JYVÄSKYLÄN YLIOPISTO
UNIVERSITY OF JYVÄSKYLÄ

Quantum Materials by Design

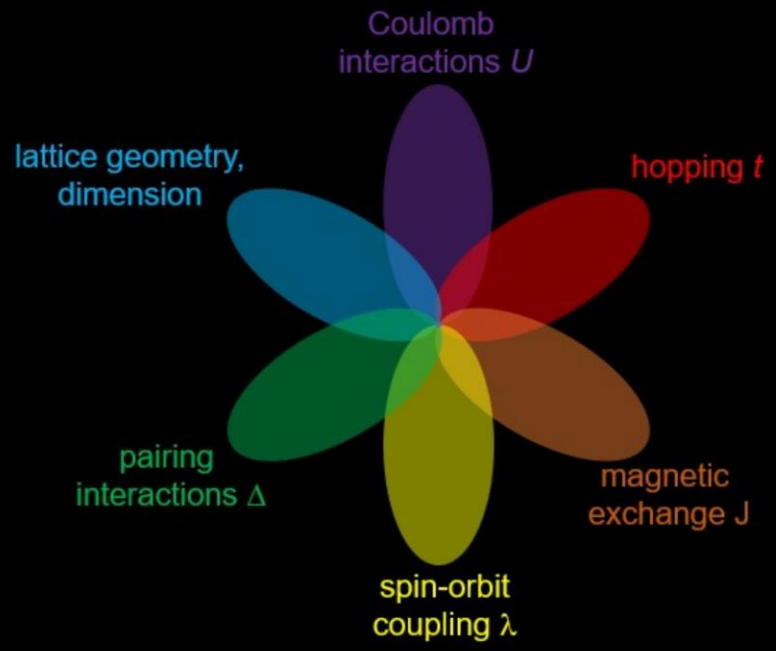
Shawulienu Kezilebieke

SPICE Workshop on Hybrid Correlated States and Dynamics in Quantum Materials, May 14th - 16th 2024

Quantum Materials ?

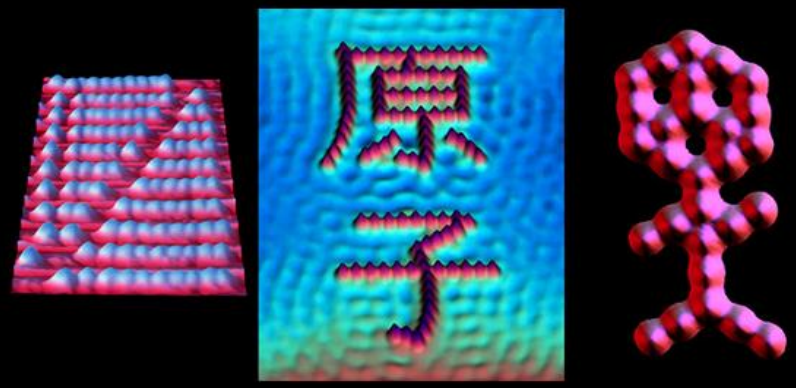
Materials displaying quantum effects on macroscopic scale, complex emergent phenomena

Method:
Designer quantum materials



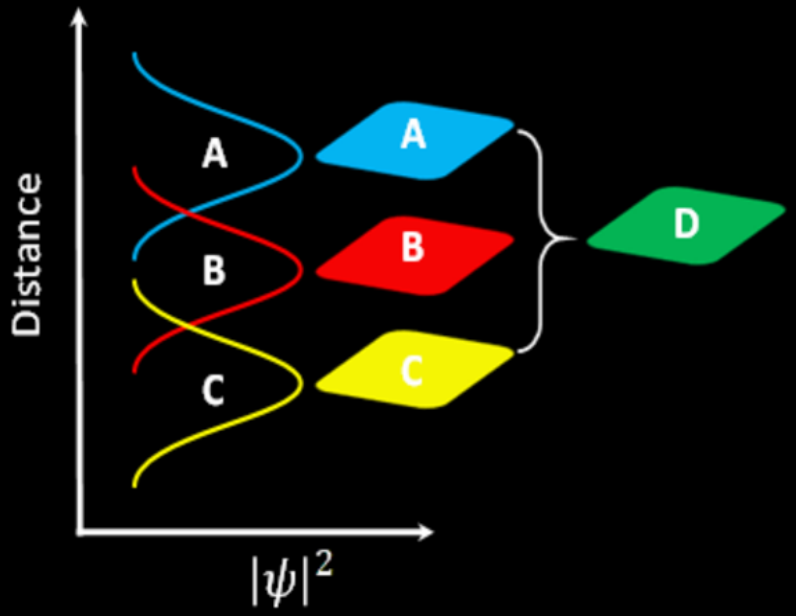
Design parameters

Platform 1:
Atom by atom



Atom manipulation

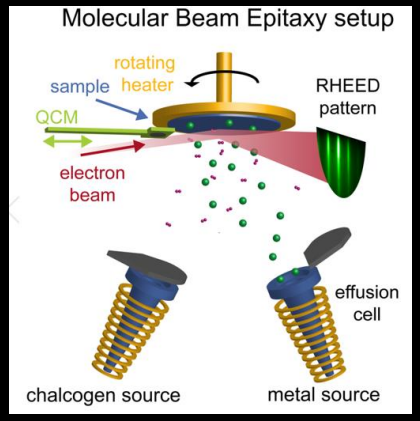
Platform 2:
Layer by layer

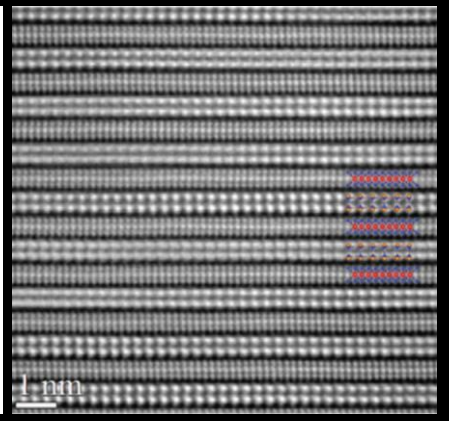


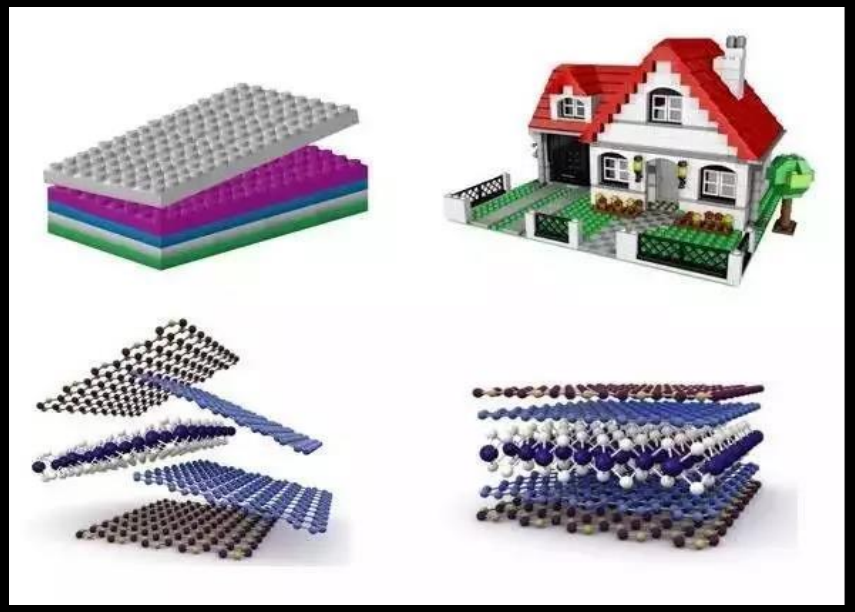
2D- Heterostructures

Tools

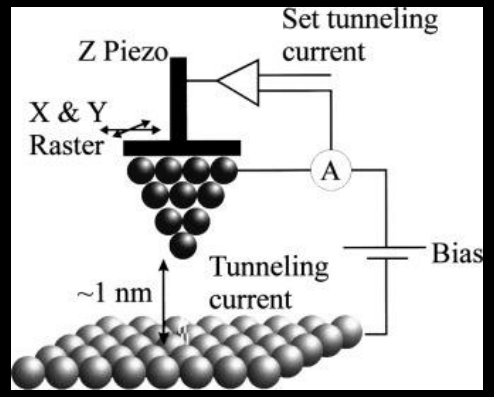
Molecular beam epitaxy MBE



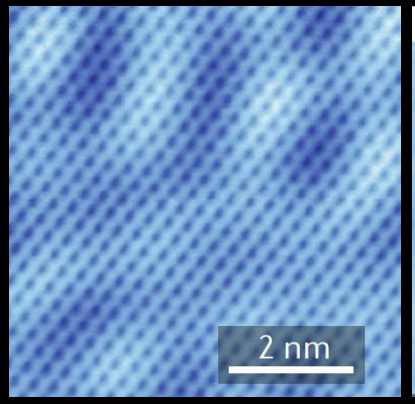




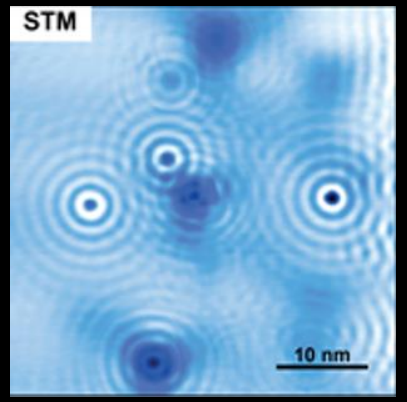
Scanning tunneling microscope STM



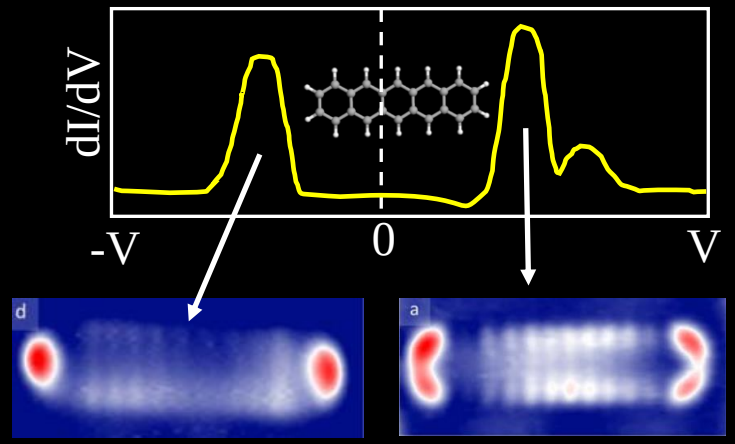
Particle



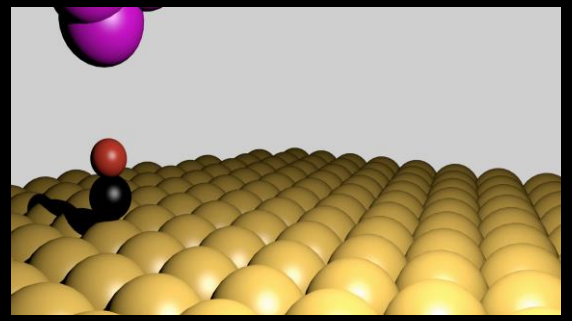
Wave



Scanning tunneling spectroscopy STS



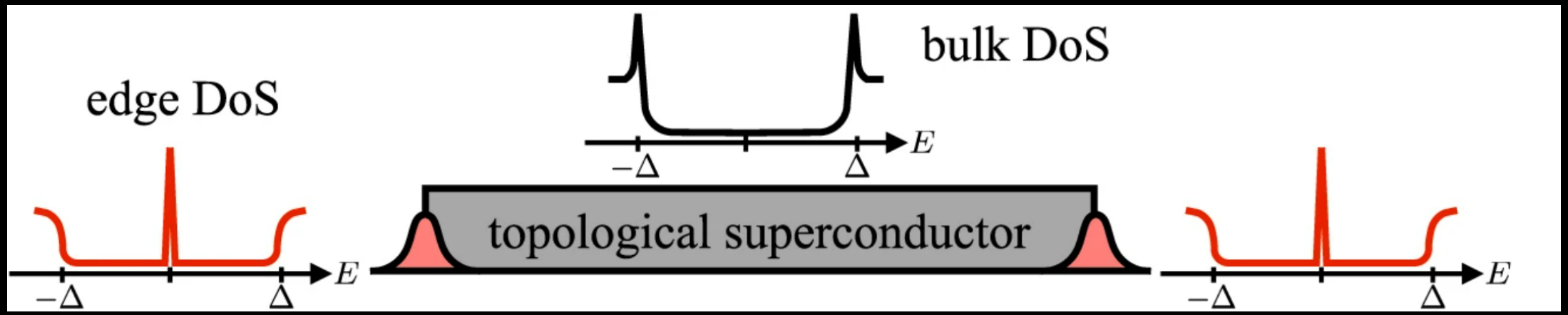
Atom Manipulation



$$\mathrm{d}I/\mathrm{d}V_\mathrm{b}(V_\mathrm{b},x,y) \propto \mathrm{LDOS}(eV_\mathrm{b},x,y) = \sum_{\delta E} |\psi_i(E_i,x,y)|^2$$

