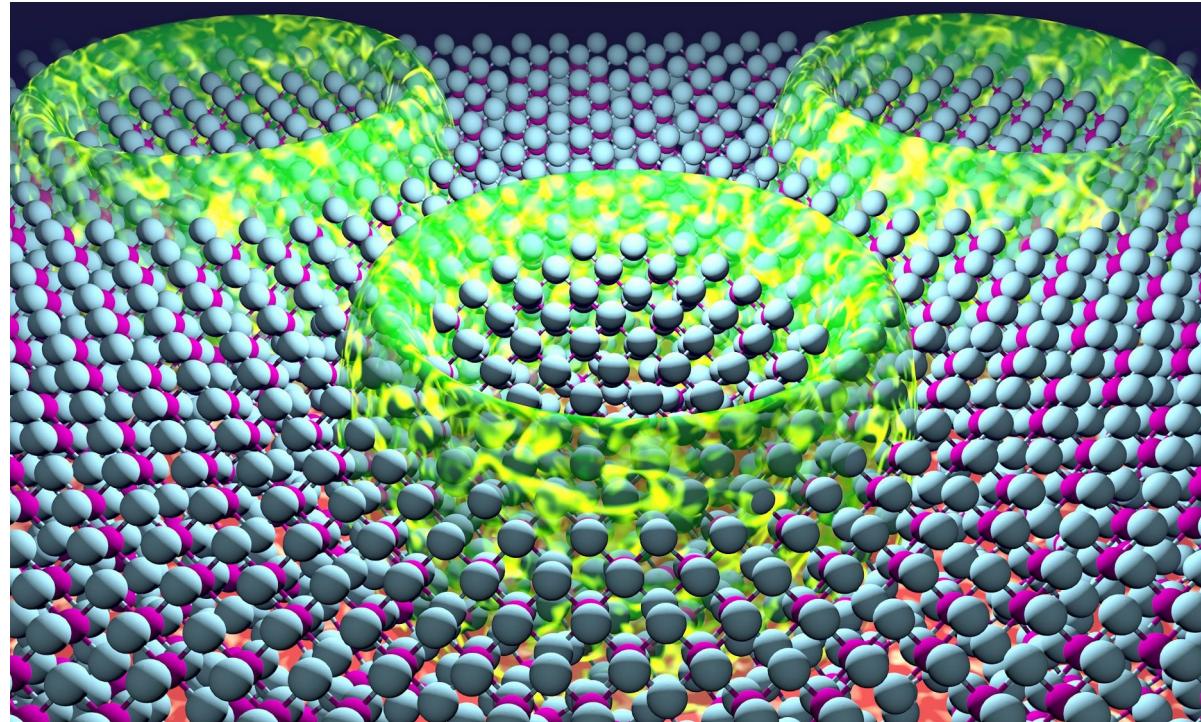


Lecture 3: Moire electronic states and twisted van der Waals heterostructures



Pedagogical School “Emergent phenomena in van der Waals heterostructures”

January 7th 2023, Tata Institute of Fundamental Research (TIFR), India

Plan for the lecture

- Moire and quasiperiodicity
- Band structure folding, unfolding and minibands
- Correlations in moire electronic structures
- Topology in moire systems
- Twisted graphene multilayers

Schedule for the lecture

- 30 min lecture
- 5 min break
- 30 min lecture

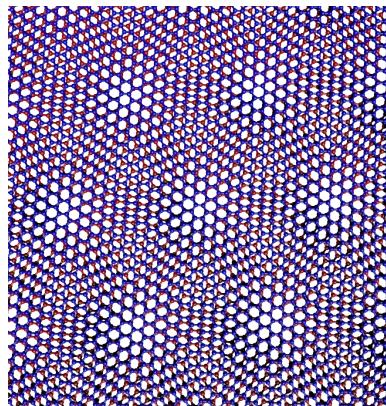
You can download the slides and software from

https://github.com/joselado/emergent_phenomena_in_van_der_Waals_school_tifr_2023



Moire materials

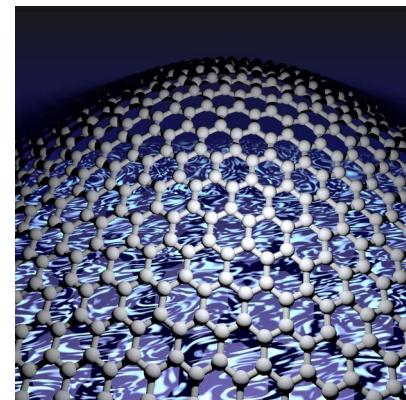
Twisted graphene multilayers



graphene

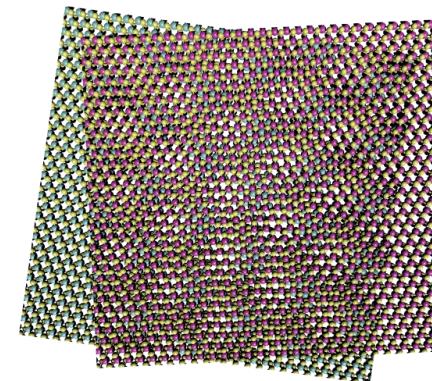
Moire states in several layers

Buckled 2D materials



Moire states in single layer

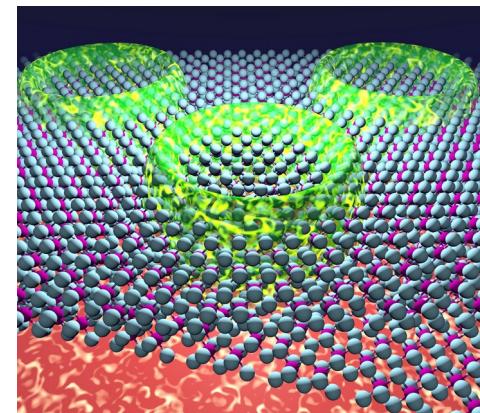
Twisted TMDCs



MoS_2 , WSe_2

Moire states in single/several layer

Twisted magnetic 2D materials



CrCl_3 , CrBr_3

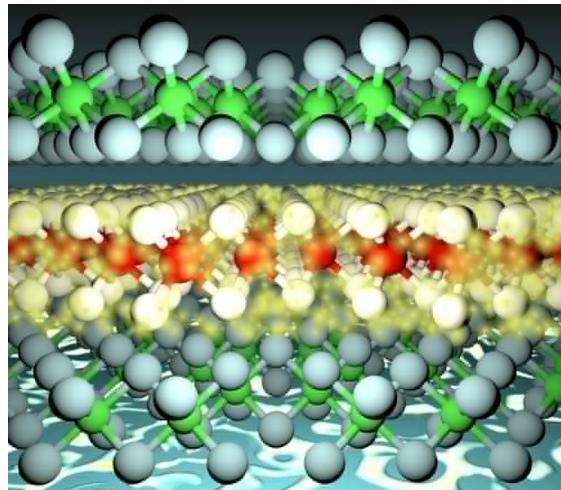
Moire magnetism

Moire in electronic properties

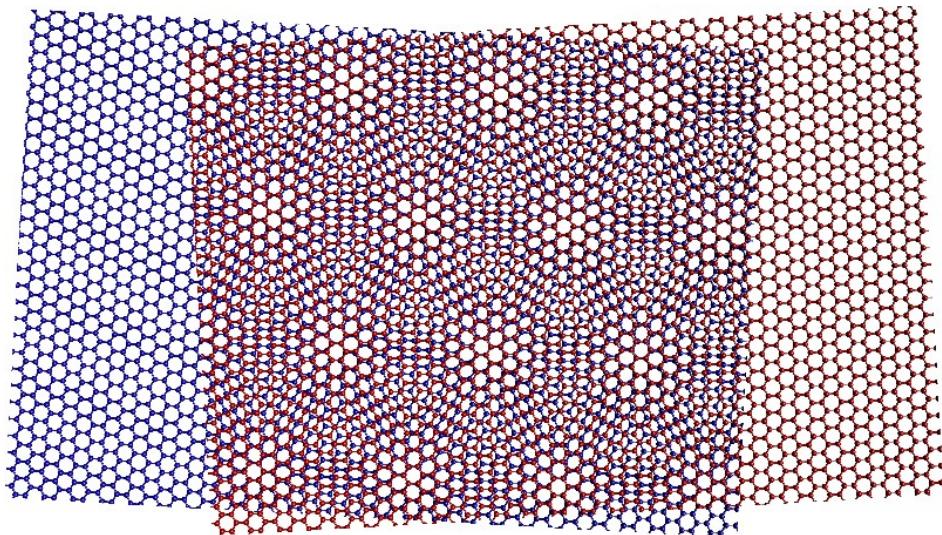
Moire in magnetic properties

How to create moire states with 2D materials

Stacking



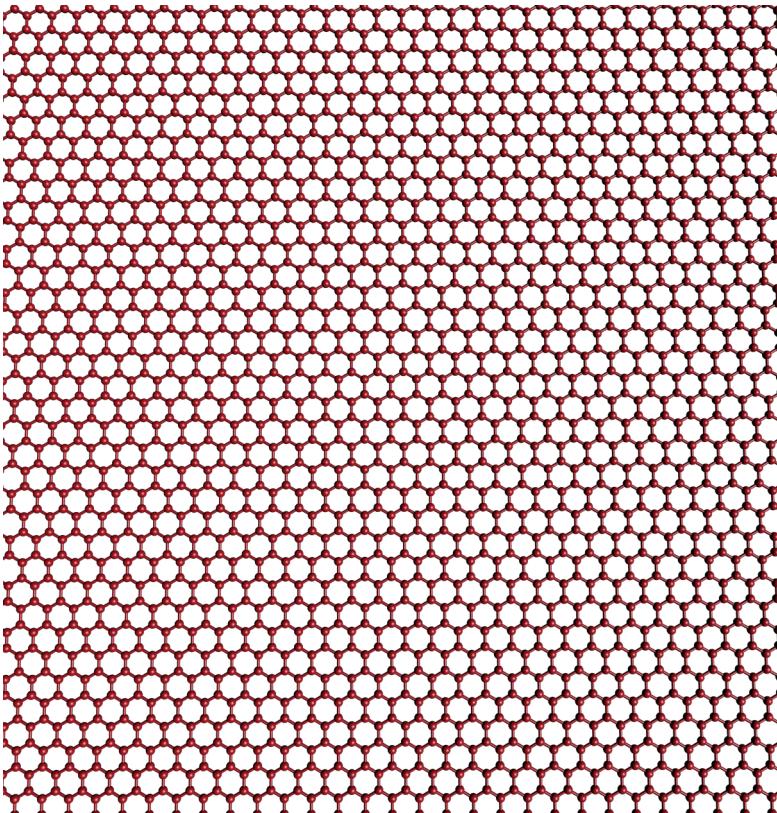
Rotating



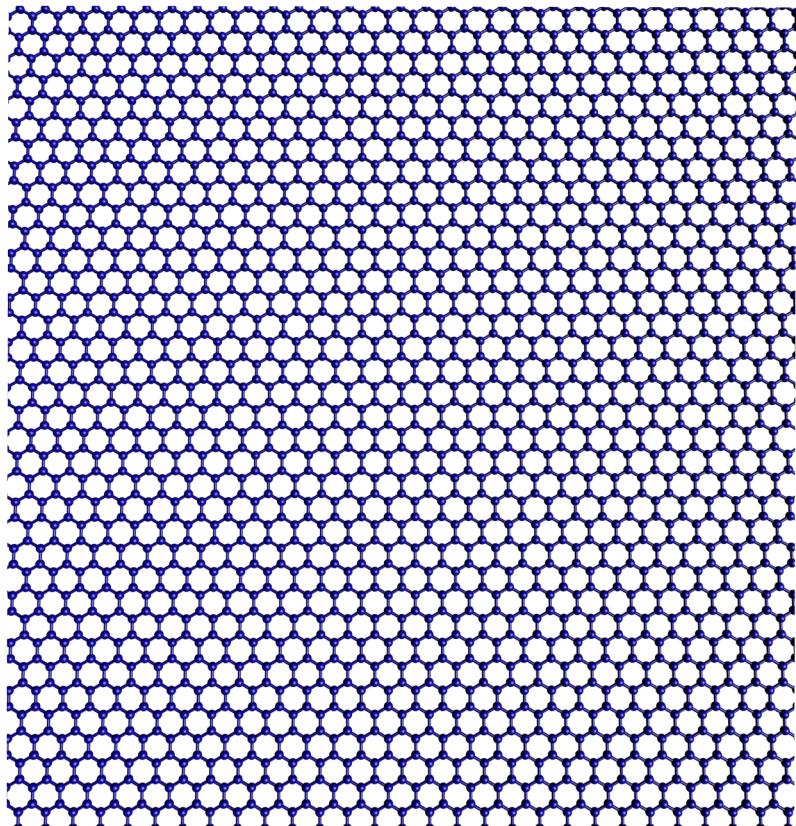
These are unique features of two-dimensional materials

A bilayer van der Waals heterostructure

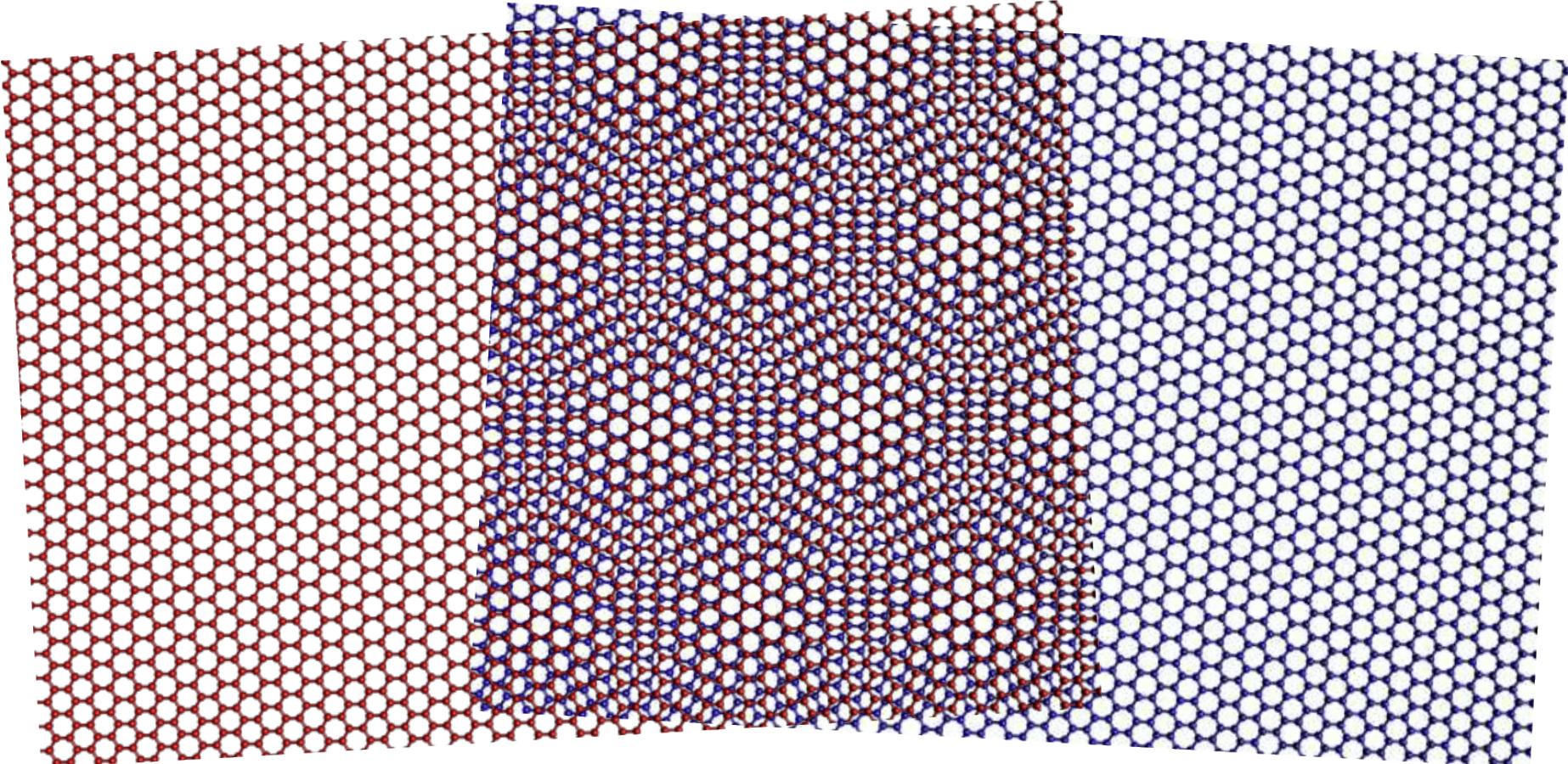
Upper graphene layer



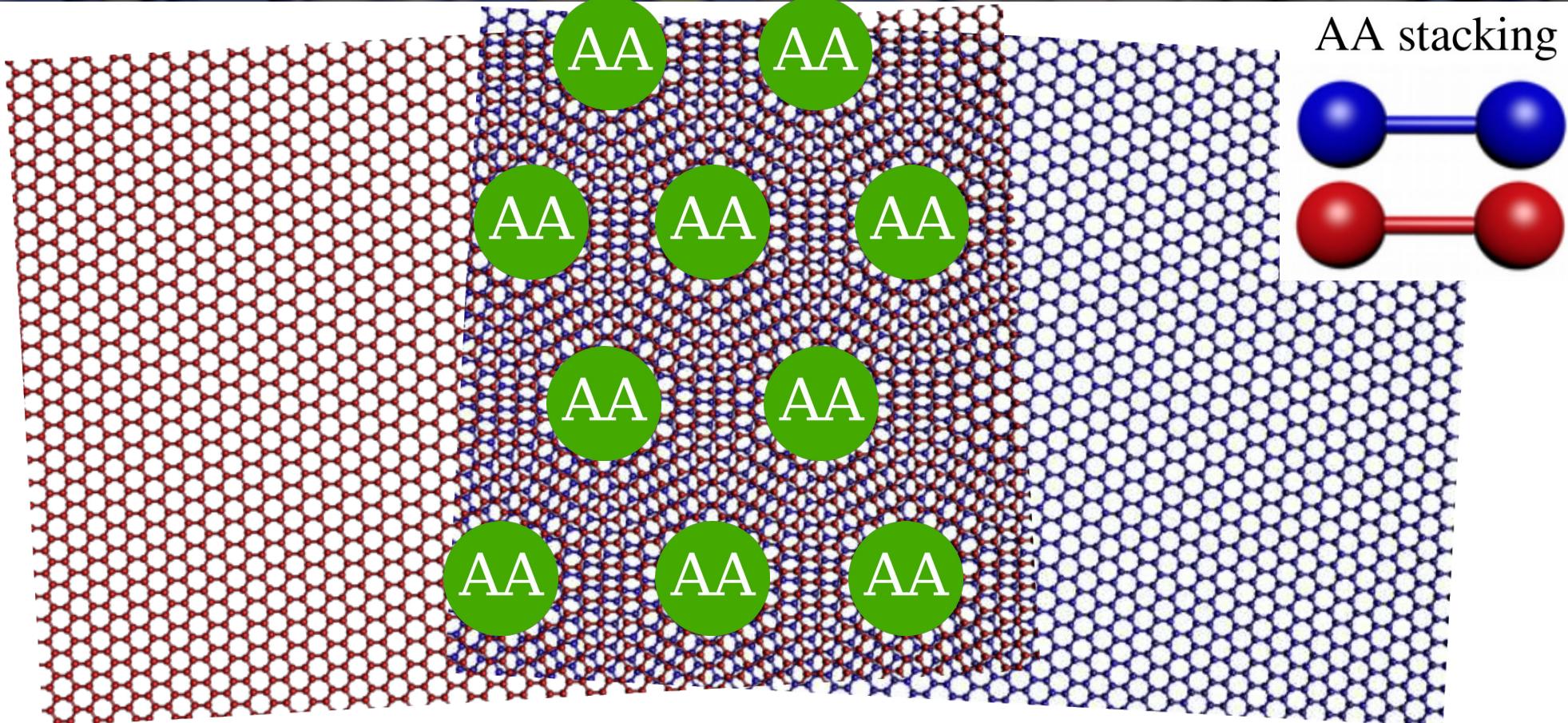
Lower graphene layer



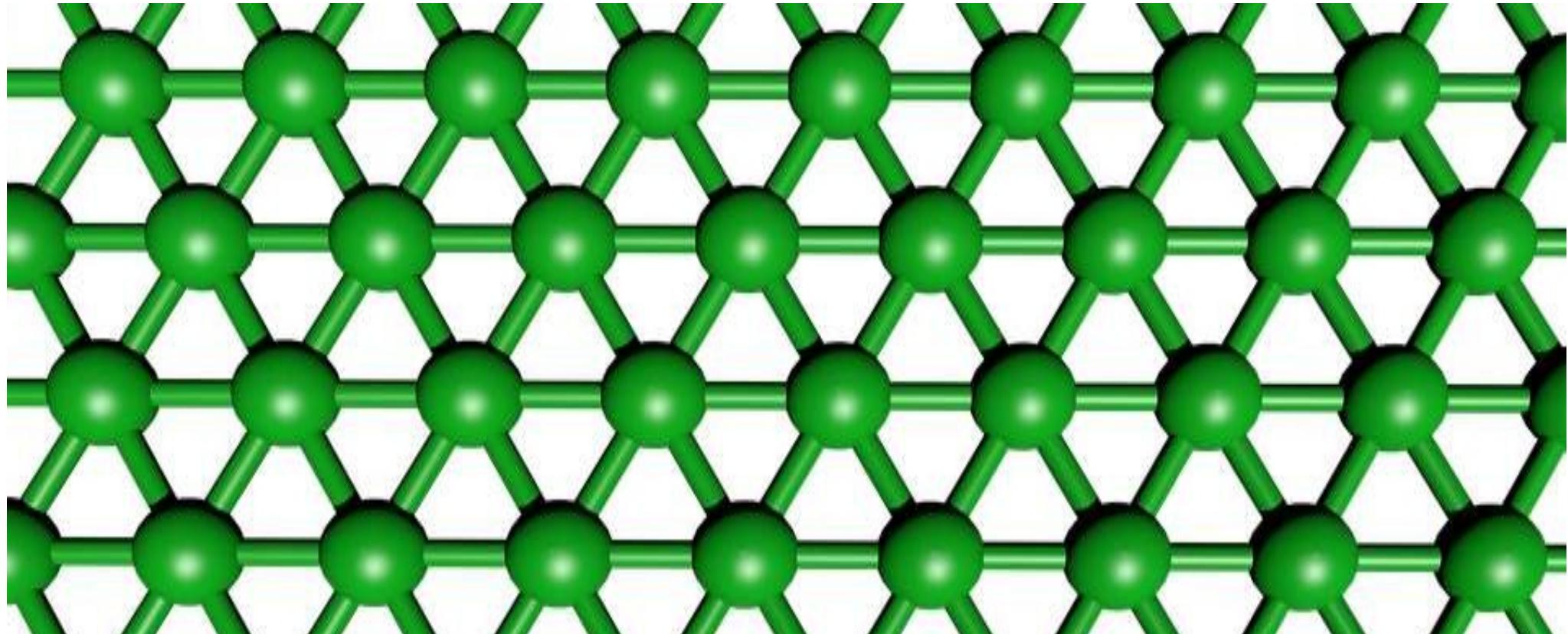
A bilayer van der Waals heterostructure



A bilayer van der Waals heterostructure

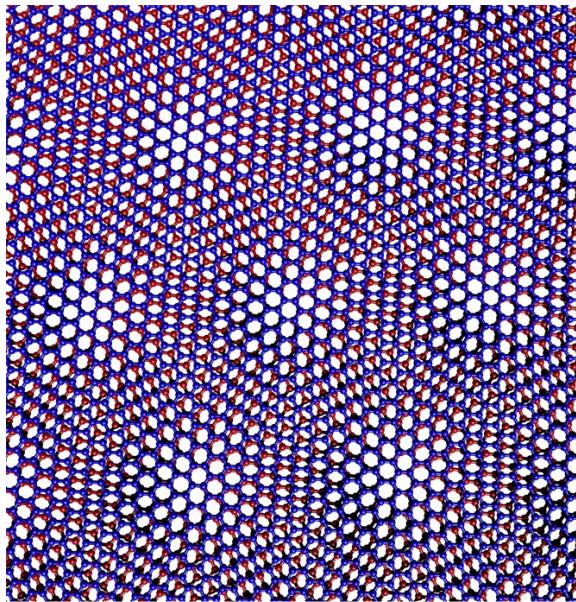


A bilayer van der Waals heterostructure

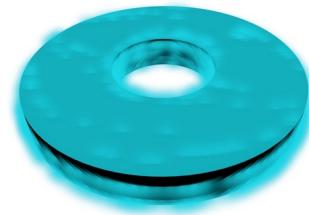


Electronic states in a single moire superlattice

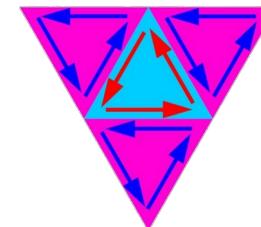
Twisted bilayer graphene



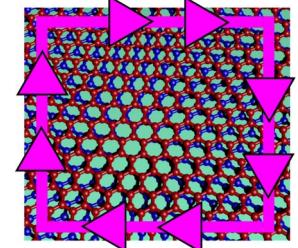
Superconductivity



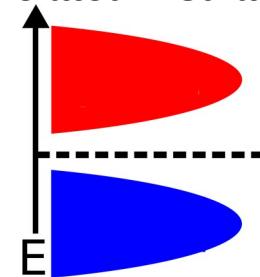
Topological networks



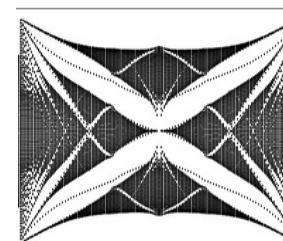
Chern insulators



Correlated insulators



Quasicrystalline physics



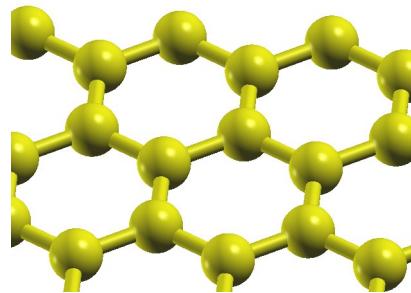
Fractional Chern insulators



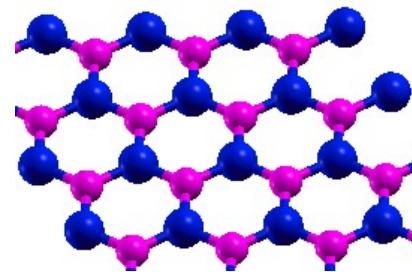
A single twisted van der Waals material realizes a variety of widely different electronic states

The building blocks for twisted van der Waals heterostructure

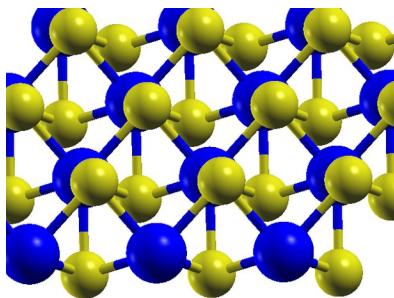
Semimetal
Graphene



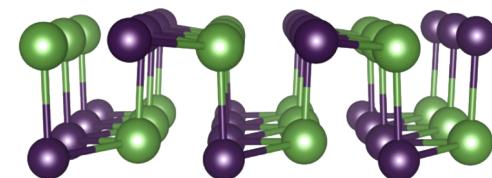
Insulator
BN



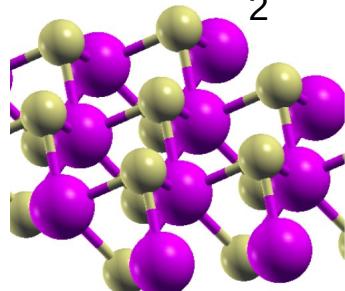
Superconductor
 NbSe_2



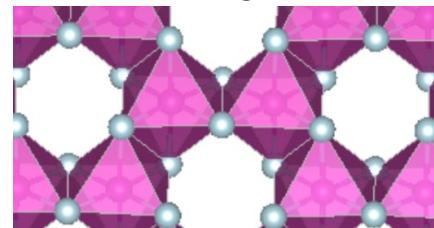
Ferroelectric
 SnTe



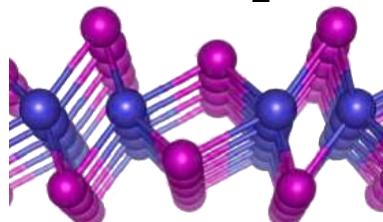
Semiconductor
 WSe_2



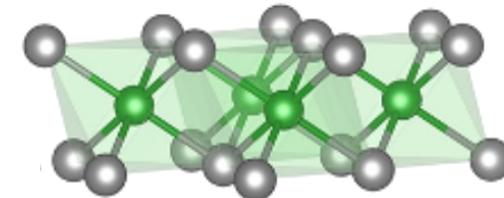
Ferromagnet
 CrI_3



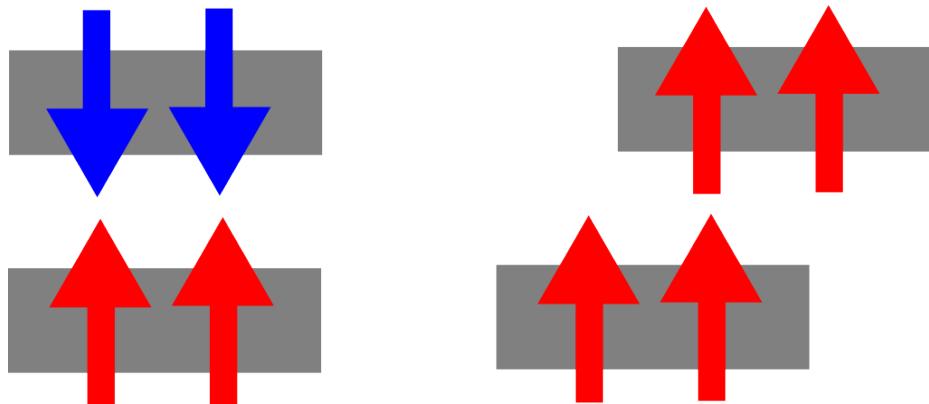
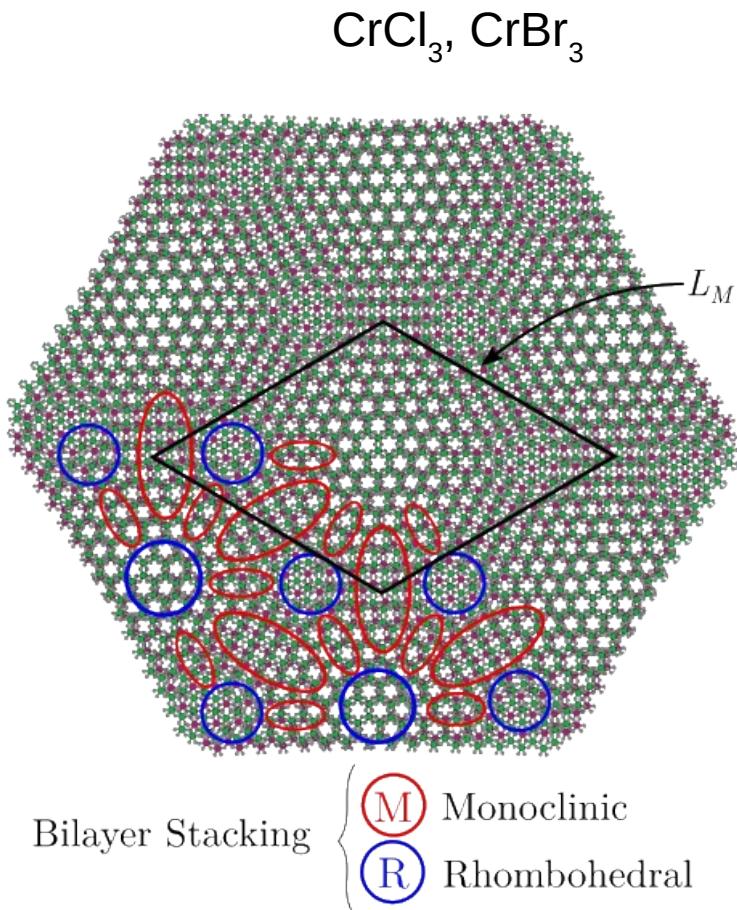
Quantum spin
Hall insulator
 WTe_2



