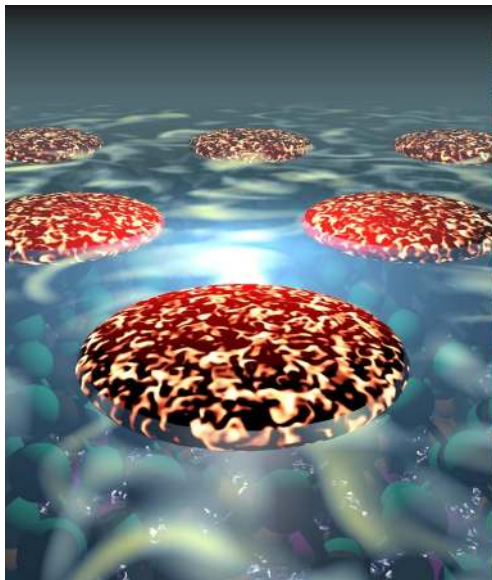


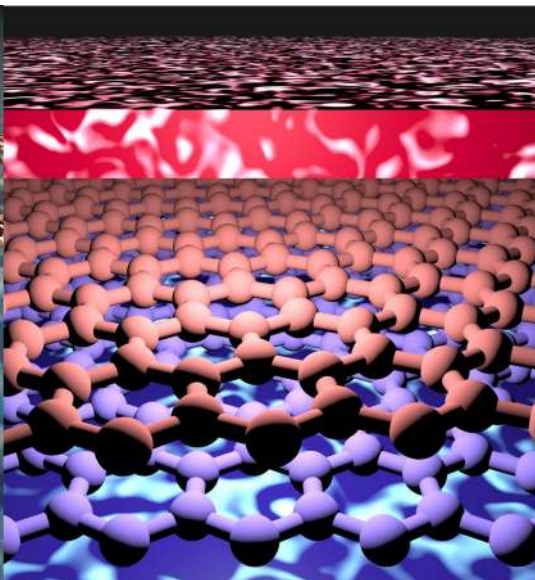
Moire-enabled topological superconductors and impurity spectroscopy in twisted van der Waals heterostructures

Jose Lado

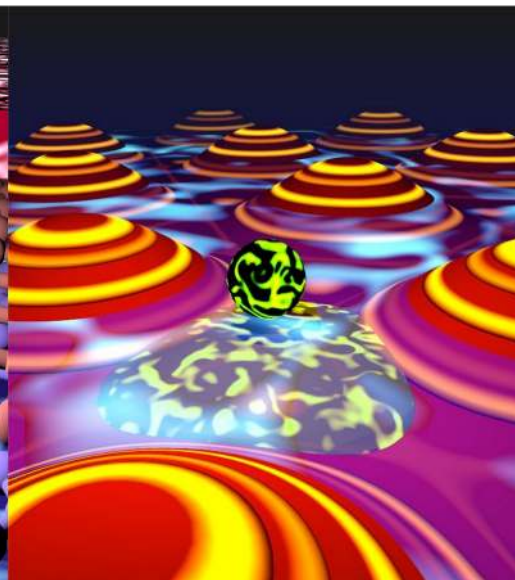
Department of Applied Physics, Aalto University, Finland



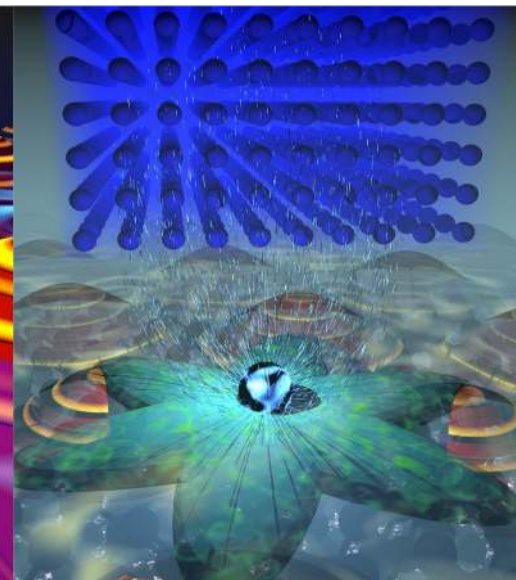
Nano Lett. 2022, 22, 1,
328–333 (2022)



arXiv:2307.04605
(2023)



Phys. Rev. Mat. 6,
094010 (2022)



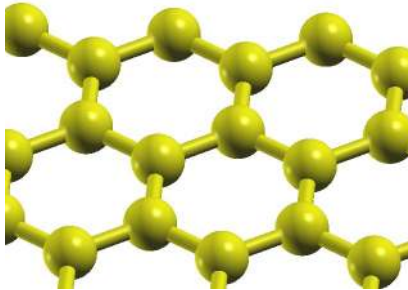
arXiv:2308.11400
(2023)

International Workshop on Superconductivity and Magnetism in Two Dimensional Films and Heterostructures
September 1st 2023, Bath, UK

The two-dimensional materials world

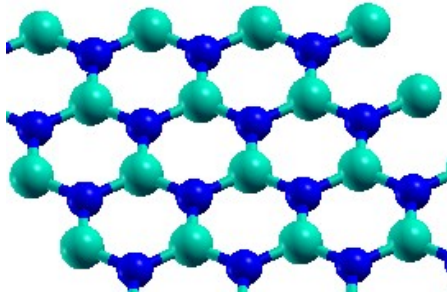
Semimetal

Graphene



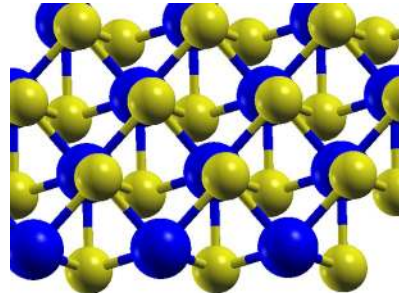
Insulator

BN



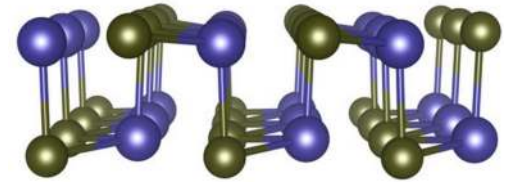
Superconductor

NbSe₂



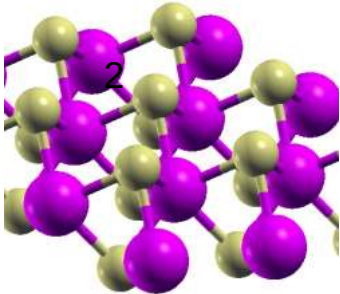
Ferroelectric

SnTe



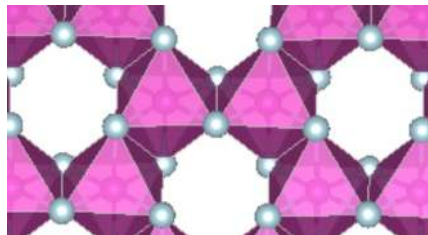
Semiconductor

WSe



Ferromagnet

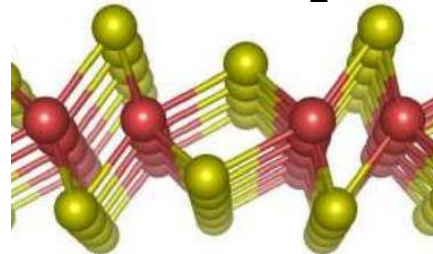
CrI₃



Quantum spin

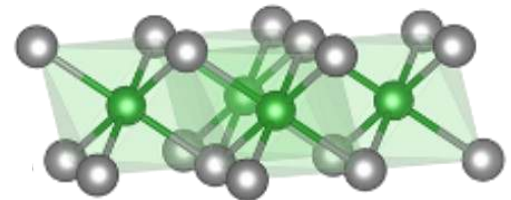
Hall insulator

WTe₂



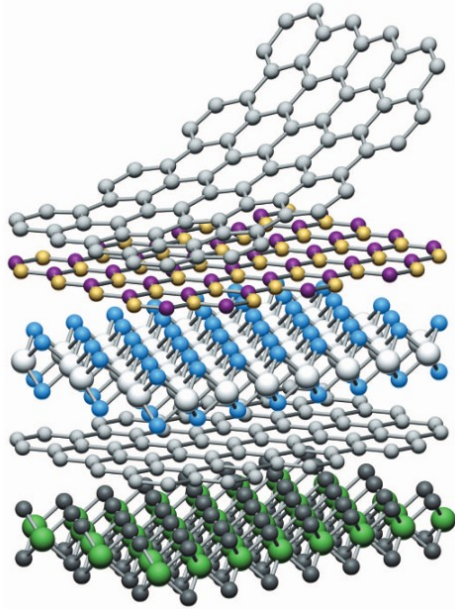
Multiferroic

NiI₂



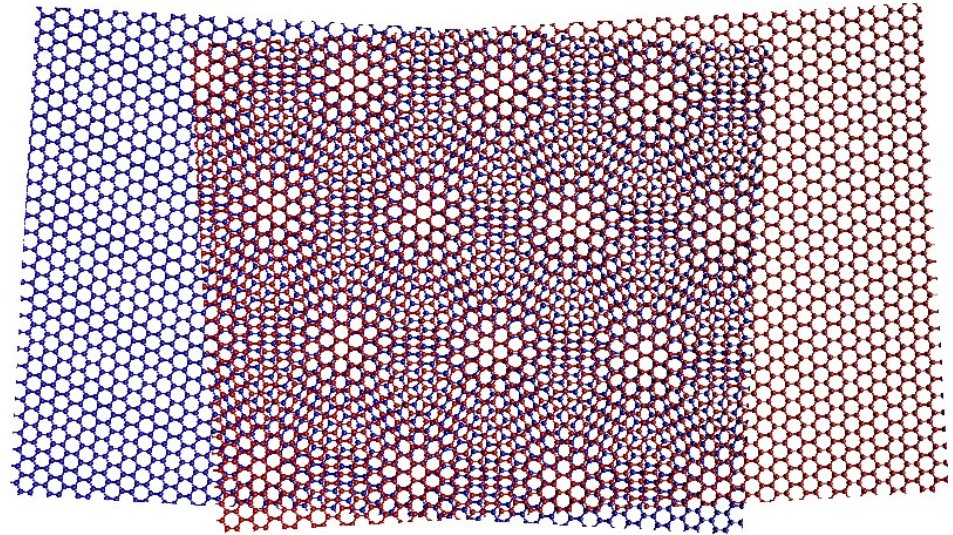
The flexibility of two-dimensional materials

They can be stacked



Nature 499, 419–425 (2013)

They can be rotated

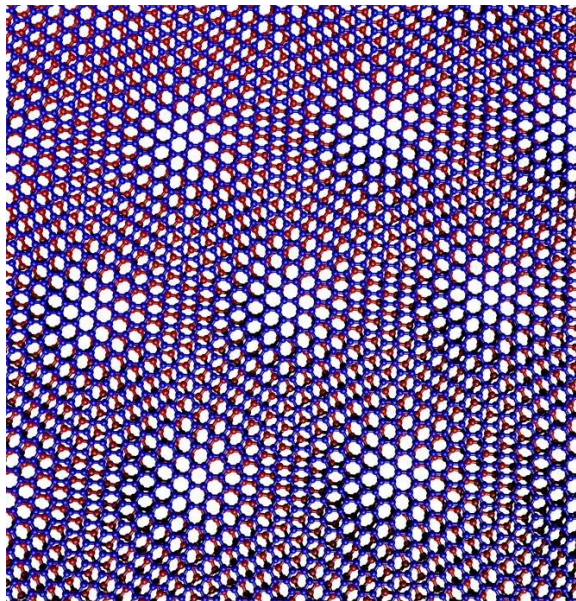


Science 361, 6403, 690-693 (2018)

These are unique features of two-dimensional materials

One material, a zoo of electronic phases

Twisted bilayer graphene

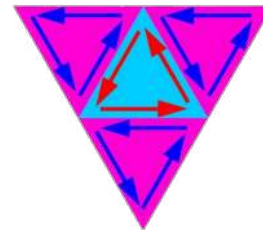


Superconductivity



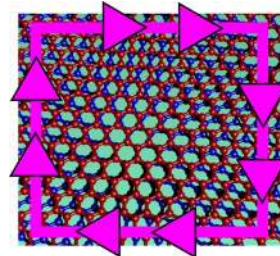
Nature 556, 43–50 (2018)

Topological networks



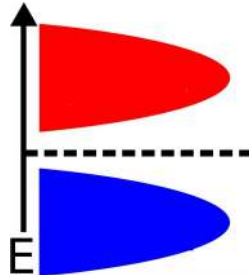
Nano Lett. 18, 11,
6725-6730 (2018)

Chern insulators



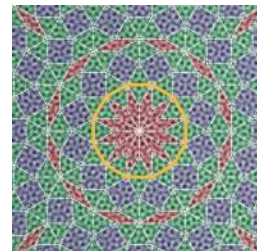
Science 365, 605-608 (2019)

Correlated insulators



Nature 556, 80–84 (2018)

Quasicrystalline physics



Science 361, 782-786 (2018)

Fractional Chern insulators

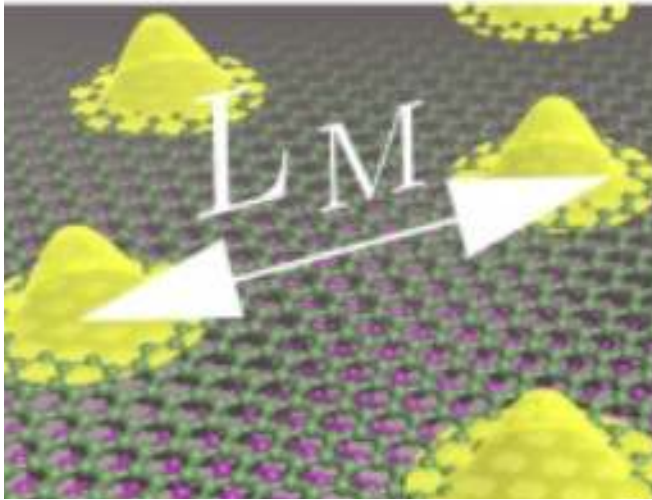


Nature 600, 439–443 (2021)

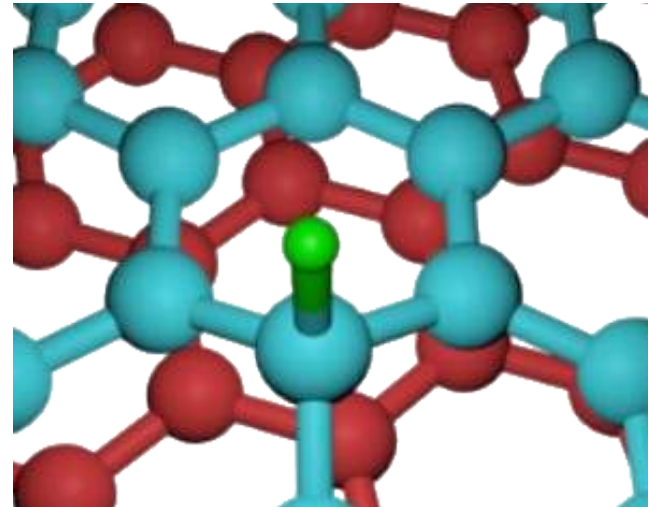
Twisted graphene multilayers provide a powerful platform for emergent phenomena

Two length scales in twisted van der Waals materials

The emergent moire scale



The original atomic scale

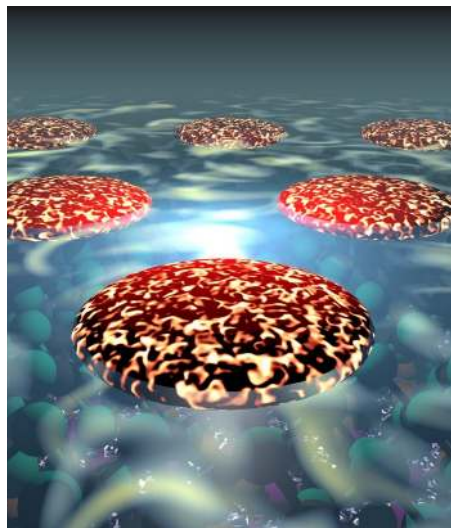


The coexistence of these two different scales is unique to moire systems

How do atomic impurities impact the physics emerging from much bigger length scales?

