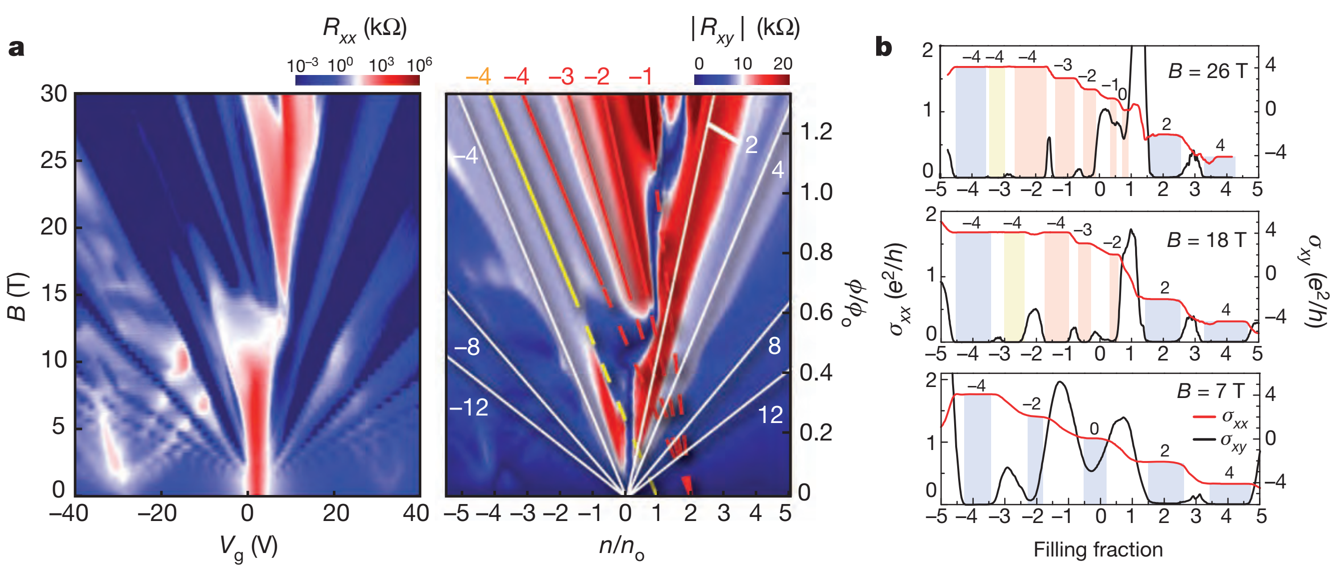
Graphene on hBN: moire superlattice



Moire wavelength:

$$\lambda = \frac{(1+\delta)a}{\sqrt{2(1+\delta)(1-\cos(\phi))+\delta^2}}$$

Hofstadter's butterfly spectrum and Fractal quantum Hall effect



See also

Ponomarenko *et al*,, Nature (2013)

Hunt *et al*,, Science (2013)

Correlated Quantum State in Twisted Graphene Bilayer

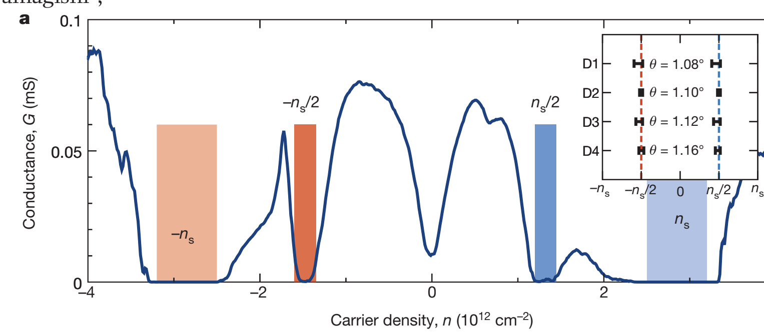
80 | NATURE | VOL 556 | 5 APRIL 2018

LETTER

doi:10.1038/nature26154

Correlated insulator behaviour at half-filling in magic-angle graphene superlattices

Yuan Cao[1], Valla Fatemi[1], Ahmet Demir[1], Shiang Fang[2], Spencer L. Tomarken[1], Jason Y. Luo[1], Javier D. Sanchez-Yamagishi[2], Kenji Watanabe[3], Takashi Taniguchi[3], Efthimios Kaxiras[2,4], Ray C. Ashoori[1] & Pablo Jarillo-Herrero[1]



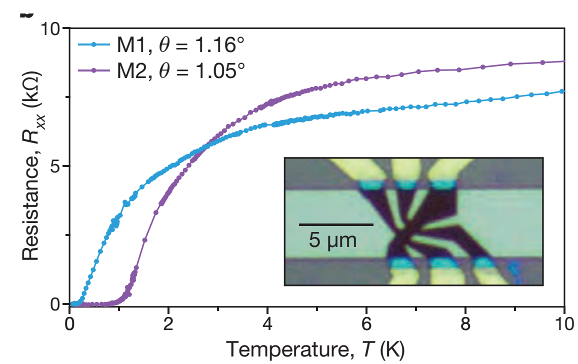
5 APRIL 2018 | VOL 556 | NATURE | 43

ARTICLE

doi:10.1038/nature26160

Unconventional superconductivity in magic-angle graphene superlattices

Yuan Cao[1], Valla Fatemi[1], Shiang Fang[2], Kenji Watanabe[3], Takashi Taniguchi[3], Efthimios Kaxiras[2,4] & Pablo Jarillo-Herrero[1]



Twistronics: 2D materials beyond Legoland

Correlated insulator

Cao et al., Nature 556, 80–84 (2018).
Burg et al., PRL 123, 197702 (2019).

Unconventional superconductivity

Cao et al., Nature 556, 43–50 (2018).
Yankowitz el al, Science 363, 1059–1064 (2019).
Lu et al, Nature 574, 653–657 (2019).

Magnetism and Quantum Anomalous Hall Effect

Sharpe et al., Science 365, 605–608 (2019).
Serlin et al., arXiv:1907.00261 (2019).

Trilayers double bilayers

Chen et al. Nature Physics 15, 237–241 (2019).
Chen et al., Nature 572, 215219 (2019).She et al., ArXiv 2019

Double bilayers

Shen et al., arXiv:1903.06952 (2019).
Liu et al, arXiv:1903.08130 (2019).
Cao et al., arXiv:1903.08596 (2019).
Adak et al., arXiv:2001.09916 (2020)

TMDC/TMDC

Tang et al. arXiv:1910.08673 (2019).
Regan et al., arXiv:1910.09047 (2019).
Wang et al., arXiv:1910.12147 (2019).

***

STM

Jiang et al., Nature 572 91-95 (2019).
Kerelsky et al., Nature 572 95-100 (2019).
Xie et al., Nature 572 101-105 (2019).

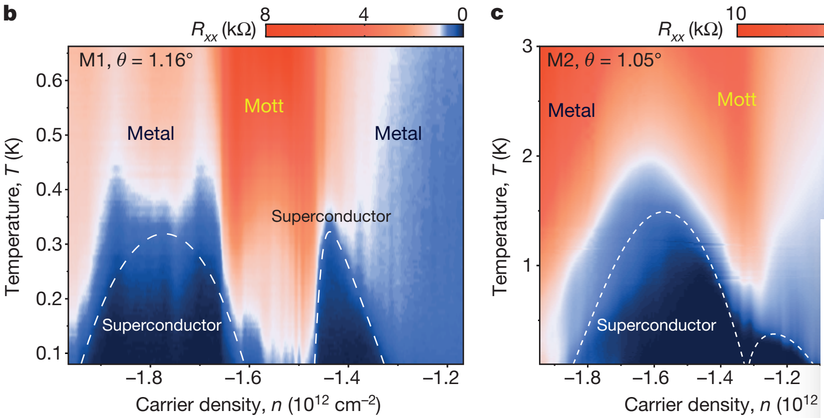
Scanning Probes

Cao et al., Nature 556, 43–50 (2018).
Yankowitz el al, Science 363, 1059–1064 (2019).
Lu et al, Nature 574, 653–657 (2019).

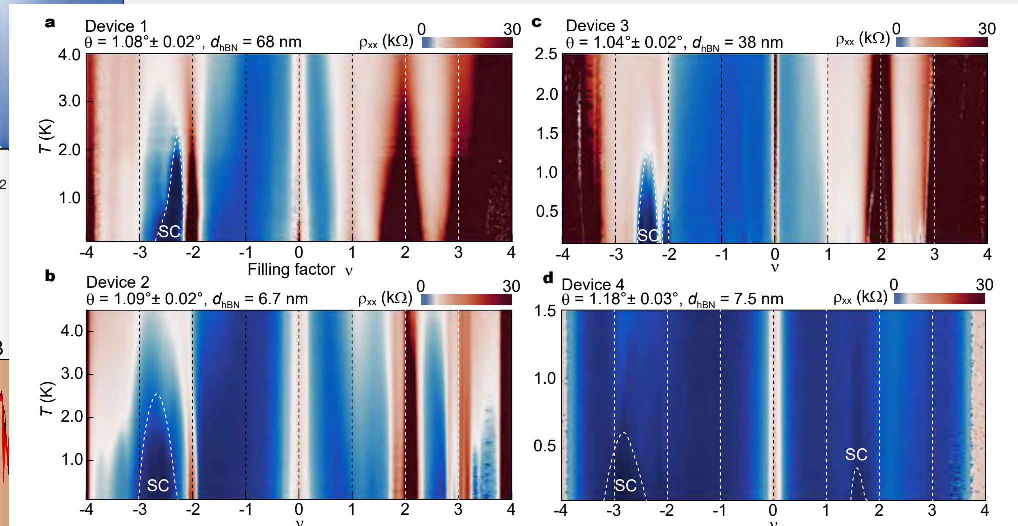
Optical Spectroscopy (excitons in moire)

Tran, K. et al. Nature 567, 71–75 (2019).
Seyler, K. L. et al. Nature 567, 66–70 (2019).
Jin, C. et al. Nature 567, 76–80 (2019).

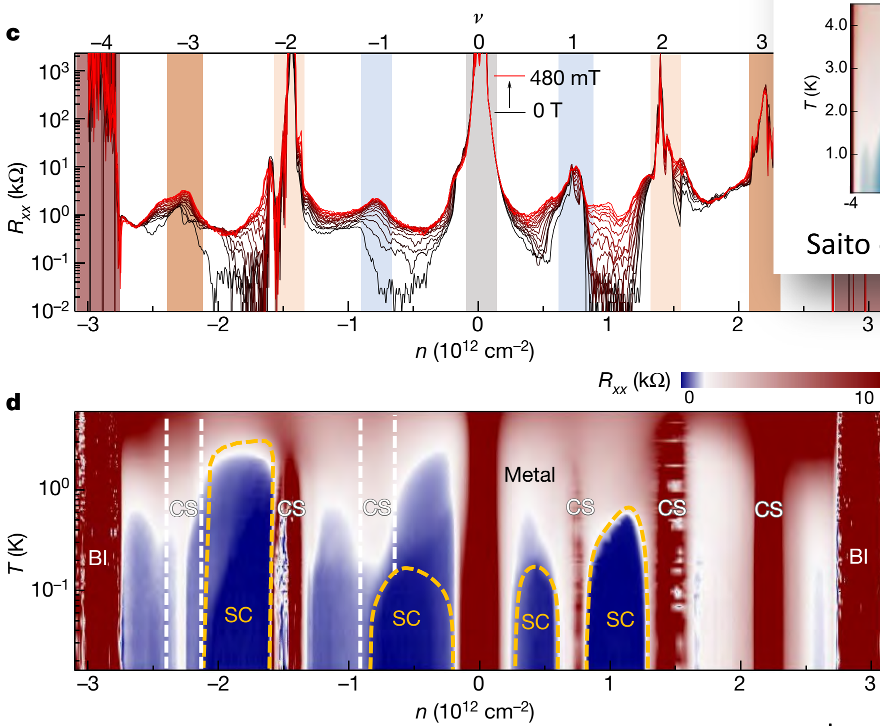
Superconducting Phase Diagram for MA TBG



Cao et al., Nature 556, 43–50 (2018).



