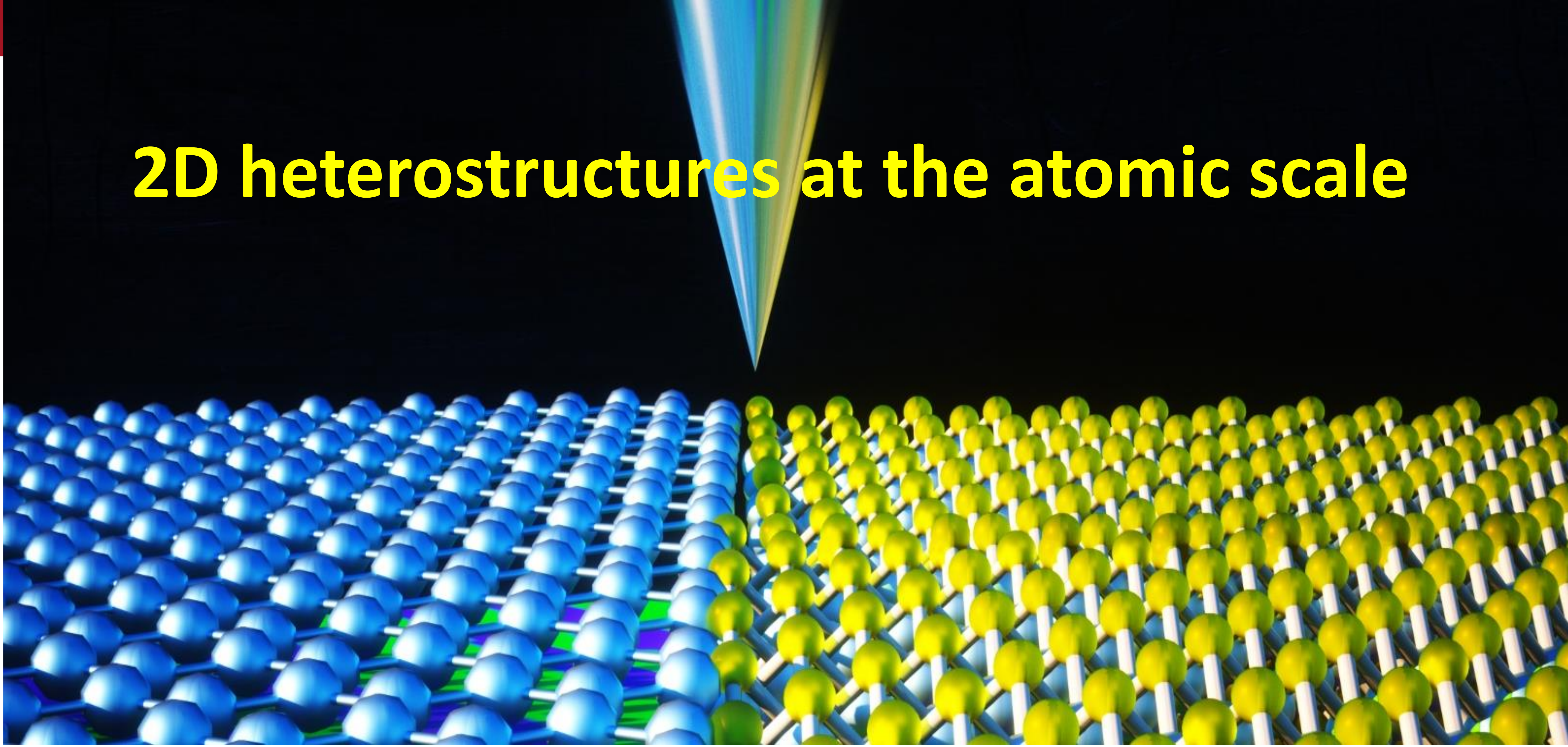
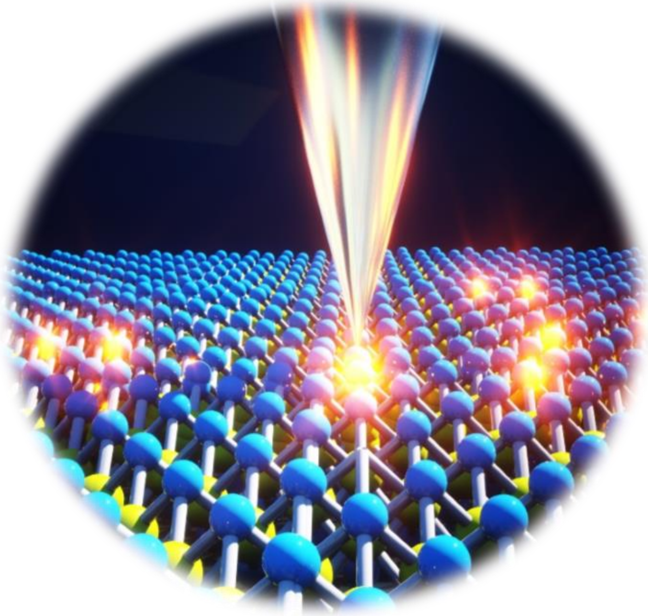
2D heterostructures at the atomic scale



Adina Luican-Mayer
Department of Physics, University of Ottawa

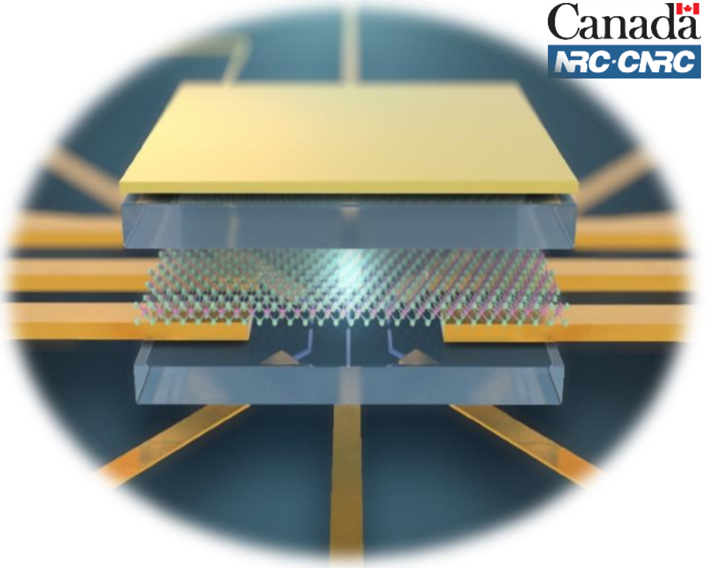
Quantum matter at the atomic scale



- Defects
- Moiré patterns
- Magnetic TI
- CDW in 1T-TaS_2

Quantum circuits in 2D materials

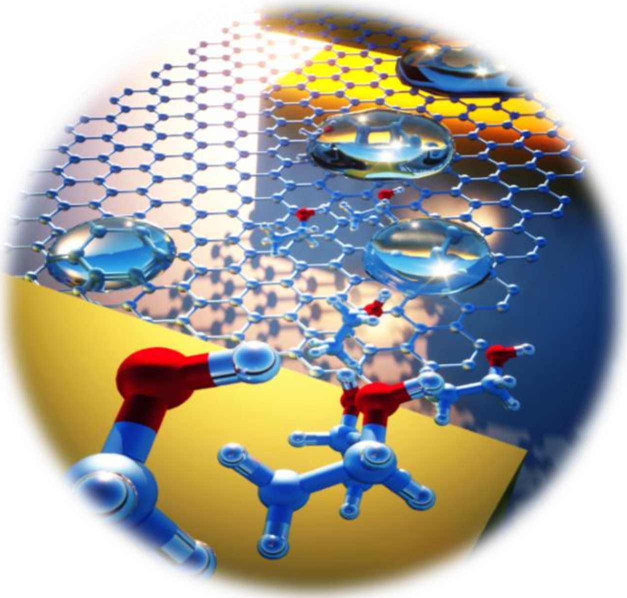
Canada
NRC·CNRC



- Quantum confined structures for quantum computing and sensing

preprint arXiv:2203.11871 ***(2022)***
Appl. Phys. Lett. 119, 133104 **(2021)**
Appl. Phys. Lett. 115, 231603 **(2019)**

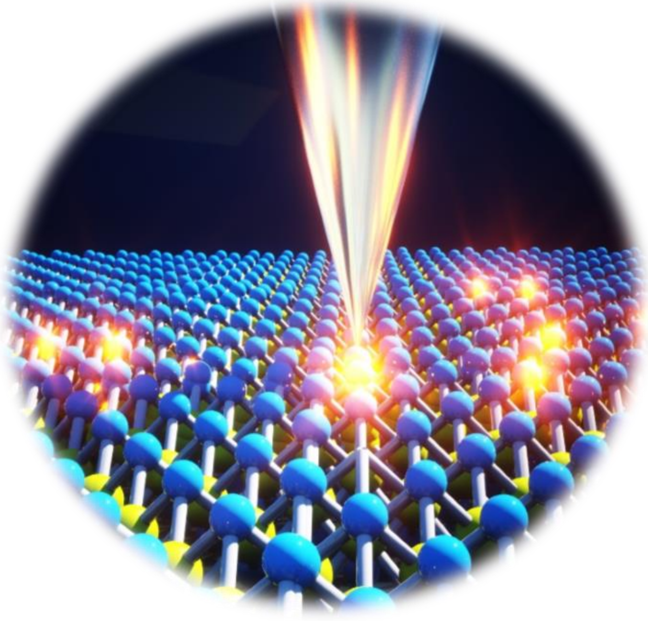
2D materials for energy, environment, and security



- Development of selective chemical noses
- Development of thermal camouflage devices/textiles

MDPI Sensors 22 (6), 2383, **(2022)**
ACS Sensors 6 (12), 4417 **(2021)**
ACS App. Mat. & Interfaces 13, 51, 6175 **(2021)**
ACS Omega 5, 21320 **(2020)**
ACS App. Mat. & Interfaces 12, 39764 **(2020)**

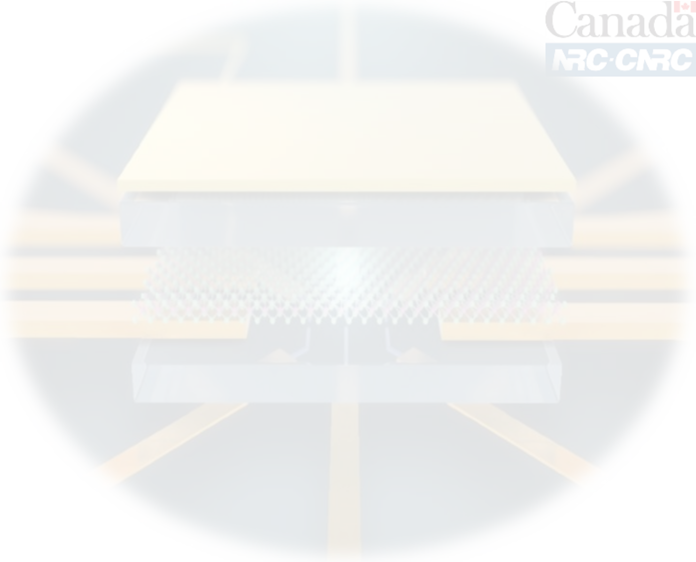
Quantum matter at the atomic scale



- Defects
- **Moiré patterns**
- Magnetic TI
- CDW

JAP 128 (4), 044303 **(2020)**
Phys. Rev. B 102, 205408 **(2020)**

Quantum circuits in 2D materials



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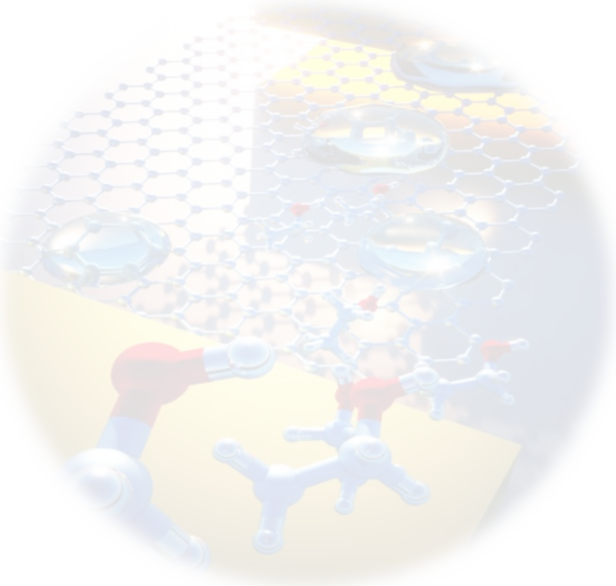

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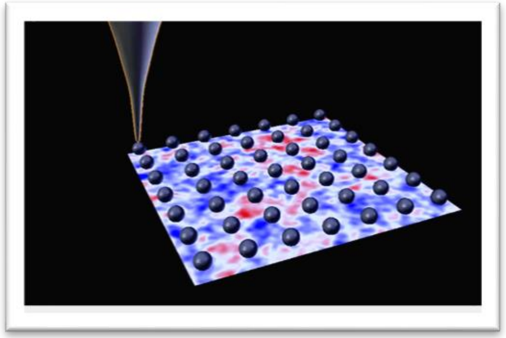
ACS App. Mat. & Interfaces 13, 51, 6175 **(2021)**
ACS Omega 5, 21320 **(2020)**
ACS App. Mat. & Interfaces 12, 39764 **(2020)**

Scanning Tunnelling Microscopy/Spectroscopy



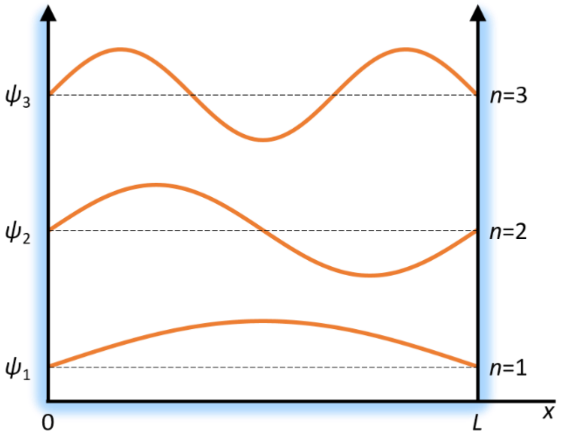
$$I \propto \frac{4\pi e}{\hbar}\int_0^{eV_B} \overbrace{\rho_S\left(E_F - eV_B + \epsilon\right)}^{\textit{Sample}} \overbrace{\rho_T\left(E_F + \epsilon\right)}^{\textit{Tip}} \overbrace{|M|^2}^{\textit{Tunnel junction}} d\epsilon$$

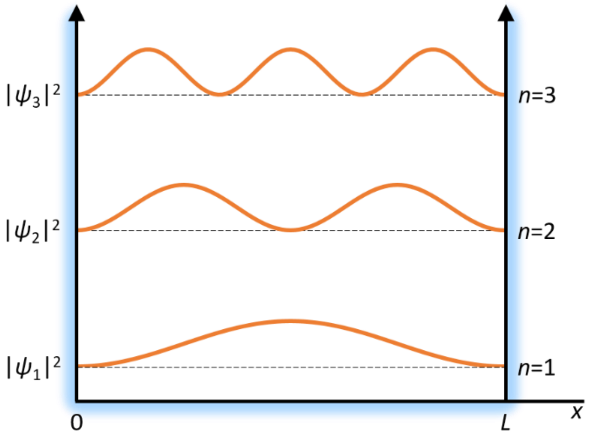
- Topography

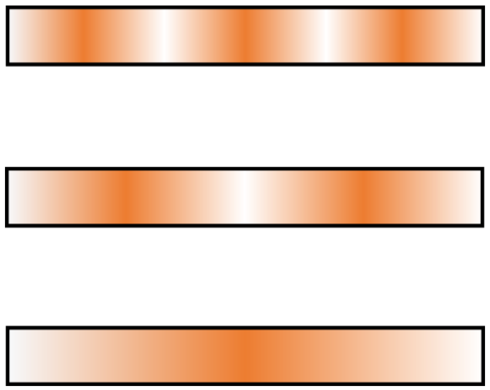
$$I \propto e^{\frac{-2d}{\hbar}\sqrt{2m\Phi}}$$