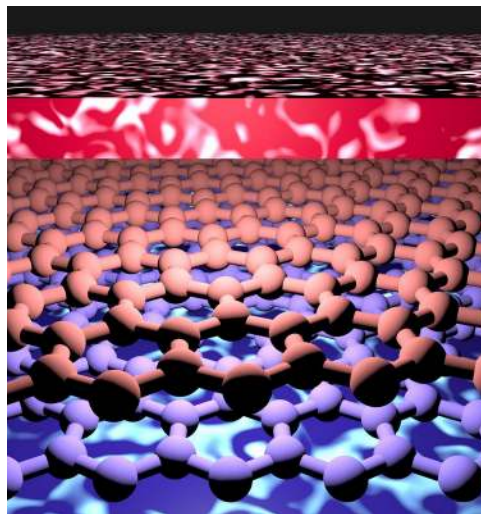
Today's plan

*Moire-enabled
topological
superconductivity
in $\text{CrBr}_3/\text{NbSe}_2$*



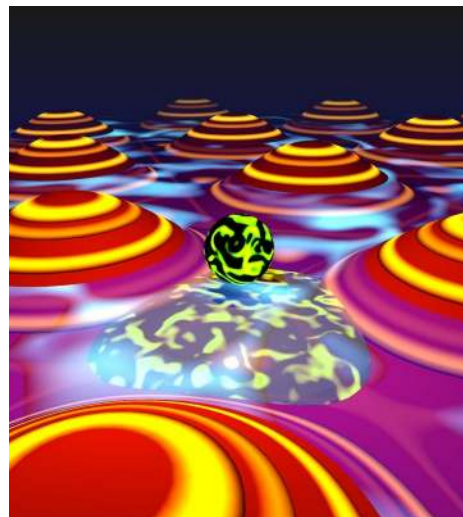
Nano Lett. 2022, 22, 1,
328–333 (2022)

*Moire-enabled
topological
superconductivity
in twisted graphene*



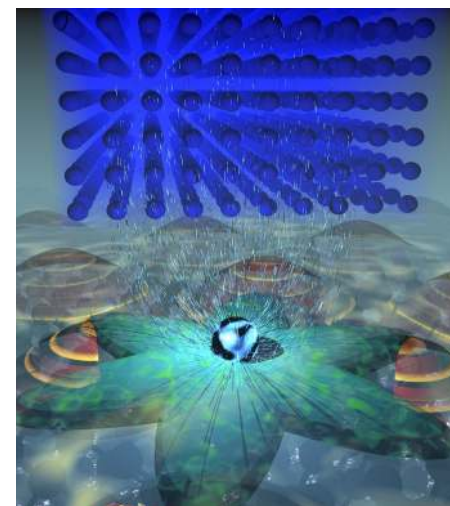
arXiv:2307.04605

*Impurities in twisted
moire topological
superconductors*



Phys. Rev. Mat. 6,
094010 (2022)

*Hamiltonian learning
from moire impurity
tomography*



arXiv:2308.11400

Behind the scenes

Experiment

S. Ganguli



M. Aapro



S. Kezilebieke



V. Vaňo



Md. Huda



P. Liljeroth



Nano Lett. 22, 1, 328-333 (2022)

Theory

E. Bascones



M. Khosravian



R. Koch

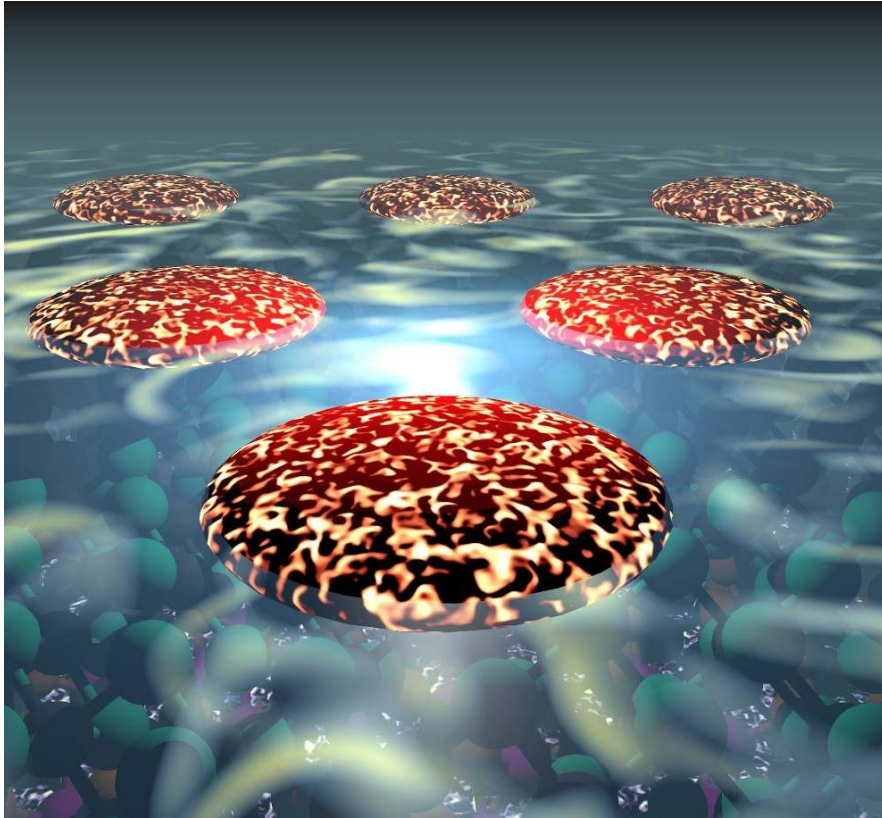


arXiv:2307.04605

arXiv:2308.11400

Phys. Rev. Materials 6, 094010 (2022)

Artificial topological moire superconductivity in $\text{NbSe}_2/\text{CrBr}_3$



S. Ganguli



M. Aapro



S. Kezilebieke



V. Vaňo



Md. Huda



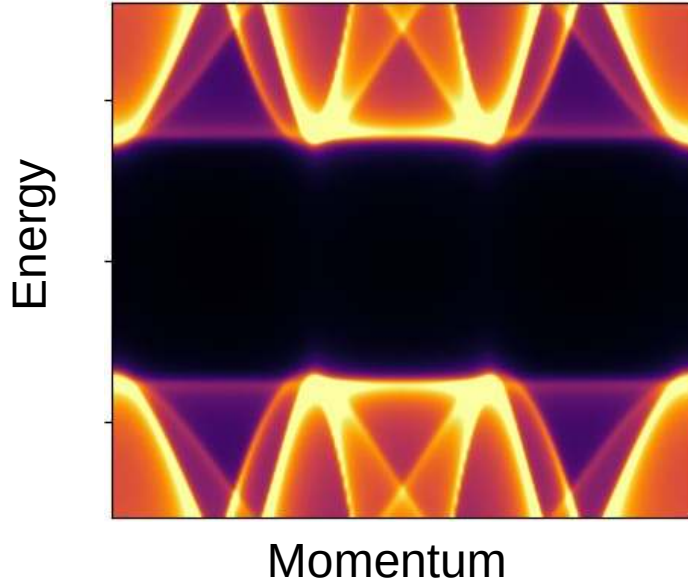
P. Liljeroth



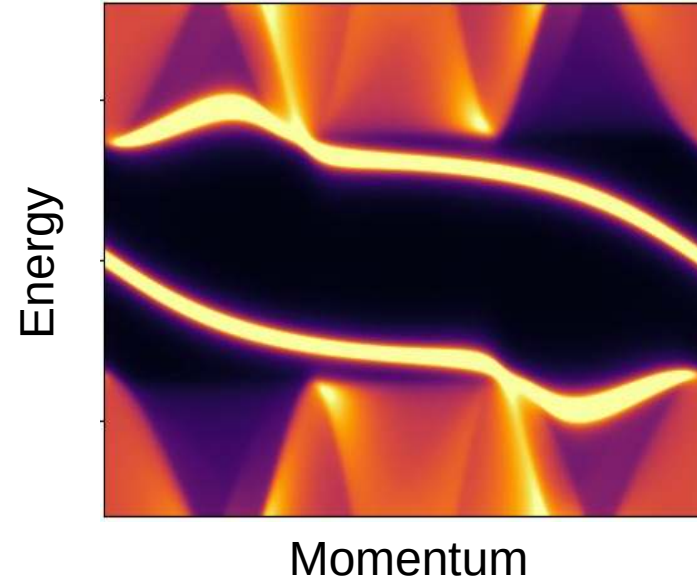
Nano Lett. 22, 1, 328-333 (2022)

Topological superconductors

Full gap in the bulk

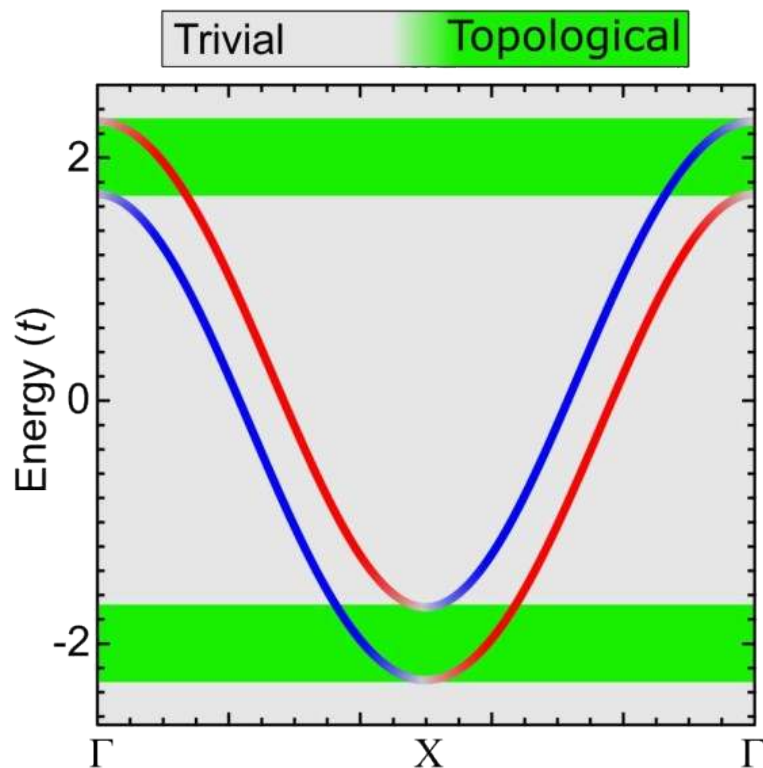


Gapless (Majorana) mode at the edge



Topological superconductors are rare in nature, and thus have to be artificially engineered

Warm up: 1D topological superconductor



$$H = H_0 + H_J + H_R$$

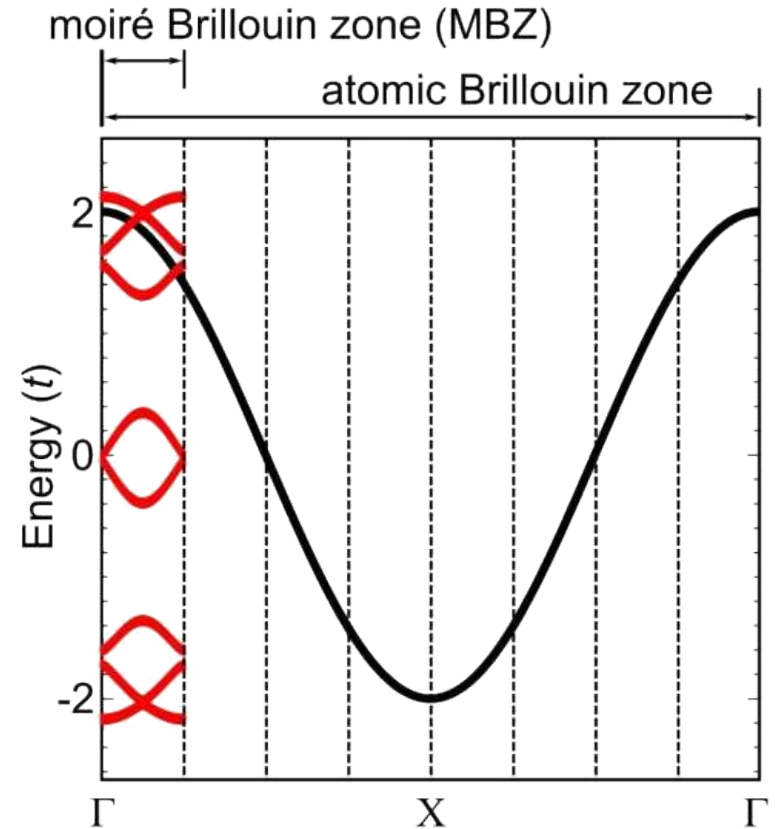
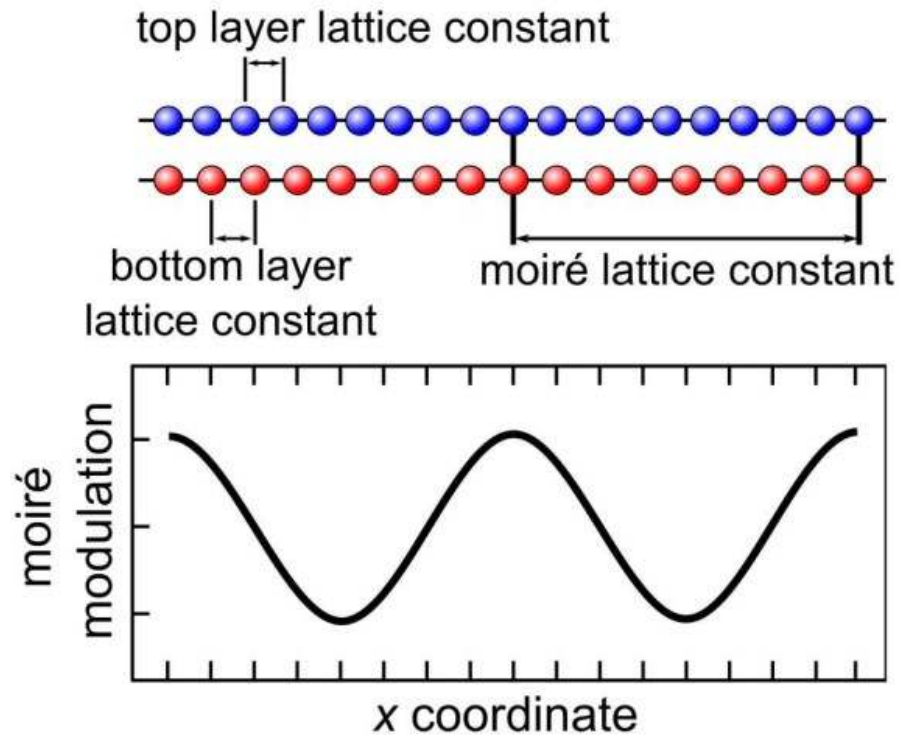
Kinetic energy