Saito et al., arXiv:1911.13302 (see also Singh et al., arXiv 2002.03003)

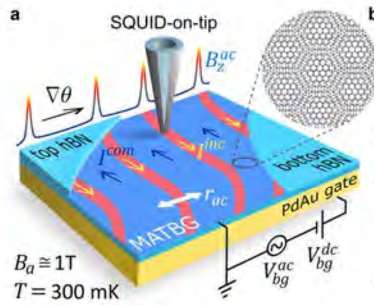


Lu et al, Nature 574, 653–657 (2019).

Local Variation of Twisting Angles

Scanning SQUID Measurement

Uri et al., arXiv:190804595 (2019)



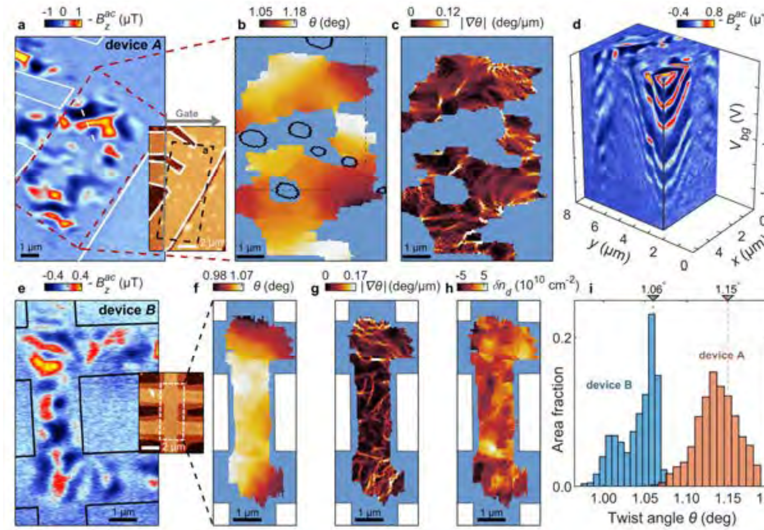
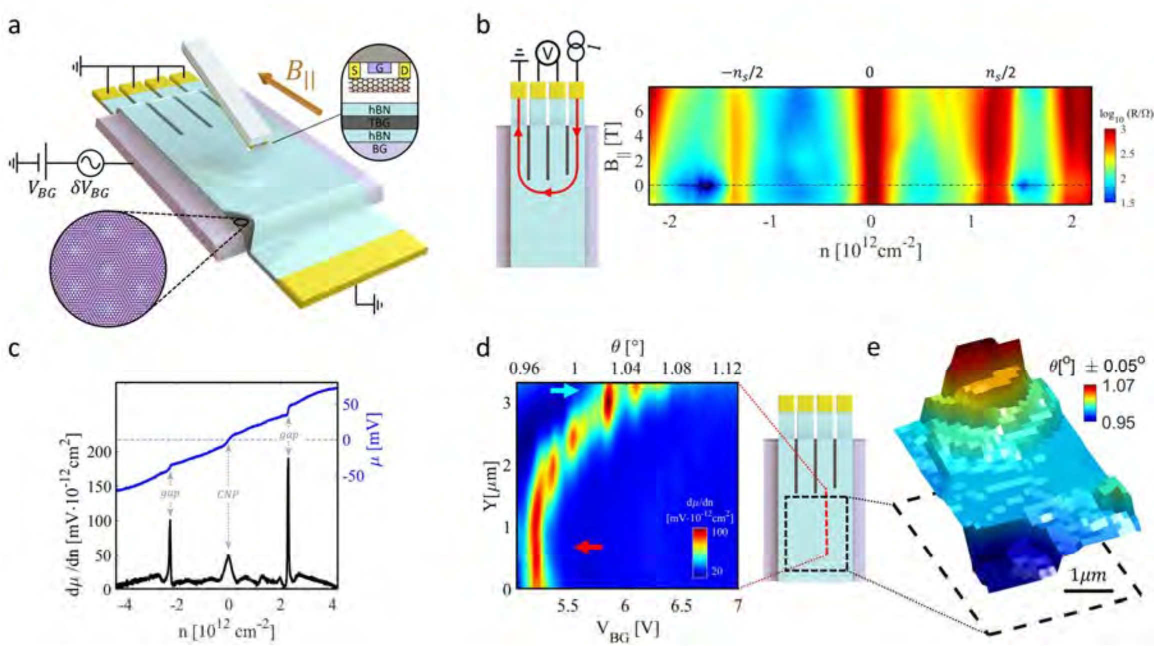


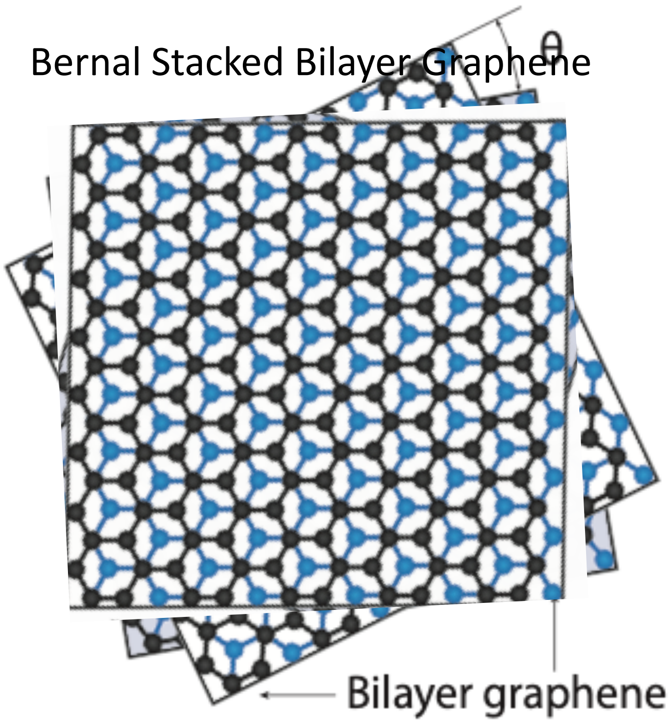
Fig. 3. Mapping the twist angle and Landau levels in MATBG. (a) B_z^{ac} image of the dashed area in the

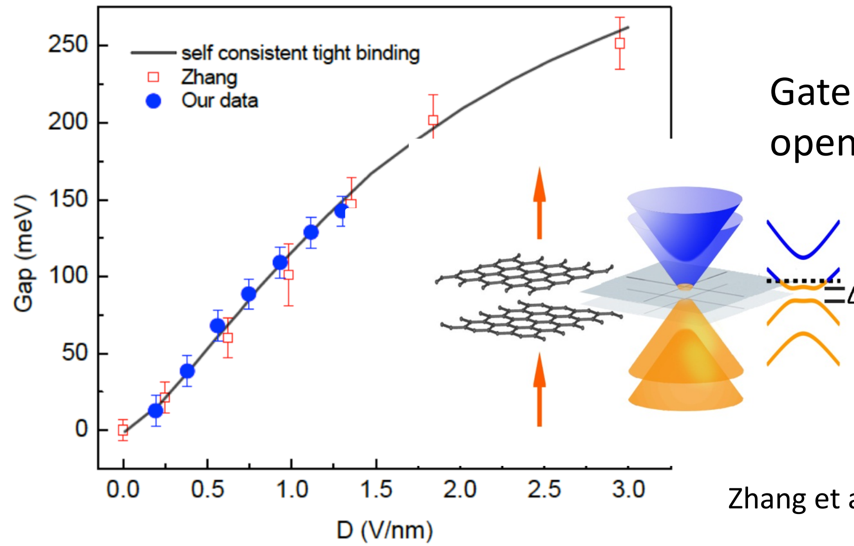


Scanning nanotube SET

Zondiner et al., arXiv:191206150 (2019)

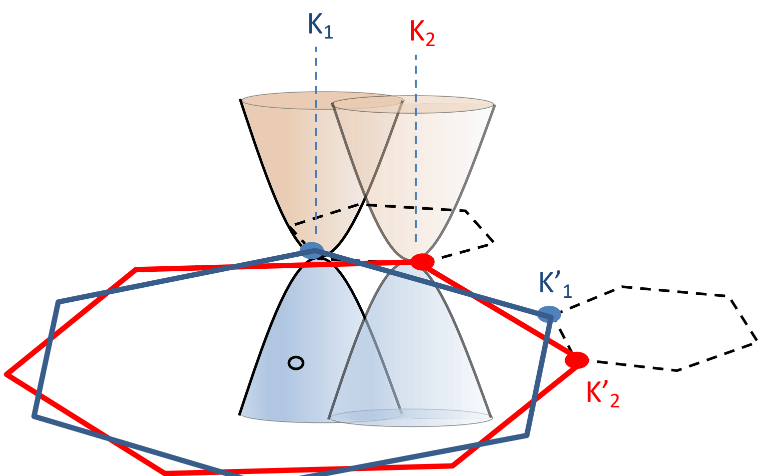
Twisted Double Bilayer Graphene



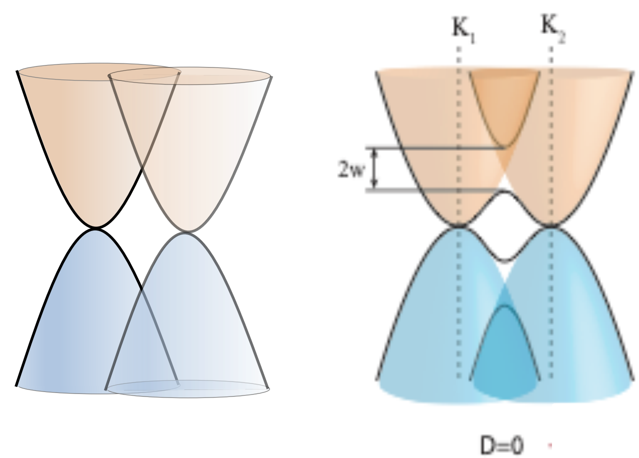


Gate tunable Gap opening in bilayer

Zhang et al. Nature (2008)