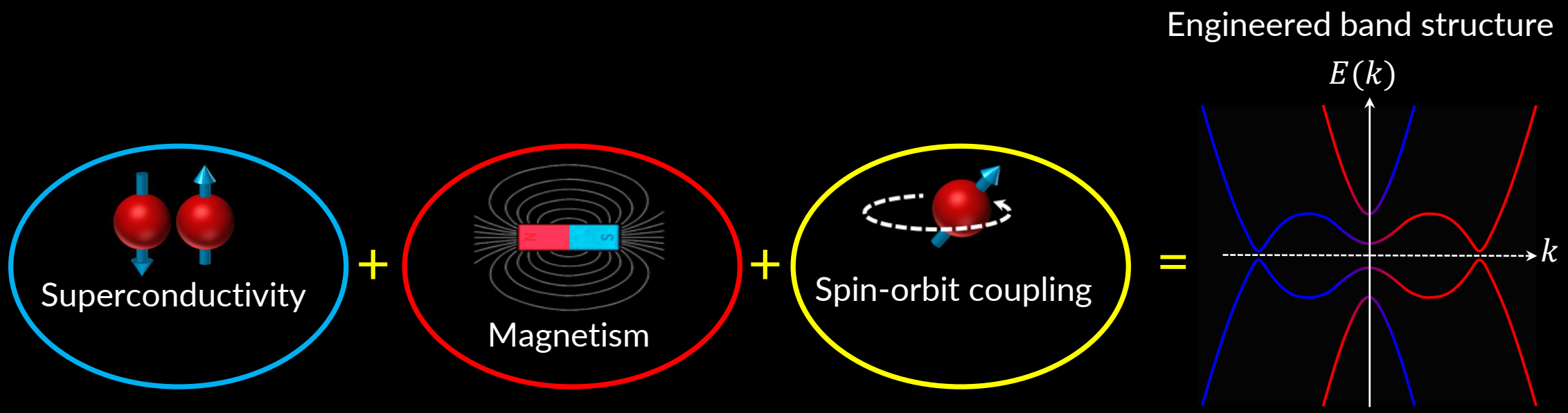
Topological superconductor

A topololological superconductors are a class of superconducting materials has a superconducting gap in the bulk but show protected metallic states on its boundaries or surfaces.



Such excitations are the condensed matter realization of Majorana fermions. Due to their topological protection against disorder and their non-Abelian statistics, Majorana modes are a prominent building block for topological quantum computers

Artificial topological superconductor



M. Sato, and Y. Ando, Topological superconductors: a review. Rep. Prog. Phys. 80, 076501(2017)

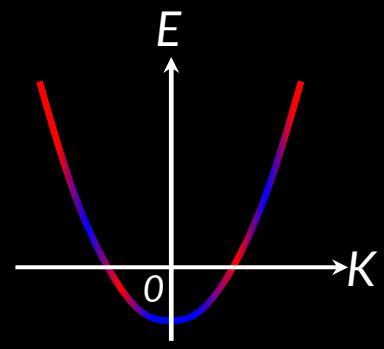
Topological superconductivity

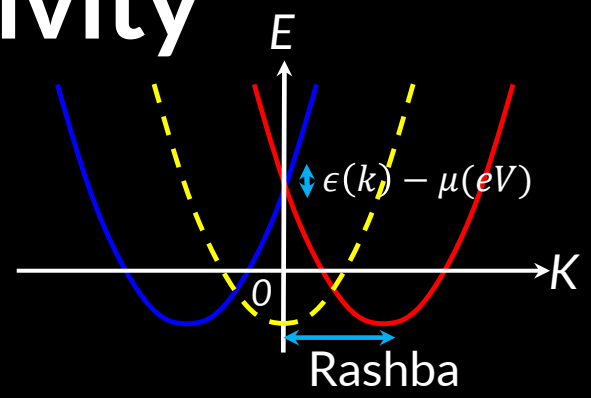
Standard recipe

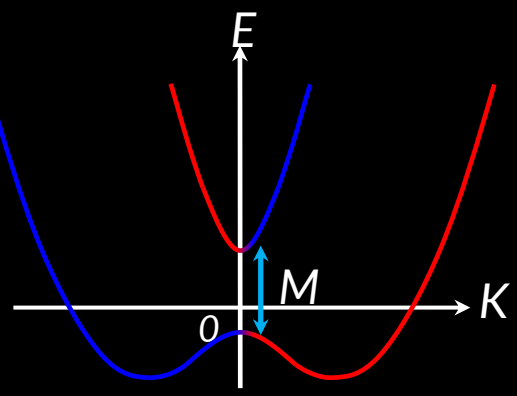
- Start with a simple parabolic band
- Add Rashba spin-orbit coupling α
- Add Zeeman term M (perpendicular to spin-orbit)
- Add superconductivity Δ

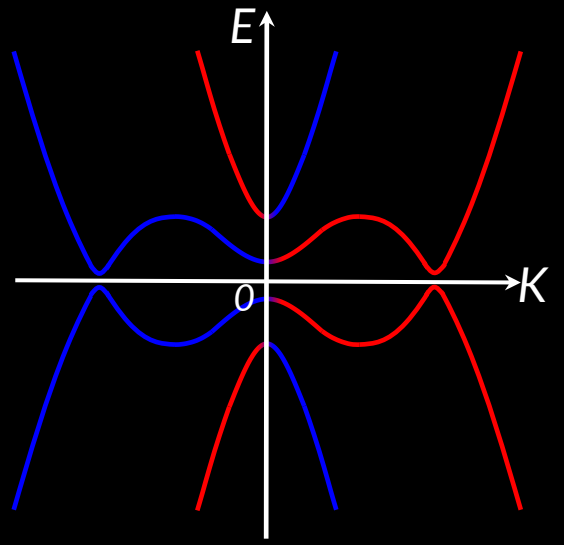
Condition for the topological phase

$$\left|\epsilon\left(\overrightarrow{k_0}\right) - \mu\right| \leq M$$

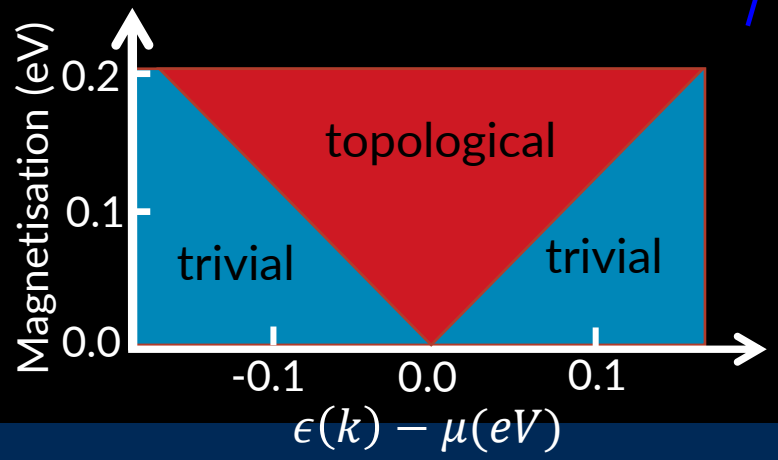








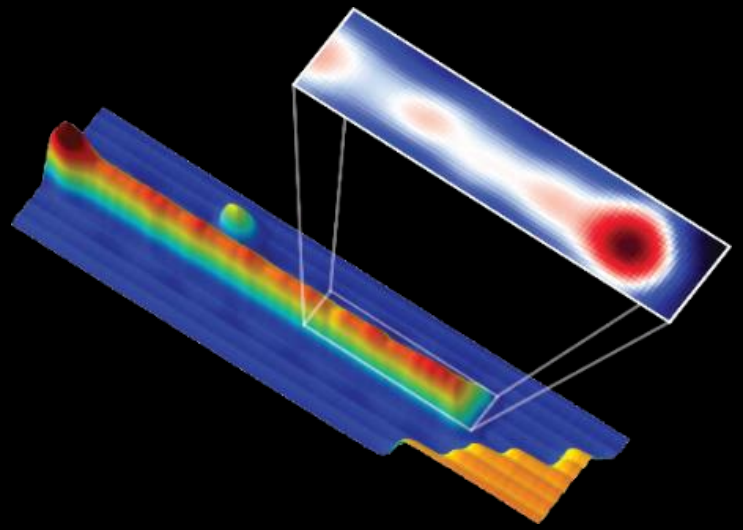
Topological phase diagram



Mixing magnetism and superconductivity

Observation of Majorana fermions in ferromagnetic atomic chains on a superconductor

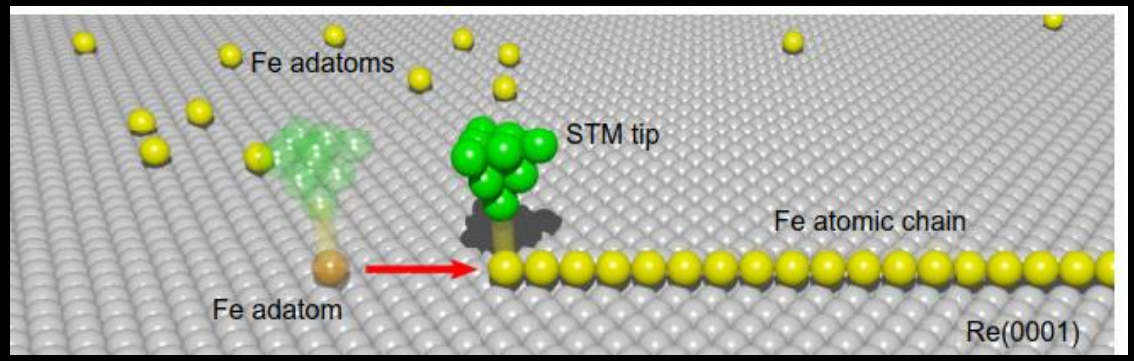
Stevan Nadj-Perge,[1*] Ilya K. Drozdov,[1*] Jian Li,[1*] Hua Chen,[2*] Sangjun Jeon,[1] Jungpil Seo,[1] Allan H. MacDonald,[2] B. Andrei Bernevig,[1] Ali Yazdani[1]†



SCIENCE 602 31 OCTOBER 2014 • VOL 346 ISSUE 6209

Toward tailoring Majorana bound states in artificially constructed magnetic atom chains on elemental superconductors

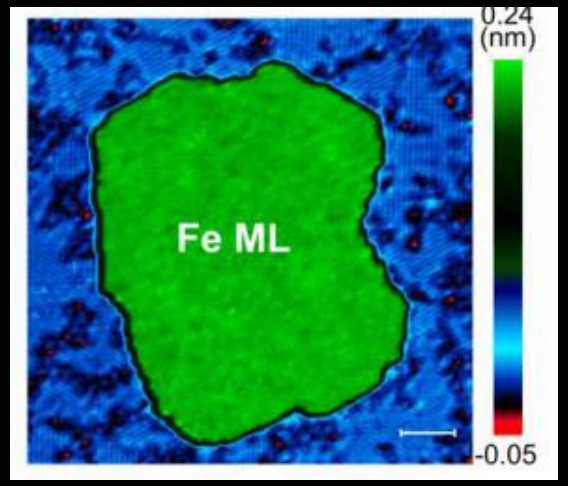
Howon Kim,[1]* Alexandra Palacio-Morales,[1] Thore Posske,[1] Levente Rózsa,[1] Krisztián Palotás,[2,3] László Szunyogh,[4] Michael Thorwart,[1] Roland Wiesendanger[1]*