Exchange field

Rashba spin-orbit coupling

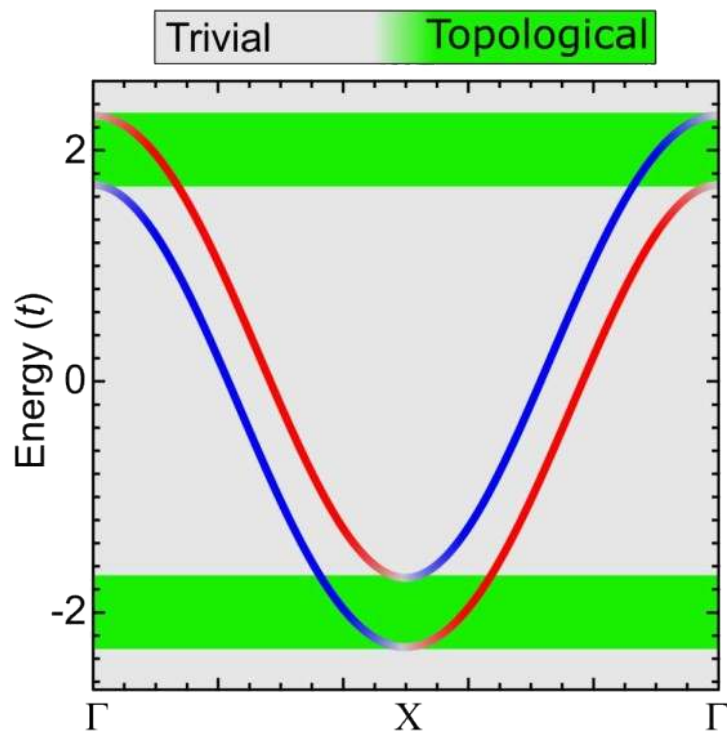
When switching on an s-wave pairing, green regions lead to topological superconductivity

Warm up: 1D moiré superconductor

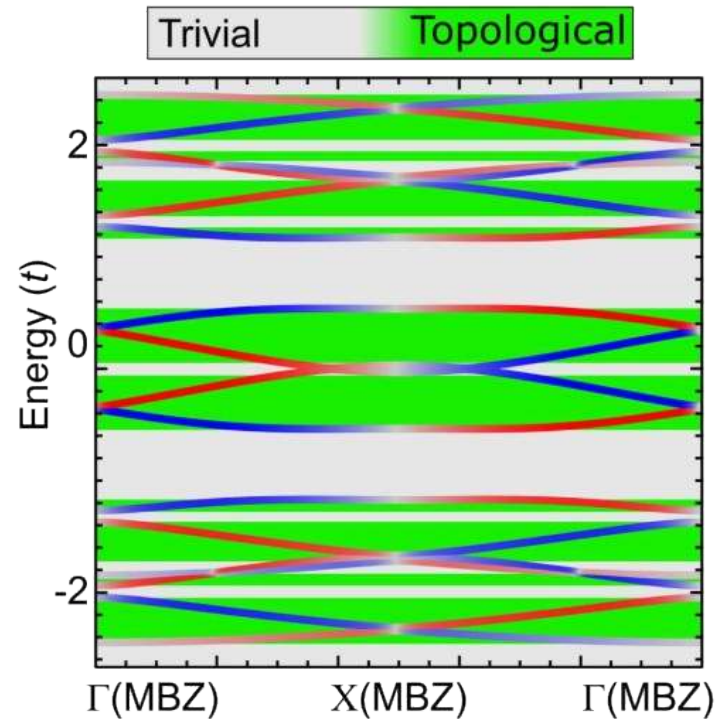


Warm up: 1D moire superconductor

Without moire



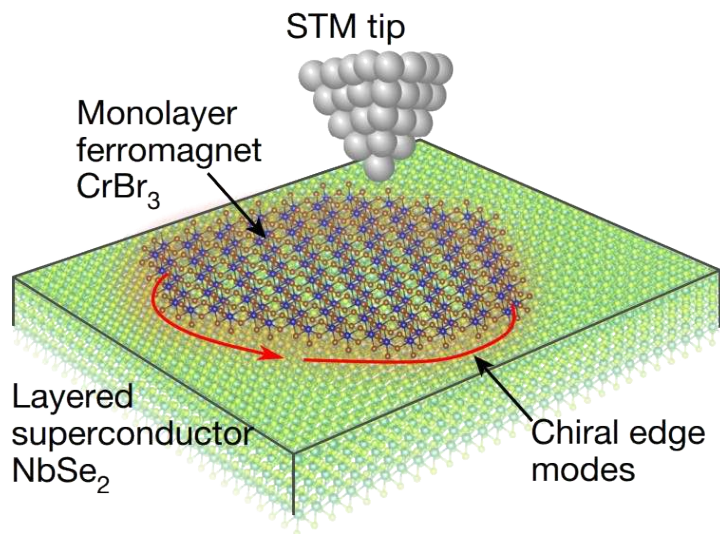
With moire



Moire pattern allow to realize topological superconductivity in otherwise forbidden energies

Topological superconductivity in a van der Waals heterostructure

CrBr₃/NbSe₂ heterostructure

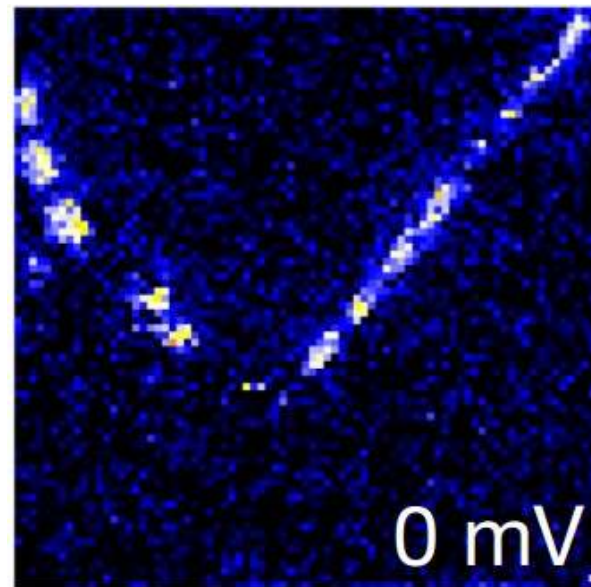


Nature 588, 424–428 (2020)

A topological superconducting state appears in CrBr₃/NbSe₂

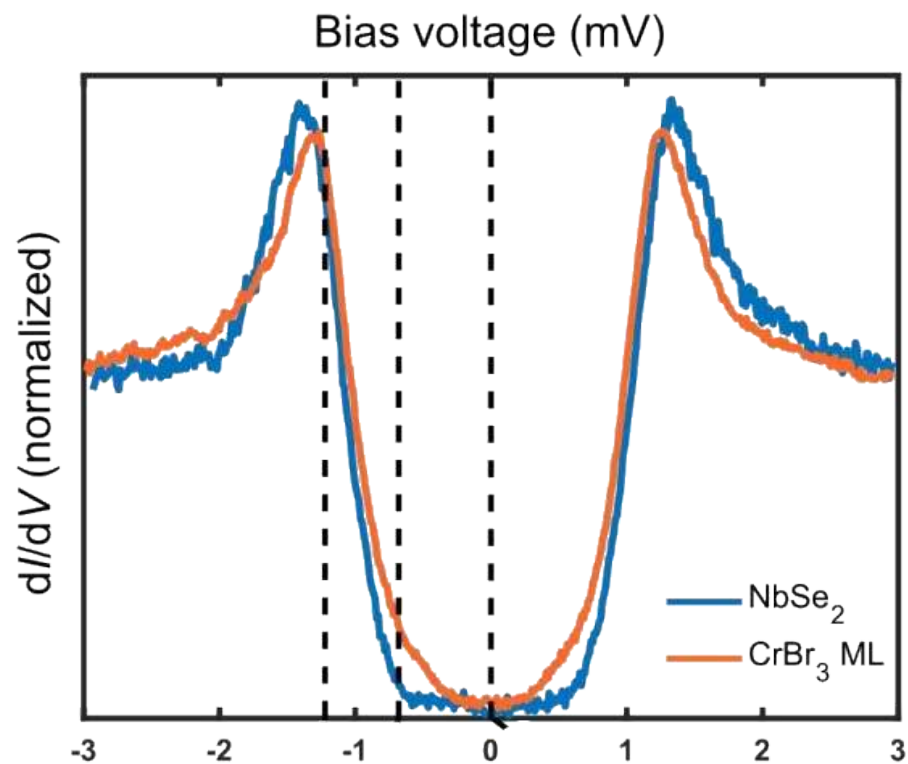
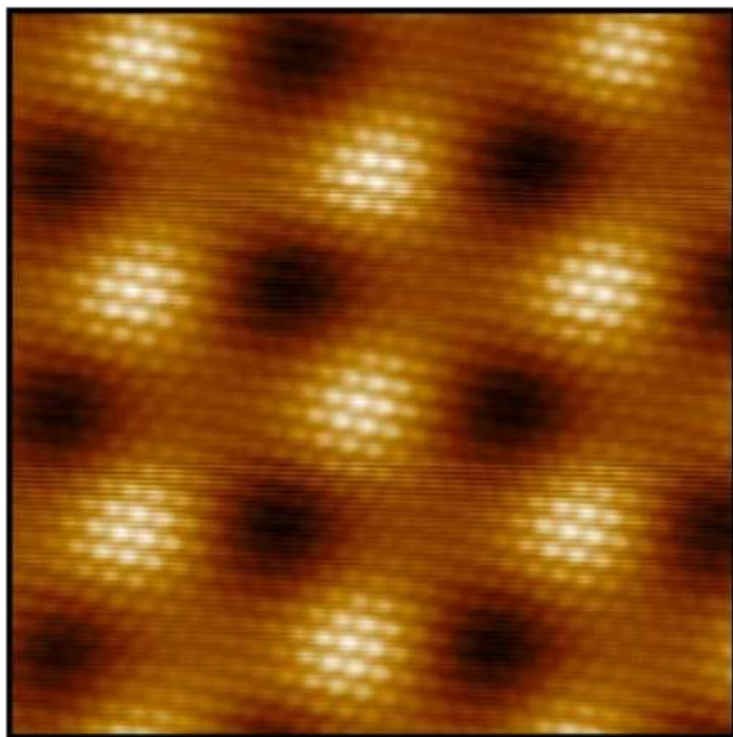
What is the role of the twist between the two van der Waals materials?

Zero bias dI/dV



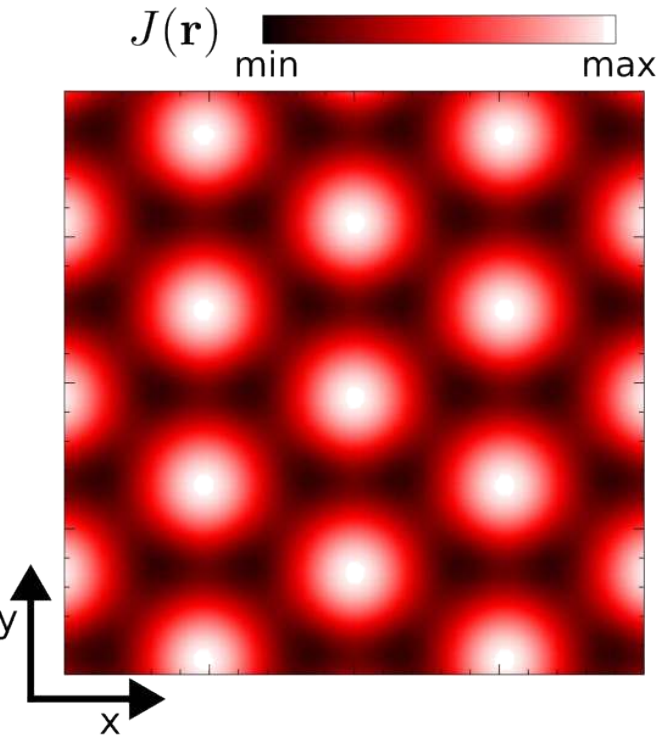
$\text{CrBr}_3/\text{NbSe}_2$ heterostructure