- Local density of states

$$\frac{dI_t}{dV_{Bias}} \propto \rho_{sample}(eV)$$

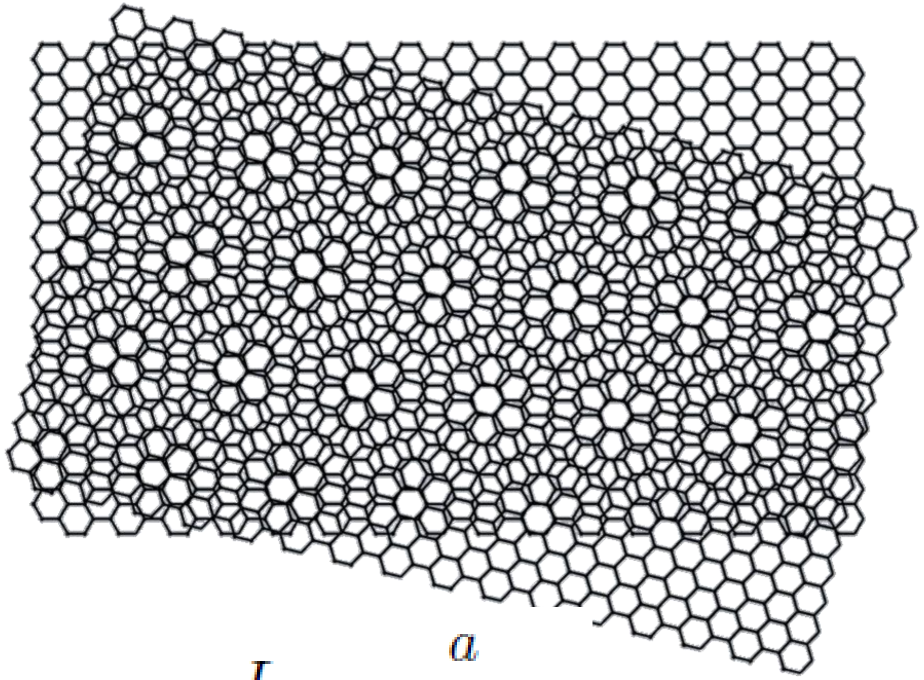






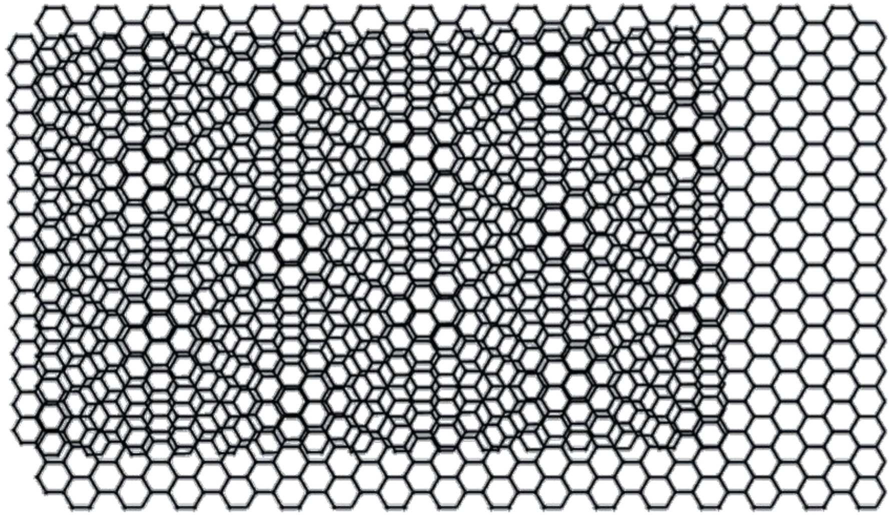
Moiré patterns in 2D materials

Twist



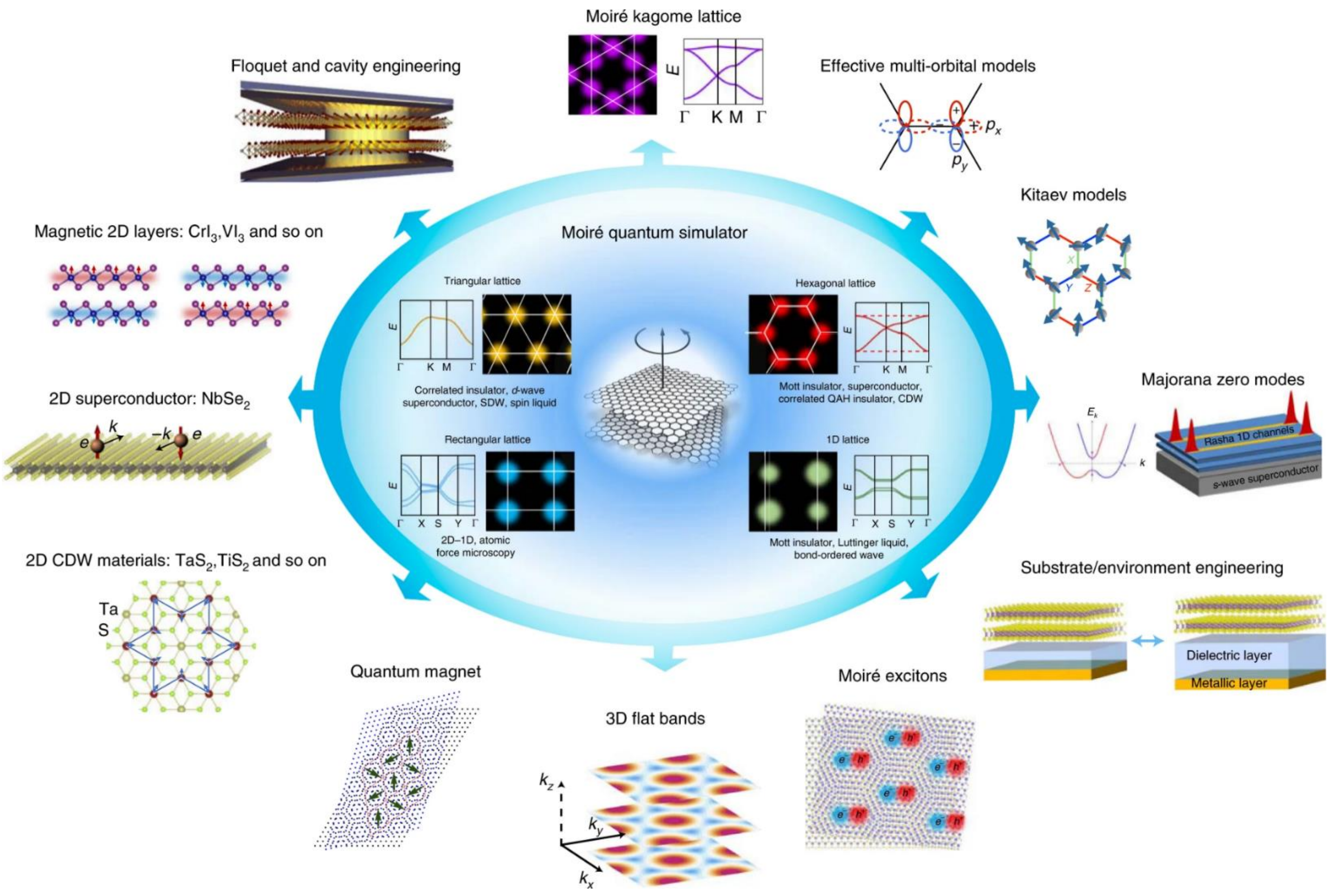
$$L = \frac{a}{2sin(\frac{\theta}{2})}$$

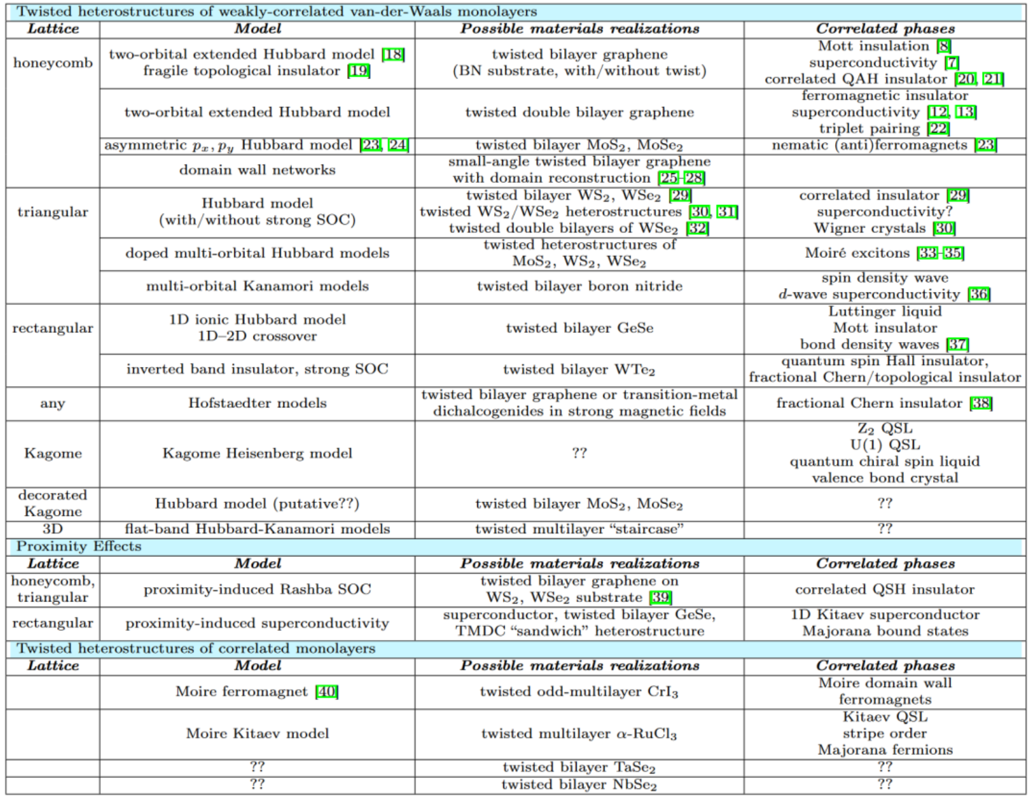
Lattice mismatch



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

2D Moiré platform





Twisted heterostructures of weakly-correlated van-der-Waals monolayers

Lattice	***Model***	***Possible materials realizations***	***Correlated phases***
honeycomb	two-orbital extended Hubbard model [18] fragile topological insulator [19]	twisted bilayer graphene (BN substrate, with/without twist)	Mott insulation [8] superconductivity [7] correlated QAH insulator [20, 21]
	two-orbital extended Hubbard model	twisted double bilayer graphene	ferromagnetic insulator superconductivity [12, 13] triplet pairing [22]
	asymmetric p_x, p_y Hubbard model [23, 24]	twisted bilayer MoS_2, $MoSe_2$	nematic (anti)ferromagnets [23]
	domain wall networks	small-angle twisted bilayer graphene with domain reconstruction [25–28]	
triangular	Hubbard model (with/without strong SOC)	twisted bilayer WS_2, WSe_2 [29] twisted WS_2/WSe_2 heterostructures [30, 31] twisted double bilayers of WSe_2 [32]	correlated insulator [29] superconductivity? Wigner crystals [30]
	doped multi-orbital Hubbard models	twisted heterostructures of MoS_2, WS_2, WSe_2	Moiré excitons [33–35]
	multi-orbital Kanamori models	twisted bilayer boron nitride	spin density wave *d*-wave superconductivity [36]
rectangular	1D ionic Hubbard model 1D–2D crossover	twisted bilayer GeSe	Luttinger liquid Mott insulator bond density waves [37]
	inverted band insulator, strong SOC	twisted bilayer WTe_2	quantum spin Hall insulator, fractional Chern/topological insulator
any	Hofstaedter models	twisted bilayer graphene or transition-metal dichalcogenides in strong magnetic fields	fractional Chern insulator [38]
Kagome	Kagome Heisenberg model	??	Z_2 QSL U(1) QSL quantum chiral spin liquid valence bond crystal
decorated Kagome	Hubbard model (putative??)	twisted bilayer MoS_2, $MoSe_2$	??
3D	flat-band Hubbard-Kanamori models	twisted multilayer "staircase"	??

Proximity Effects

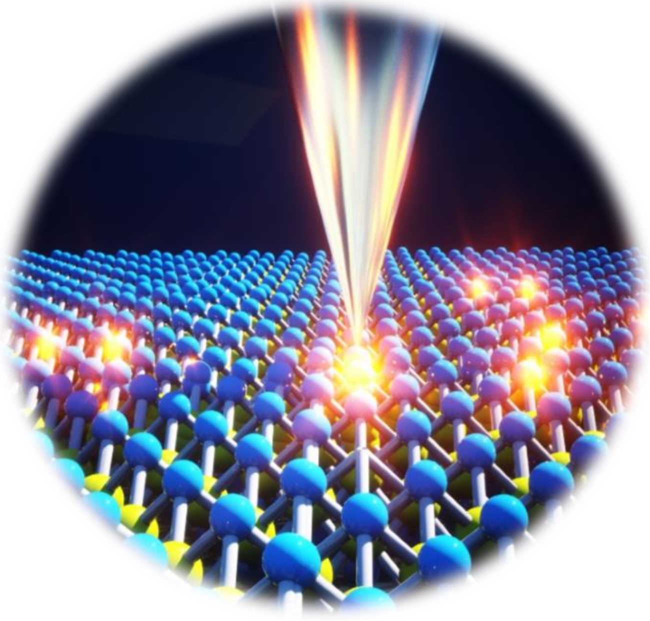
Lattice	***Model***	***Possible materials realizations***	***Correlated phases***
honeycomb, triangular	proximity-induced Rashba SOC	twisted bilayer graphene on WS_2, WSe_2 substrate [39]	correlated QSH insulator
rectangular	proximity-induced superconductivity	superconductor, twisted bilayer GeSe, TMDC "sandwich" heterostructure	1D Kitaev superconductor Majorana bound states

Twisted heterostructures of correlated monolayers

Lattice	***Model***	***Possible materials realizations***	***Correlated phases***
	Moire ferromagnet [40]	twisted odd-multilayer CrI_3	Moire domain wall ferromagnets
	Moire Kitaev model	twisted multilayer α-$RuCl_3$	Kitaev QSL stripe order Majorana fermions
	??	twisted bilayer $TaSe_2$	??
	??	twisted bilayer $NbSe_2$	??