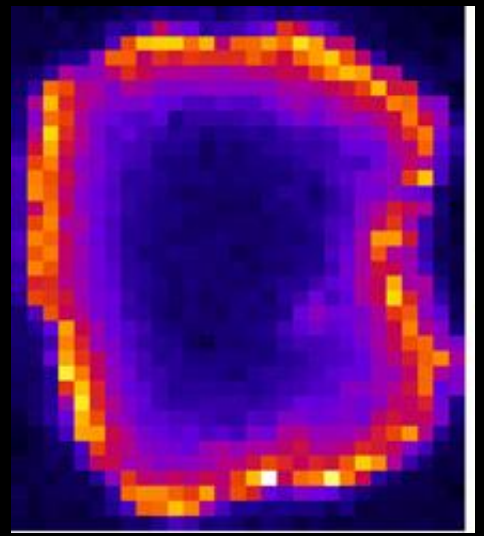


Kim *et al.*, *Sci. Adv.* 2018;**4**:eaar5251

Topological superconductivity in 2D

- 1D edge modes
- Depends on substrate spin-orbit and magnetic texture of the lattice
- Potentially a rich variety of different Chern numbers





A. Palacio-Morales et al., Sci. Adv. 5, eaav6600 (2019)

PRL 114, 236803 (2015) PHYSICAL REVIEW LETTERS week ending 12 JUNE 2015

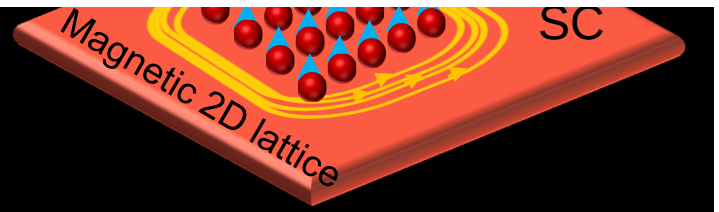
Topological Superconductivity and High Chern Numbers in 2D Ferromagnetic Shiba Lattices

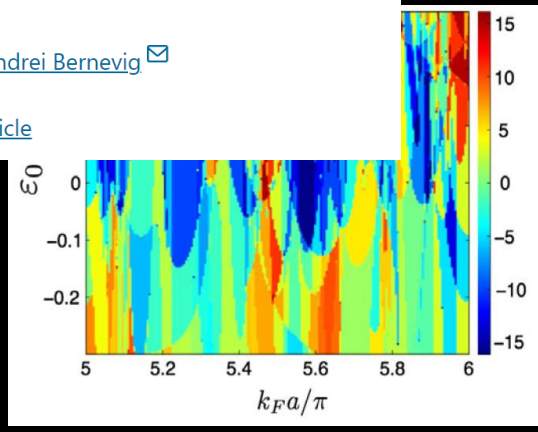
Joel Röntynen and Teemu Ojanen*
O. V. Lounasmaa Laboratory (LTL), Aalto University, P. O. Box 15100, FI-00076 AALTO, Finland
(Received 18 December 2014; published 12 June 2015)

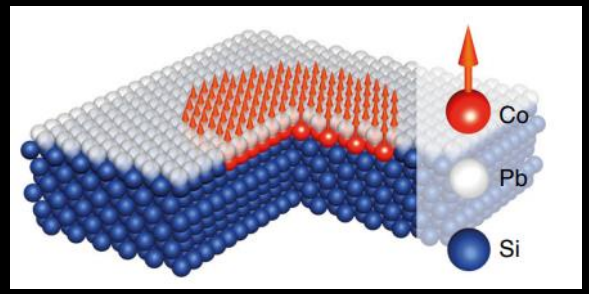
Two-dimensional chiral topological superconductivity in Shiba lattices

Jian Li, Titus Neupert, Zhijun Wang, A. H. MacDonald, A. Yazdani & B. Andrei Bernevig

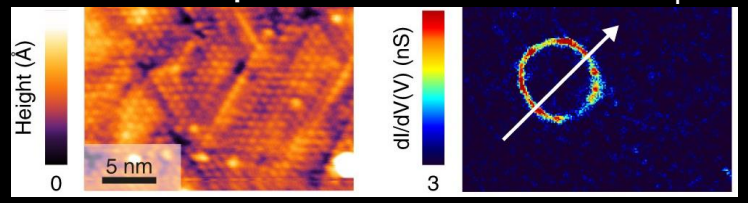
Nature Communications **7**, Article number: 12297 (2016) | Cite this article

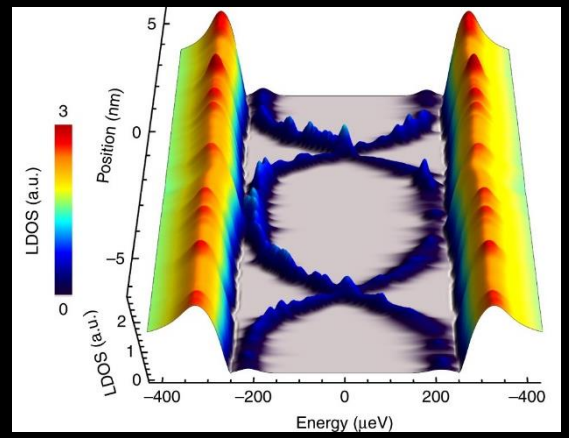






STM topo LDOS at E_F



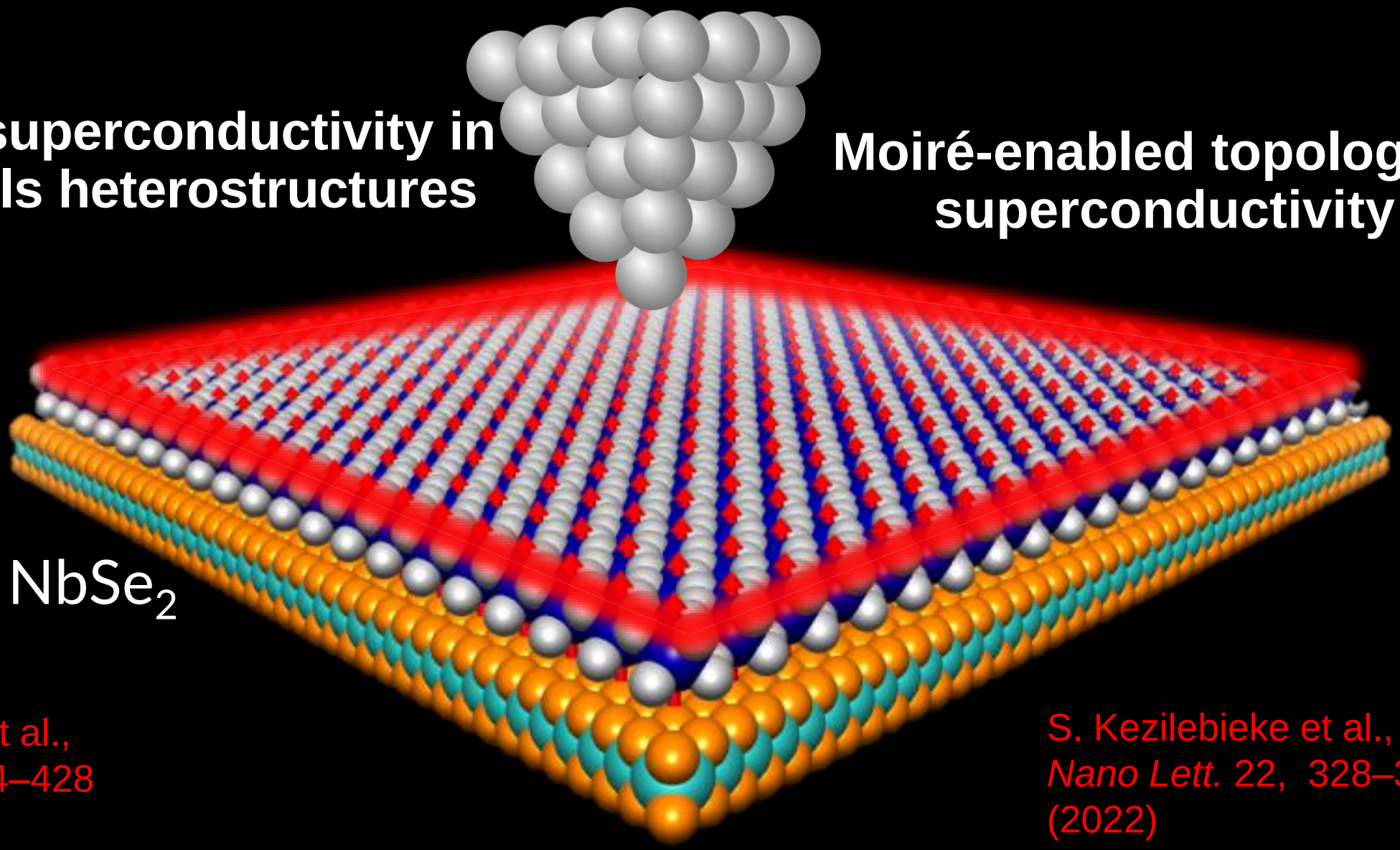


G. Ménard et al. Nat. Commun. 8, 2040 (2017)

Outline

Topological superconductivity in van der Waals heterostructures

Moiré-enabled topological superconductivity



FM= $CrBr_3$

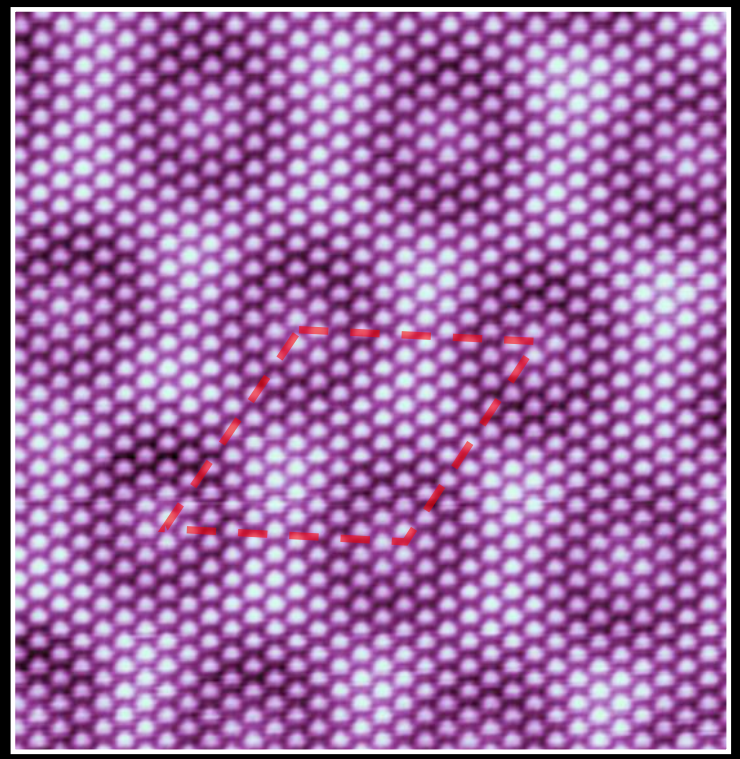
SC= $NbSe_2$

S. Kezilebieke et al., Nature, 588, 424–428 (2020)

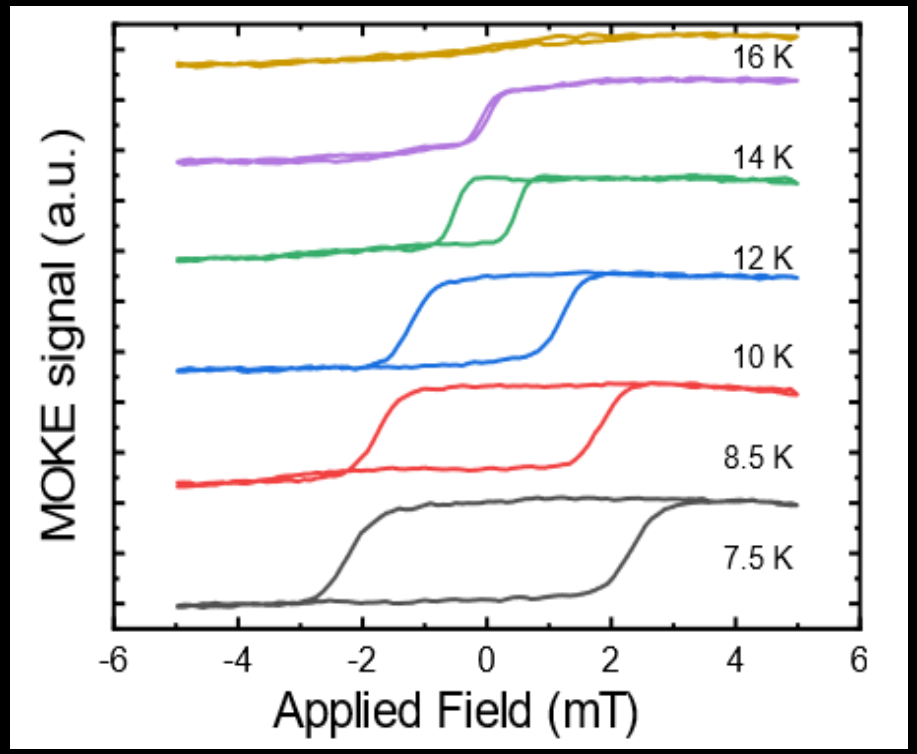
S. Kezilebieke et al., *Nano Lett.* 22, 328–333 (2022)