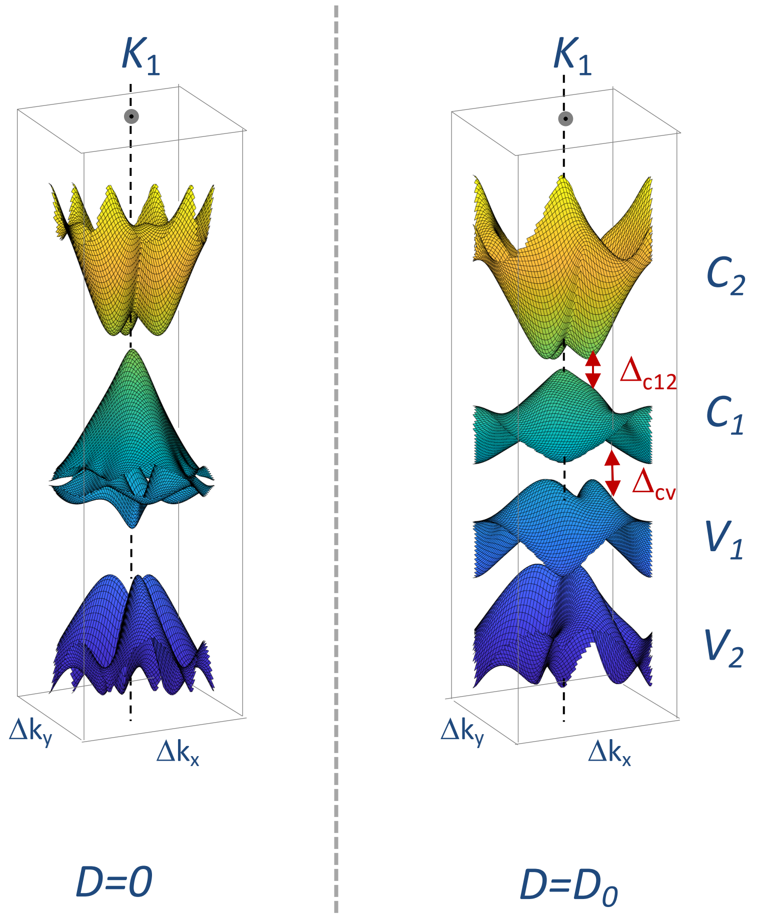
Twisted Double Bilayer Graphene (tDBG)



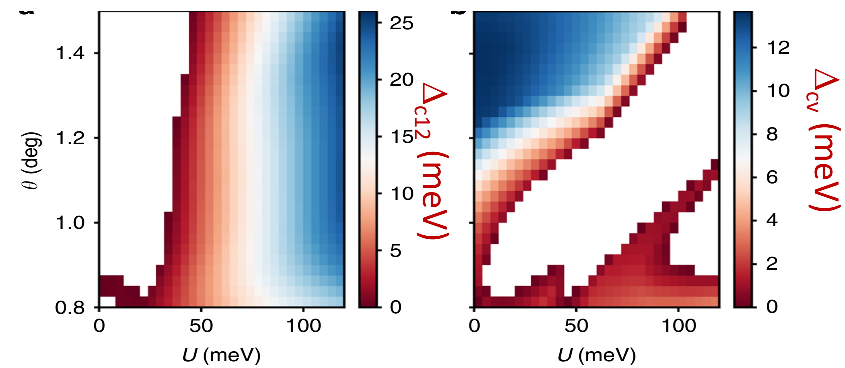
Gate tunable flat bands, no exact angle control needed!

Twisted Double Bilayer Graphene: Tunability

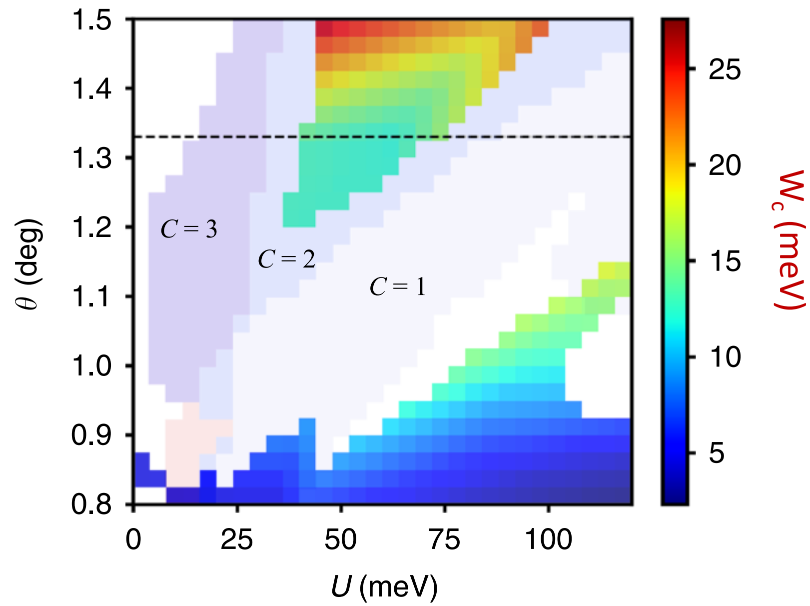
Tight binding with effective Wannier orbits



Band Gaps

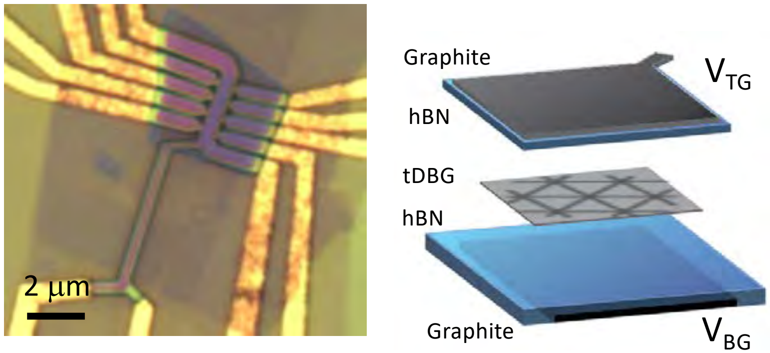


Isolated Conduction band width

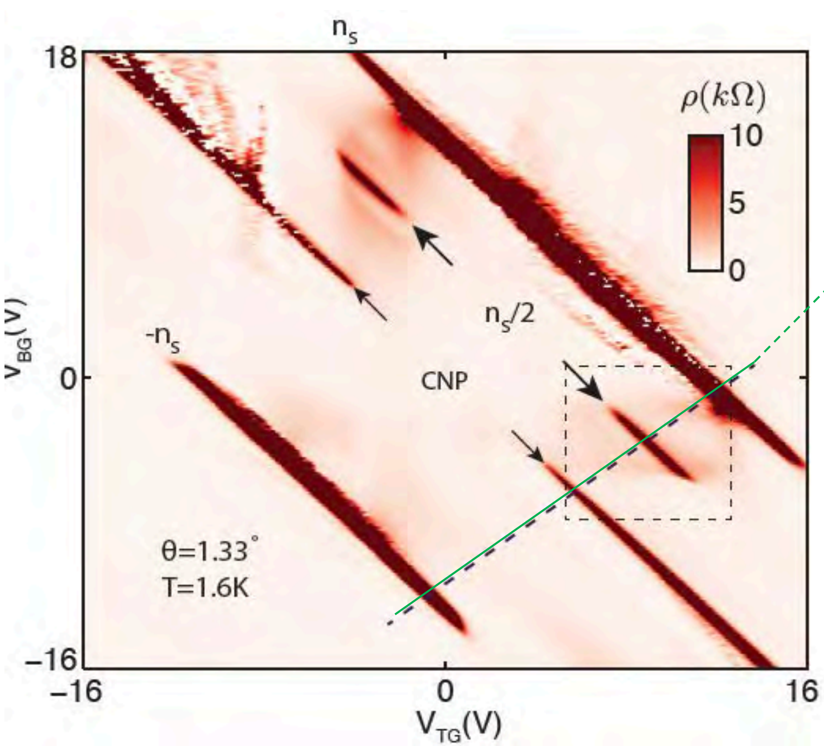


J. Y. Lee et al., Nature Comm (2019)

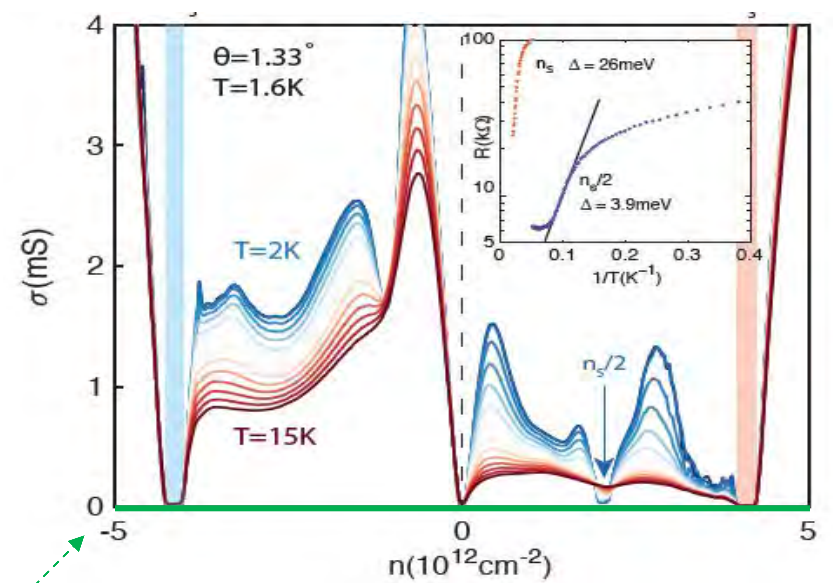
Mott Insulators in tDBG: $\theta = 1.33^{\circ}$

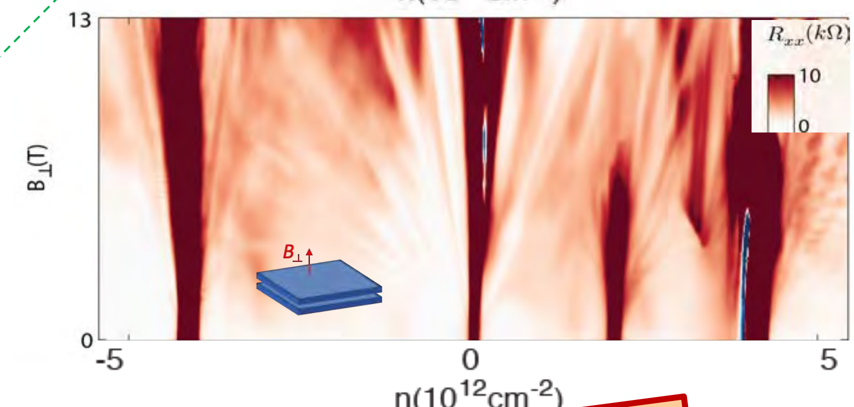


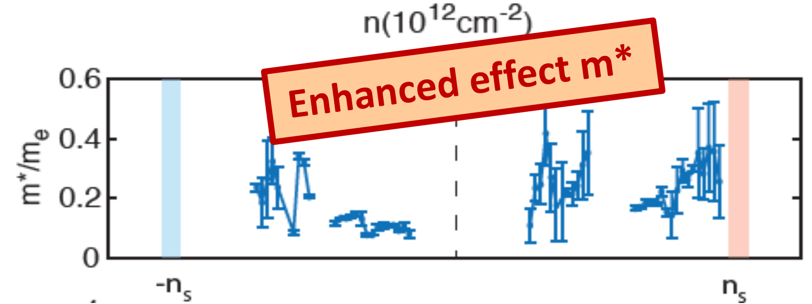
Top and bottom Gate dependent 4-terminal ρ