Nature Physics 17, 155–163 (2021)

Quantum matter at the atomic scale

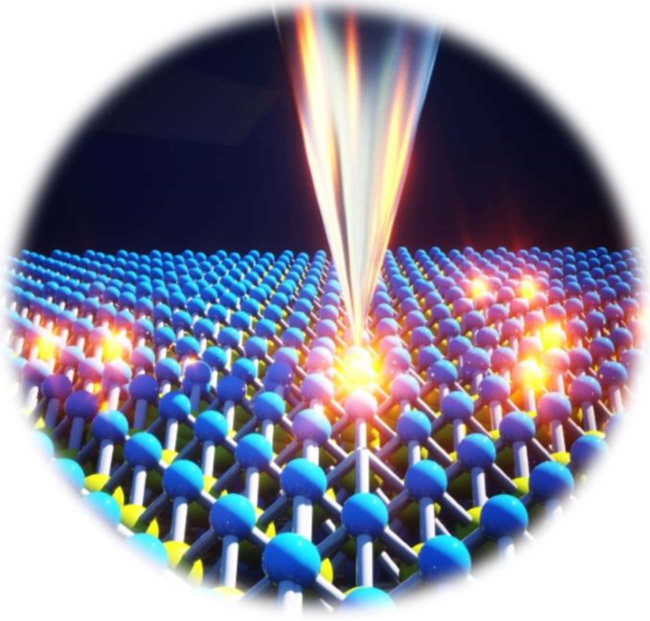


- Defects
- **Moiré patterns**
- Magnetic TI
- CDW

1. Realizing mixed symmetry moiré patterns

2. Reversible control of ferroelectric domains in twisted TMDS

Quantum matter at the atomic scale



- Defects
- **Moiré patterns**
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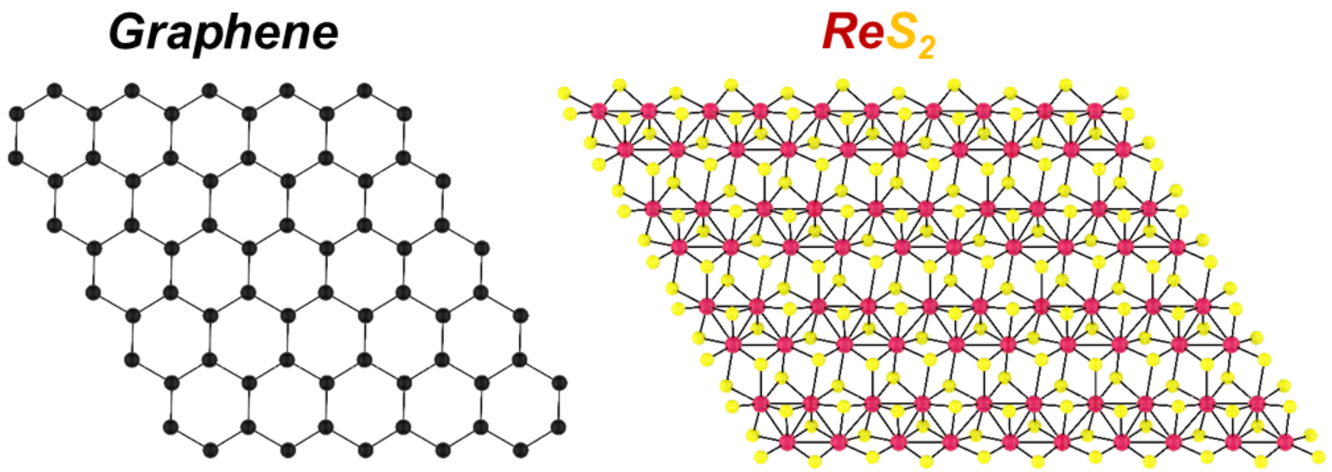
1. Realizing mixed symmetry moiré patterns

2. Reversible control of ferroelectric domains in twisted TMDS

Moiré patterns from mixed symmetry systems



- For two materials with different crystal structures, the moiré patterns emerge due to the interference of extended unit cells

M. Le Ster, et al. 2D Mater. 7(1), 011005 (2020).

Moiré patterns from mixed symmetry systems

Primitive Unit Cells:

$\{a_1, a_2\}$

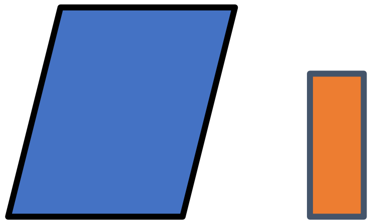
$\{b_1, b_2\}$

→

Extended Unit Cells:

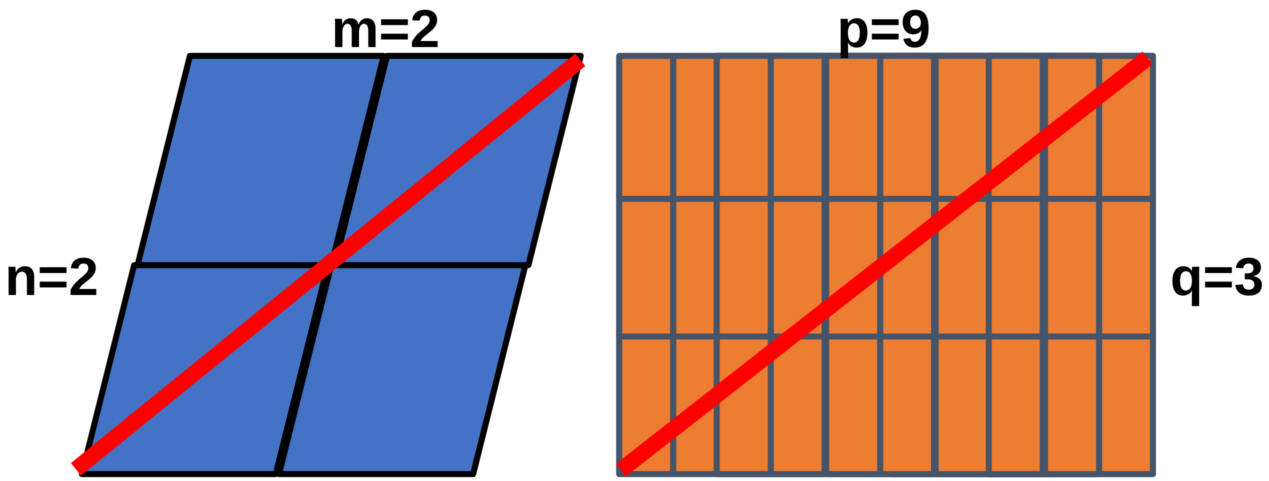
$\{m*a_1, n*a_2\}$

$\{p*b_1, q*b_2\}$



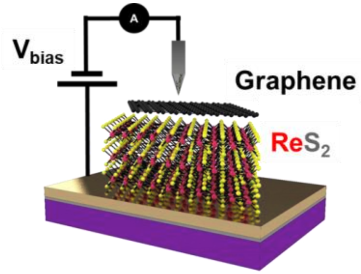
Primitive Unit Cells
(Mismatched)

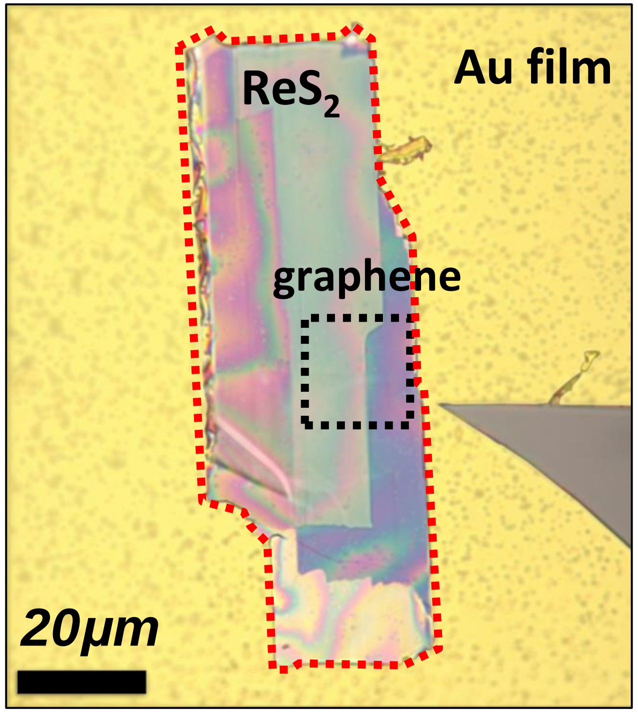
→

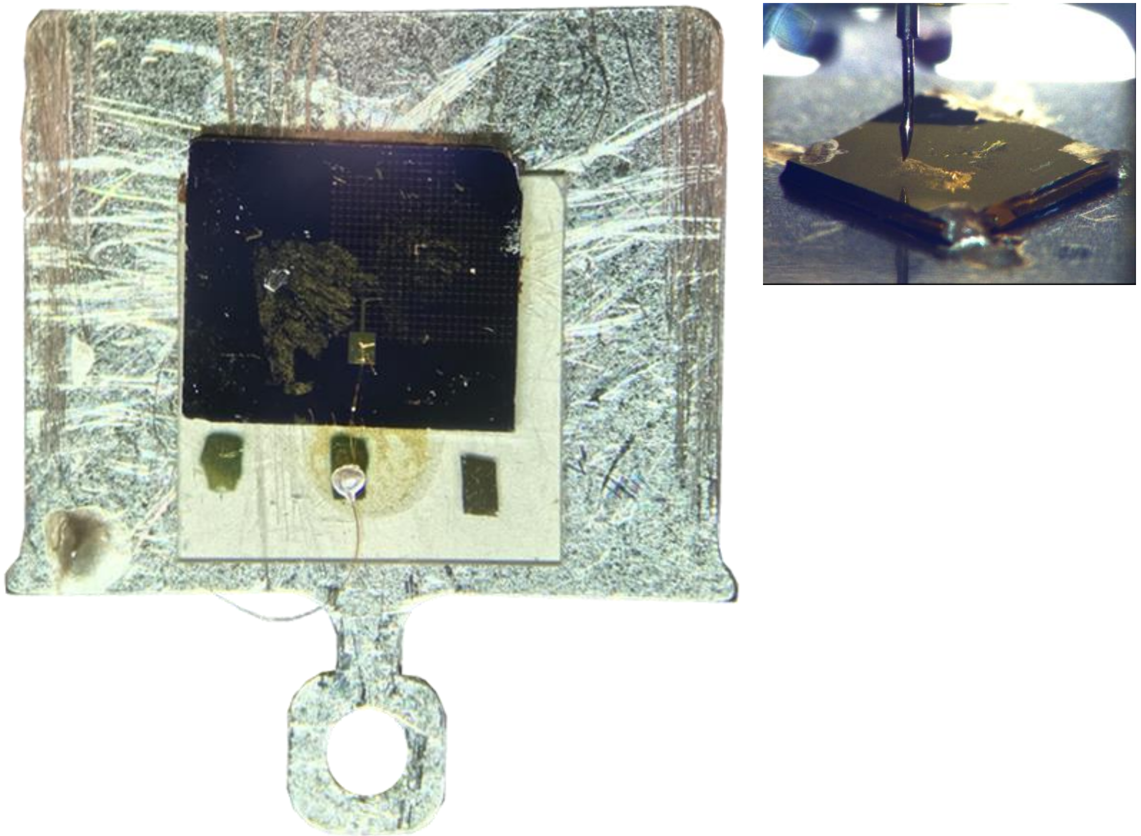


Extended Unit Cells
(Nearly the same on the diagonal)

Graphene - Rhenium Disulfide vertical heterostructures



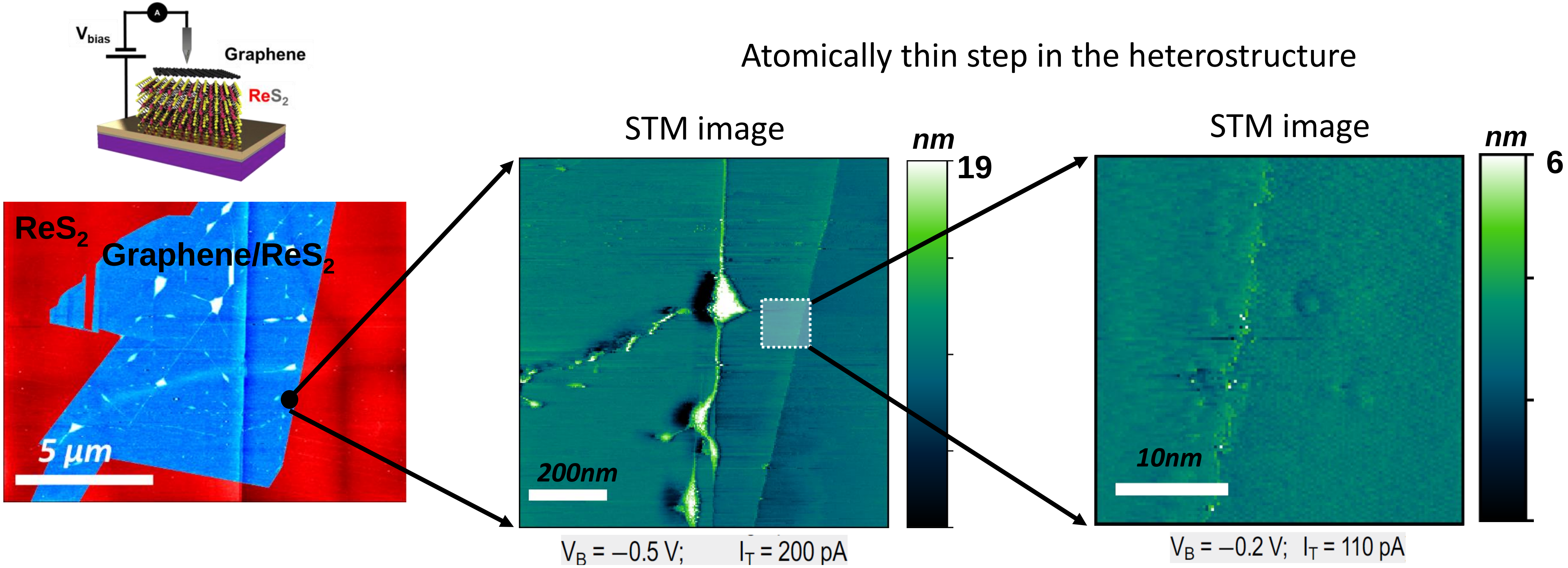




JAP 128 (4), 044303 **(2020)**

Graphene - Rhenium Disulfide vertical heterostructures

Atomically thin step in the heterostructure

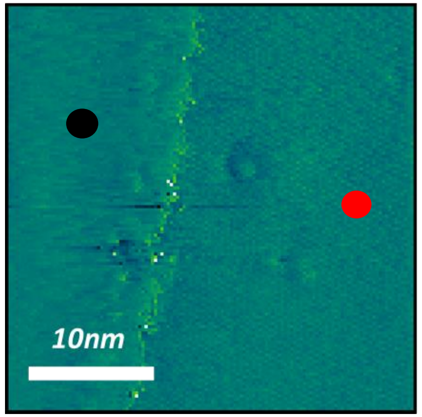


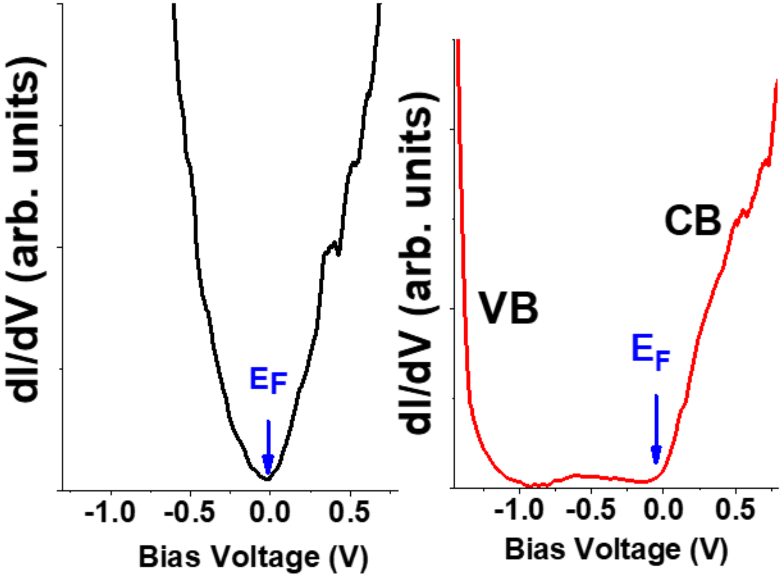
JAP 128 (4), 044303 **(2020)**

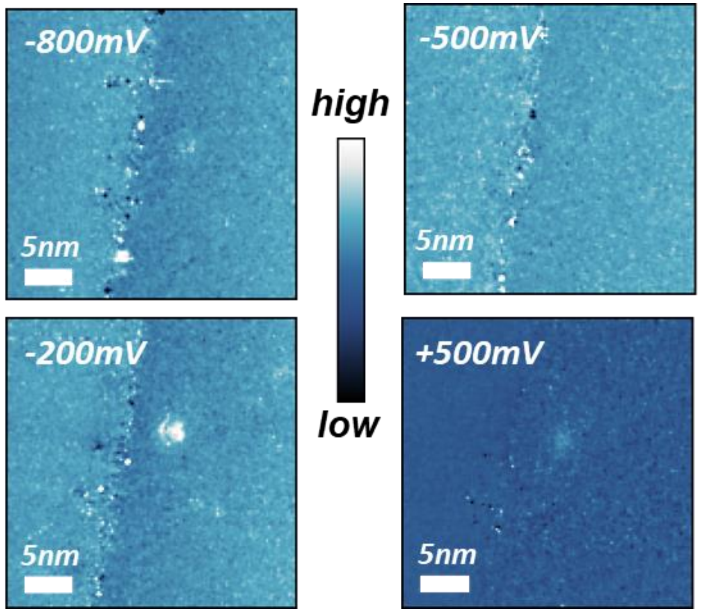
Graphene - Rhenium Disulfide vertical heterostructures

Band alignment at the interface
Scanning Tunneling Spectroscopy

STM image



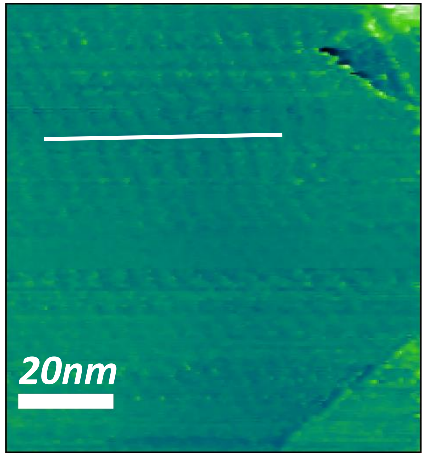




JAP 128 (4), 044303 **(2020)**

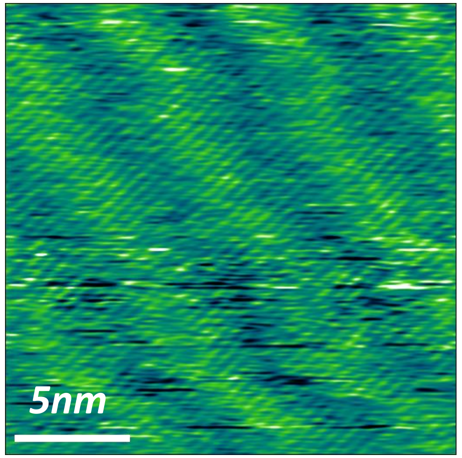
Graphene - Rhenium Disulfide vertical heterostructures

STM image

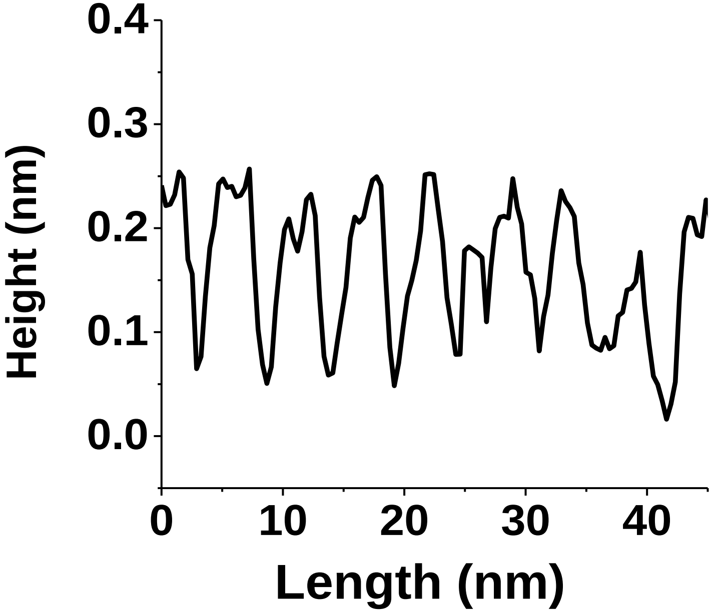


$V_B = -1.0\ V;\ I_T = 100\ pA$

STM image



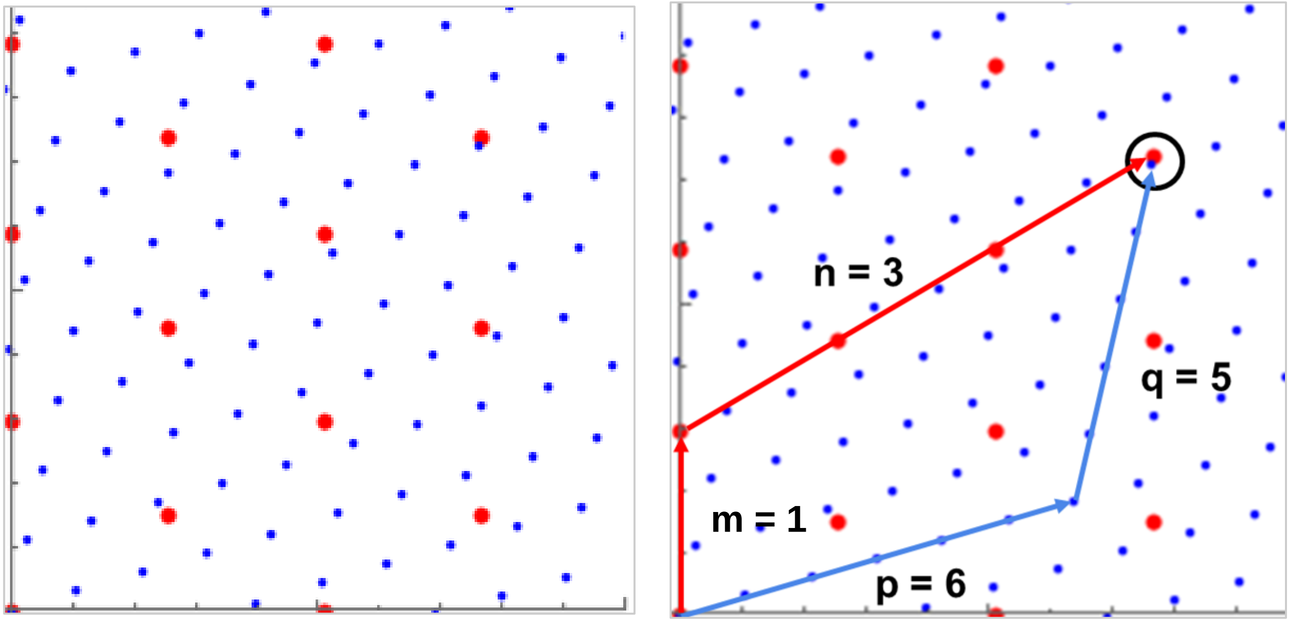
$V_B = -1.0\ V;\ I_T = 100\ pA$



JAP 128 (4), 044303 **(2020)**

Moiré patterns from mixed symmetry systems

Graphene, ReS_2



Mohammed Ezzi, Shaffique Adam. (National University of Singapore)

Moiré wavelength as a function of angle

$G_{mn} = m^*G_1 + n^*G_2$

$S_{pq}(\theta) = p^*S_1(\theta) + q^*S_2(\theta)$

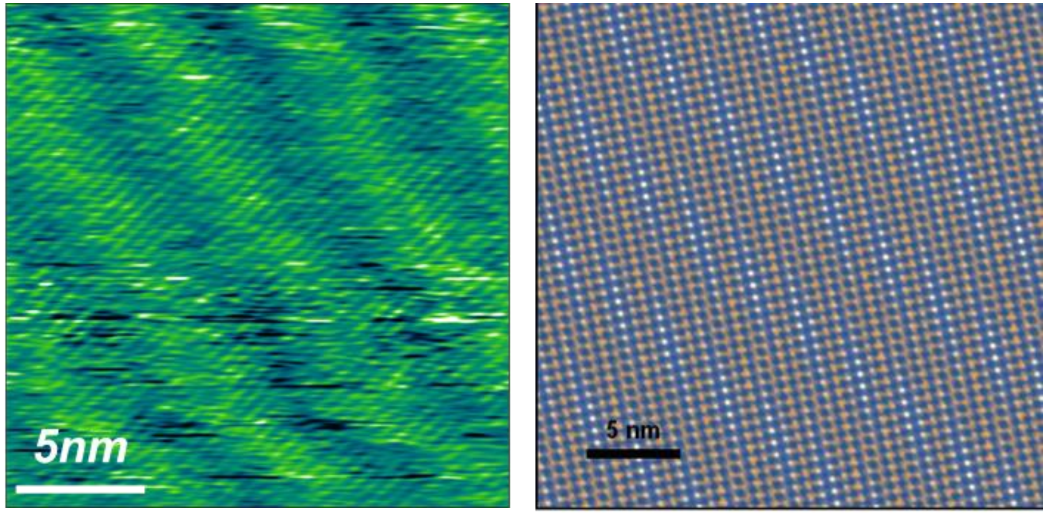
$$\boxed{\lambda_{mnpq}(\theta) = |G_{mn} - S_{pq}(\theta)|^{-1}}$$

Theory: Mohammed Ezzi, Shaffique Adam.
(National University of Singapore)

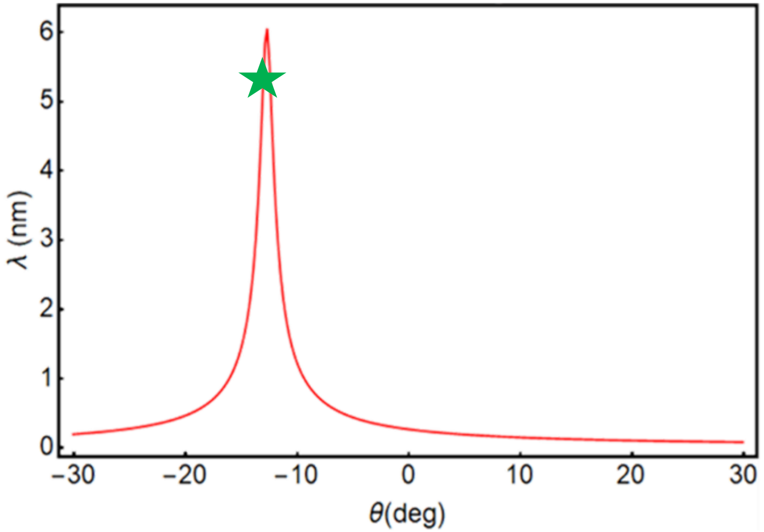
M. Le Ster, T. Märkl, and S. A. Brown, 2D Mater. 7(1), 011005 (2020)

Graphene - Rhenium Disulfide vertical heterostructures

12° twist with periodicity 5.2 nm.



$$\lambda_{mnpq} = |K_{mnpq}|^{-1}$$



$$(m, n, p, q) = (3, 1, 6, 5)$$

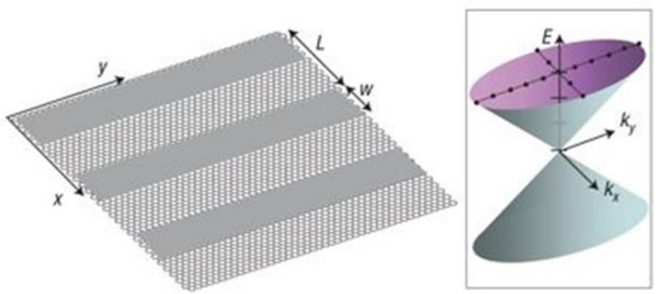
{a1 , a2} , {b1 , b2} Basic unit cells

{m a1, n a2}, {p b1, q b2} Extended unit cells

JAP 128 (4), 044303 **(2020)**

Mixed symmetry patterns

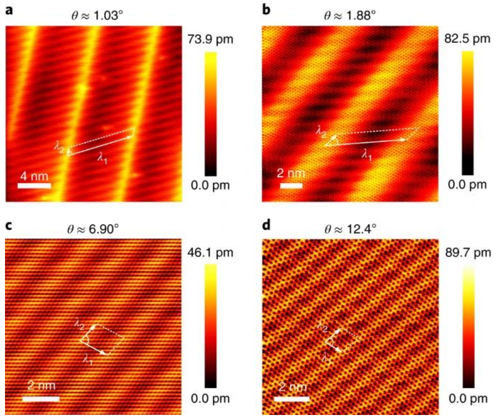
Anisotropic Dirac cone?



Park et al. Nature Physics **volume 4**, pages 213–217 (2008)

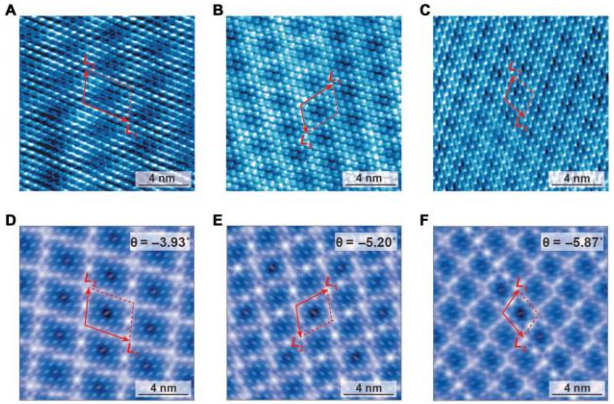
Nature Nanotechnology volume 16, pages 525–530 (2021)

Graphene/BP



Nat. Nano. 13(9), 828–834 (2018).

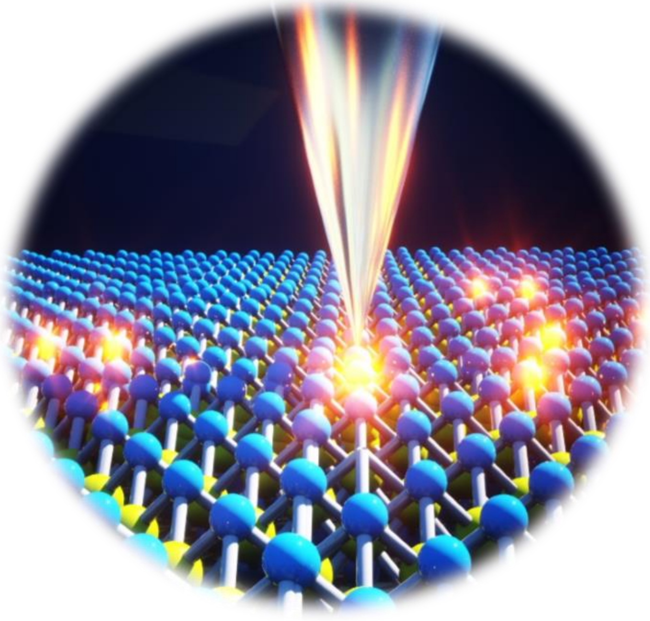
$ReSe_2$/Graphene



Sci. Adv. 5(7), 2347 (2019)

JAP 128 (4), 044303 **(2020)**

Quantum matter at the atomic scale

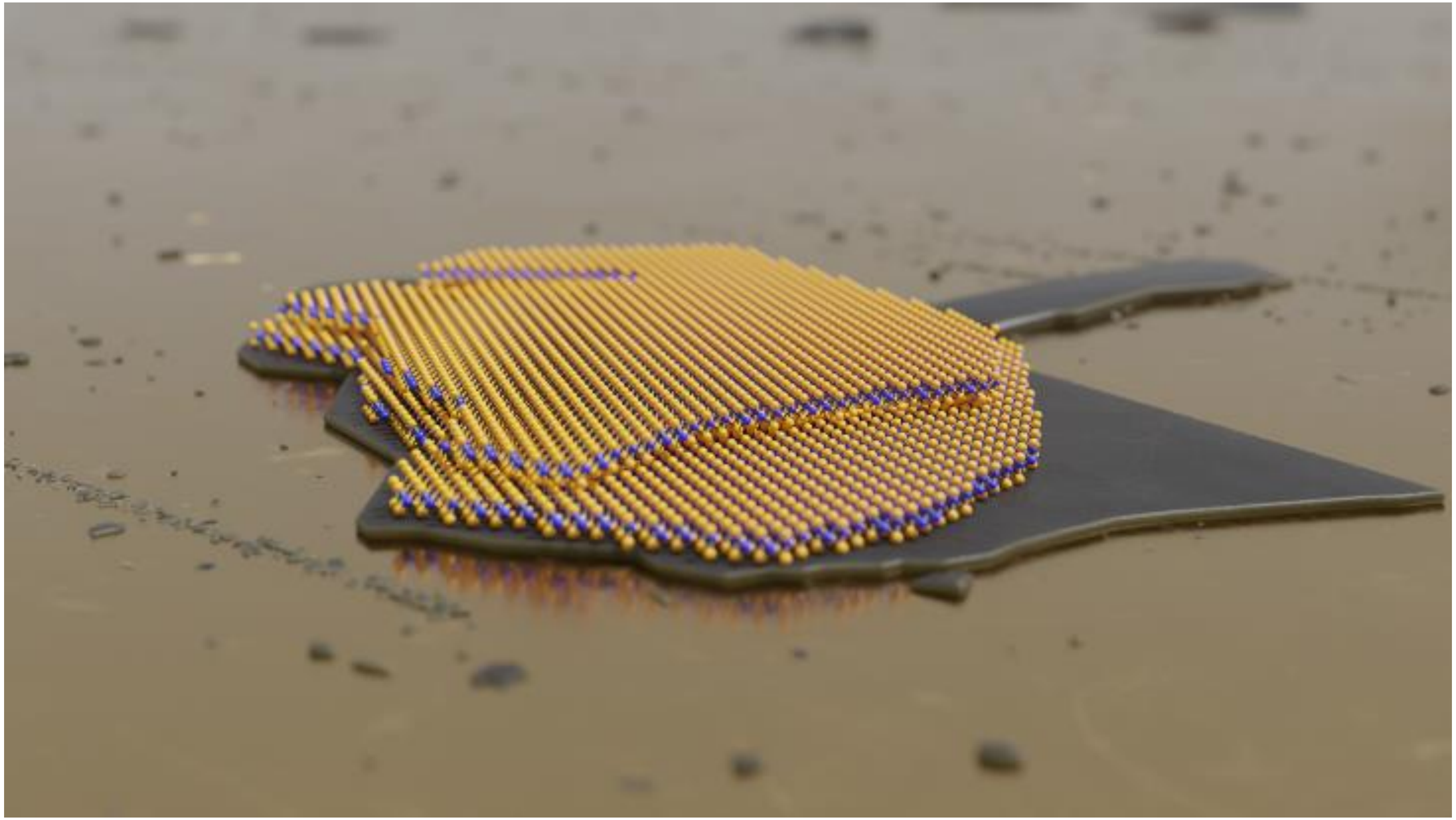


- Defects
- **Moiré patterns**
- Magnetic TI
- CDW

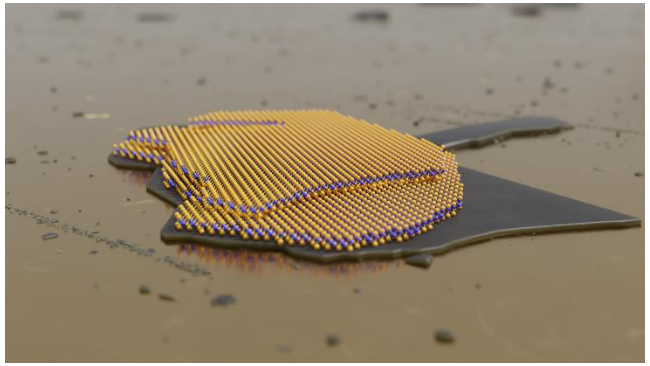
1. Realizing mixed symmetry moiré patterns

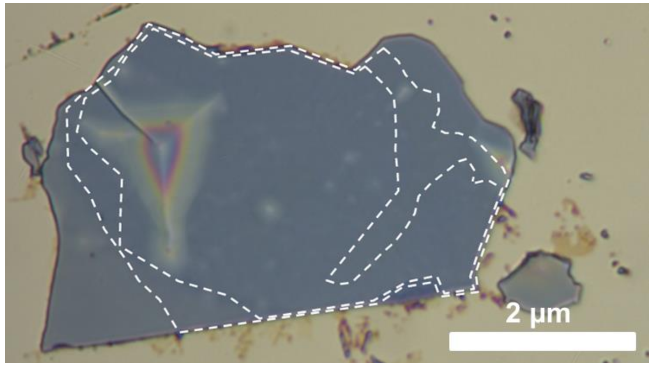
2. Reversible control of ferroelectric domains in twisted TMDS

Twisted transition metal dichalcogenides

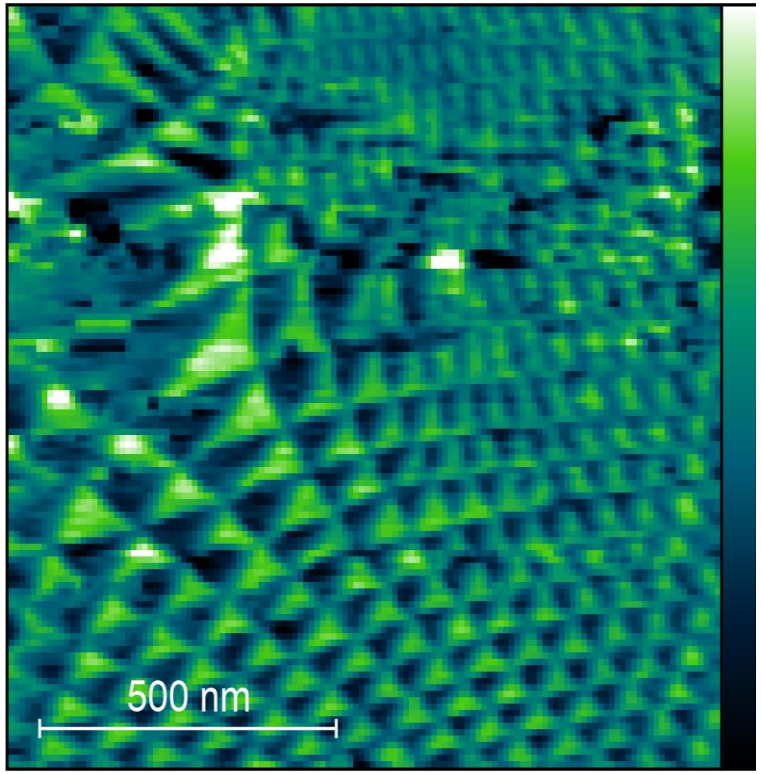


Twisted transition metal dichalcogenide WS_2

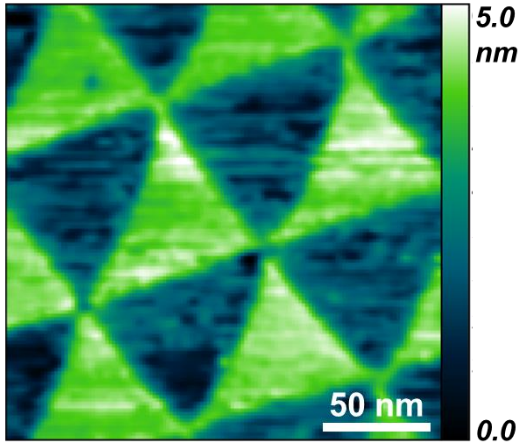


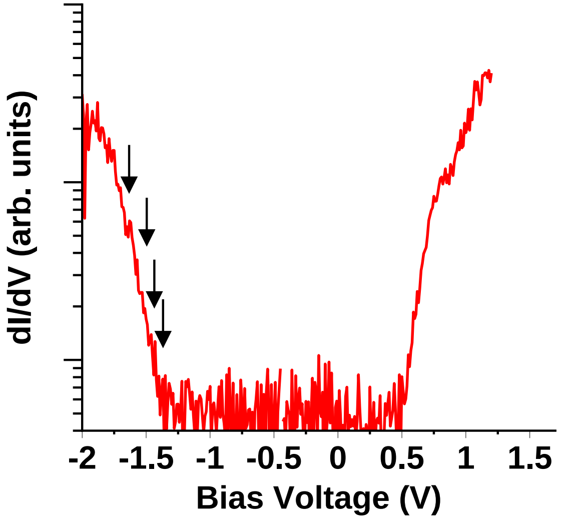


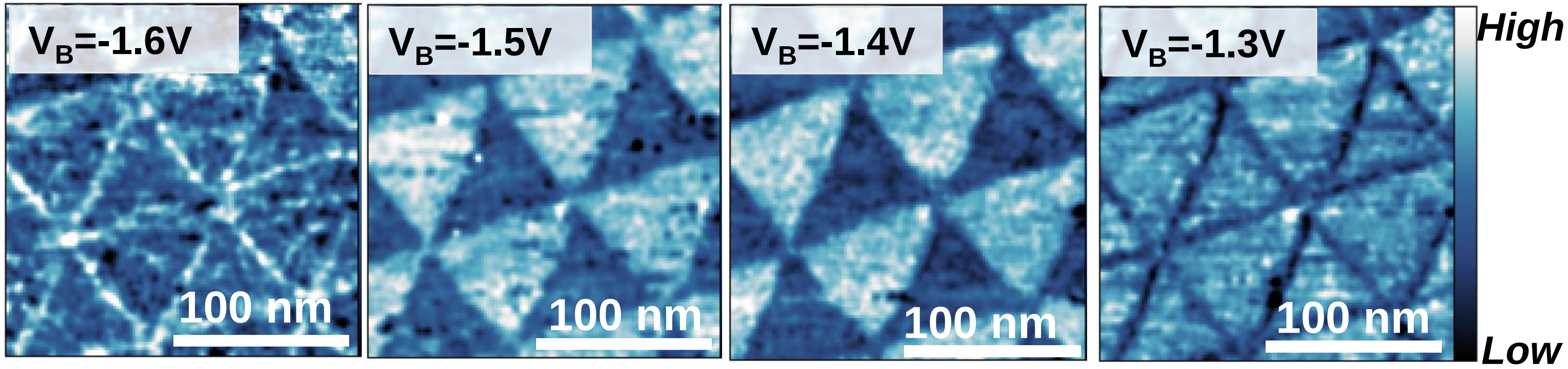
Scanning Tunneling Microscopy (STM)



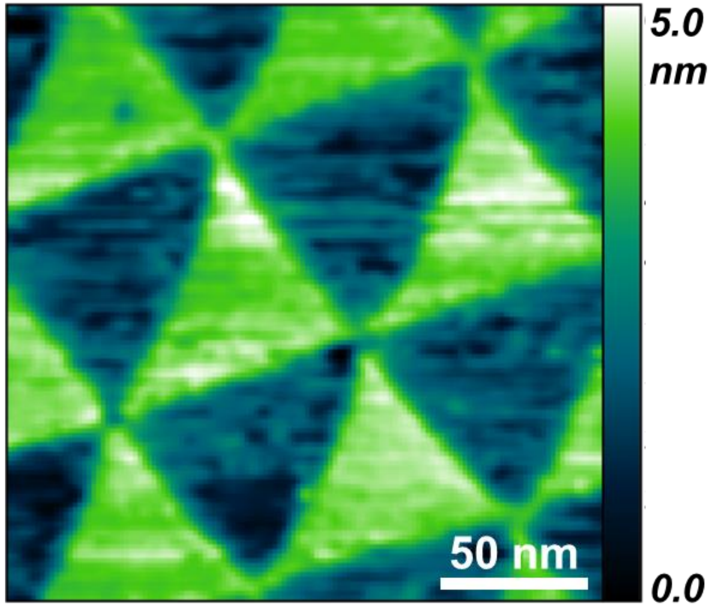
Twisted transition metal dichalcogenides - WS$_2$

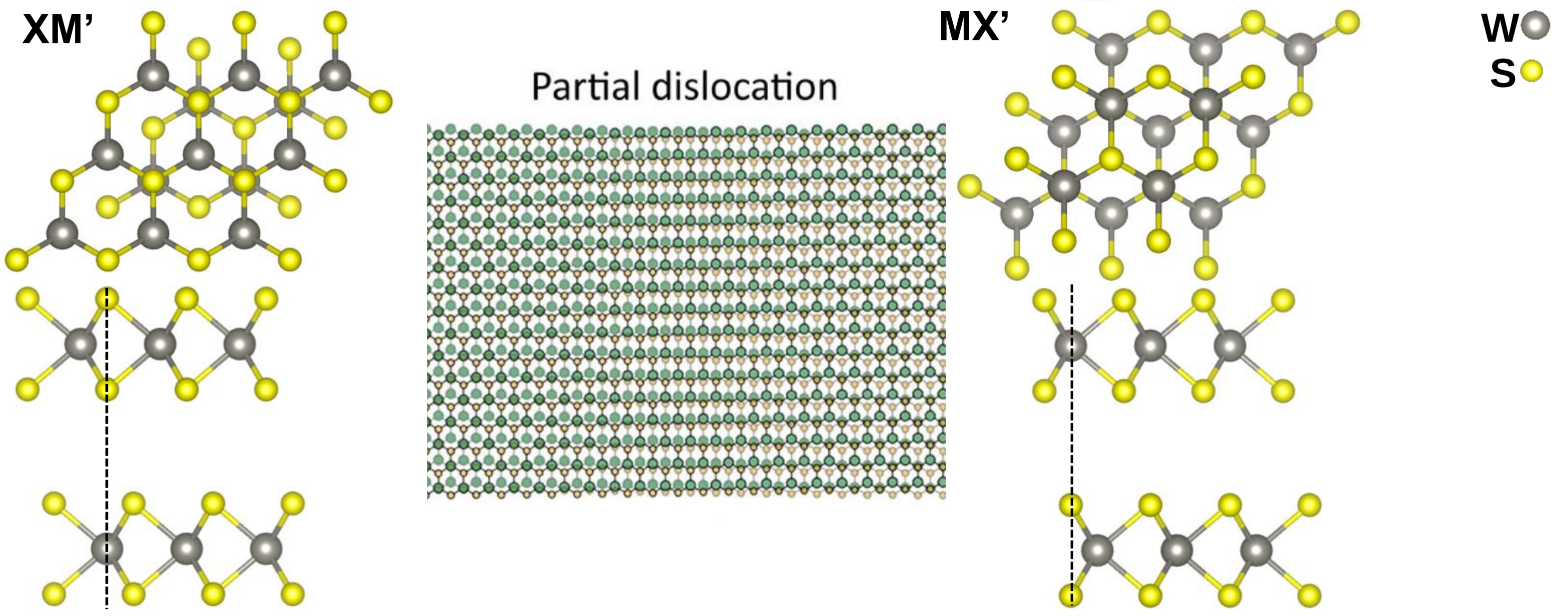






Twisted transition metal dichalcogenides – reconstruction domains

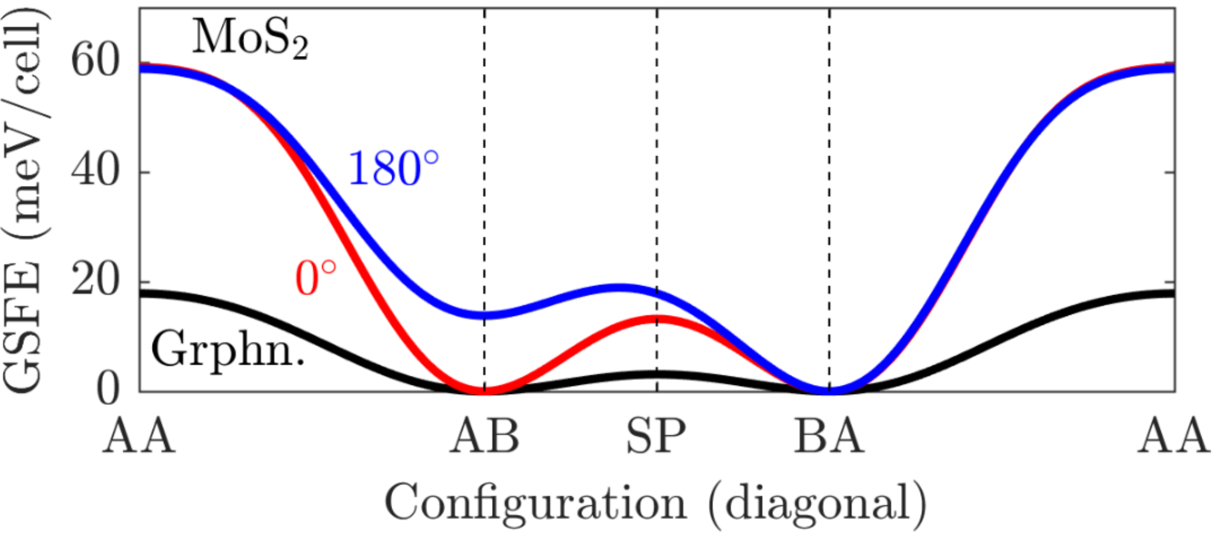




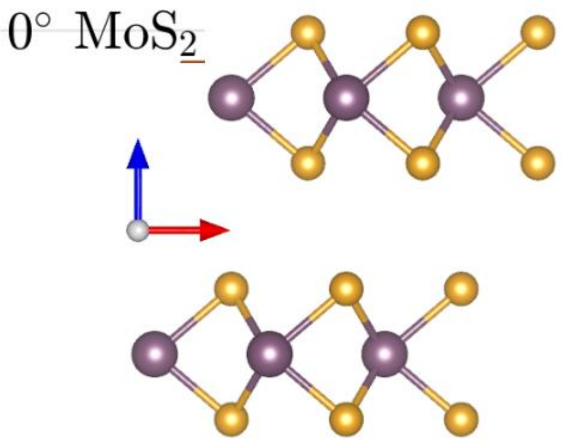
Periodicity 78 nm → twist angle 0.23°

Twisted transition metal dichalcogenides – reconstruction domains

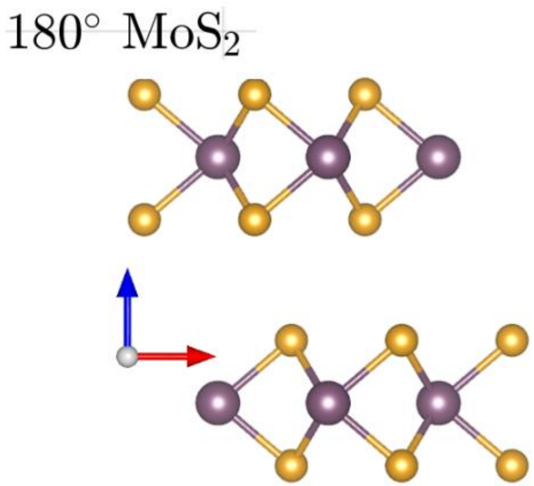
atomic relaxation → minimize the additional energy due to misalignment



parallel (P)



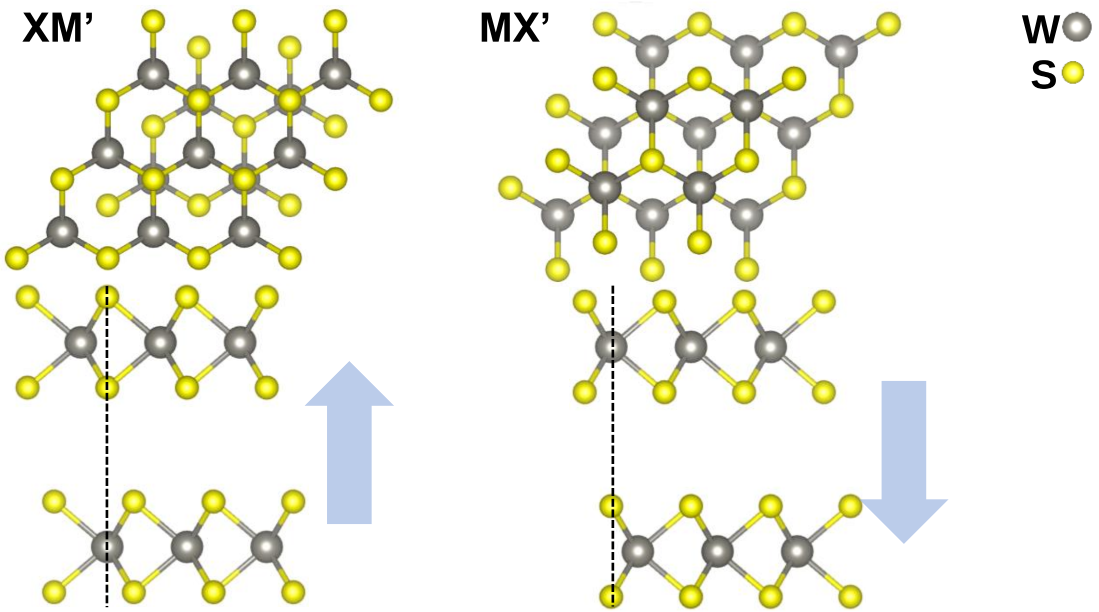
antiparallel (AP)



Enaldiev V. et al. *Phys. Rev. Lett.* **124**, 206101 (2020).
Weston, A. *et al. Nat. Nanotechnol.* **15**, 592–597 (2020).
Rosenberger, M. R. *et al. ACS Nano* **14**, 4550–4558 (2020).

Naik, M. H. & Jain, M. *Phys. Rev. Lett.* **121**, 266401 (2018).
Wang, X. *et al. Nat. Nanotechnol.* (2022)
Carr, S. *et al. Phys. Rev. B* **98**, 1–7 (2018).

Twisted transition metal dichalcogenides – polarization domains



Spontaneous interlayer charge transfer → **out-of-plane ferroelectric polarisation**

Ferreira, F., *et al. Sci. Rep.* **11**, 1–10 (2021).
Enaldiev, V. *et al. Nano Lett.* **22**, 1534–1540 (2022)
Wang, X. *et al. Nat. Nanotechnol.* (2022)

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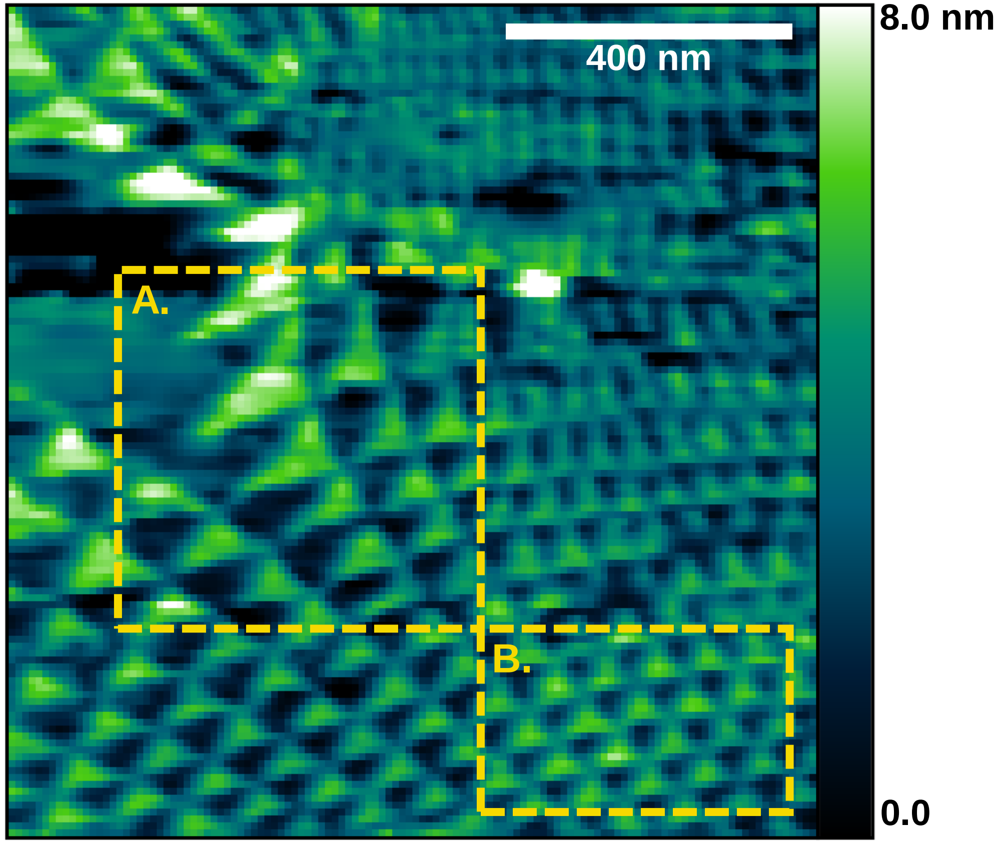
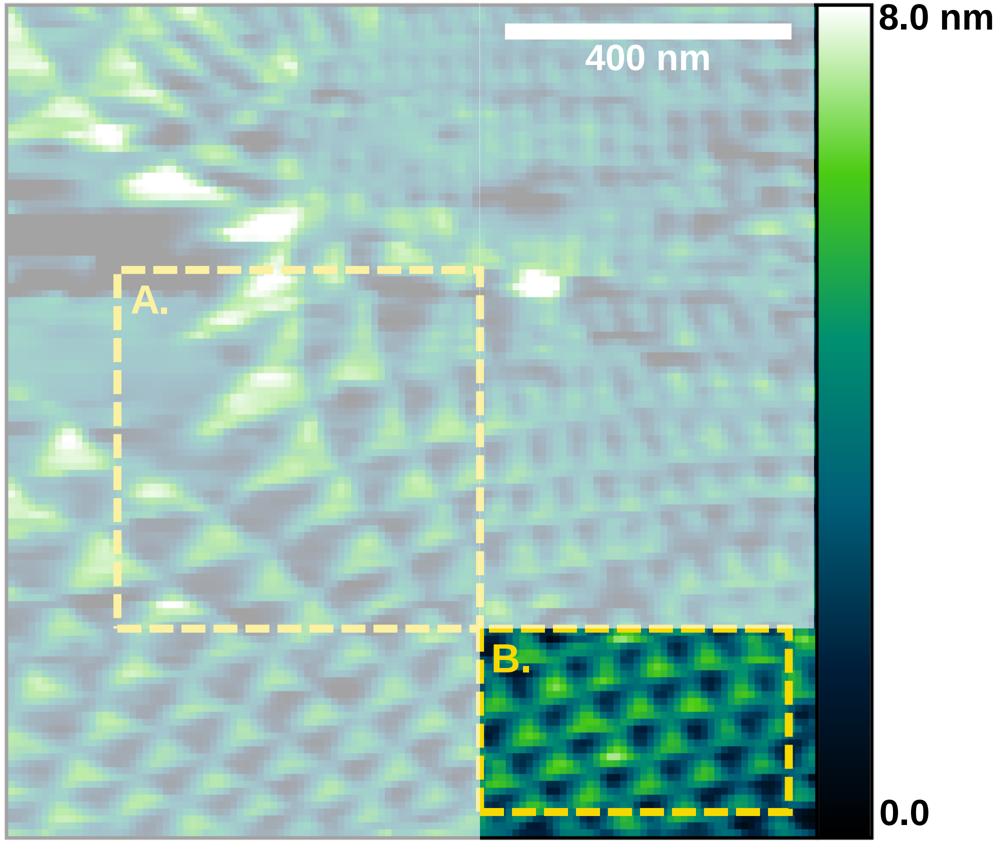
Weston, A. *et al. Nature Nano*. (2021)

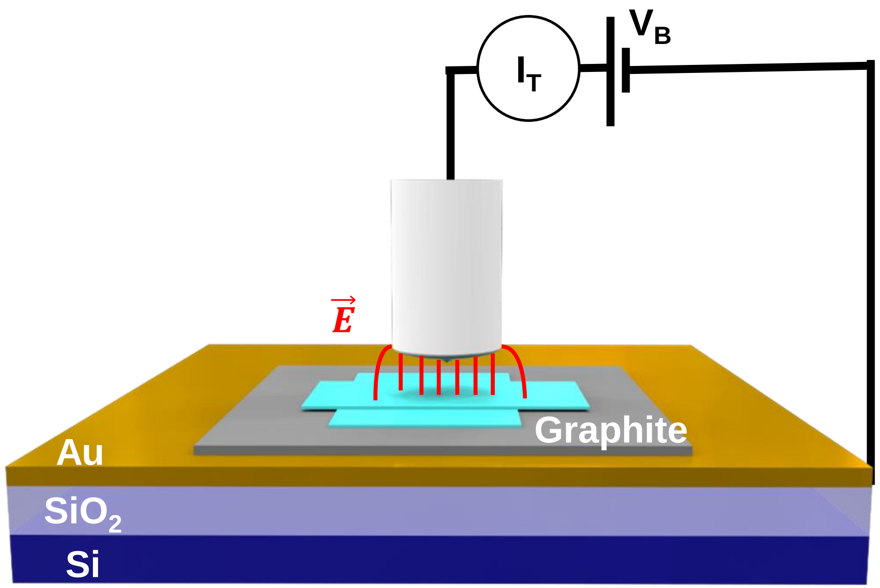
Twisted transition metal dichalcogenides WS_2



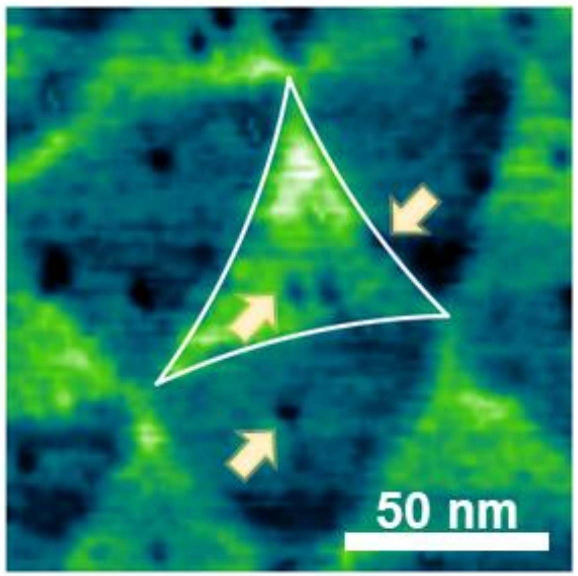
Twisted transition metal dichalcogenides WS_2



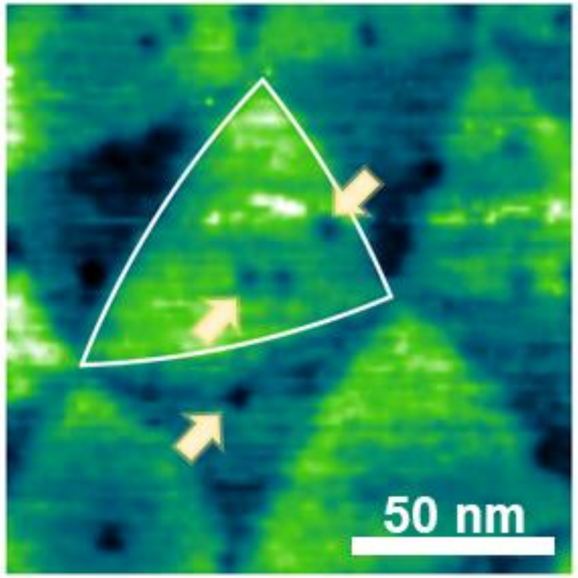
Electric field control over the ferroelectric domains



$V_B<0$



$V_B>0$

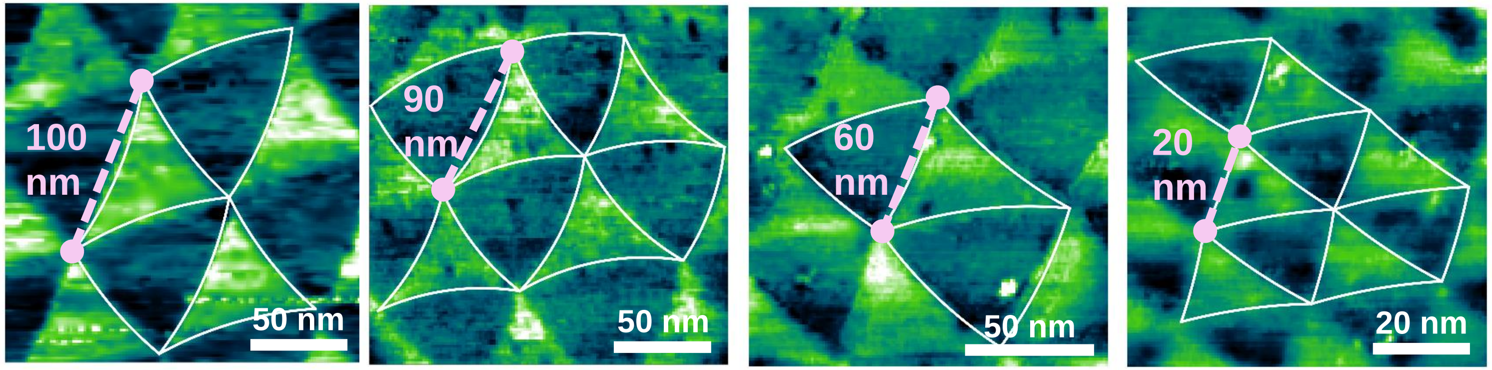


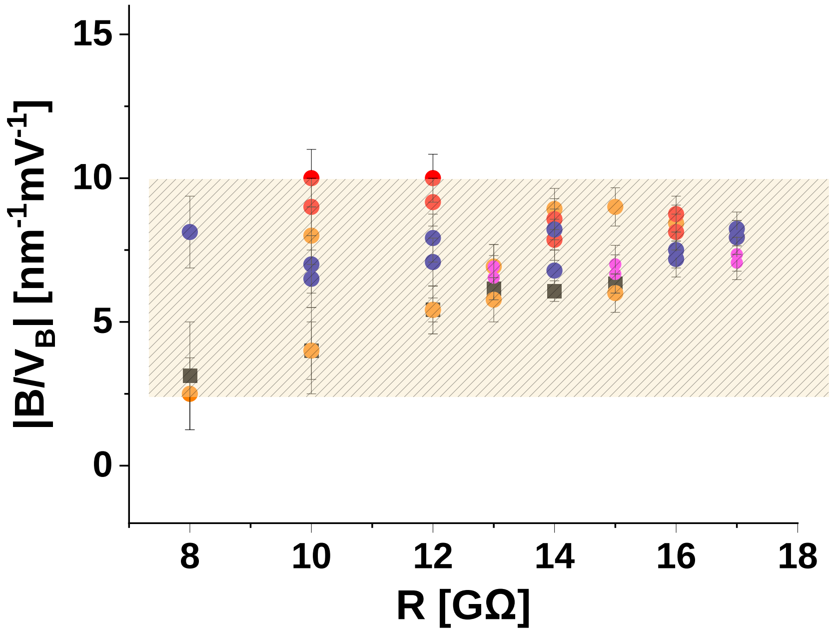
Twisted transition metal dichalcogenides

$$F(x) = \int_0^x \frac{f(x')}{\sqrt{1 - f^2(x')}} dx'$$

$$f^3 - Af - B\left(x - \frac{\ell}{2}\right) = 0$$

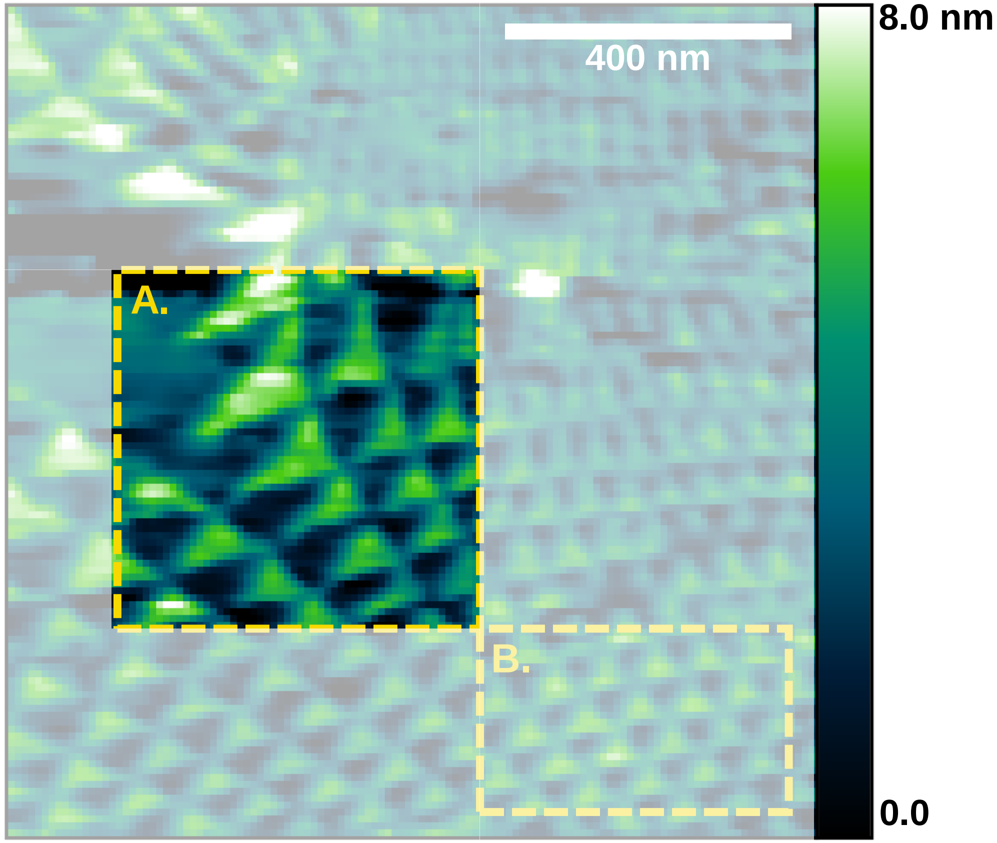
$$A = \frac{\omega}{\tilde{\omega}} + 2,\ B = \frac{2D\Delta}{\tilde{\omega}}$$



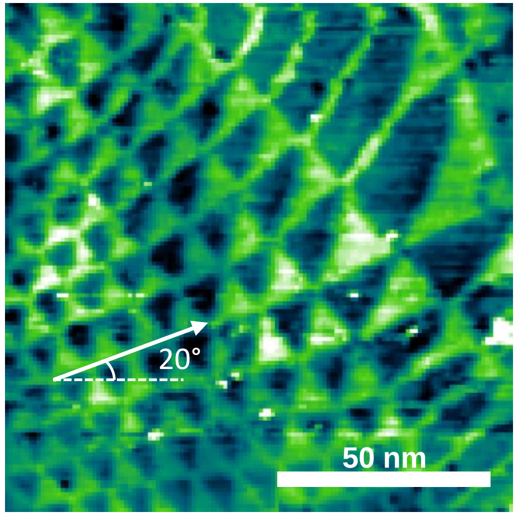


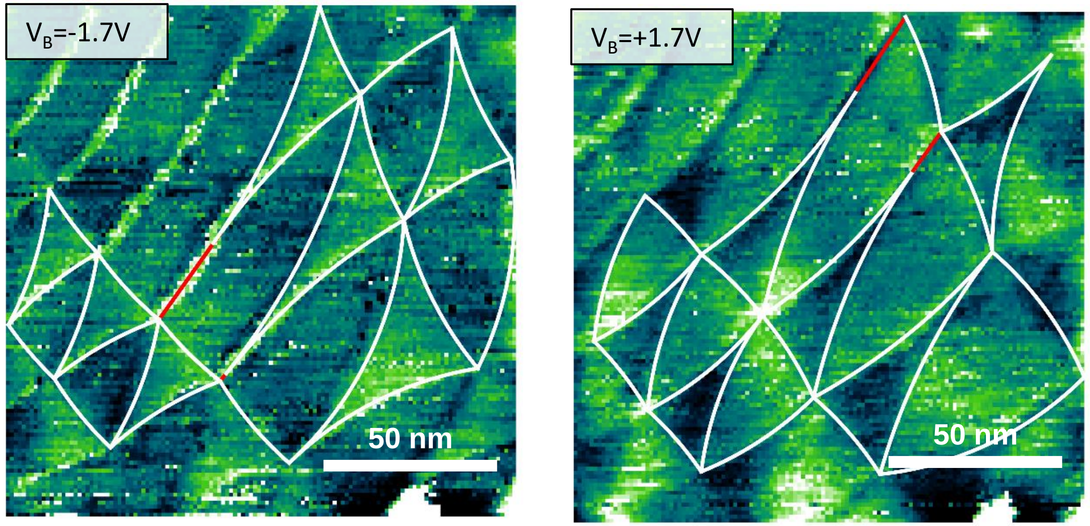
Model by: Vladimir Enaldiev, Vladimir Falko *University of Manchester, UK*

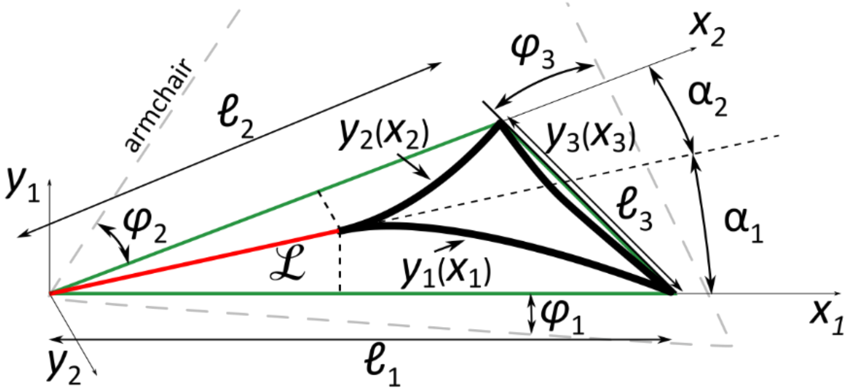
Twisted transition metal dichalcogenides WS_2

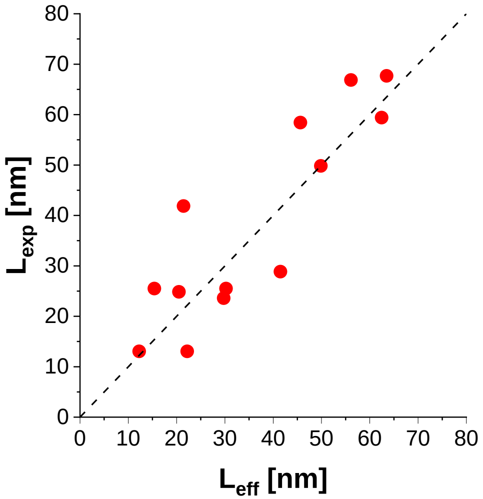


Twisted transition metal dichalcogenides

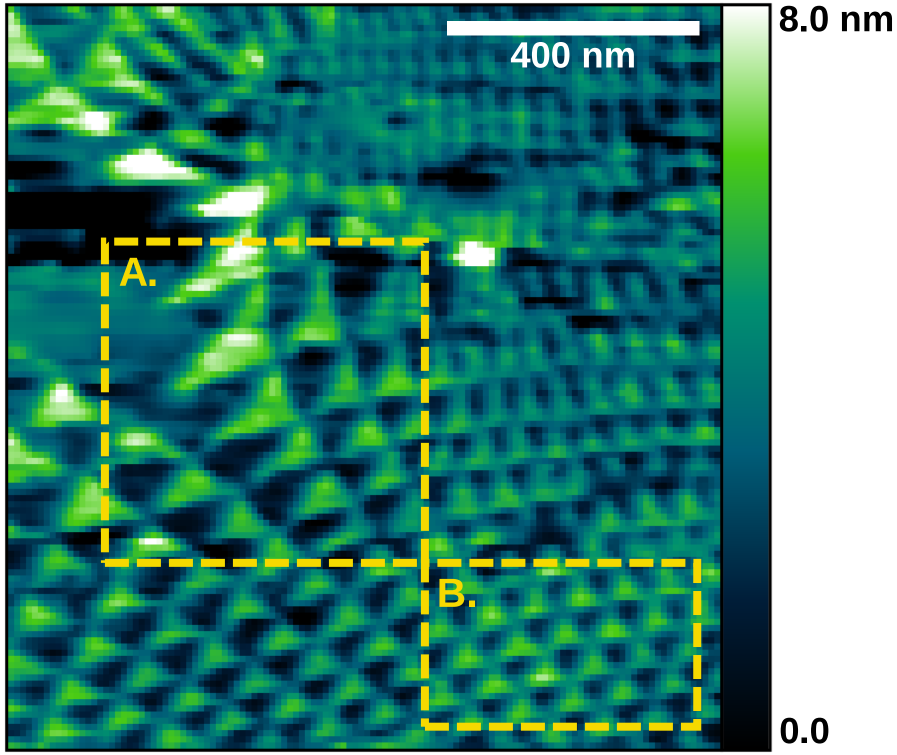


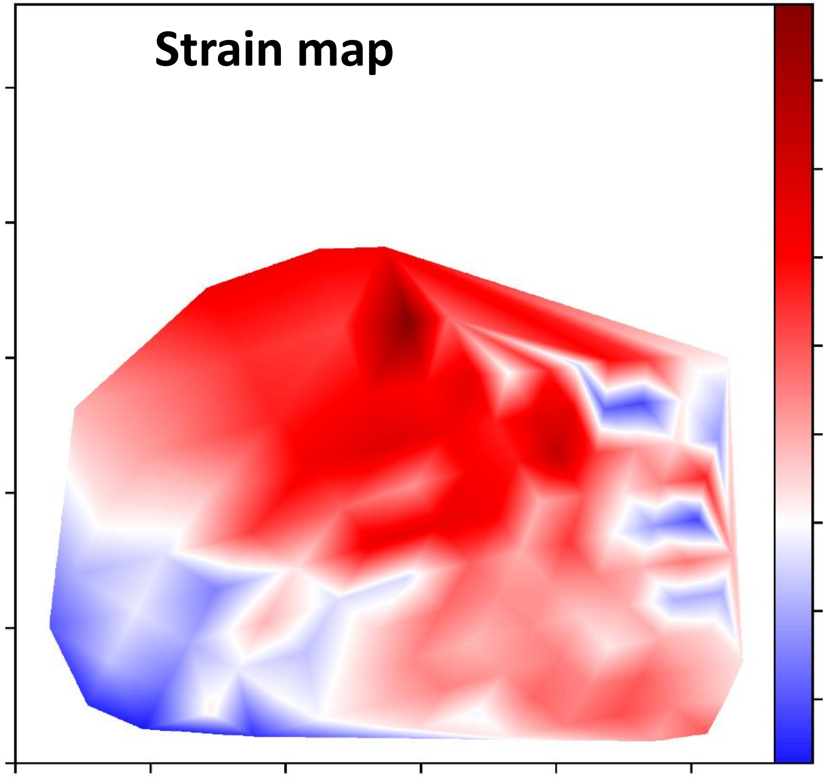




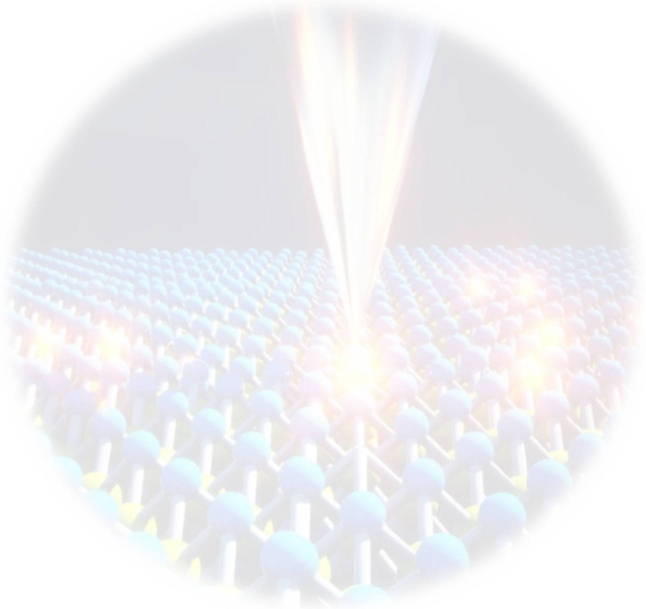


Twisted transition metal dichalcogenides





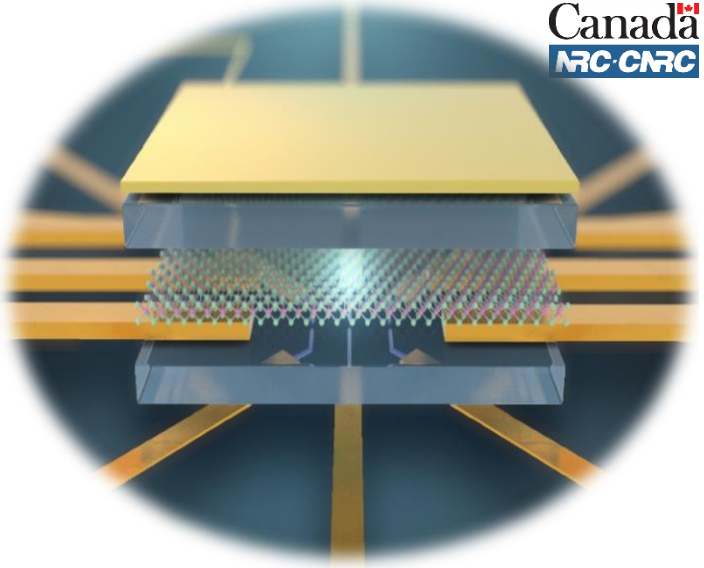
Quantum matter at the atomic scale



- Defects, edges, boundaries
- **Moiré patterns**

JAP 128 (4), 044303 **(2020)**
Phys. Rev. B 102, 205408 **(2020)**

Quantum circuits in 2D materials



- Quantum confined structures for quantum computing and sensing

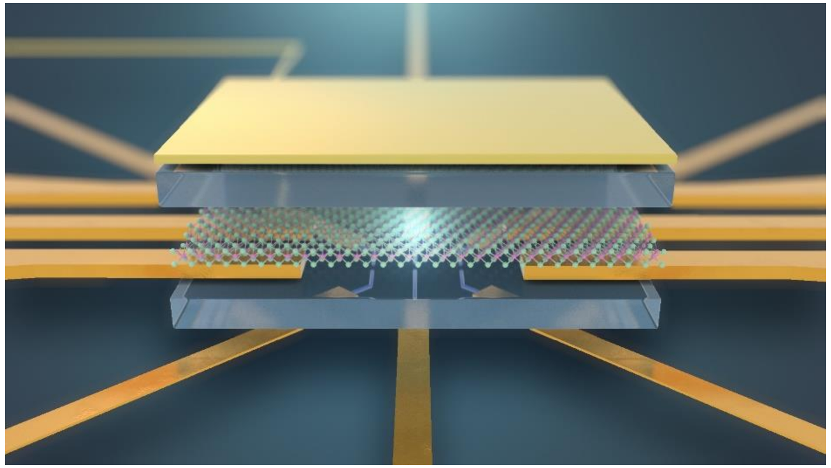
preprint arXiv:2203.11871 ***(2022)***
Appl. Phys. Lett. 119, 133104 **(2021)**
Appl. Phys. Lett. 115, 231603 **(2019)**