$CrBr_3$ monolayer on $NbSe_2$

157 ×157 nm²



19 ×19 nm²

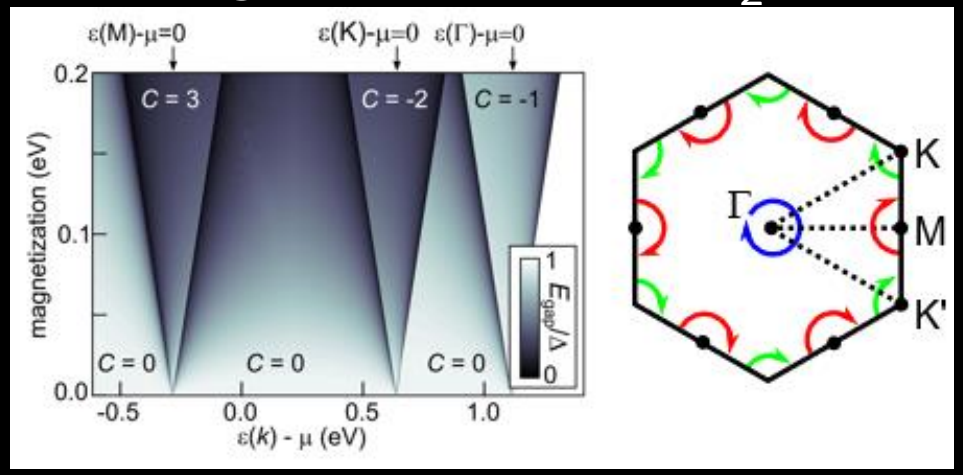


- ✓ Compound source MBE on freshly cleaved (under vacuum) $NbSe_2$ in UHV.
- ✓ Samples characterized with low-temperature STM, magneto-optical Kerr effect measurements.
- ✓ $CrBr_3$ monolayer ferromagnetic with out-of-plane magnetization. Curie temperature ca. 16 K.

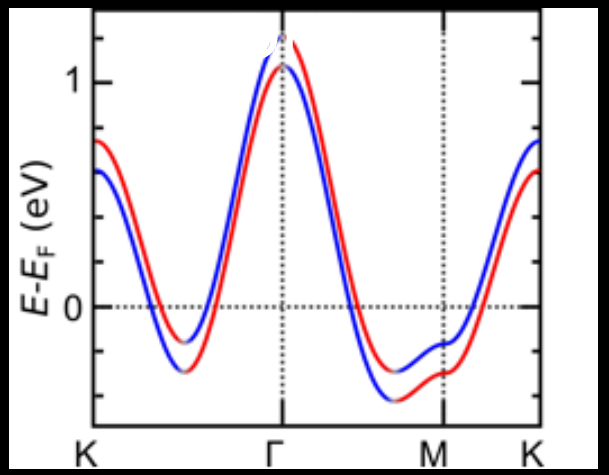
S. Kezilebieke et al. *Adv. Mater.* 2021, 2006850

Topological phase VS chemical potential

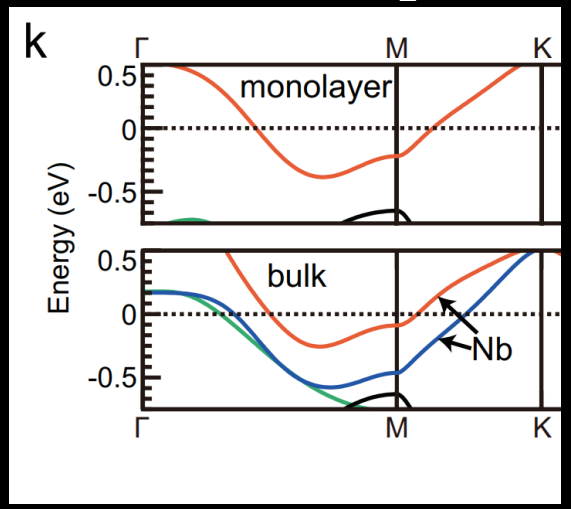
Topological phase diagram for a triangular lattice ($NbSe_2$)



M-point closest to Fermi according to

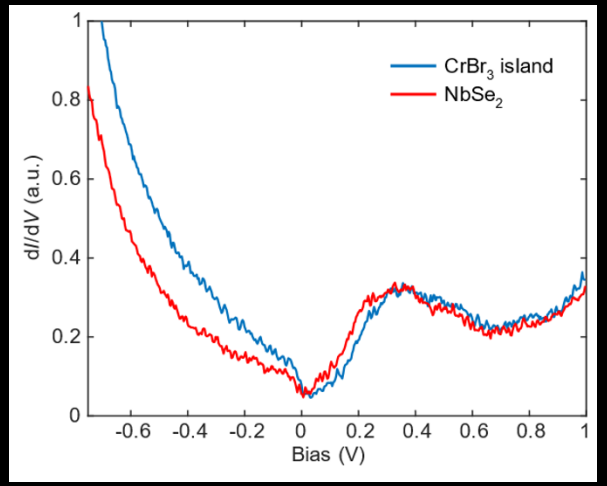


50-100 meV below E_F for bulk $NbSe_2$

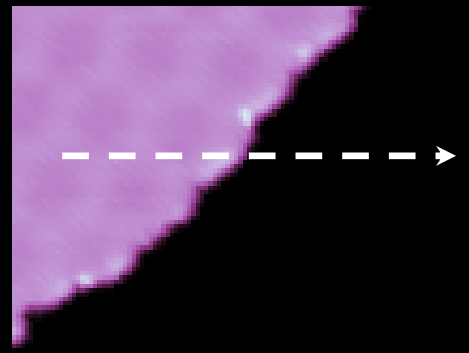


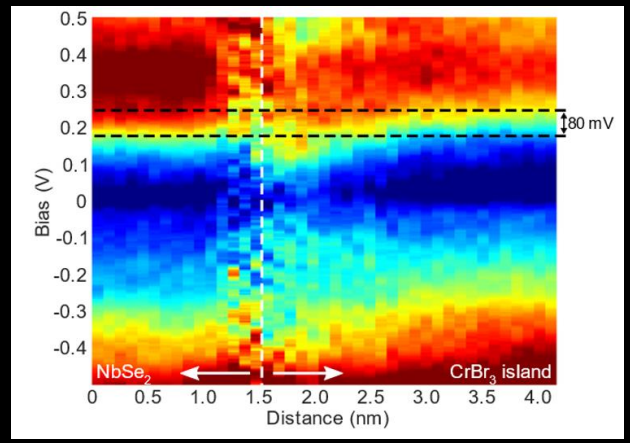
Nat. Phys. **12**, 92–97 (2016)

$NbSe_2$ + Rashba + Zeeman



Shift of the $NbSe_2$ states under $CrBr_3$



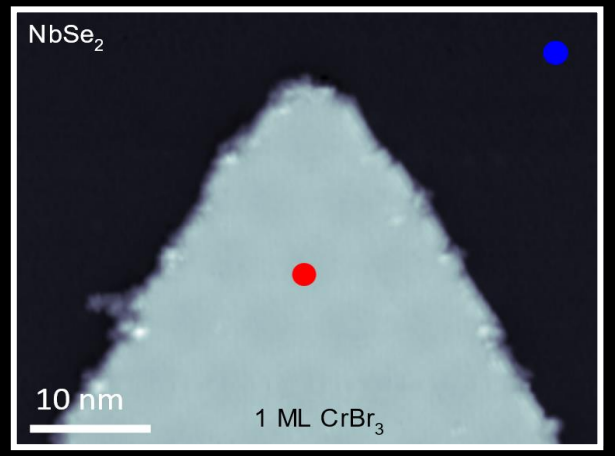


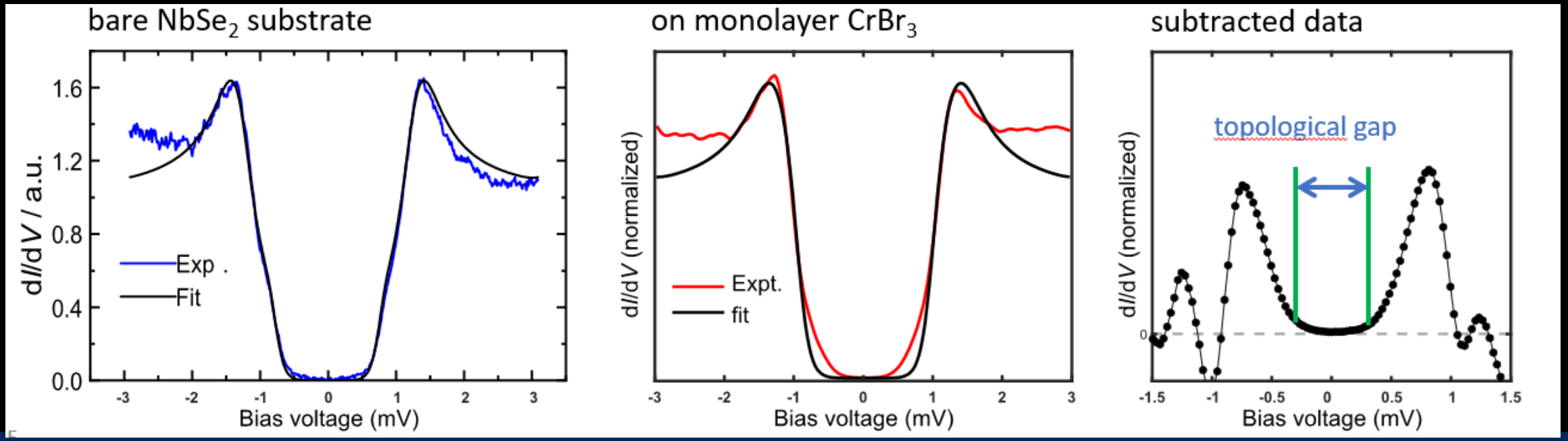
Overall shift makes it more plausible

Low-bias spectroscopy

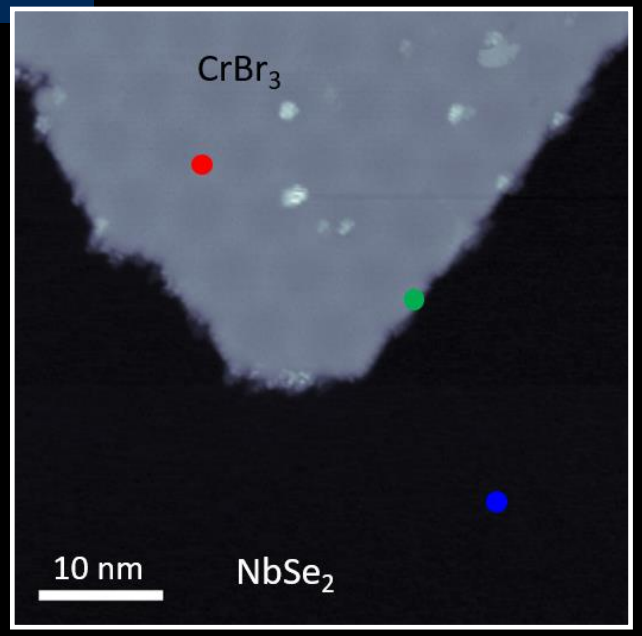
- Combining the required ingredients for topological superconductivity
- On the island, there is signal inside the SC gap: formation of Shiba bands due to the magnetic layer
- Gap between the Shiba bands