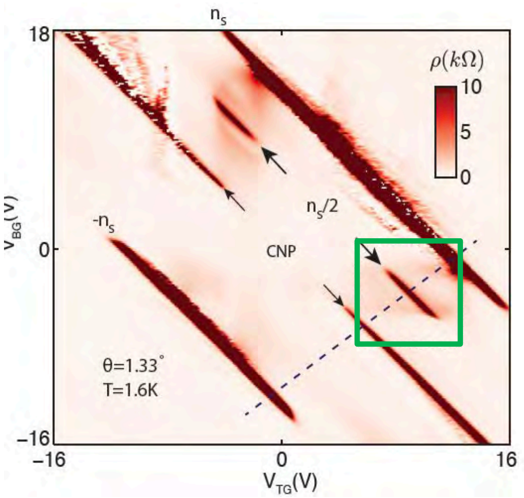
Temperature dependent 2-p conductance

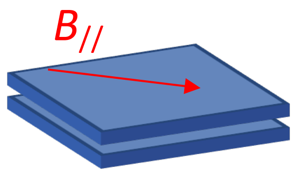


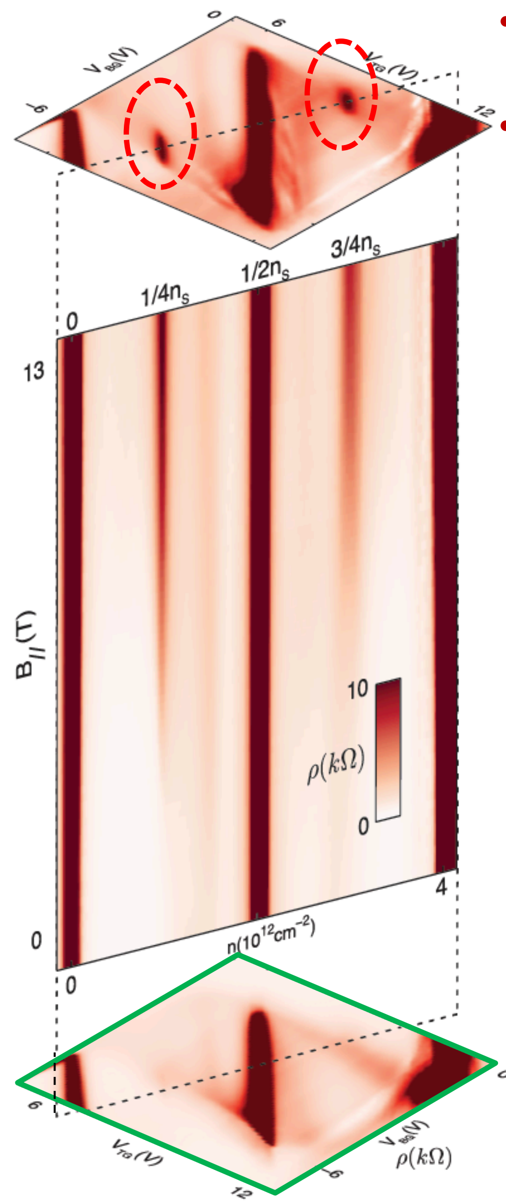




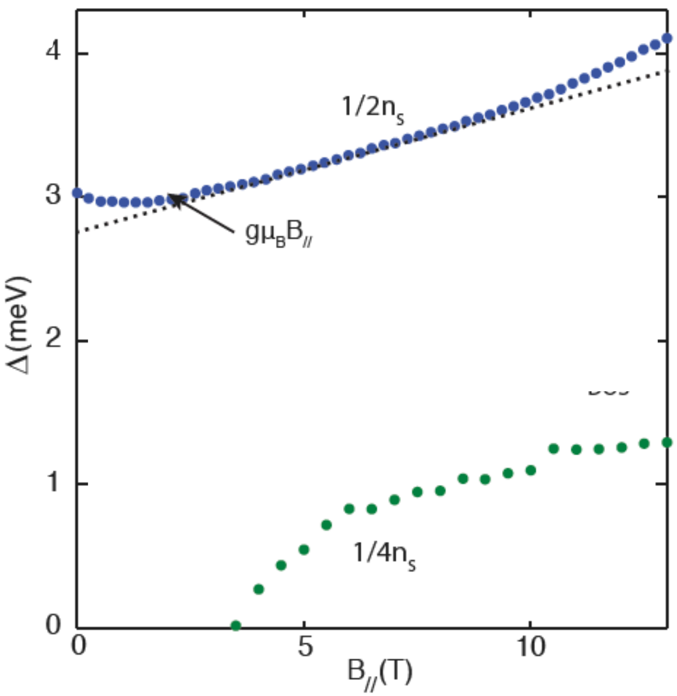
Ferromagnetic Mott Insulators in tDBG $\theta = 1.33^{o}$







- $n_s/4$ & $3n_s/4$ gaps appear at finite $B_{//}$
- $n_s/2$ states become stronger

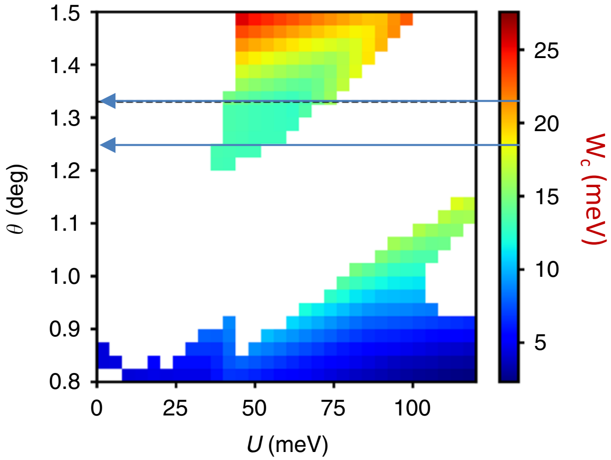


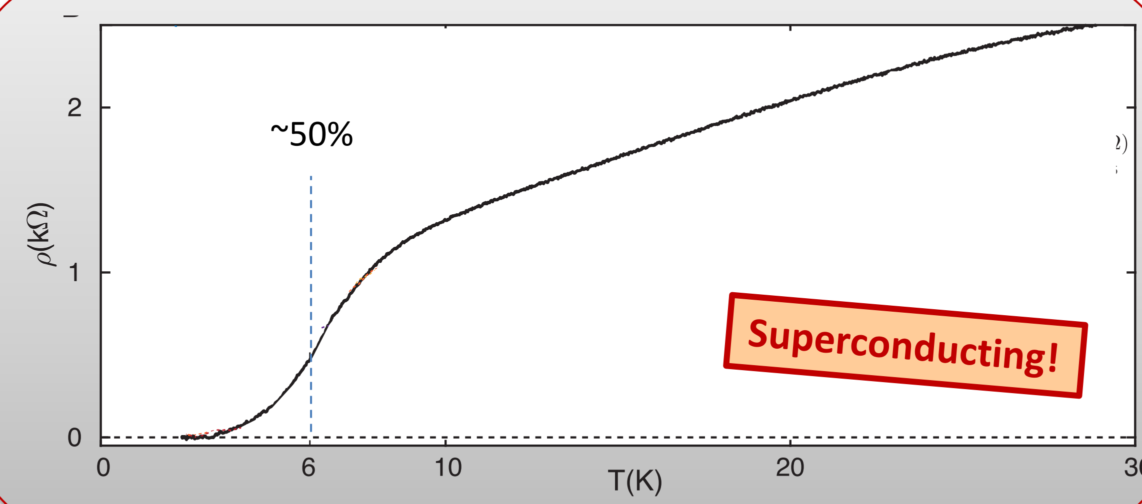
- Gap increases with $B_{//}$
- $g \approx 2$

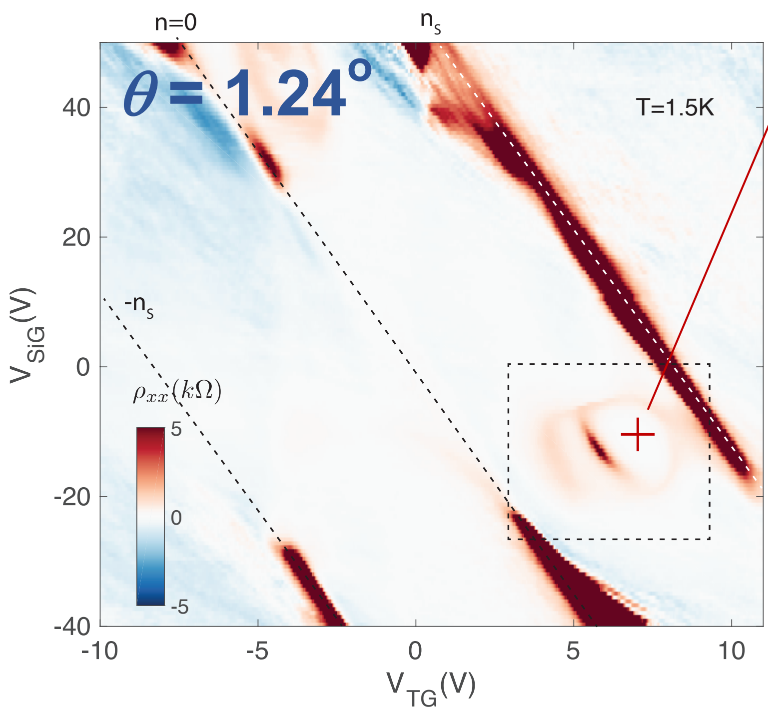
Spin polarized Mott State!