Multiferroic
 NiI_2



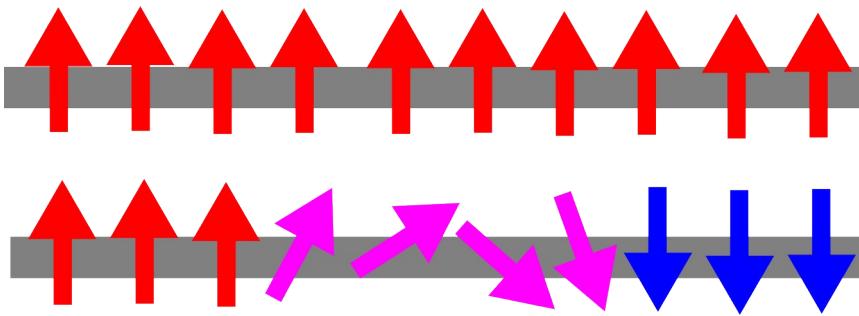
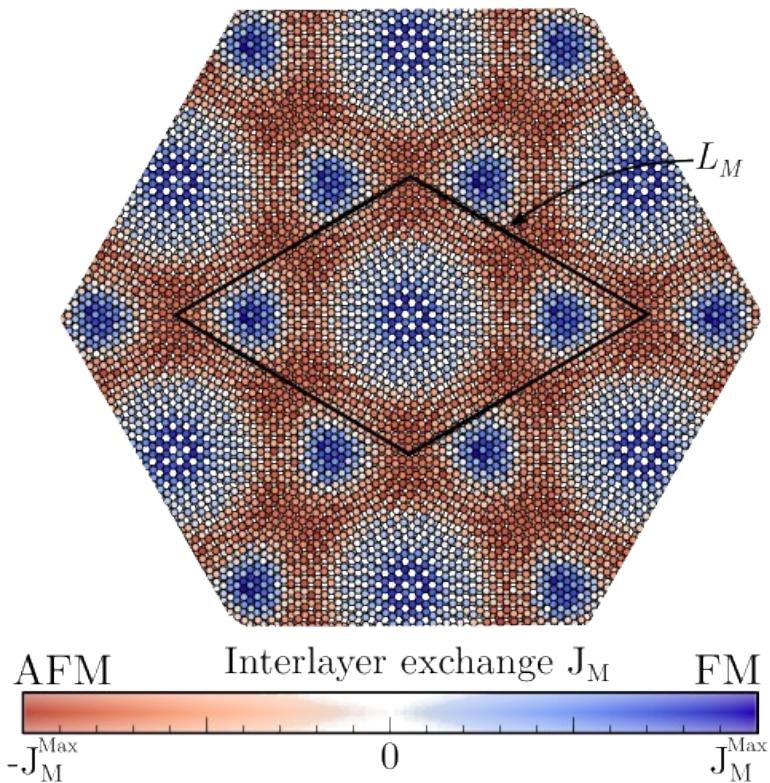
Twisted 2D magnetic materials



The local stacking determines the coupling between layers

Twisted 2D magnetic materials

Non-collinear magnetism and multiferroic order appear due to the moire



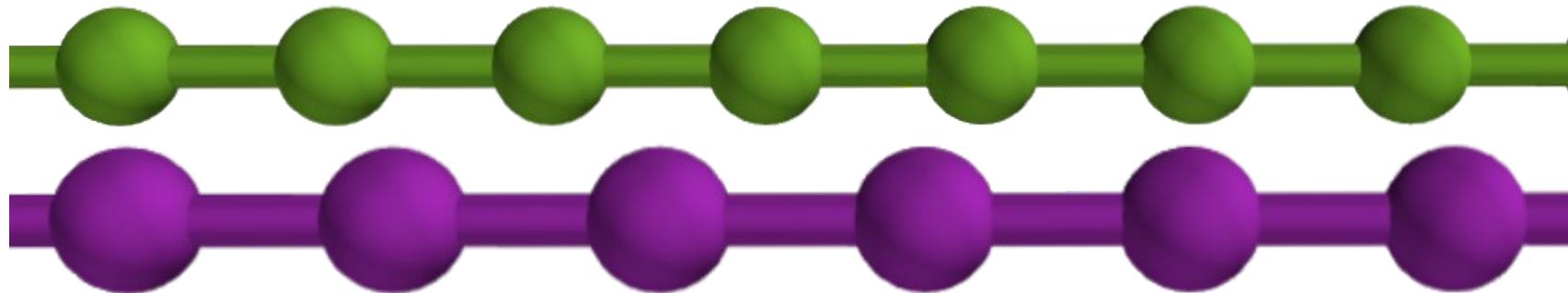
$$\mathbf{P} = \xi \mathbf{q} \times \mathbf{e}$$

Electric polarization SOC driven Spin rotation axis
Wavevector of the spin spiral

Superpotentials and quasiperiodicity

A minimal moire potential

Let us now take a one dimensional superlattice



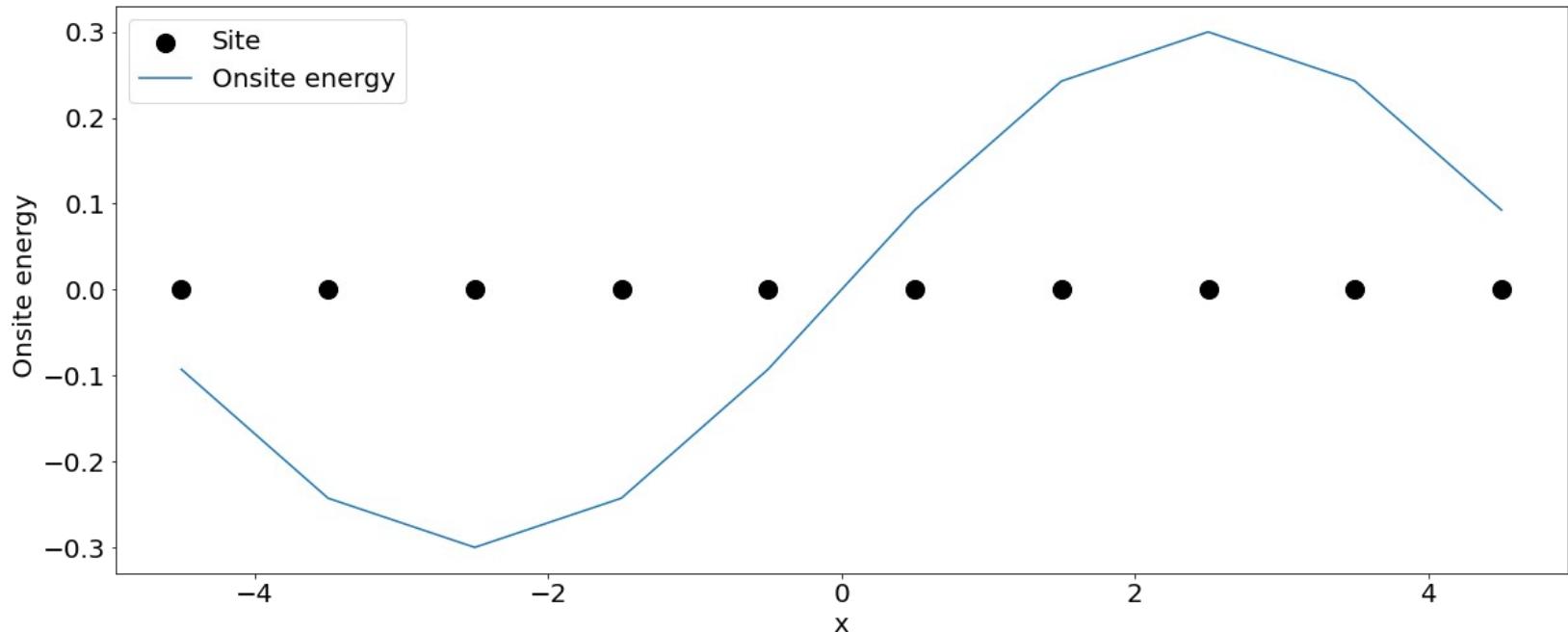
We have now two length scales

- The lattice constant of the top system
- The lattice constant of the bottom

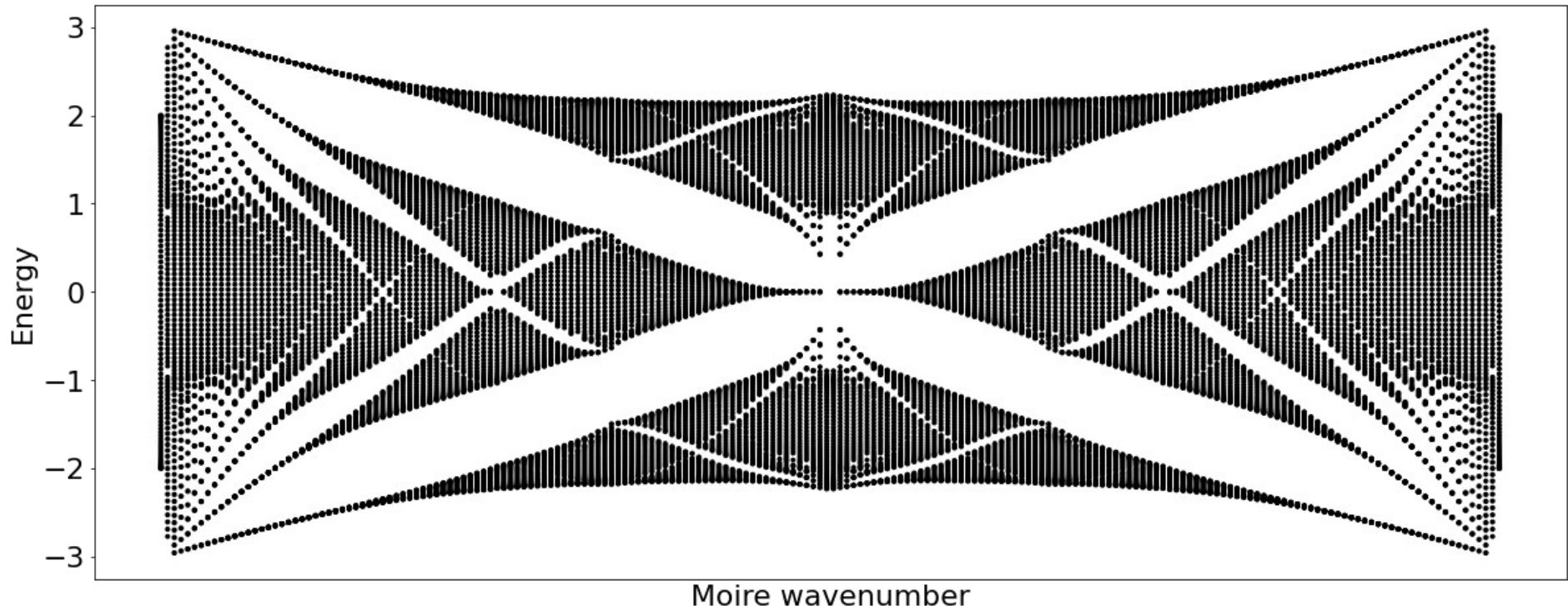
Let us see how the electronic structure gets modified by the superlattice effect

A minimal moire potential

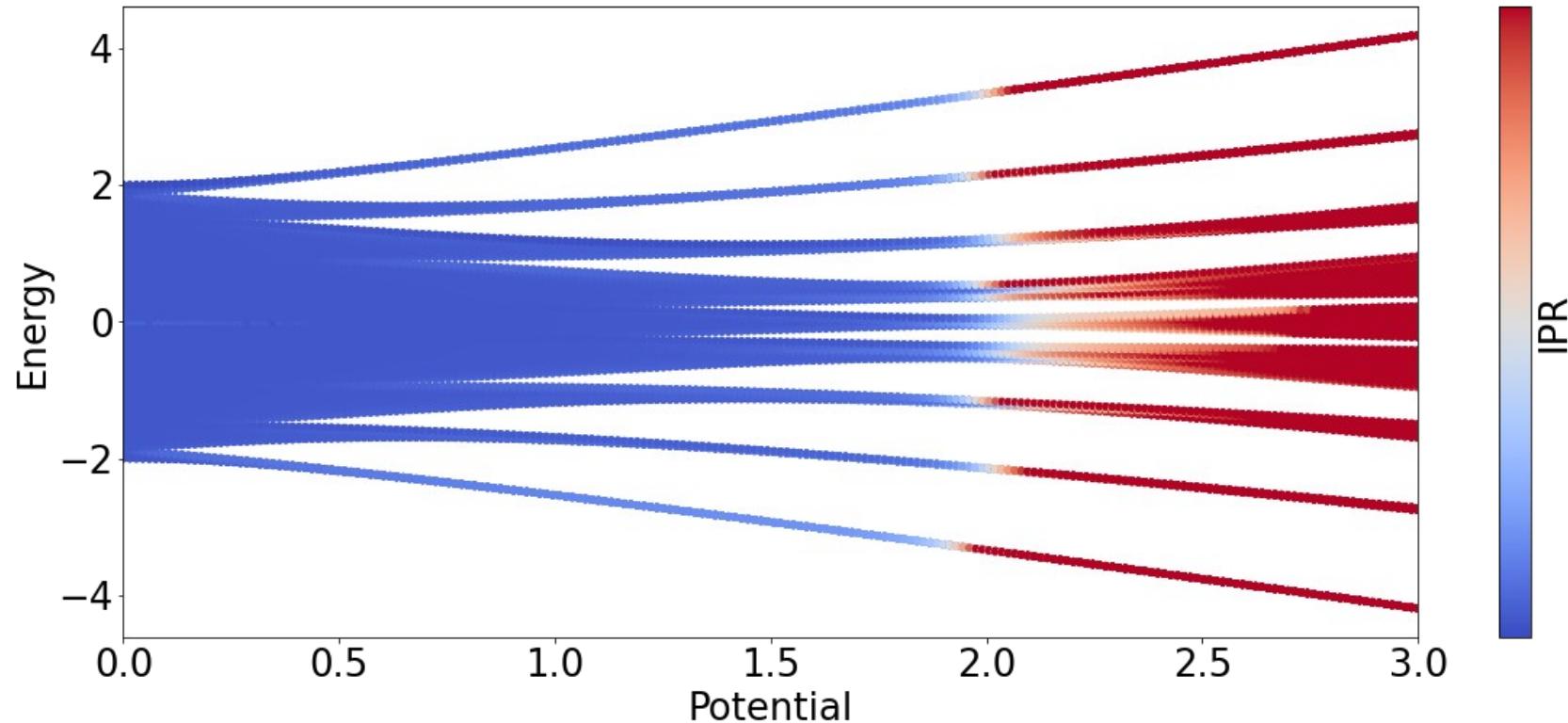
$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + \lambda \sum_n \cos(qn) c_n^\dagger c_n$$



Spectrum as a function of the moire wavevector



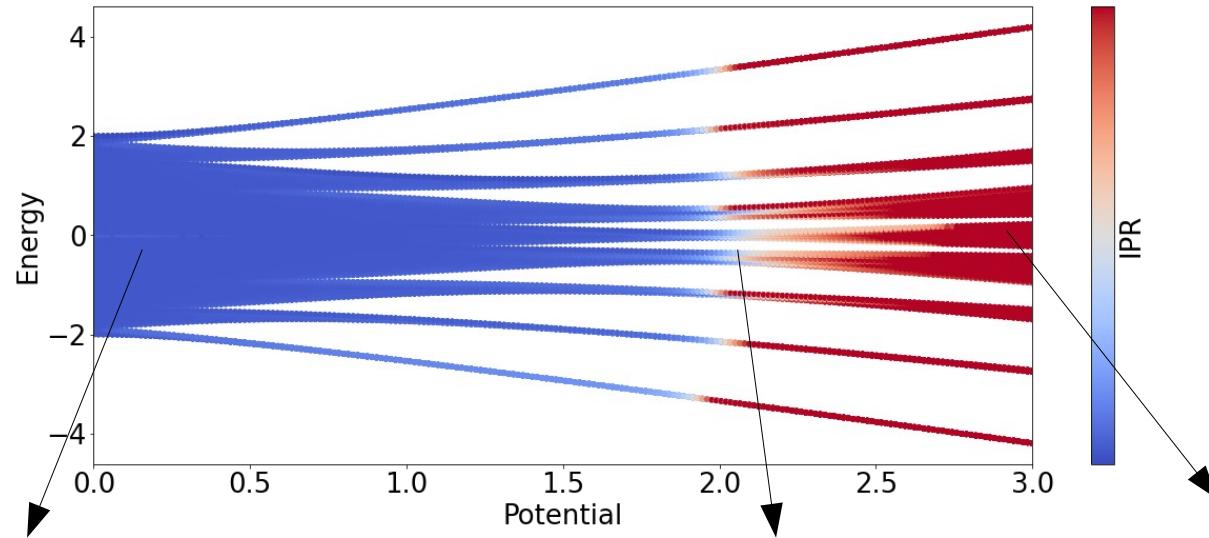
Superpotentials and criticality



Moire potentials can give rise to critical wavefunctions

$$IPR = \sum_r |\Psi(r)|^4$$

Superpotentials and criticality



$$IPR = \sum_r |\Psi(r)|^4$$

Extended states

$$|\Psi(\mathbf{r})| = 1/N$$

Critical states

$$|\Psi(\mathbf{r})| = |r|^{-\alpha}$$

Localized states

$$|\Psi(\mathbf{r})| = e^{-\lambda|r|}$$

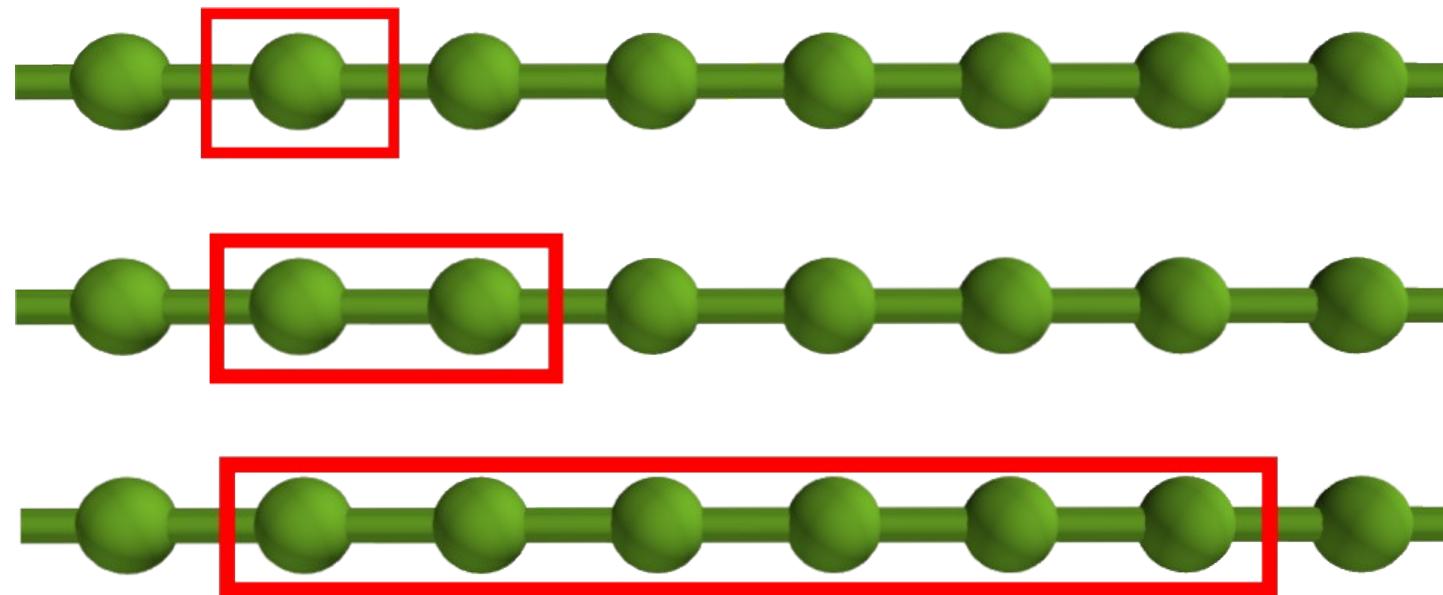
Minibands and band structure unfolding

Supercells and band folding

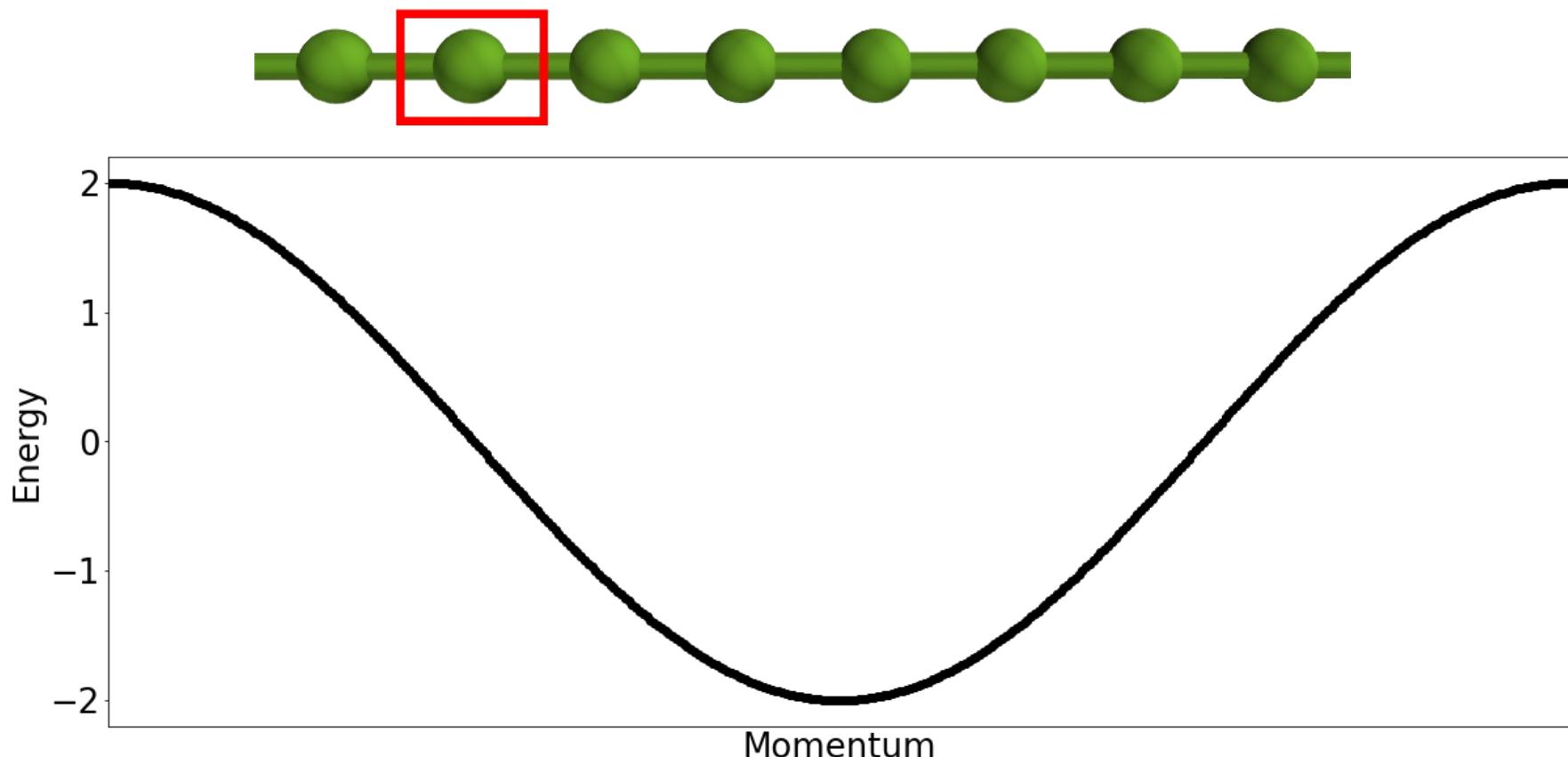
Let us take a 1D chain

$$H = \sum_n c_n^\dagger c_{n+1} + h.c.$$

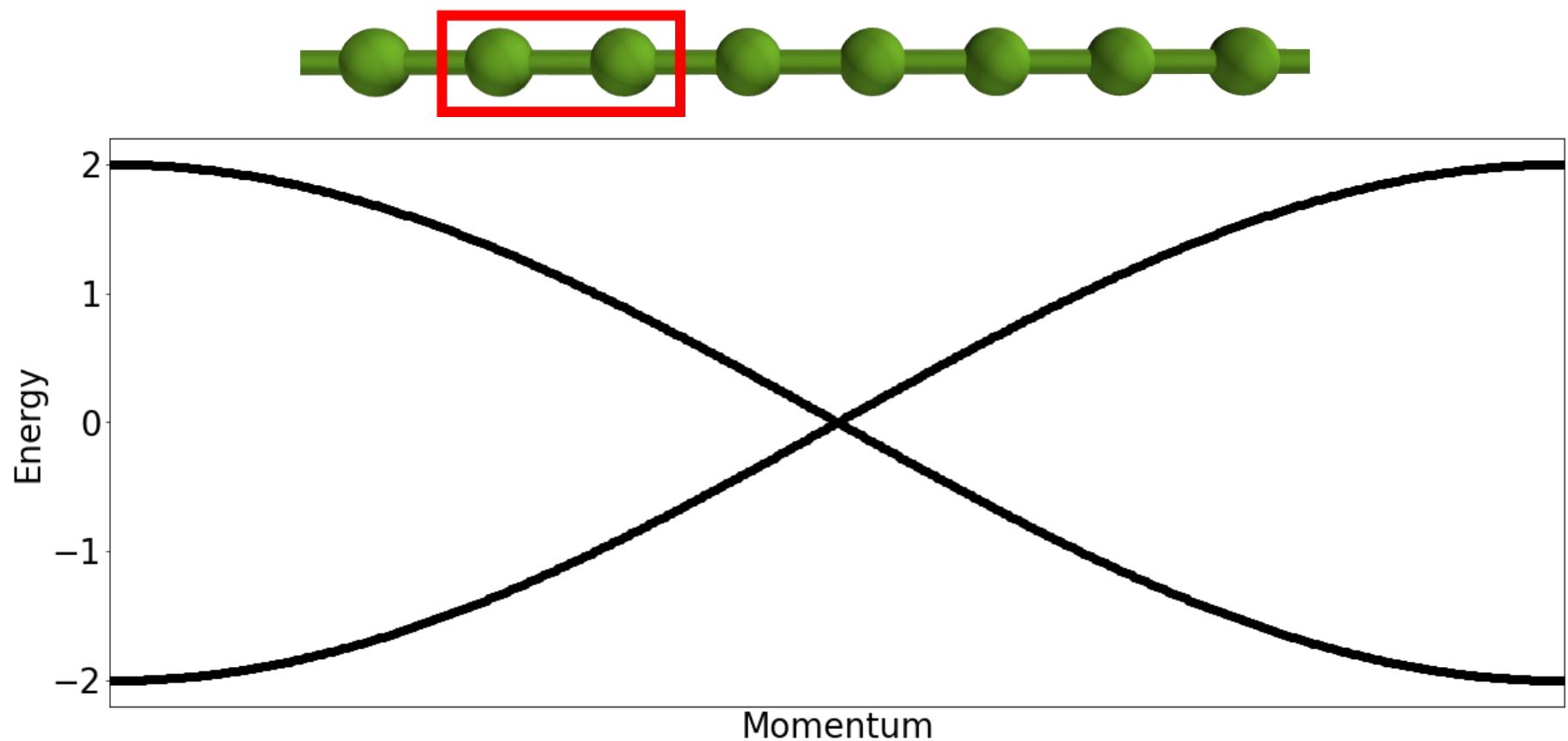
Let us see how the electronic structure changes with the unit cell