Canada
NRC·CNRC

With Dr. Louis Gaudreau

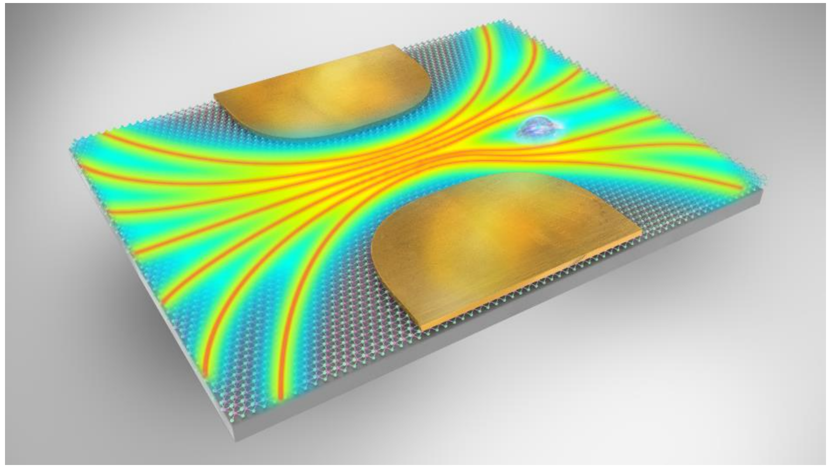
Tungsten Diselenide (WSe_2)

Gated Quantum Dots



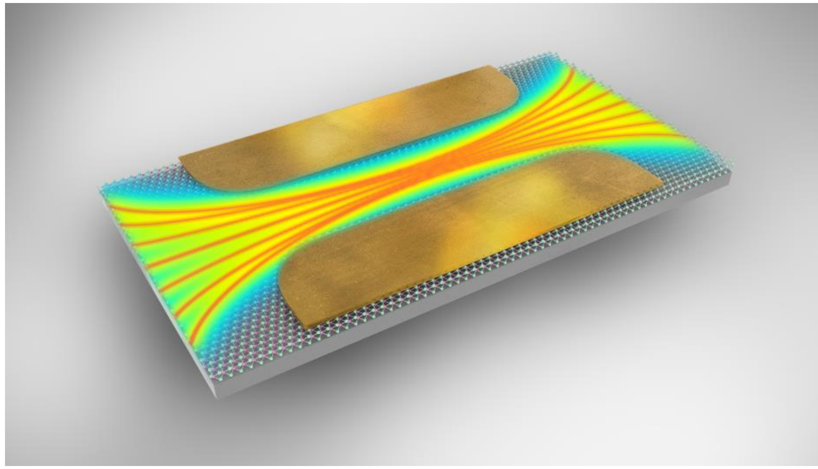
Appl. Phys. Lett. 119, 133104 **(2021)**
Appl. Phys. Lett. 115, 231603 **(2019)**

Nano-Constriction for Charge Detection



preprint arXiv:2203.11871 ***(2022)***

Quantized Transport in a 1D Channel



In preparation

uOttawa

Wafer-scale growth

✓ uOttawa instrument capabilities:

Graphene on sapphire (c-plane 0001)

Gases: H2, CH4, Ar

Boron Nitride on sapphire (c-plane 0001)

Gases: H2, Ar

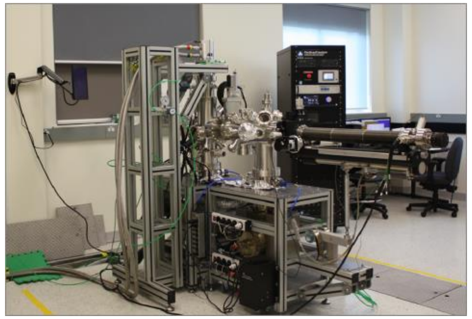
MO: Borazine

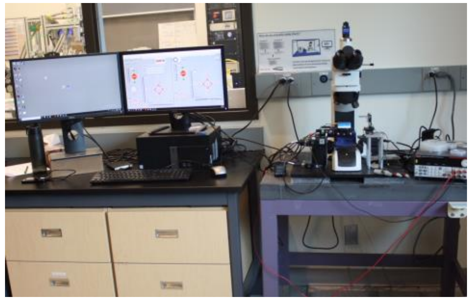
Tungsten Disulfide on sapphire (c-plane 0001)

Gases: H2, Ar

MO: Tungsten hexacarbonyl, Ditertiarybutylsulfide

Merci! Thank you!





Cleanroom user facility

CRPuO

Access to nanofab cleanroom facilities

Materials characterization user facility

CAMaR

Access to materials characterization facilities

uOttawa

NSERC CRSNG

Ontario Research Fund

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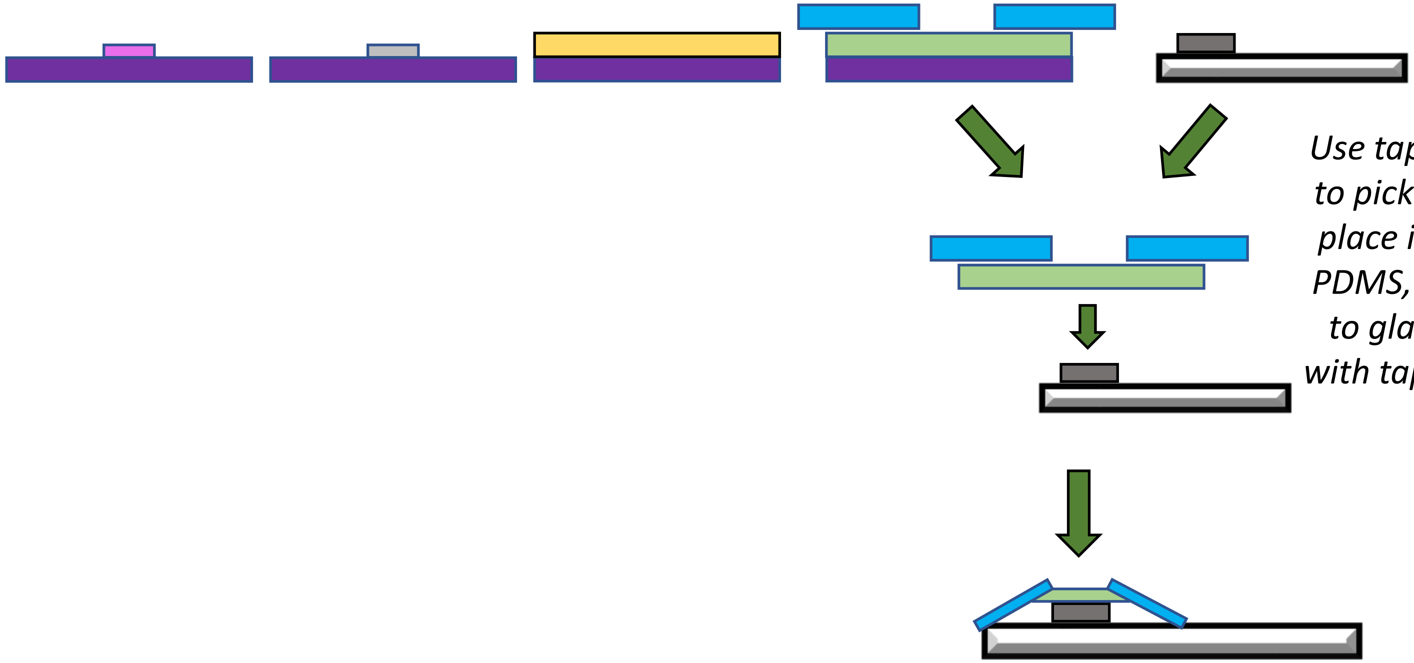
INNOVATION POUR LA DÉFENSE, L'EXCELLENCE ET LA SÉCURITÉ

Canada
NRC·CNRC

Part 1: Prepare Ingredients



Flake 1 on substrate

Flake 2 on substrate

Gold-coated substrate

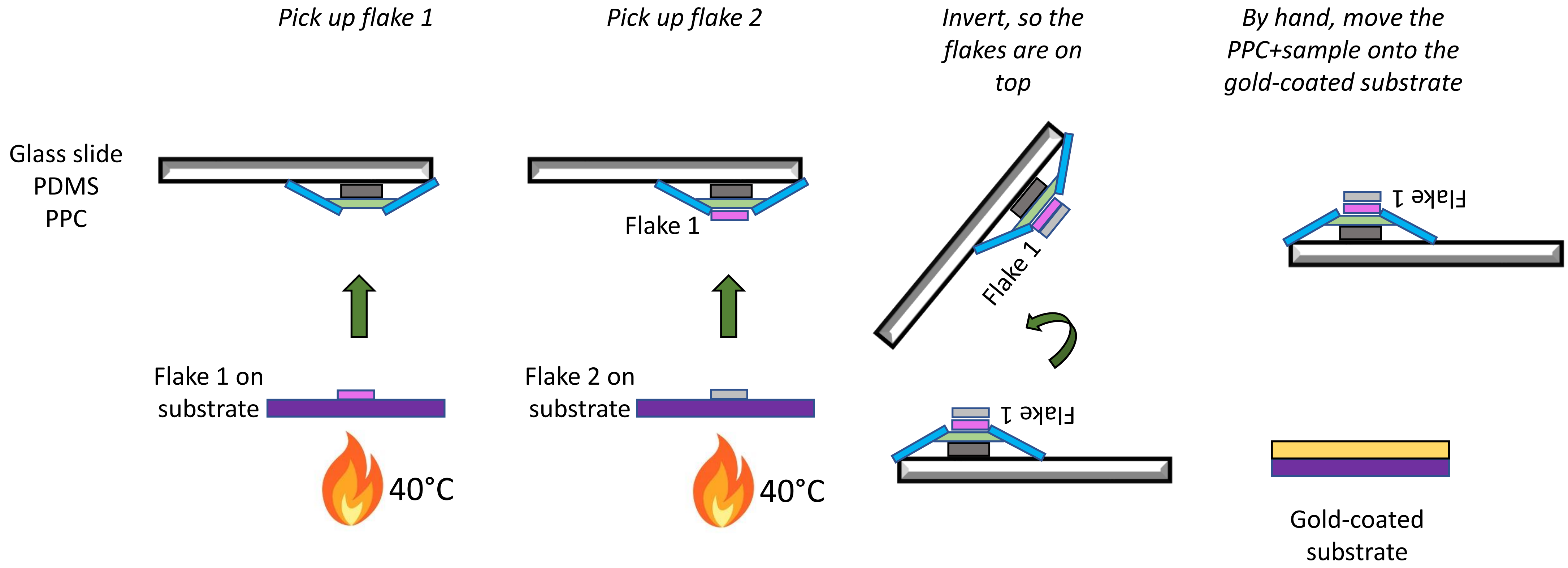
Spin-coat PPC on substrate → *add tape frame*

Cut PDMS square and place on glass slide → *plasma etch*

Use tape frame to pick up PPC, place it on the PDMS, secured to glass slide with tape frame

The stamp

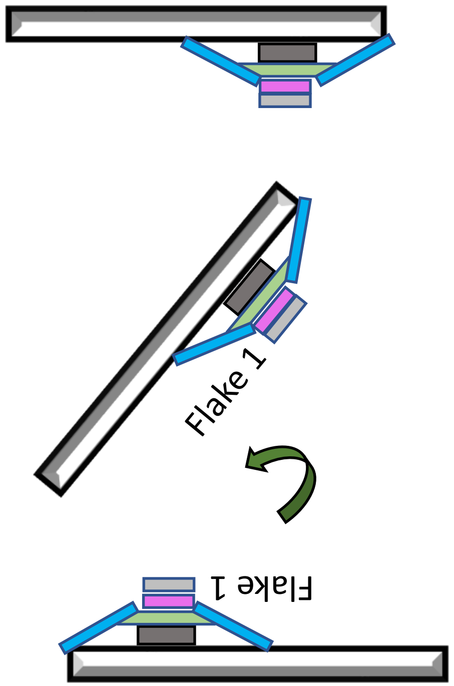
Part 2: Assemble the heterostructure



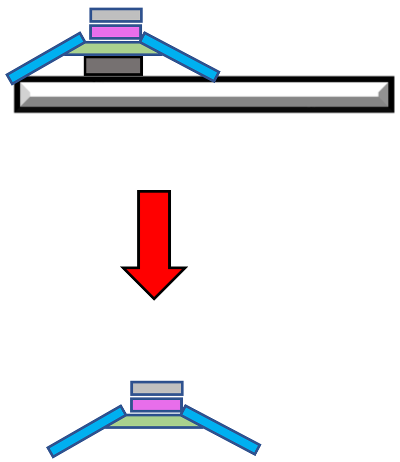
Part 3: Invert

Glass slide
PDMS
PPC
Flake 1
Flake 2

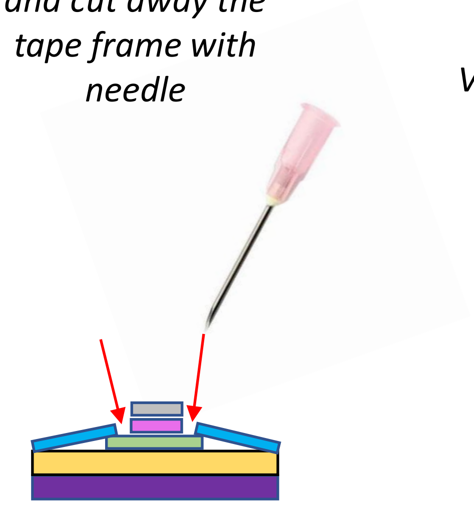
Invert, so the flakes are on top



By hand, remove the PPC+sample using the tape frame



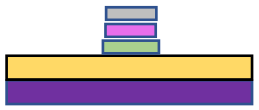
Place onto substrate and cut away the tape frame with needle



Gold-coated substrate

Part 4: Cleaning Steps

Hot plate (160°C for a few seconds)
Annealing (300°C for 10H in 60sccm H_2/Ar)
Vacuum furnace (300°C for 30m)
AFM Brooming (~100-300nN)



STM clean ✓