Superconductivity in tDBG

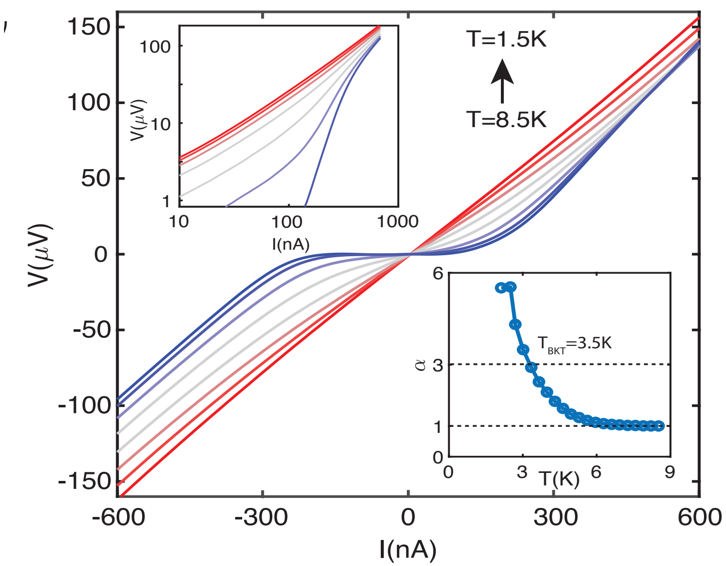
Isolated Conduction band width







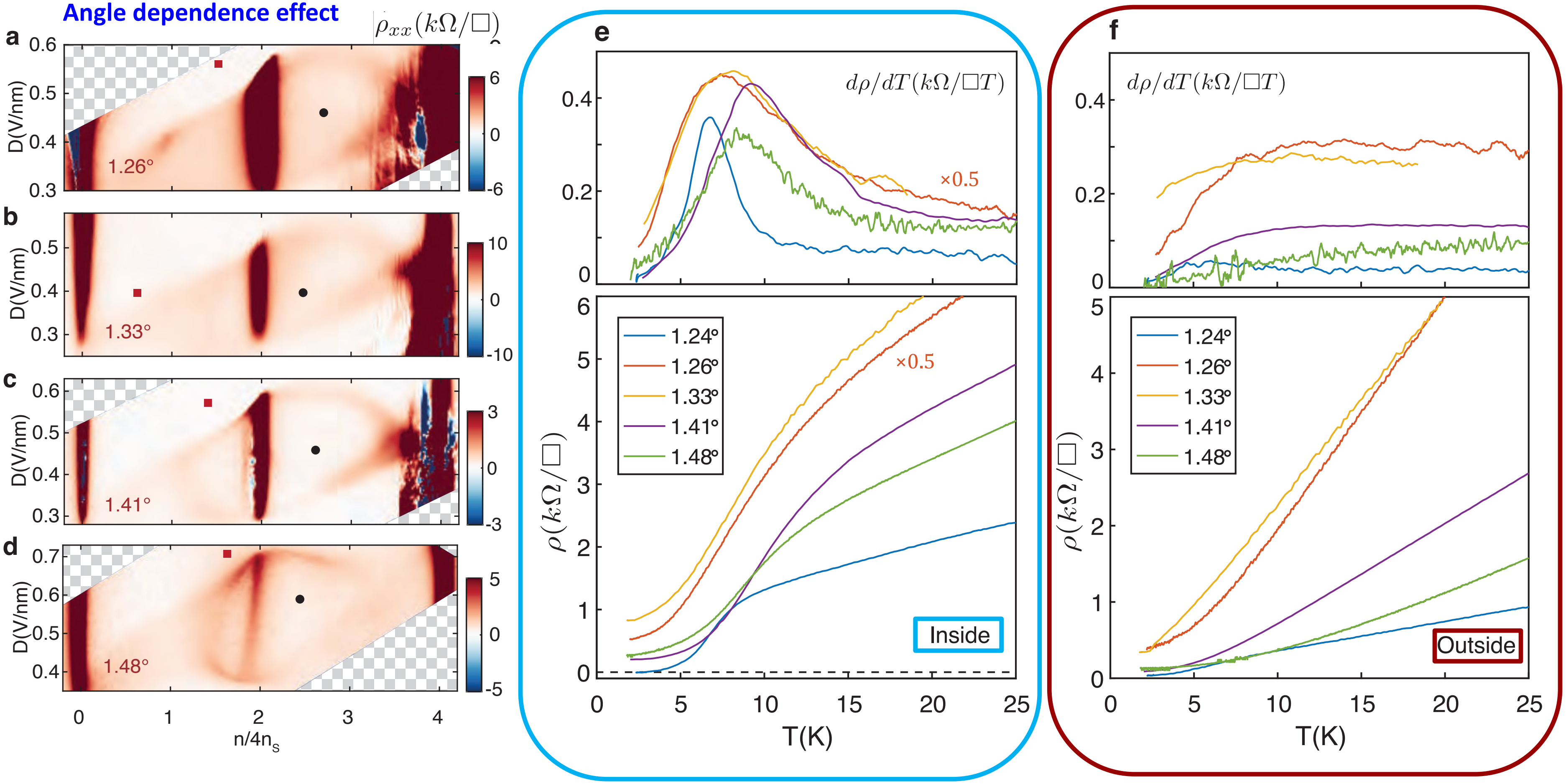
I-V characteristics: BTK Transition



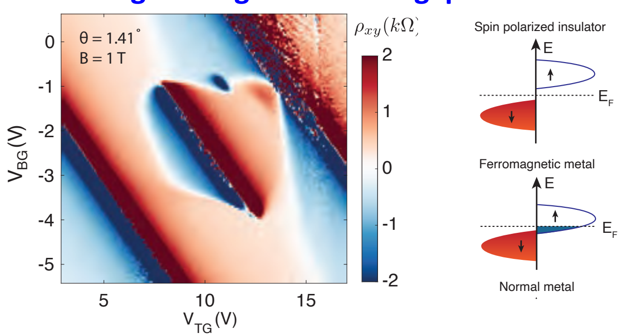
T_{BTK} =3.5 K

Superconducting Or Not Superconducting?

Angle dependence effect



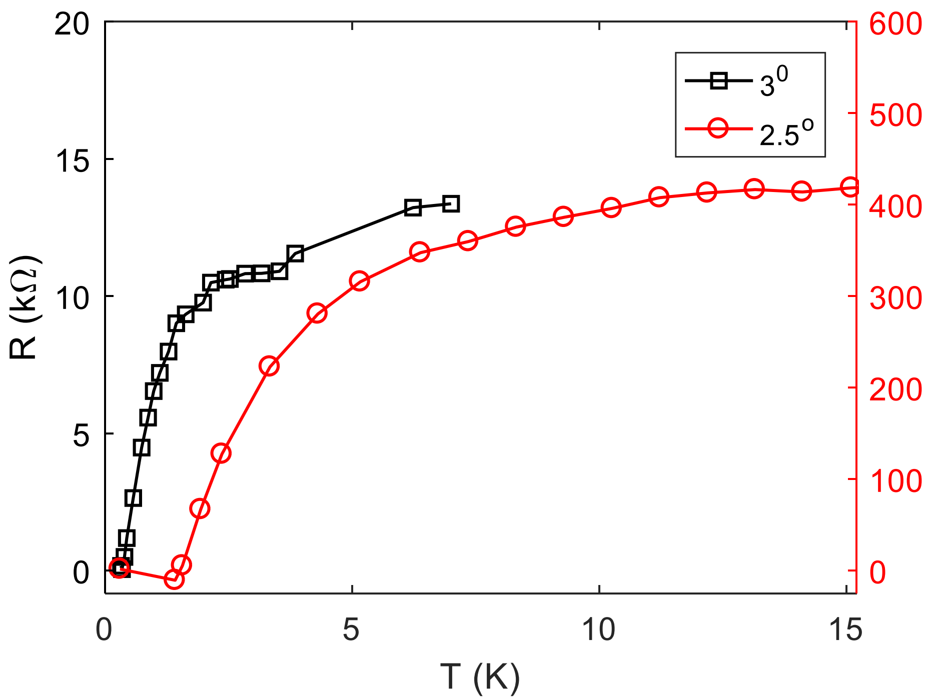
Hall sign change across the gap

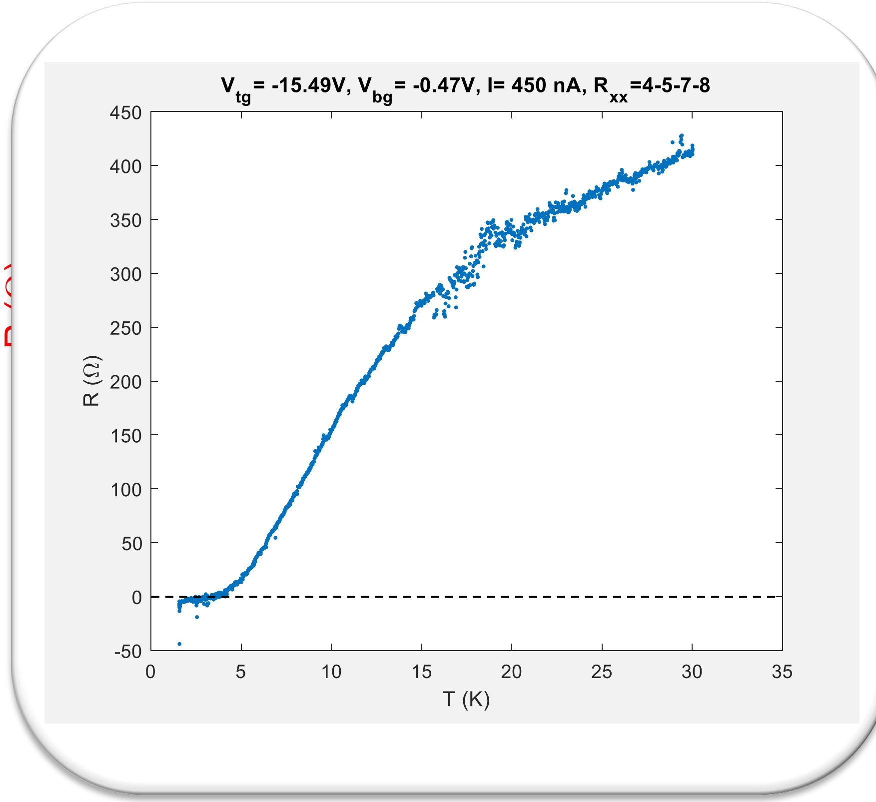


- Critical transition behavior near the spin polarized gaps
- However, we have just one sample showing ~zero resistance.

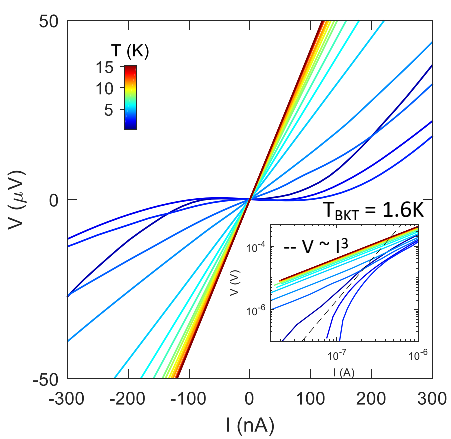
See also similar data in He *et al.*, arXiv:2002.08904

Superconducting(?) Twisted bilayer WSe_2

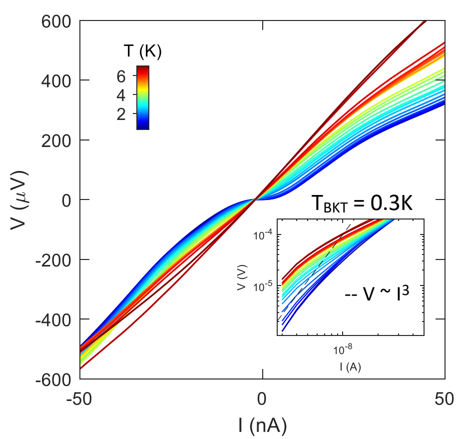




Angle : 2.5°



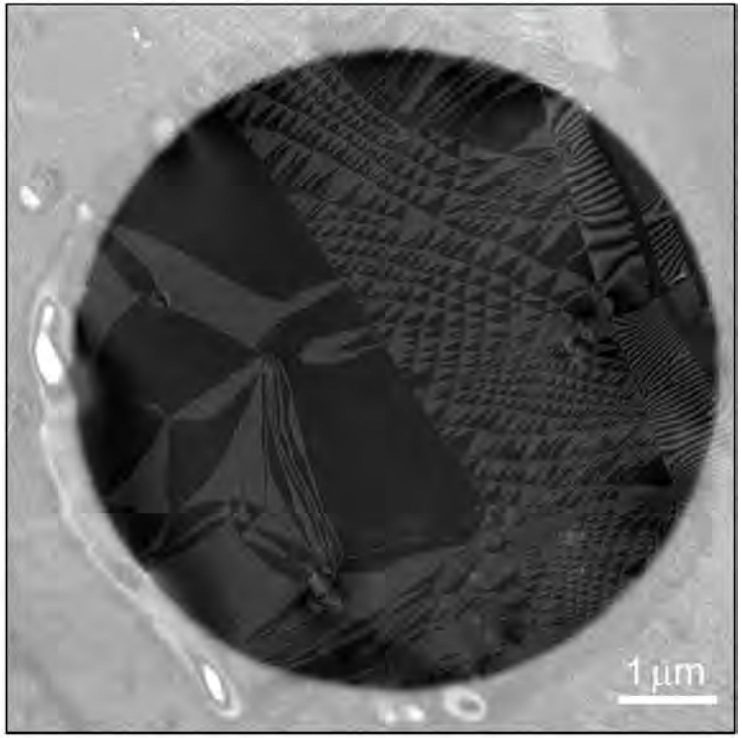
Angle : 3°



Superconducting-like state T_c ~ 0.3 - ~~3 K~~ ~ 8 K
has been realized in a wide angle range!