STM experiments at T = 350 mK

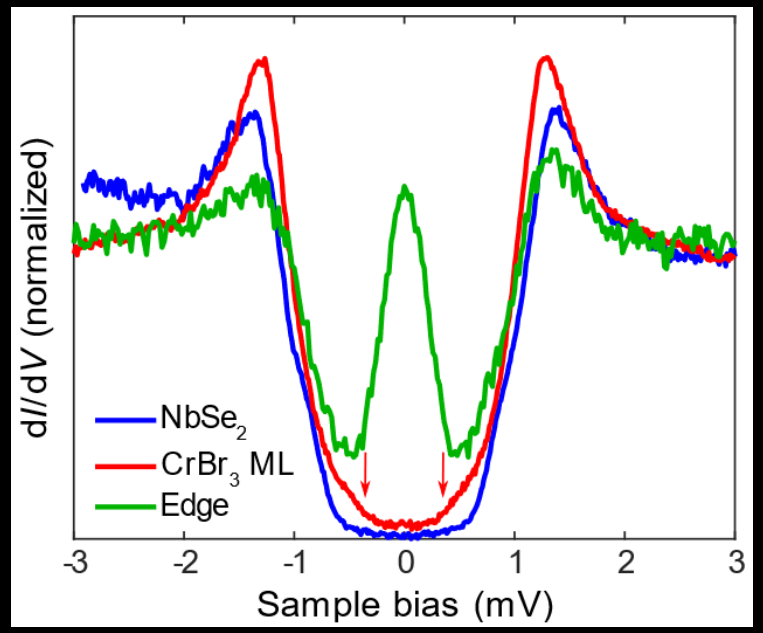




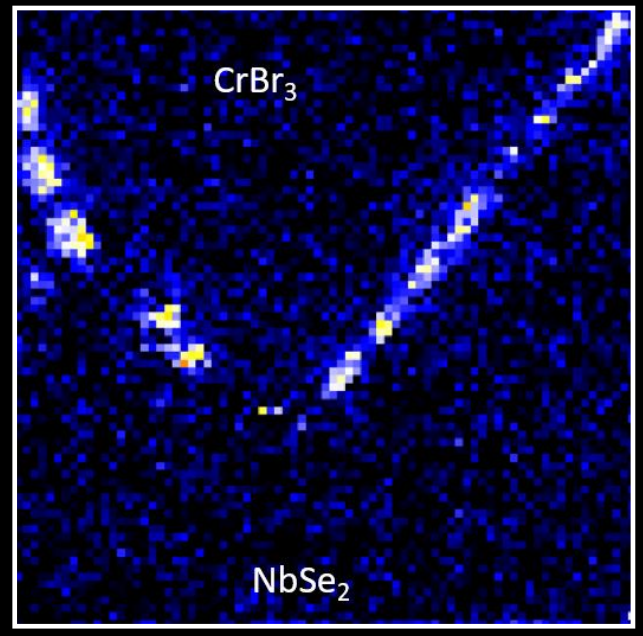
Island edges



STM image



STS

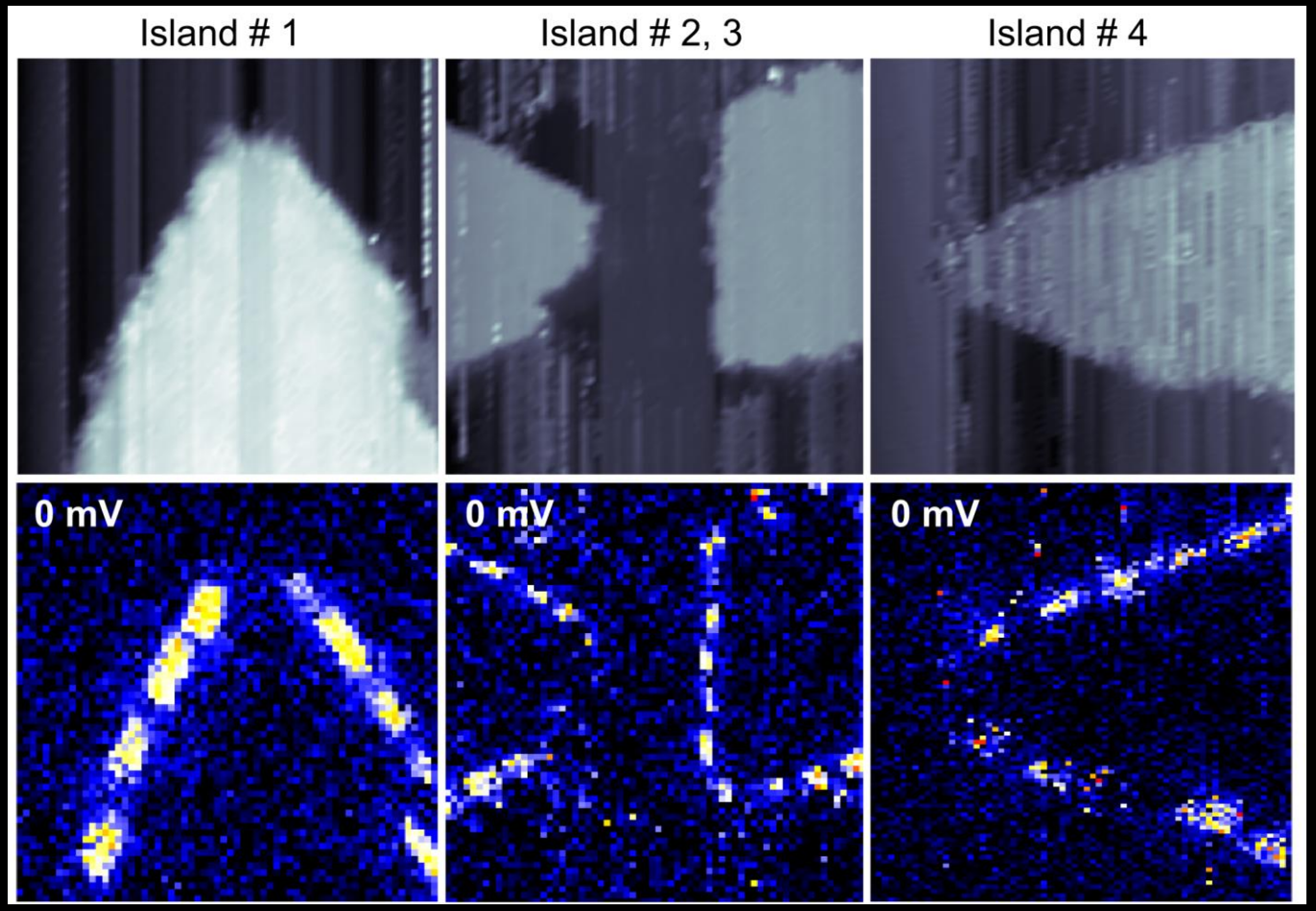


LDOS map at E_F

- Distinct zero bias signature at the island edges
- Spatial mapping: localized edge modes

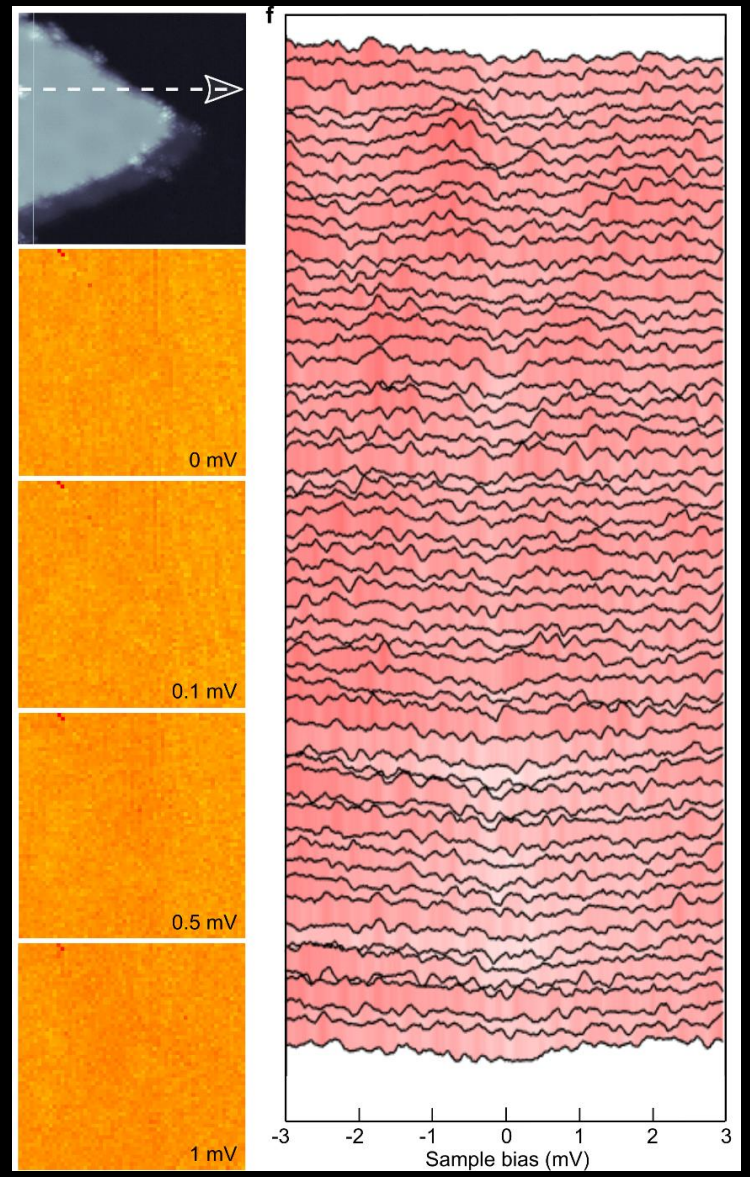
Is it topological superconductivity?

- Appears on all island edges



Is it topological superconductivity?

- Appears on all island edges
- Removing superconductivity (quenching with an external magnetic field) also removes the edge state completely
- Not Kondo, not standard edge state



External field 4T

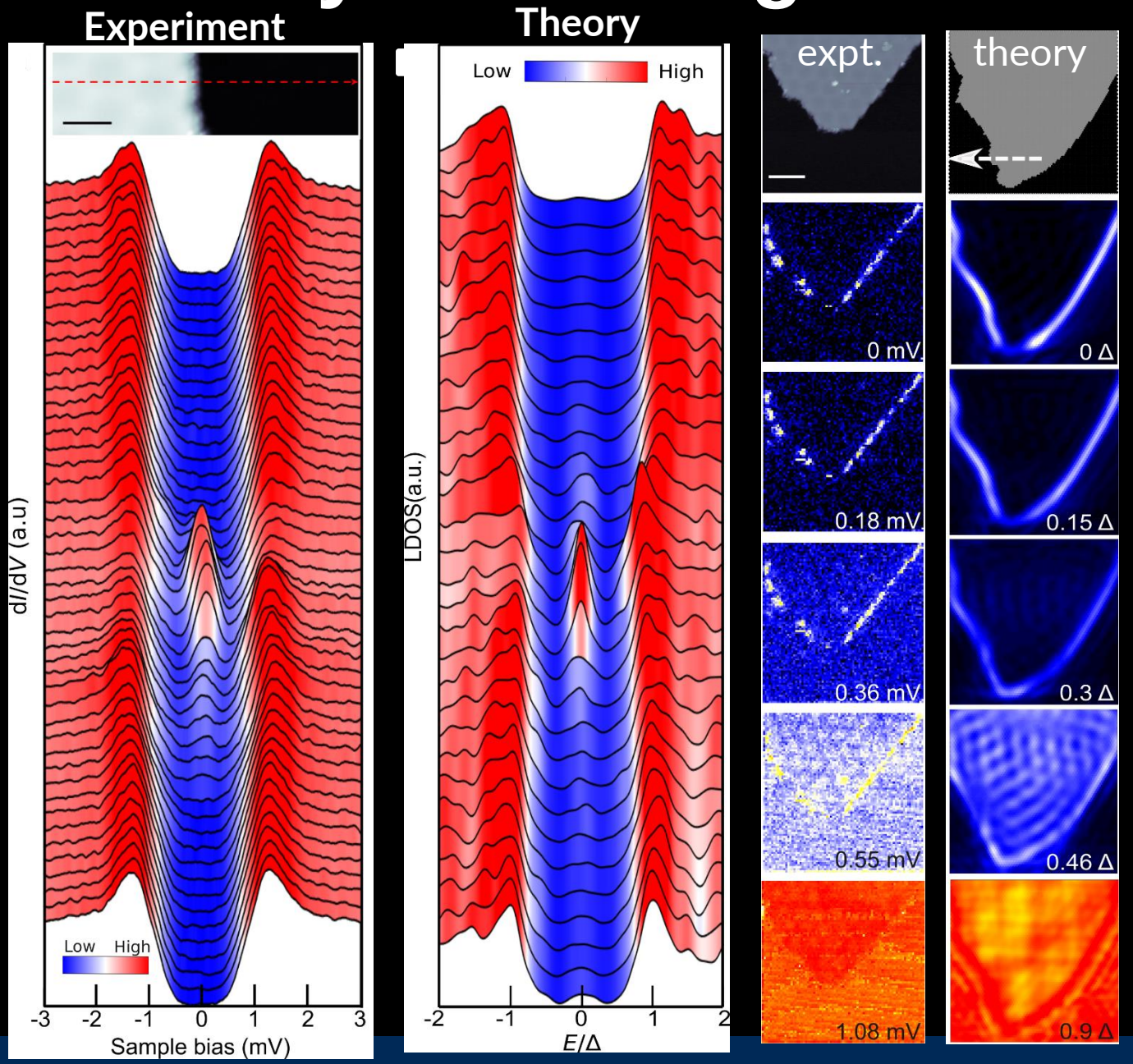
Comparison with theory at the edge

Experiment: grid spectroscopy over an edge of a $CrBr_3$ island

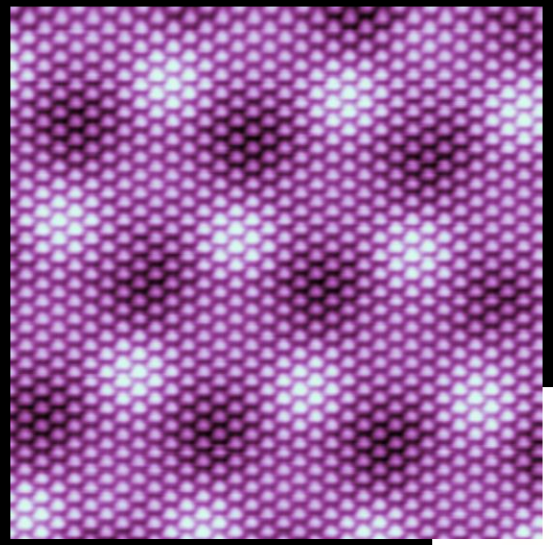
The edge modes coexist with Shiba bands at higher energies