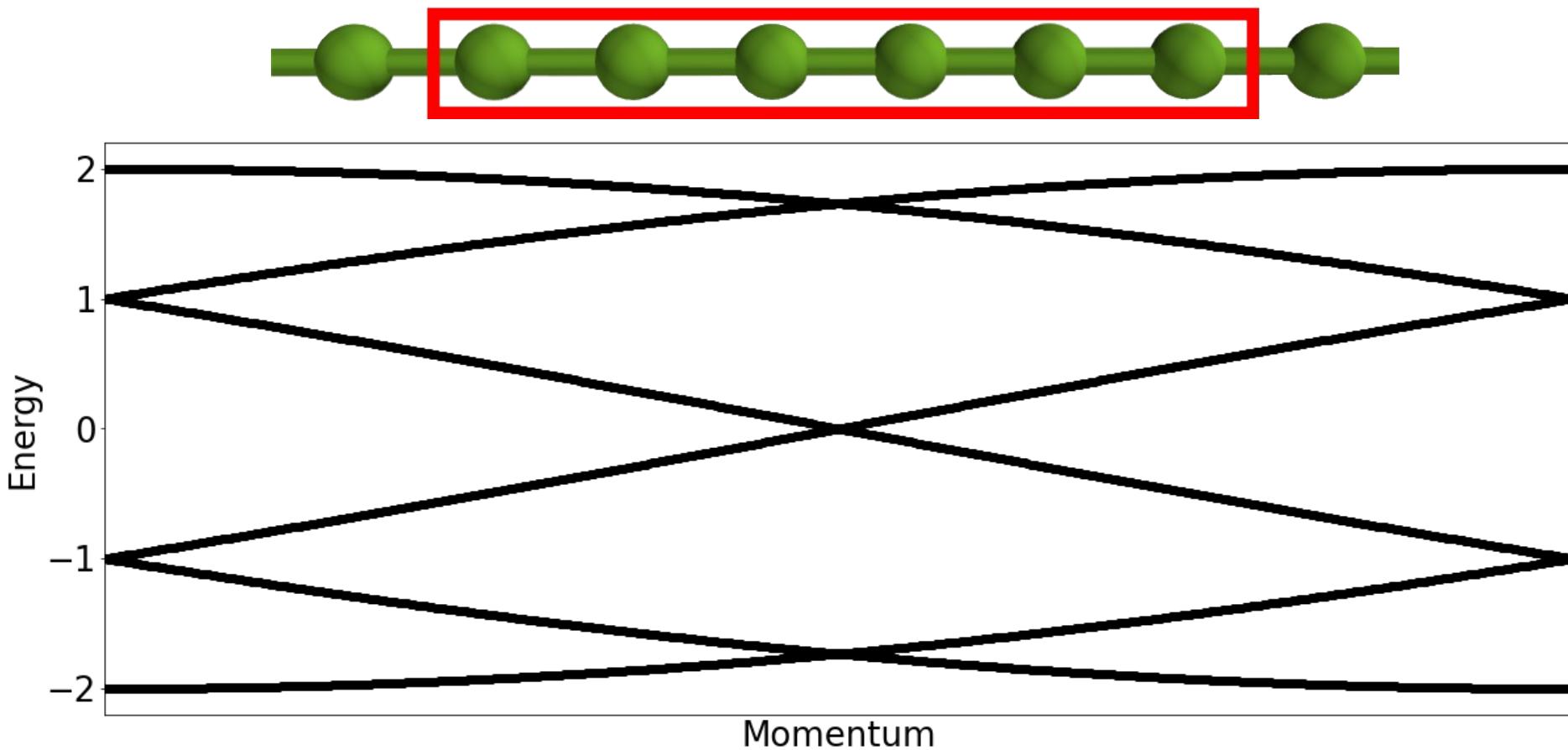
Supercells and band folding



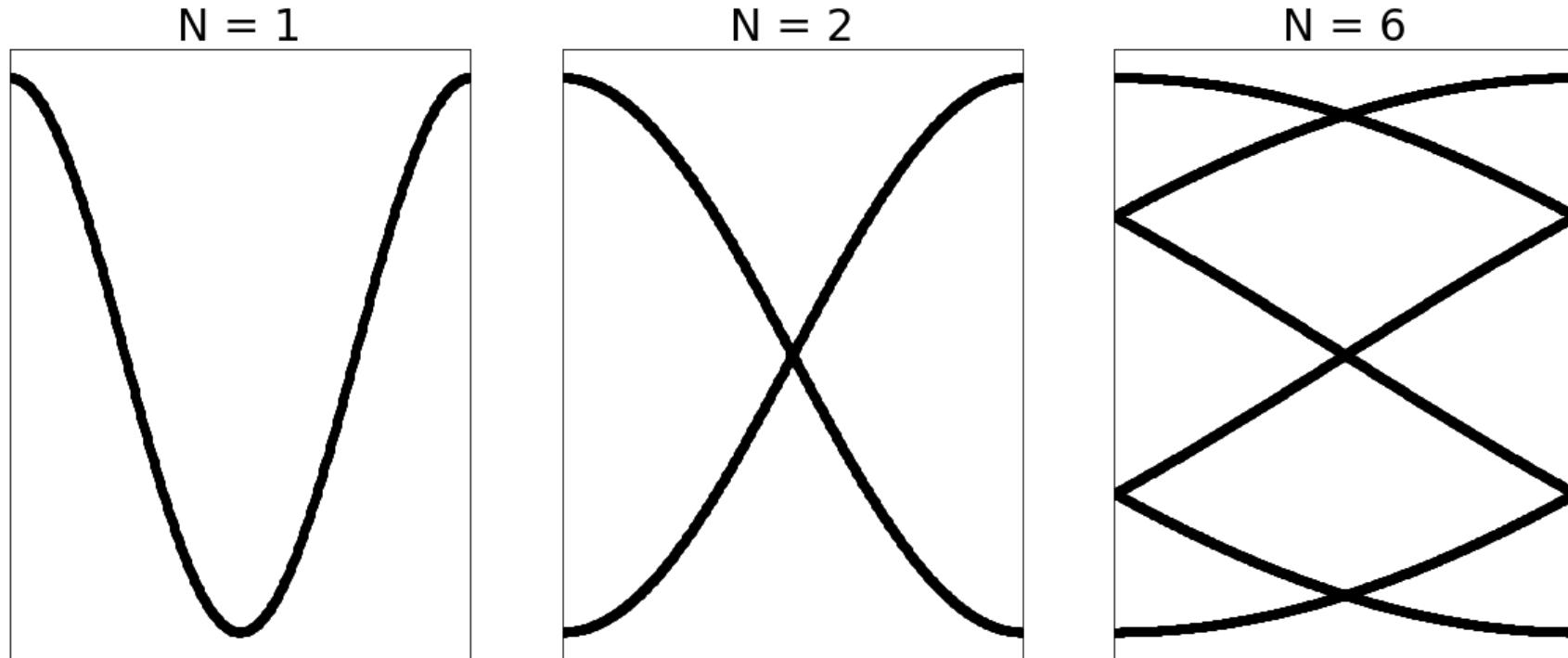
Supercells and band folding



Supercells and band folding

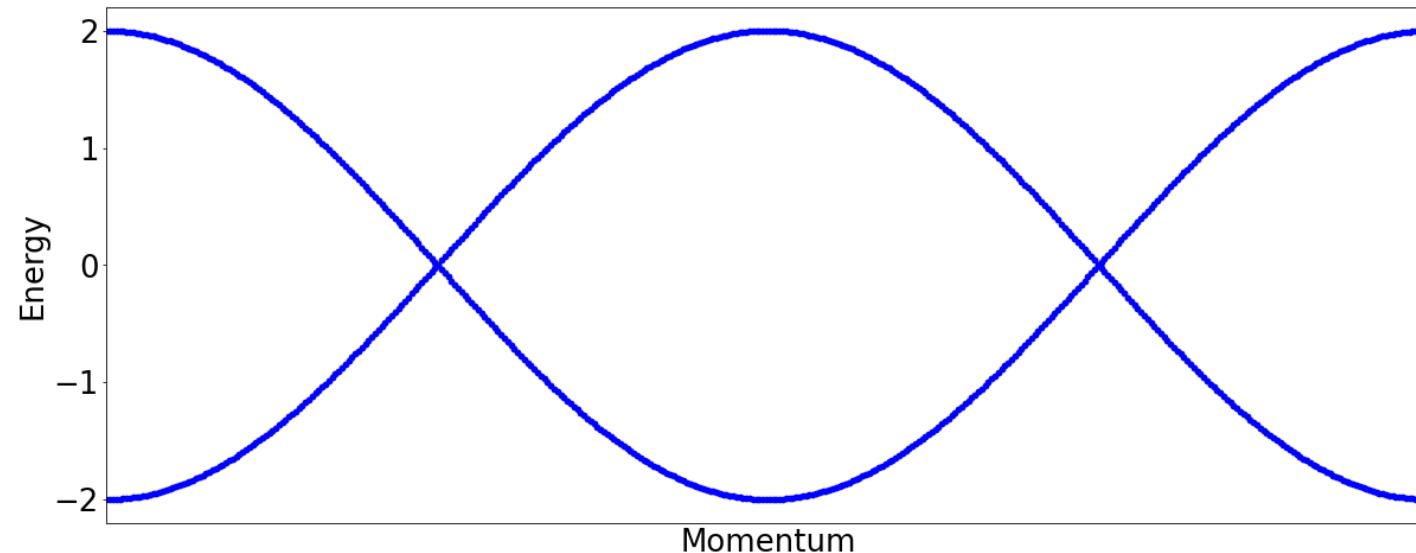
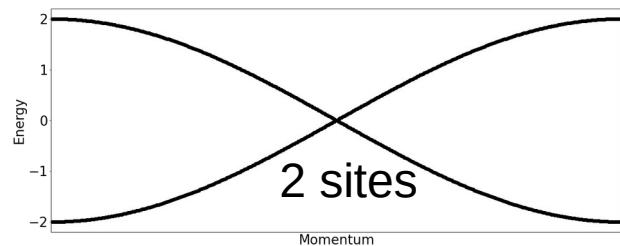
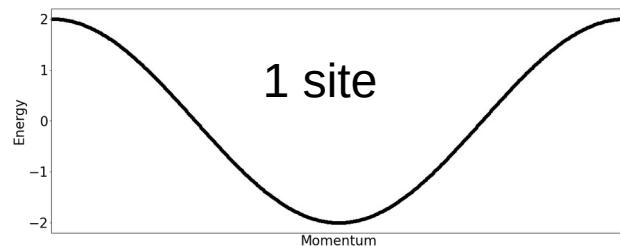


Supercells and band folding



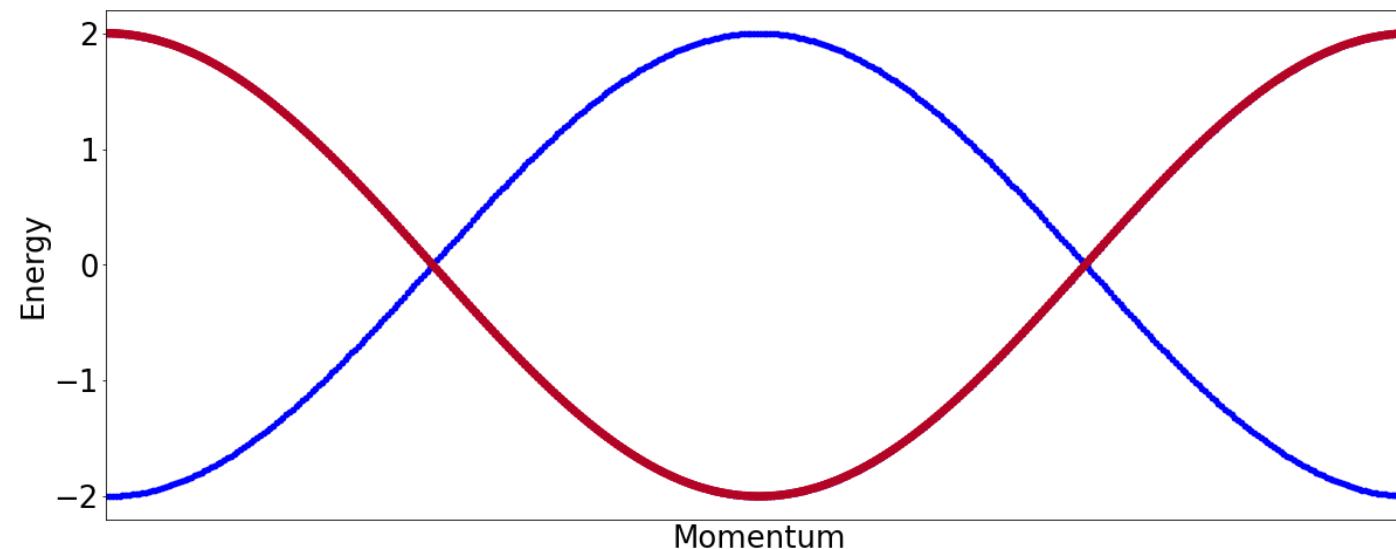
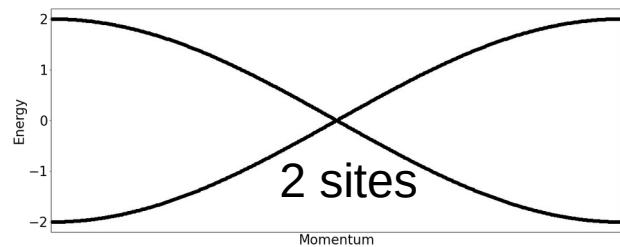
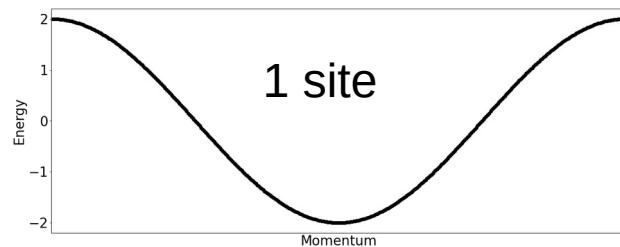
All these electronic structures represent the same physical system, but how do we see that?

Supercells and band folding



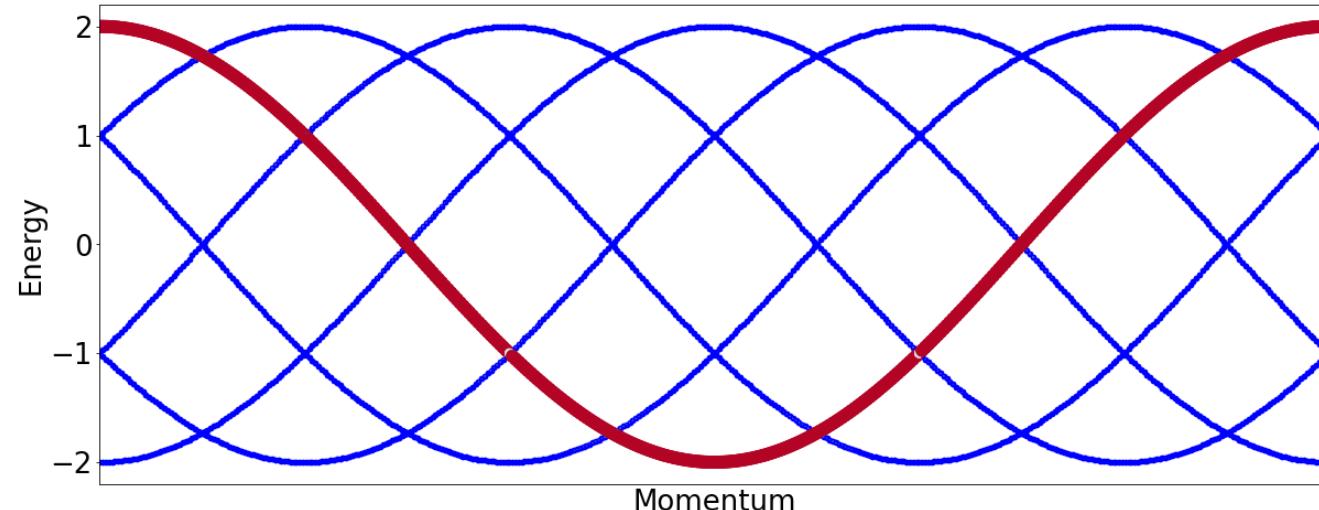
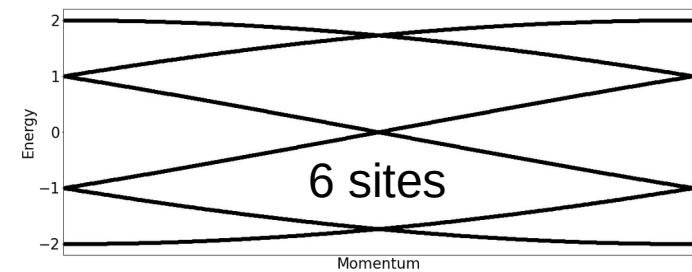
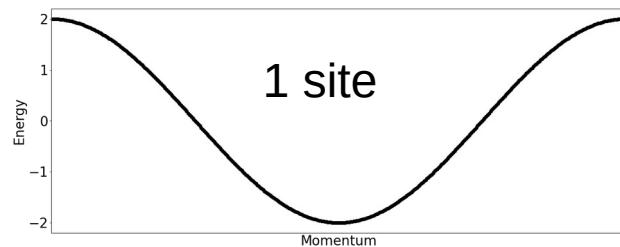
Repeating the electronic structure recovers the original electronic dispersion

Supercells and band folding



Repeating the electronic structure recovers the original electronic dispersion

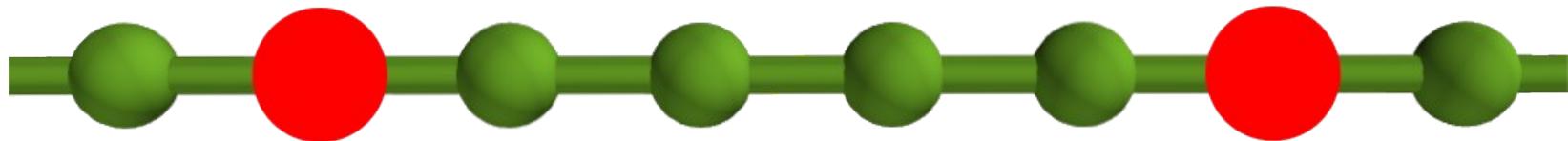
Supercells and band folding



Repeating the electronic structure recovers the original electronic dispersion

Unfolding and anticrossings in superlattices

Let us now put an impurity every 6 sites (once in a supercell 6)

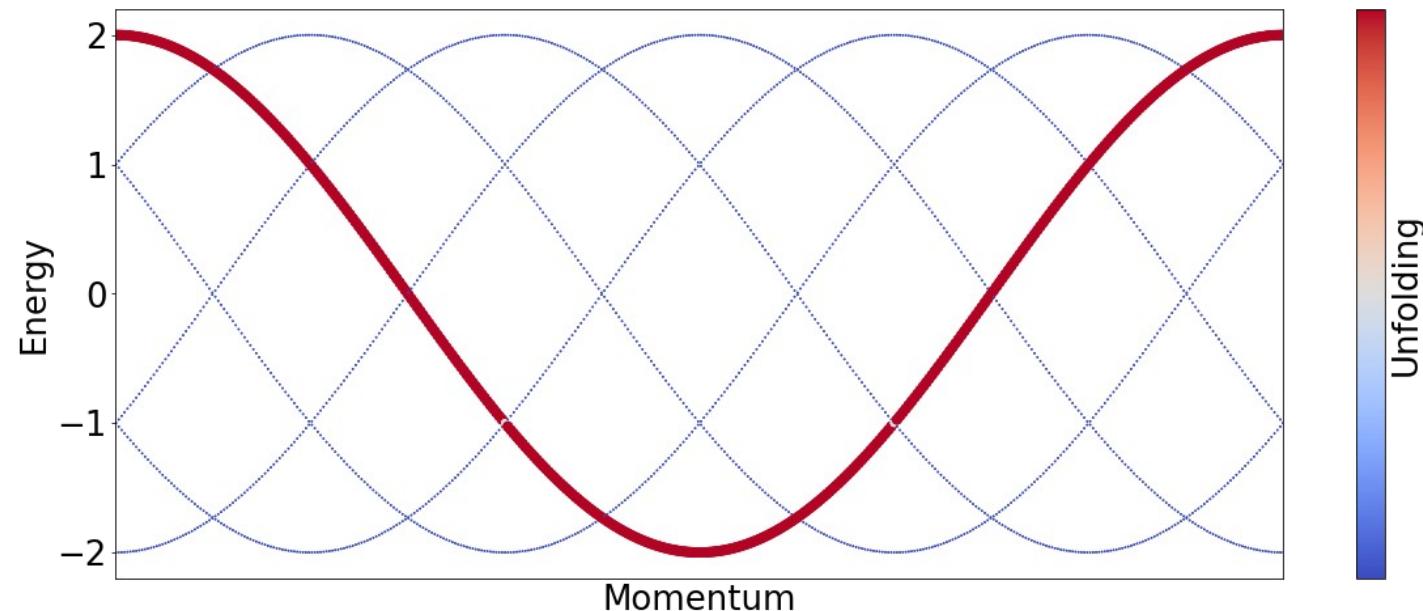


$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V_0 \sum_\alpha c_\alpha^\dagger c_\alpha \quad \alpha \equiv 0 \pmod{6}$$

Unfolding and anticrossings in superlattices

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V_0 \sum_\alpha c_n^\dagger c_n$$

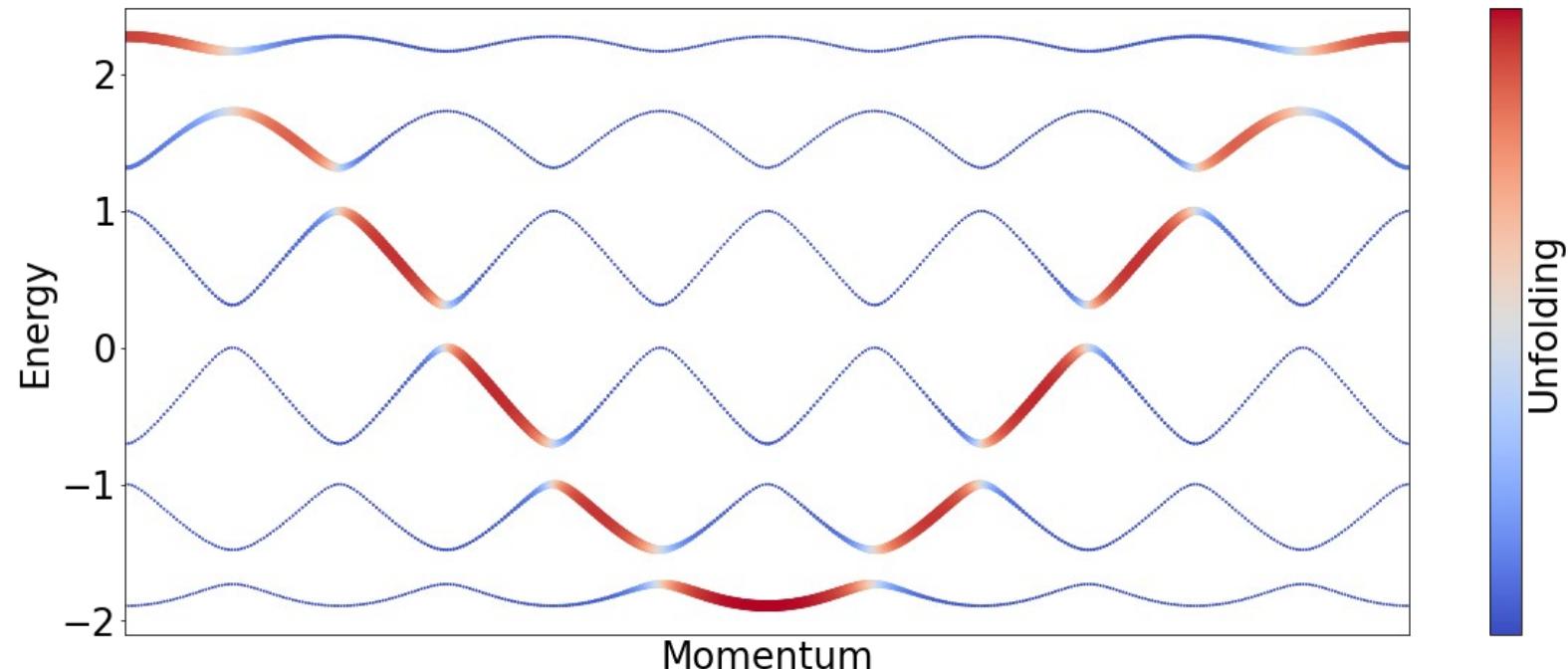
$$V_0 = 0$$



Electronic structure unfolding

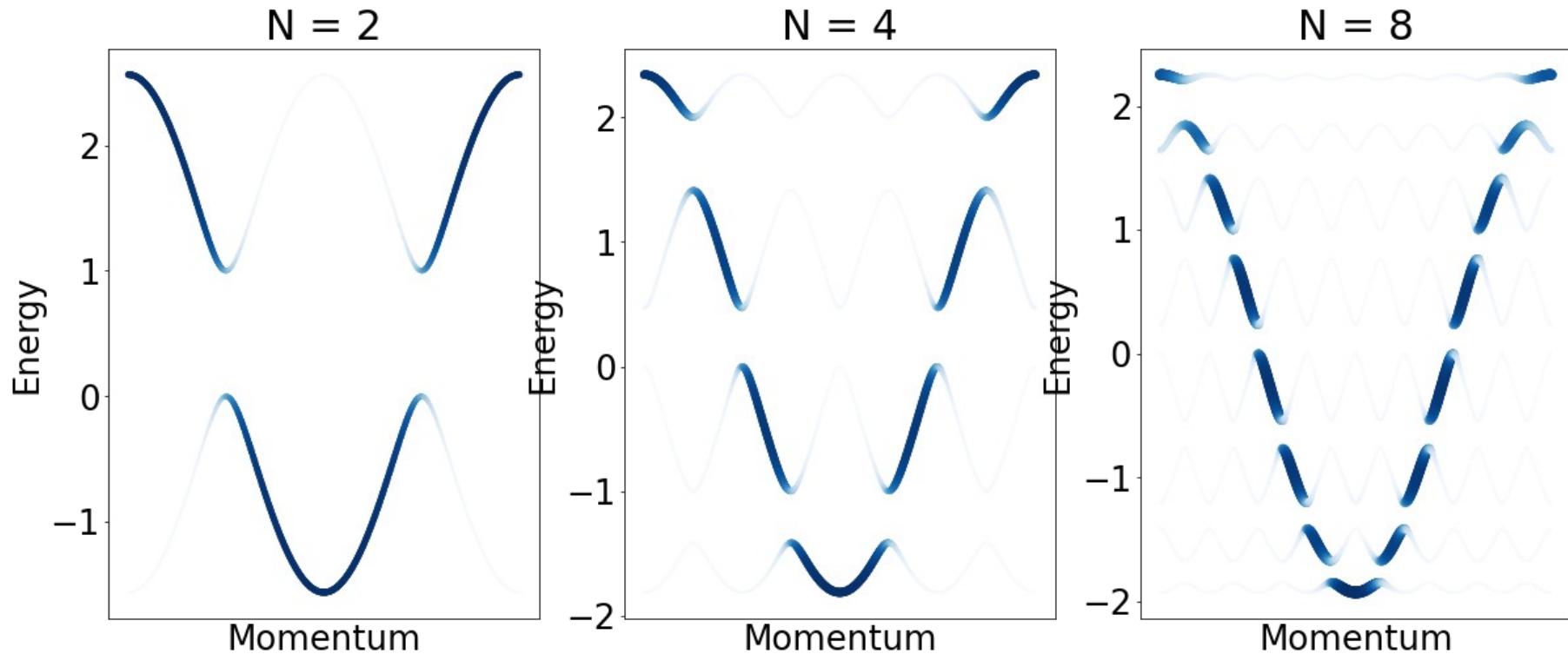
$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V_0 \sum_\alpha c_n^\dagger c_n$$

$$V_0 \neq 0$$



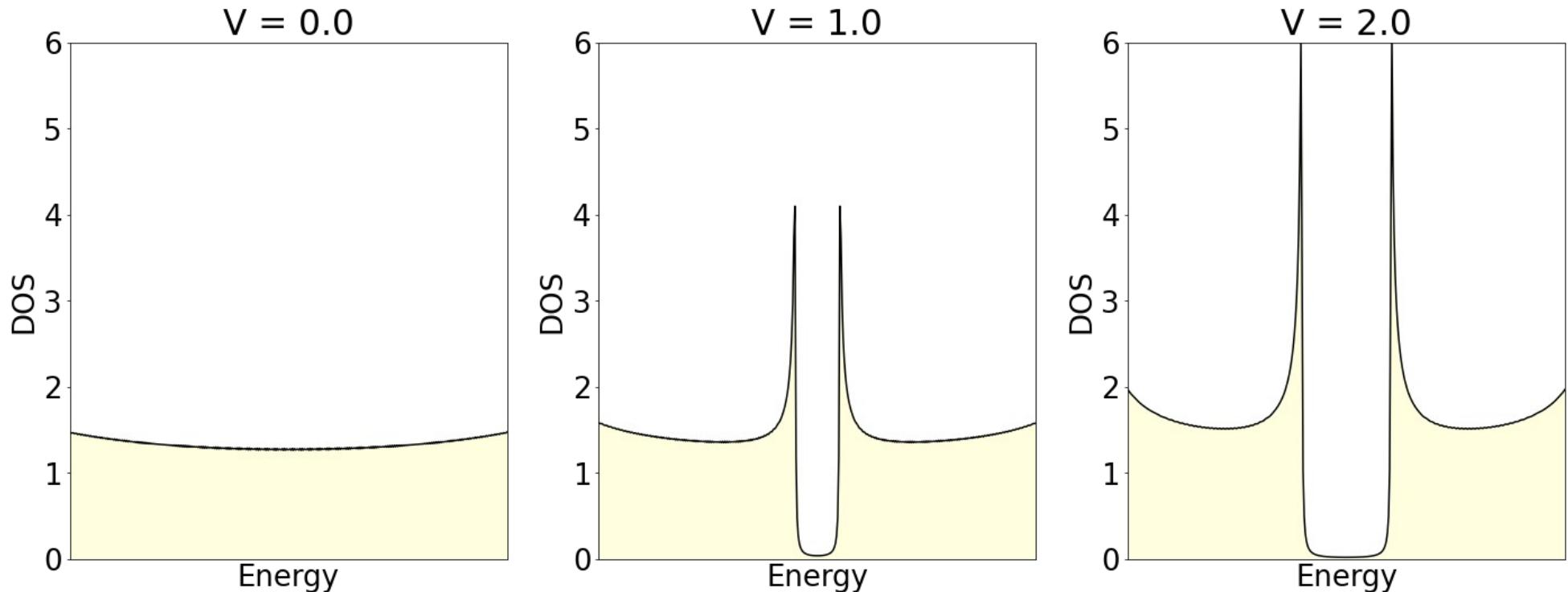
Anticrossing between the bands appear due to the superlattice potential

Electronic structure unfolding



As the periodicity of the superlattice is increased, more minibands appear

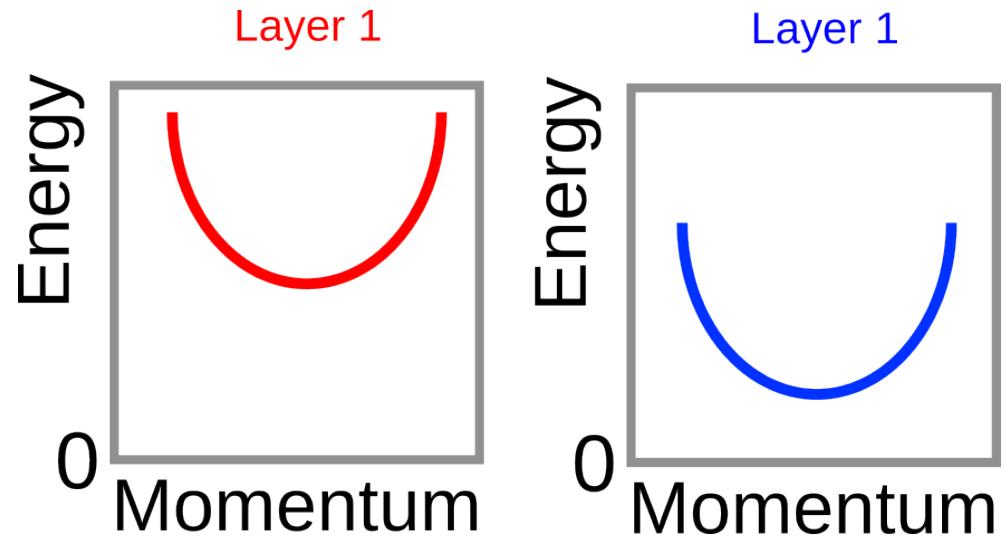
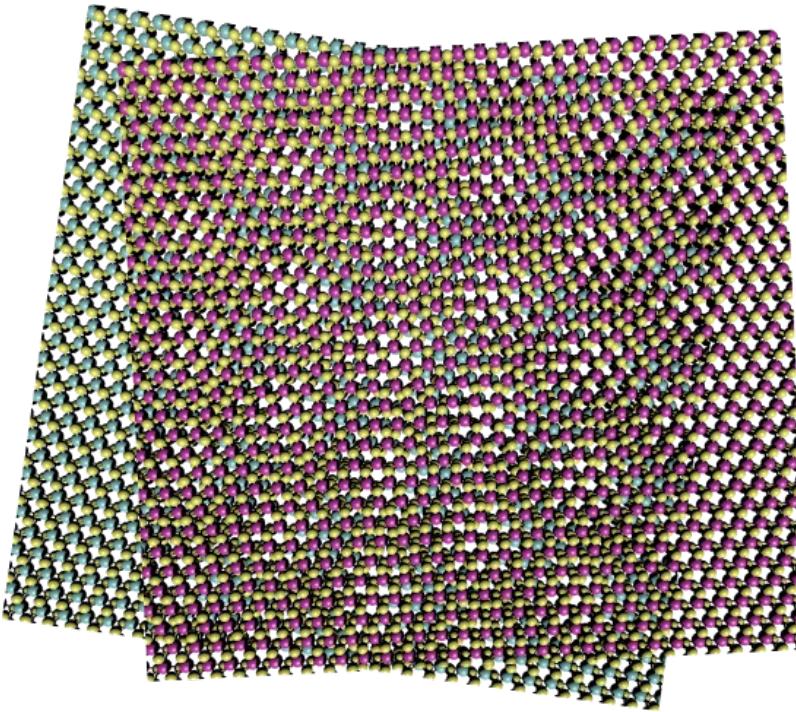
Moire electronic structure



As the strength of the moire potential increases, the density of states gets enhanced

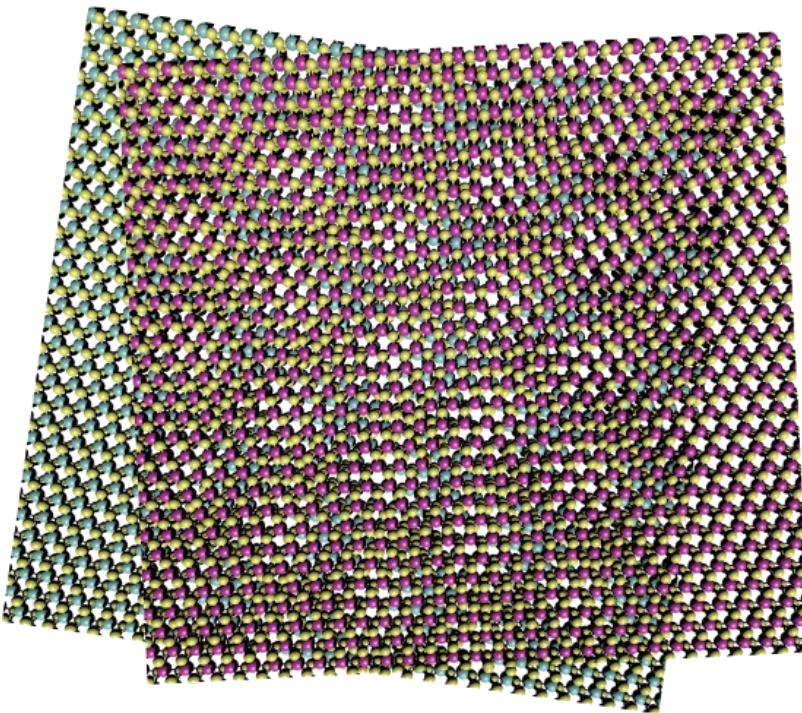
Moire in twisted TMDC

In twisted TMDC heterobilayers, the moire modulates the band off set of one layer

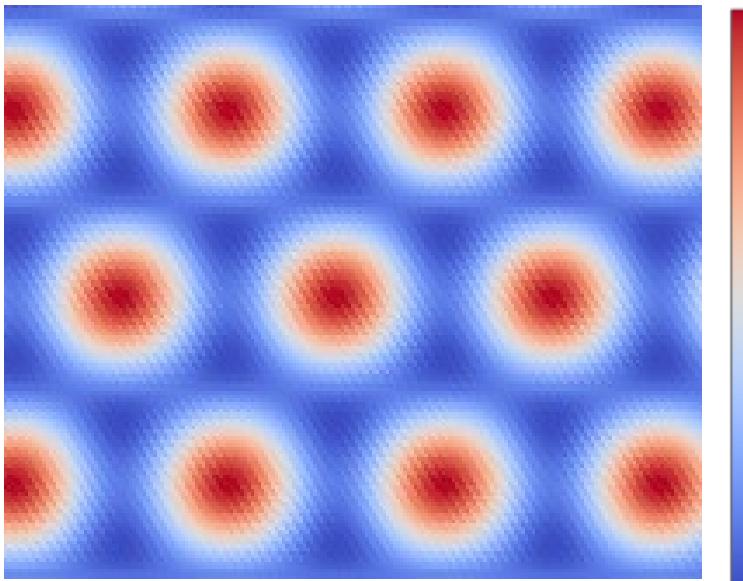


Moire in twisted TMDC

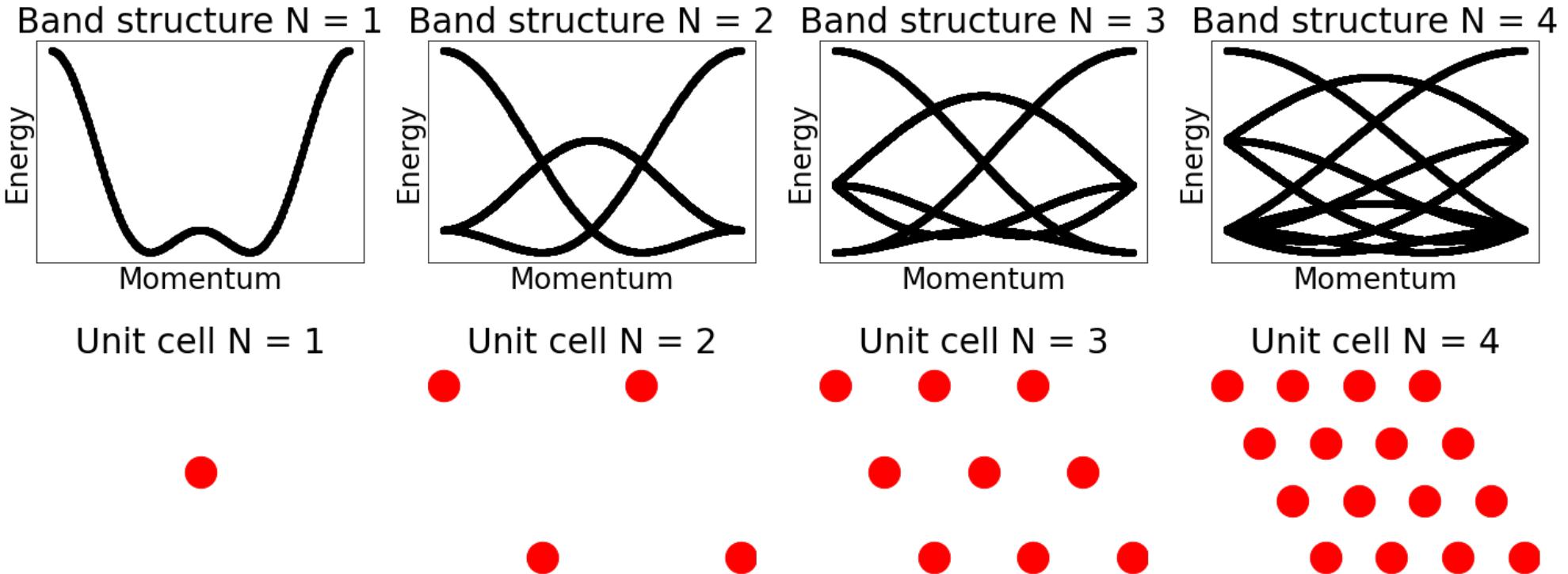
In twisted TMDC heterobilayers, the moire modulates the band off set of one layer



$$H = \sum_{ij} c_i^\dagger c_j + h.c. + \sum_n V(\mathbf{r}_n) c_n^\dagger c_n$$



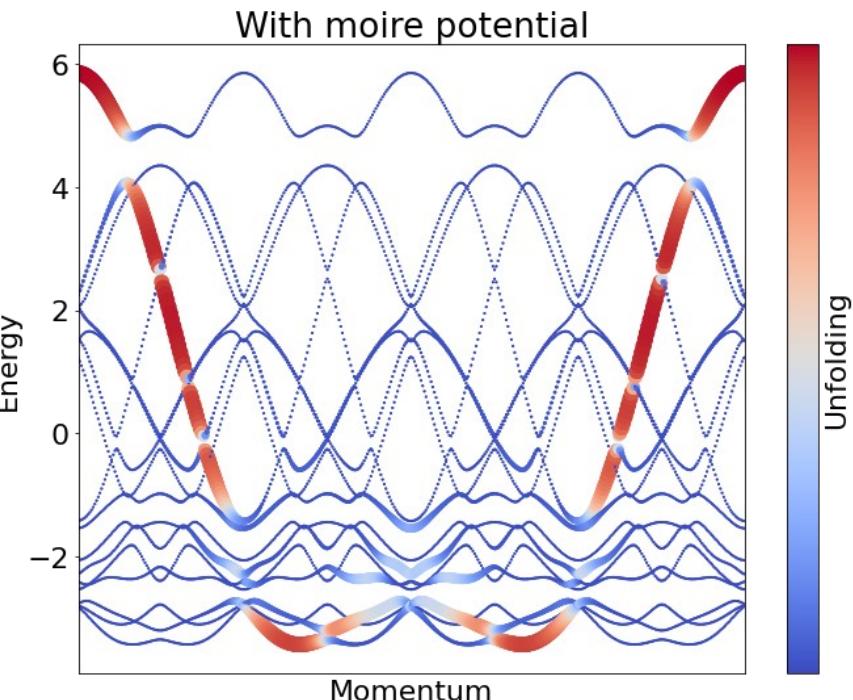
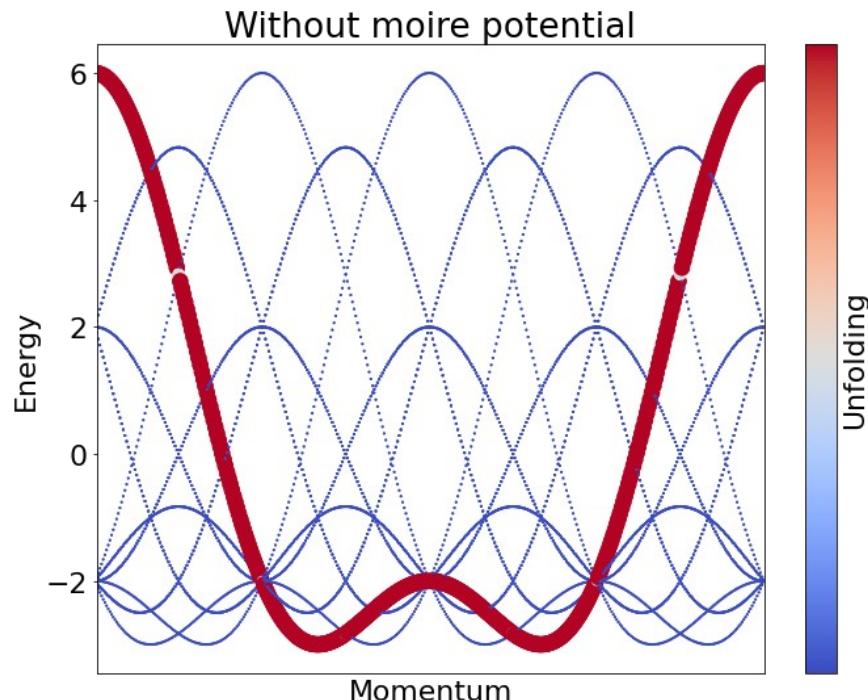
Band structure folding in 2D superlattices



A 2D superlattice gives rise to a complex folding of the electronic structure

Band structure folding in 2D superlattices

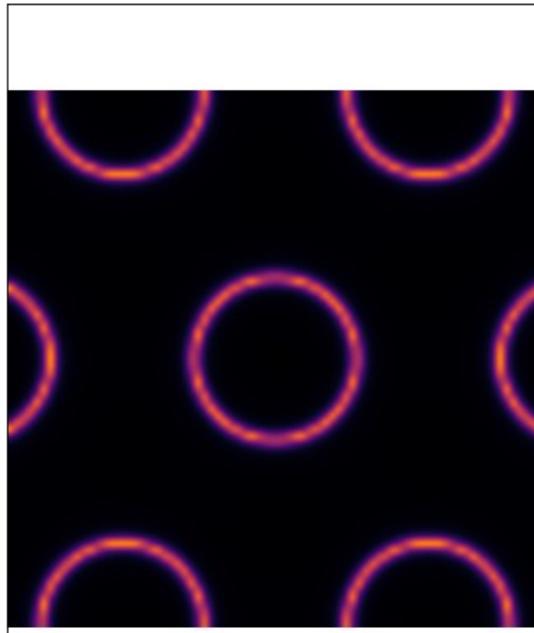
Mini-bands appear due to the moire in one of the layers



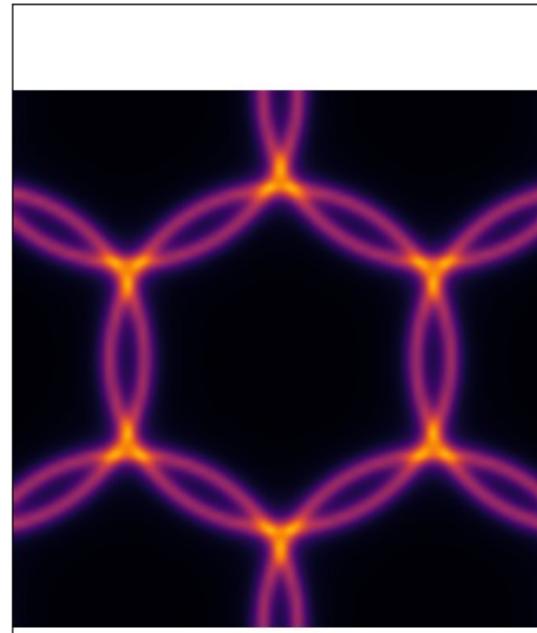
Fermi surface folding in superlattices

The Fermi surface in 2d supercell gets folder, turning one Fermi surface into many

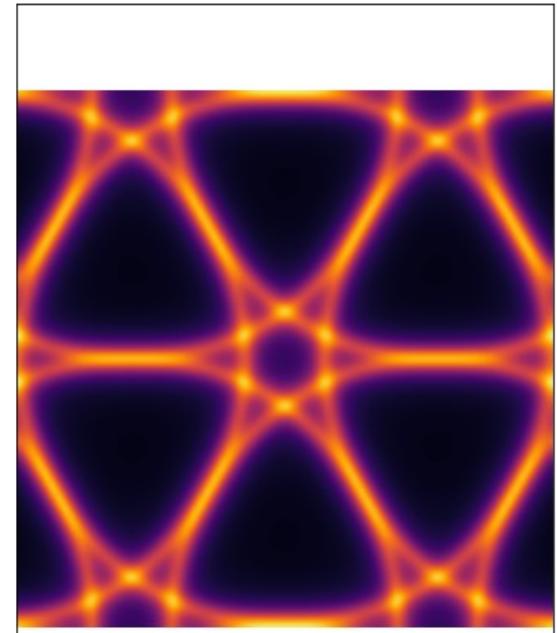
$N = 1$



$N = 2$

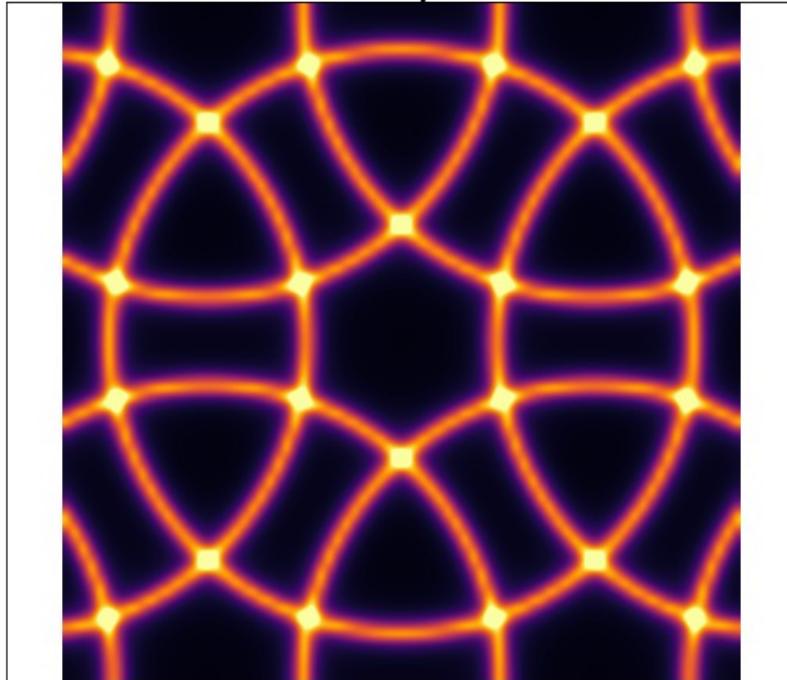


$N = 3$

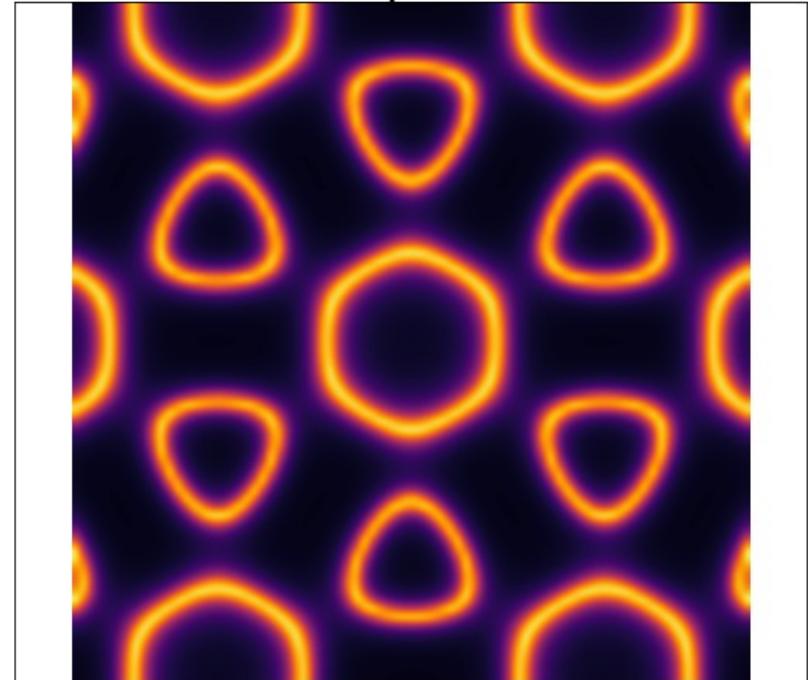


Fermi surface folding in superlattices

Without superlattice



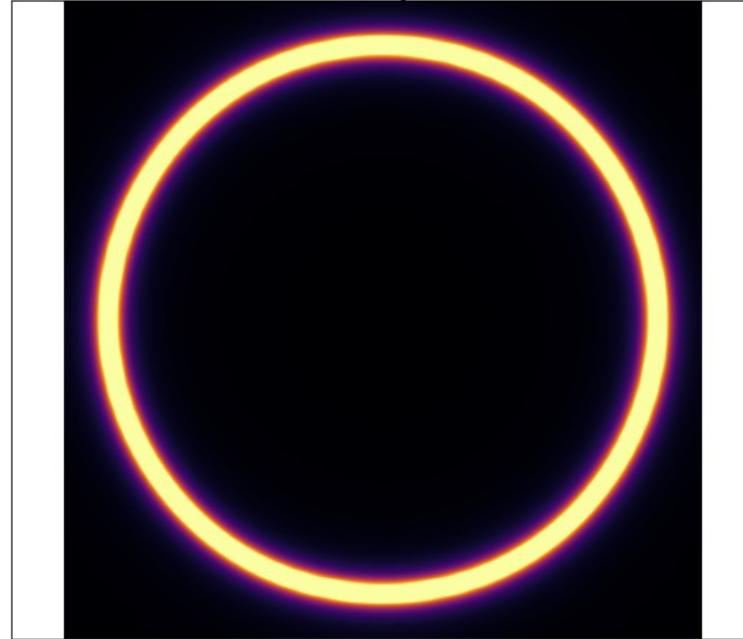
With superlattice



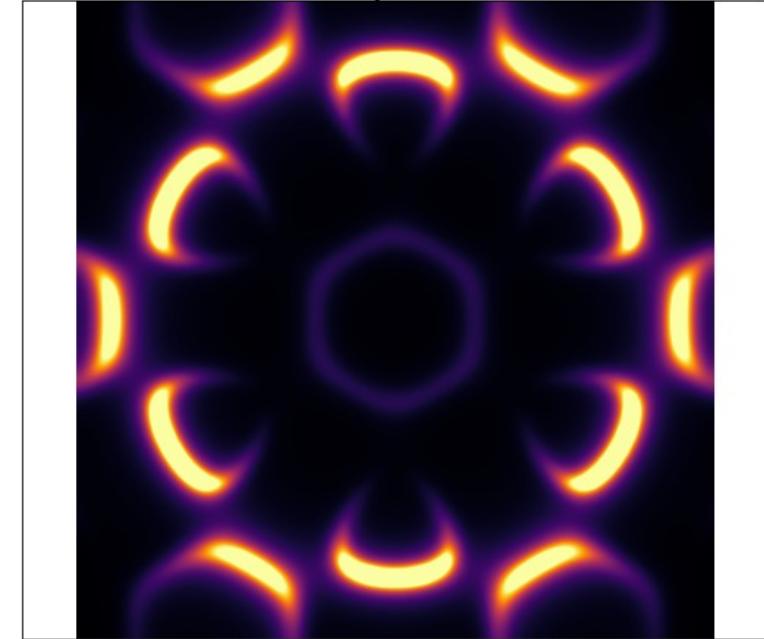
The superlattice changes the Fermi surface topology on the underlying 2D material

Fermi surface unfolding in superlattices

Without superlattice



With superlattice



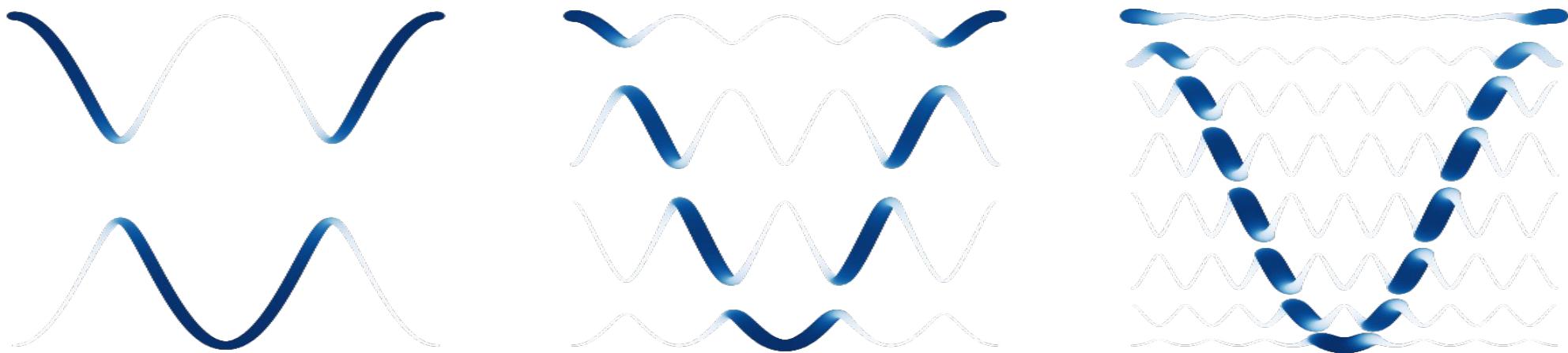
Superlattices fragment the original Fermi surface when unfolded to the original unit cell

Break

5 min break

(optional) to discuss during the break

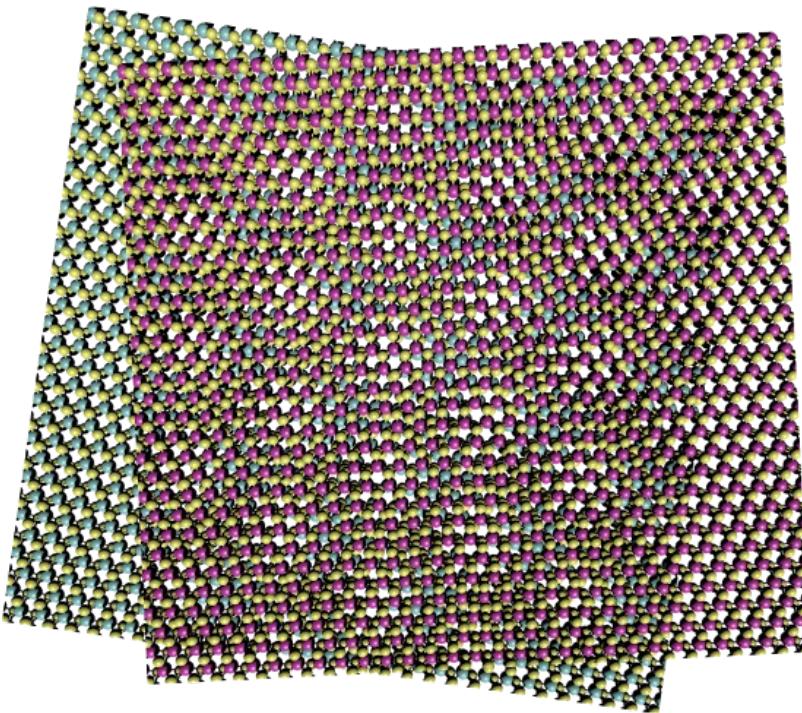
Which band structure has more van Hove singularities?



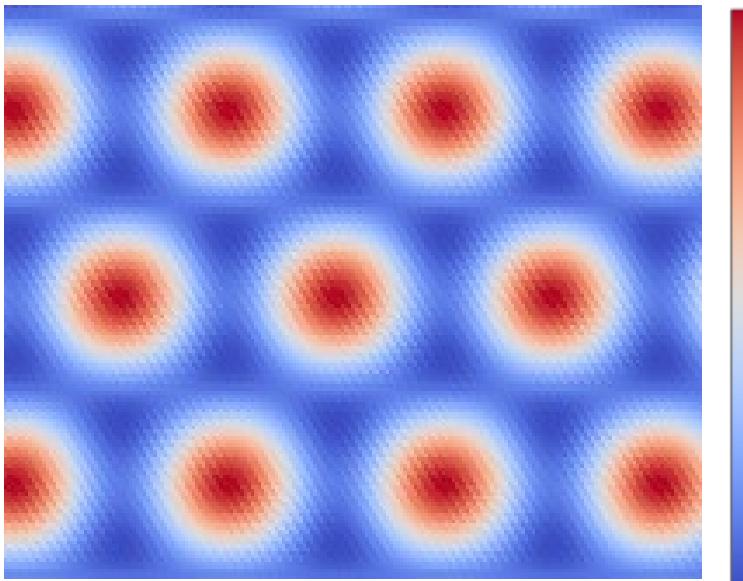
Moire-driven correlated states

Moire in twisted TMDC

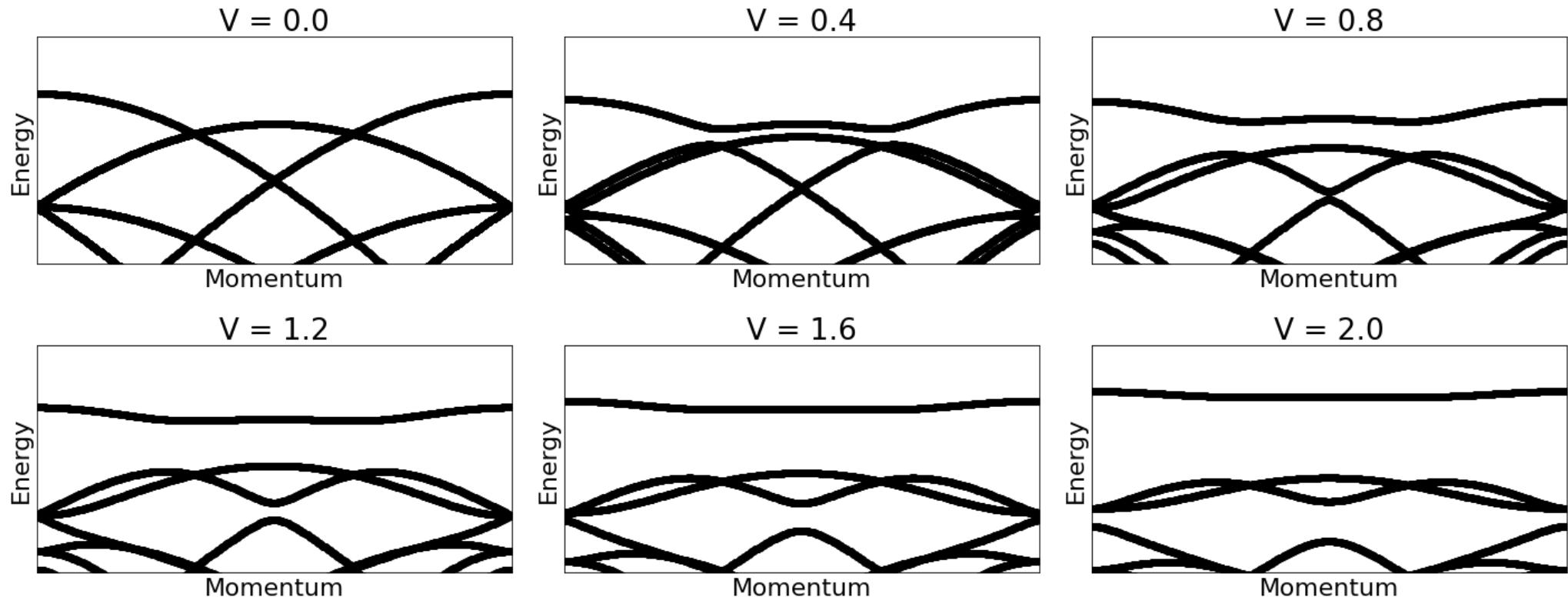
In twisted TMDC heterobilayers, the moire modulates the band off set of one layer



$$H = \sum_{ij} c_i^\dagger c_j + h.c. + \sum_n V(\mathbf{r}_n) c_n^\dagger c_n$$

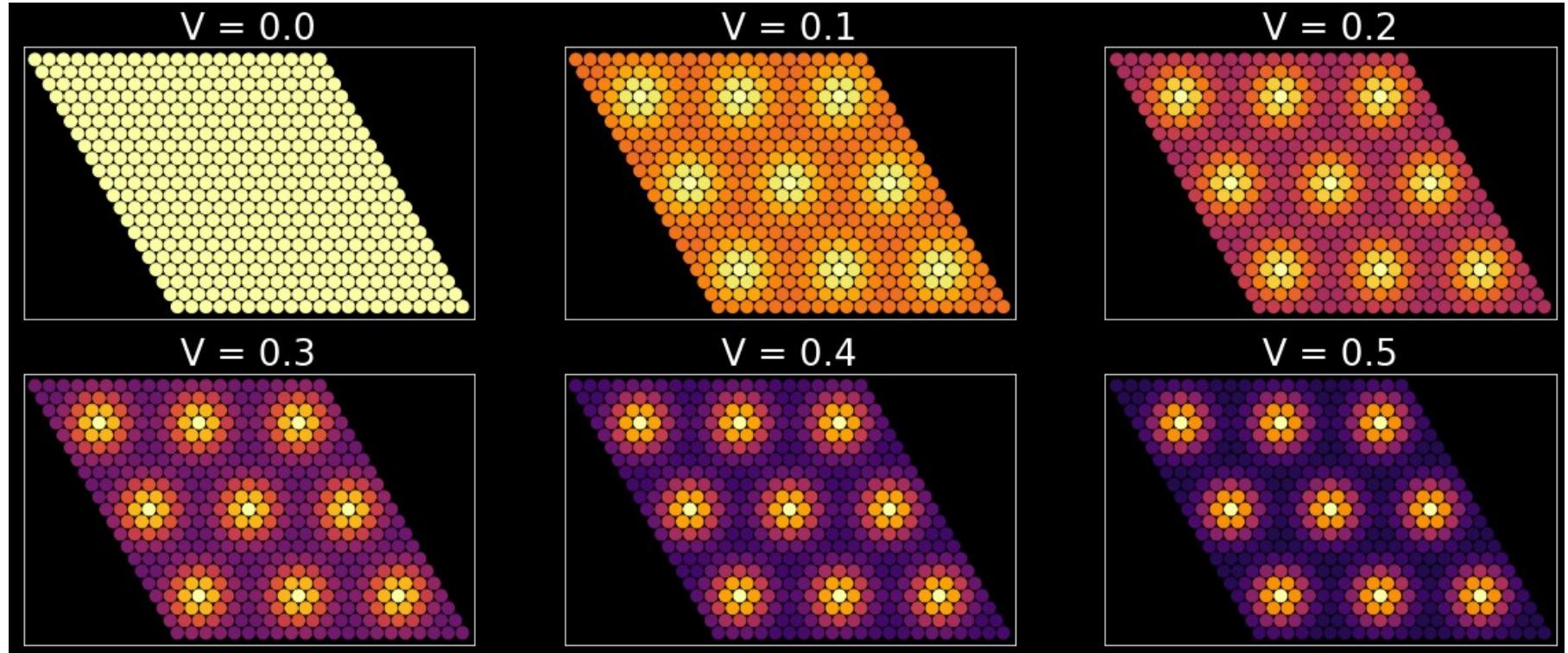


Band flattening by a moire



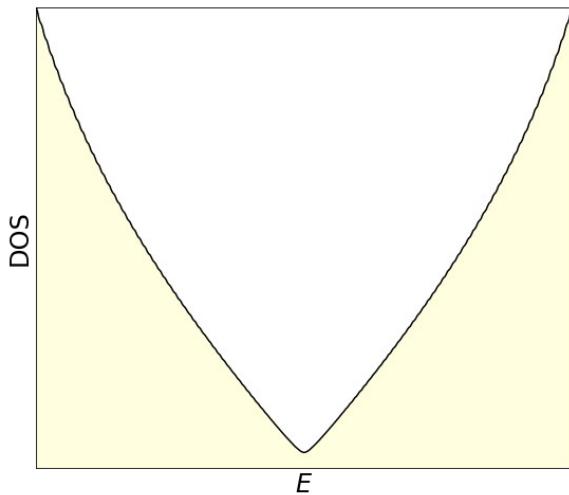
As the strength of a modulation is increased, flat bands appear

Emergence of moire states

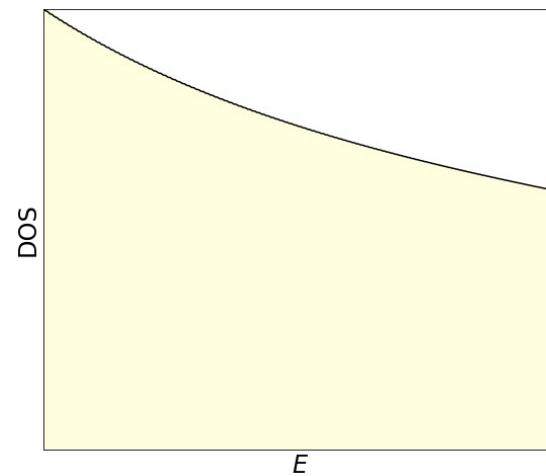


Controlling the electronic spectra with the moire angle

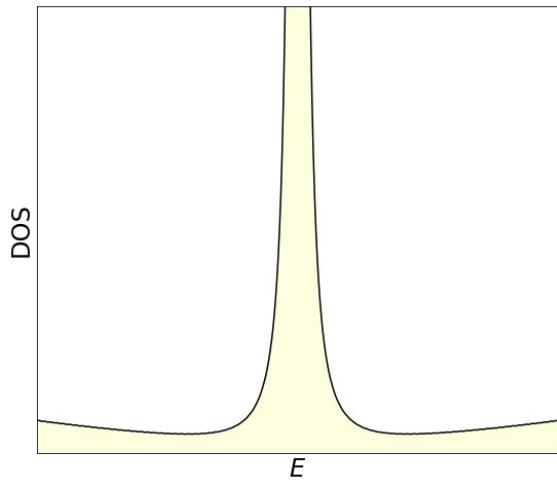
Semimetals



Metals



Flat bands



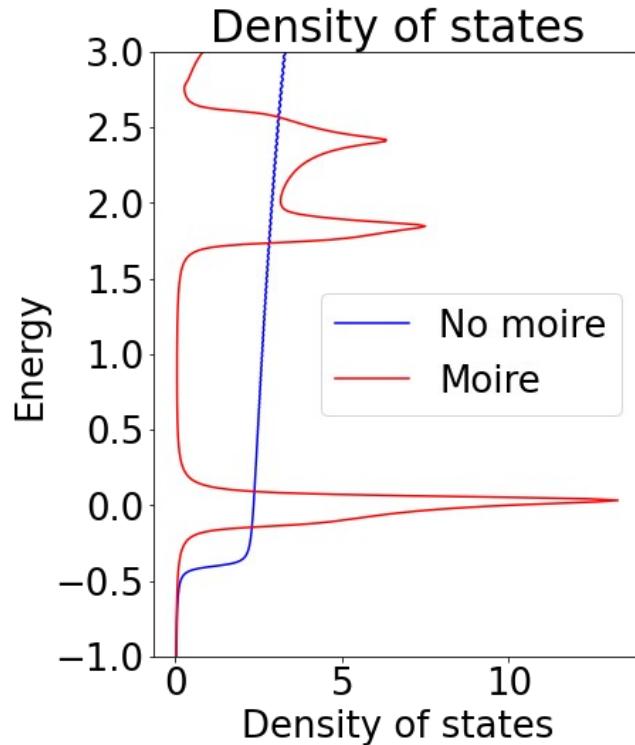
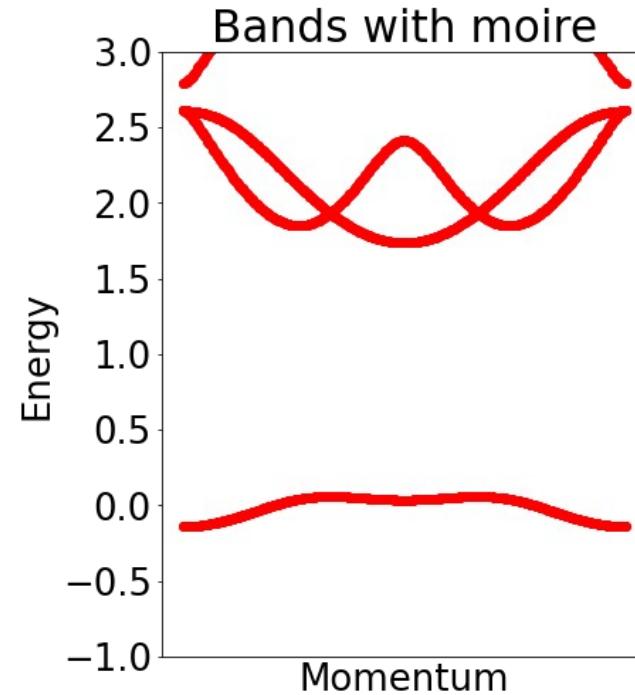
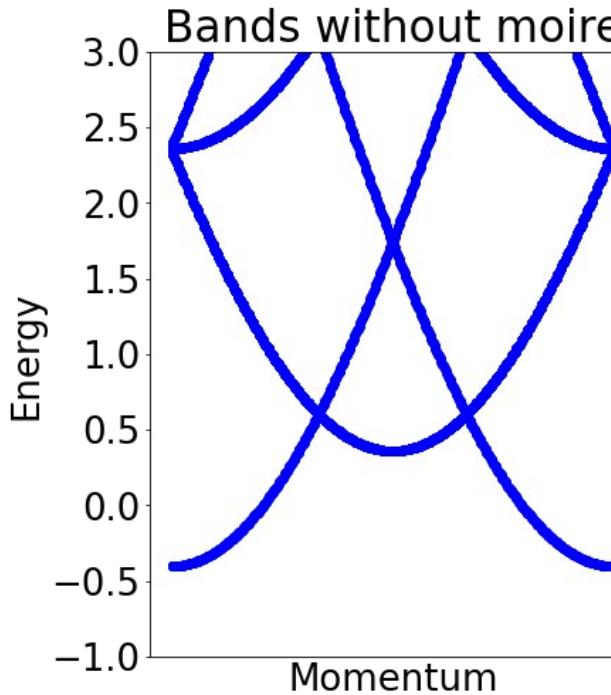
Moire/twist angle



Moire potentials allow driving systems to the correlated limit

$$U_C \sim \frac{1}{D(E_F)}$$

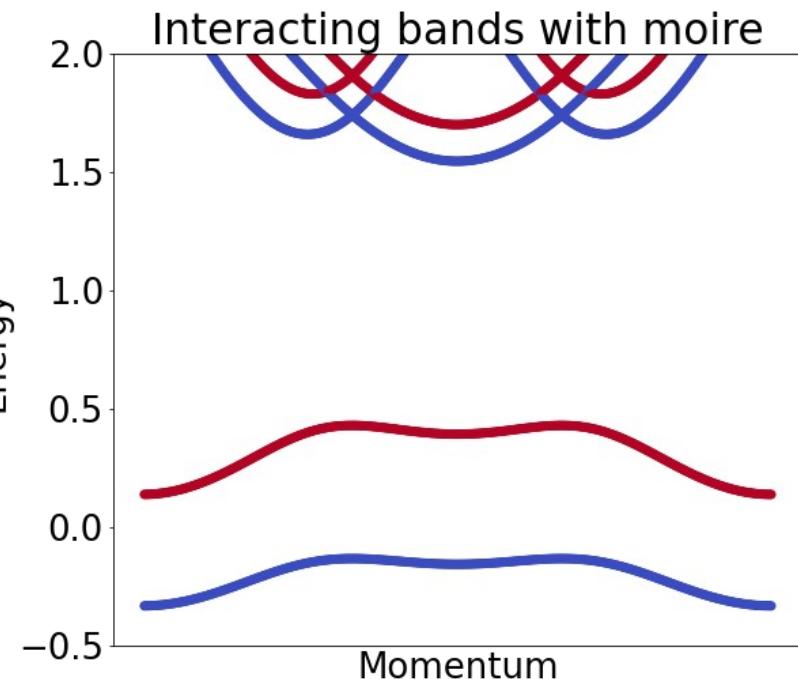
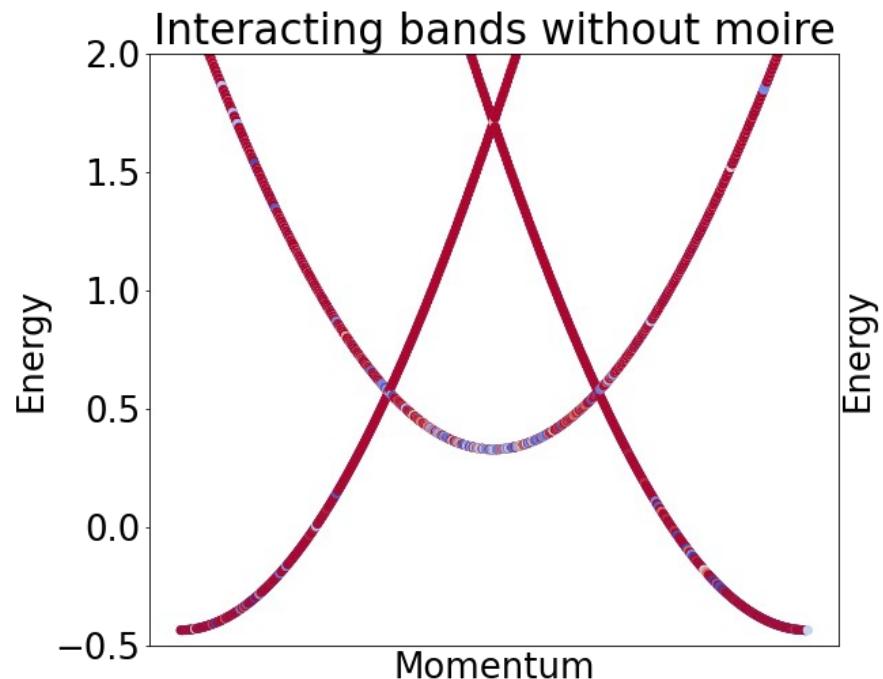
Moire-enhanced DOS



The moire potential gives rise to an enhanced DOS

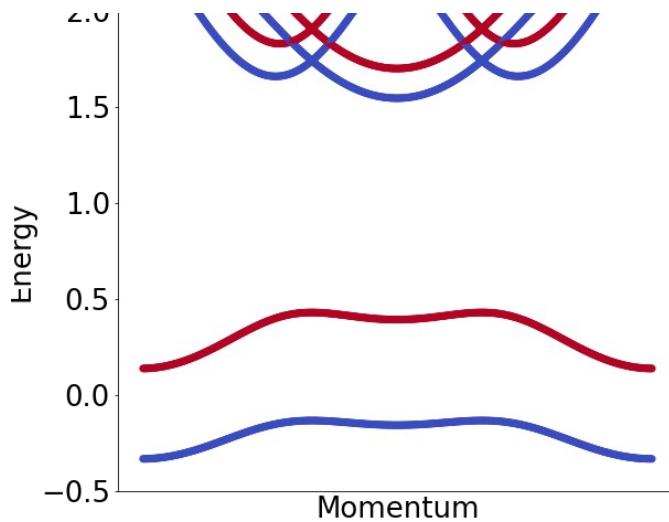
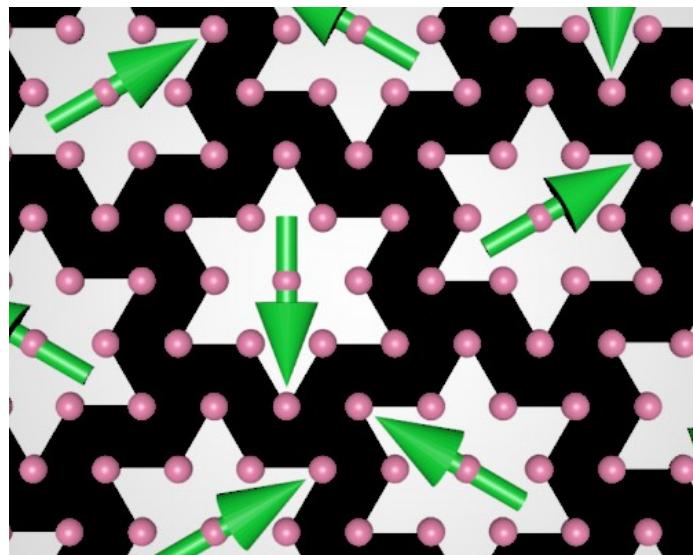
Interactions in the absence and presence of a moire

$$H = \sum_{ij,s} t_{ij} c_{i,s}^\dagger c_{j,s} + \sum_i U c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} + h.c.$$



Correlated state in 1T-TaS₂ from miniband formation

Charge-density wave reconstruction, leading to a localized orbital in a $\sqrt{13} \times \sqrt{13}$ unit cell



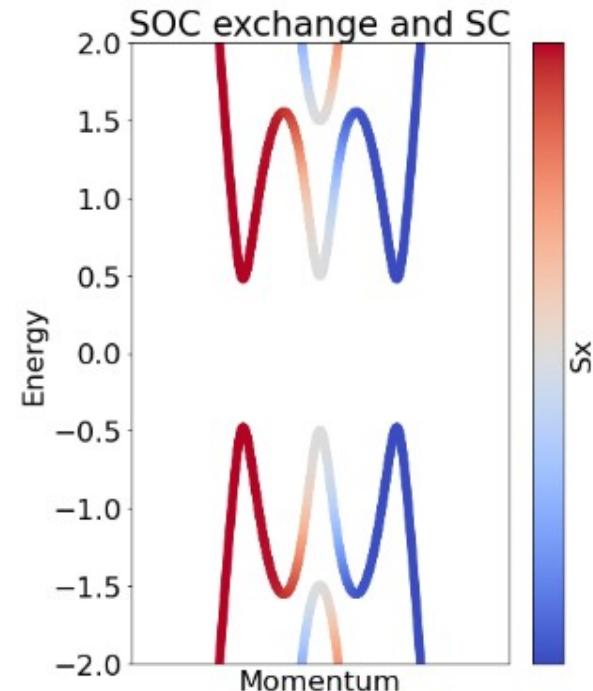
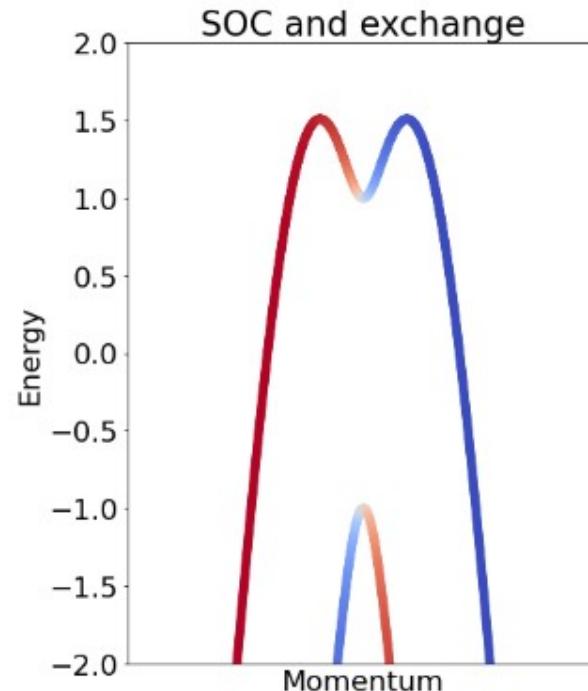
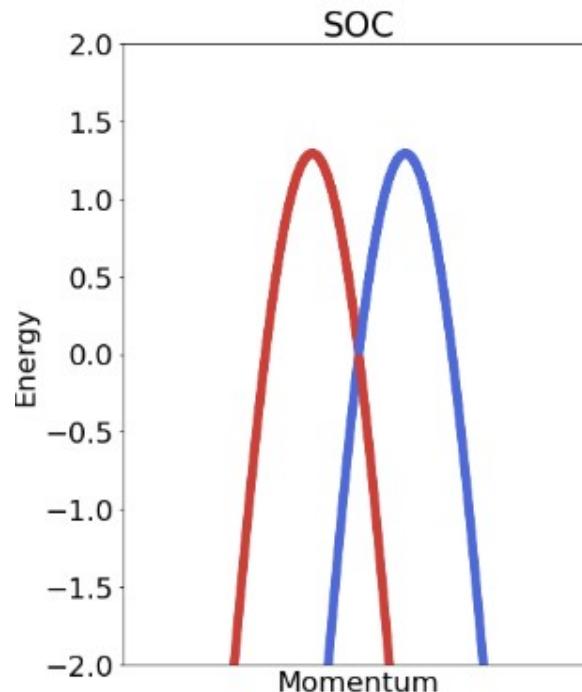
A charge density wave distortion acts as a superlattice modulation

Strong interactions give rise to local moment formation in the mini-bands

Moire-driven topological states

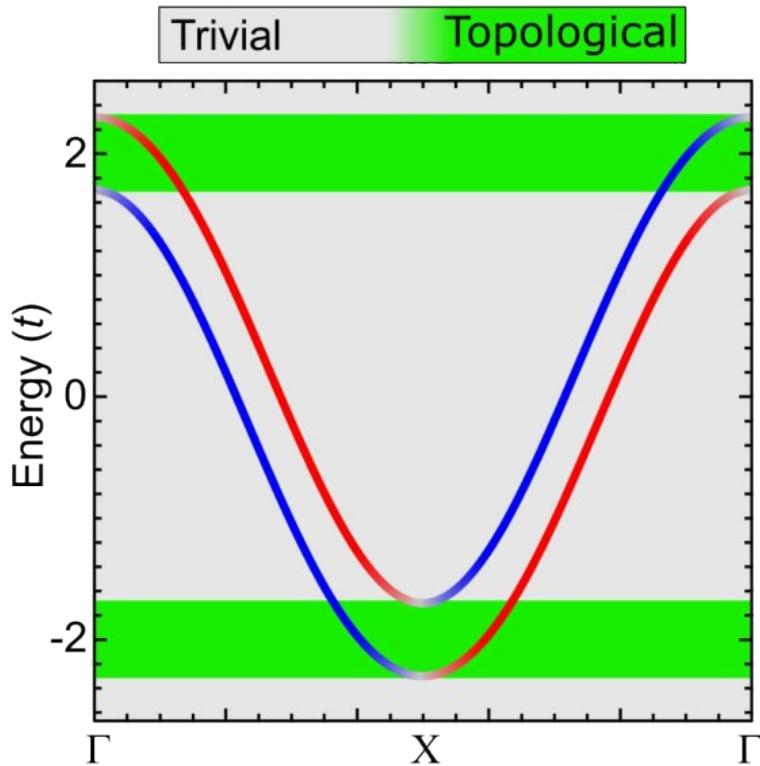
Artificial topological superconductivity

Bulk electronic structure



The combination of SOC and exchange creates helical states
Superconductivity gaps out the helical states in a non-trivial way

Artificial topological superconductor



$$H = H_0 + H_J + H_R$$

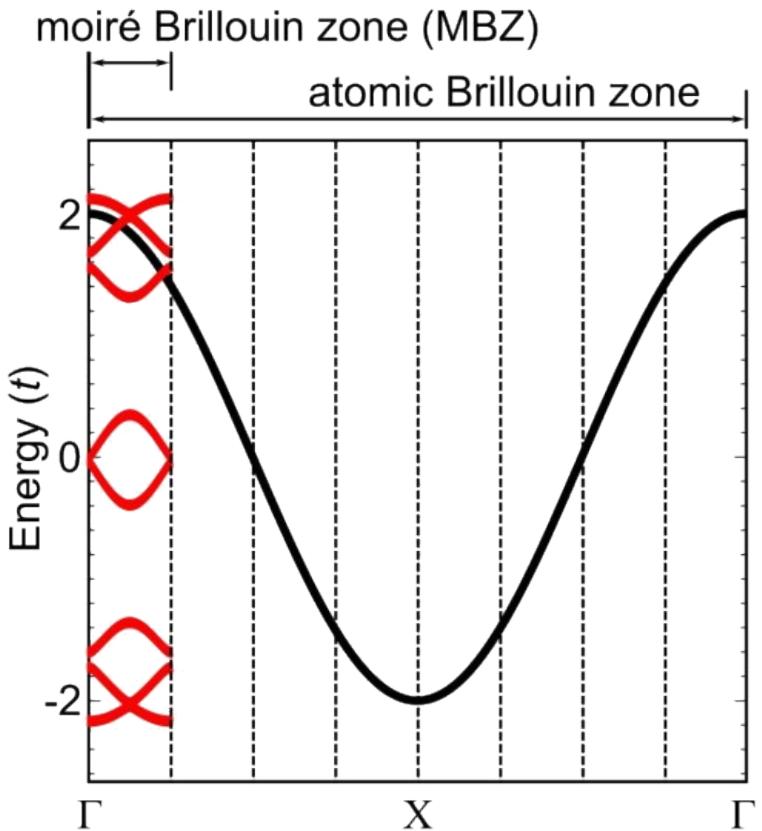
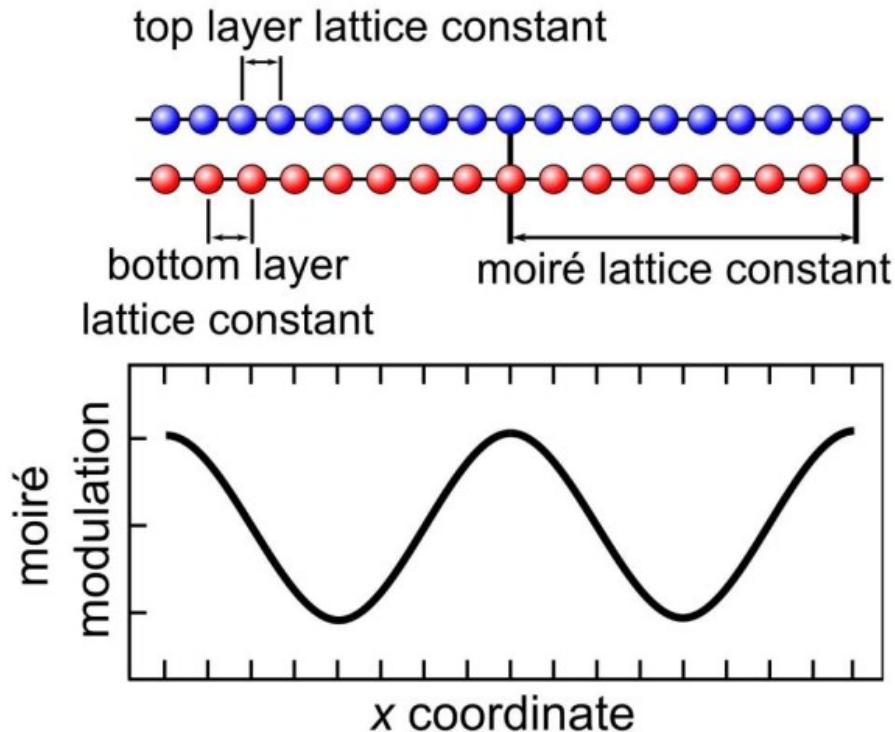
Kinetic energy

Exchange field

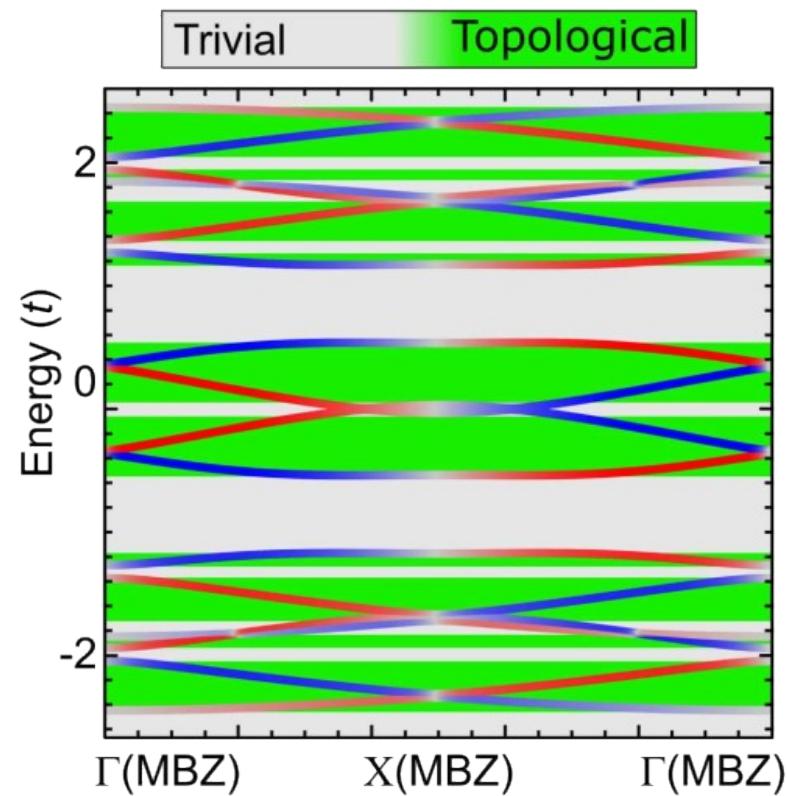
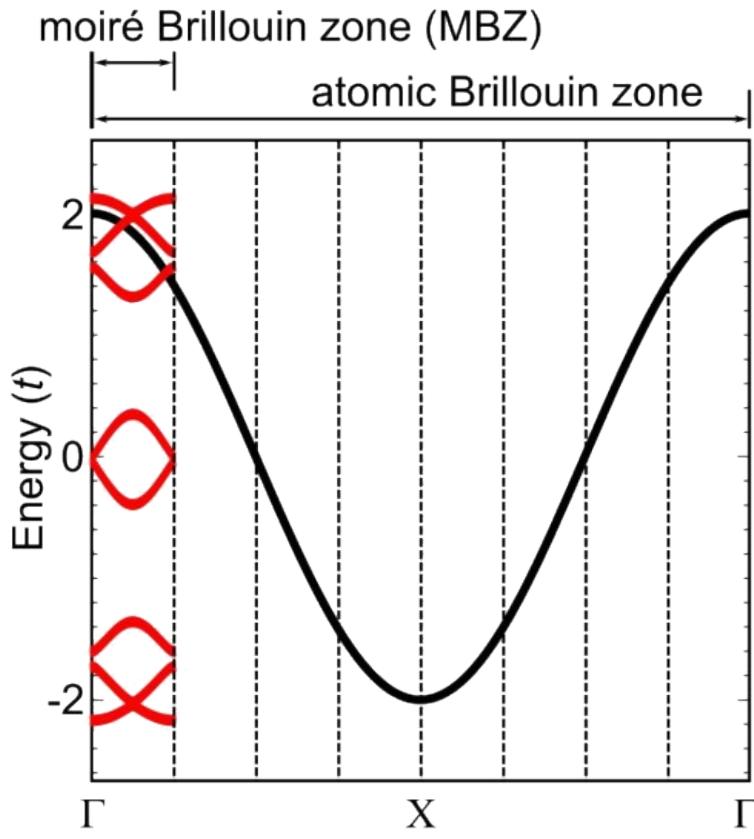
Rashba spin-orbit coupling

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

Artificial moire topological superconductor

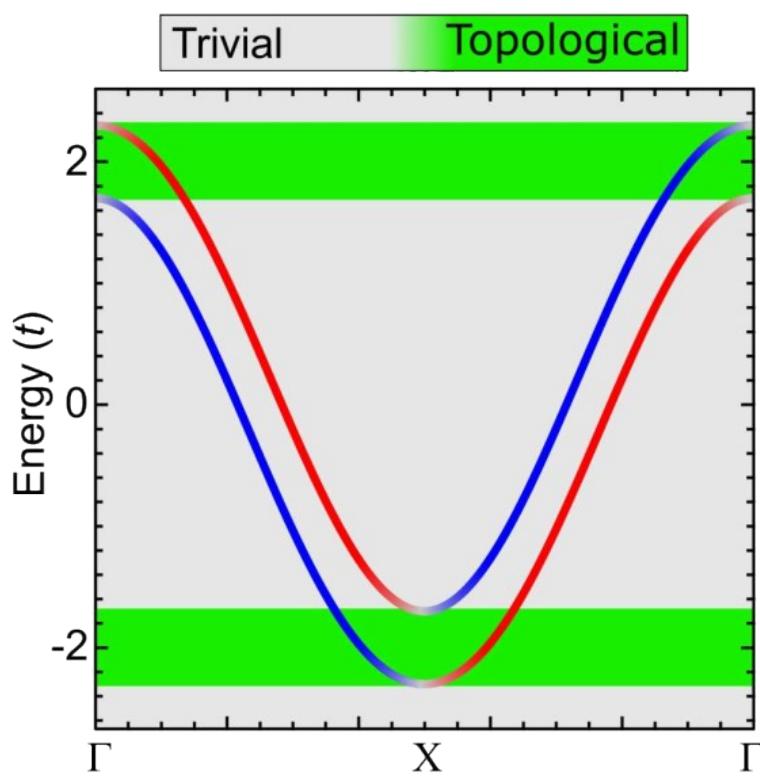


Artificial moire topological superconductor

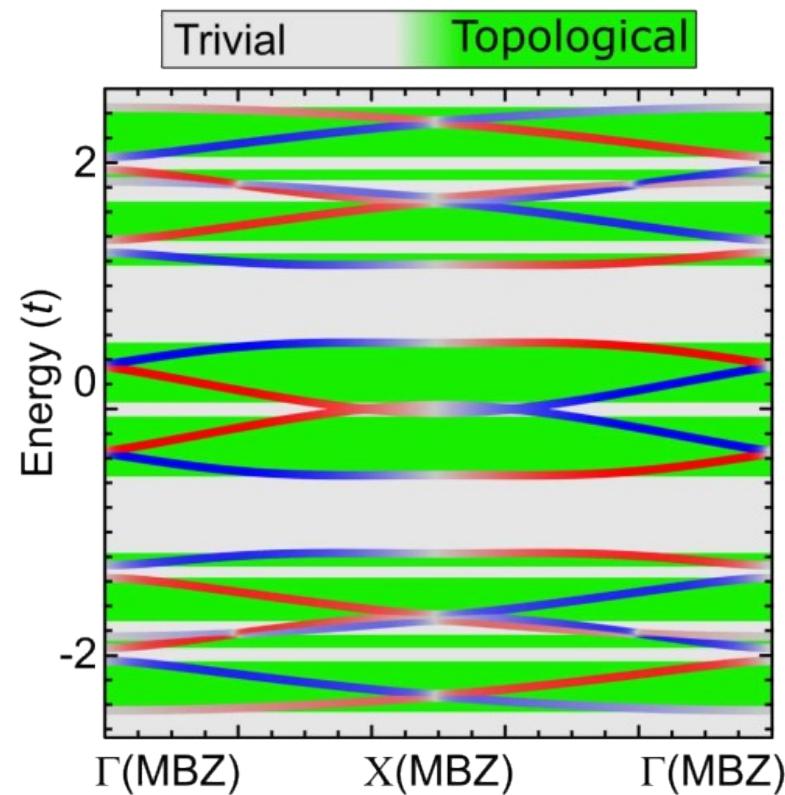


Artificial moire topological superconductor

Without moire

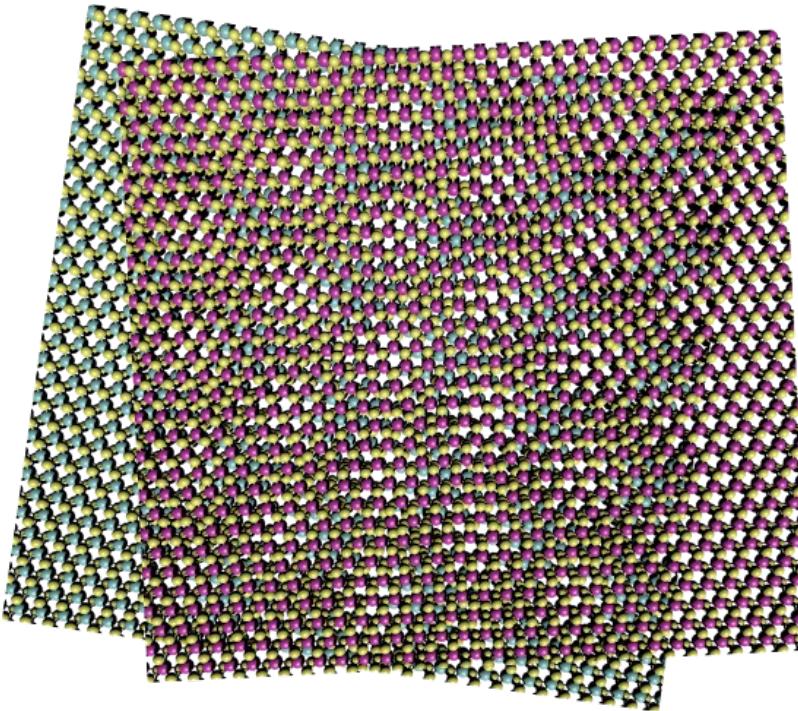


With moire



Moire driven gaps in the band structure

In twisted TMDC heterobilayers, the moire modulates the band off set of one layer



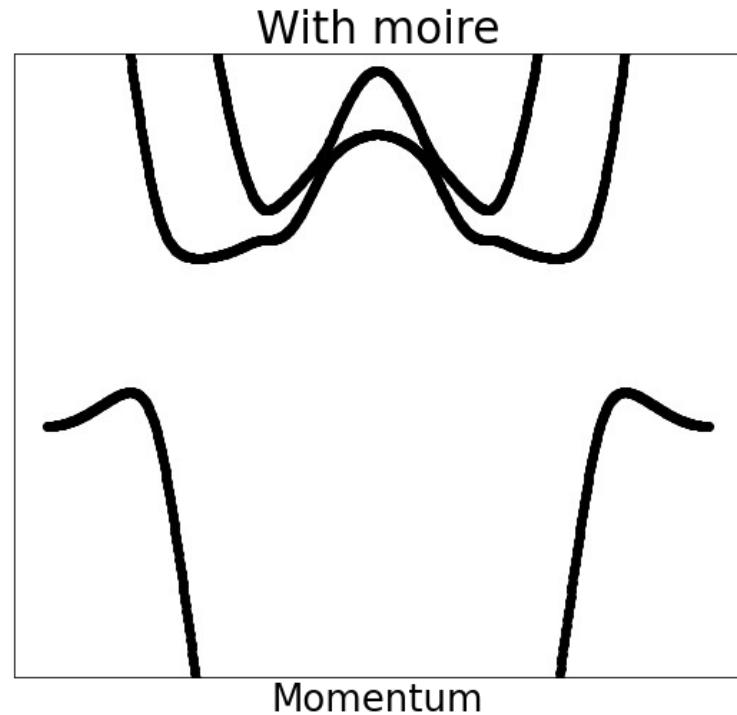
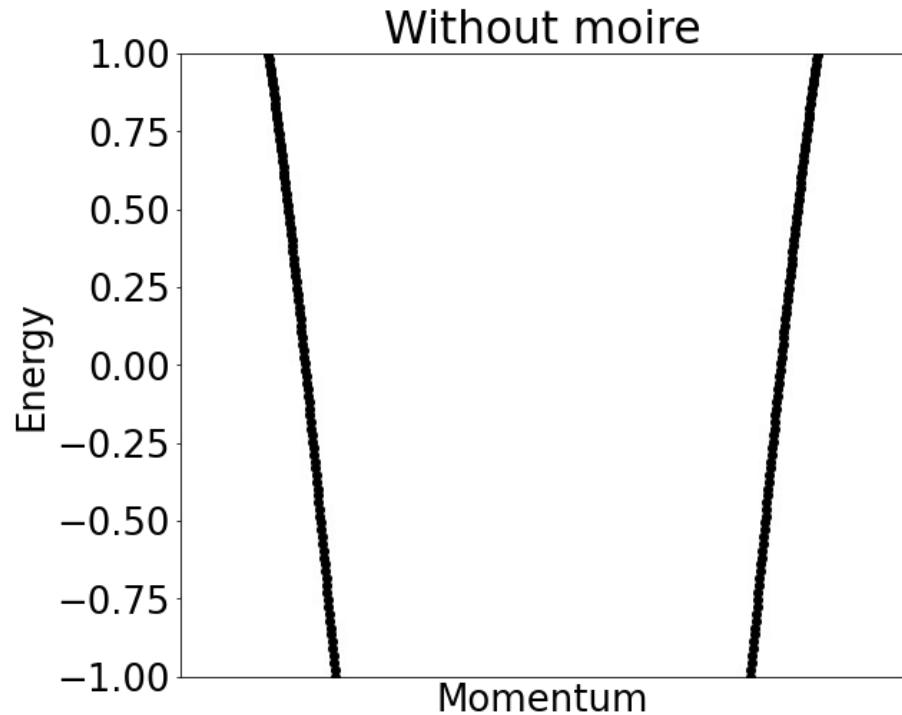
$$H = H_0 + H_J + H_R$$

Kinetic energy

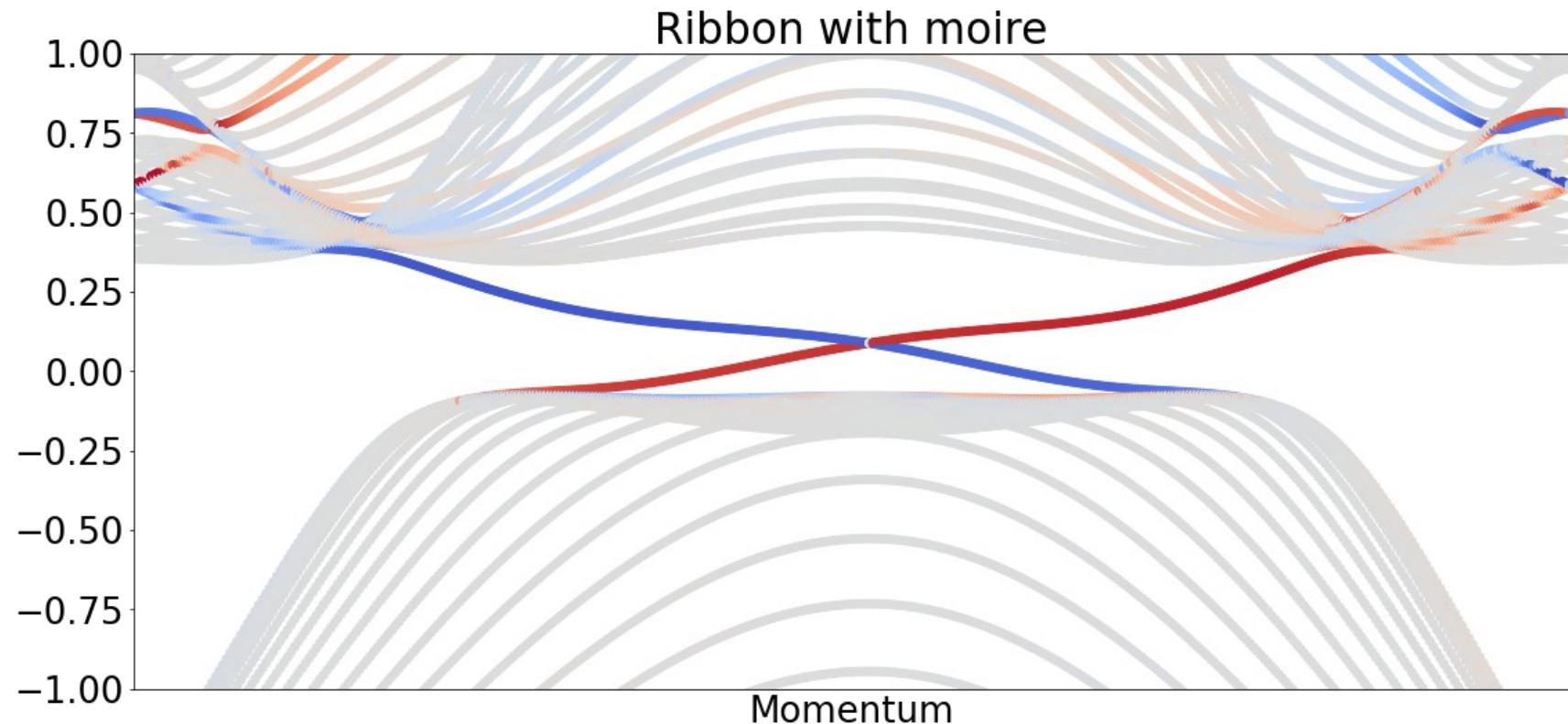
Exchange field

Rashba spin-orbit coupling

Moire driven gaps in the band structure



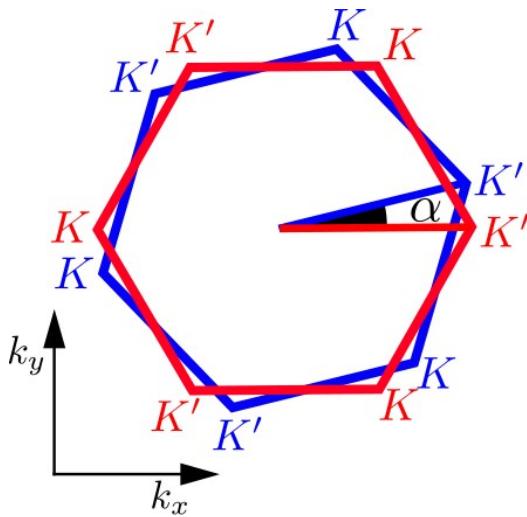
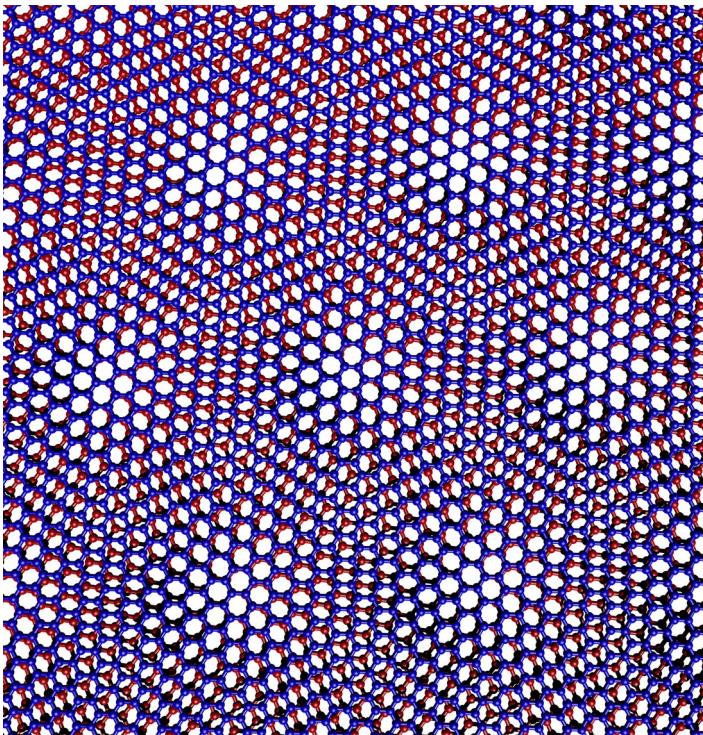
Moire driven gaps in the band structure



Chiral states appear in a ribbon driven by the moire

Electronic structure of twisted graphene multilayers

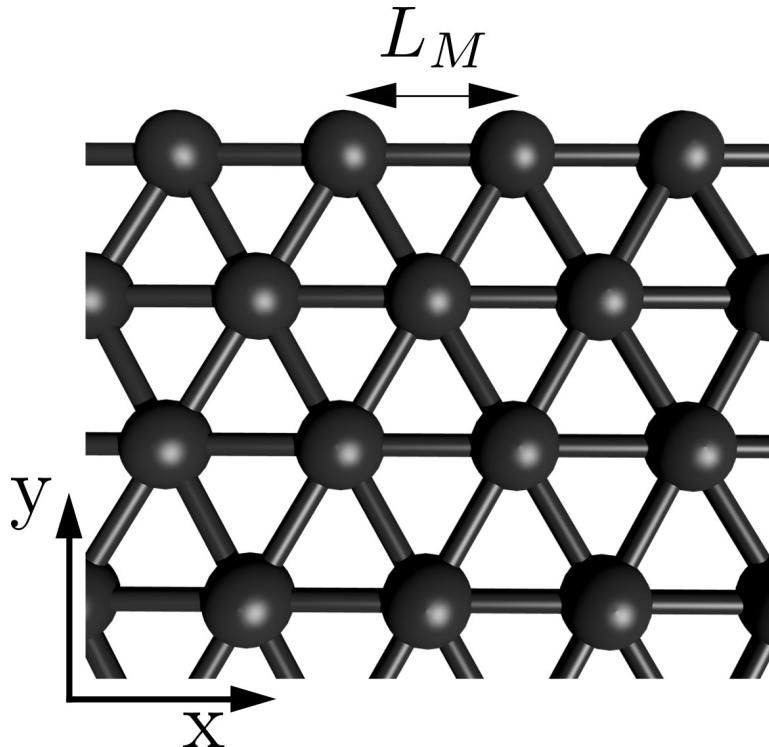
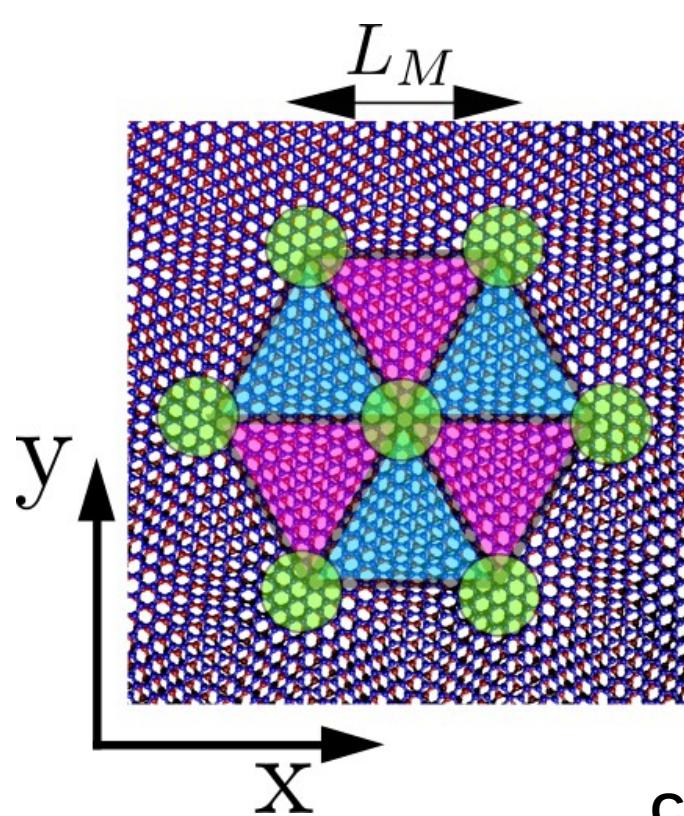
Twisted bilayer graphene



Additional parameters in the system

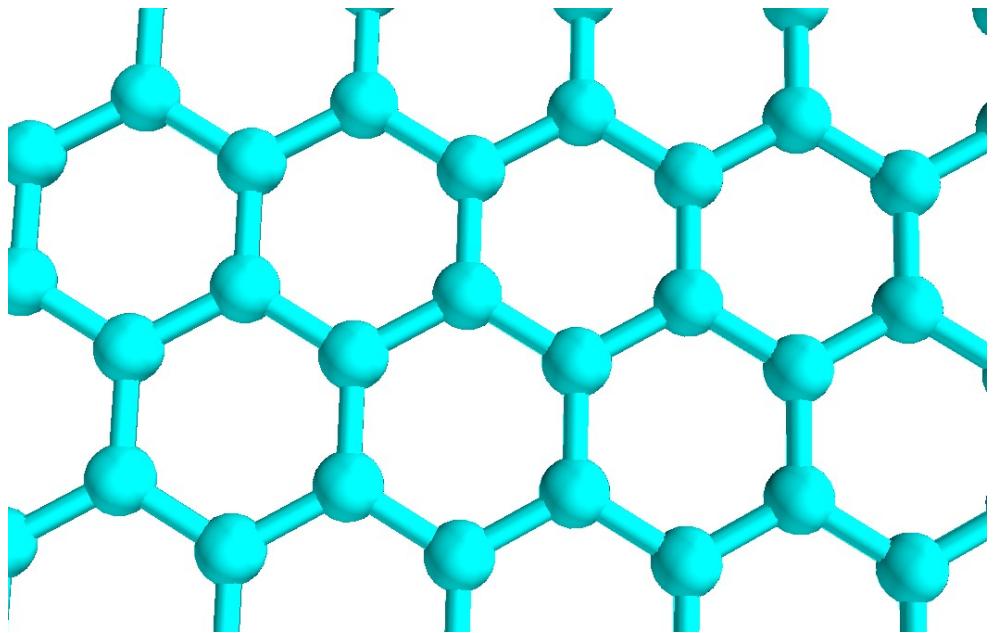
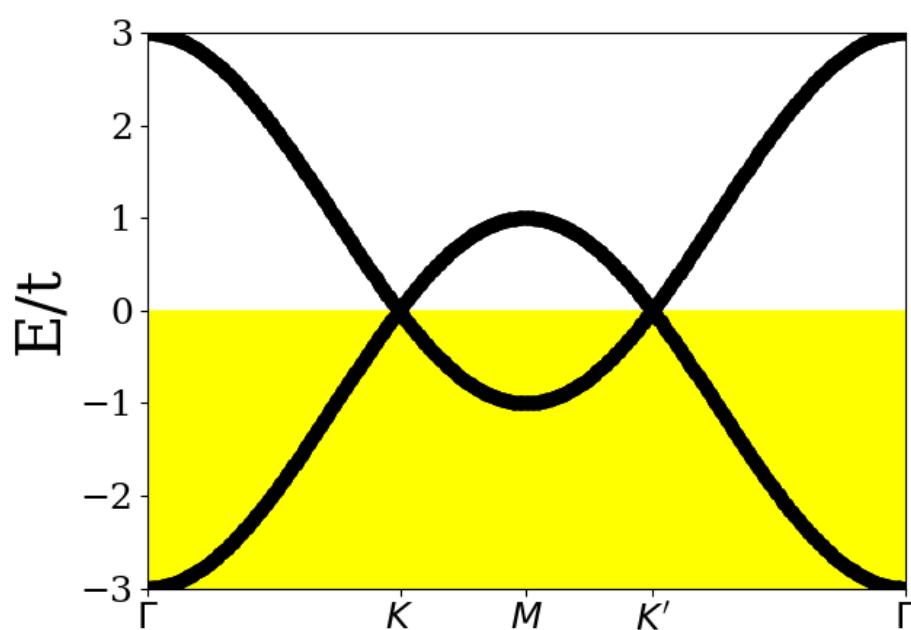
Angle between the layers α
Bias between the layers U

A new length scale: the moire length



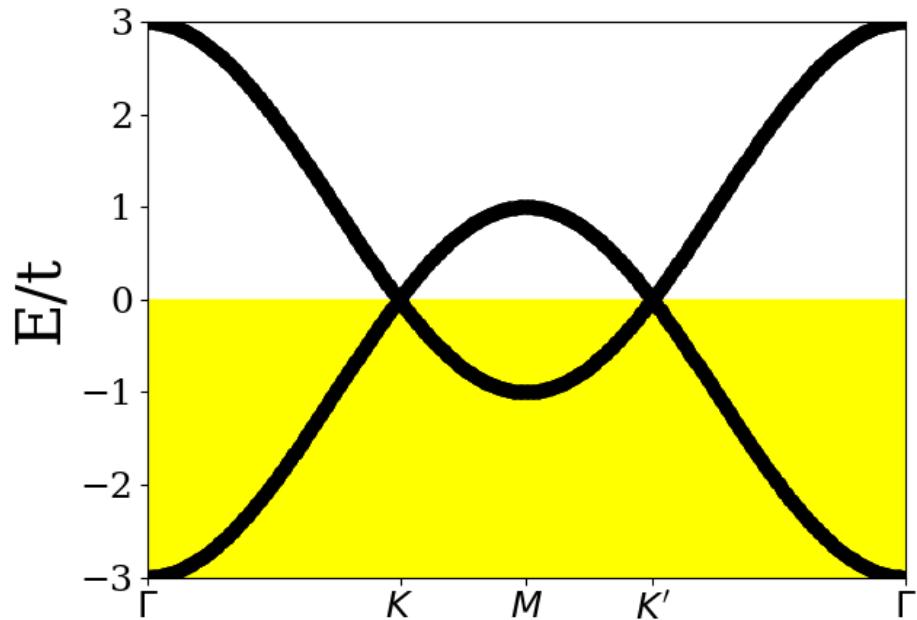
Creating effective lattices with tunable lattice constants

Structure of graphene



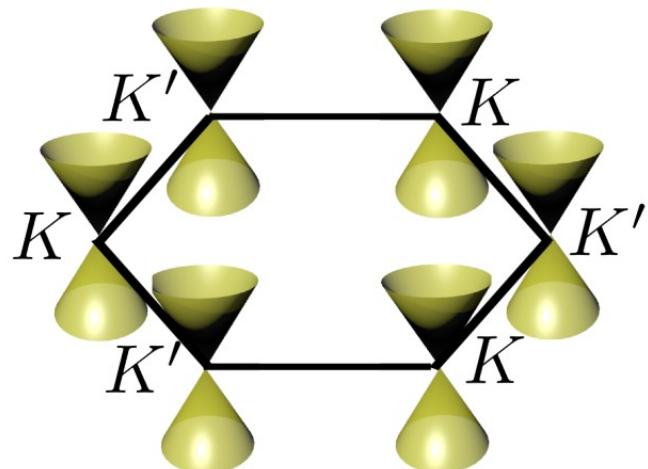
Minimal model: Single orbital in a honeycomb lattice

The electronic structure of graphene

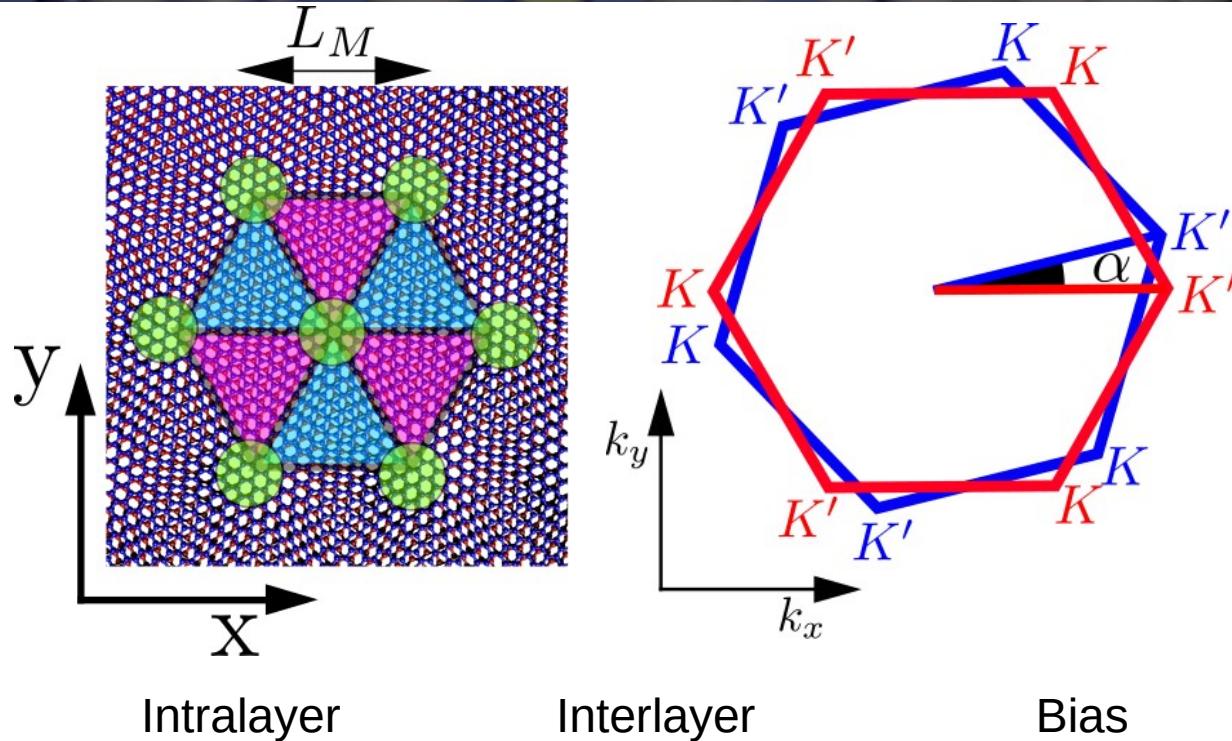


$$H = \begin{pmatrix} 0 & p_x \pm ip_y \\ p_x \mp ip_y & 0 \end{pmatrix}$$

$$H = p_x \sigma_x \pm p_y \sigma_y$$



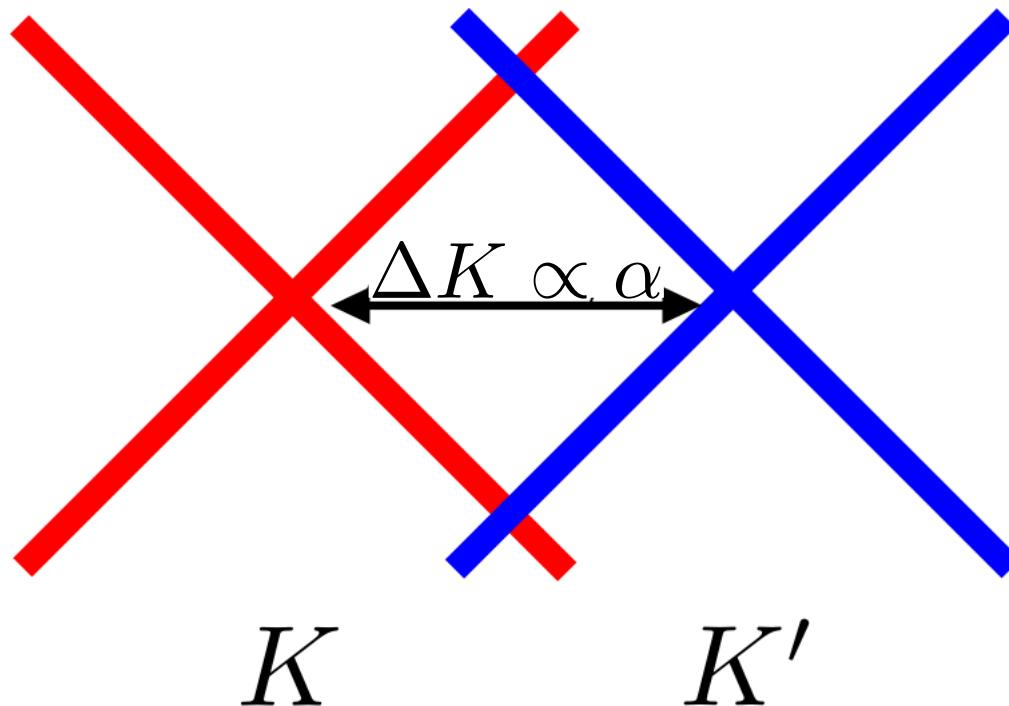
Real and reciprocal space in twisted bilayer graphene



$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j + \sum_{ij} \hat{t}_\perp(\mathbf{r}_i, \mathbf{r}_j) c_i^\dagger c_j + U \sum_i \tau_z^{ii} c_i^\dagger c_i,$$

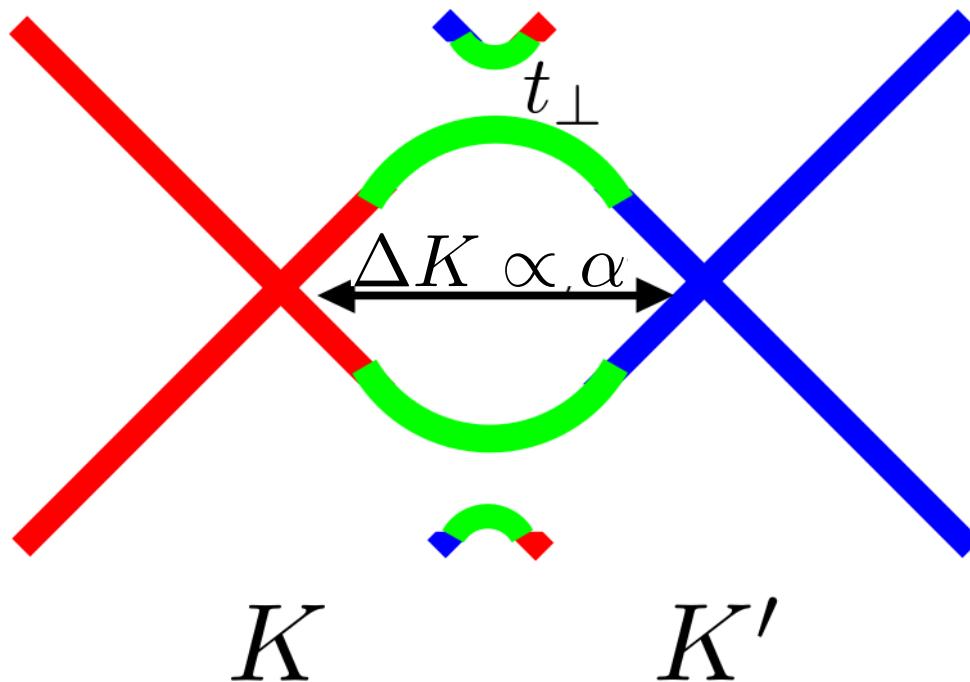
Velocity renormalization at large angle

$$\bar{v}_F/v_F = 1 - 9[t_\perp/v_F \Delta K]$$



Velocity renormalization at large angle

$$\bar{v}_F/v_F = 1 - 9[t_\perp/v_F \Delta K]$$

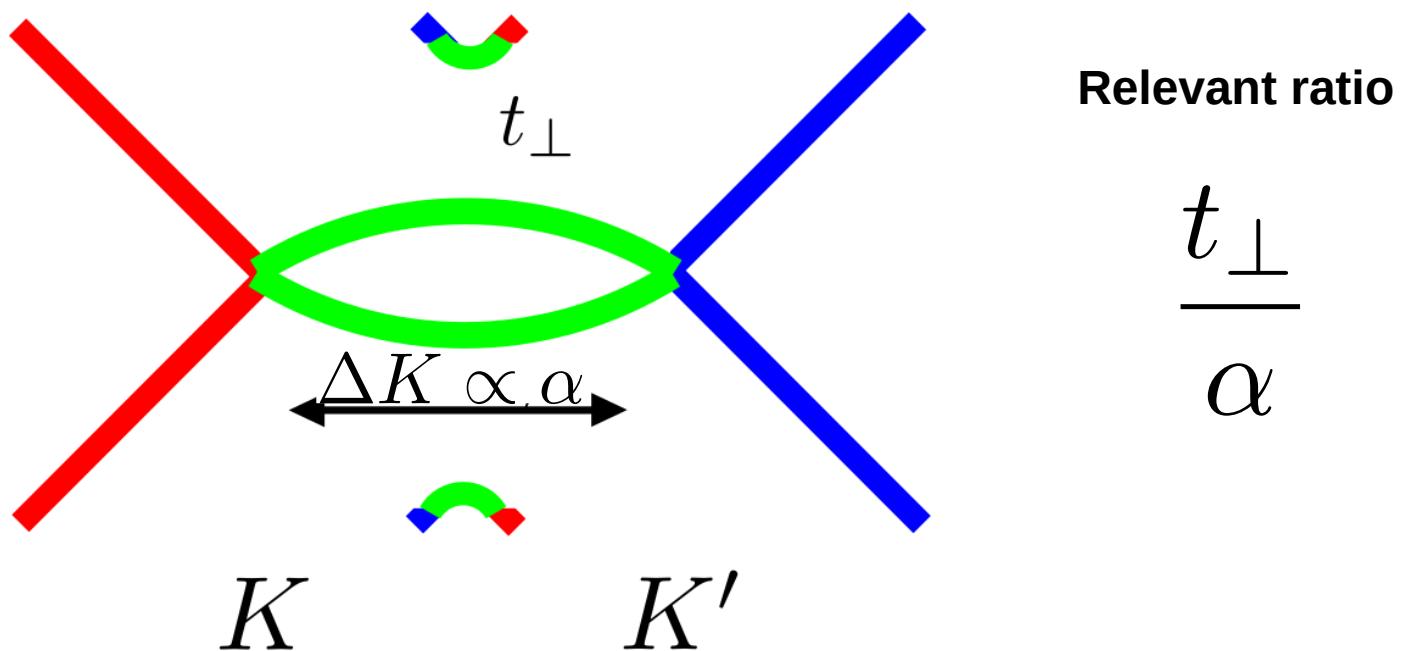


Relevant ratio

$$\frac{t_\perp}{\alpha}$$

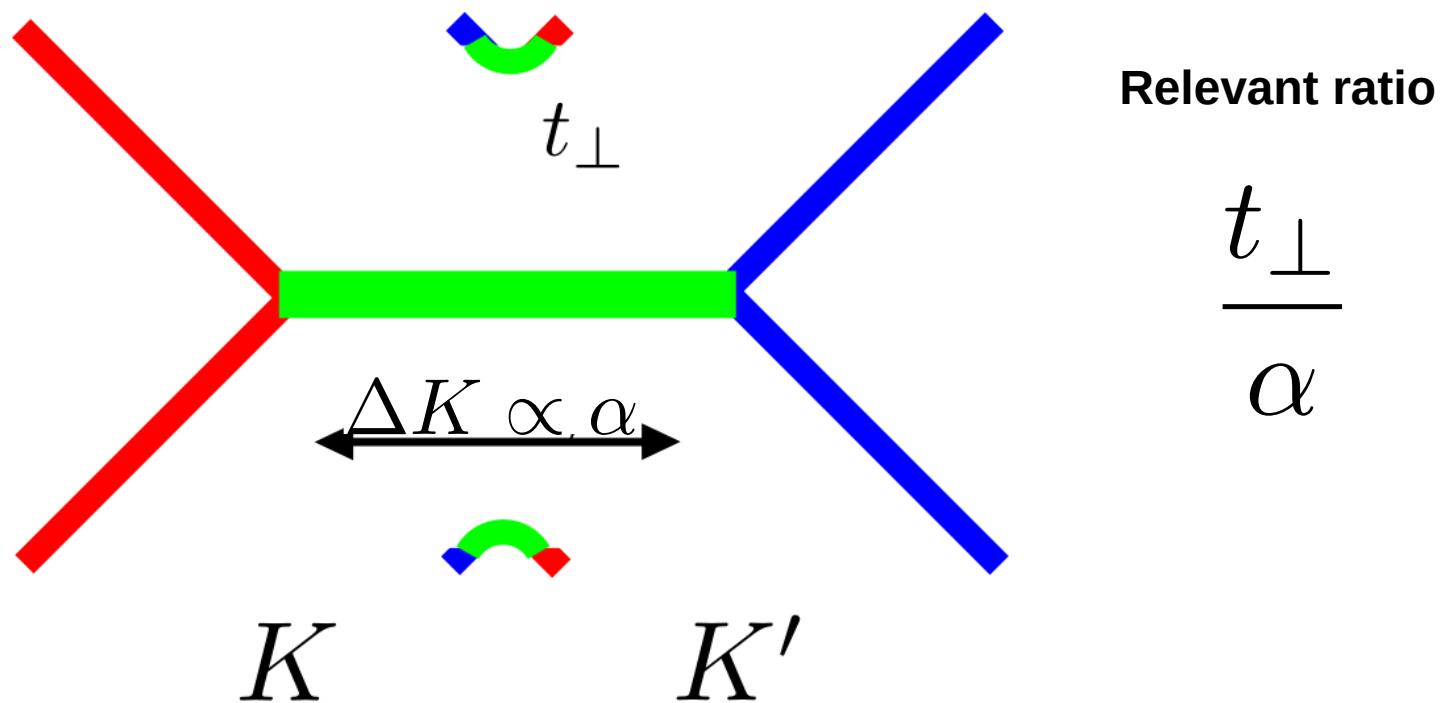
Velocity renormalization at large angle

$$\bar{v}_F/v_F = 1 - 9[t_\perp/v_F \Delta K]$$

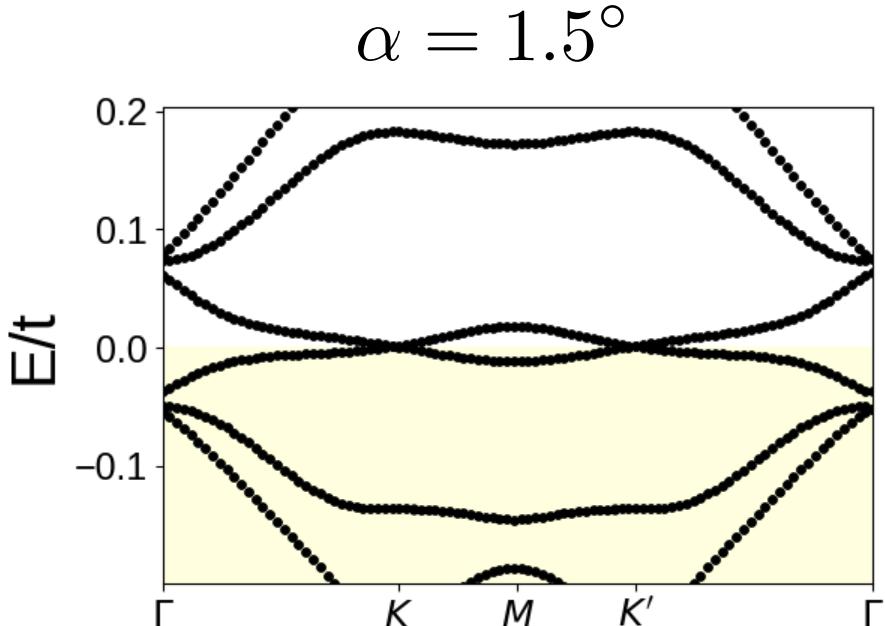
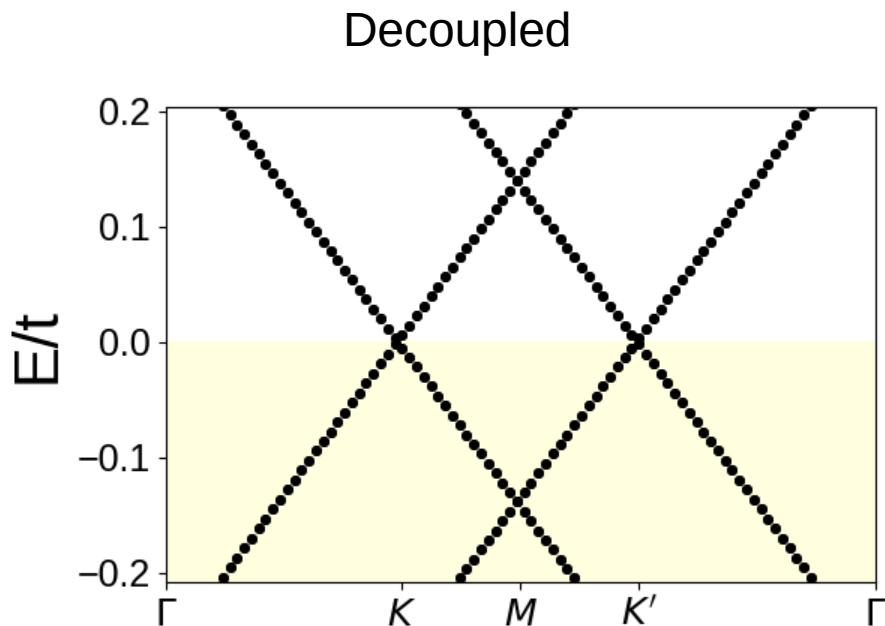


Velocity renormalization

$$\bar{v}_F/v_F = 1 - 9[t_\perp/v_F \Delta K]$$

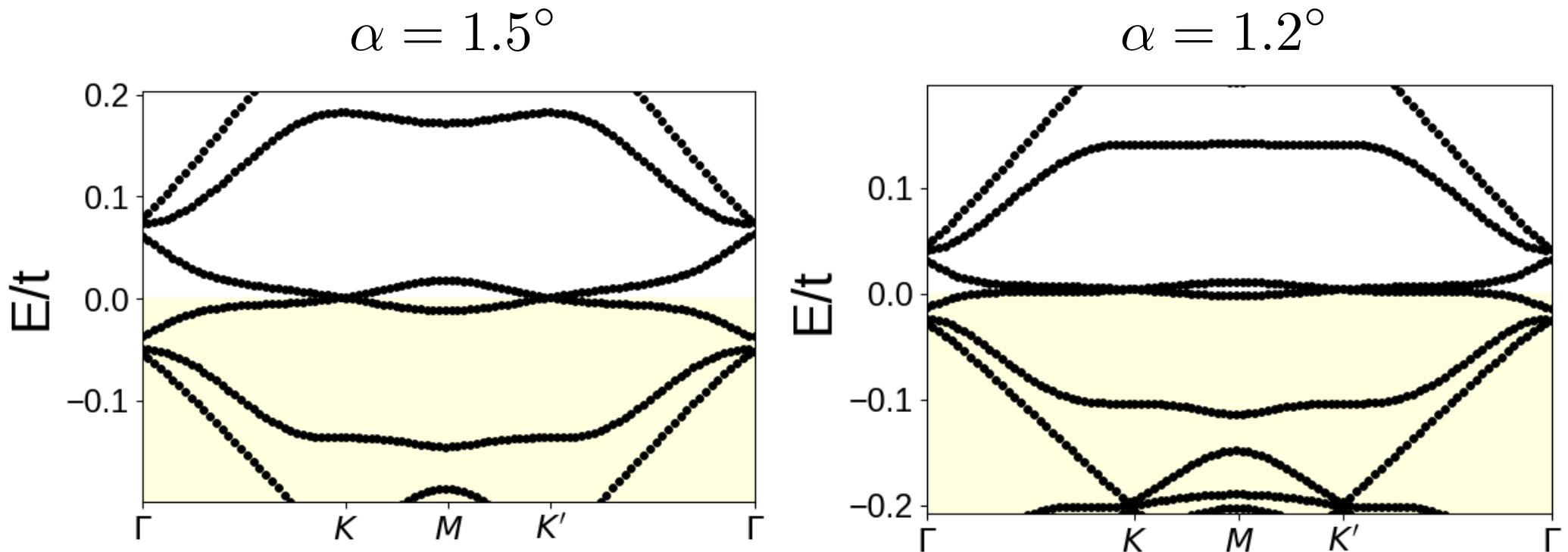


Band structure of twisted bilayer graphene



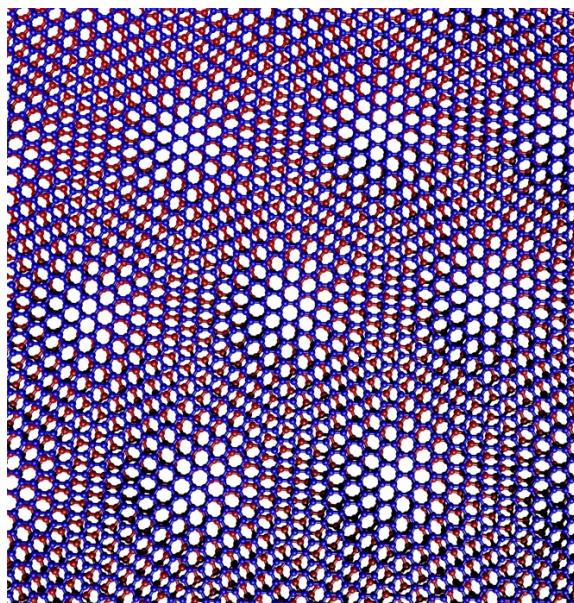
As the angle between layers is decreased, the bands become flatter

Band structure of twisted bilayer graphene

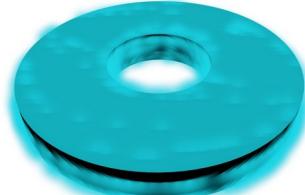


As the rotation angle approached 1 degree, the lowest band becomes flatter

Correlations in twisted bilayer graphene flat bands

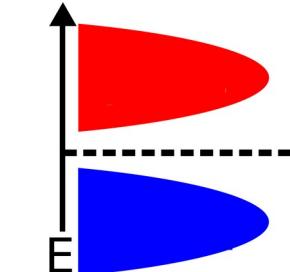


Superconductivity



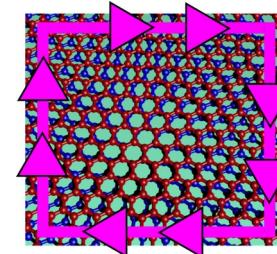
Nature 556, 43–50 (2018)

Correlated insulators



Nature 556, 80–84
(2018)

Chern insulators



Science 365, 605-608
(2019)

Fractional Chern insulators

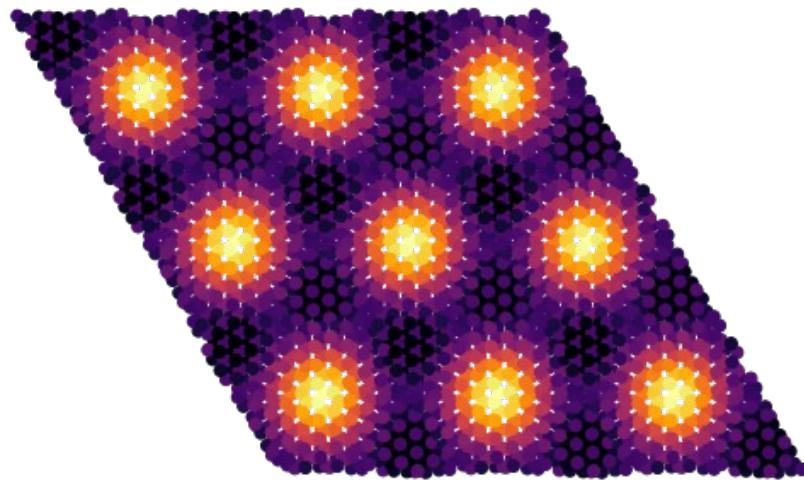


Nature 600, 439–443
(2021)

Correlated states in flat bands give rise to a wide variety of phenomena

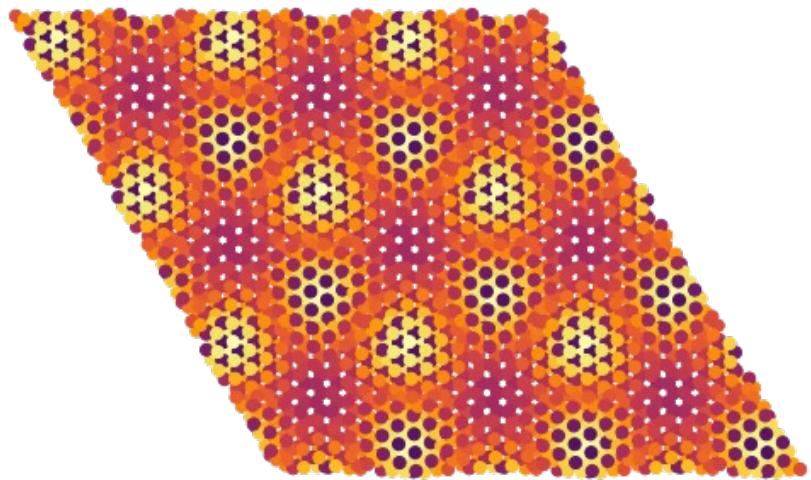
Distribution of states in the twisted graphene bilayer

$E = 0.0$



Triangular

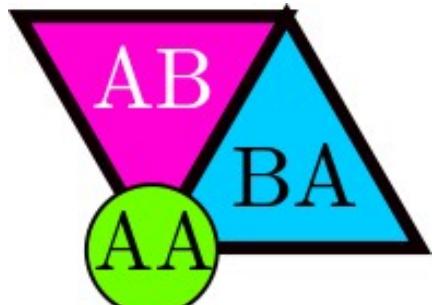
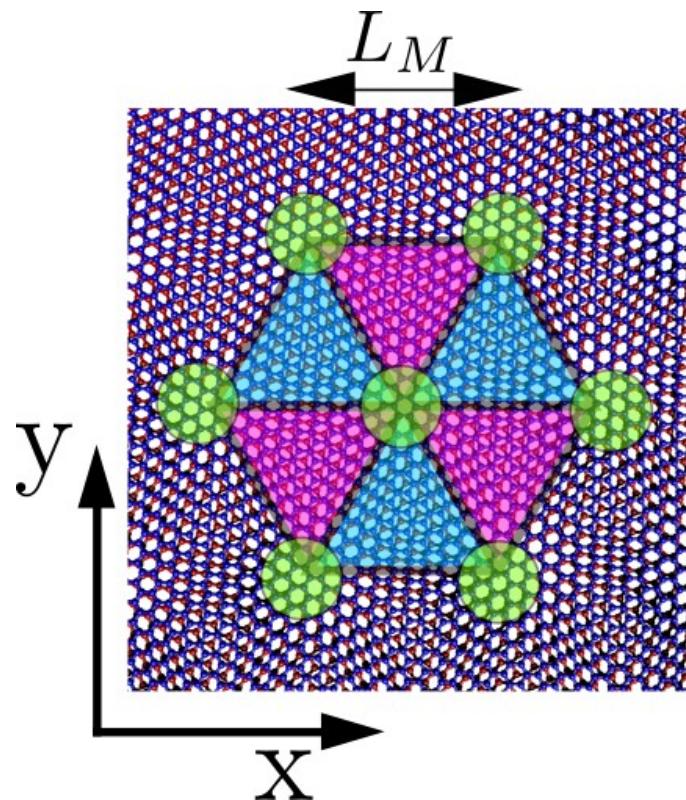
$E = 0.25$



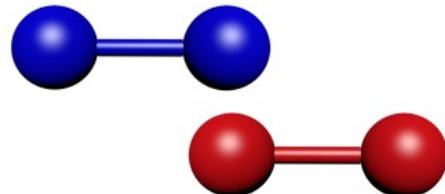
Hexagonal

The spatial distribution of the states is highly dependent on the energy

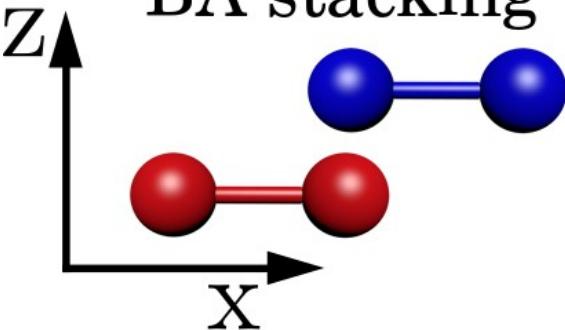
Stacking of twisted bilayer graphene



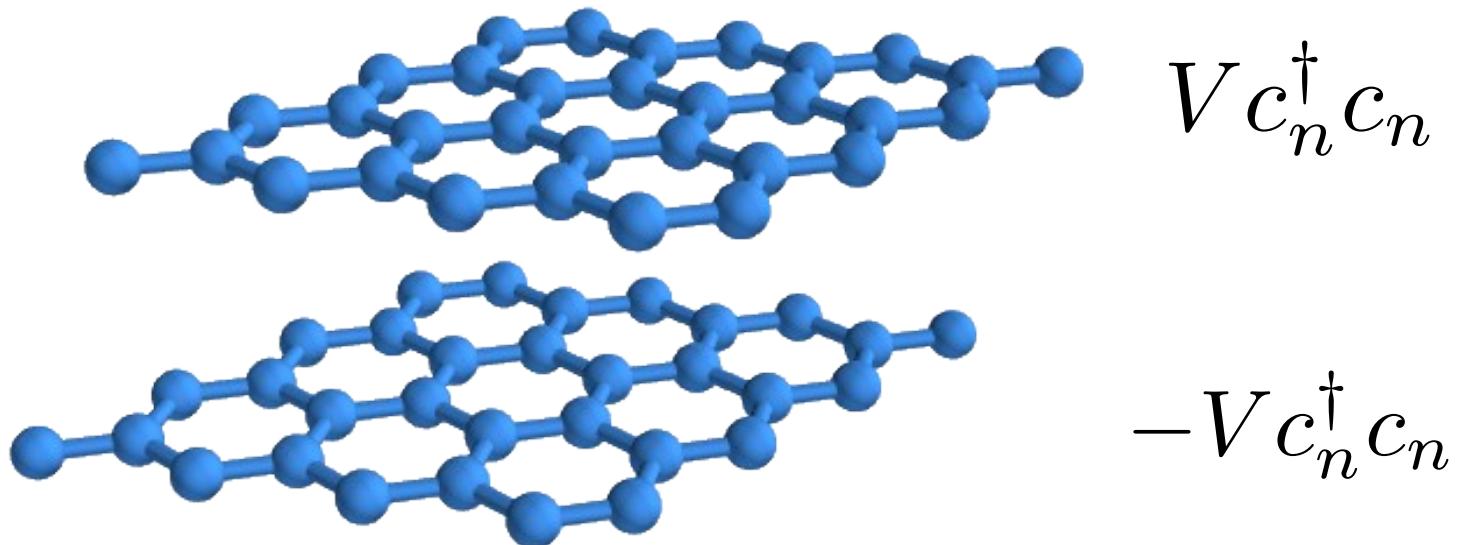
AB stacking



BA stacking



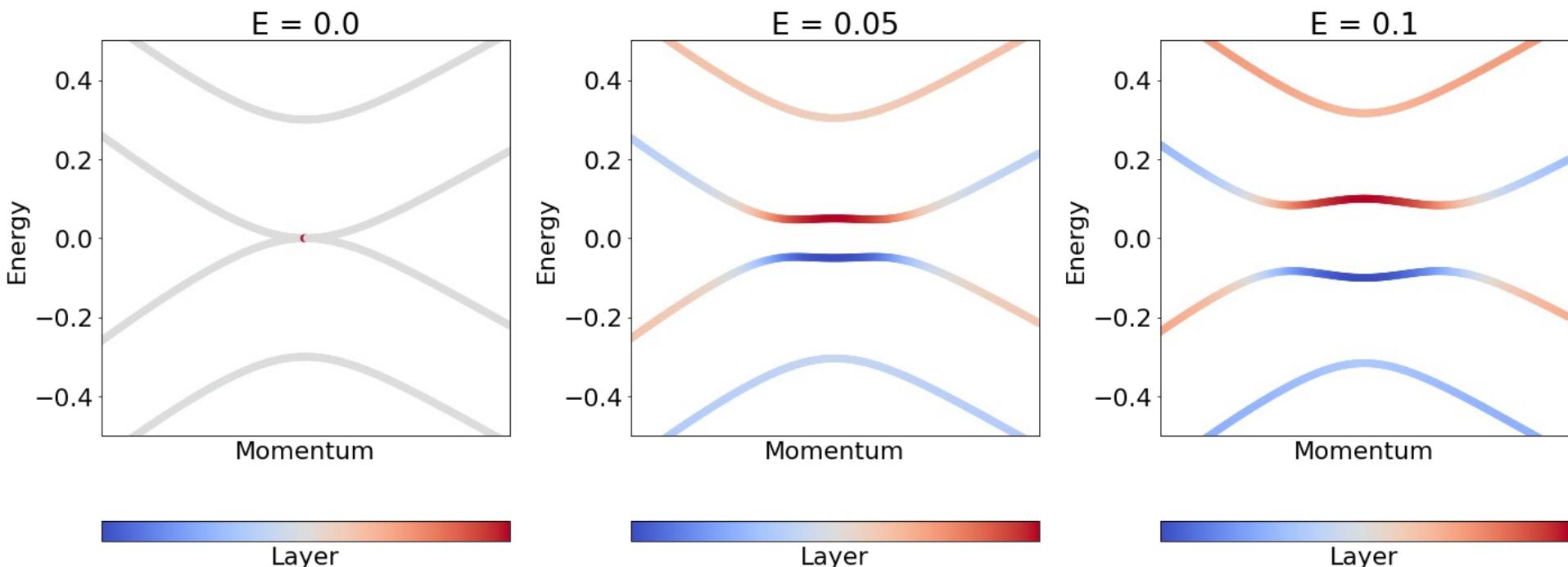
Bias in AB bilayer graphene



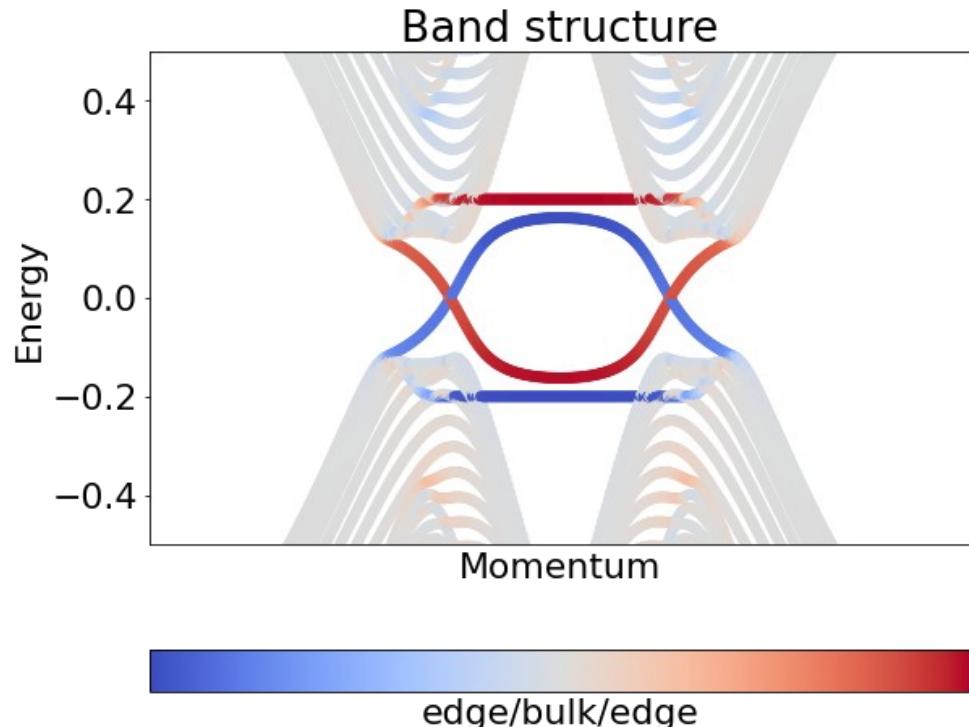
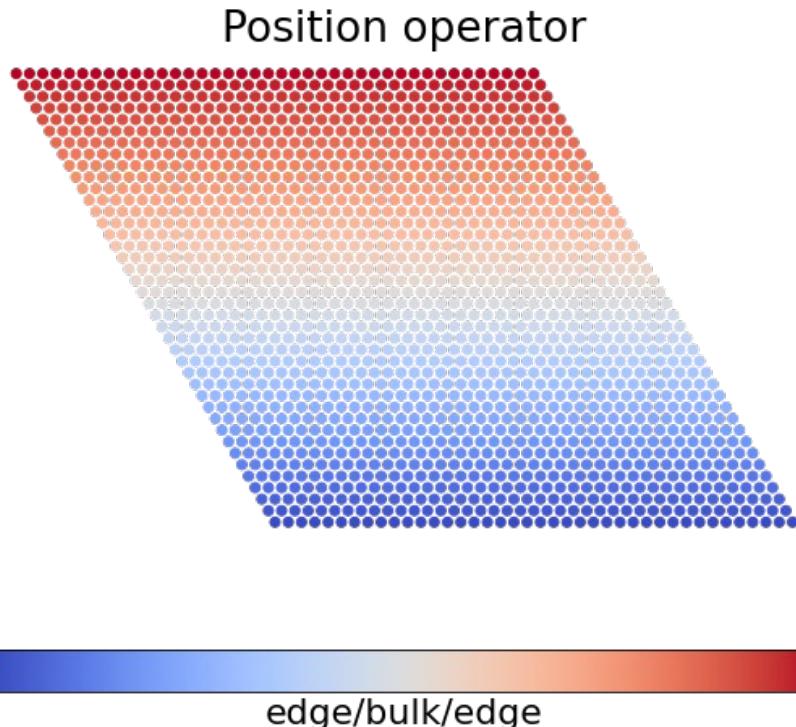
Let us look at the impact of a bias in an aligned graphene bilayer

The electronic structure of bilayer graphene

Graphene bilayers open a gap when an interlayer bias is applied

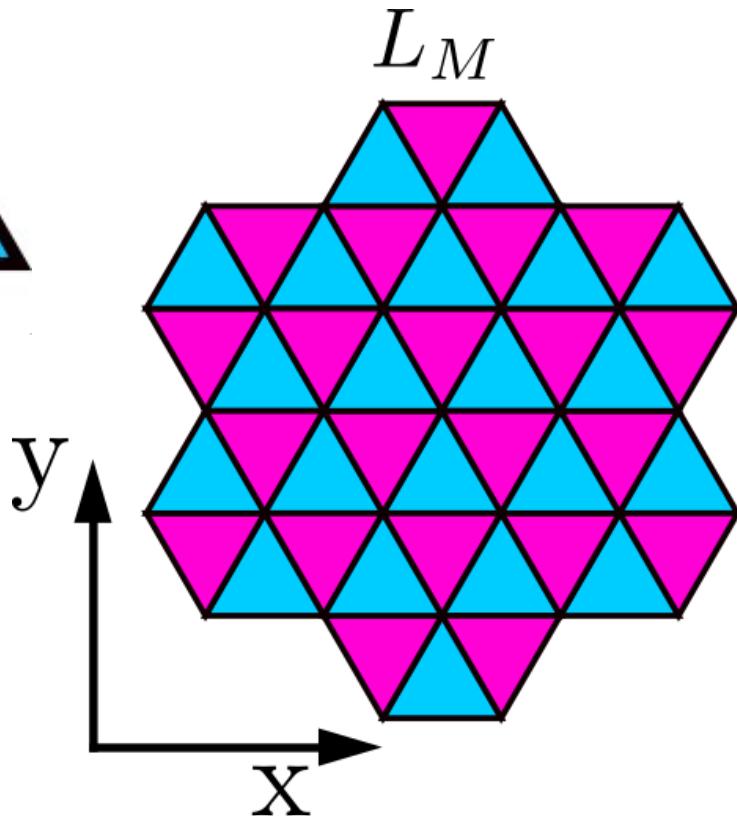
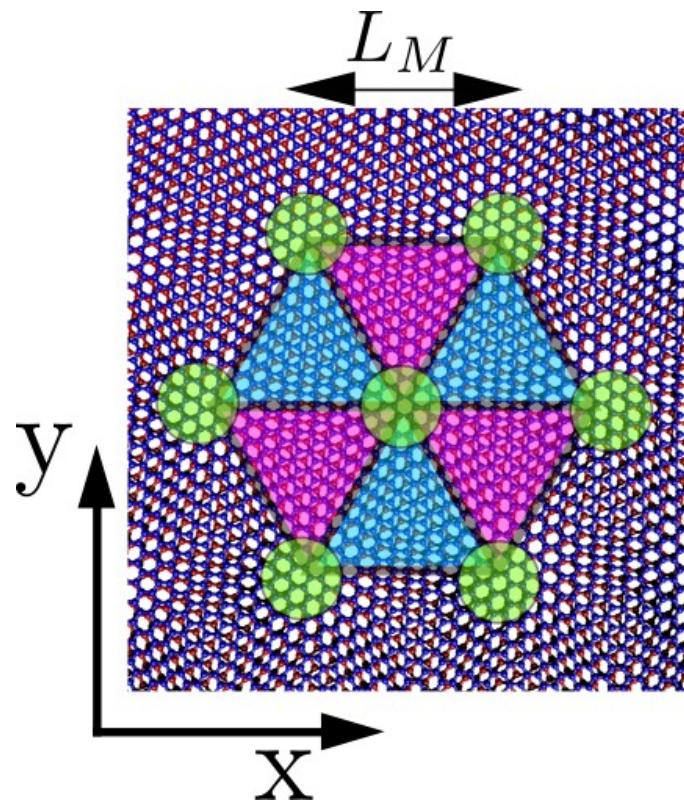


Biased bilayer graphene, pseudo-helical states

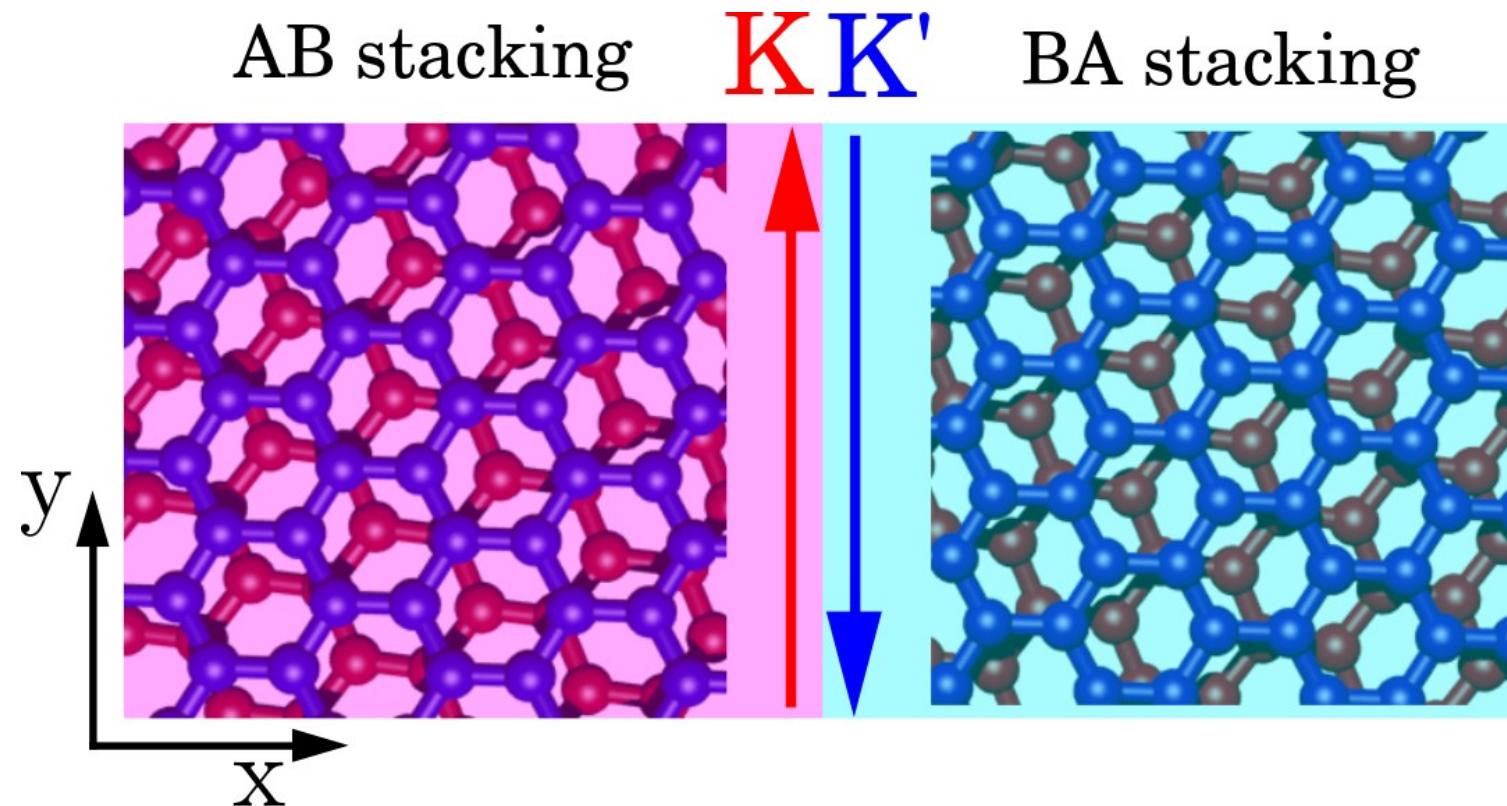


Edge states appear in the presence of a bias between layers

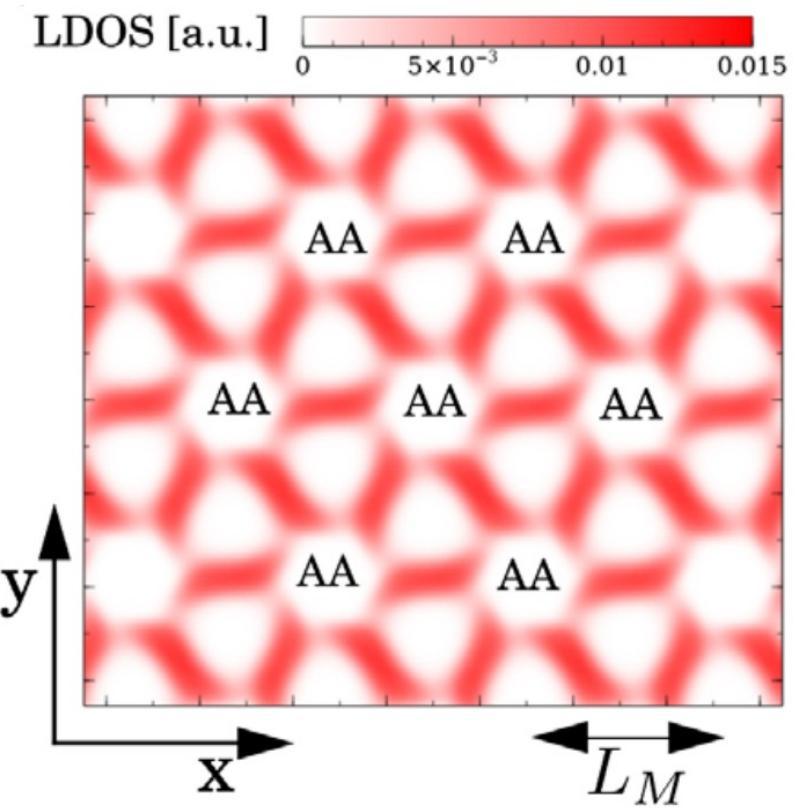
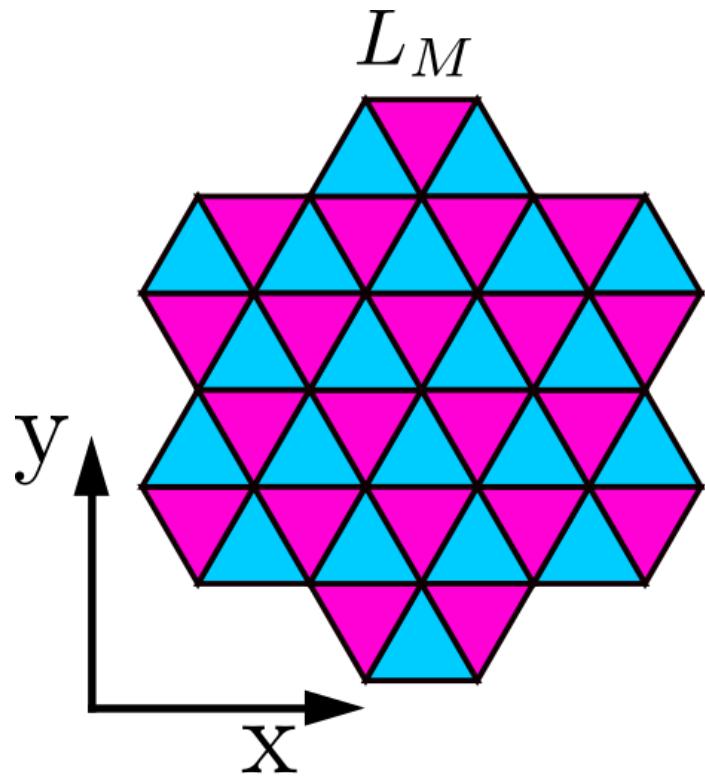
Stacking of twisted bilayer graphene



Interfacial modes in biased TBG

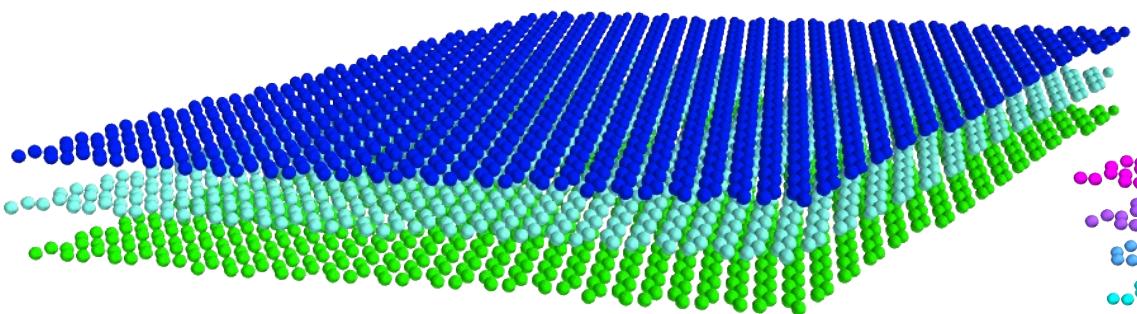


Helical networks in TBG

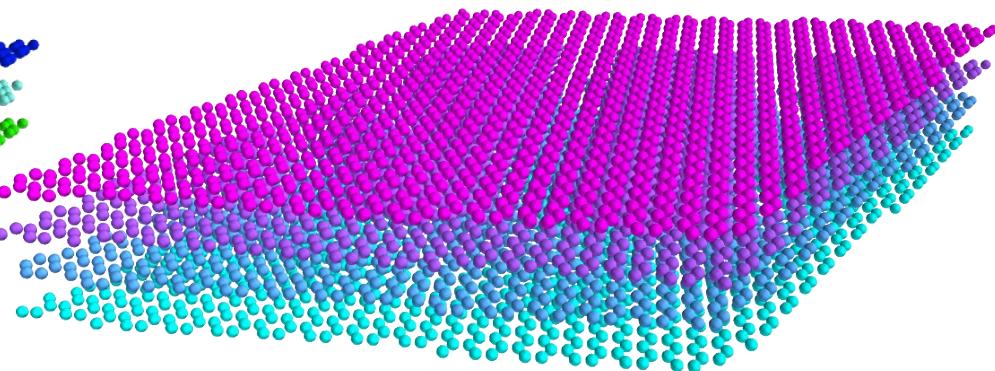


Other twisted graphene multilayers

Twisted graphene trilayer

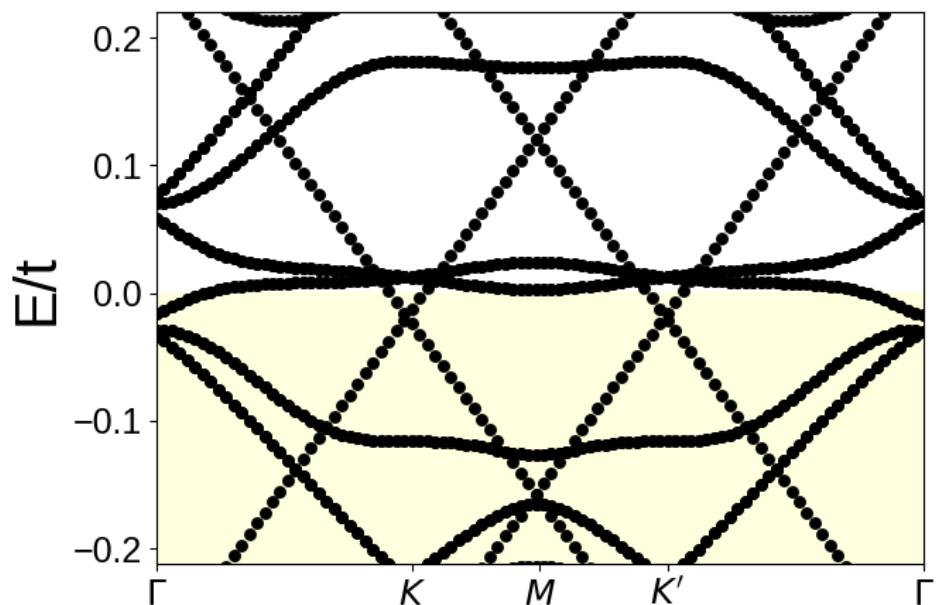


Twisted graphene double bilayer

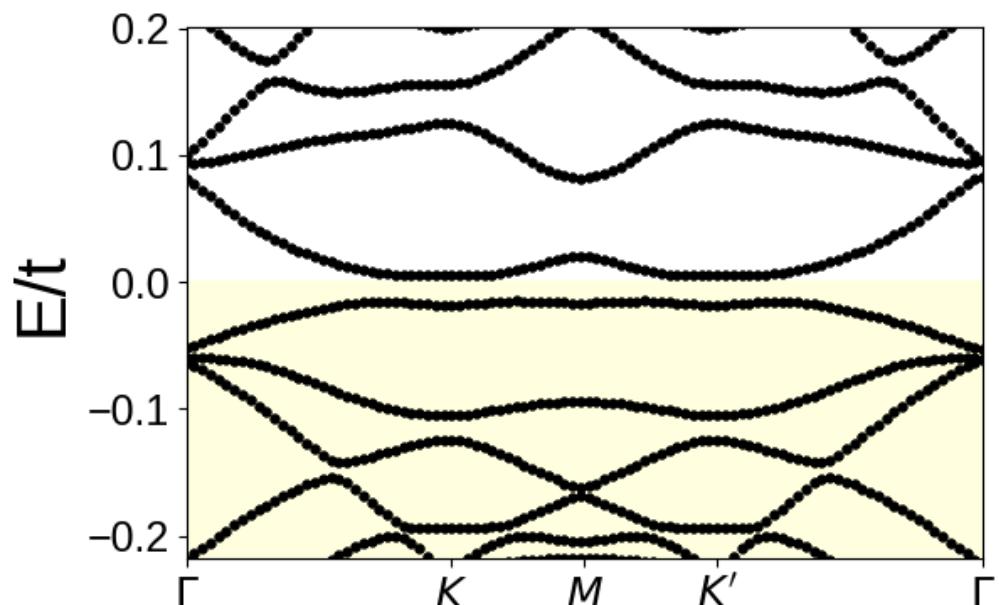


Other twisted graphene multilayers

Twisted graphene trilayer



Twisted graphene double bilayer



Flat and dispersive moire bands appear in generic twisted graphene multilayers

(Optional) Exercise session

Download the Jupyter-notebook from

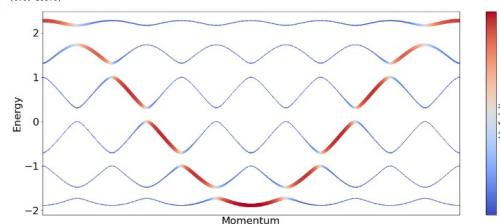
https://github.com/joselado/emergent_phenomena_in_van_der_Waals_school_tifr_2023

You will see examples with the code

```
In [17]: # let us now add an impurity in the previous supercell, and see how it leads to anticrossings in the bands
from pygula import geometry
g = geometry.Chain() # generate chain
h = g.get_hamiltonian()
g = g.get_supercell(N=store_primal=True) # generate a supercell, store_primal is required for unfolding
g = g.get_hamiltonian() # and generate the Hamiltonian

# let us define a potential for an impurity
r0 = np.array([0,0,0])
fpot = lambda r: 1.0*((r-r0).dot(r-r0)<=2) # impurity in site r0
# from pygula import potentials
# fpot = potentials.lennard_jones(r0=v+1.) # this is equivalent

h.add_potential(fpot) # now add the impurity potential
kpath = g.get_kpath() # compute in the original Brillouin zone, just by extending the reciprocal vectors
(k,e,c) = h.get_bandoperator("unfold",kpath=kpath) # compute band structure
plt.figure(figsize=(5,5)); plt.xlabel("Momentum"); plt.ylabel("Energy"); plt.xticks([]); plt.yticks([-2,-1,0,1,2])
plt.colorbar(label="Unfolding", ticks=[-2,-1,0,1,2])
plt.xlim([min(k),max(k)])
Out[17]: (0.0, 399.0)
```



You can modify them, and answer questions

Exercise

- Change the size of the supercell. Do the anticrossings appear at the same energies?
- If the strength of the impurity becomes very large, what happens to the electronic structure? Discuss why it has the behavior observed