See also similar data in An *et al.*, arXiv:1907.03966

Random Moire: Domain and Domains Boundaries



Random domains in WSe_2/WSe_2 with small angel

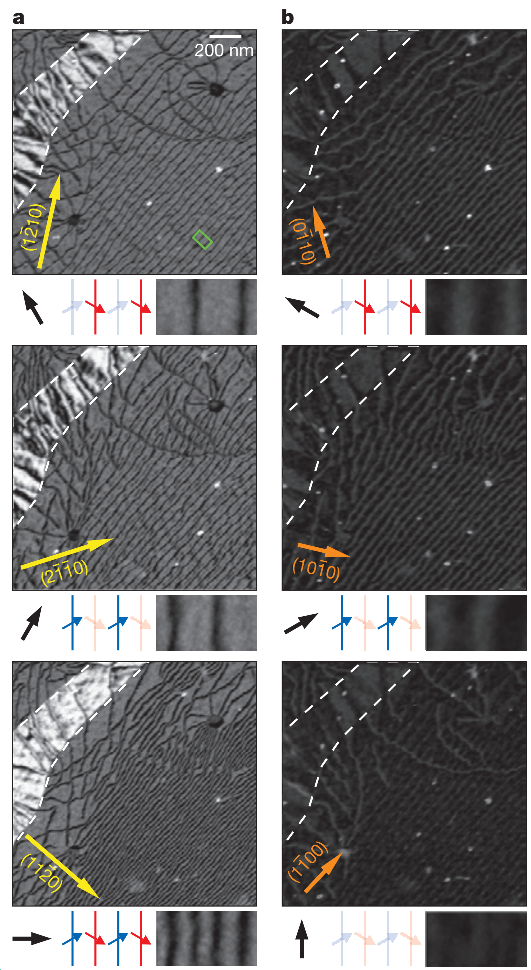
Moire lattice can be viewed as 2D network of dislocation lines.

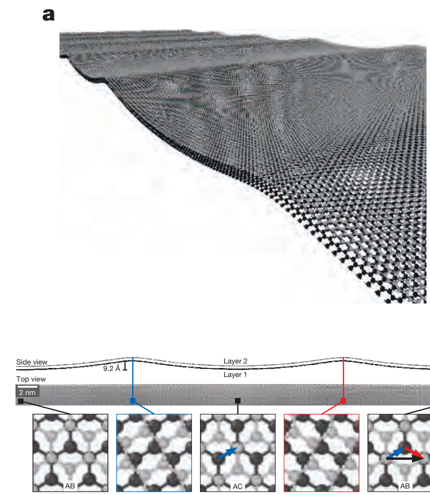
23 JANUARY 2014 | VOL 505 | NATURE | 533

doi:10.1038/nature12780

Dislocations in bilayer graphene

Benjamin Butz[1], Christian Dolle[1], Florian Niekiel[1], Konstantin Weber[2], Daniel Waldmann[3], Heiko B. Weber[3], Bernd Meyer[2] & Erdmann Spiecker[1]

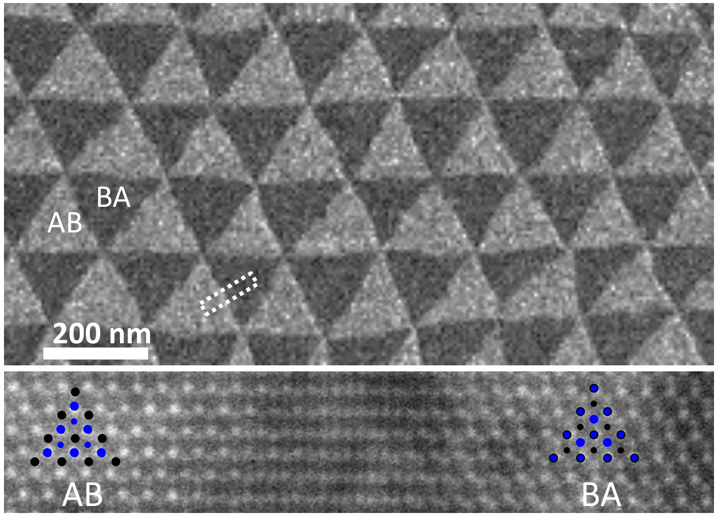




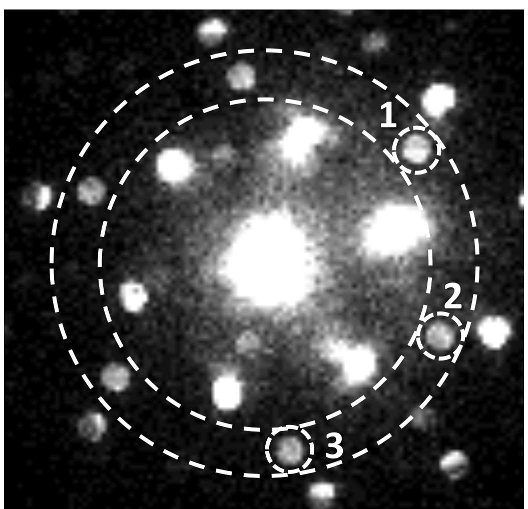
Arrays of 2D dislocation network by relative interlayer atomic registry shift

Burgers Vector for Moire Boundaries in TBG

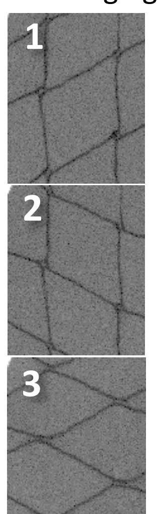
Dark field TEM/ Atomic-resolution Scanning TEM



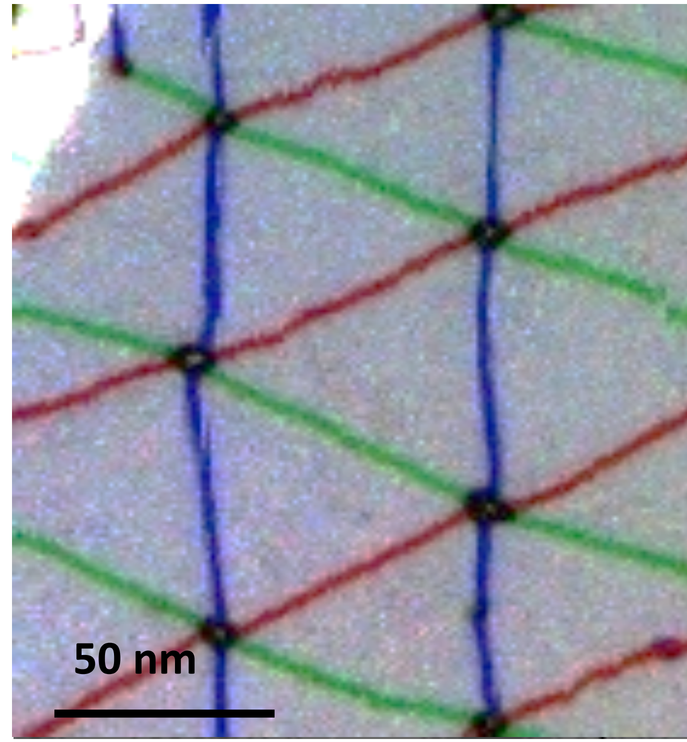
Electron diffraction



Second Order Brag Peak
Dark field imaging



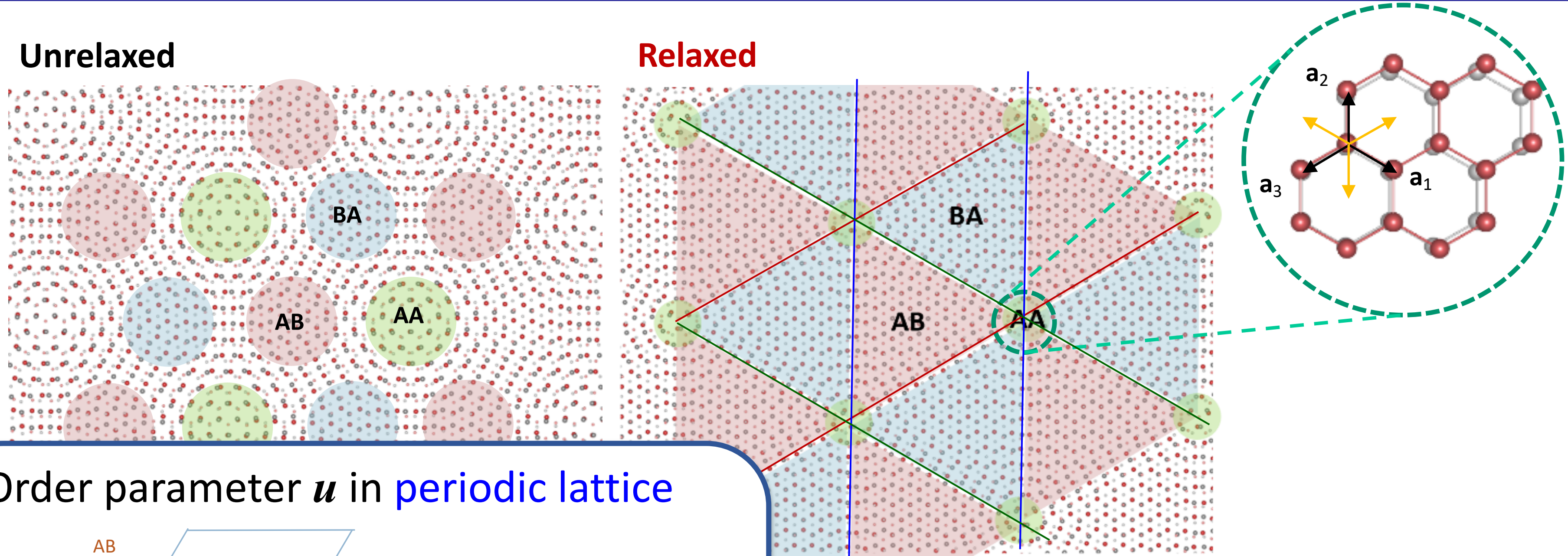
Domain Boundary Coloring by Burgers Vector



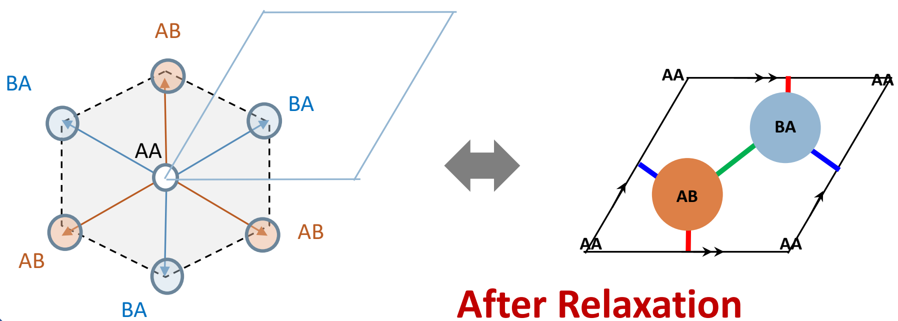
After the lattice relaxation, AA site is a junction for three dislocation lines intersect!