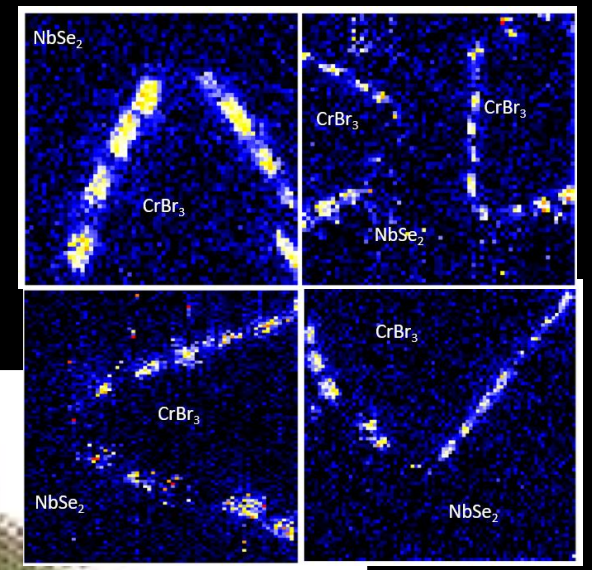
Quantitative match between theory and experiment:

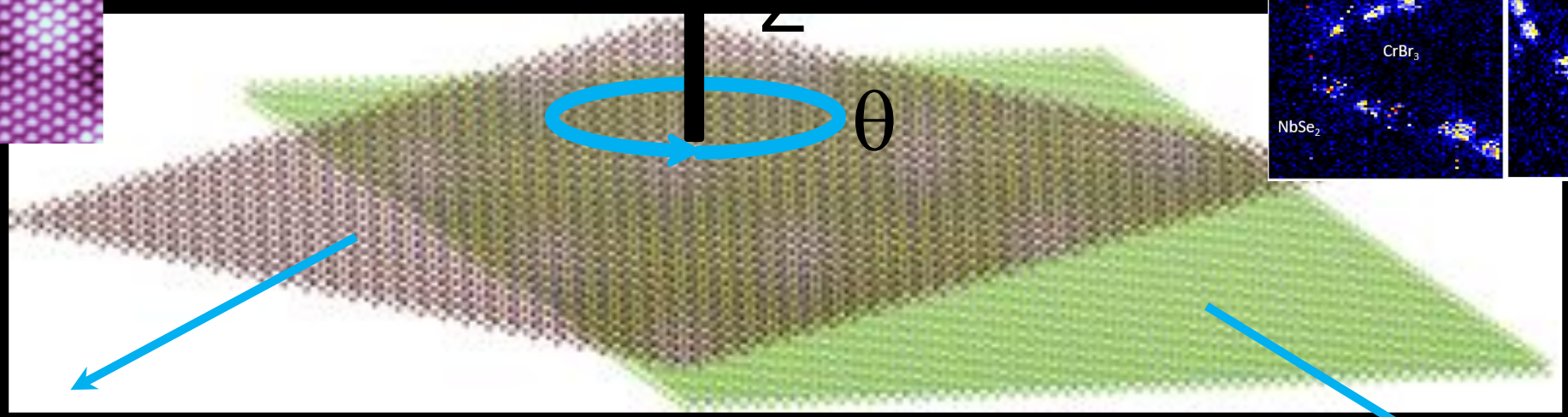
1. the correct edge mode penetration depth of ~2.5nm (orders of magnitude smaller than simple estimates)
2. the specific form of the subgap local density of states (depends on system-specific dispersion of the topological edge modes)
3. coexistence of the topological edge modes and bulk states in a substantial energy window
4. non-uniform distribution of the edge-mode spectral weight (stems from geometric irregularities of the island boundary)



Does the moiré modulation lead to a new emergent response in designer topological superconductors?







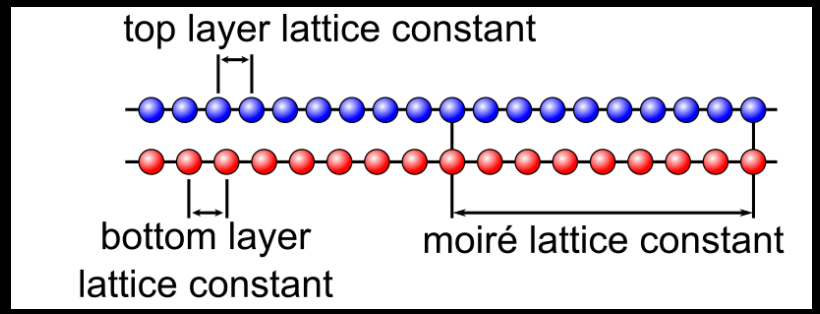
Ferromagnet

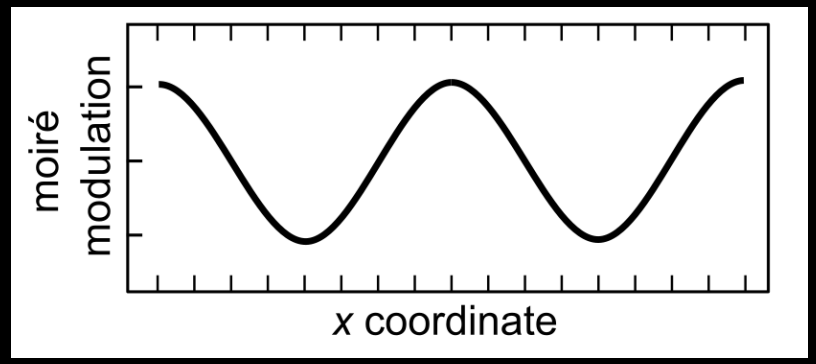
Superconductor

S. Kezilebieke et al. Nano Lett. 2022, 22, 1, 328−333

Moiré superlattice

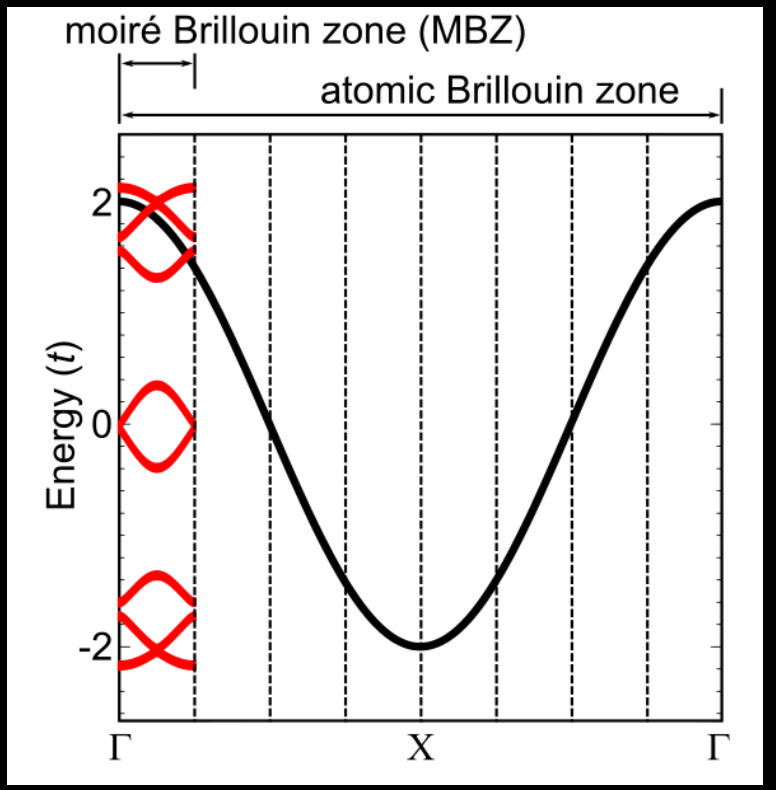
- A moiré pattern results from the projection of one periodic pattern to another with relative lattice constant or misalignment.
- It creates periodic potential to modify the electronic properties of pristine materials.





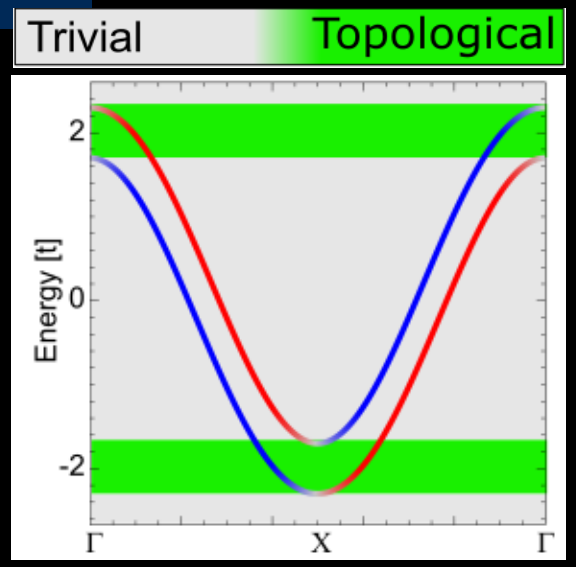
Schematic of the moiré pattern set up by the lattice mismatch

Moiré folds the bands (moiré Brillouin zone)

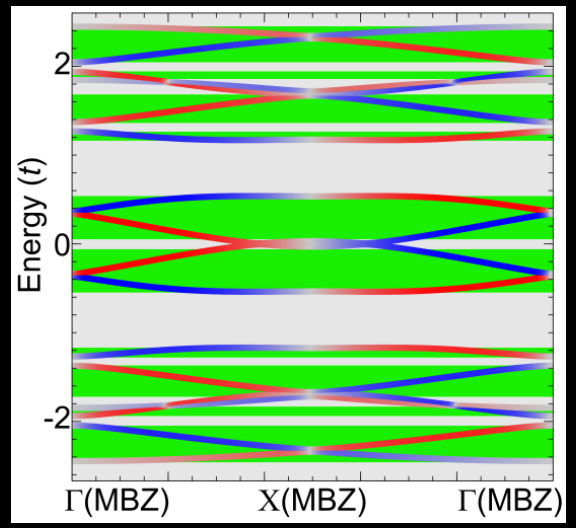


1D moiré-driven topological superconductivity

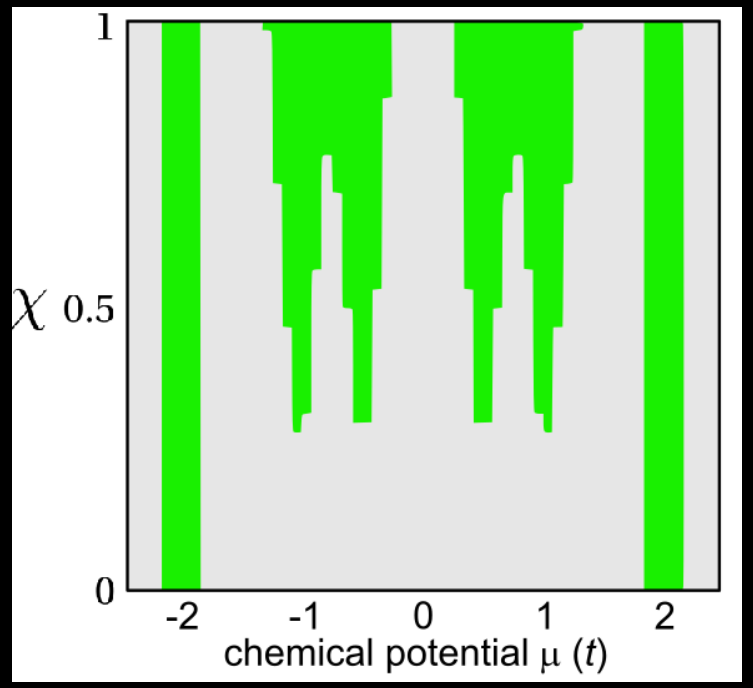
Without moiré



With moiré



Topological phase diagram

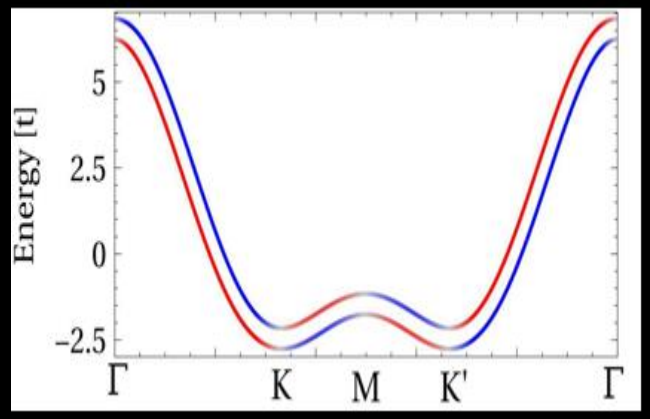


- Moiré modulation open topological regions in the phase diagram at parameter values corresponding to the trivial state in the absence of the moiré

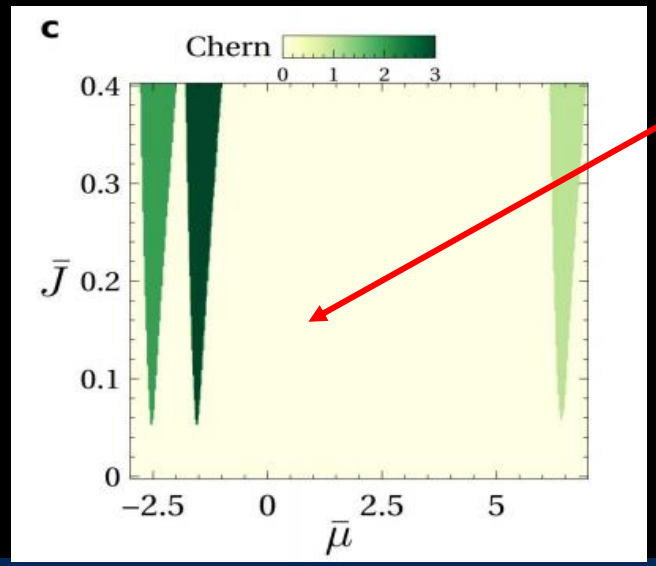
Modulation χ of exchange coupling, electrostatic potential etc..

2D moiré-driven topological superconductivity

Band structure for a triangular lattice

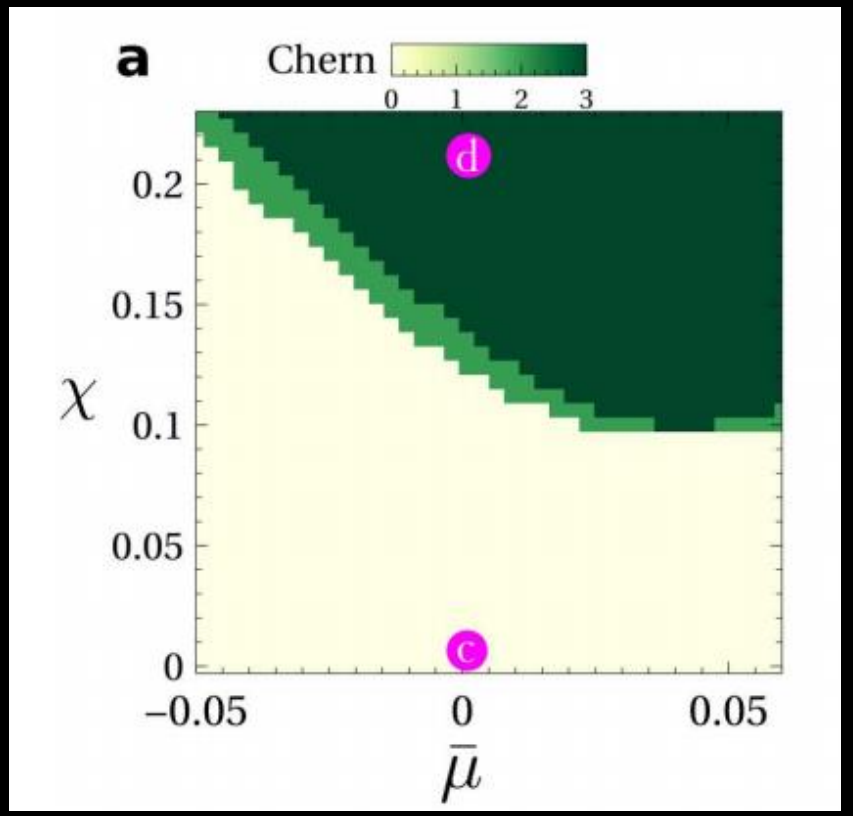


Topological phase diagram



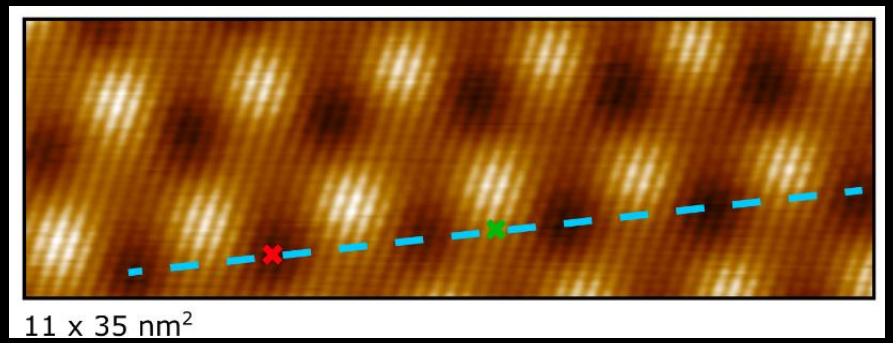
Close to charge neutrality no topological state appears by increasing the exchange coupling.

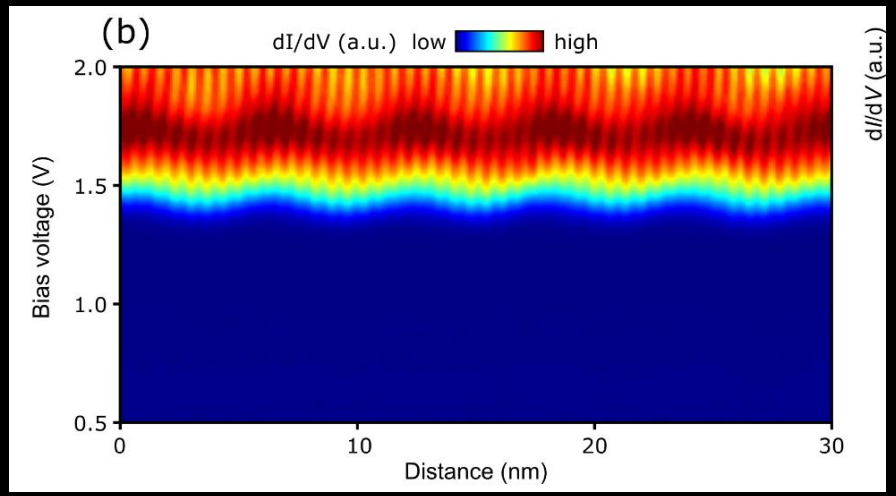
Topological phase diagram with moiré

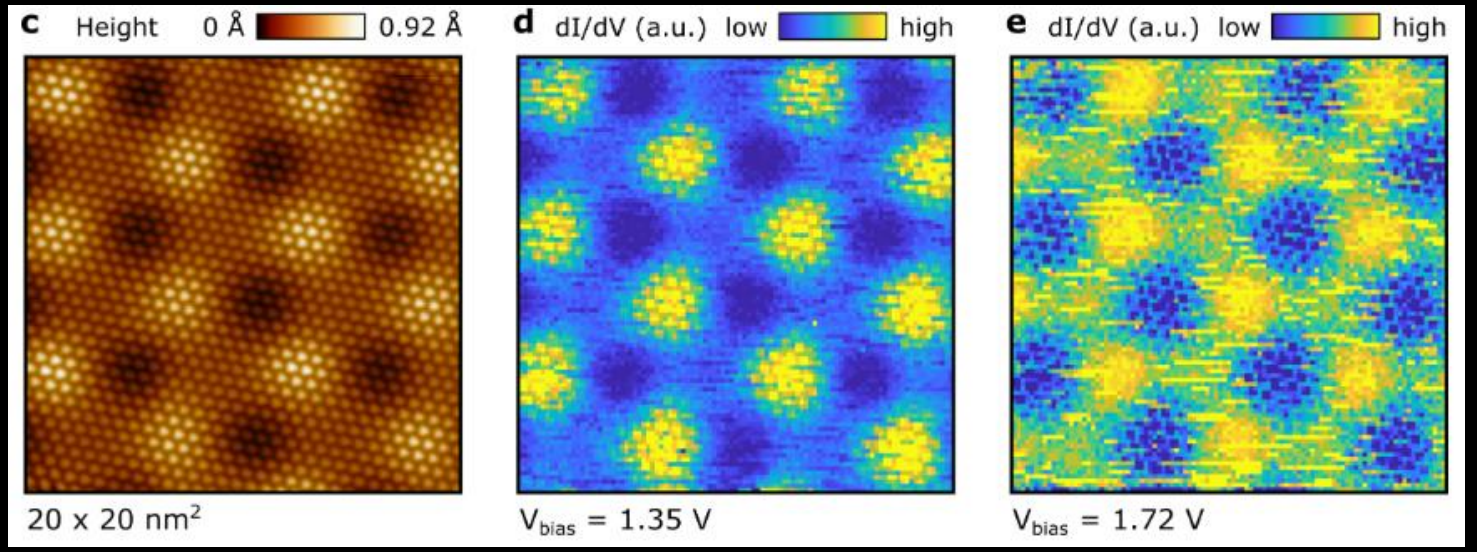


It is clearly observed that as the modulation is switched on, a new topological state appears

Large bias *dI/dV* spectroscopy of $CrBr_3$ monolayer on $NbSe_2$

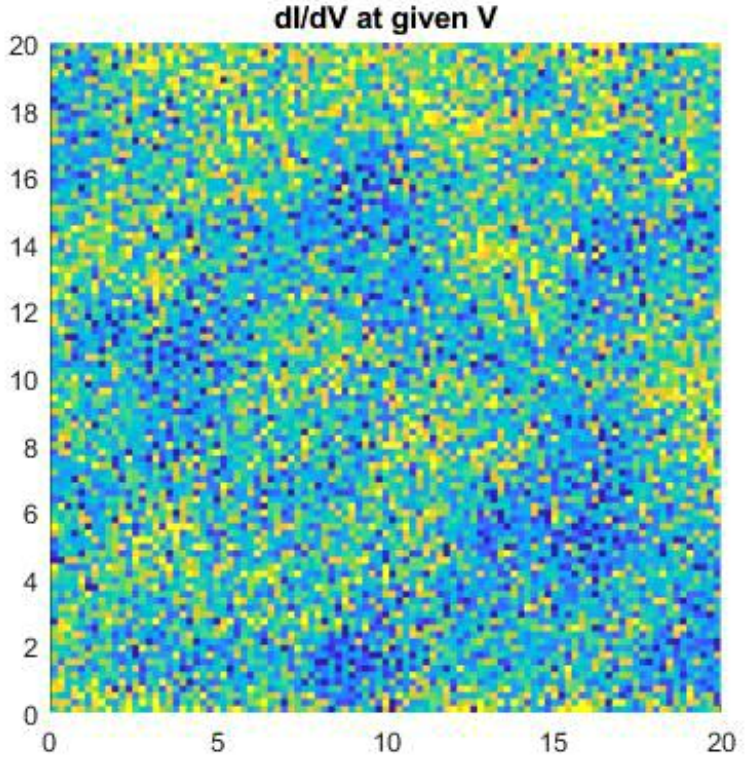


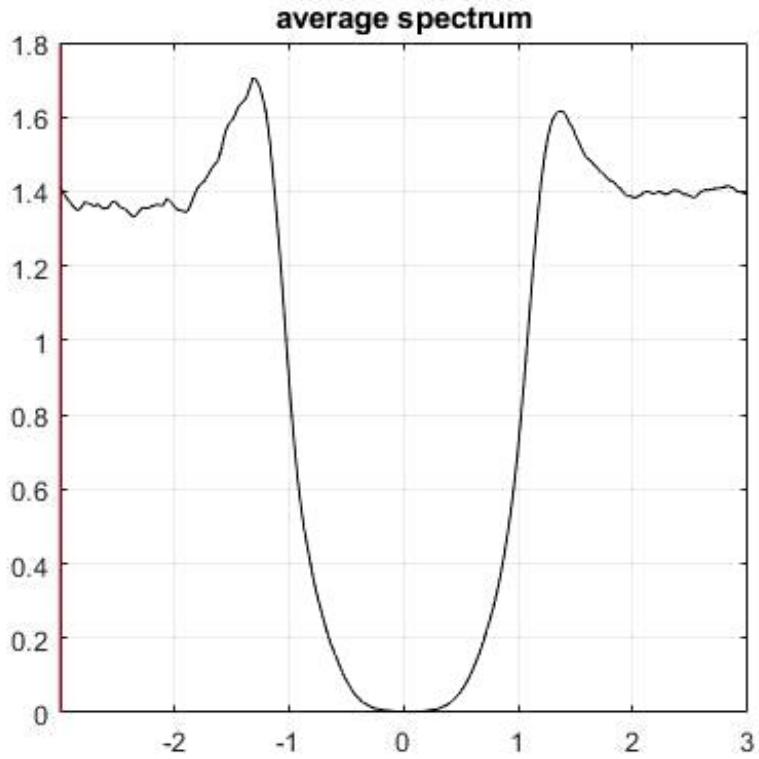




The conduction band edge of $CrBr_3$ is modulated with exactly the periodicity of the moiré pattern of $CrBr_3/NbSe_2$ heterostructure, with magnitude of the modulation around 50mV

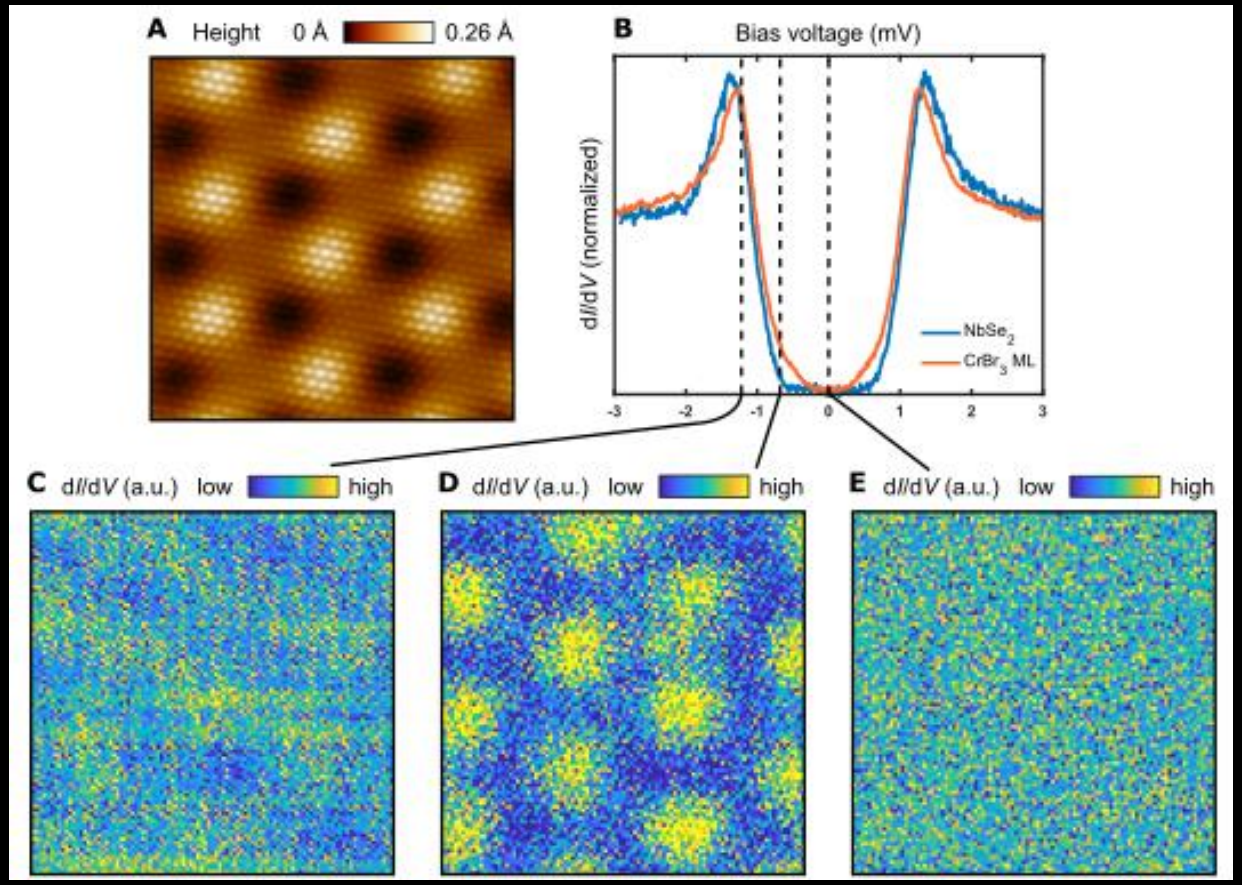
Correlation between moiré pattern and YSR bands





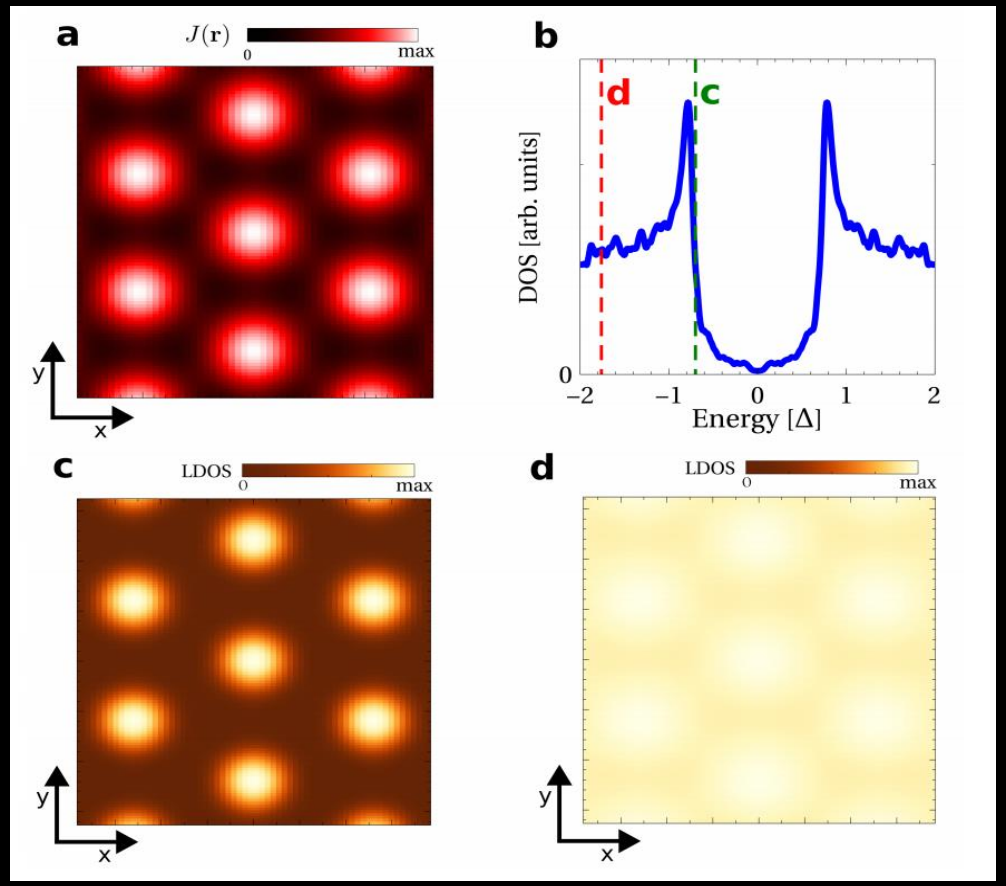
Correlation between moiré pattern and YSR bands

Experiment



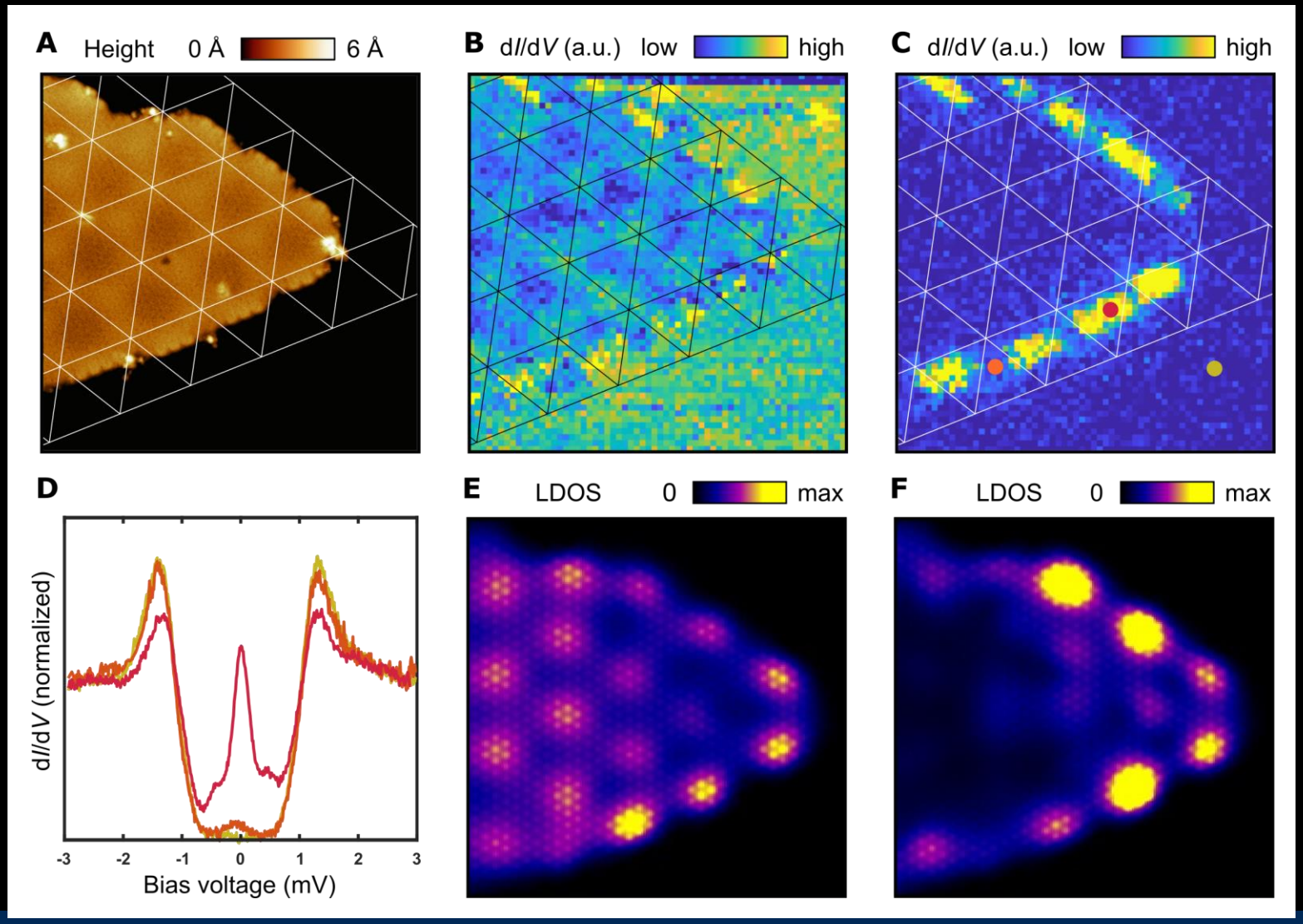
A clear correlation between the moiré pattern and dI/dV map only appears at the energy of the YSR bands.

Theory



The modulations of the YSR band LDOS due to the modulated exchange J.

Edge states of the topological superconductor with a moiré pattern



- Moiré-modulations also modulate the edge modes.
- "Simple" modelling predicts modulation with the moiré period.
- More details – Nano Lett. 2022, 22, 1, 328–333

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