Height 0 Å  0.26 Å

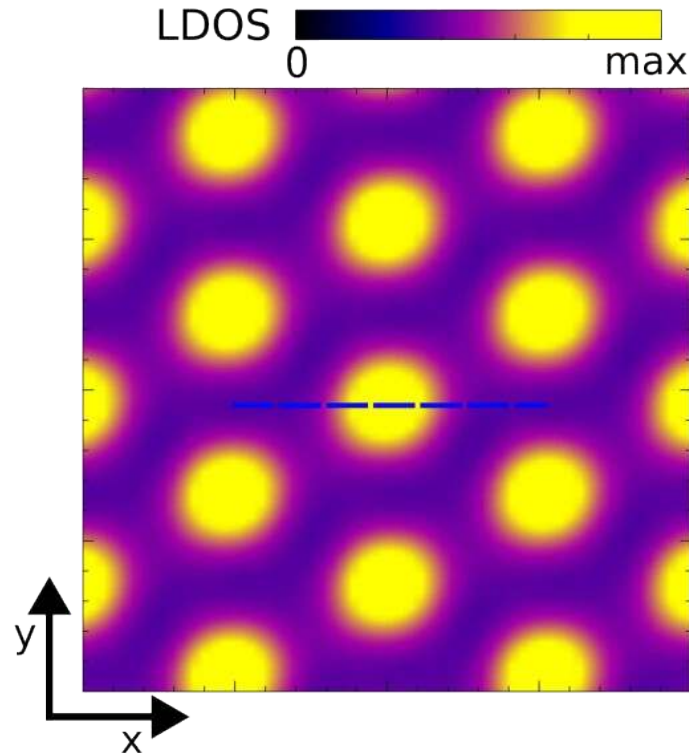


Bulk Yu-Shiba-Rusinov states

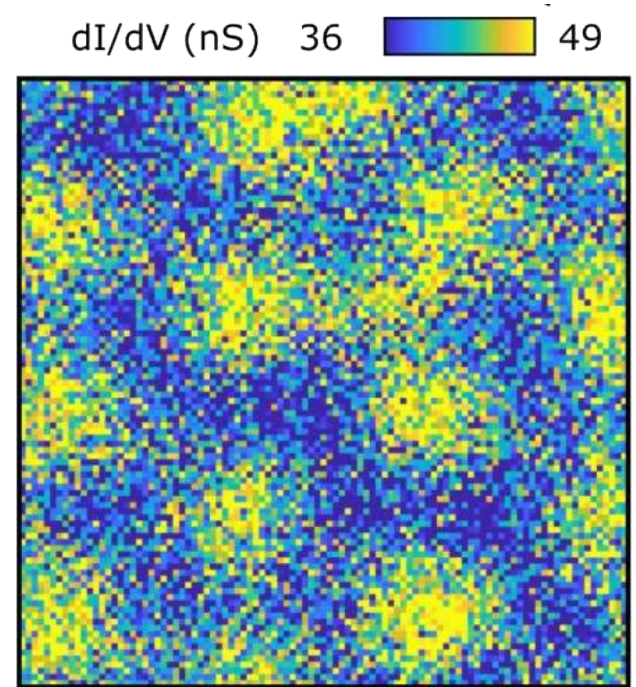
Exchange profile



Theoretical LDOS



Experimental dI/dV

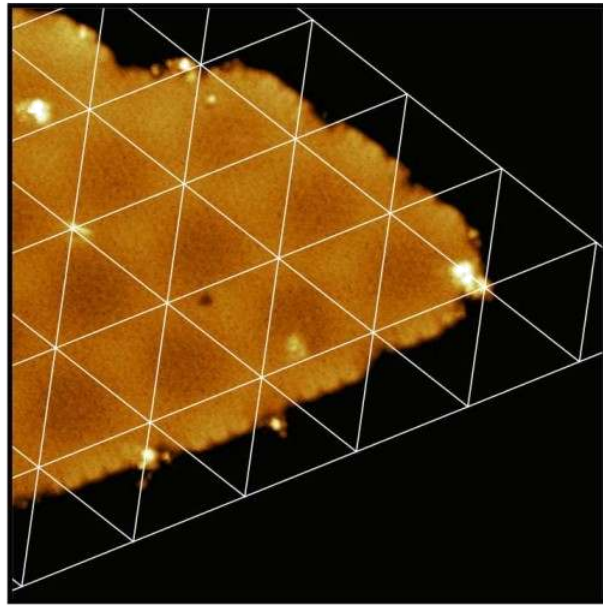


Bulk Yu-Shiba-Rusinov states are imprinted by the modulated exchange profile

Bulk Yu-Shiba-Rusinov states

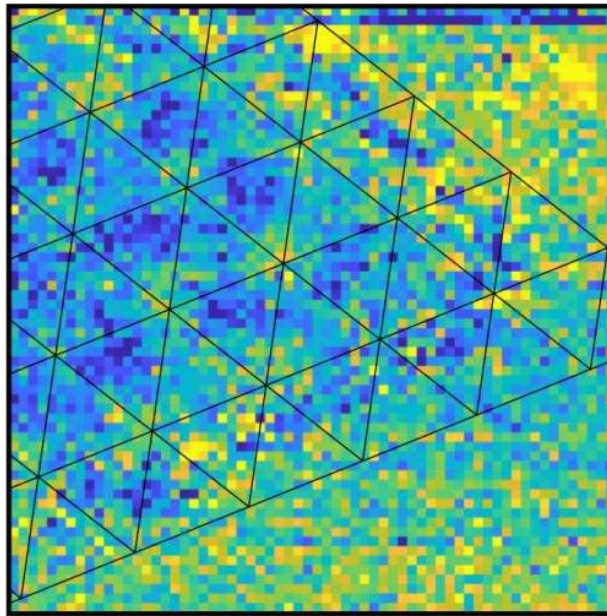
Topography

Height 0 Å  6 Å



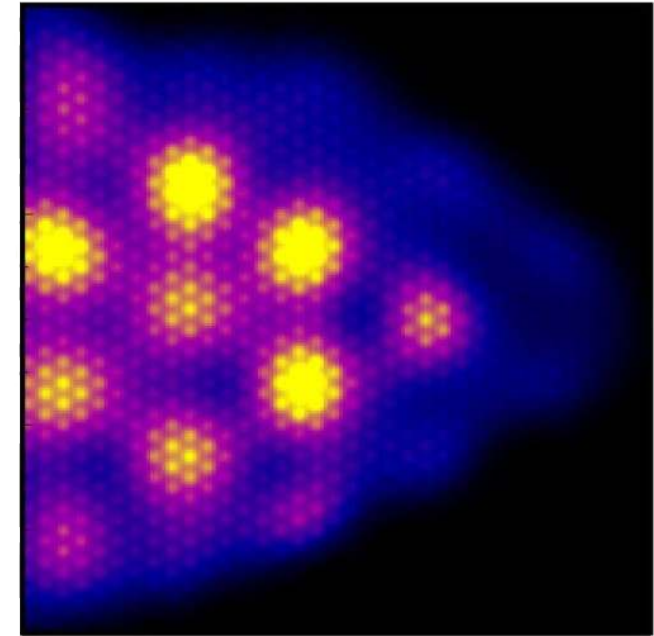
Experimental dIdV

dI/dV (nS) 19  36



Theoretical dIdV

LDOS 0  max

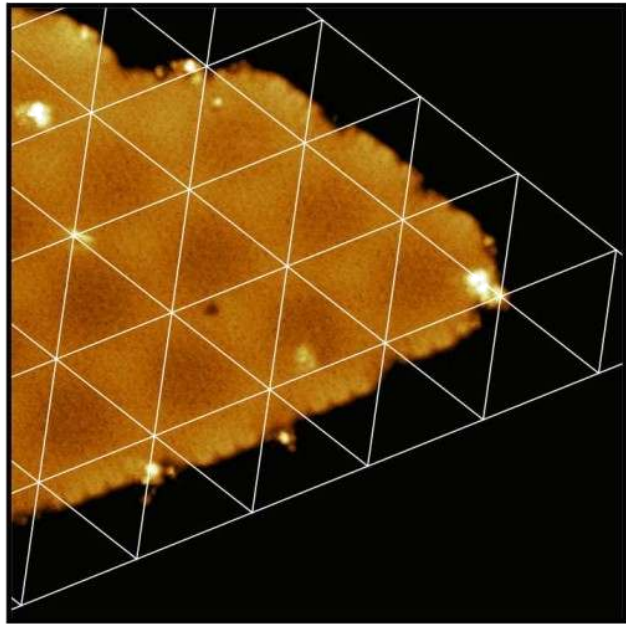


Bulk Yu-Shiba-Rusinov states are imprinted by the modulated exchange profile

Topological moire edge states

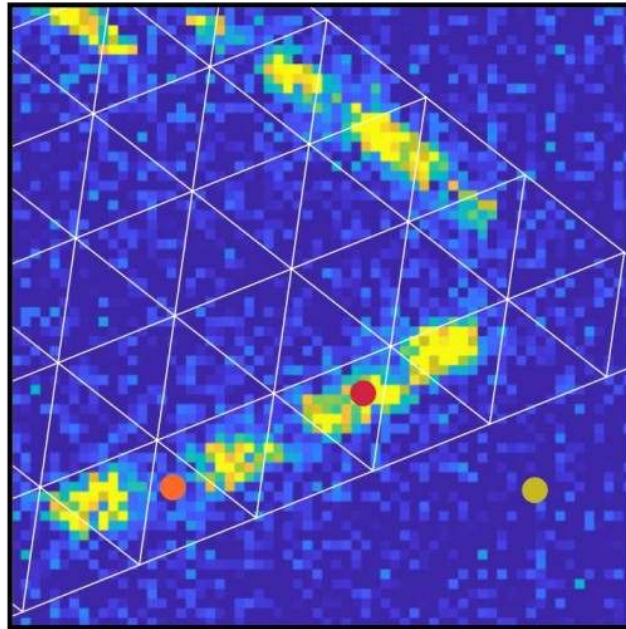
Topography

Height 0 Å  6 Å



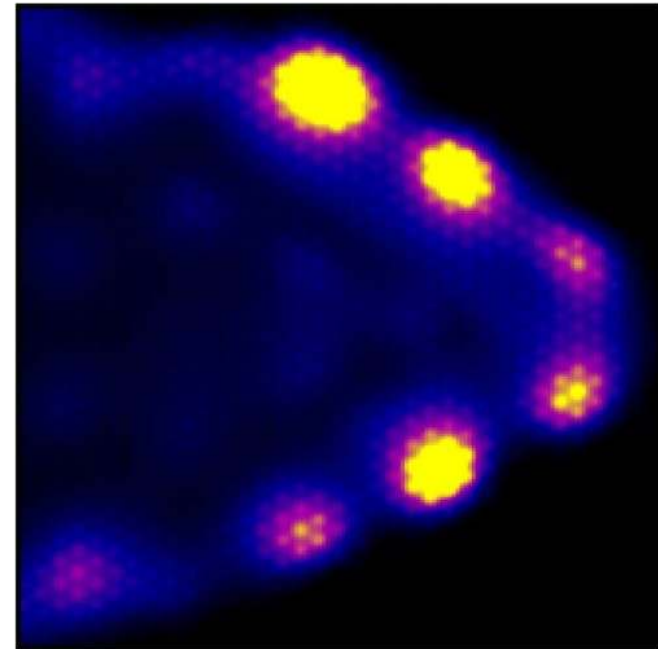
Experimental dIdV

dI/dV (nS) 1  20



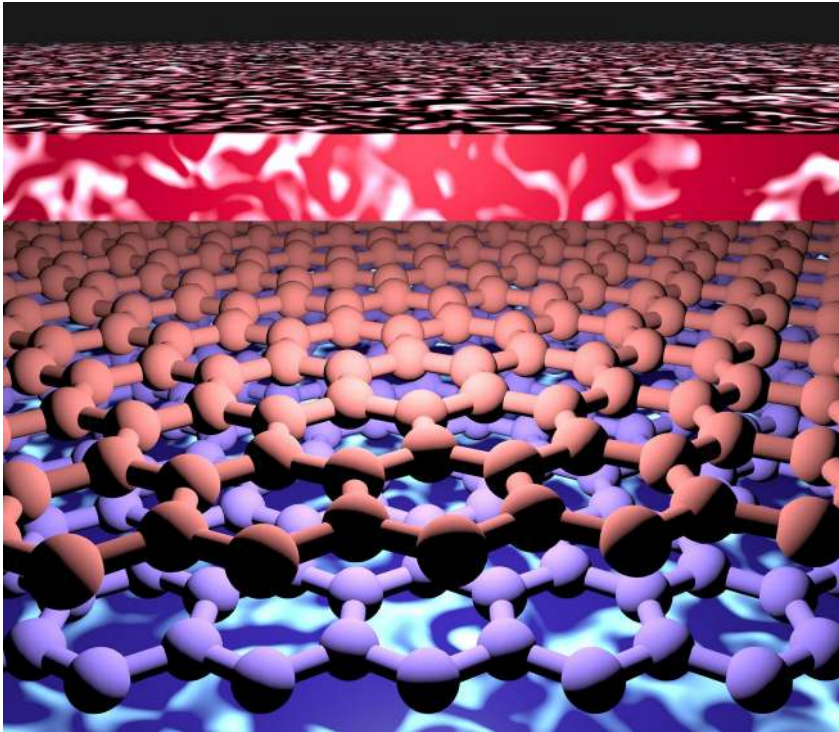
Theoretical dIdV

LDOS 0  max



Topological edge modes are imprinted by the modulated exchange profile

Moire-enabled artificial superconductors in twisted bilayer graphene



Maryam Khosravian

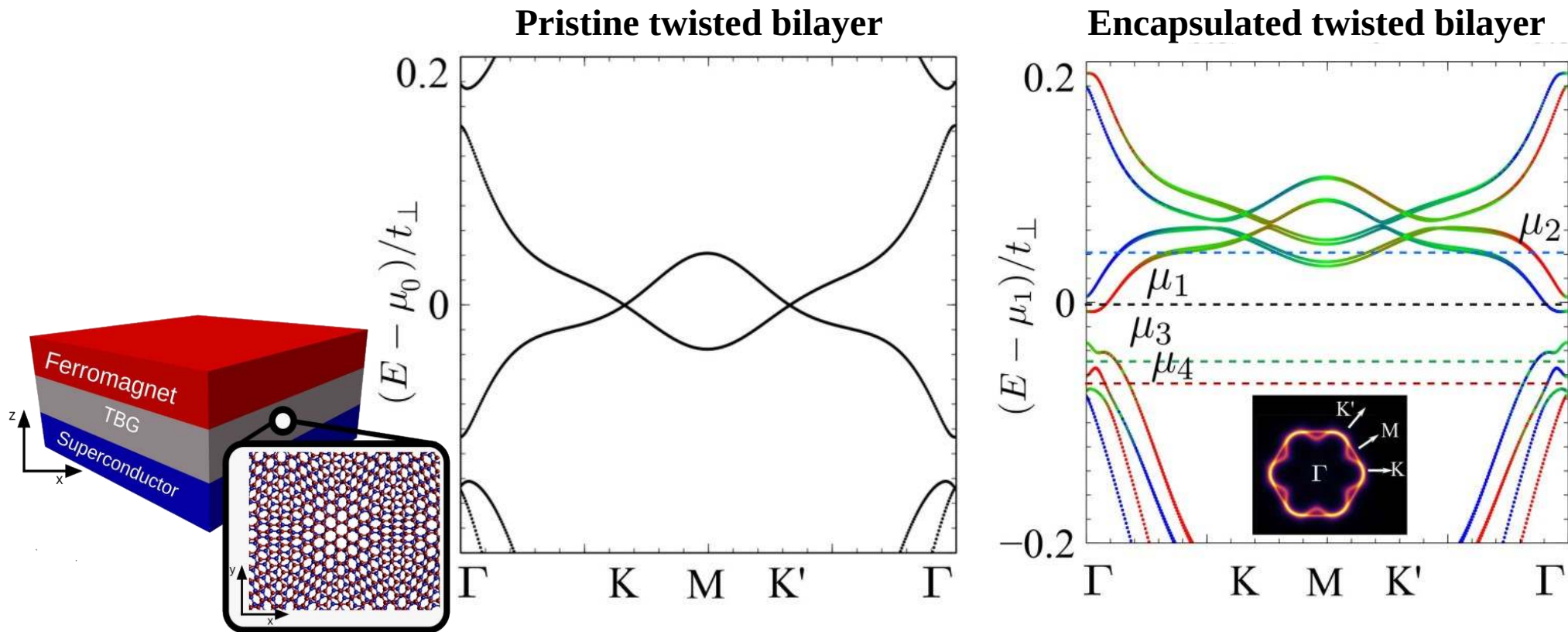


Elena Bascones



arXiv:2307.04605

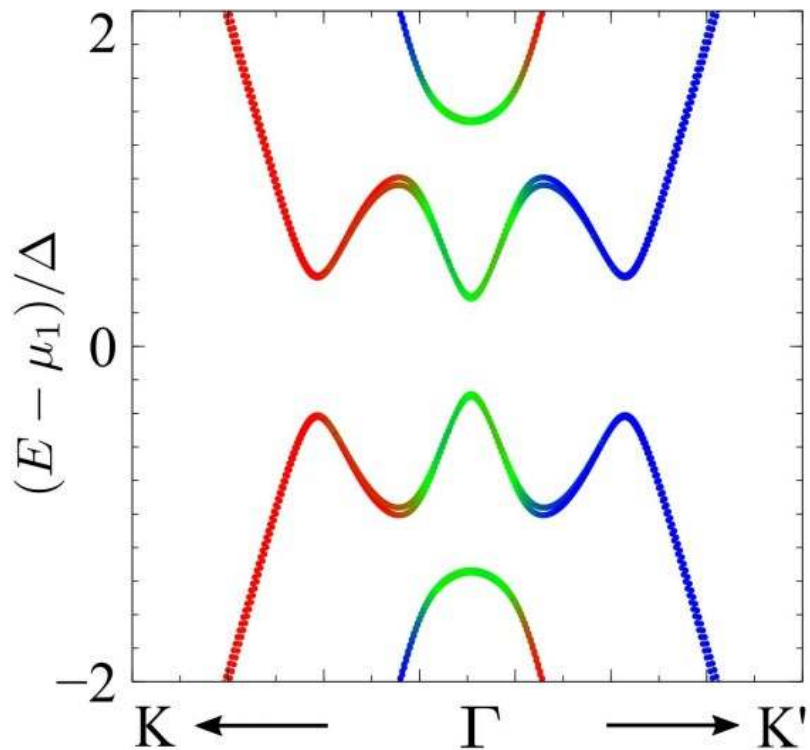
Moire-enabled artificial superconductors in twisted bilayer graphene



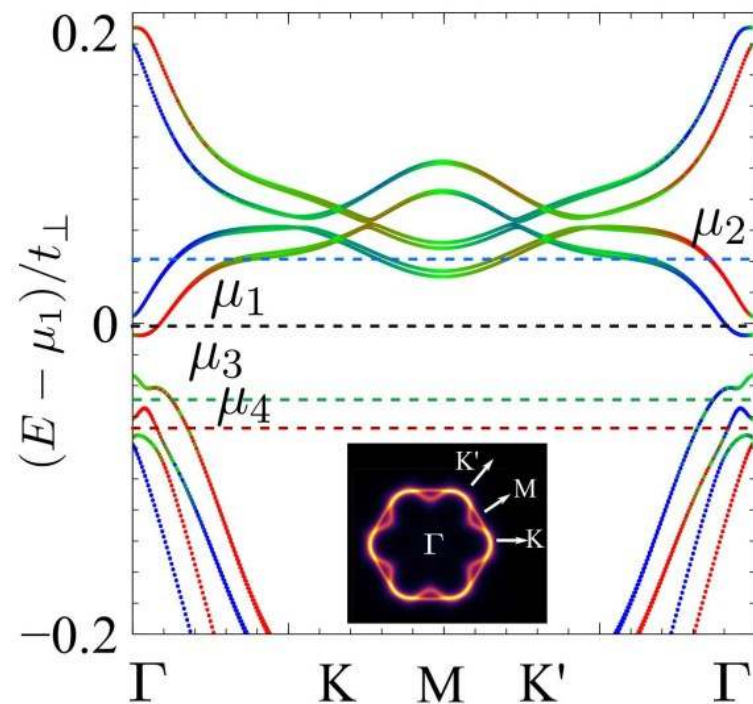
Moire effect gives rise to minigaps featuring helical states with encapsulation

Moire-enabled artificial superconductors in twisted bilayer graphene

With superconductivity



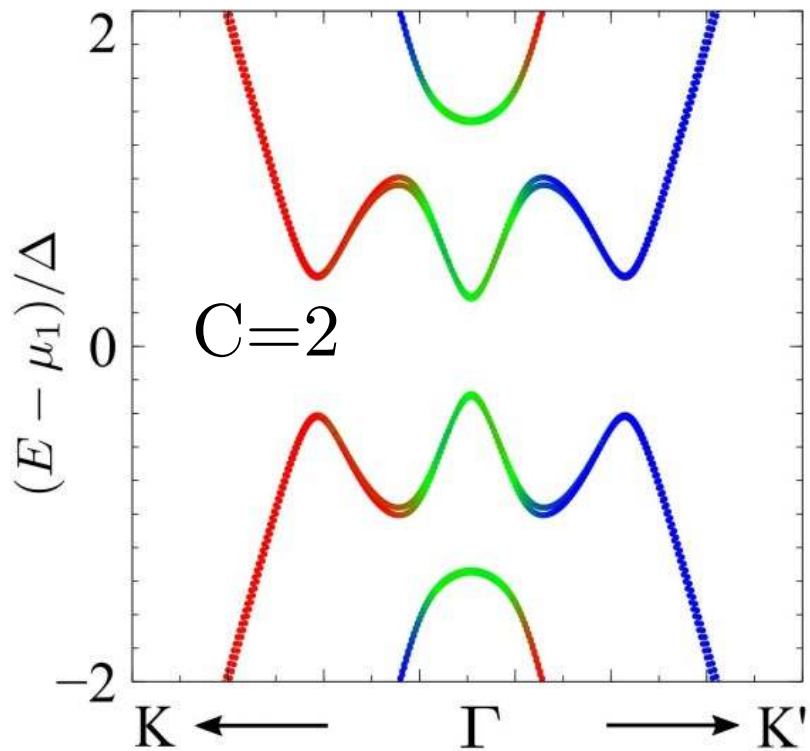
Without superconductivity



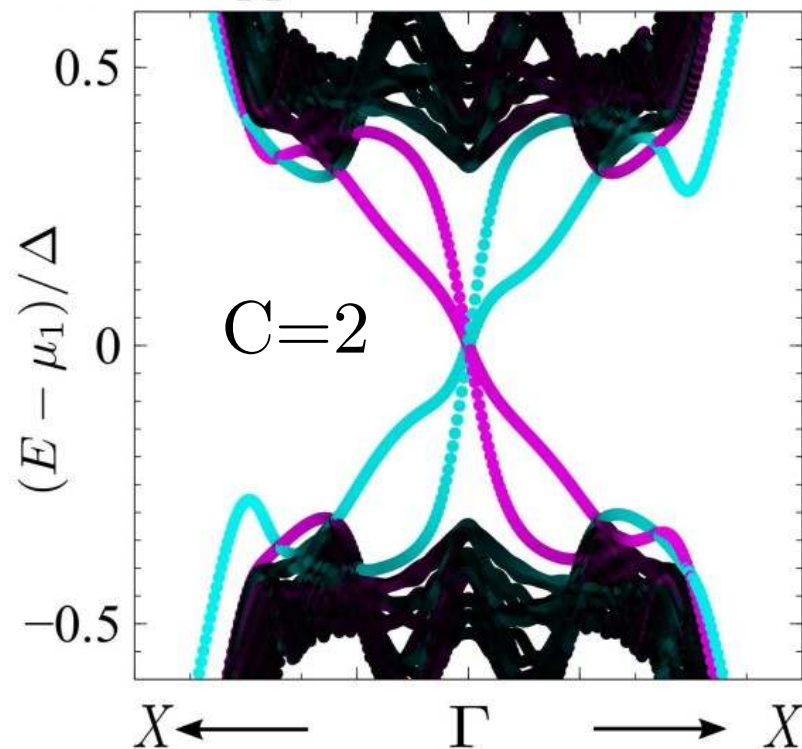
Switching on superconductivity gives rise to a topological superconducting state

Moire-enabled artificial superconductors in twisted bilayer graphene

Bulk band structure

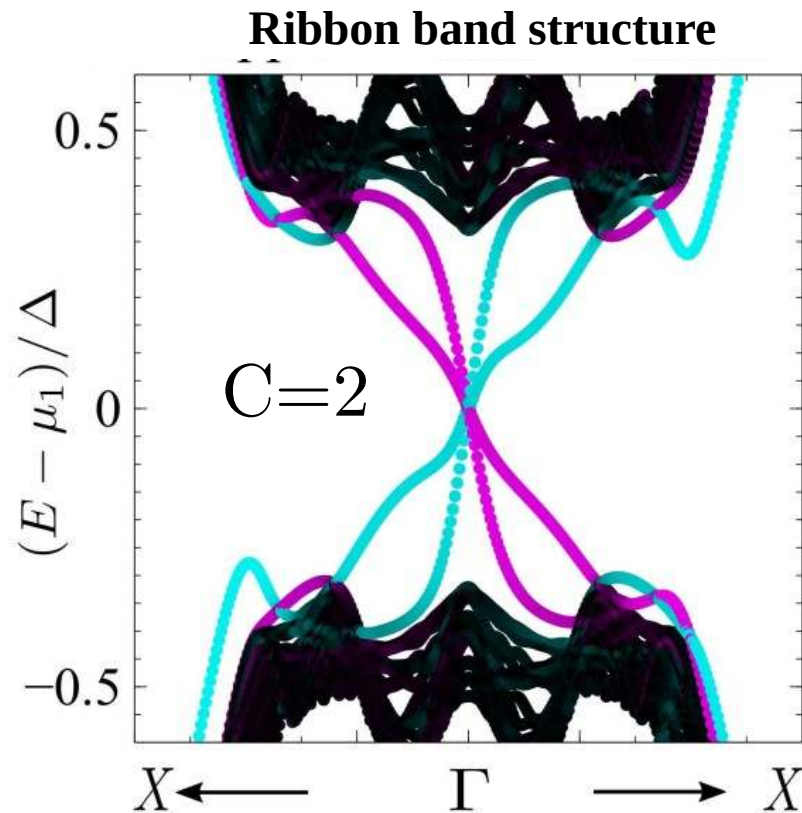
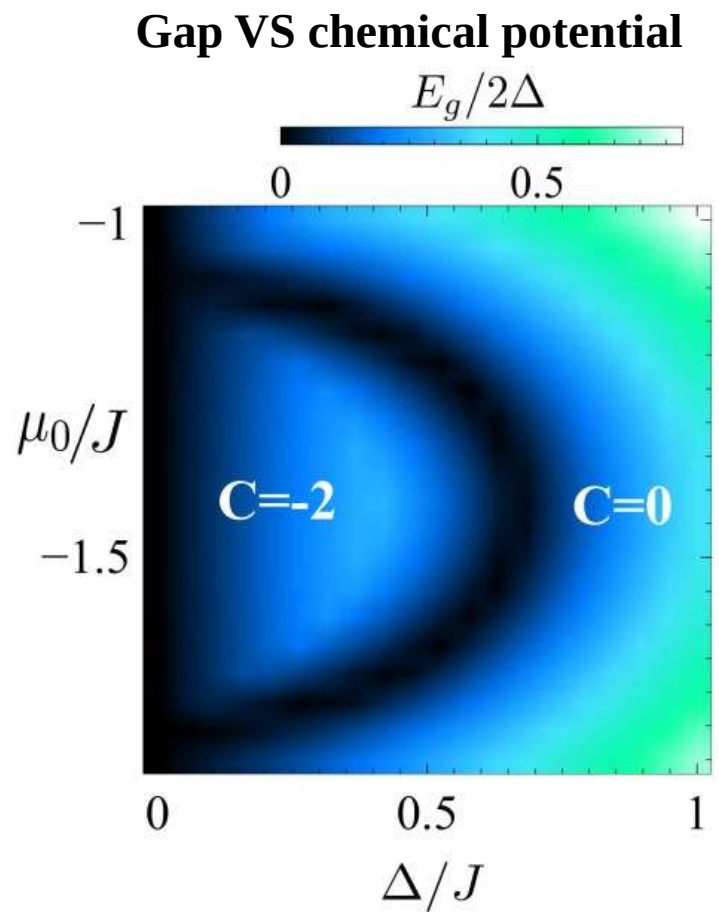


Ribbon band structure



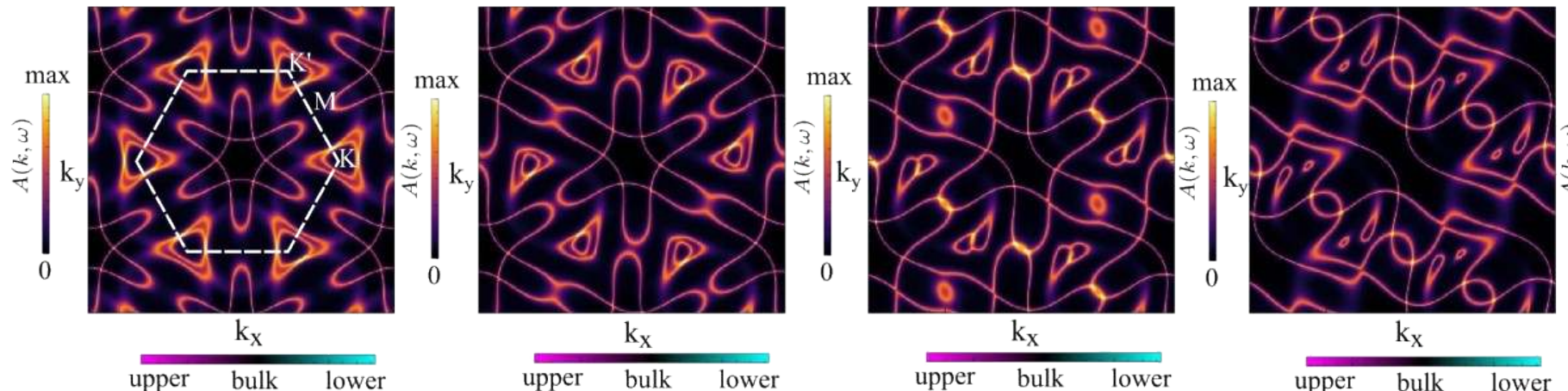
The topological state features chiral Majorana modes in a ribbon geometry

Moire-enabled artificial superconductors in twisted bilayer graphene

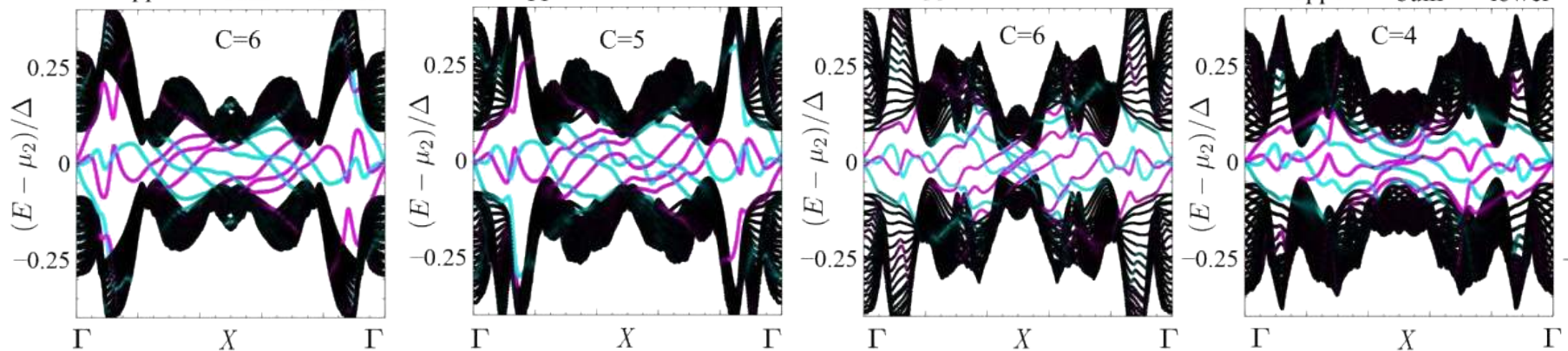


Multiple topological phases tunable by strain

Fermi surface

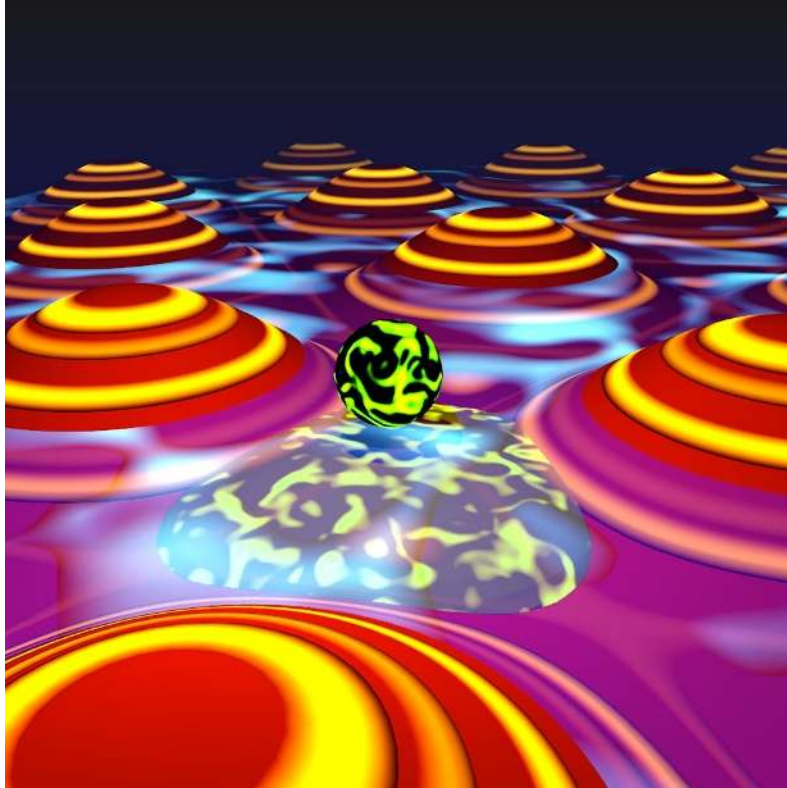


Ribbon bands



Strain allows to realize topological states with different Chern numbers

Impurities in twisted moire topological superconductors



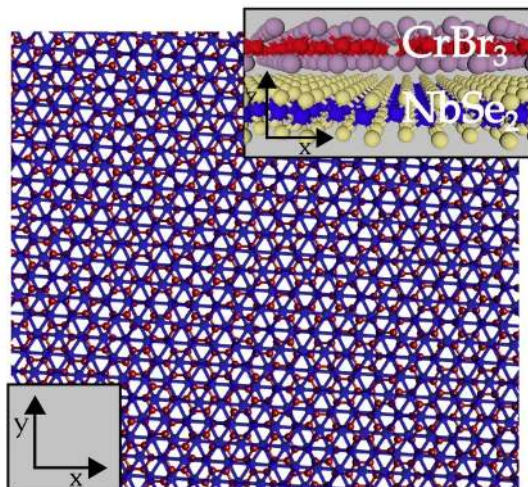
Maryam Khosravian



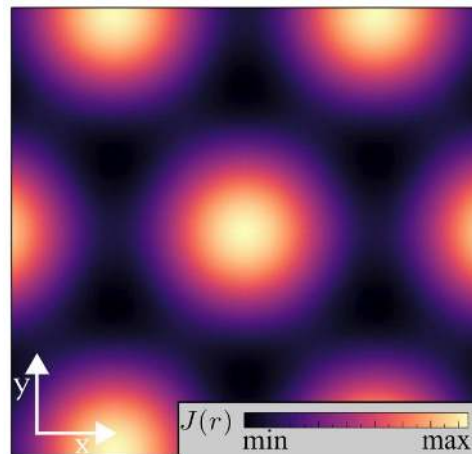
Phys. Rev. Materials 6, 094010 (2022)

Hamiltonian for the pristine moire topological superconductor

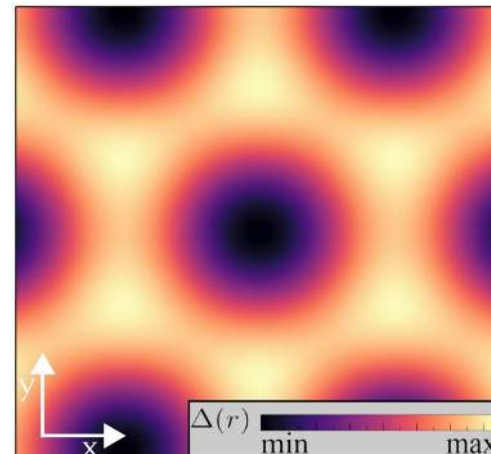
Structure



Exchange profile



Superconducting profile



$$\mathcal{H}_0 = \mathcal{H}_{\text{kin}} + \mathcal{H}_J + \mathcal{H}_R + \mathcal{H}_{\text{SC}}$$

Kinetic
energy

Exchange
coupling

Rashba
SOC

s-wave
superconductivity

Hamiltonian for the defective moire topological superconductor

Full Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{imp}}$$

Local impurity in the moire system

$$\mathcal{H}_{\text{imp}} = w \sum_s c_{n,s}^\dagger c_{n,s}$$

Weak impurity

$$w \rightarrow 0$$

Strong impurity

$$w \rightarrow \infty$$

$$\mathcal{H}_0 = \mathcal{H}_{\text{kin}} + \mathcal{H}_J + \mathcal{H}_R + \mathcal{H}_{\text{SC}}$$

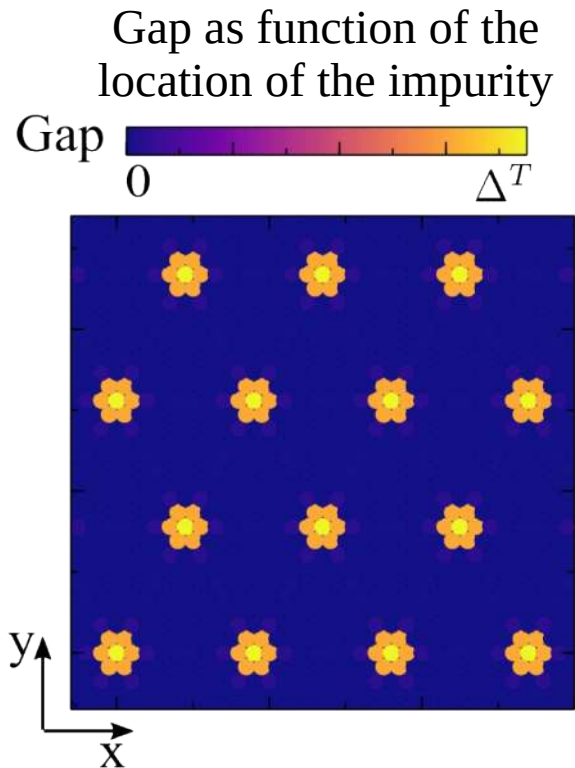
Kinetic
energy

Exchange
coupling

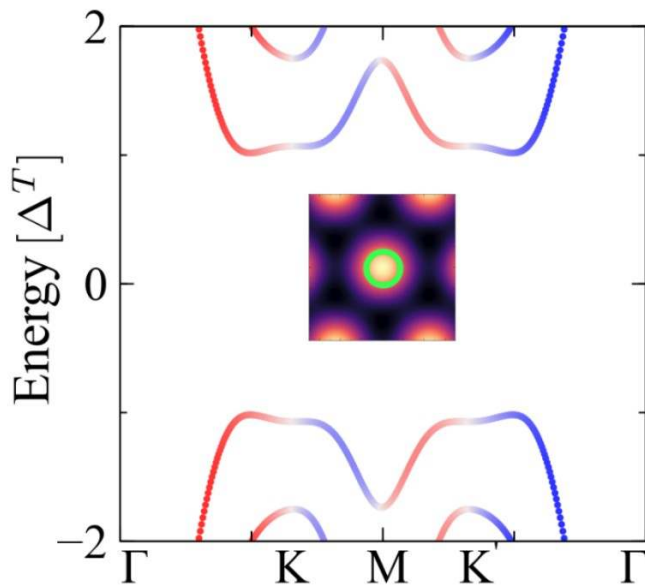
Rashba
SOC

s-wave
superconductivity

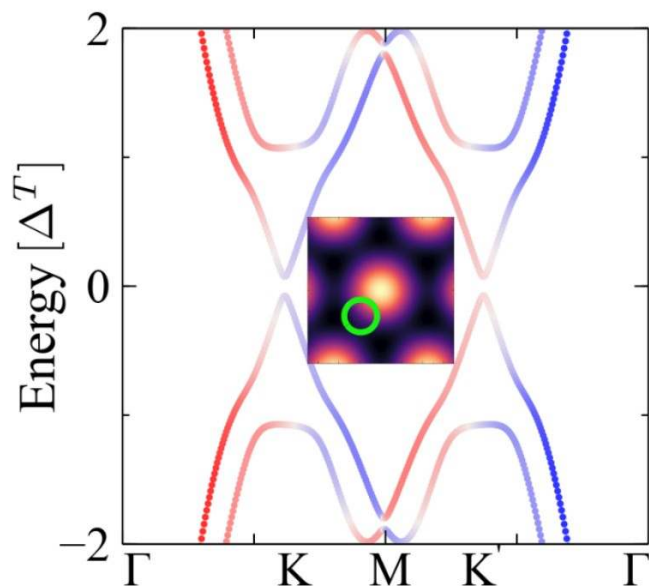
Gap as a function of the location of a strong impurity



Band structure
for impurity at the center



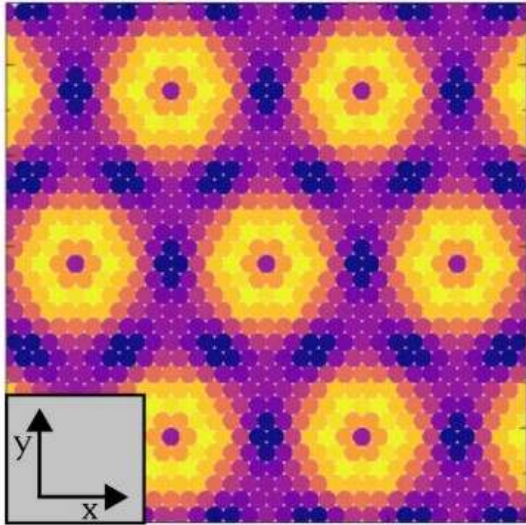
Band structure for
impurity away from the center



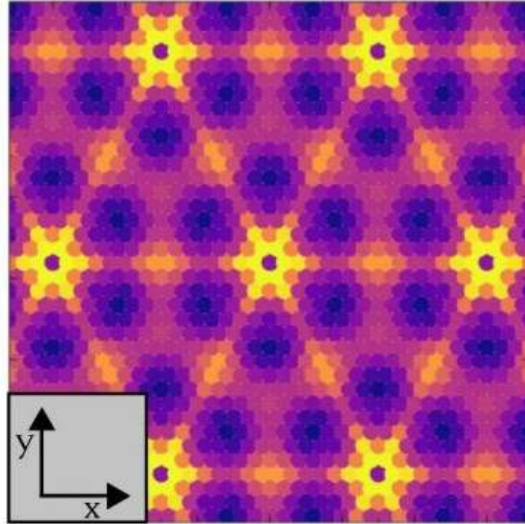
The location of the impurity strongly affects the resulting gap

Gap as function of location for different moire unit cells

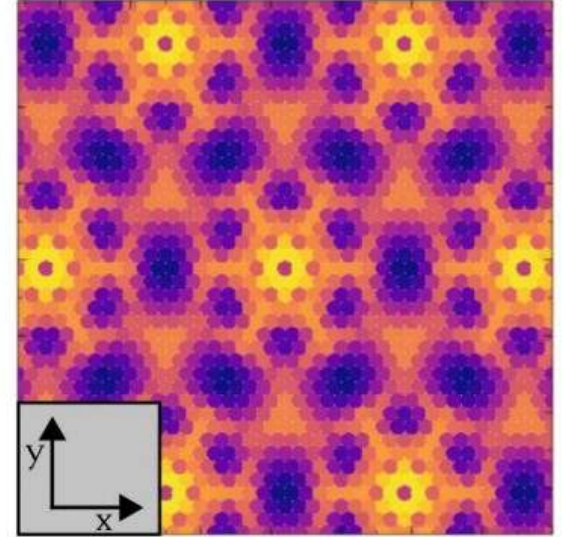
11x11 supercell
Gap 
 $0.95\Delta^T$ $1.09\Delta^T$



15x15 supercell
Gap 
 $0.79\Delta^T$ $1.01\Delta^T$



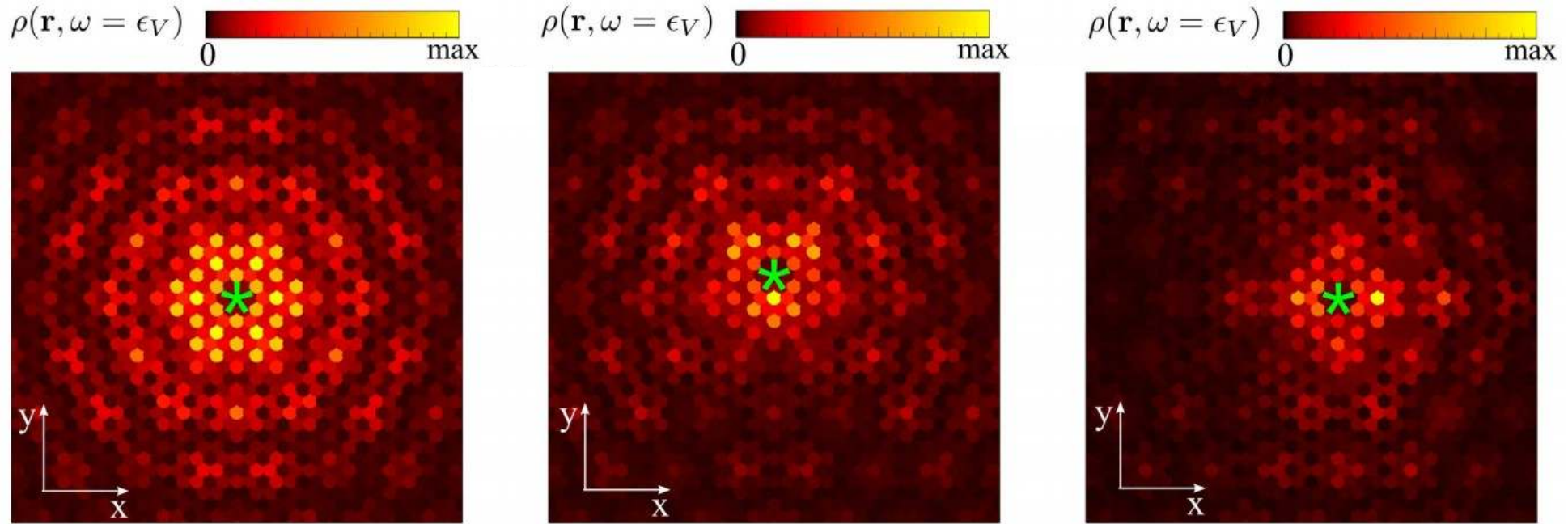
17x17 supercell
Gap 
 $0.87\Delta^T$ $0.98\Delta^T$



Detrimental locations for impurities depend on the specific moire supercell

Single impurity in a topological moire superconductor

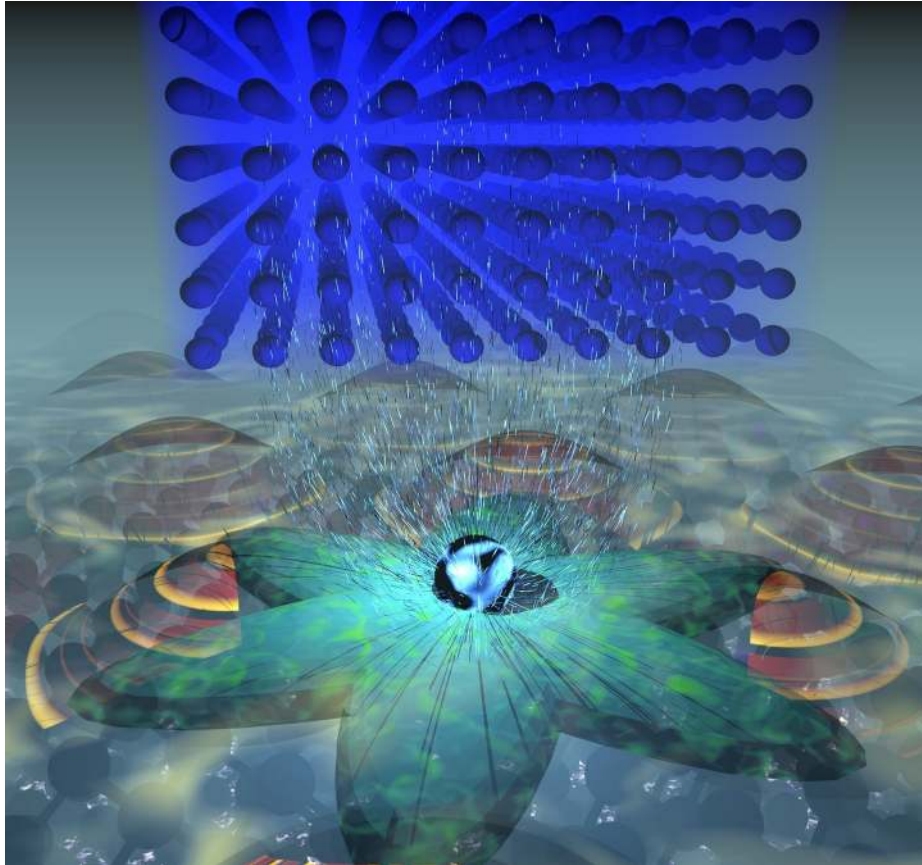
Wavefunction of the YSR state for different impurity locations



The YSR state wavefunction and the moire give rise to interference effects

Could we learn physics of the system by exploiting these interference effects?

Hamiltonian learning from impurity tomography in moire superconductors



Maryam Khosravian

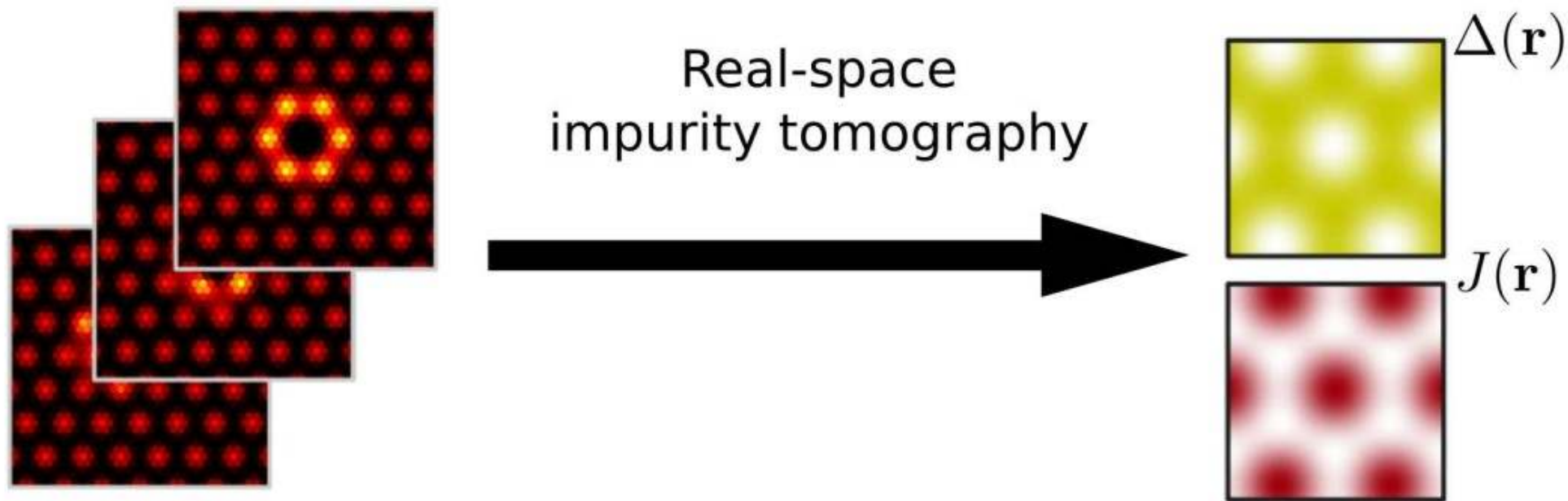


Rouven Koch



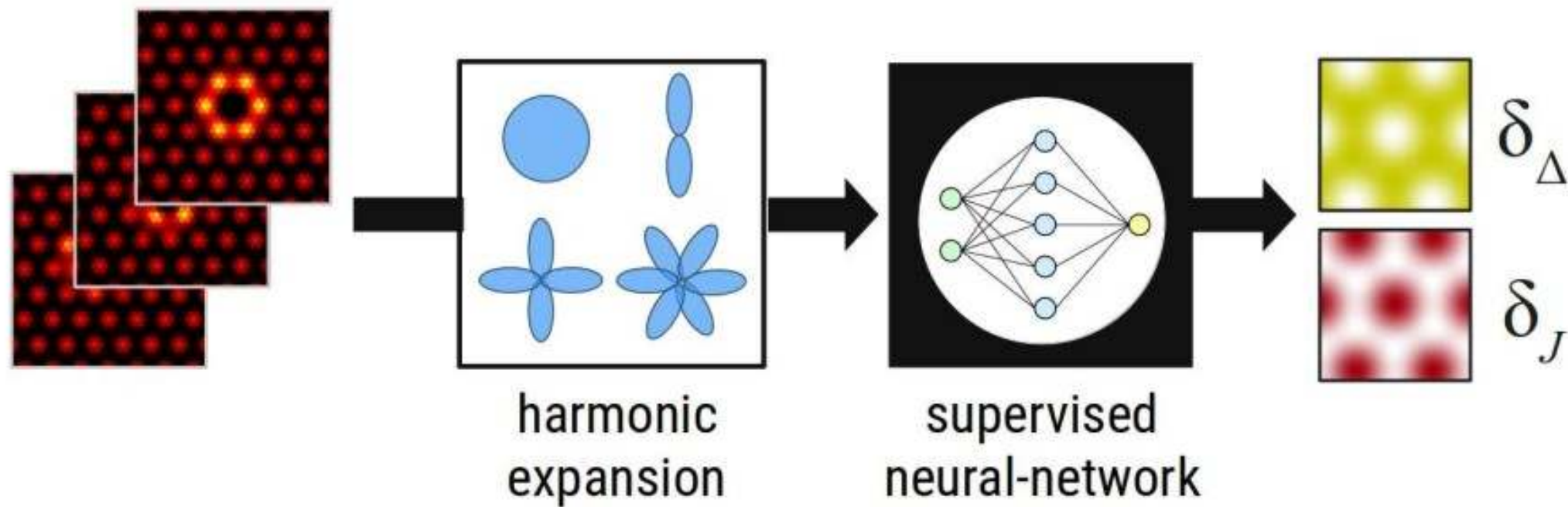
arXiv:2308.11400

Real-space impurity tomography



Can we learn real-space superconducting and exchange profiles directly from spectroscopy?

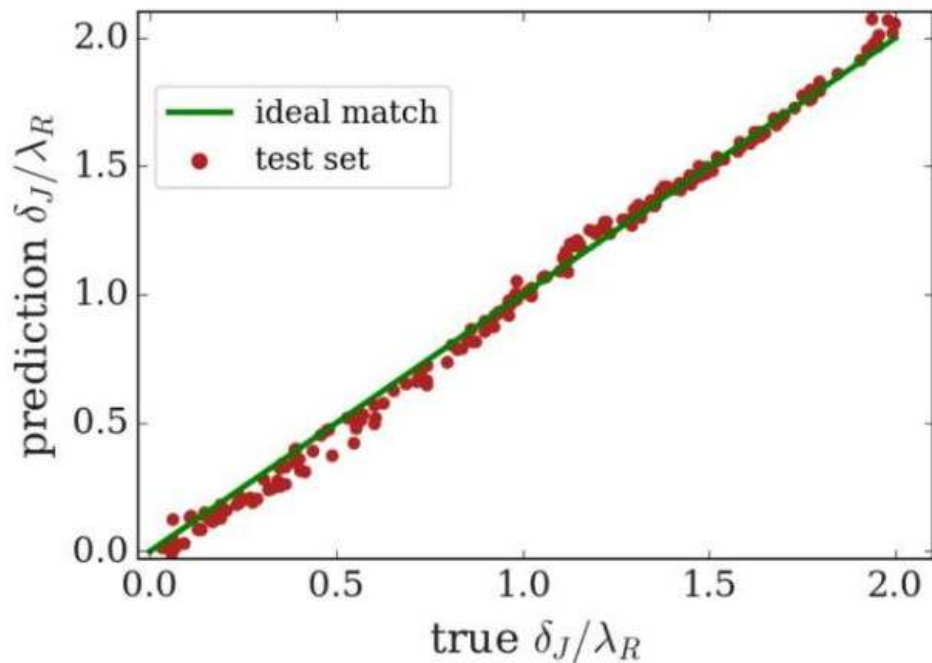
Real-space impurity tomography



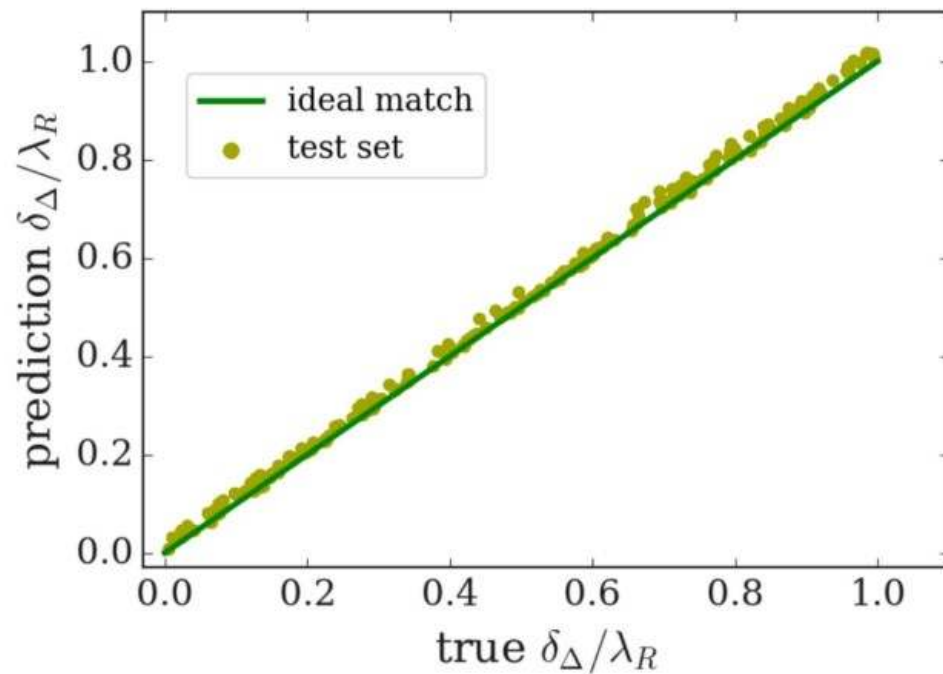
$$c_{ln} = \sum_{\alpha} \rho(\mathbf{r}_{\alpha}) e^{il\phi_{\alpha}} r_{\alpha}^n e^{-r_{\alpha}/\lambda}$$

Moire Hamiltonian learning with real-space impurity tomography

Exchange profile prediction



Superconducting profile prediction



Impurity tomography allow to extract the superconducting and exchange profiles

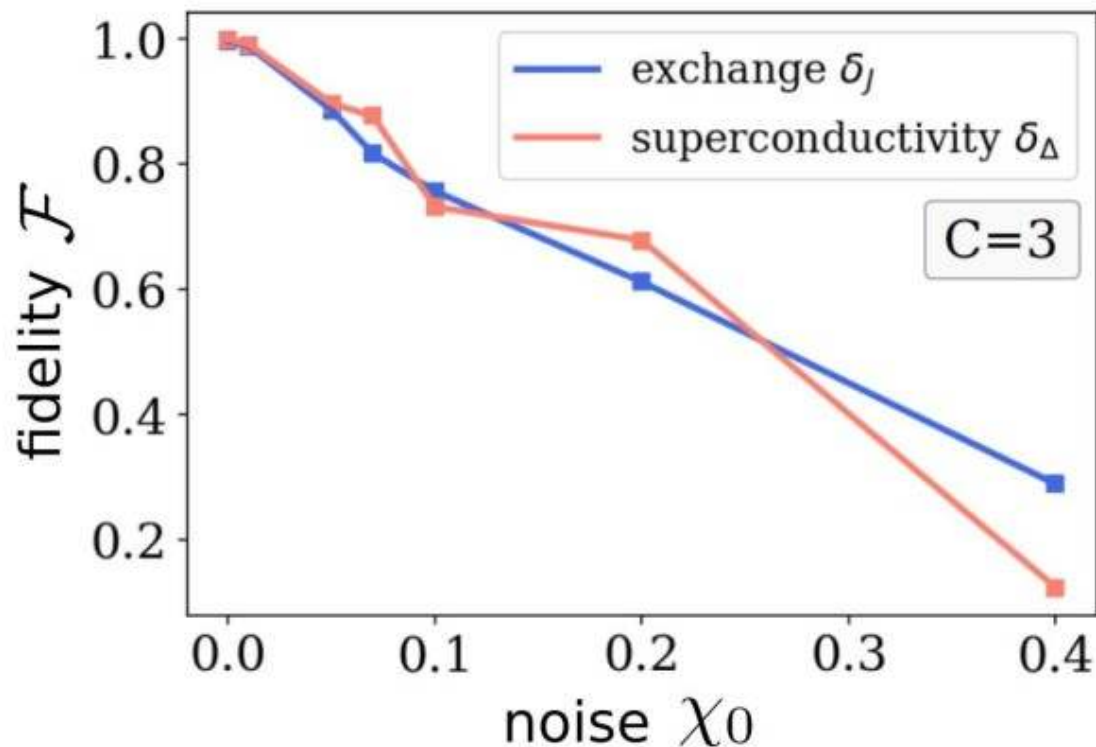
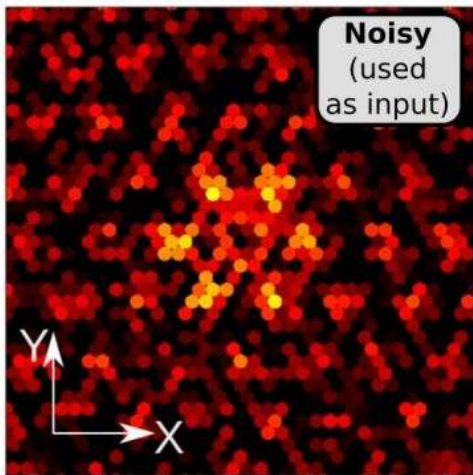
Hamiltonian learning with noisy spectroscopy

Prediction accuracy (fidelity)

$F = 1$ Perfect prediction

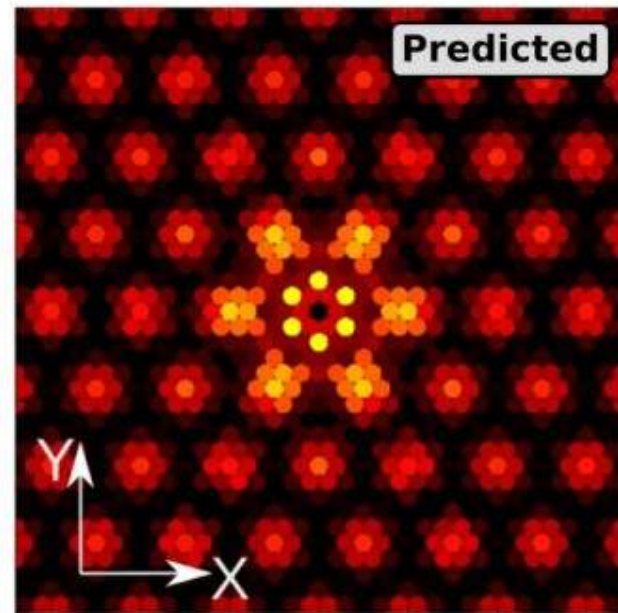
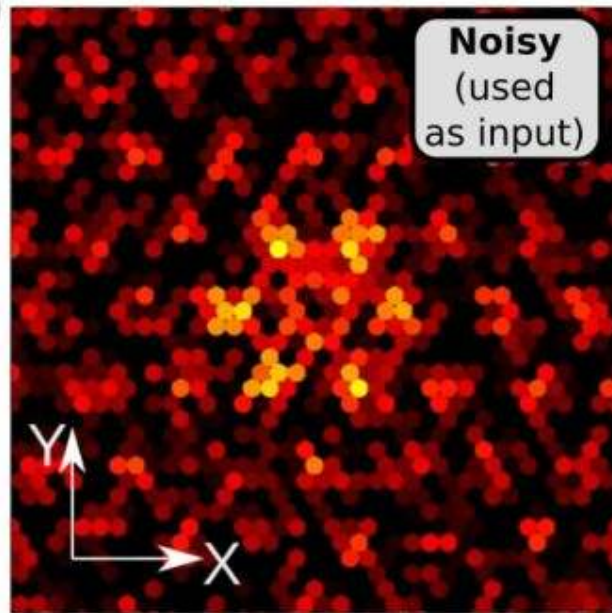
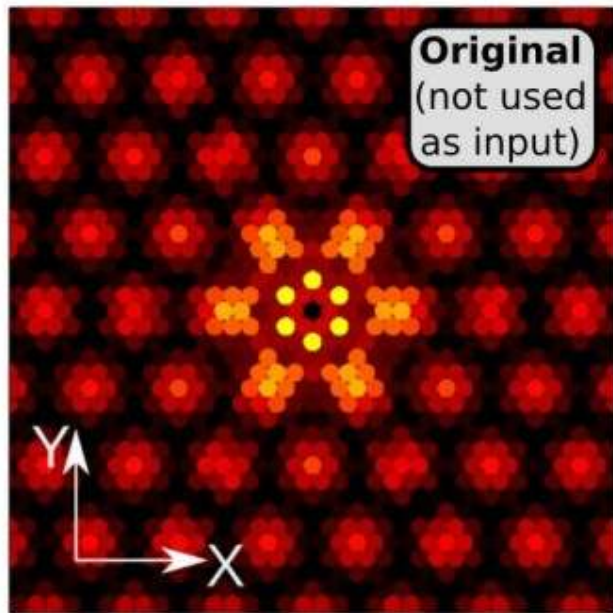
$F = 0$ No predictive power

Noise $\chi_0 = 0.2$



Hamiltonian learning is partially successful even with strong noise

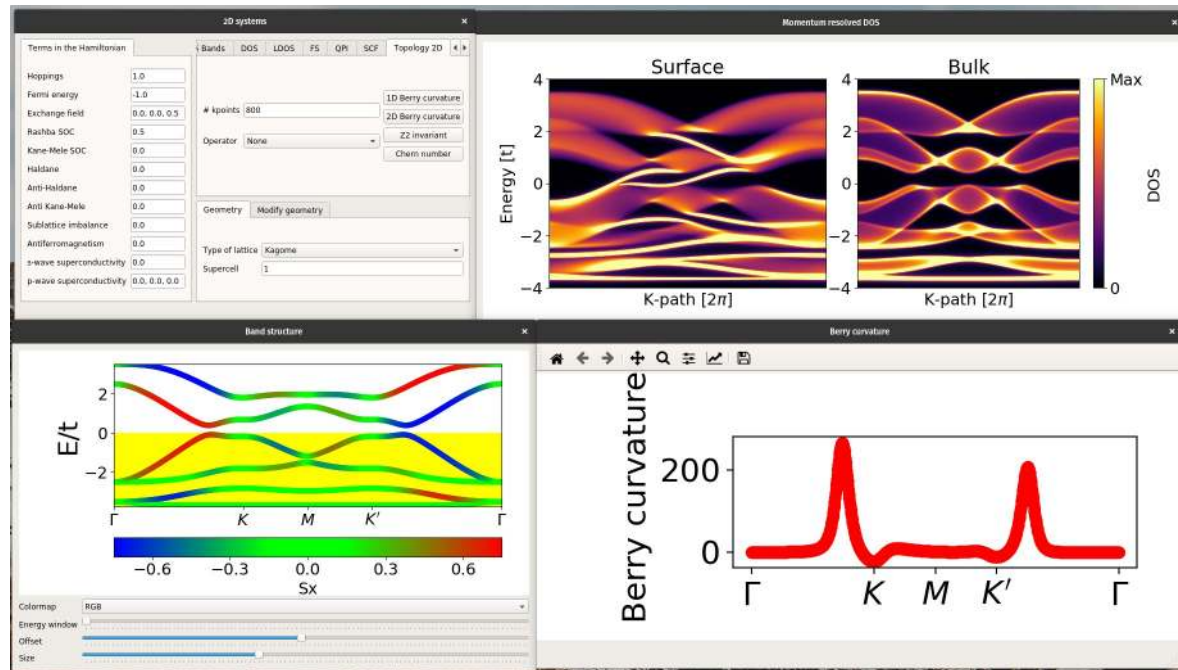
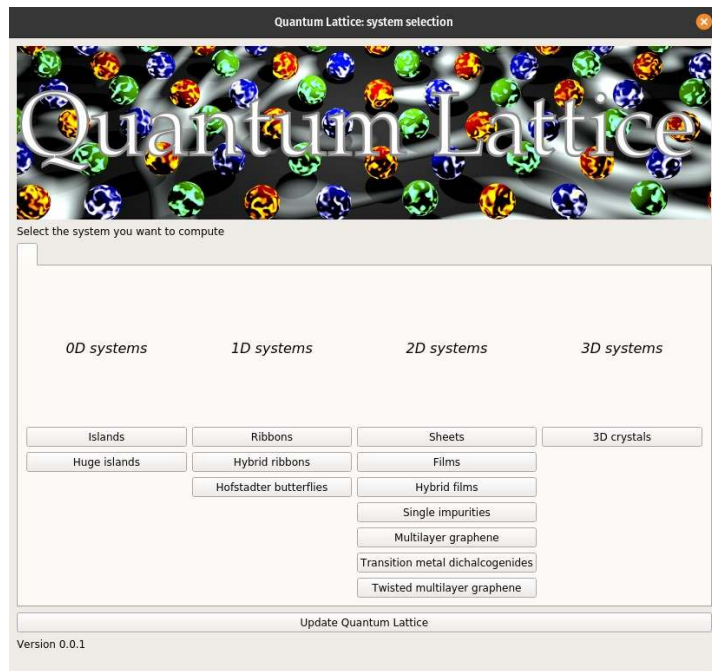
Noisy Hamiltonian reconstruction



A reconstructed Hamiltonian from noisy data reproduced the original noiseless in-gap modes

Computing electronic
properties

Quantum Lattice: A user interface to compute electronic properties

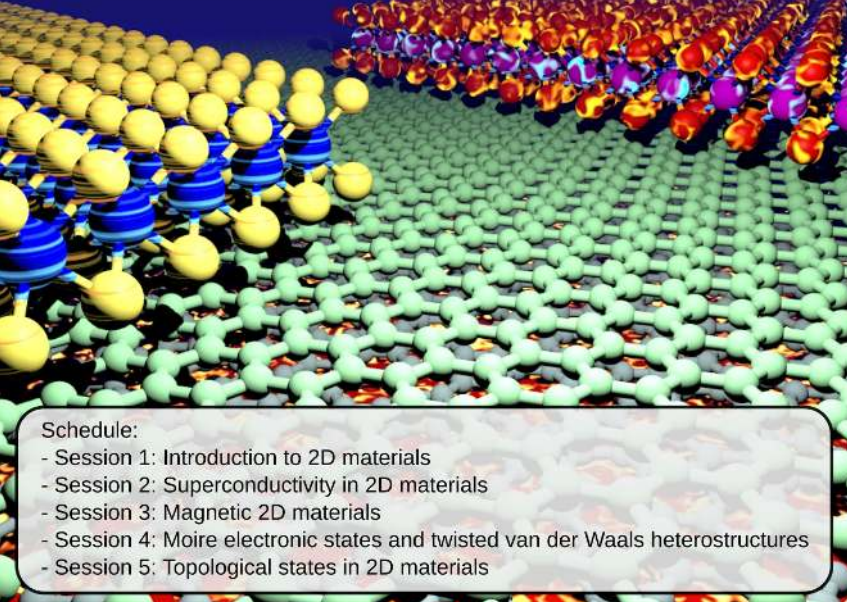


Quantum Lattice: open source interactive interface for tight binding modeling

<https://github.com/joselado/quantum-lattice>

Quantum matter in van der Waals materials school

University of Jyväskylä 31st Jyväskylä Summer School
Emergent quantum matter in
artificial two-dimensional materials
August 8th-12th 2022



Schedule:

- Session 1: Introduction to 2D materials
- Session 2: Superconductivity in 2D materials
- Session 3: Magnetic 2D materials
- Session 4: Moire electronic states and twisted van der Waals heterostructures
- Session 5: Topological states in 2D materials

Recordings available at

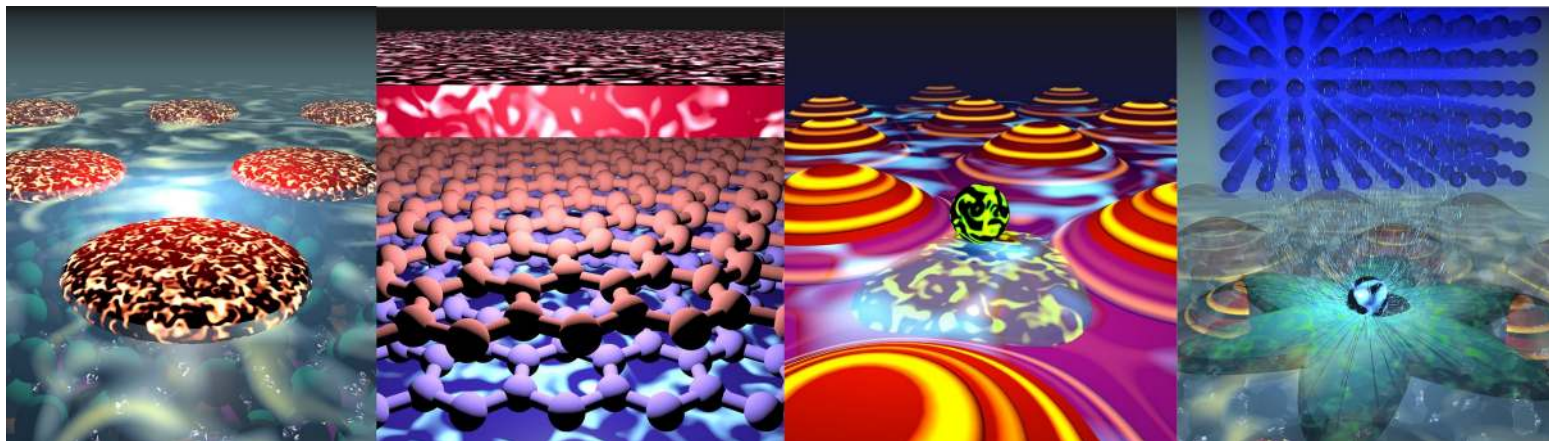


<https://www.youtube.com/channel/UCgnB-4CcqRQnvTi7P0cUakQ>

- Session 1: Introduction to 2D materials
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Take home

The interplay of moire and atomic length scales offers new possibilities to engineer topological superconductors, with impurity effects allowing us to perform Hamiltonian extraction



Thank you!

Nano Lett. 2022, 22, 1, 328–333 (2022)
arXiv:2307.04605 (2023)
Phys. Rev. Mat. 6, 094010 (2022)
arXiv:2308.11400 (2023)

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