Following Alden et al., PNAS (2013)

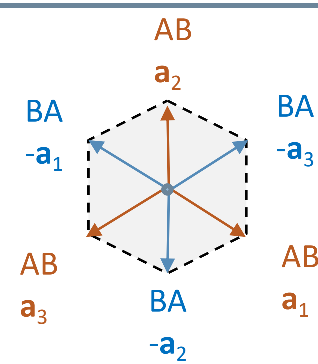
Lattice Shift Vector: Order Parameter for Relaxation Process



Order parameter $\boldsymbol{u}$ in periodic lattice



After Relaxation



Shift vector: $\boldsymbol{u}$

Order parameter
Configuration space
(periodic unit cell)

Define Lattice Shift Vector:

$$\boldsymbol{u} = [\mathbf{R}(\text{upper layer}) - \mathbf{R}(\text{lower layer})]_{\text{unit cell}}$$

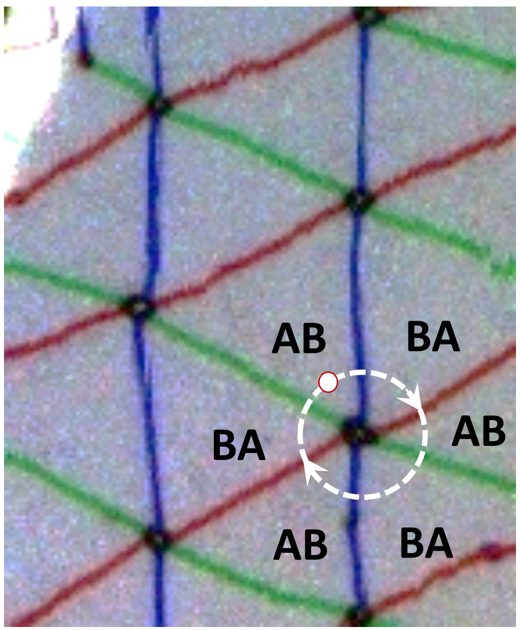
We also define $\boldsymbol{u}$ = 0 for untwisted sample and **u** = 0 for a AA site as a rotational center.

Following Alden et al., PNAS (2013)

Topology of Moire Network

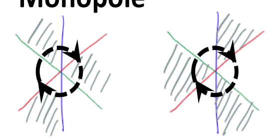
Han et al., preparation

Real Space Dark Field Moire Images

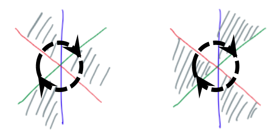


Topology of F2 Free Group Elements

Monopole

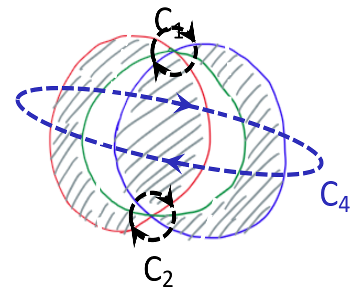


Vortices: $RLR^{-1}L^{-1} = T$



Anti-vortices: $LRL^{-1}R^{-1} = T^{-1}$

Dipole



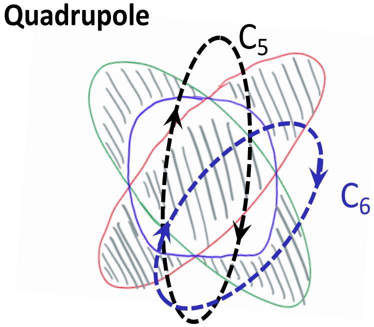
C_1: $LRL^{-1}R^{-1} = T^{-1}$

C_2: $RLR^{-1}L^{-1} = T$

C_3: $RR^{-1} = T^0$

C_4: $LR^{-1}RL^{-1} = T^0$

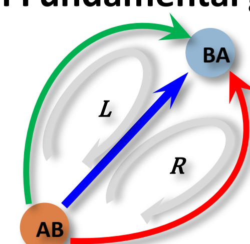
Quadrupole



C_5: $LRL^{-1}R^{-1}LRL^{-1}R^{-1} = T^{-2}$

C_6: $LR^{-1}L^{-1}LRL^{-1} = T^0$

Topological Fundamental group of order parameter space



Free group on 2 generators

$\rightarrow RL \neq LR$

$\boldsymbol{L} = gb^{-1}$

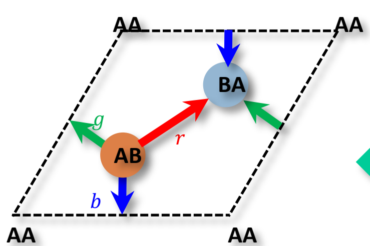
$\boldsymbol{R} = br^{-1}$

A loop around AA site corresponds to

$\boldsymbol{RLR^{-1}L^{-1}} = br^{-1}\, gb^{-1} r g^{-1}$

Equivalent to the topology of punctured torus

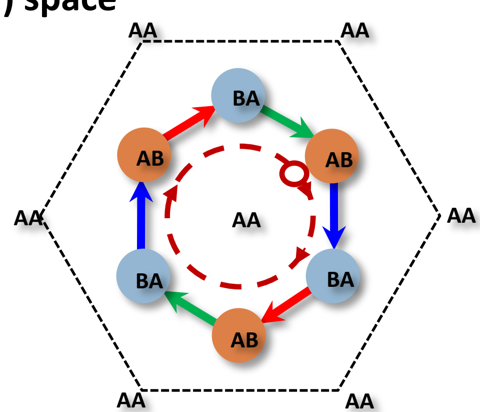
Order parameter (shift vector) space



$r = a/3[0110]$

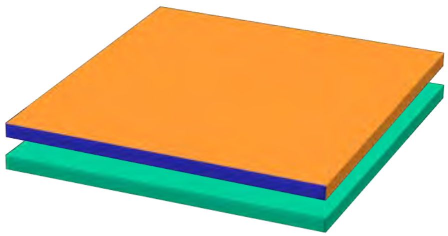
$g = a/3[1100]$

$b = a/3[1010]$



Vortex and Anti-Vortex Pair

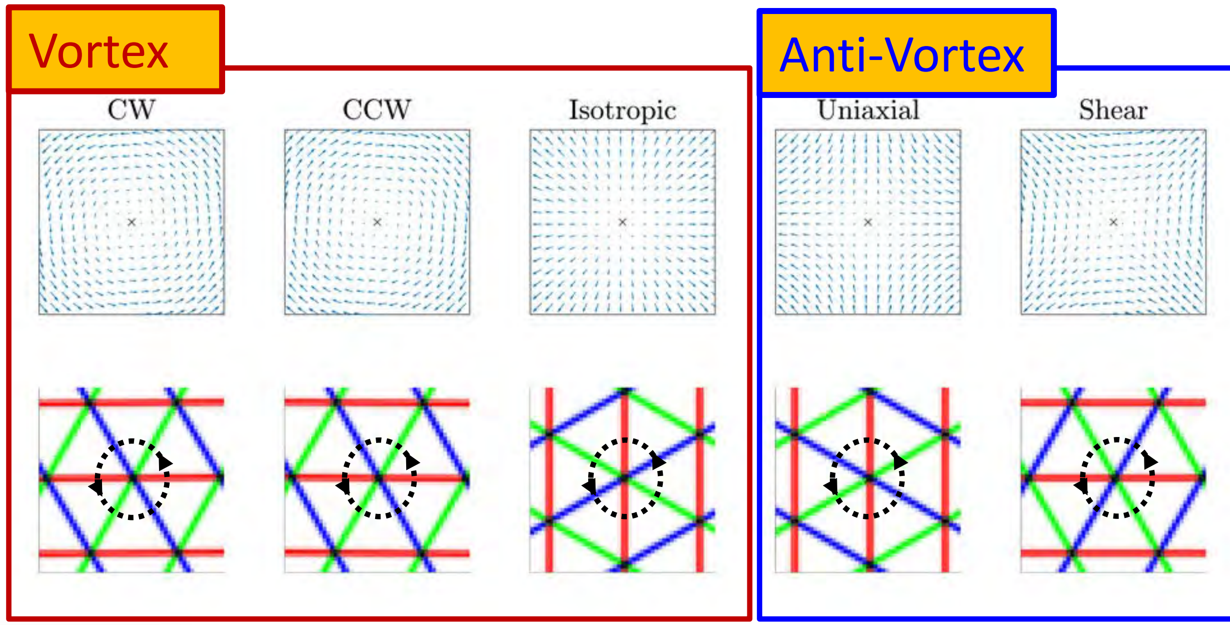
Interlayer relative elastic deformation



$$\boldsymbol{u}(\boldsymbol{r}) = \left(\mathbf{1} + \frac{\partial u_i}{\partial r_j}\right)\boldsymbol{r} = \begin{cases} \begin{pmatrix} \cos(\theta)-1 & -\sin(\theta) \\ \sin(\theta) & \cos(\theta)-1 \end{pmatrix} & \text{Rotation} \\ \begin{pmatrix} \alpha & 0 \\ 0 & \alpha \end{pmatrix} & \text{Isotropic} \\ \begin{pmatrix} \beta_1 & 0 \\ 0 & -\beta_1 \end{pmatrix} & \text{Uniaxial} \\ \begin{pmatrix} 0 & \beta_2 \\ \beta_2 & 0 \end{pmatrix} & \text{Shear} \end{cases}$$

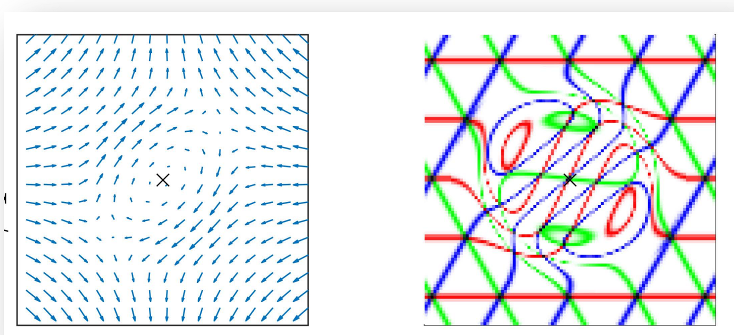
u(r) map in different elastic deformation

Corresponding dislocation network



$RLR^{-1}L^{-1} = br^{-1}\, gb^{-1}rg^{-1}$

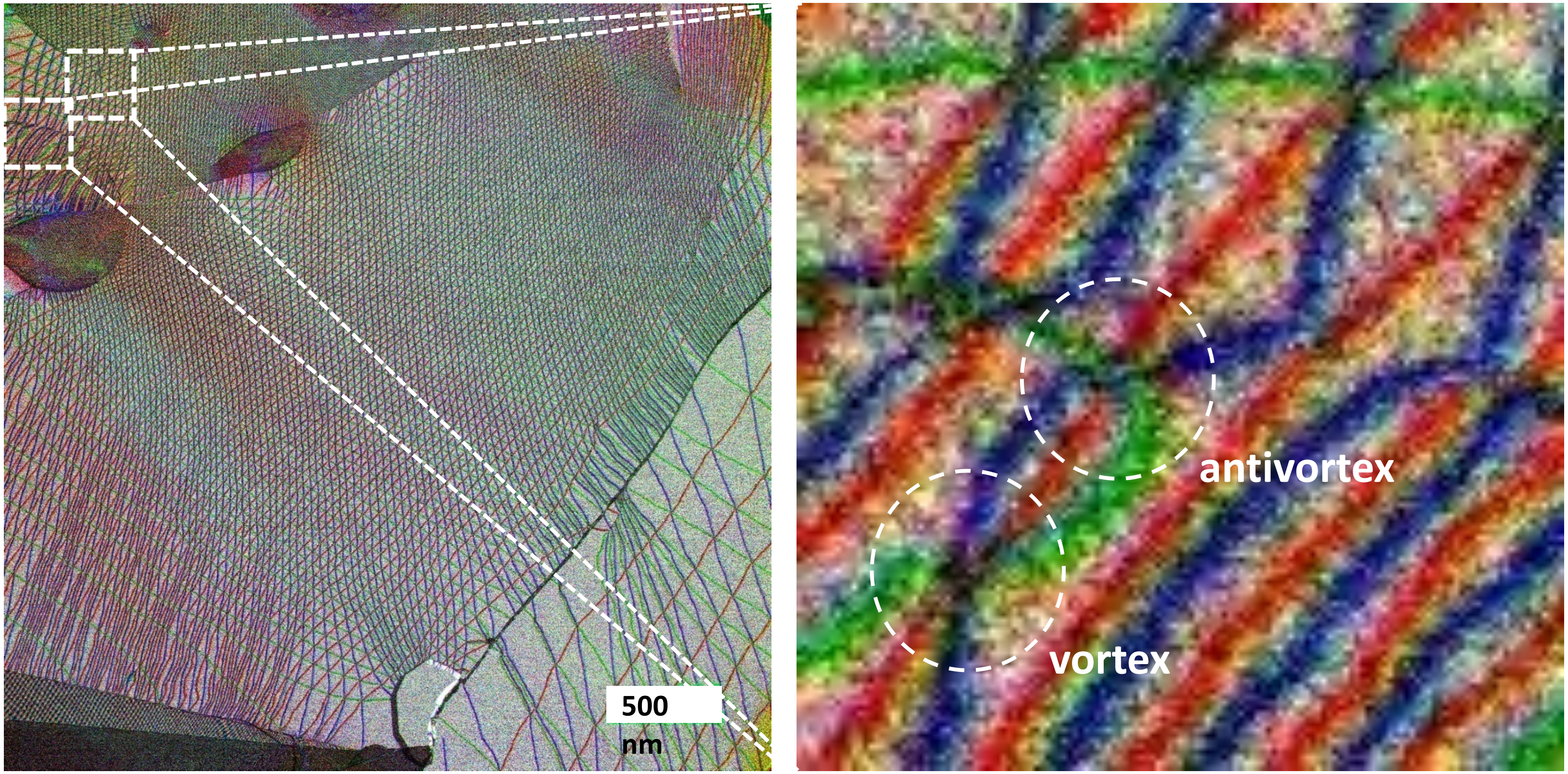
$LRL^{-1}R^{-1} = gr^{-1}bg^{-1}rb^{-1}$



Vortices and Antivortices in mixed (shear + rotation) elastic deformation

Carr et al., preparation

Realization of Vortex and Anti-Vortex Pair

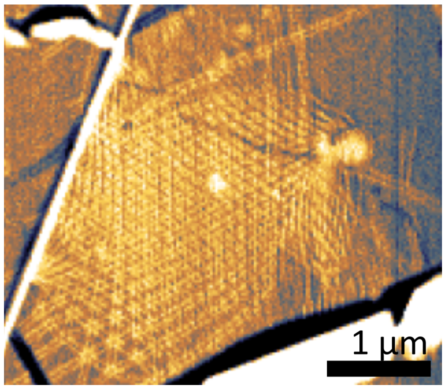


Vortex: rgbrgb, antivortex: rbgrbg

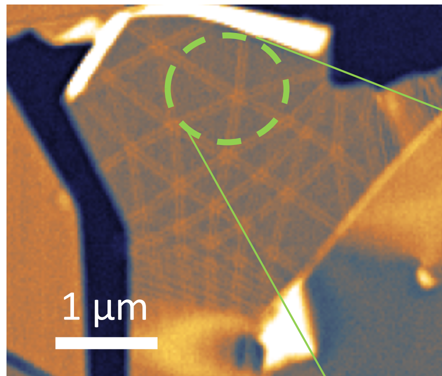
Toward Transport Through A Vortex

Designing with ultra-small twist angles

~0.1° twist

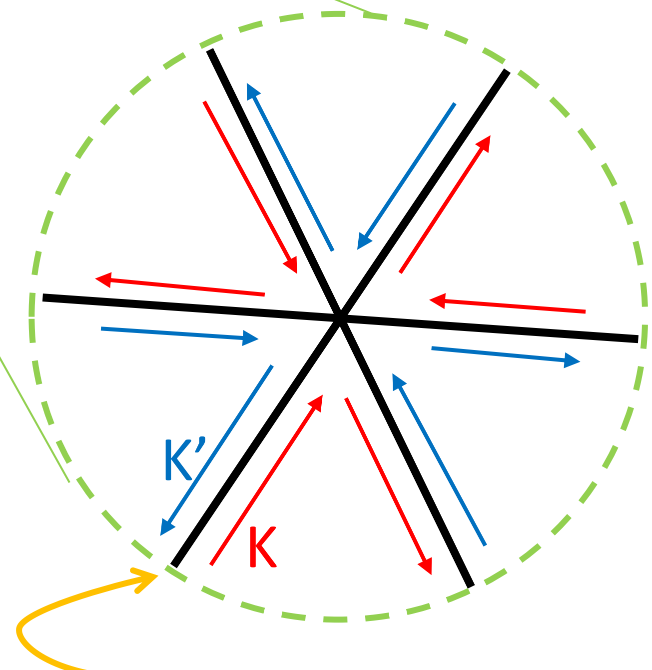


~0.01° twist



Near field IR scanning microscopy by Yue Luo

Investigate transport at vortex formed by intersecting domain walls

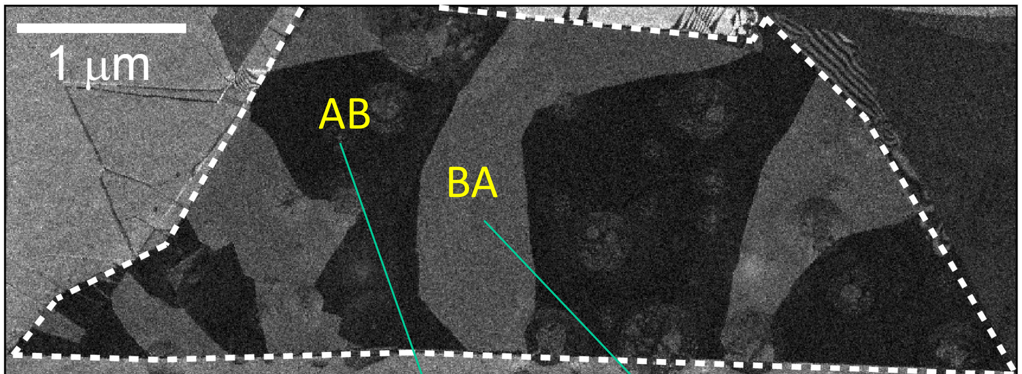


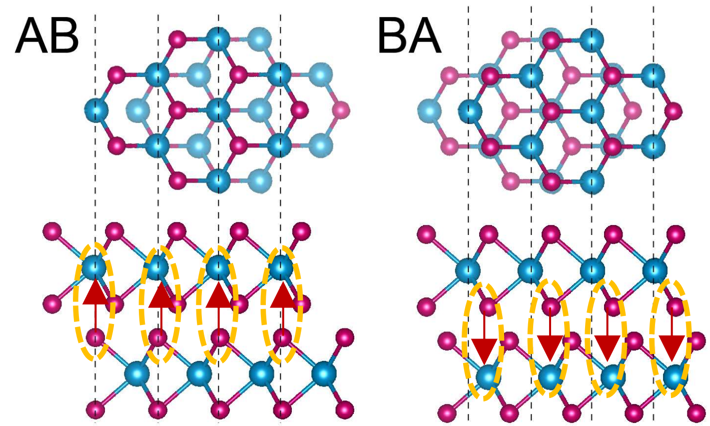
Valley-selective topologically protected modes

Imaging -> rational device design based on structure

Broken Mirror Symmetry and Spontaneous Dipoles

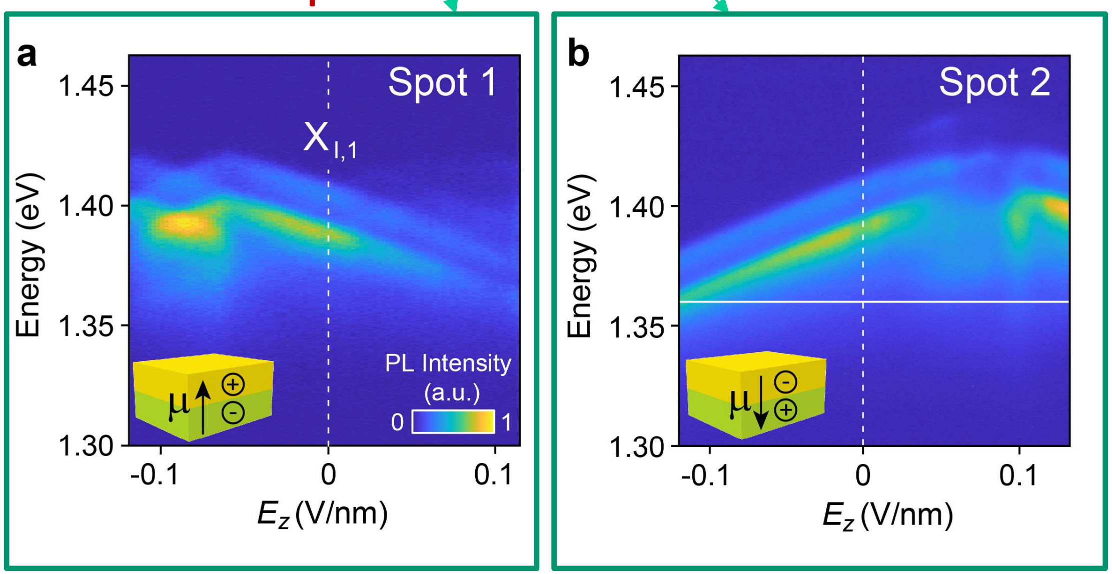
$MoSe_2/MoSe_2$ near 0 degree



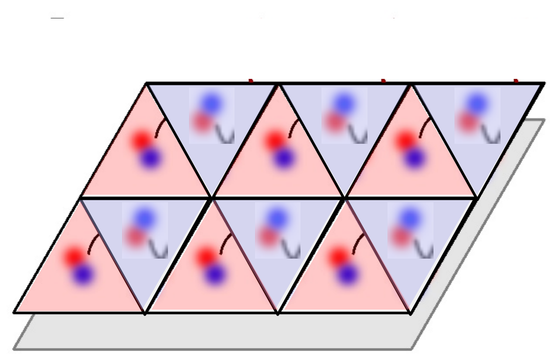


Interlayer dipole moment due to charge transfer!

Electric Field Dependent Photoluminescence



Arrays of alternating dipole moment interlayer excitons due to broken mirror/inversion symmetry in the AB and BA domains.



J. Sung et al., arXiv:2001.01157 (Collaboration with H. Park Group)

Summary and Outlook

- Moire superlattice fabrication in vdW interfaces provide band structure engineering in nanometer length scale.
- Correlated physical states appear in magic angle twisted bilayer graphene.
- Spin polarized correlated insulator in twisted double bilayers.
- AA site of moire lattice can be considered as topological defects.

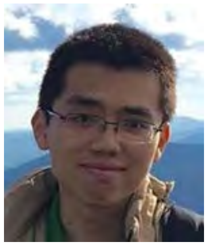
Going Forward:

- Symmetry elements in the materials can be engineered by twist angle control.
- Can we generate topologically non-trivial electronic structures from twisted vdW stacks?

Acknowledgement

Experiments

Double bilayer



Xiaomeng Liu

Zeyu Hao

WSe2/WSe2

Louis Jauregui, Andres Mire-Valdivia

2D dislocation network

Hyobin Yoo, Rebecca Engelke

BSCCO/BSCCO

Frank Zhao, Nicola Poccia

Theory

Ashvin Vishwanath

Jong Yeon Lee

Eslam khalaf

Efthimios Kaxiras

Shiang Fang

Steven Carr

Jung Hoon Han (SKKU); Minyoung Kim (Oxford)

hBN

T. Taniguchi, K. Watanabe

Funding: