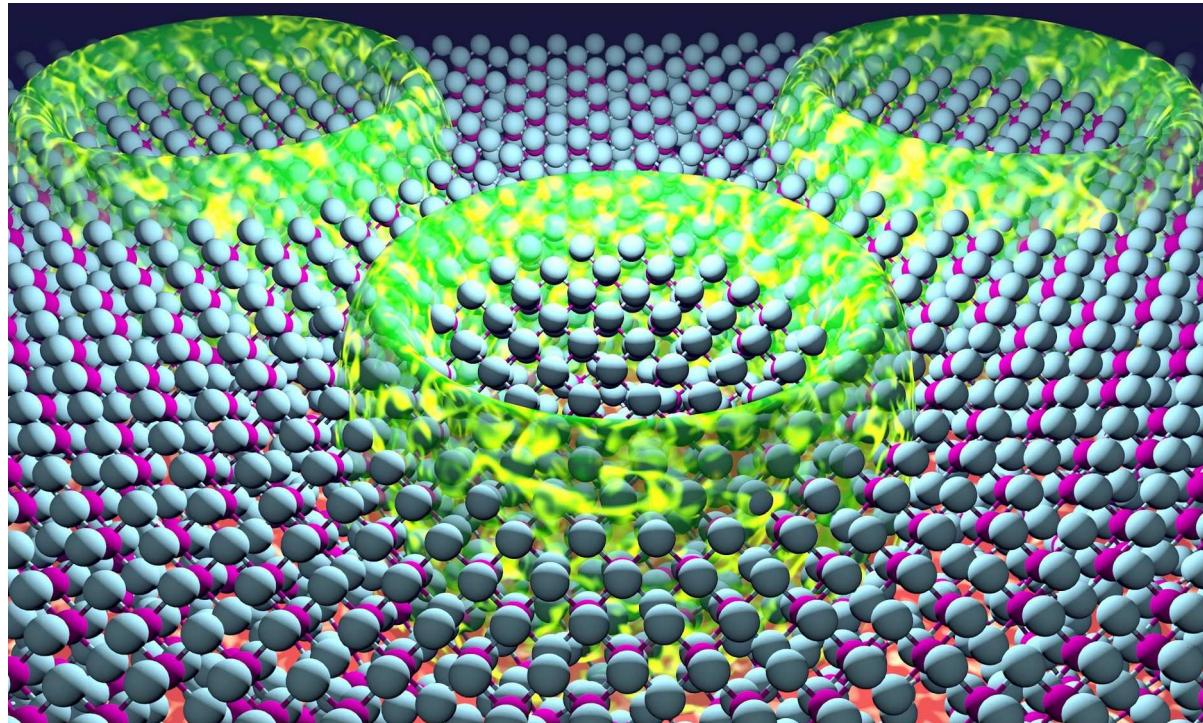


# Lecture 3: Moire electronic states and twisted van der Waals heterostructures



*Pedagogical School “Emergent phenomena in van der Waals heterostructures”*

January 7<sup>th</sup> 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

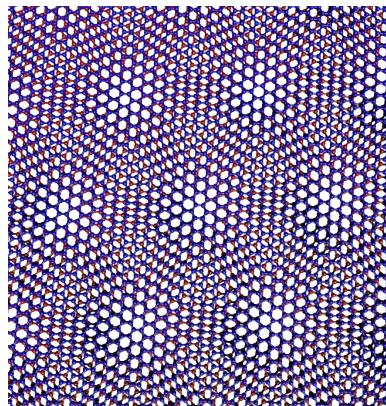
*You can download the slides and software from*

[https://github.com/joselado/emergent\\_phenomena\\_in\\_van\\_der\\_Waals\\_school\\_tifr\\_2023](https://github.com/joselado/emergent_phenomena_in_van_der_Waals_school_tifr_2023)

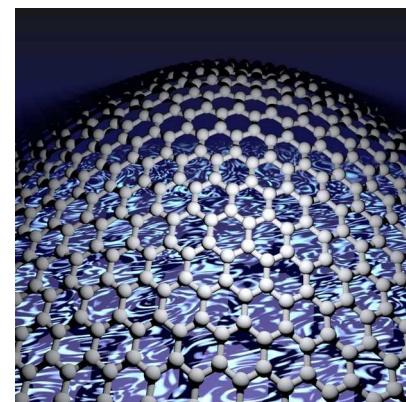


# Moire materials

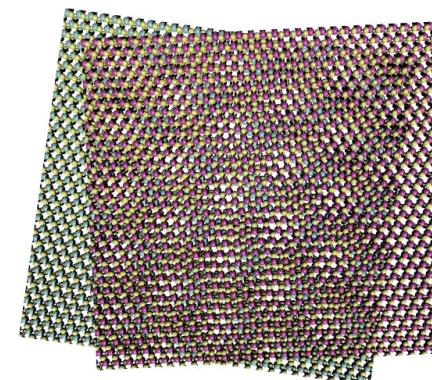
Twisted graphene multilayers



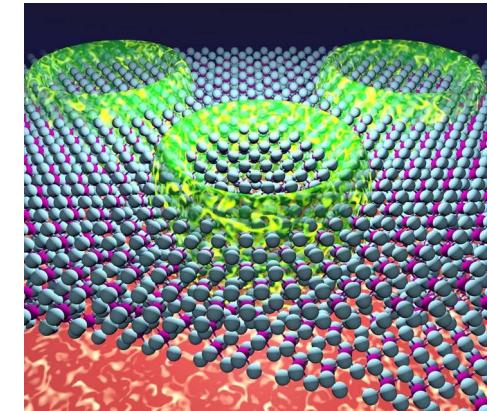
Buckled 2D materials



Twisted TMDCs



Twisted magnetic 2D materials



Moire states in several layers

graphene

Moire states in single layer

***Moire in electronic properties***

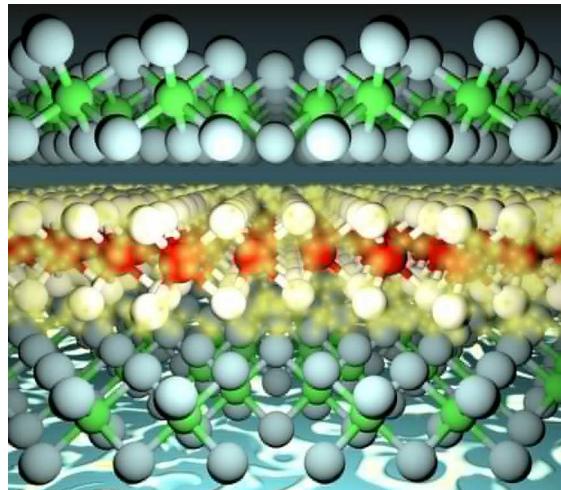
MoS<sub>2</sub>, WSe<sub>2</sub>  
Moire states in single/several layer

CrCl<sub>3</sub>, CrBr<sub>3</sub>  
Moire magnetism

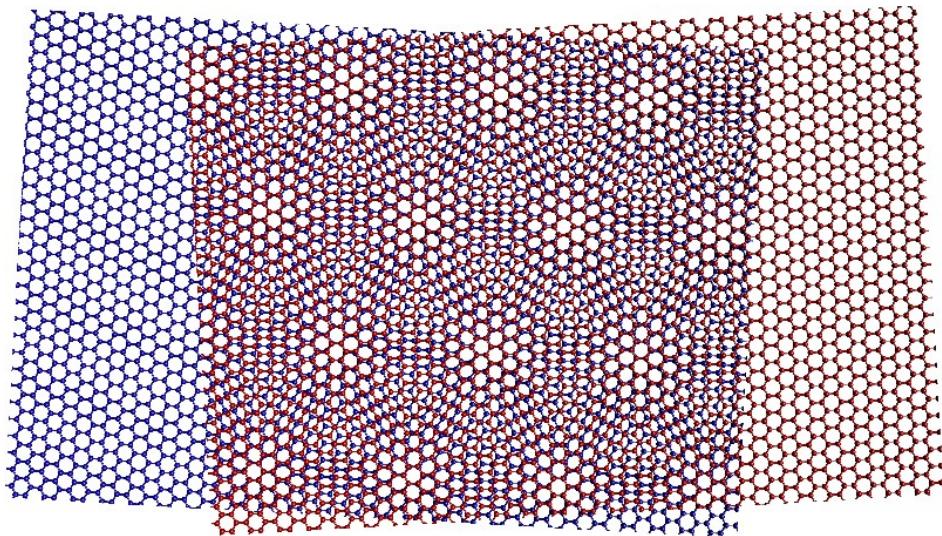
***Moire in magnetic properties***

# How to create moire states with 2D materials

**Stacking**



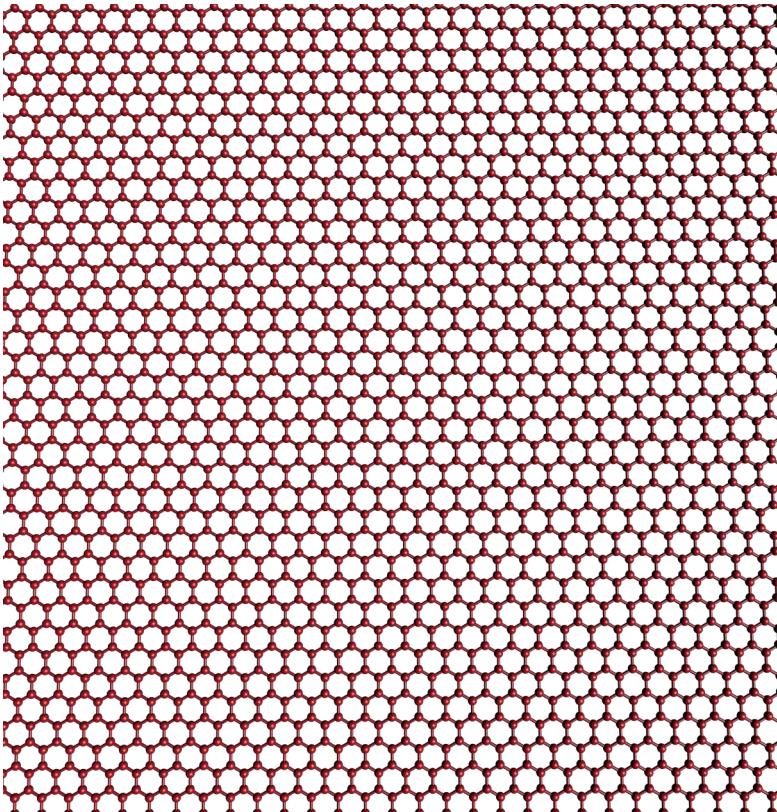
**Rotating**



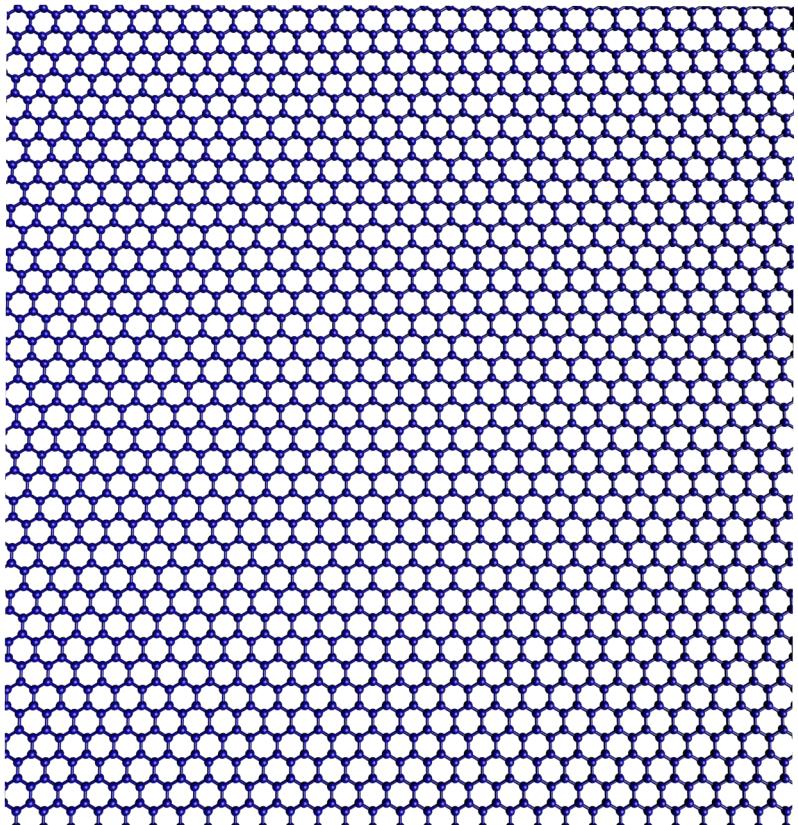
**These are unique features of two-dimensional materials**

# A bilayer van der Waals heterostructure

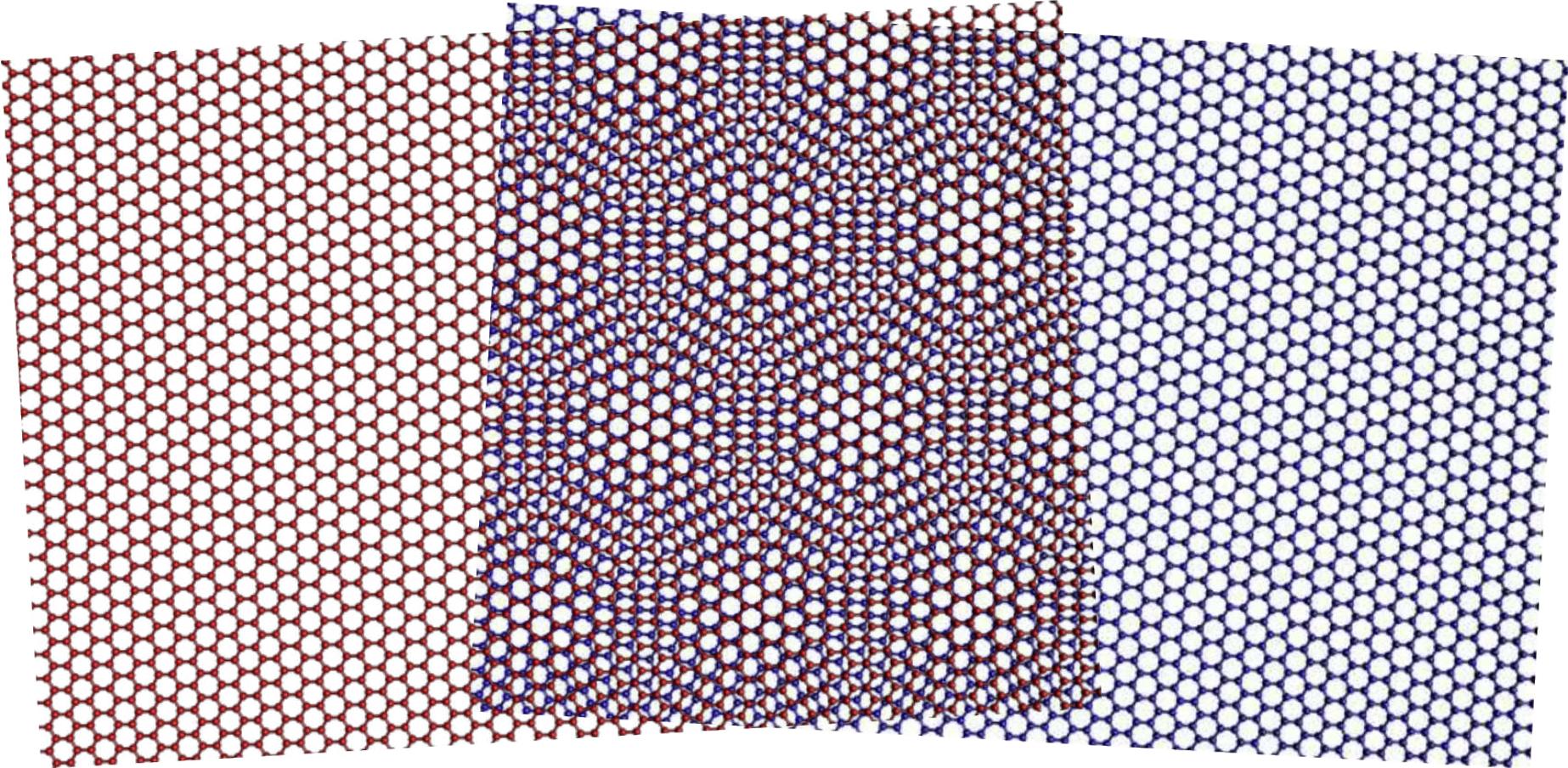
Upper graphene layer



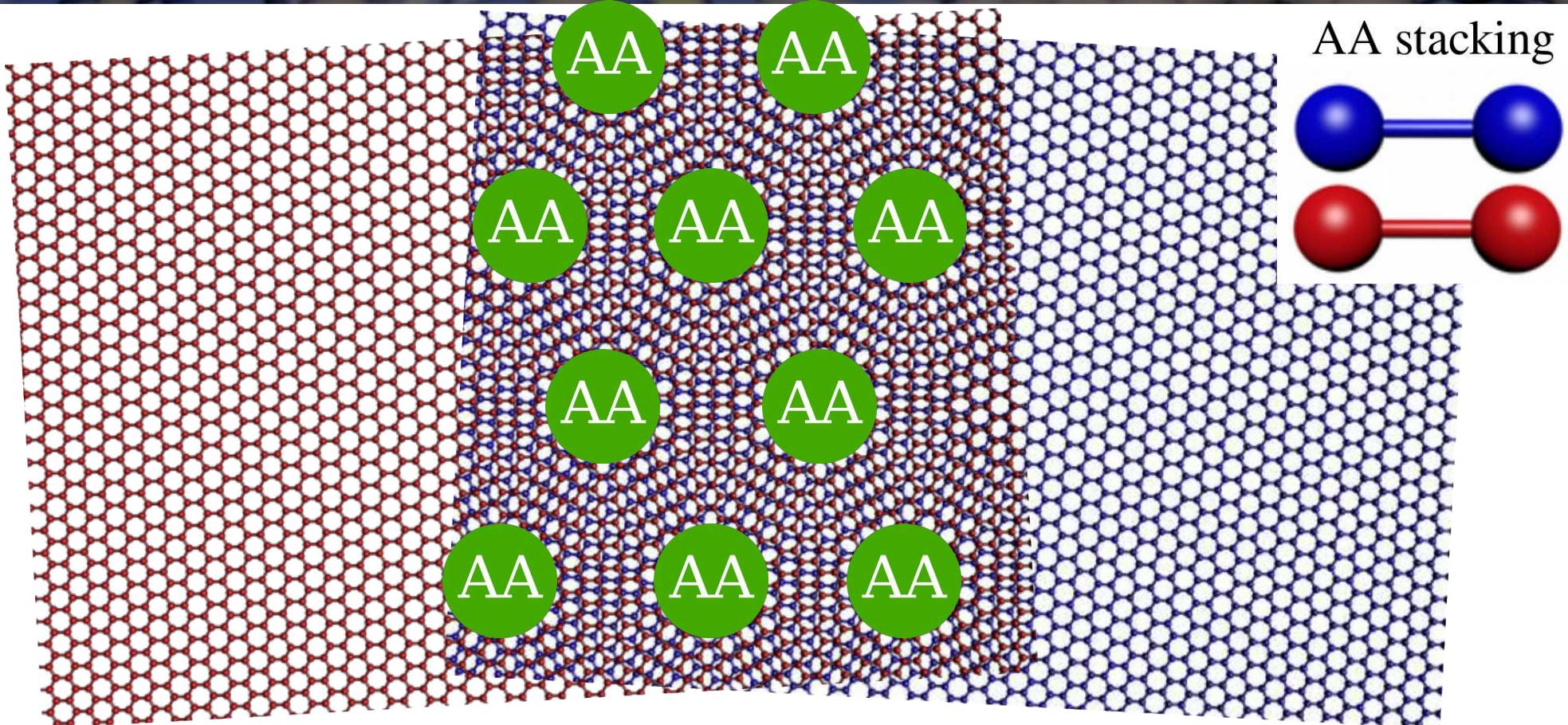
Lower graphene layer



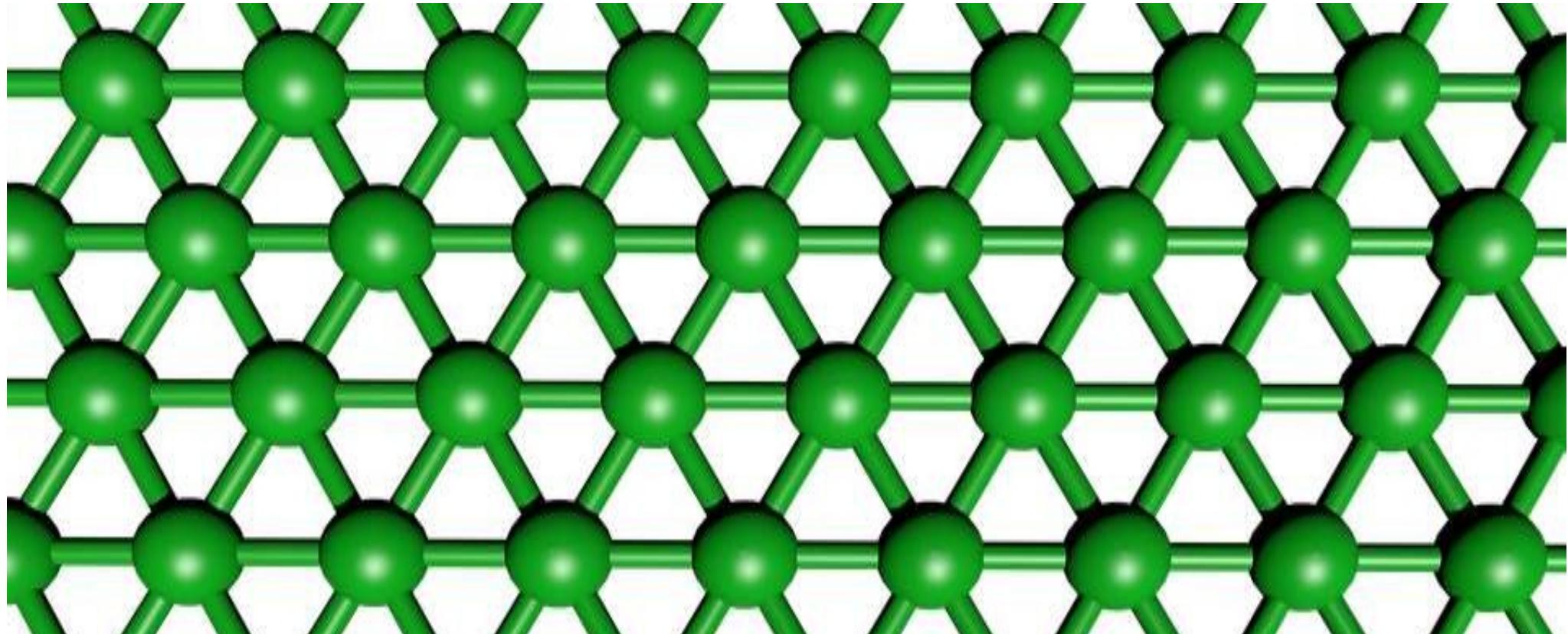
# A bilayer van der Waals heterostructure



# A bilayer van der Waals heterostructure

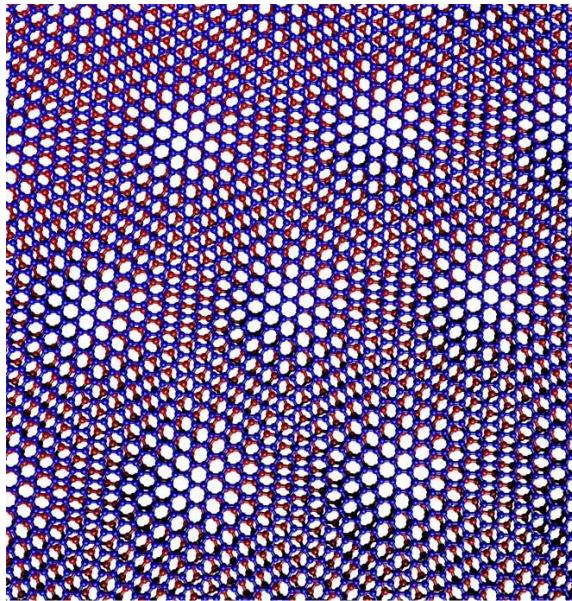


# A bilayer van der Waals heterostructure

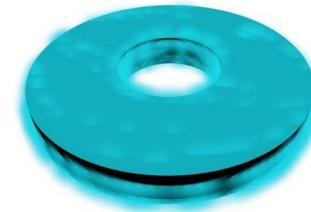


# Electronic states in a single moire superlattice

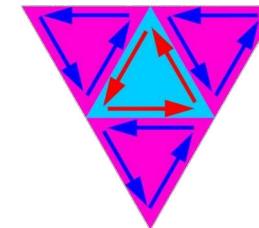
*Twisted bilayer graphene*



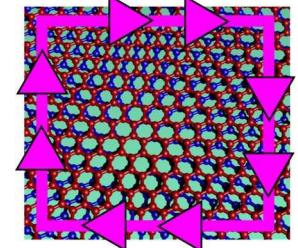
*Superconductivity*



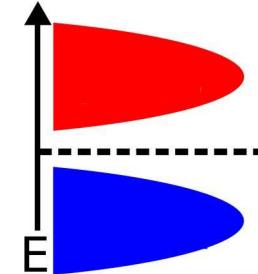
*Topological networks*



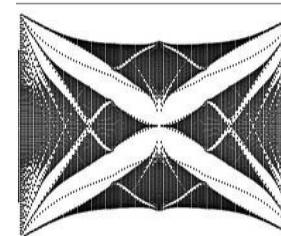
*Chern insulators*



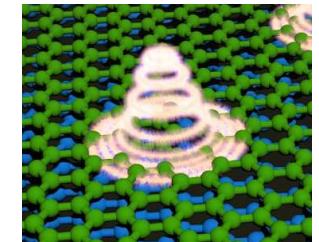
*Correlated insulators*



*Quasicrystalline physics*



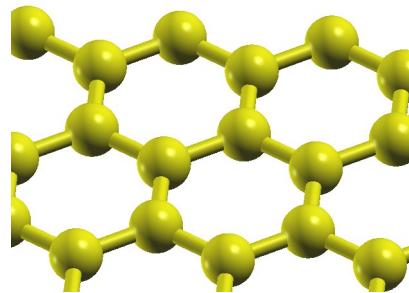
*Fractional Chern insulators*



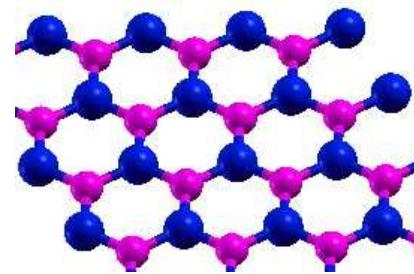
*A single twisted van der Waals material realizes a variety of widely different electronic states*

# The building blocks for twisted van der Waals heterostructure

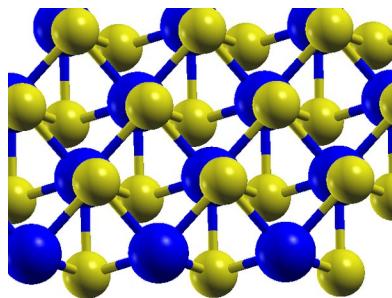
Semimetal  
Graphene



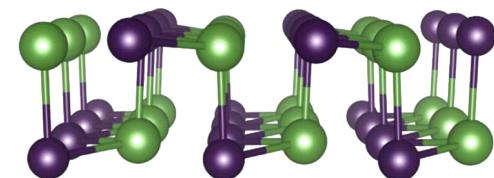
Insulator  
BN



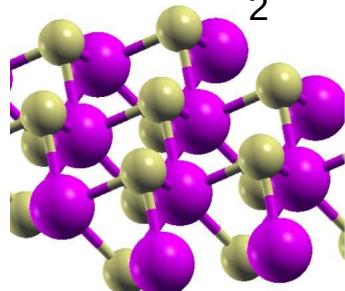
Superconductor  
 $\text{NbSe}_2$



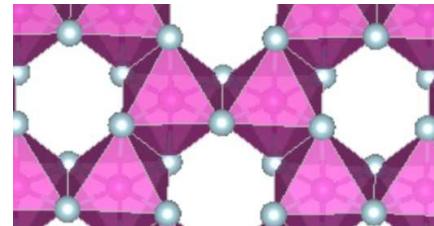
Ferroelectric  
 $\text{SnTe}$



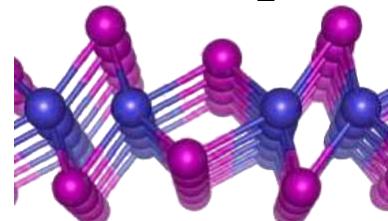
Semiconductor  
 $\text{WSe}_2$



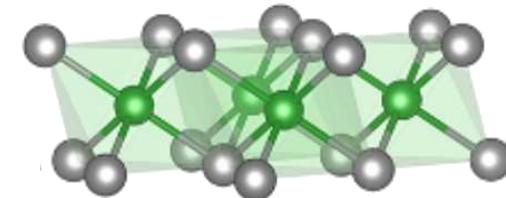
Ferromagnet  
 $\text{CrI}_3$



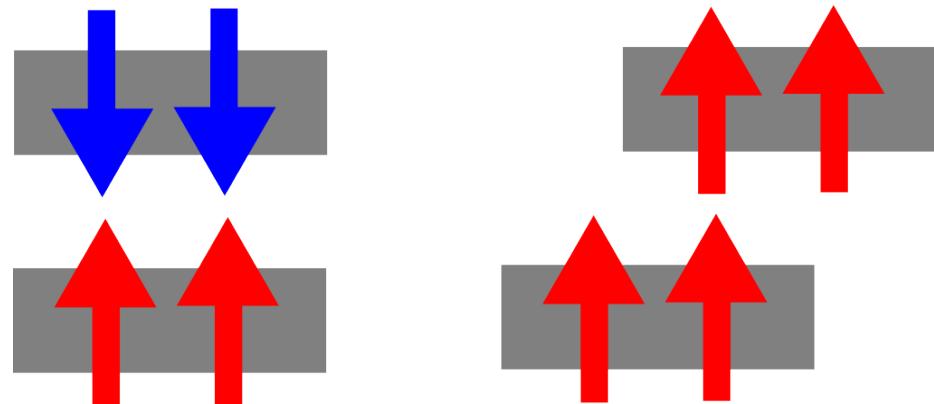
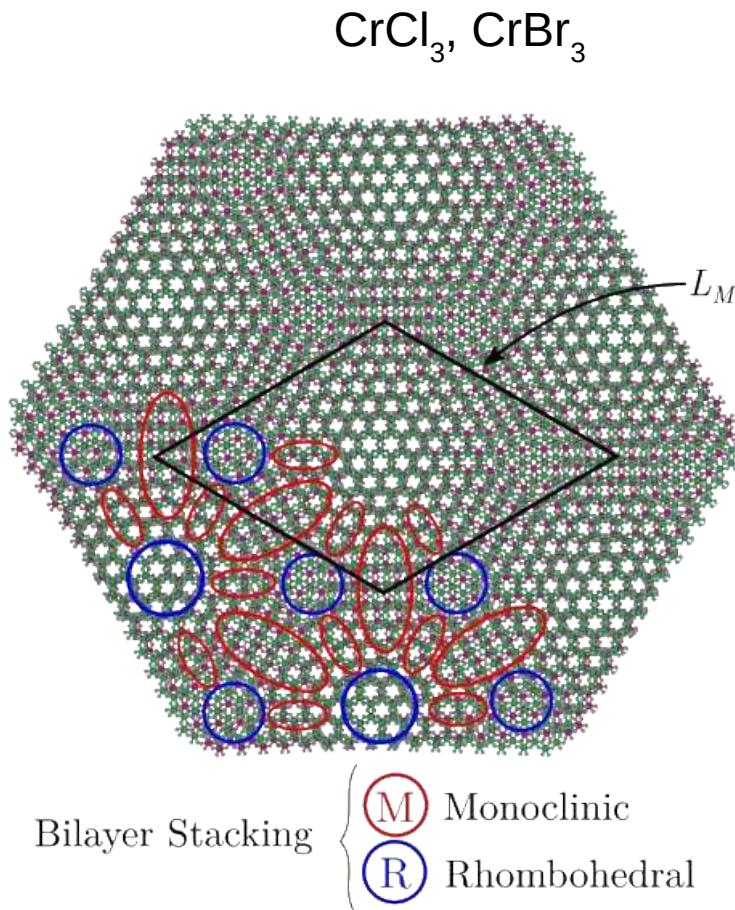
Quantum spin  
Hall insulator  
 $\text{WTe}_2$



Multiferroic  
 $\text{NiI}_2$



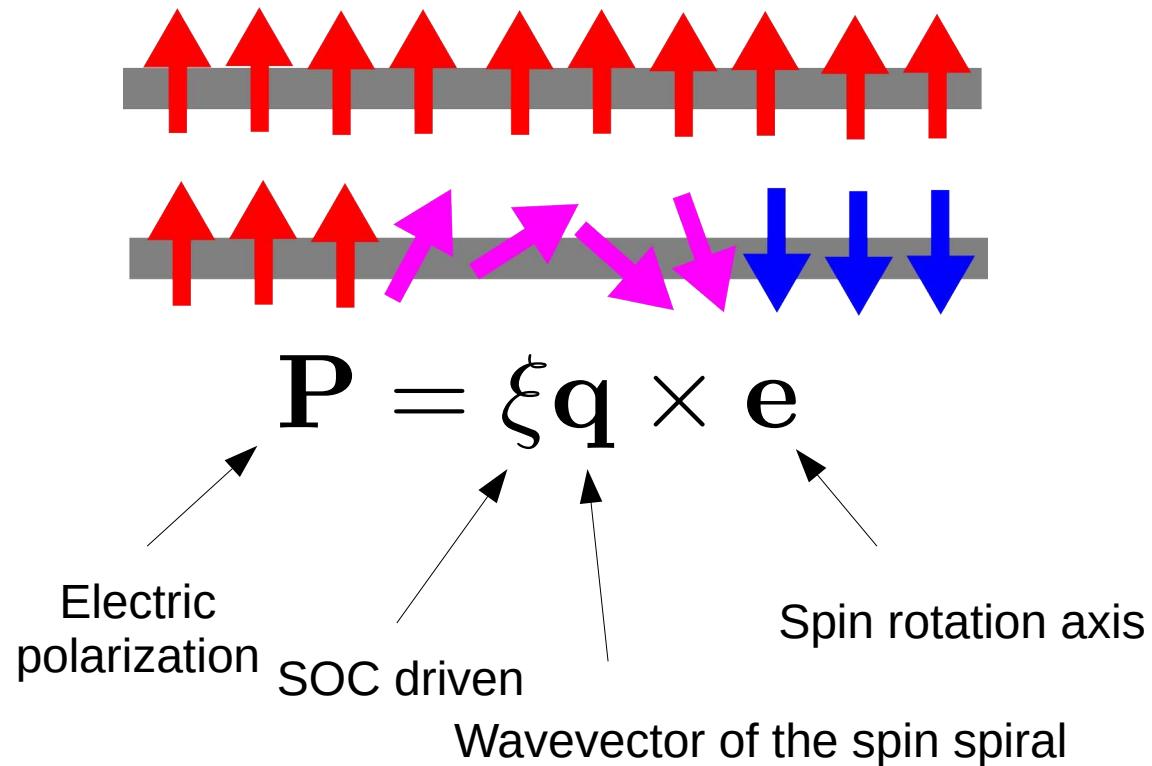
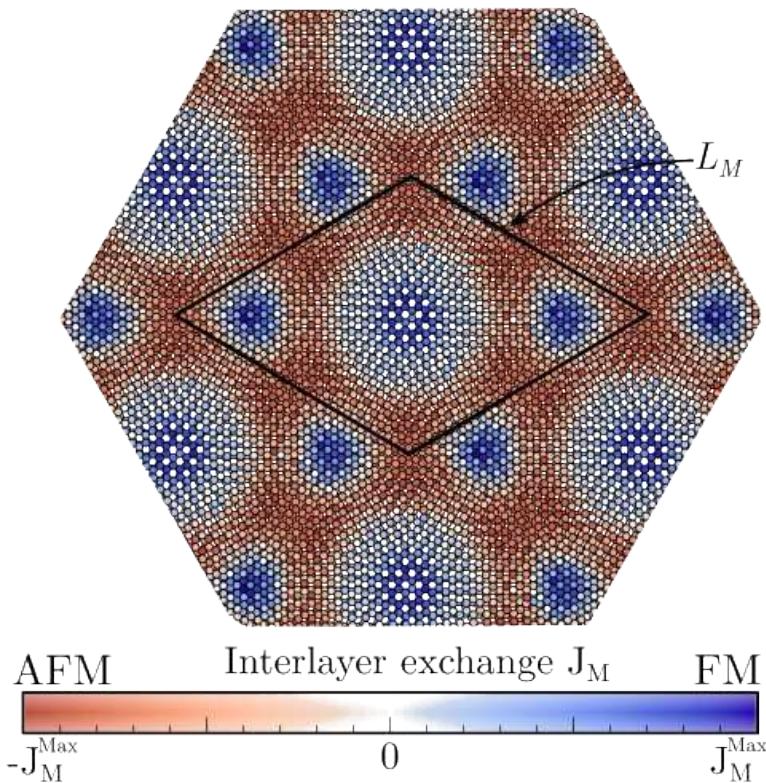
# Twisted 2D magnetic materials



The local stacking determines the coupling between layers

# Twisted 2D magnetic materials

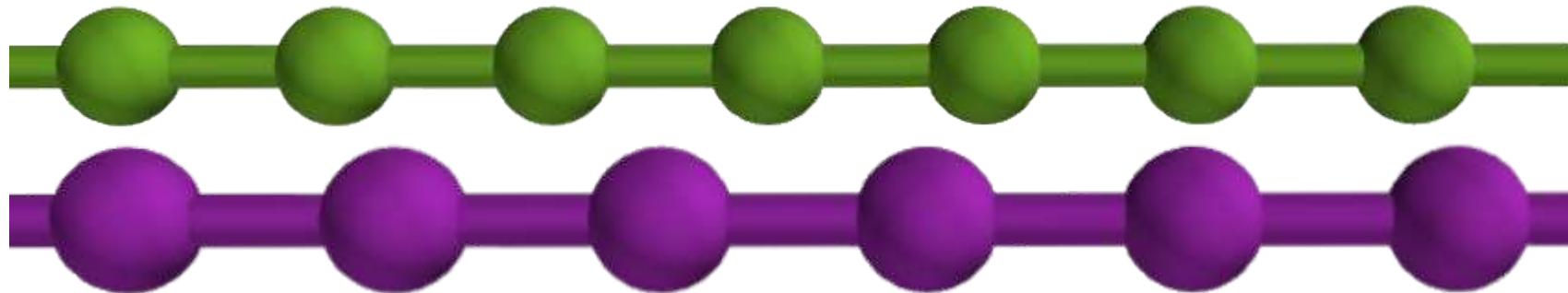
Non-collinear magnetism and multiferroic order appear due to the moire



# Superpotentials and quasiperiodicity

# A minimal moire potential

Let us now take a one dimensional superlattice



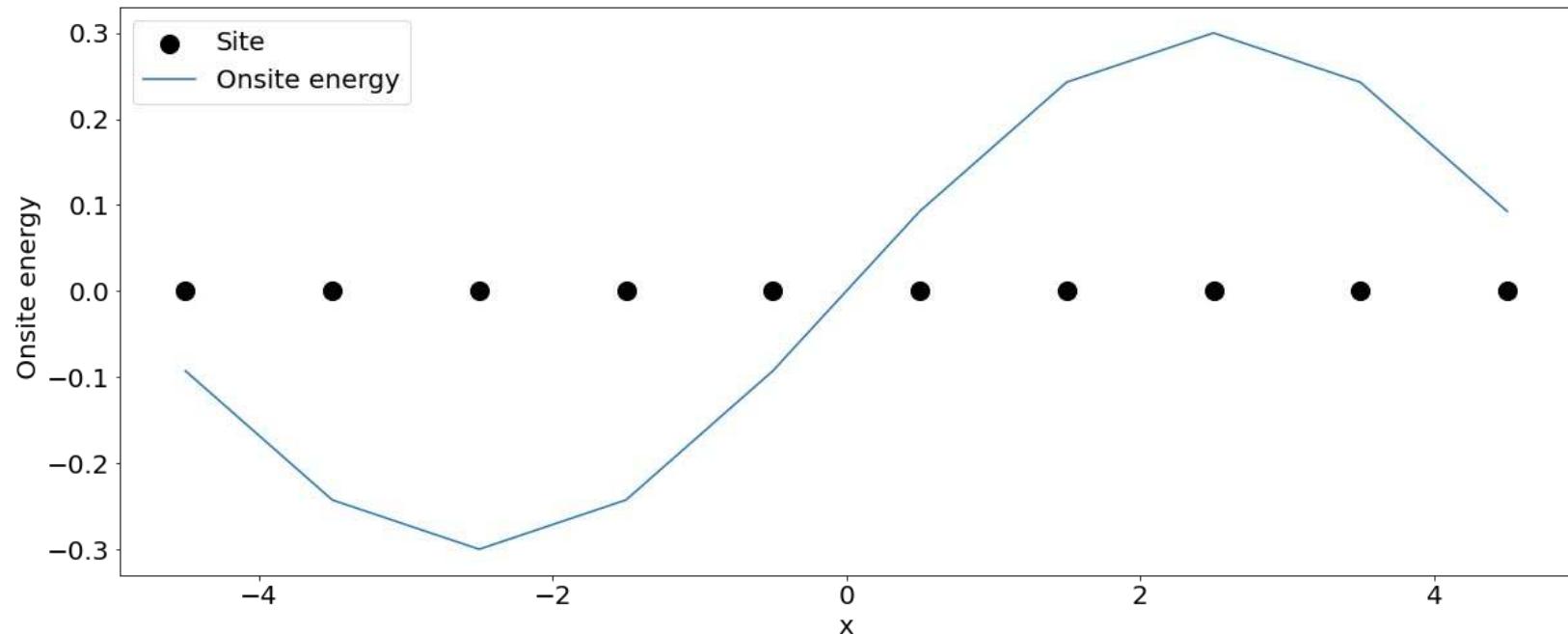
We have now two length scales

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

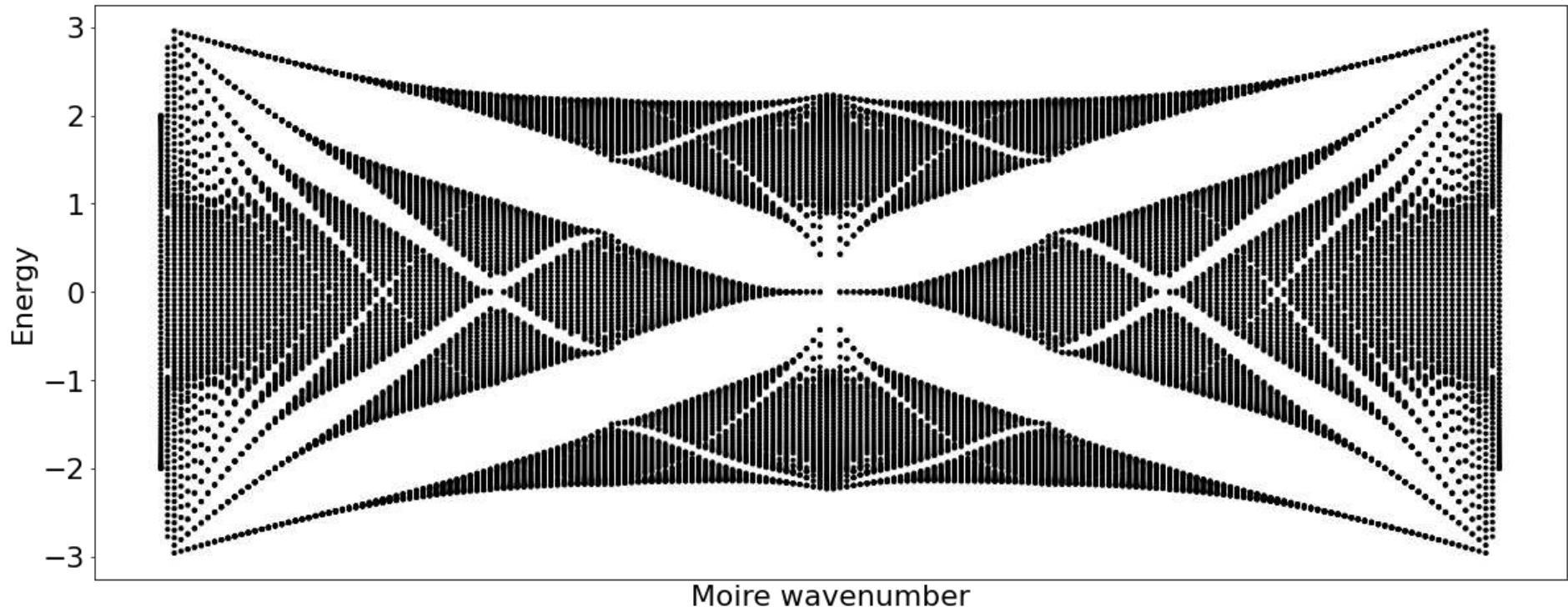
Let us see how the electronic structure gets modified by the superlattice effect

# A minimal moire potential

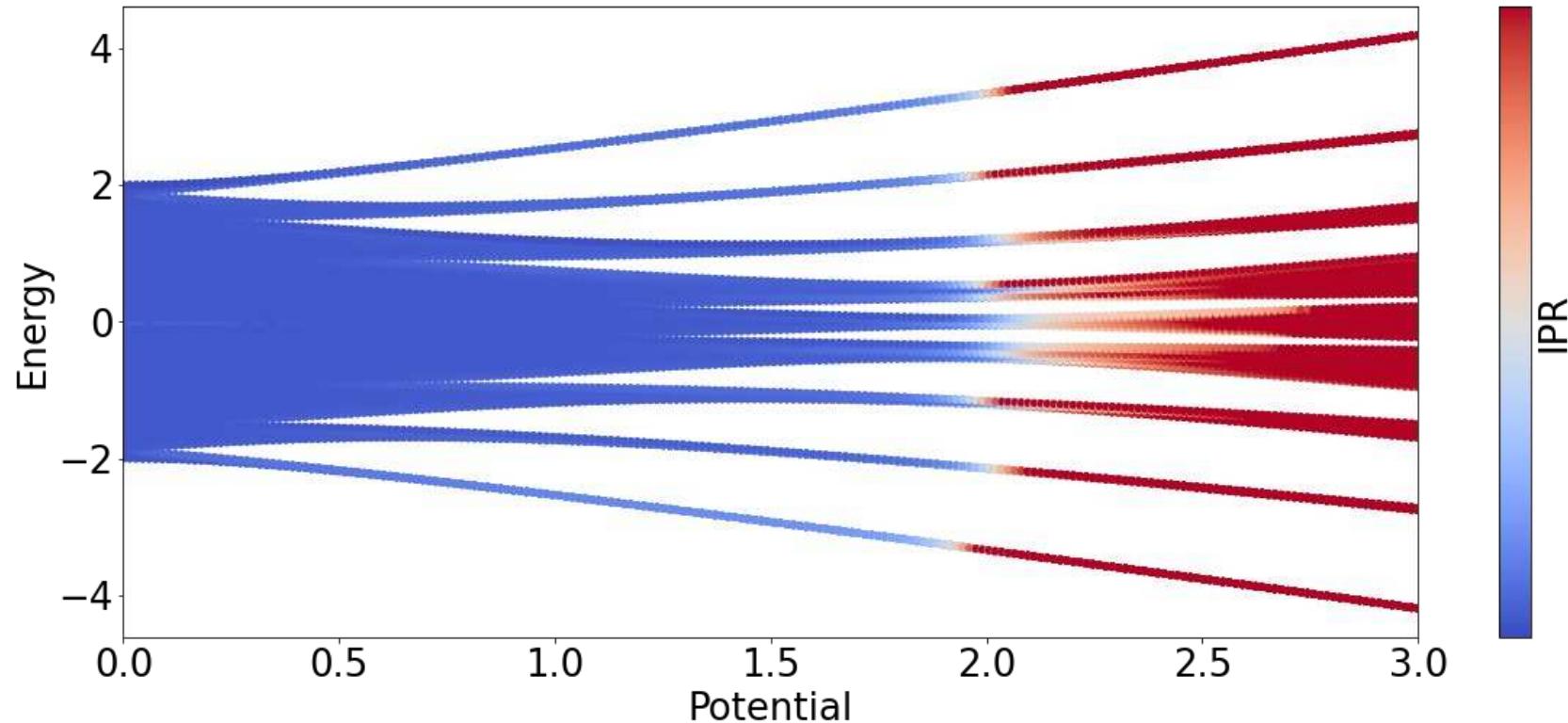
$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + \lambda \sum_n \cos(qn) c_n^\dagger c_n$$



# Spectrum as a function of the moire wavevector



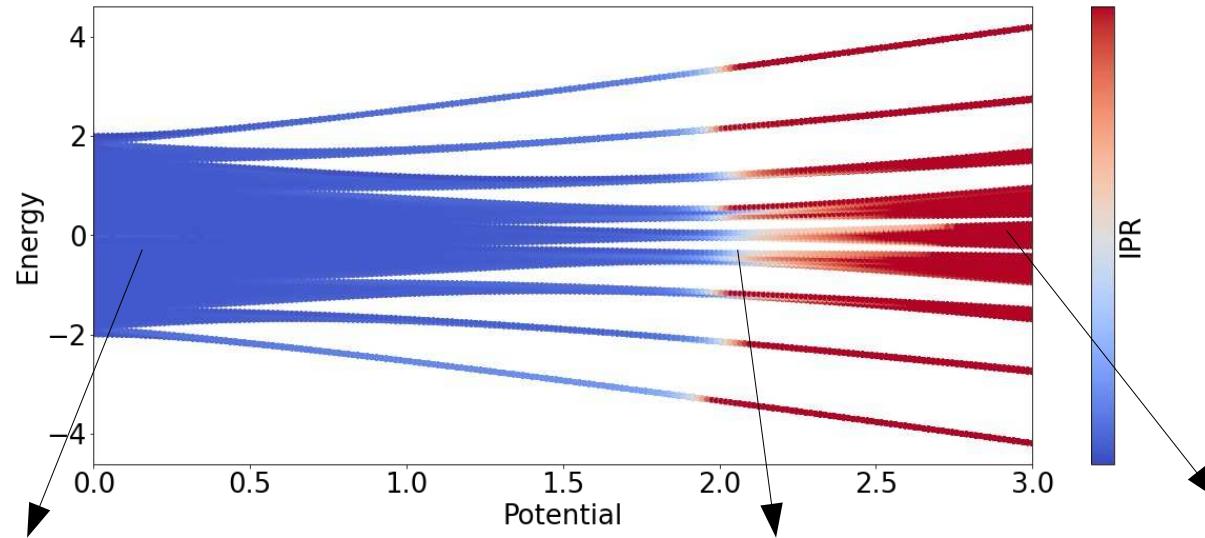
# Superpotentials and criticality



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

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

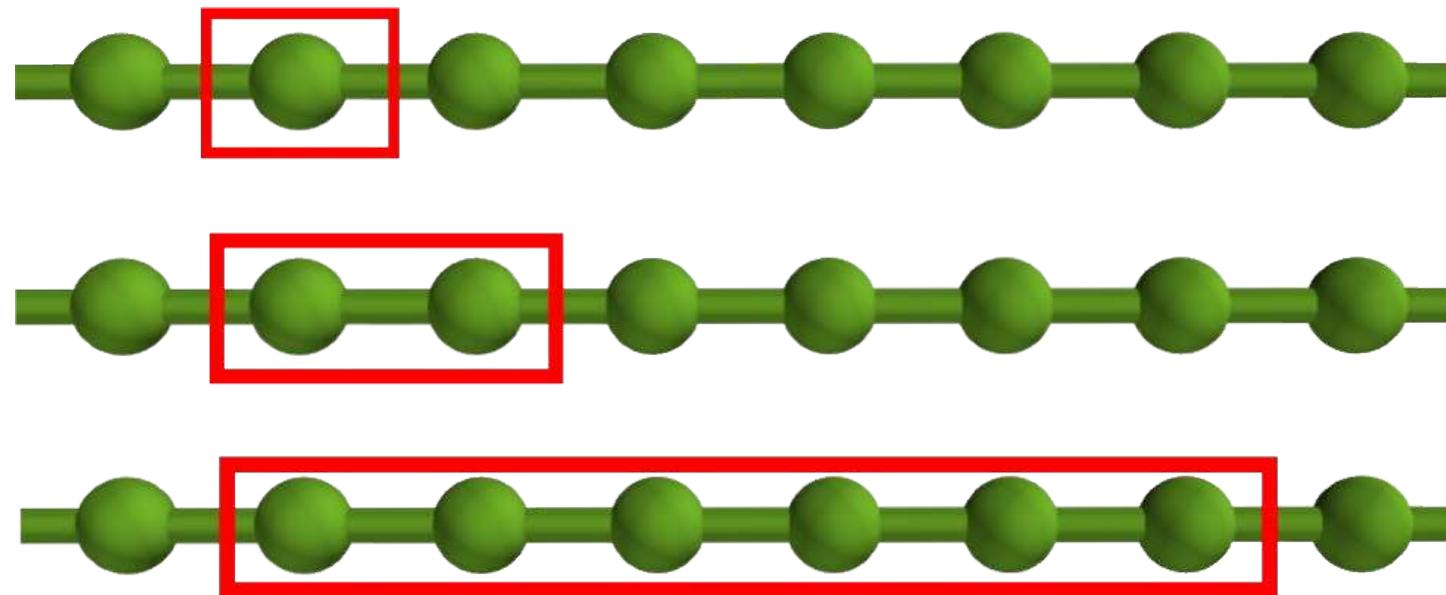
# Minibands and band structure unfolding

# Supercells and band folding

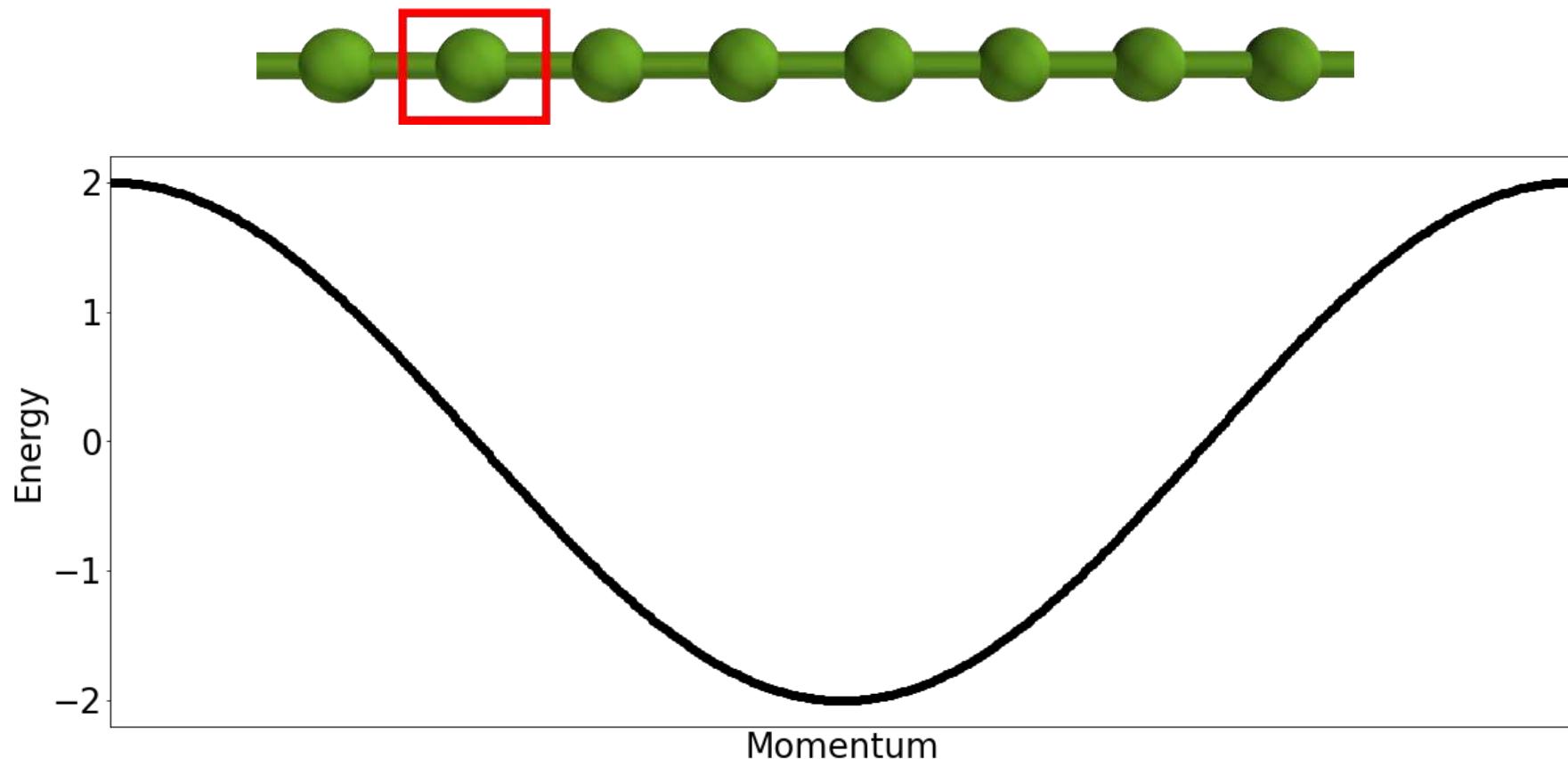
Let us take a 1D chain

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

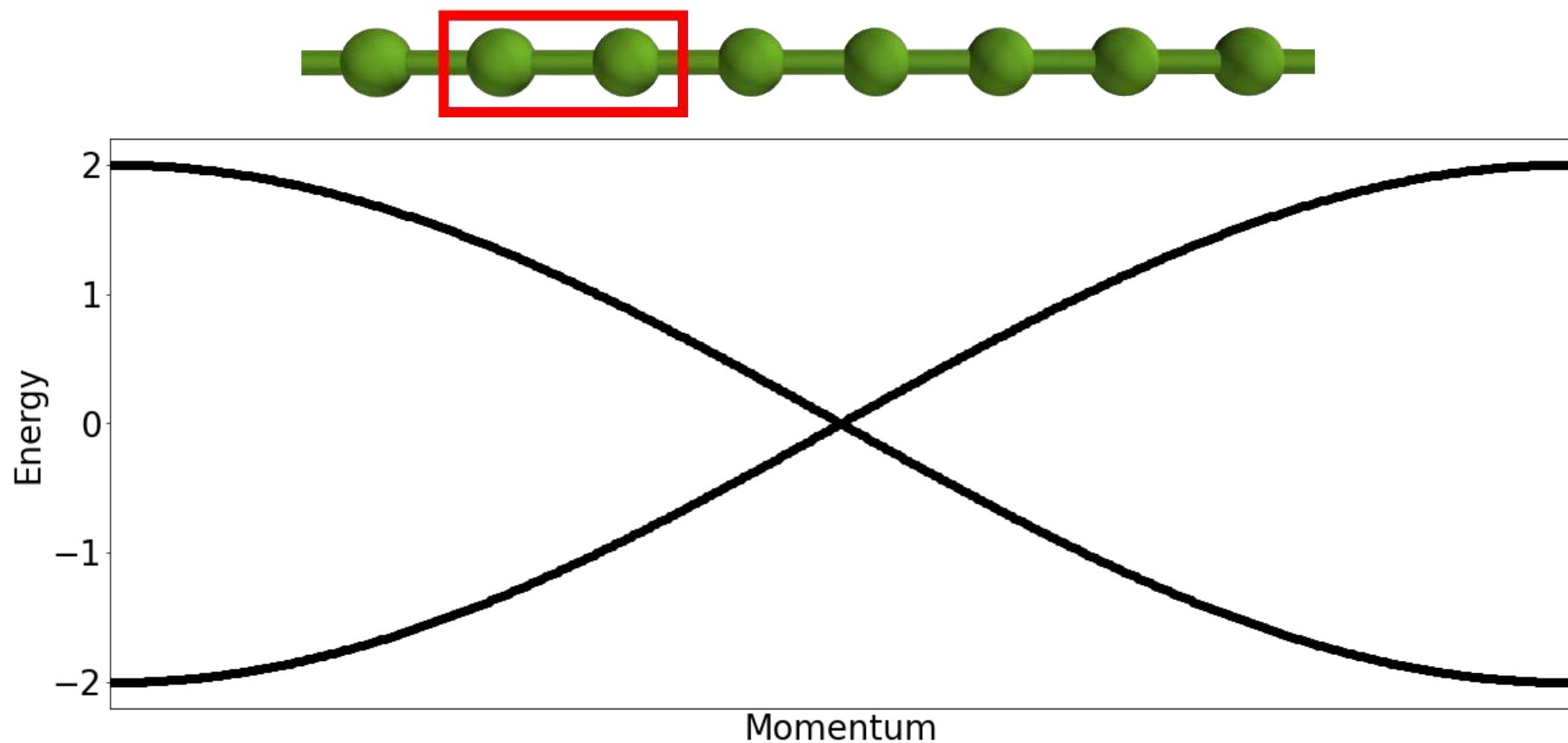
Let us see how the electronic structure changes with the unit cell



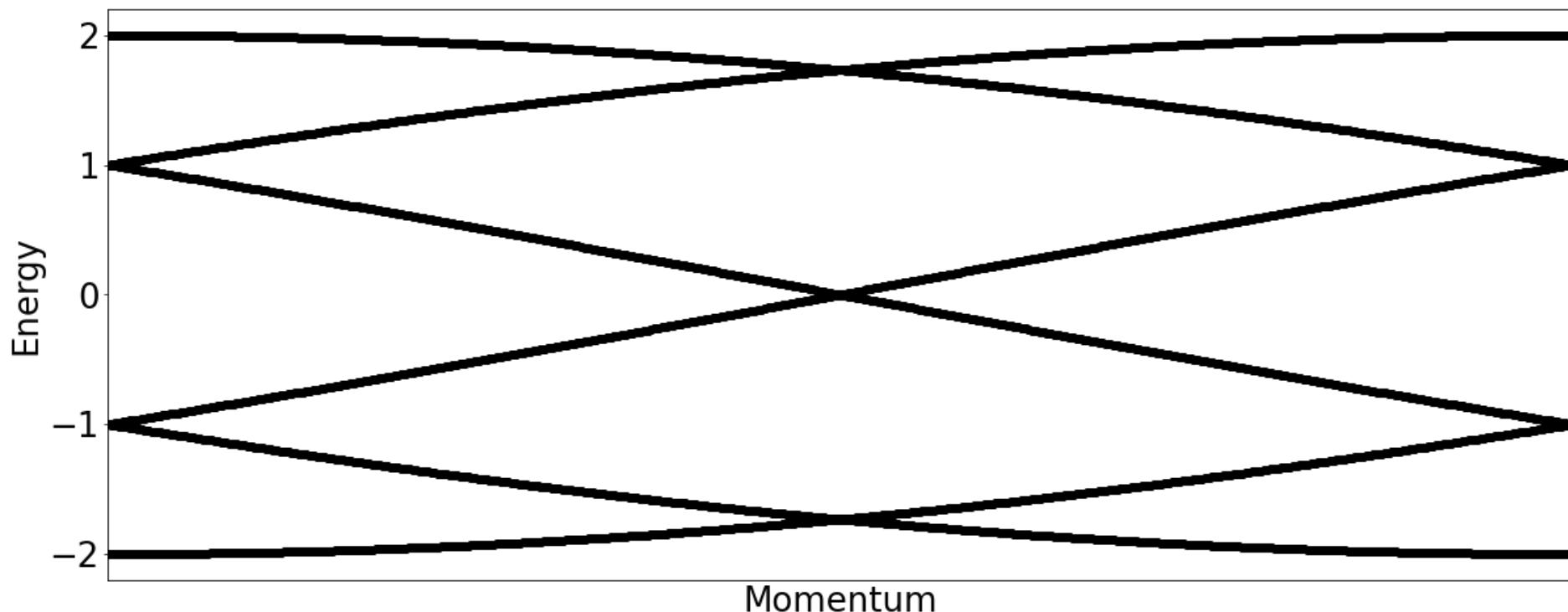
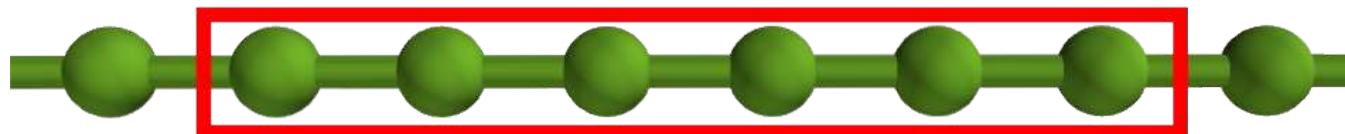
# Supercells and band folding



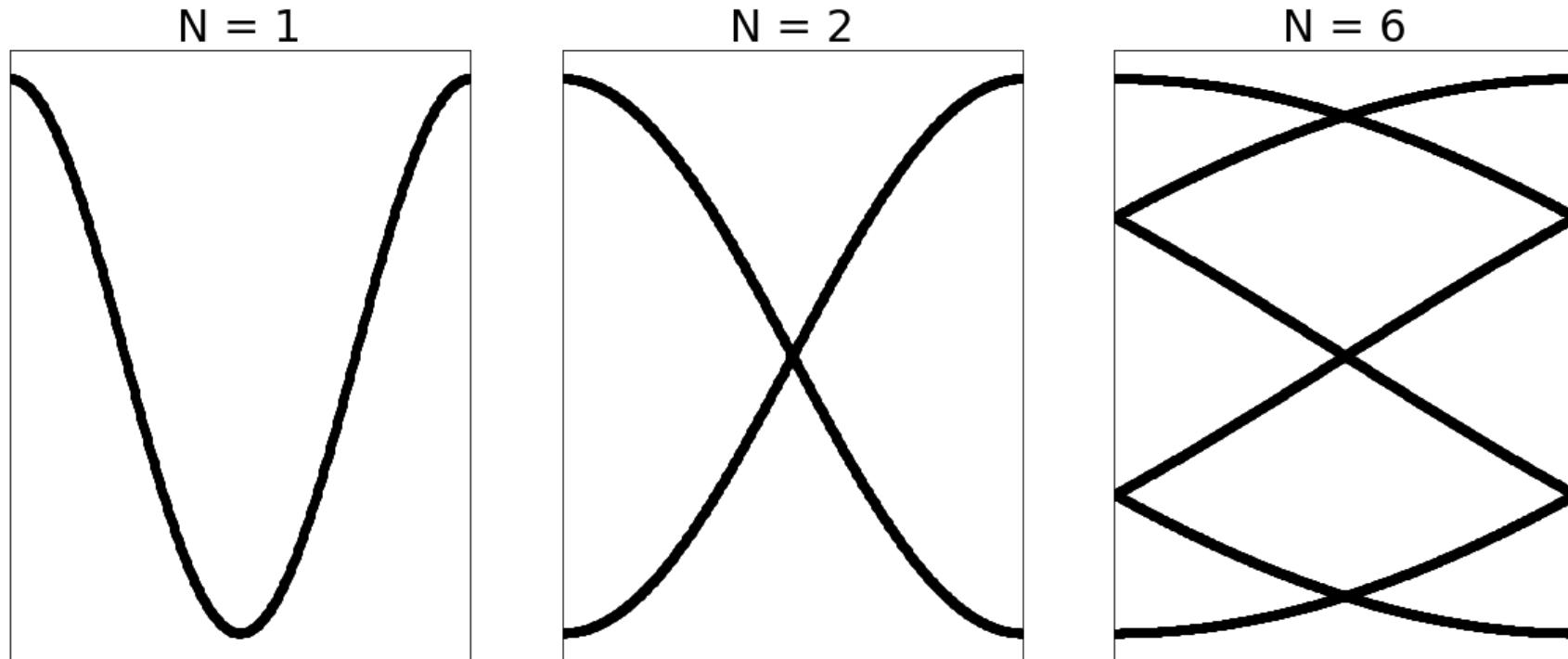
# Supercells and band folding



# Supercells and band folding

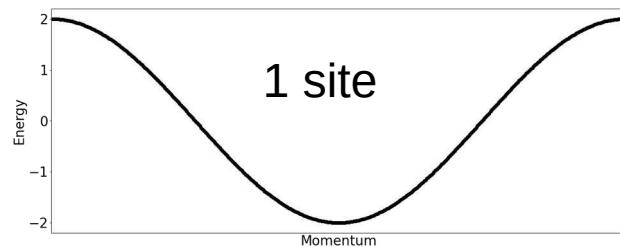


# Supercells and band folding

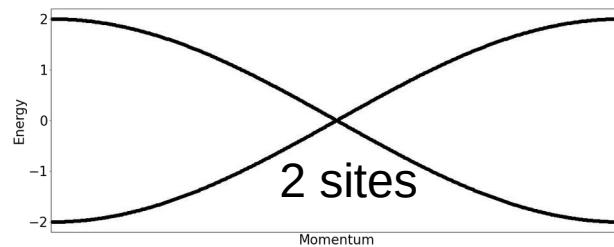


All these electronic structures represent the same physical system, but how do we see that?

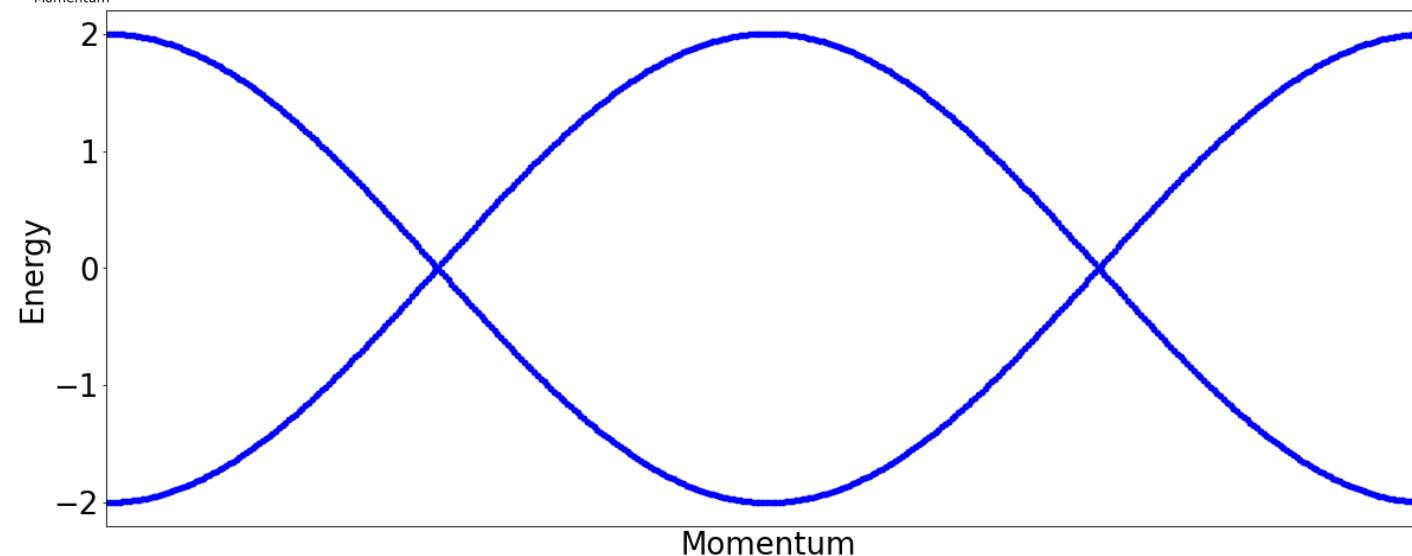
# Supercells and band folding



1 site

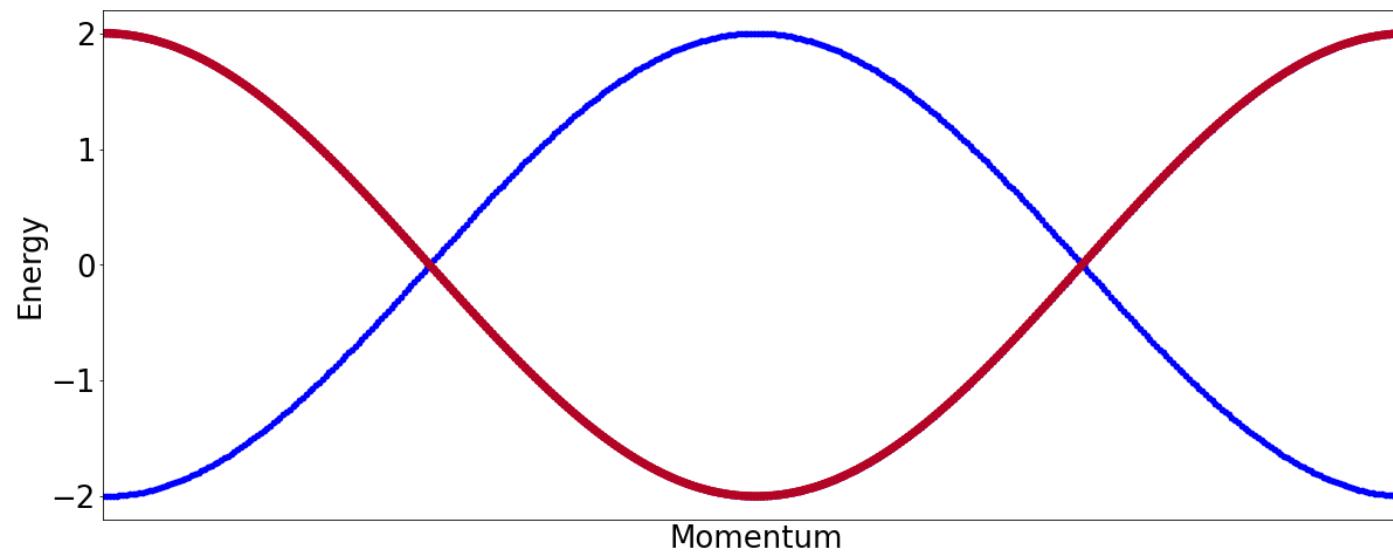
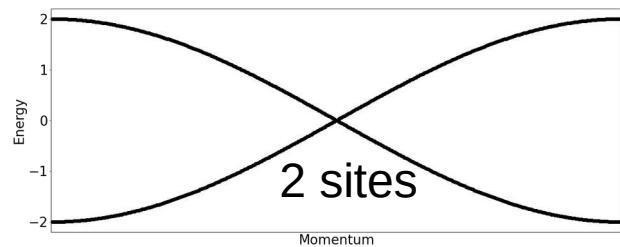
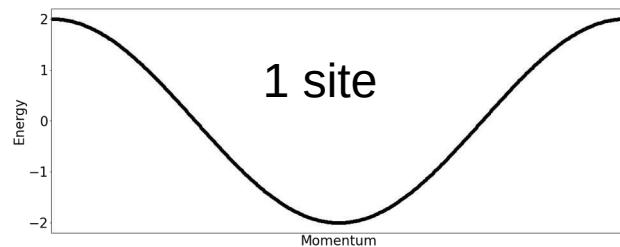


2 sites



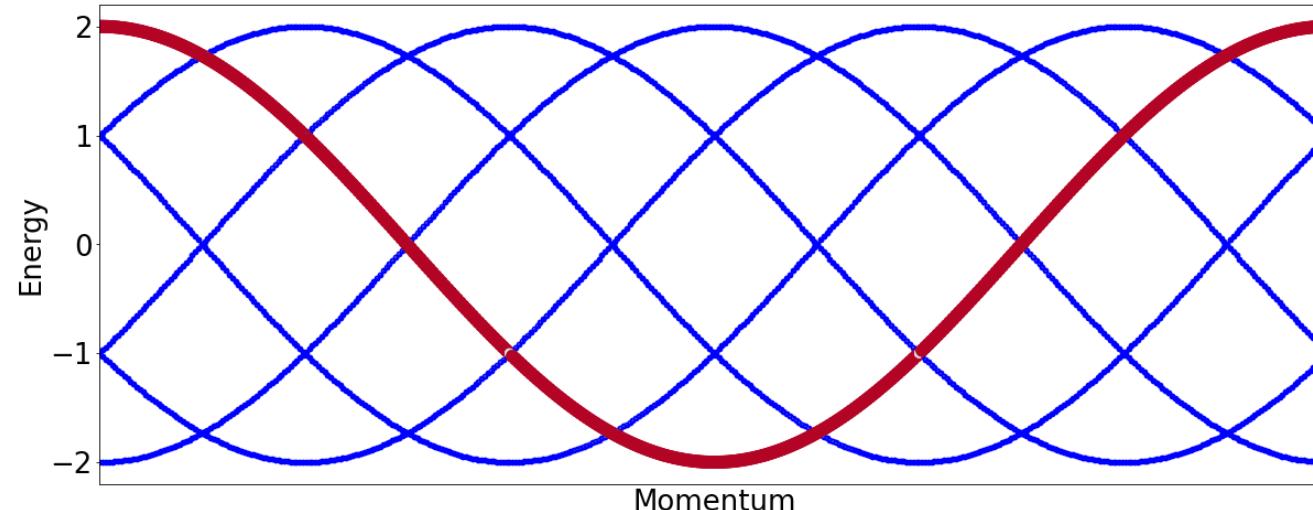
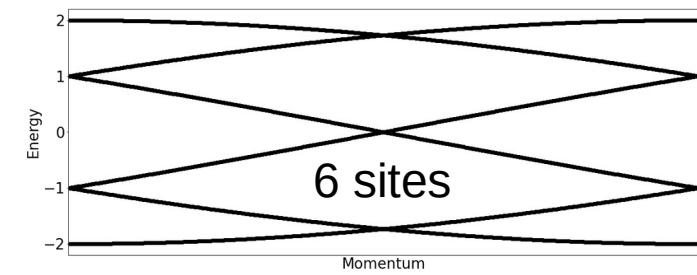
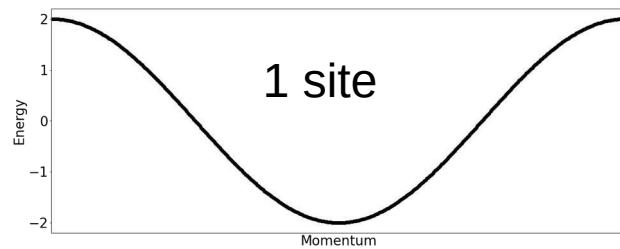
Repeating the electronic structure recovers the original electronic dispersion

# Supercells and band folding



Repeating the electronic structure recovers the original electronic dispersion

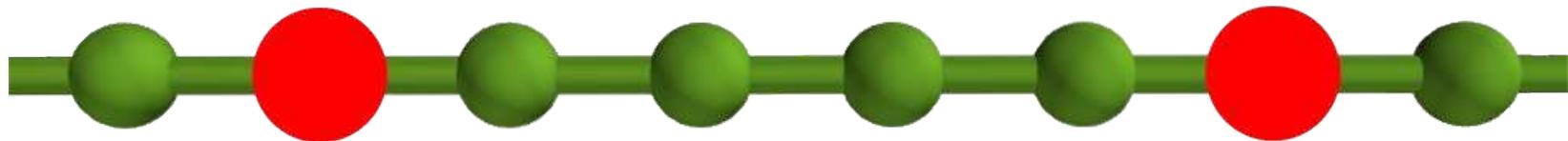
# Supercells and band folding



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)

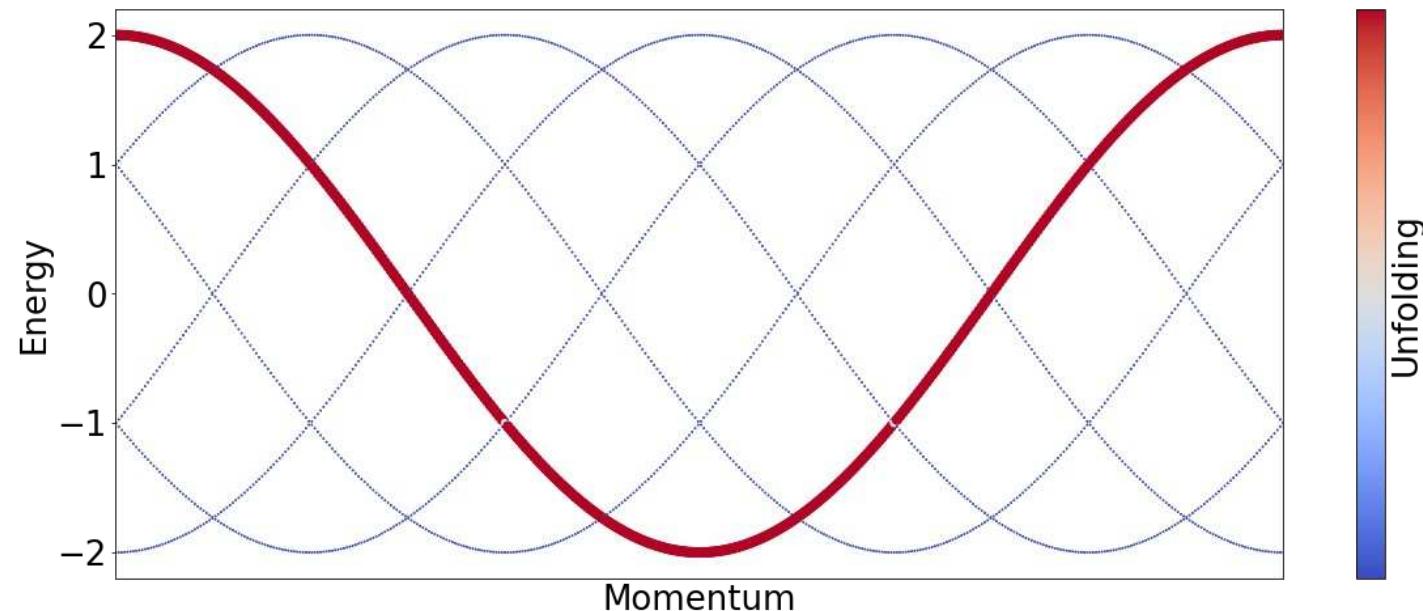


$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V_0 \sum_\alpha c_\alpha^\dagger c_\alpha \quad \alpha \equiv 0 \pmod{6}$$

# Unfolding and anticrossings in superlattices

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

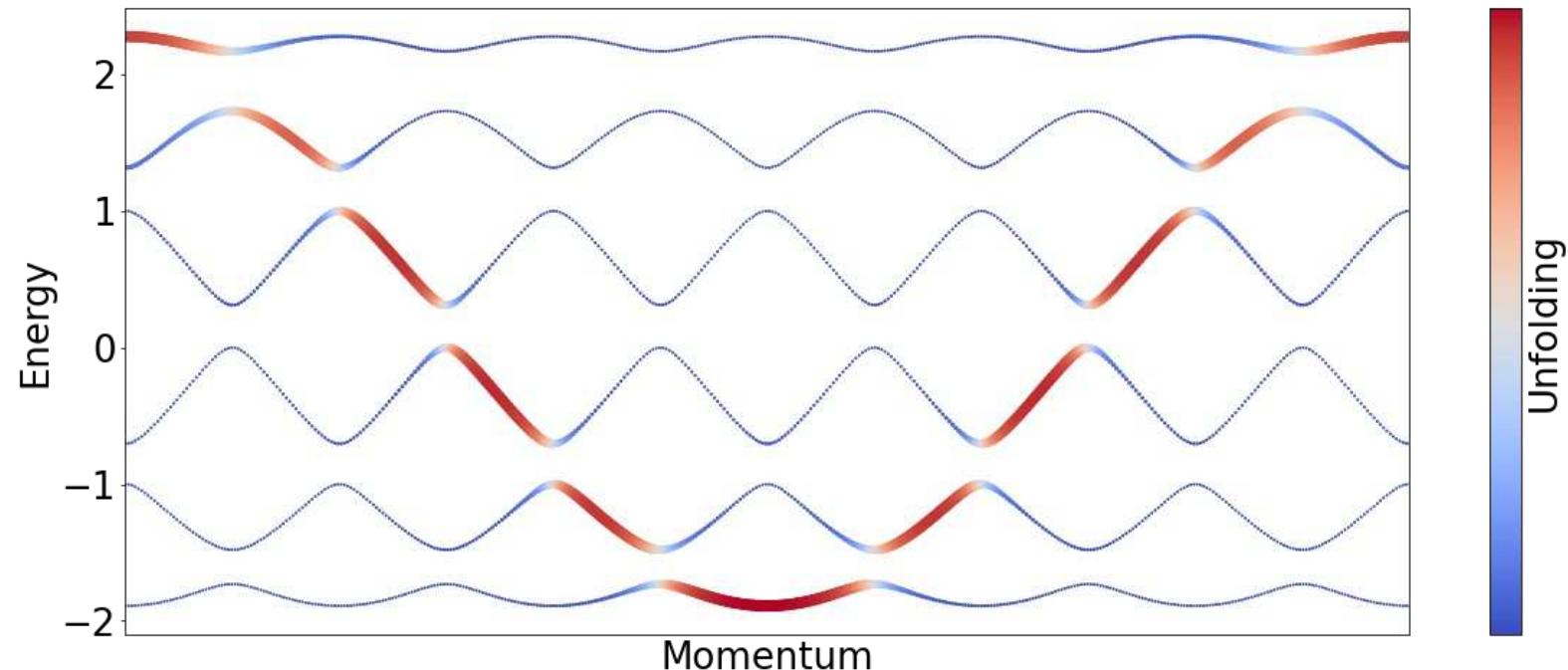
$$V_0 = 0$$



# Electronic structure unfolding

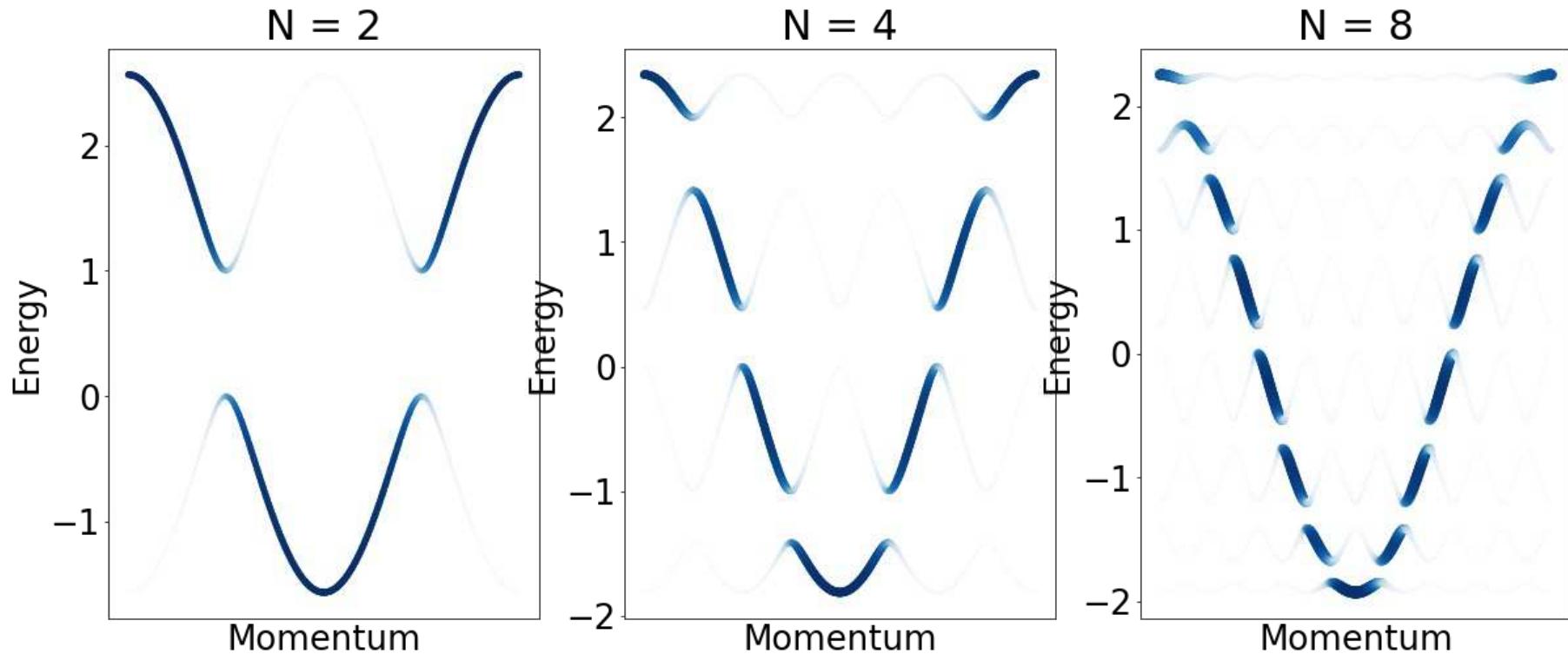
$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V_0 \sum_\alpha c_n^\dagger c_n$$

$$V_0 \neq 0$$



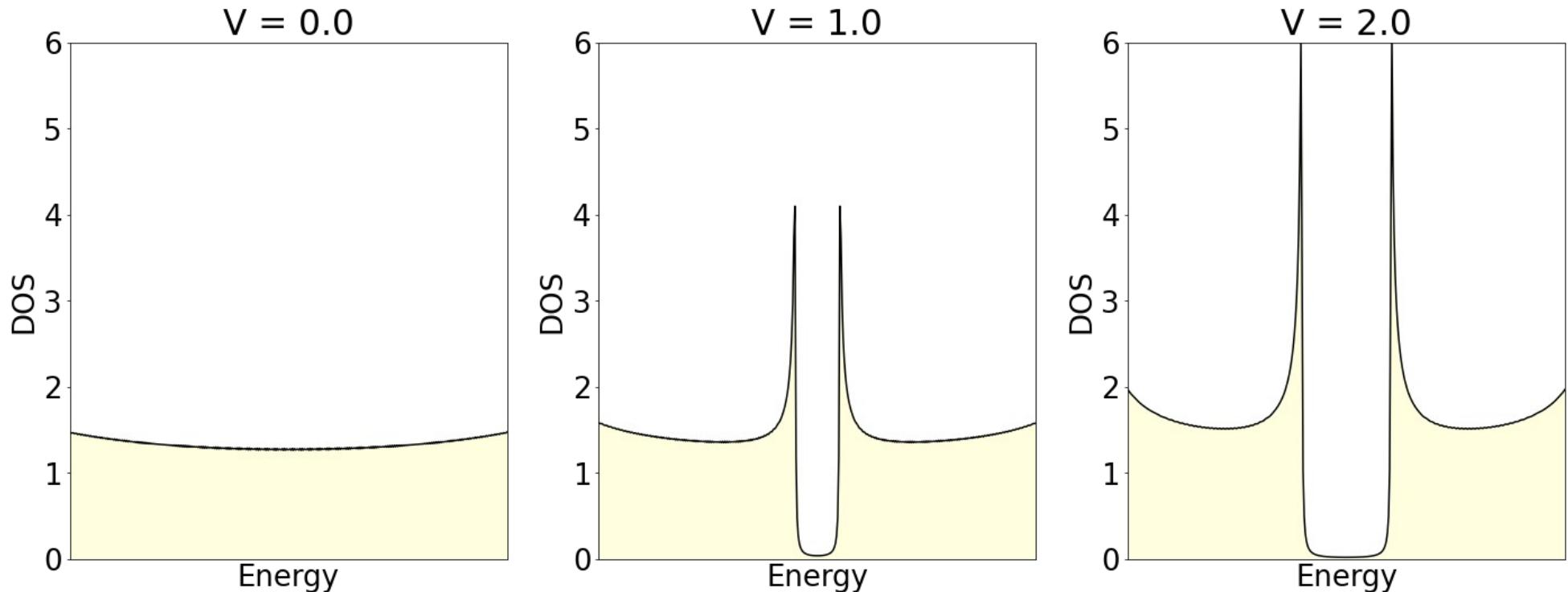
Anticrossing between the bands appear due to the superlattice potential

# Electronic structure unfolding



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

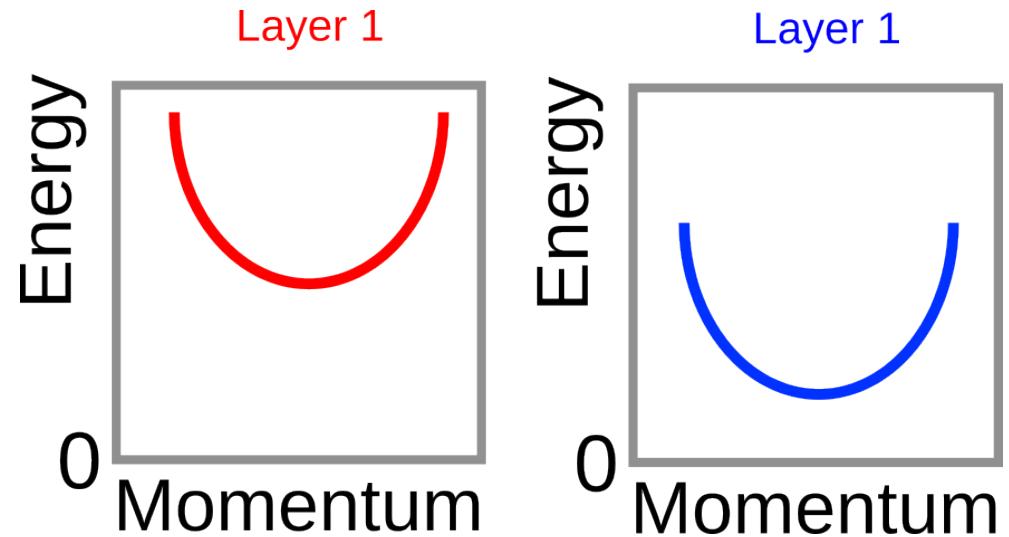
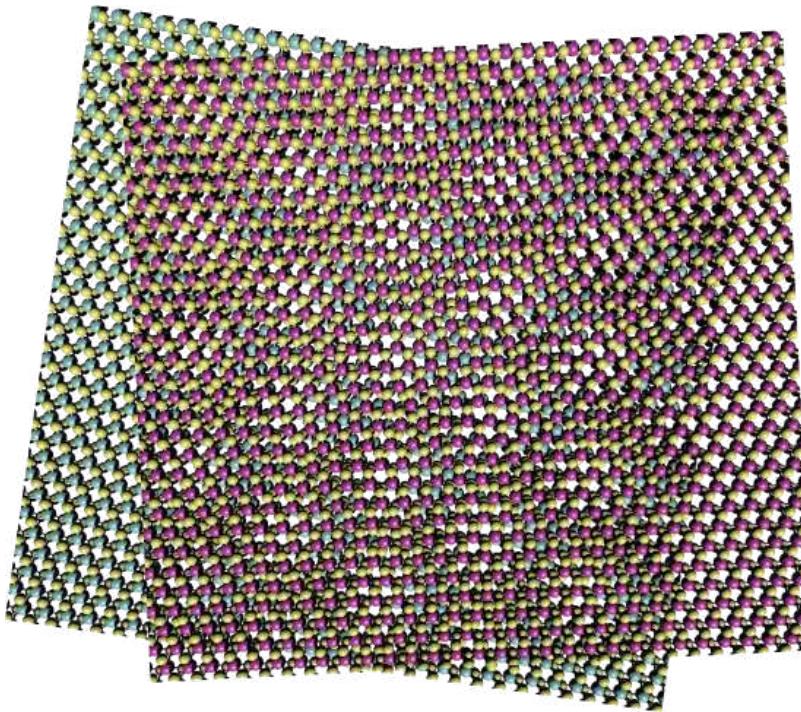
# Moire electronic structure



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

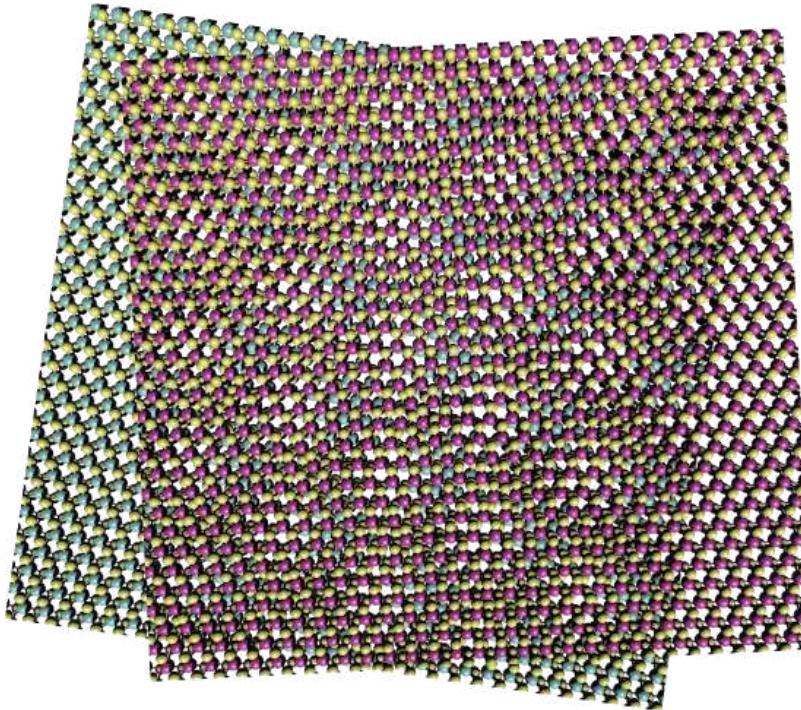
# Moire in twisted TMDC

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

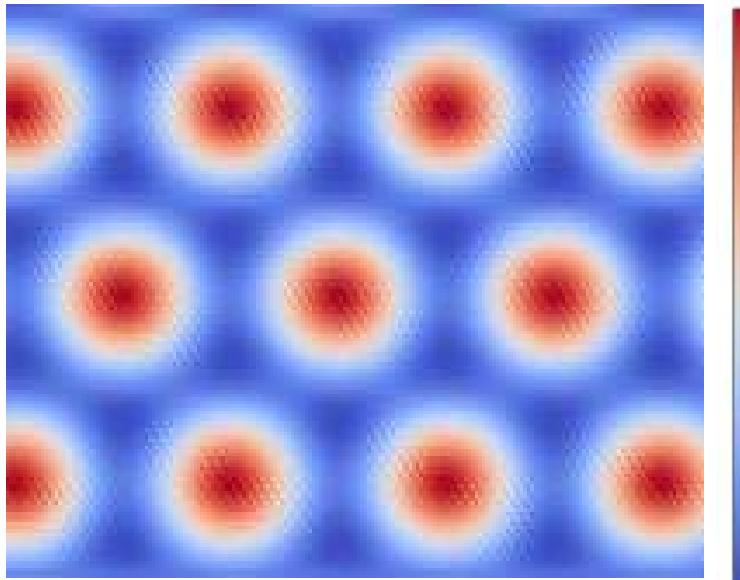


# Moiré in twisted TMDC

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

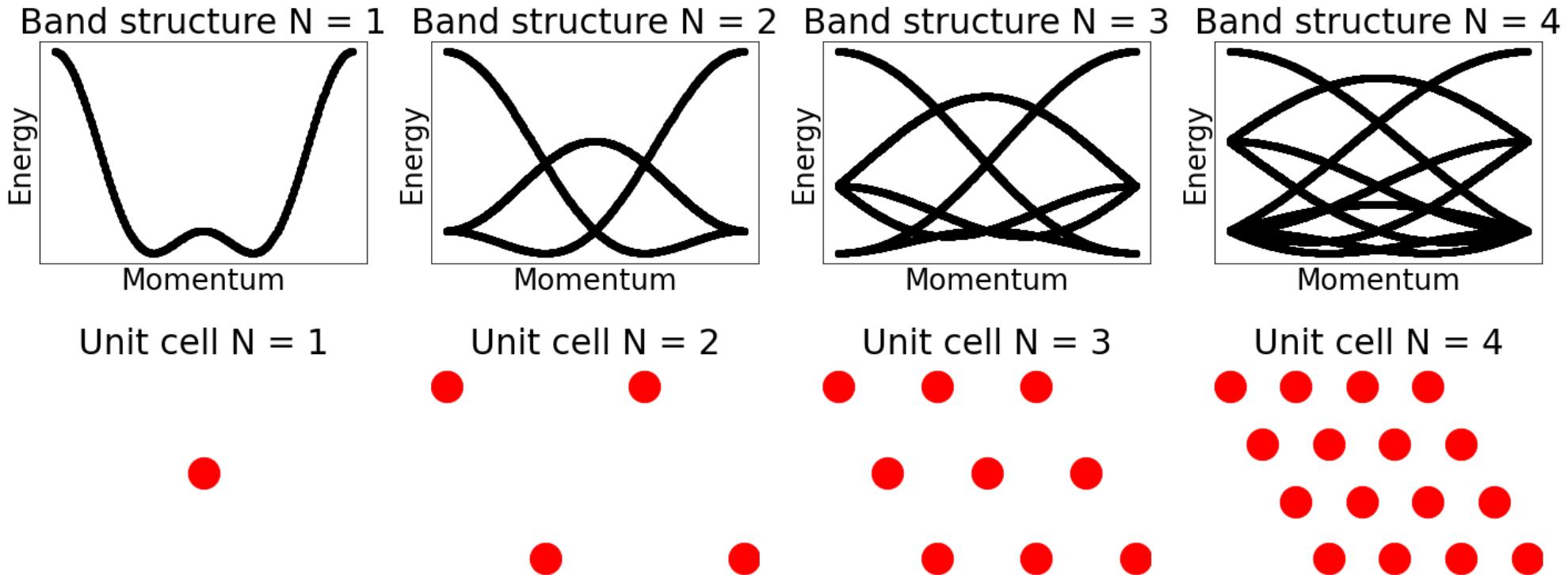


$$H = \sum_{ij} c_i^\dagger c_j + h.c. + \sum_n V(\mathbf{r}_n) c_n^\dagger c_n$$



$$V(\mathbf{r})$$

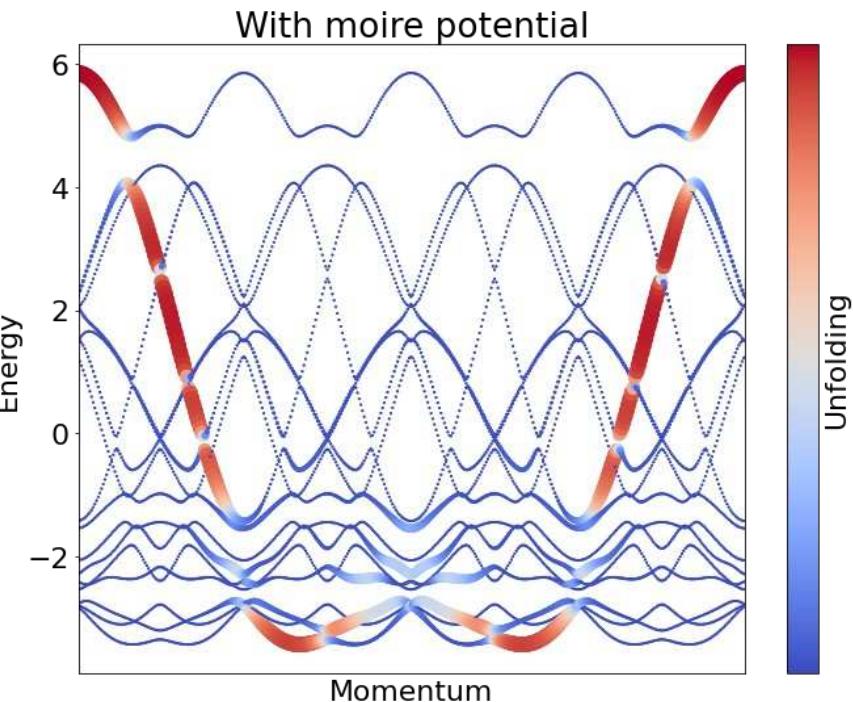
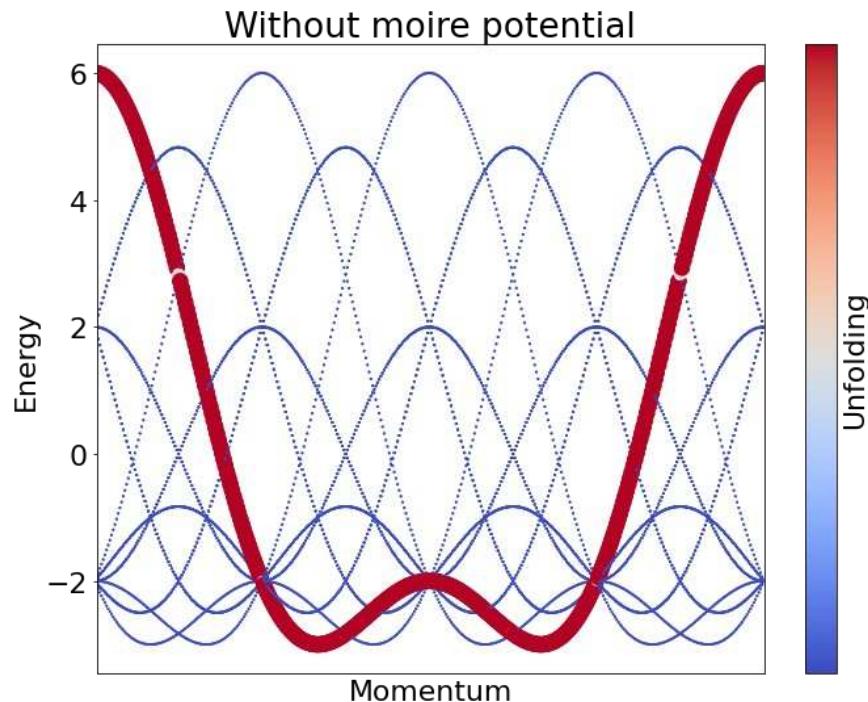
# Band structure folding in 2D superlattices



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

# Band structure folding in 2D superlattices

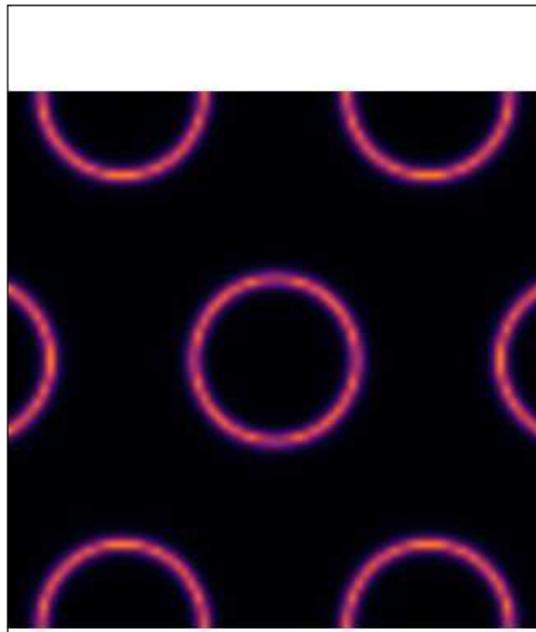
Mini-bands appear due to the moire in one of the layers



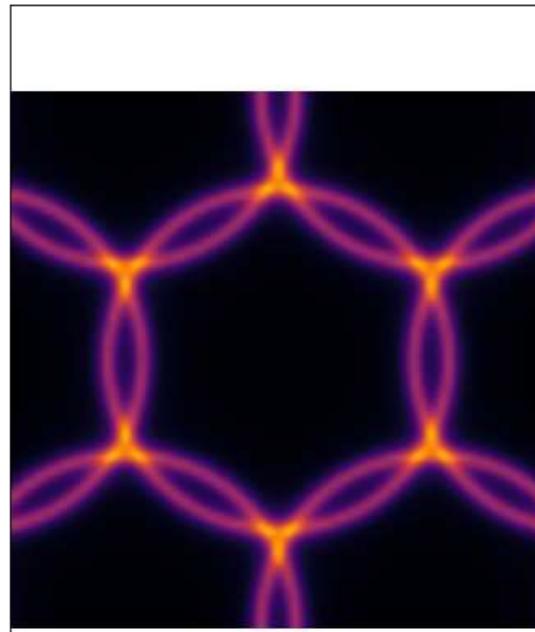
# Fermi surface folding in superlattices

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

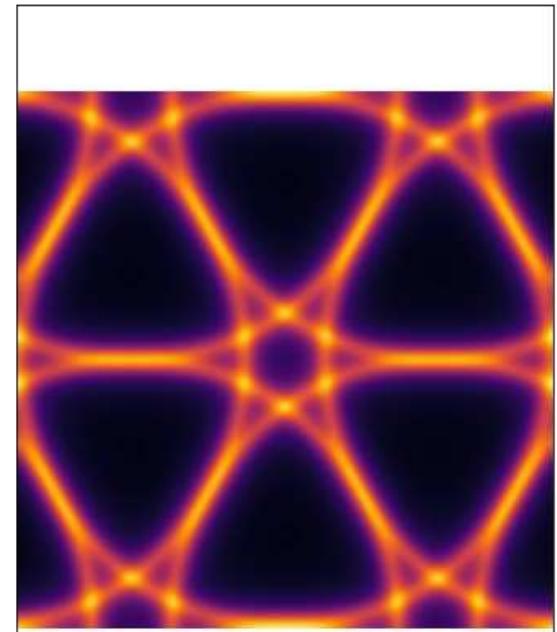
$N = 1$



$N = 2$

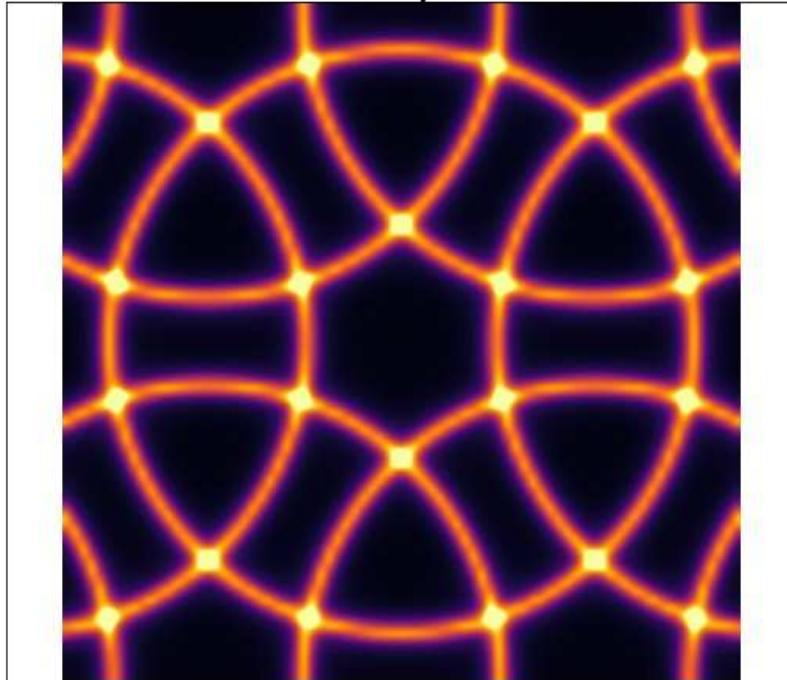


$N = 3$

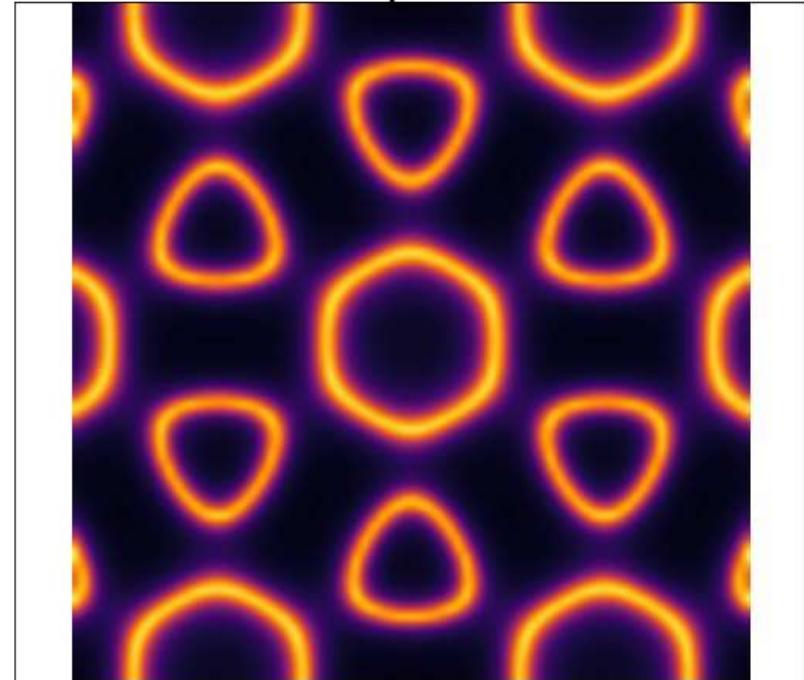


# Fermi surface folding in superlattices

Without superlattice



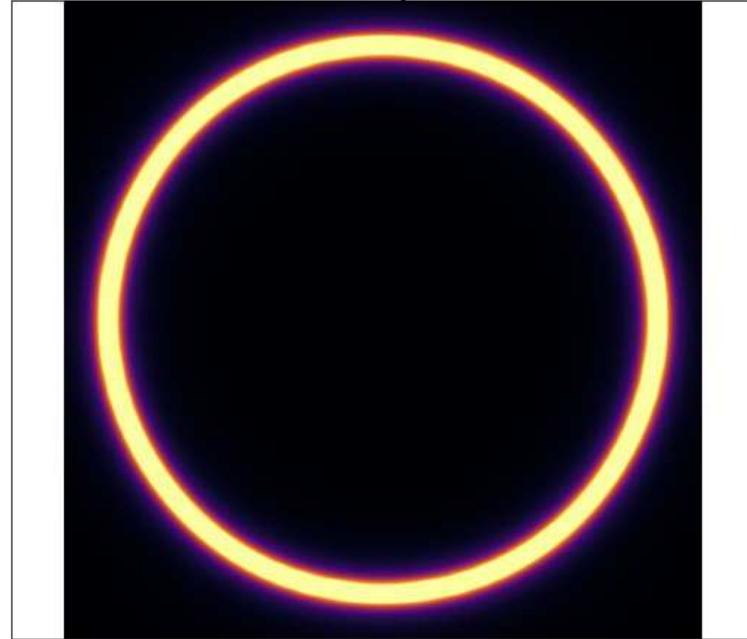
With superlattice



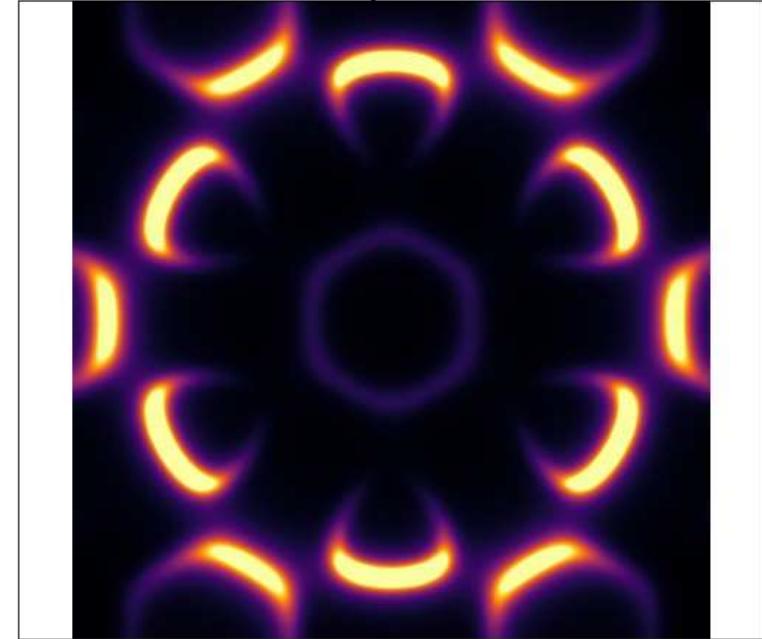
The superlattice changes the Fermi surface topology on the underlying 2D material

# Fermi surface unfolding in superlattices

Without superlattice



With superlattice



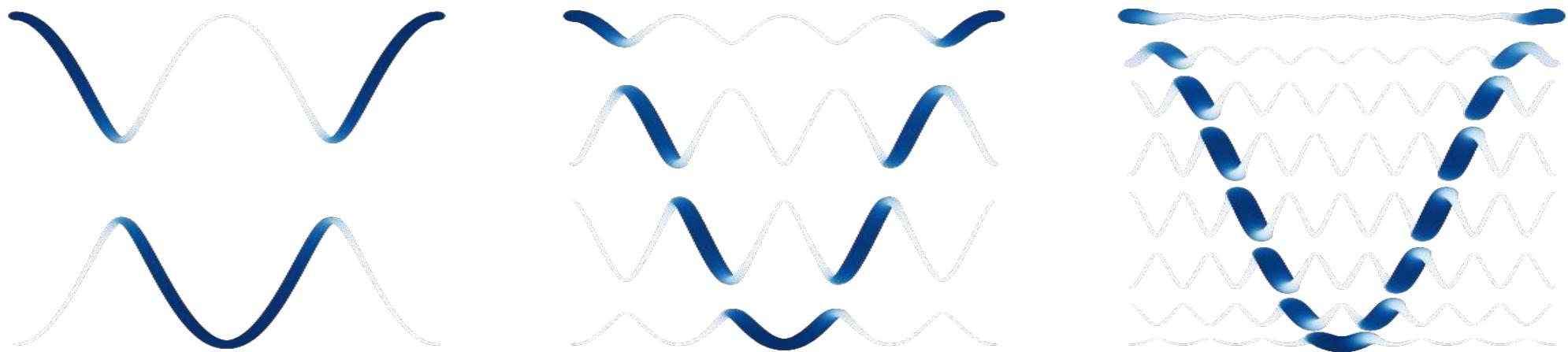
Superlattices fragment the original Fermi surface when unfolded to the original unit cell

# Break

5 min break

*(optional) to discuss during the break*

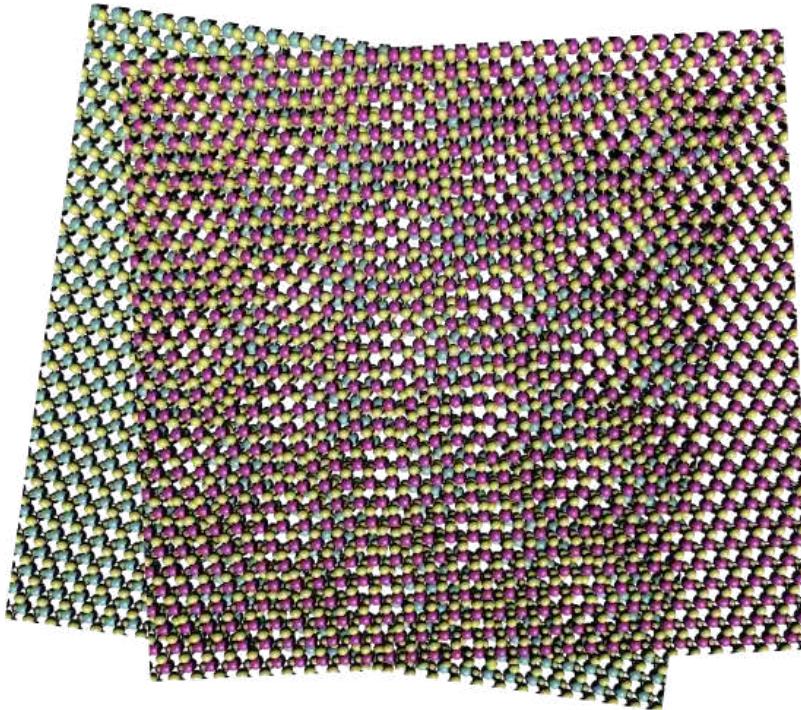
Which band structure has more van Hove singularities?



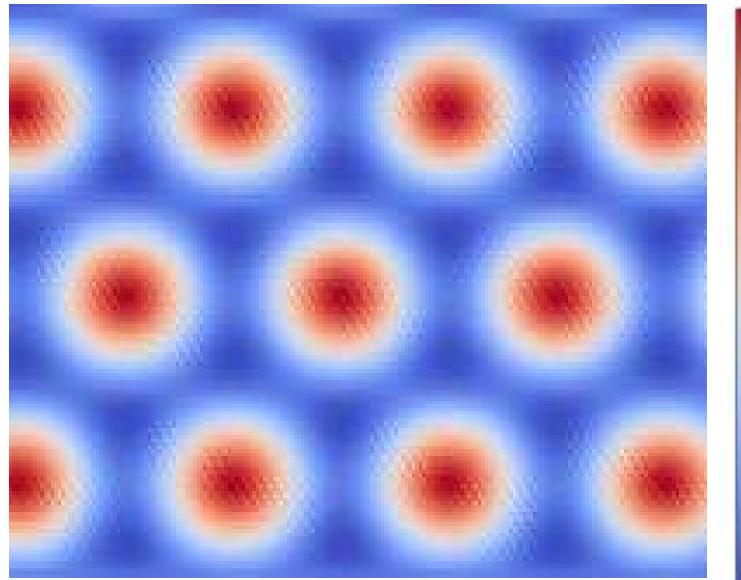
# Moire-driven correlated states

# Moiré in twisted TMDC

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

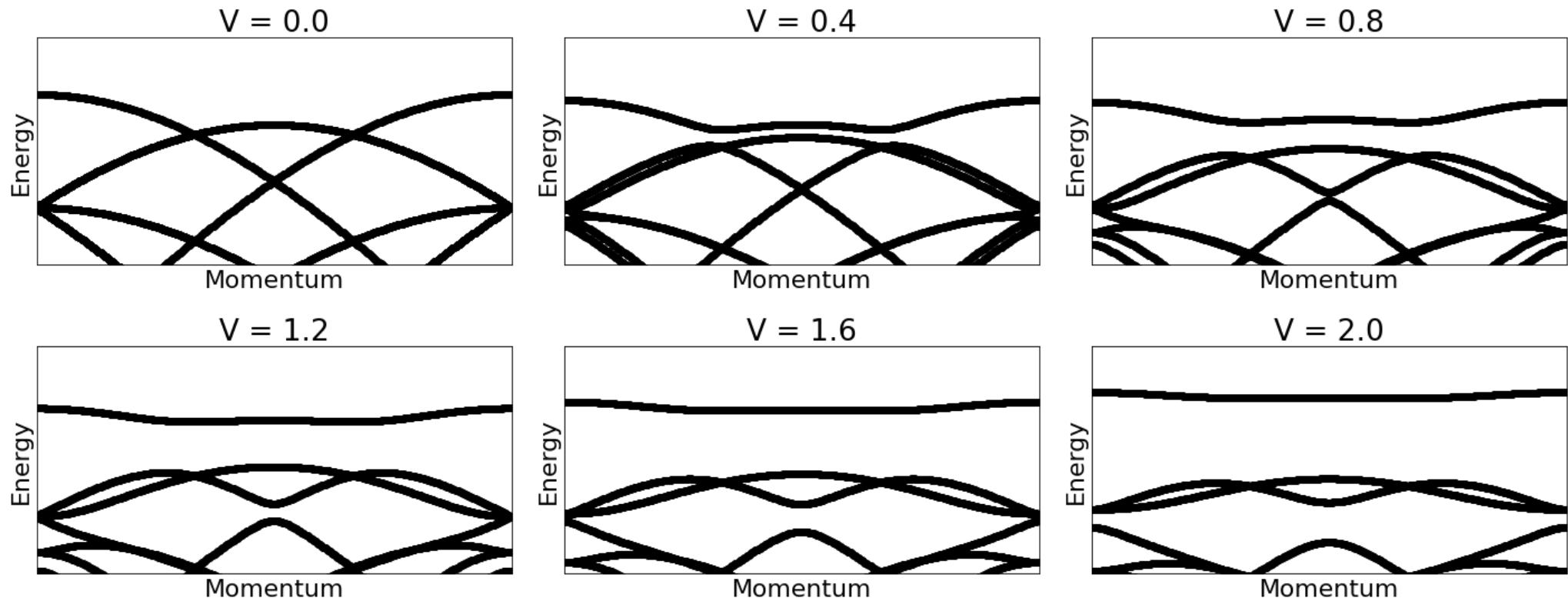


$$H = \sum_{ij} c_i^\dagger c_j + h.c. + \sum_n V(\mathbf{r}_n) c_n^\dagger c_n$$



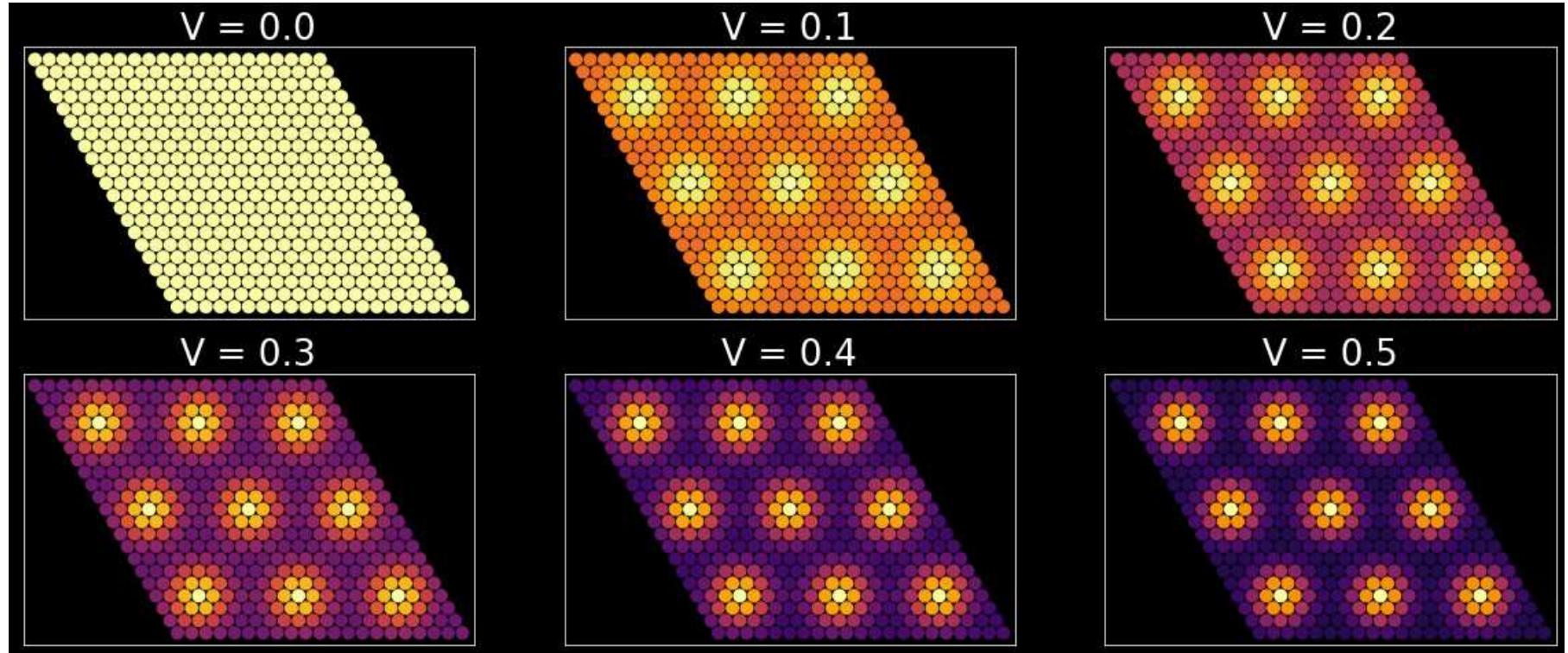
$$V(\mathbf{r})$$

# Band flattening by a moire



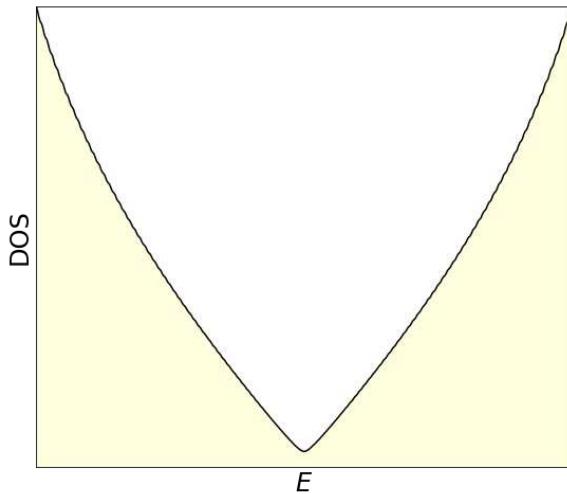
As the strength of a modulation is increased, flat bands appear

# Emergence of moire states

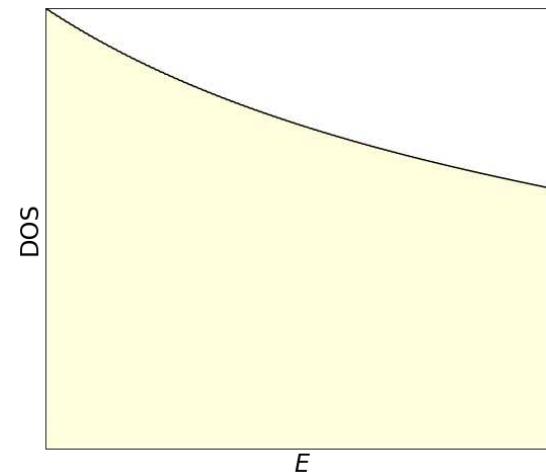


# Controlling the electronic spectra with the moire angle

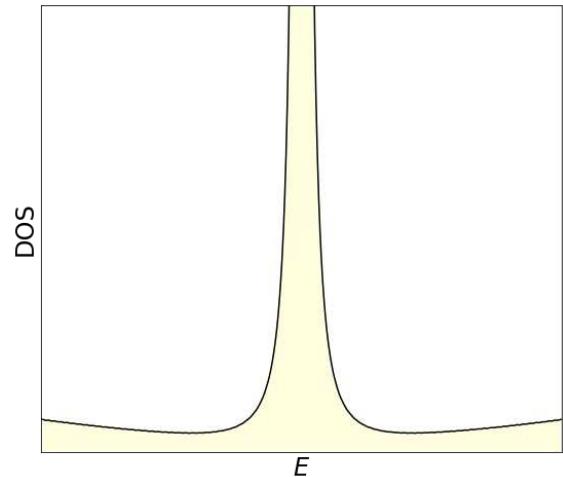
Semimetals



Metals



Flat bands



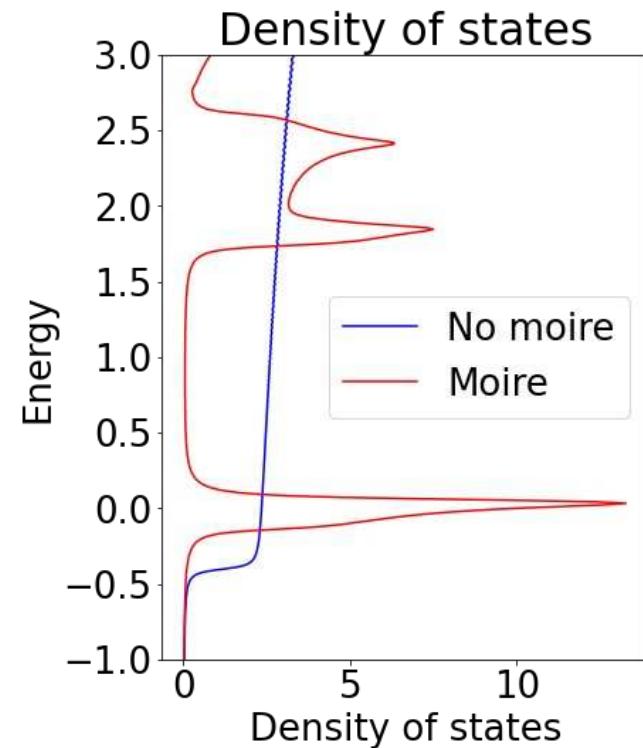
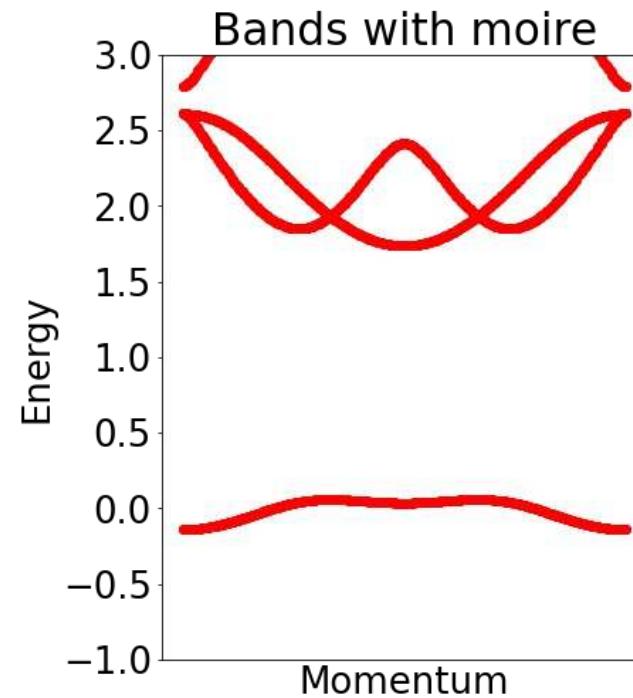
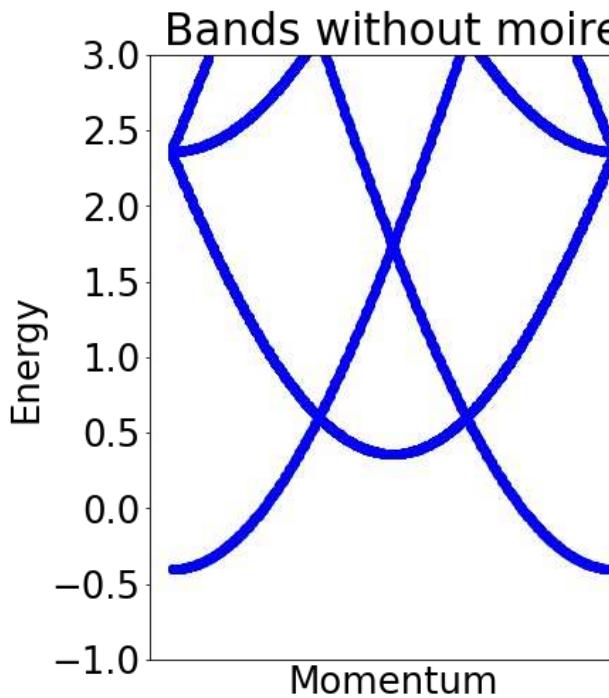
Moire/twist angle



Moire potentials allow driving systems to the correlated limit

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

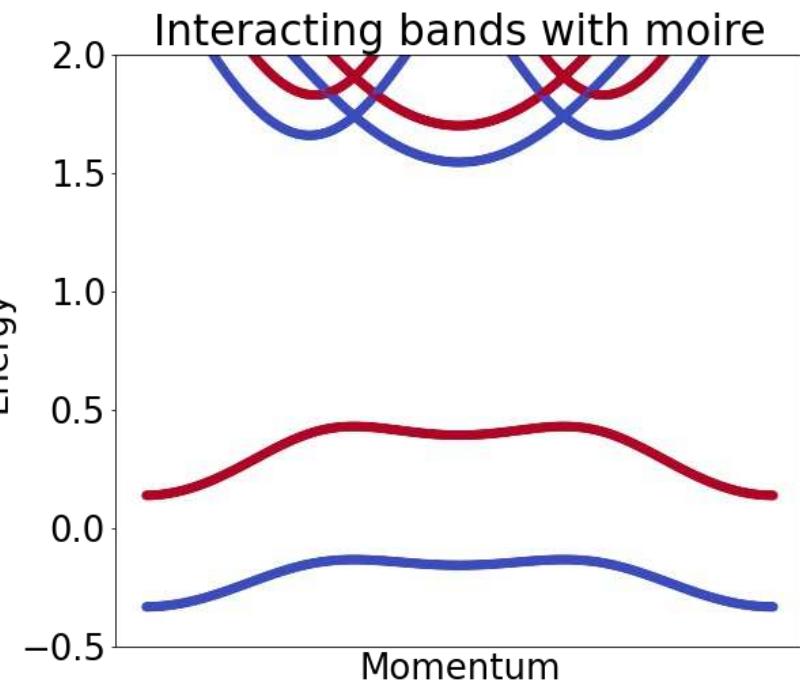
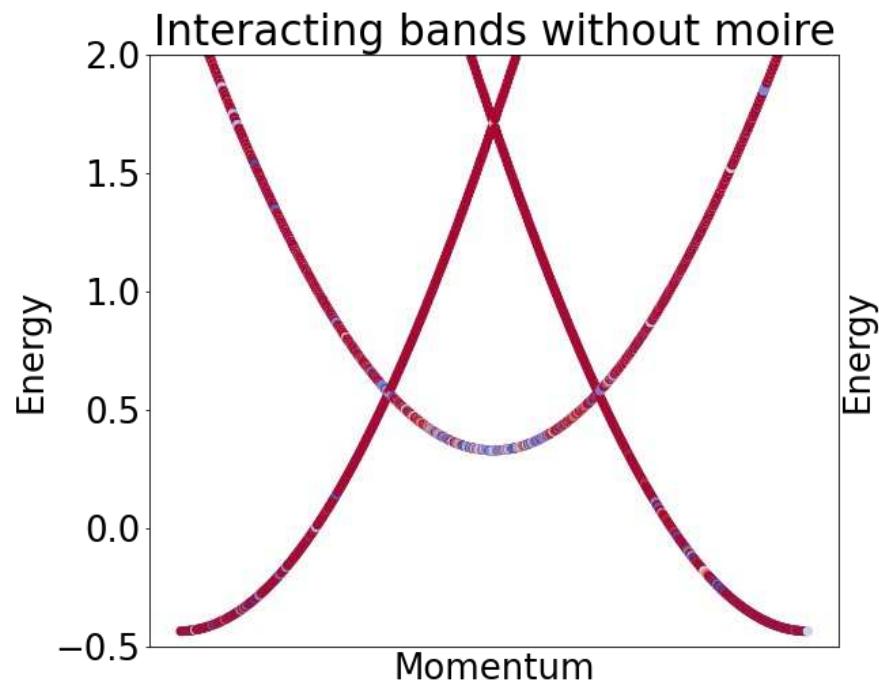
# Moire-enhanced DOS



The moire potential gives rise to an enhanced DOS

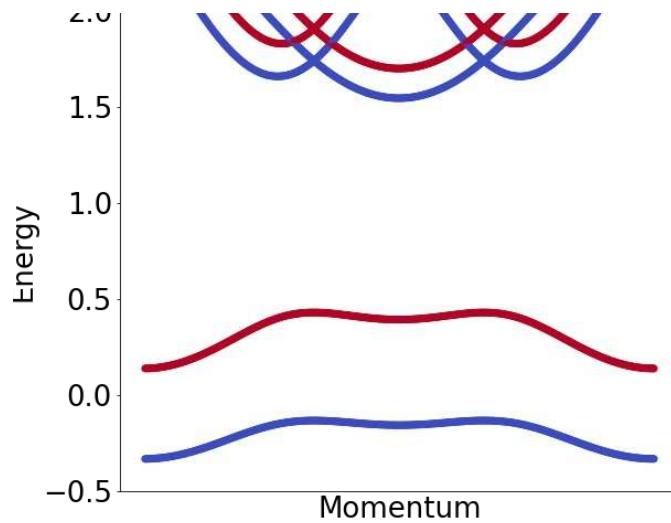
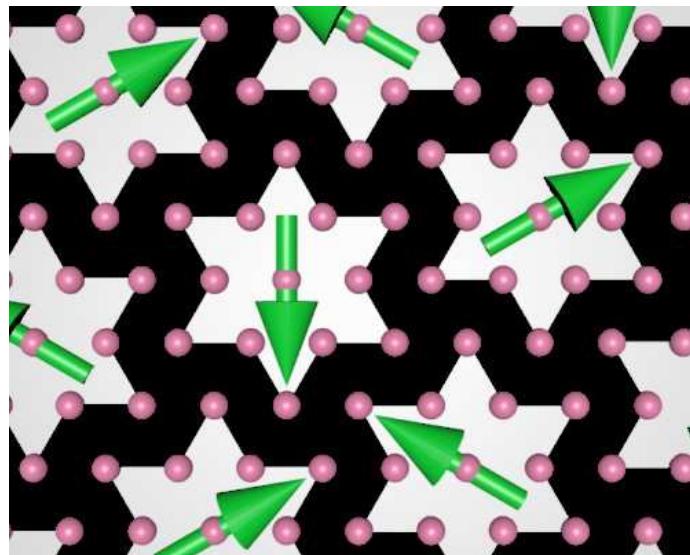
# Interactions in the absence and presence of a moire

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



# Correlated state in 1T-TaS<sub>2</sub> from miniband formation

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



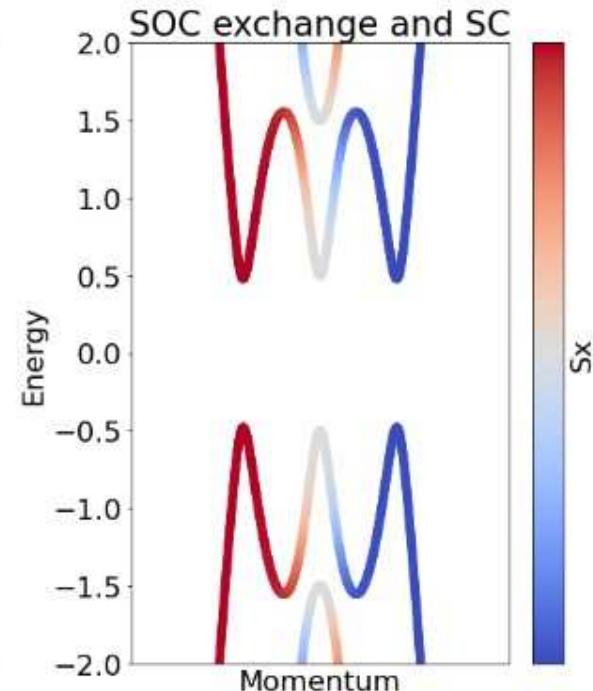
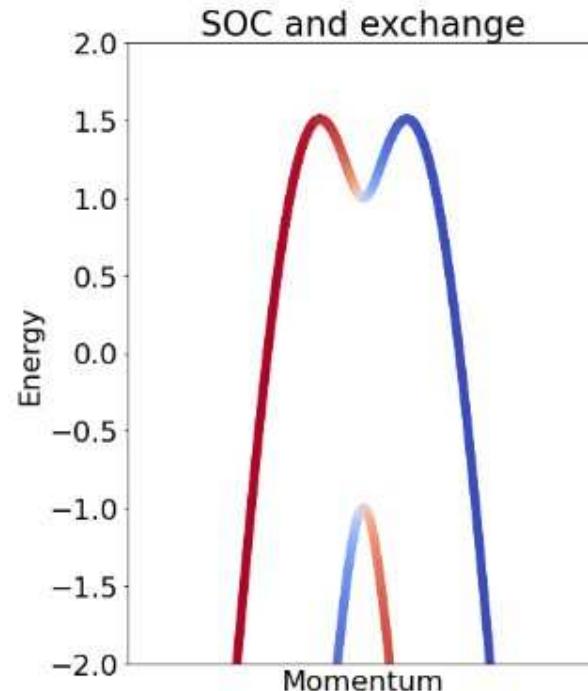
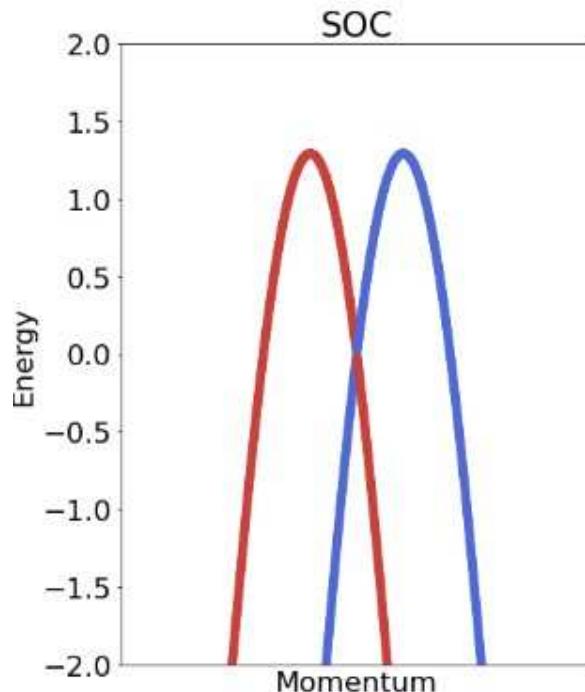
A charge density wave distortion acts as a superlattice modulation

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

# Moire-driven topological states

# Artificial topological superconductivity

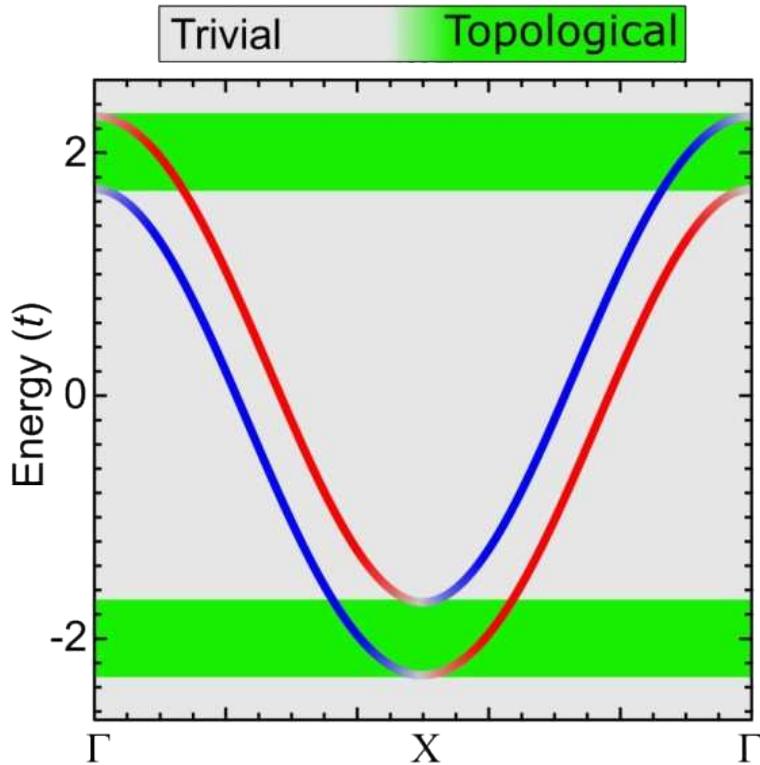
Bulk electronic structure



$S_x$

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

# Artificial topological superconductor



$$H = H_0 + H_J + H_R$$

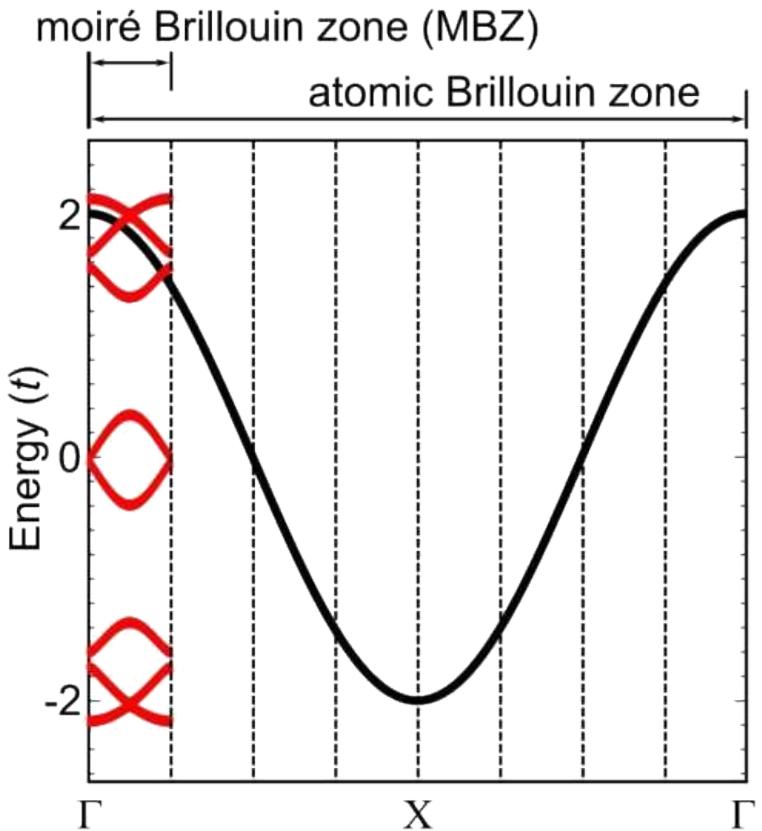
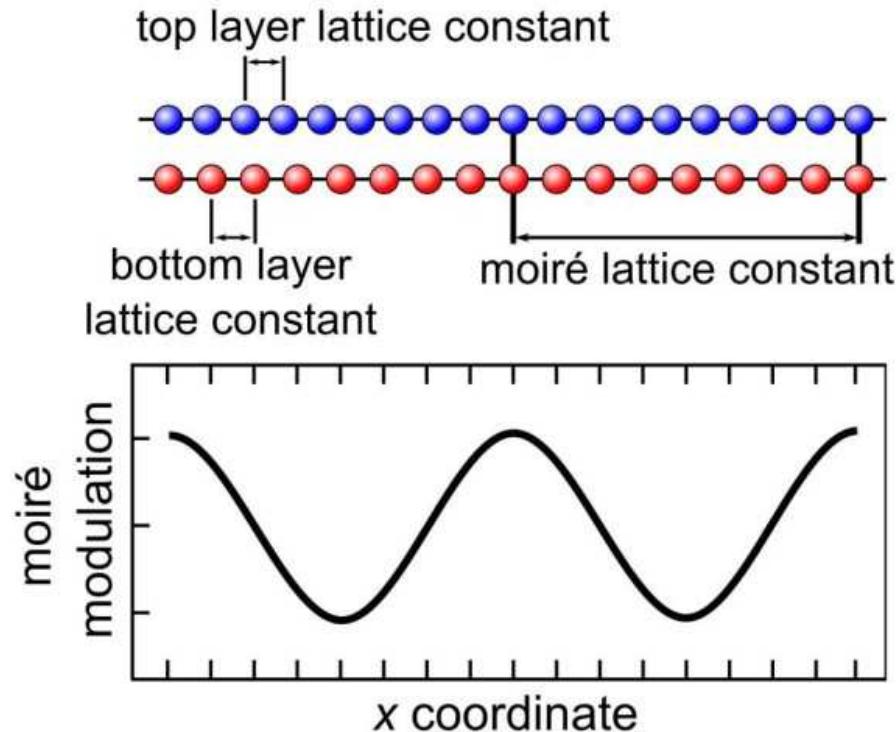
Kinetic energy

Exchange field

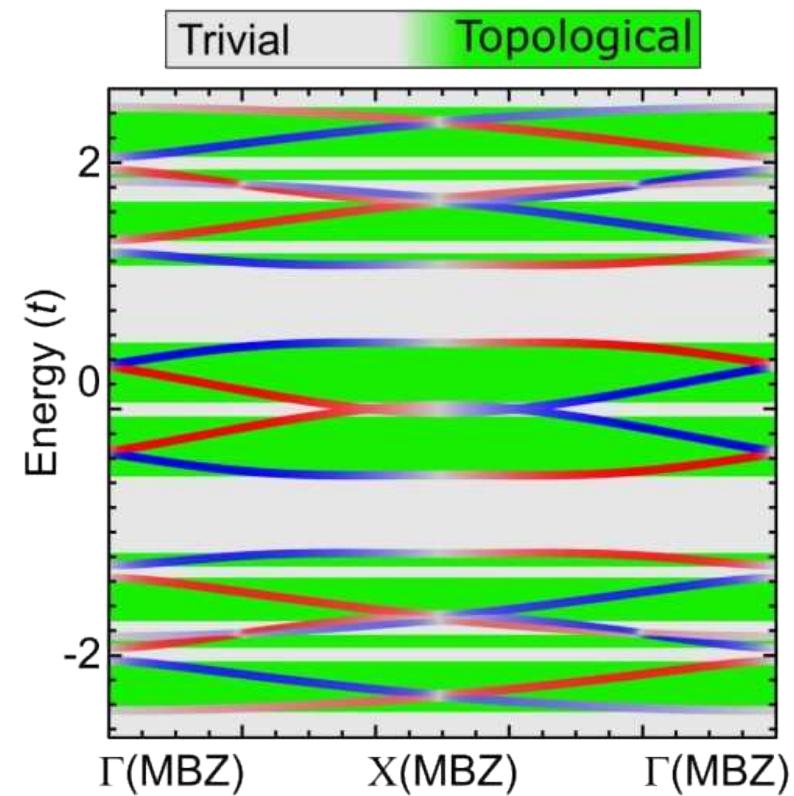
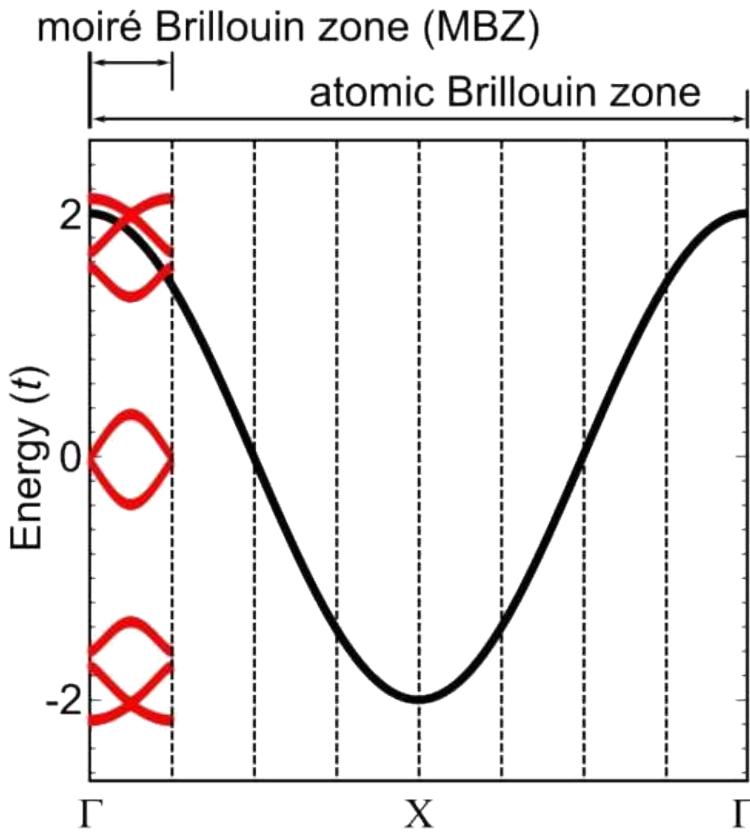
Rashba spin-orbit coupling

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

# Artificial moire topological superconductor

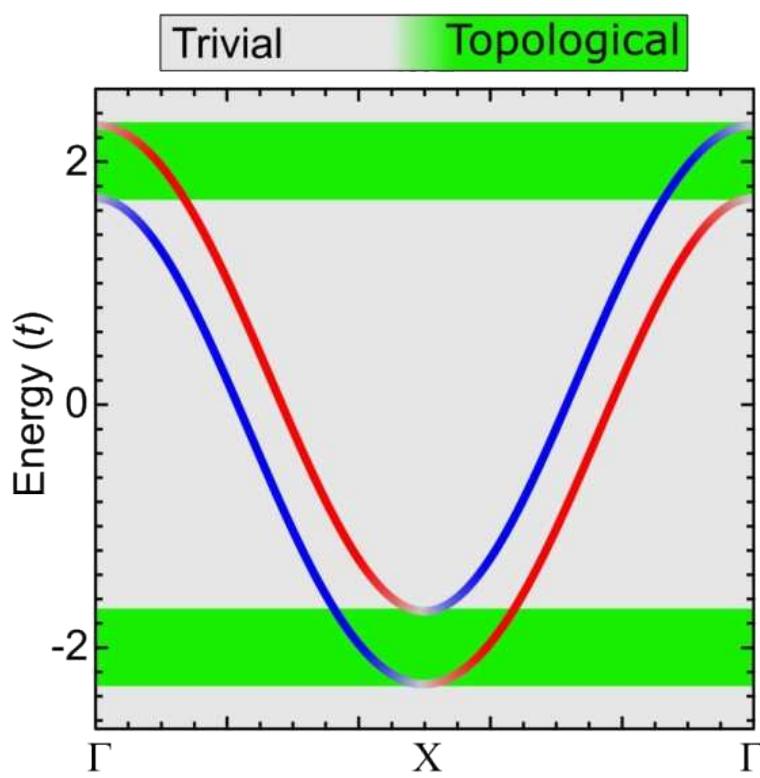


# Artificial moiré topological superconductor

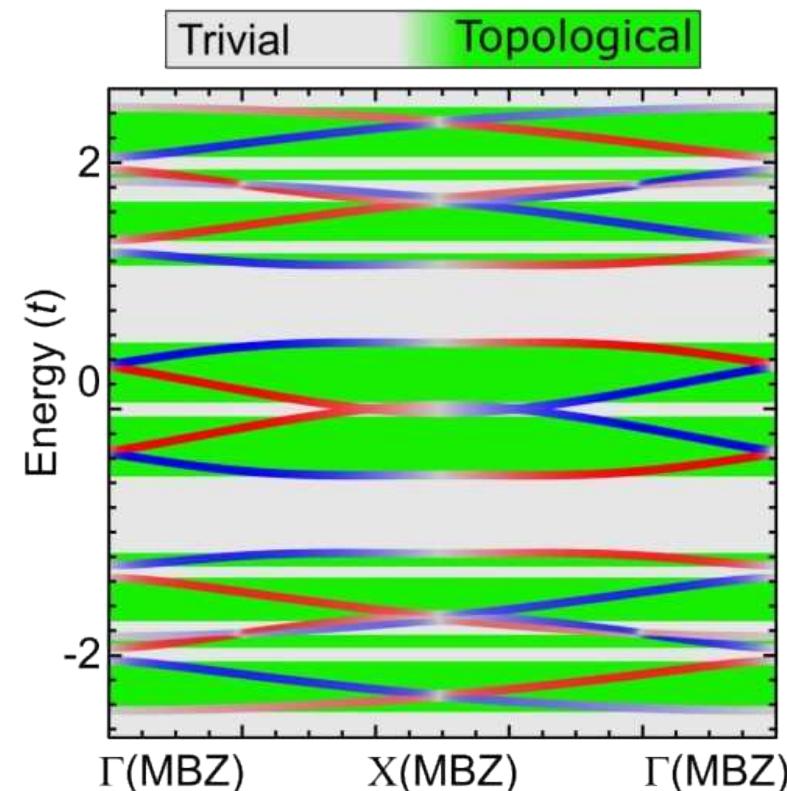


# Artificial moire topological superconductor

Without moire

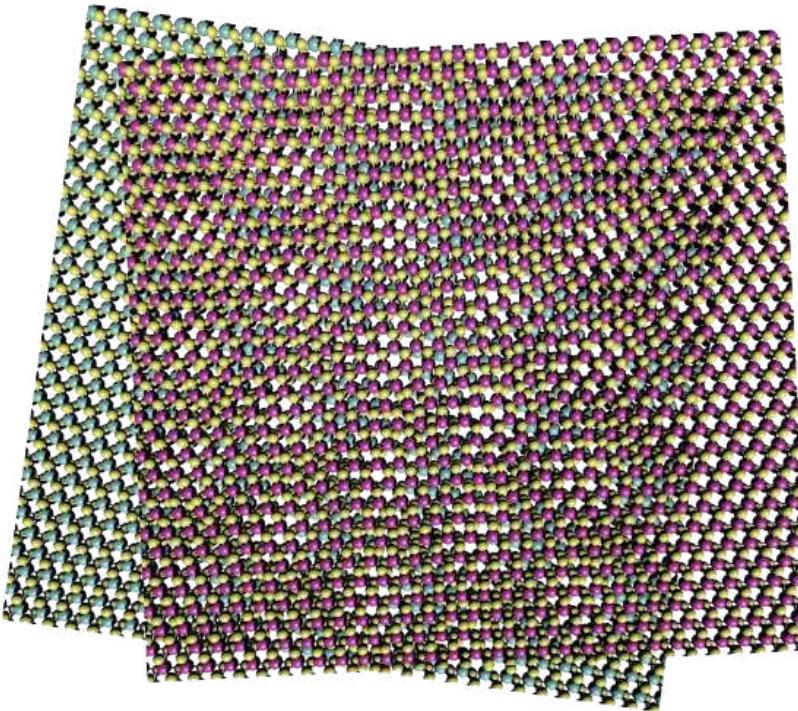


With moire



# Moire driven gaps in the band structure

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



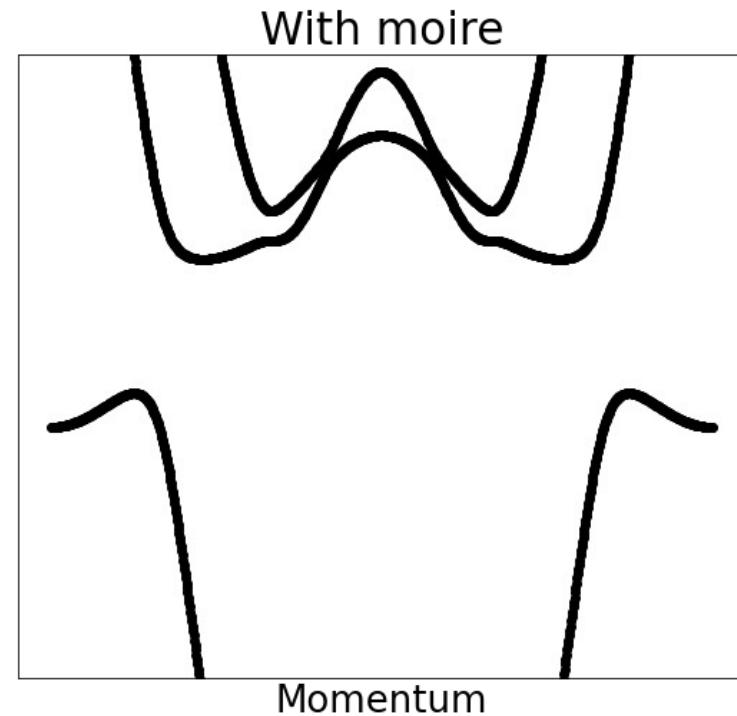
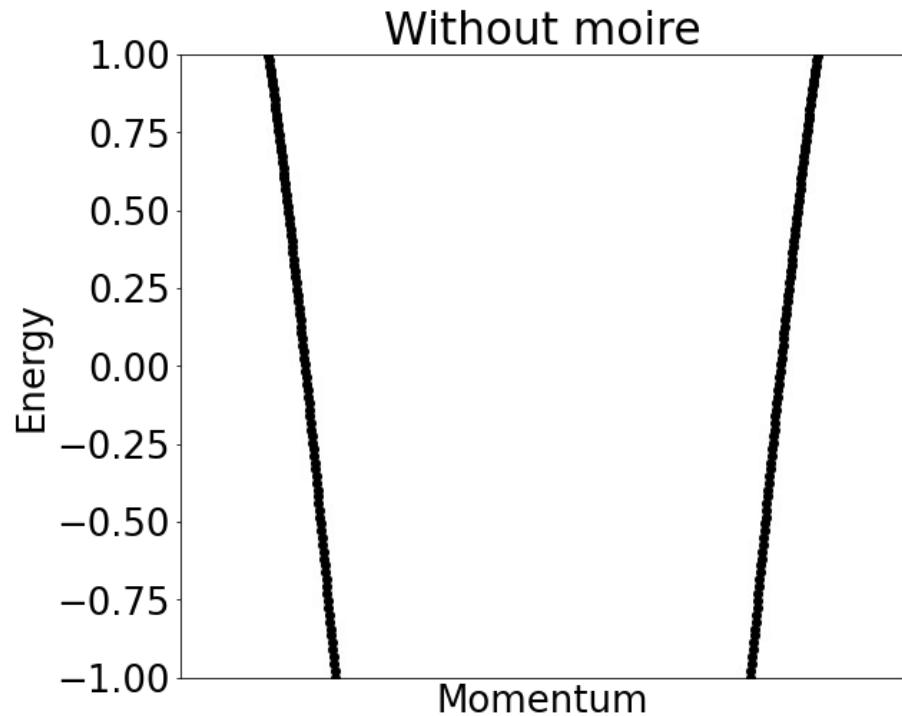
$$H = H_0 + H_J + H_R$$

Kinetic energy

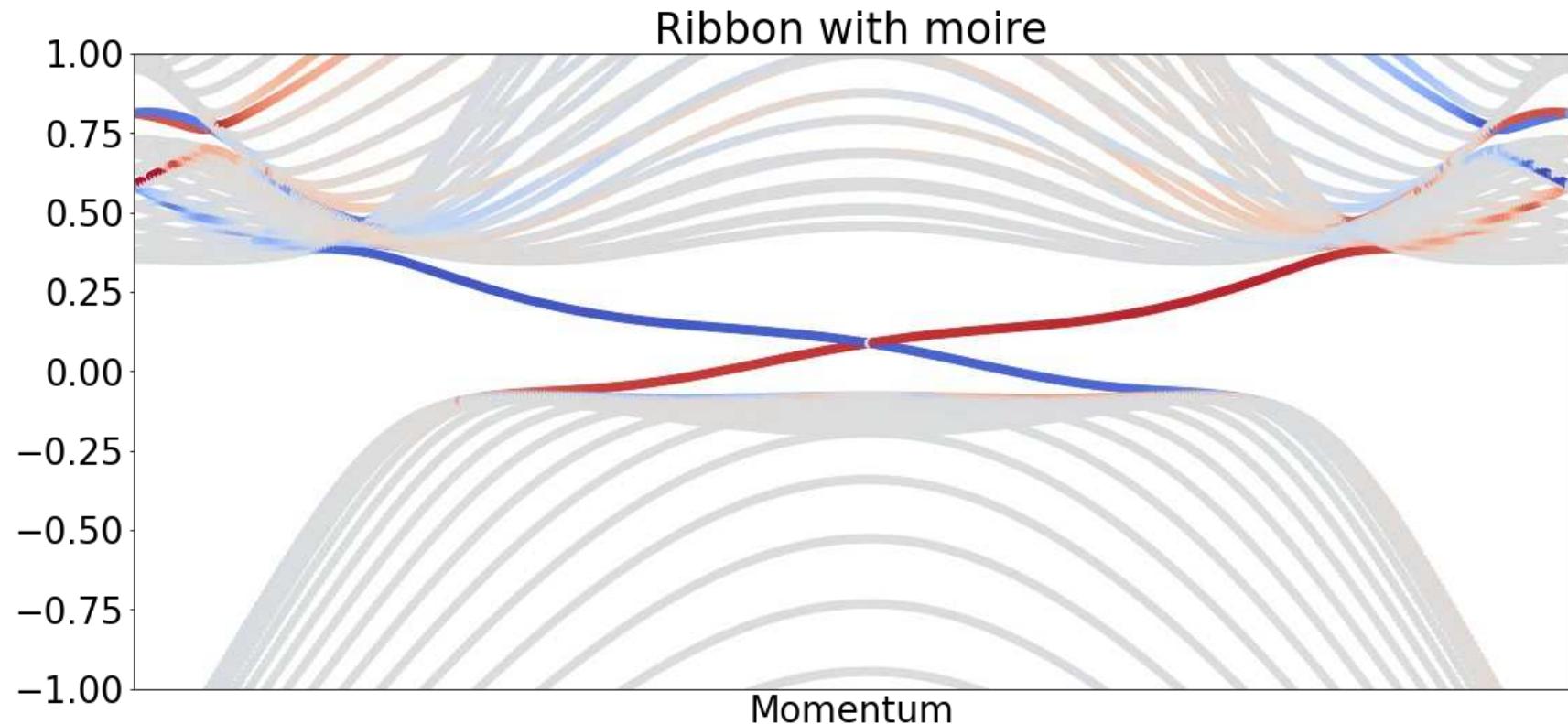
Exchange field

Rashba spin-orbit coupling

# Moire driven gaps in the band structure



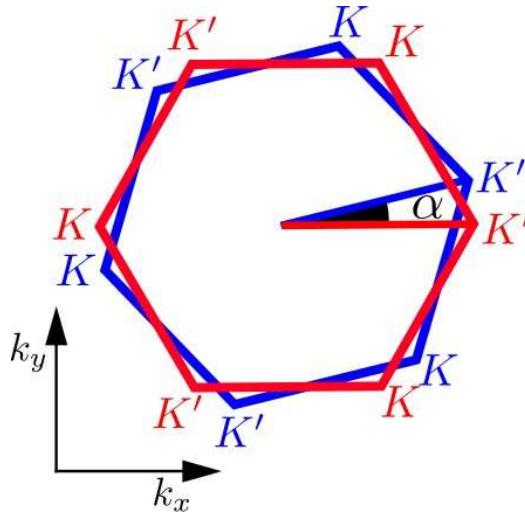
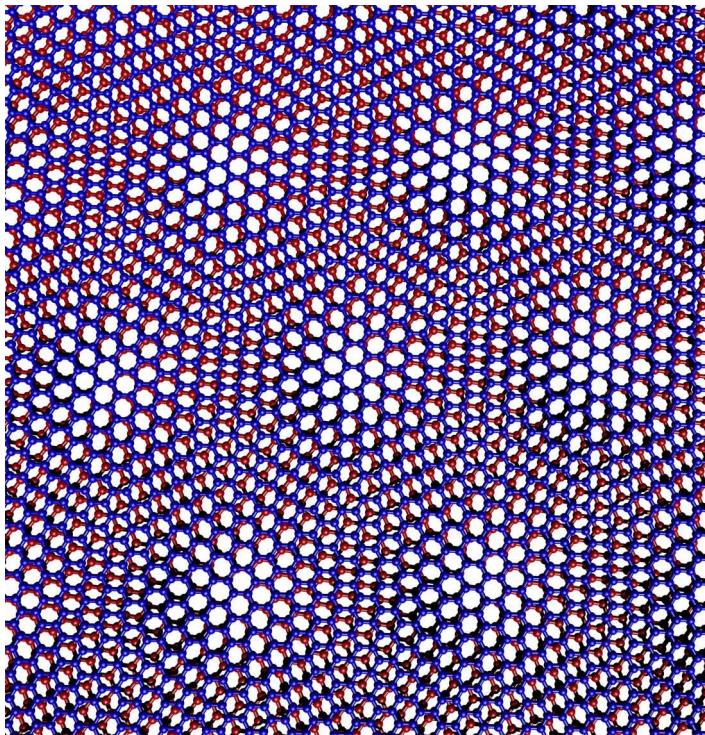
# Moire driven gaps in the band structure



Chiral states appear in a ribbon driven by the moire

# Electronic structure of twisted graphene multilayers

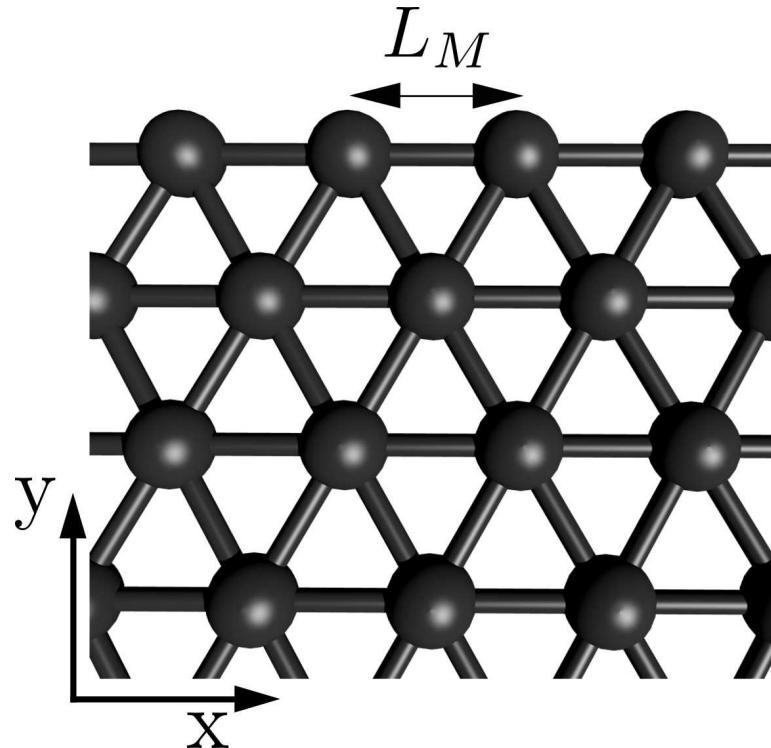
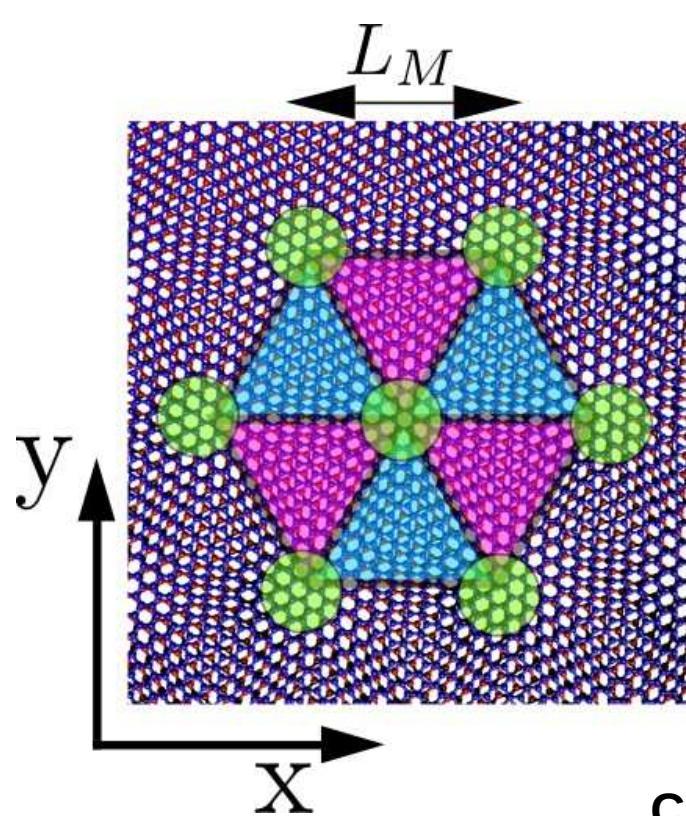
# Twisted bilayer graphene



**Additional parameters in the system**

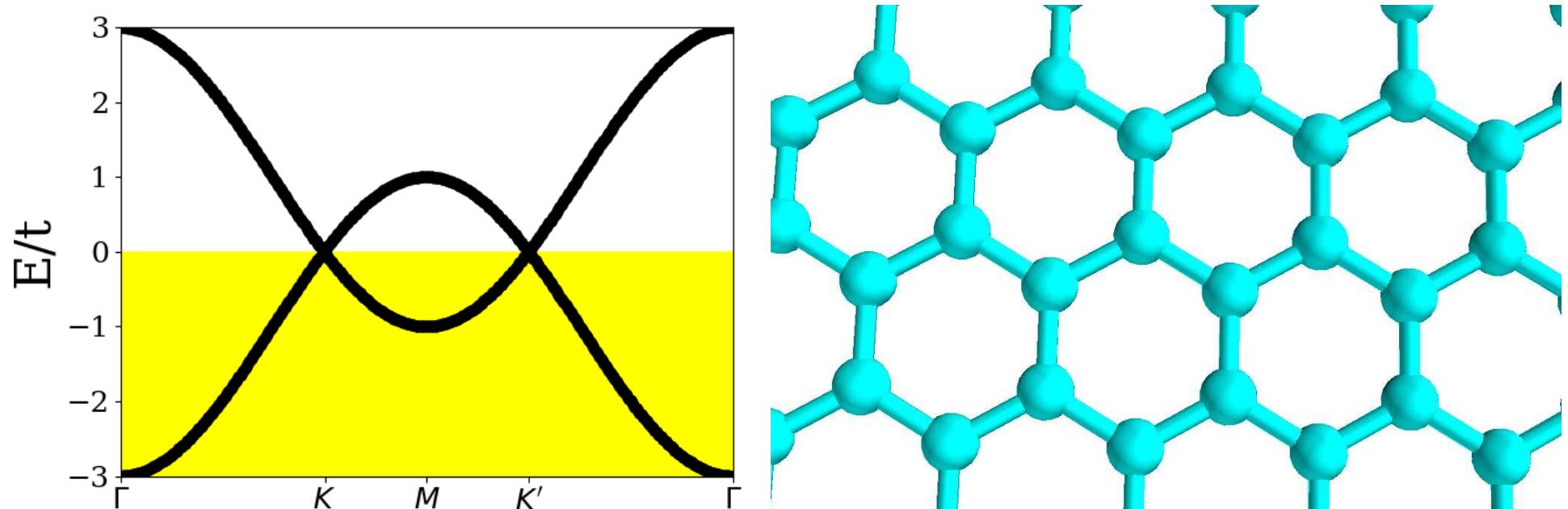
Angle between the layers  $\alpha$   
Bias between the layers  $U$

# A new length scale: the moire length



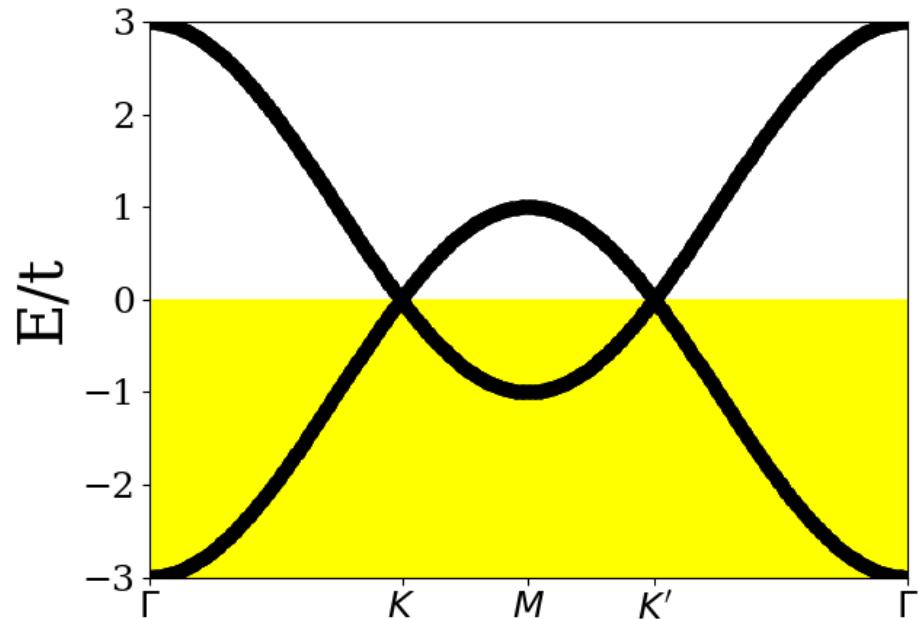
Creating effective lattices with tunable lattice constants

# Structure of graphene



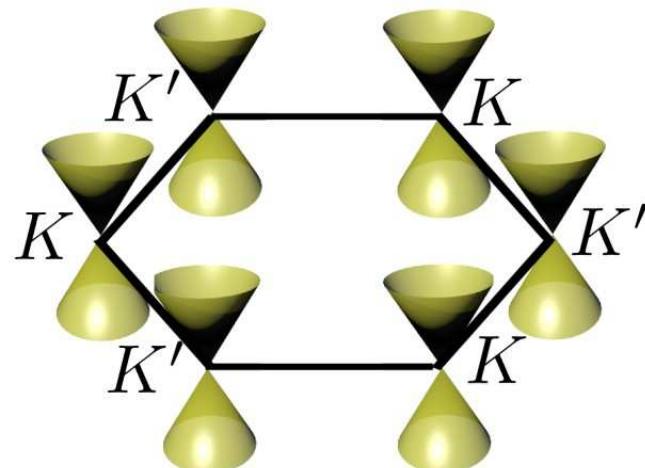
Minimal model: Single orbital in a honeycomb lattice

# The electronic structure of graphene

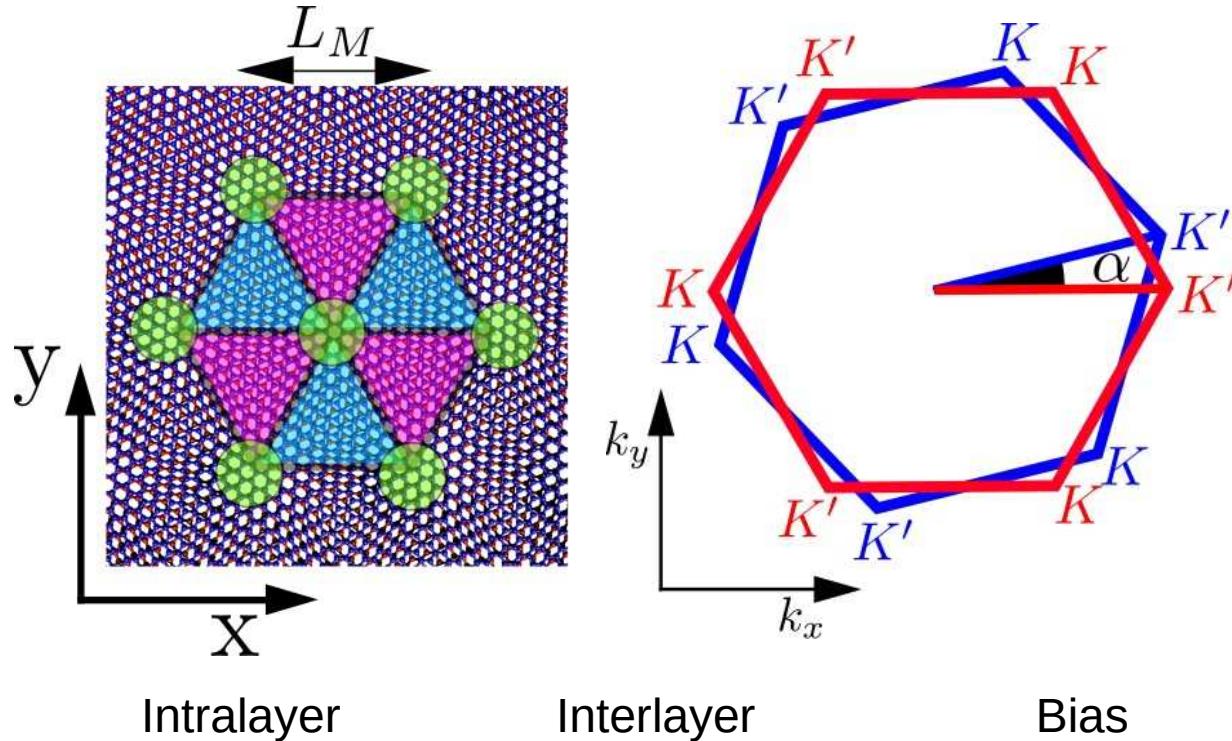


$$H = \begin{pmatrix} 0 & p_x \pm ip_y \\ p_x \mp ip_y & 0 \end{pmatrix}$$

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



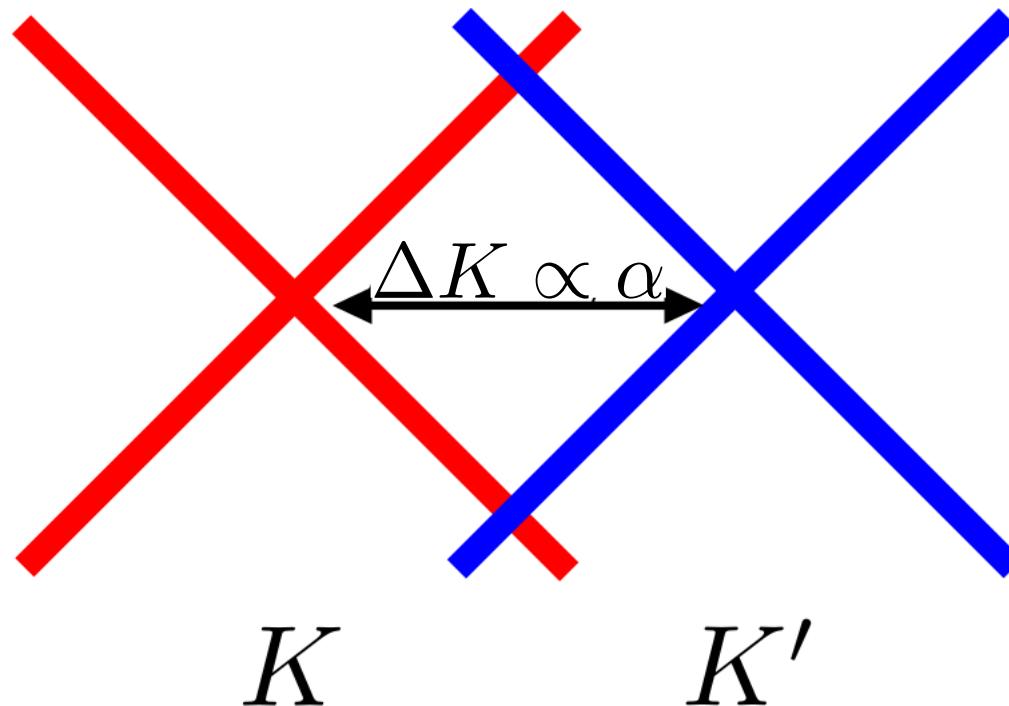
# Real and reciprocal space in twisted bilayer graphene



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

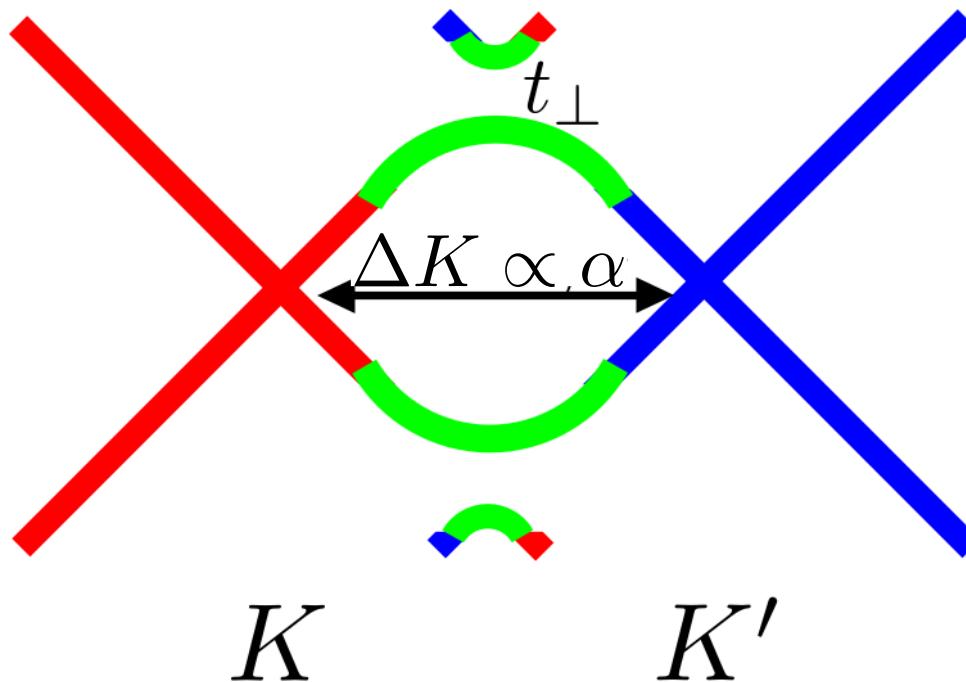
# Velocity renormalization at large angle

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



# Velocity renormalization at large angle

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

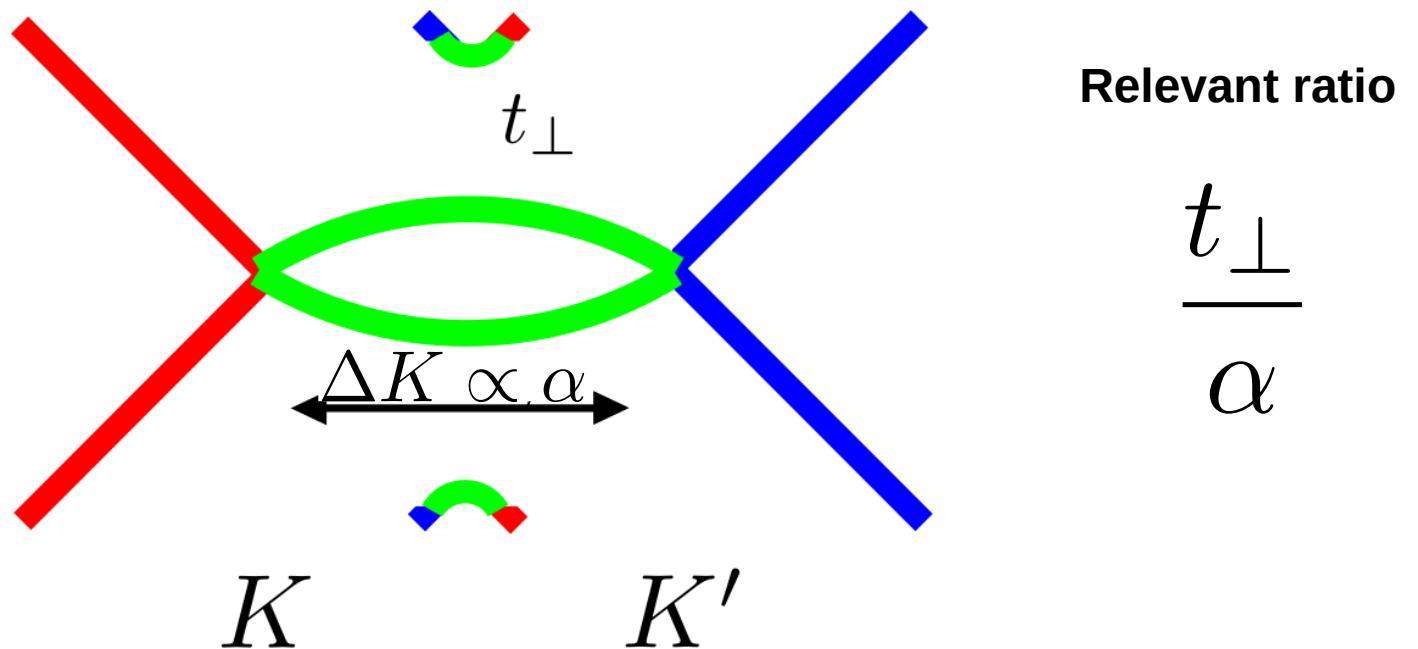


Relevant ratio

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

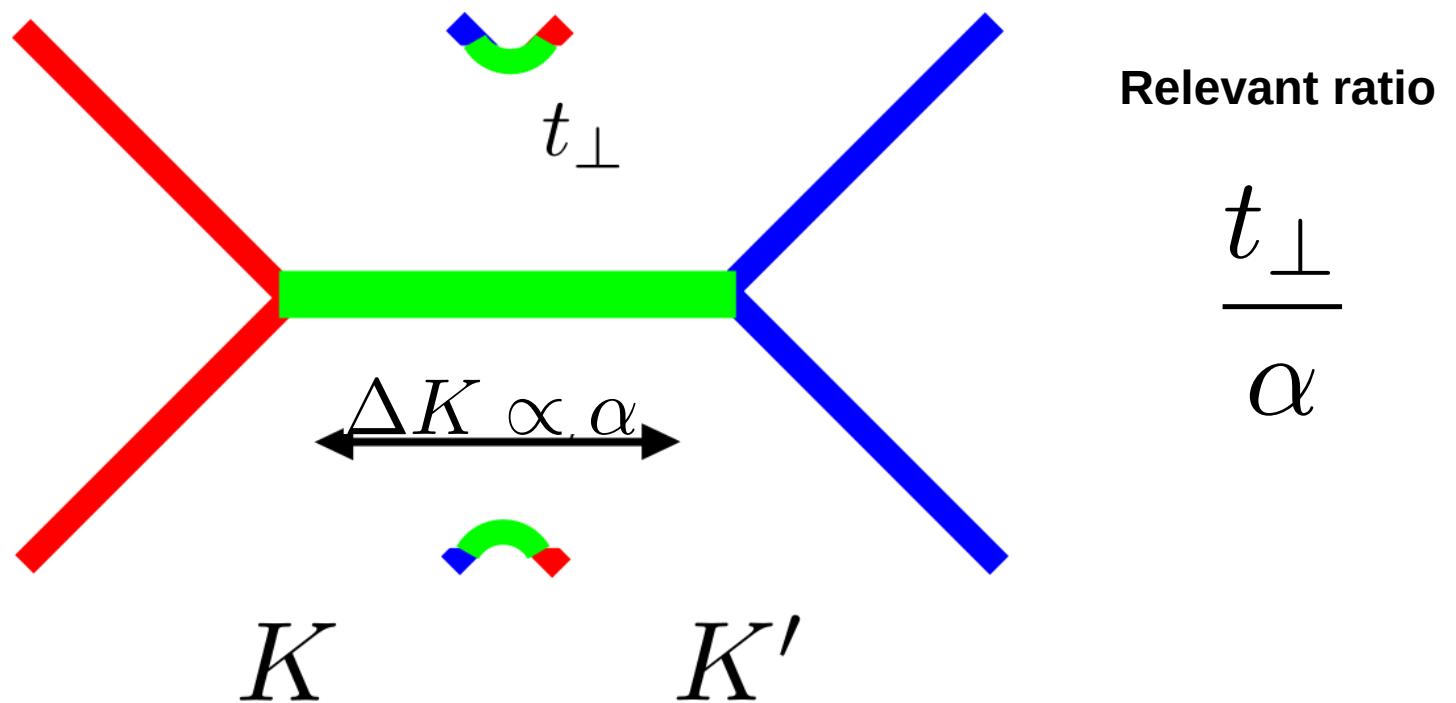
# Velocity renormalization at large angle

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

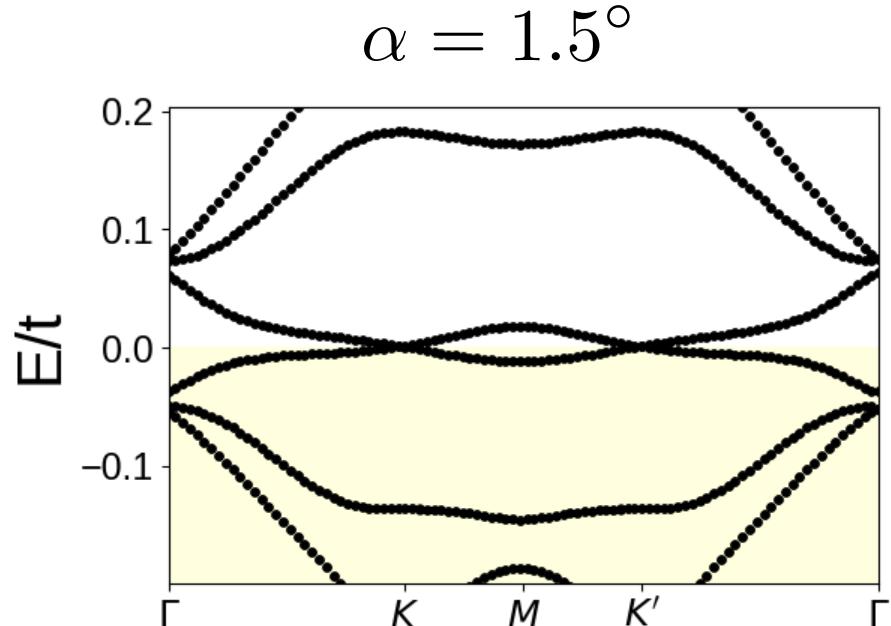
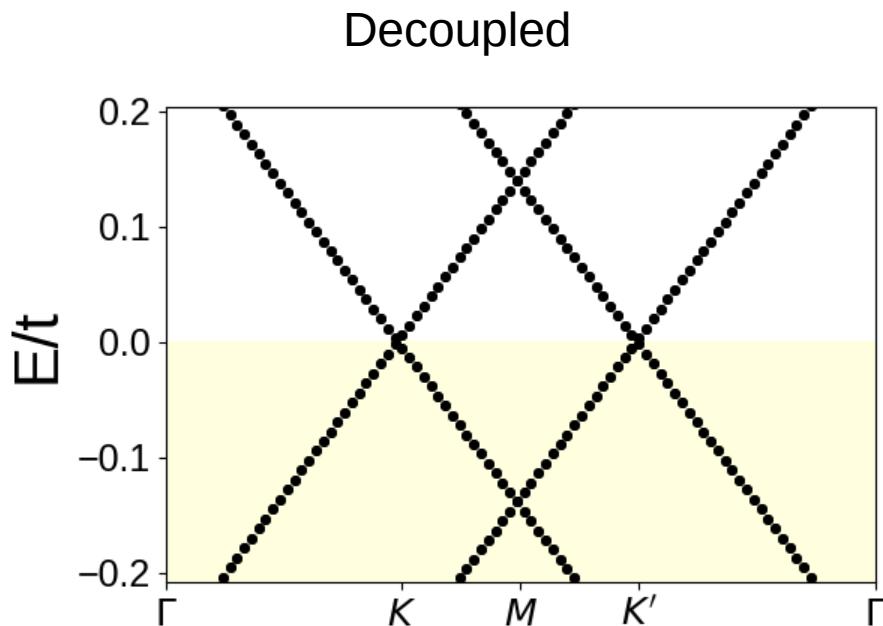


# Velocity renormalization

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

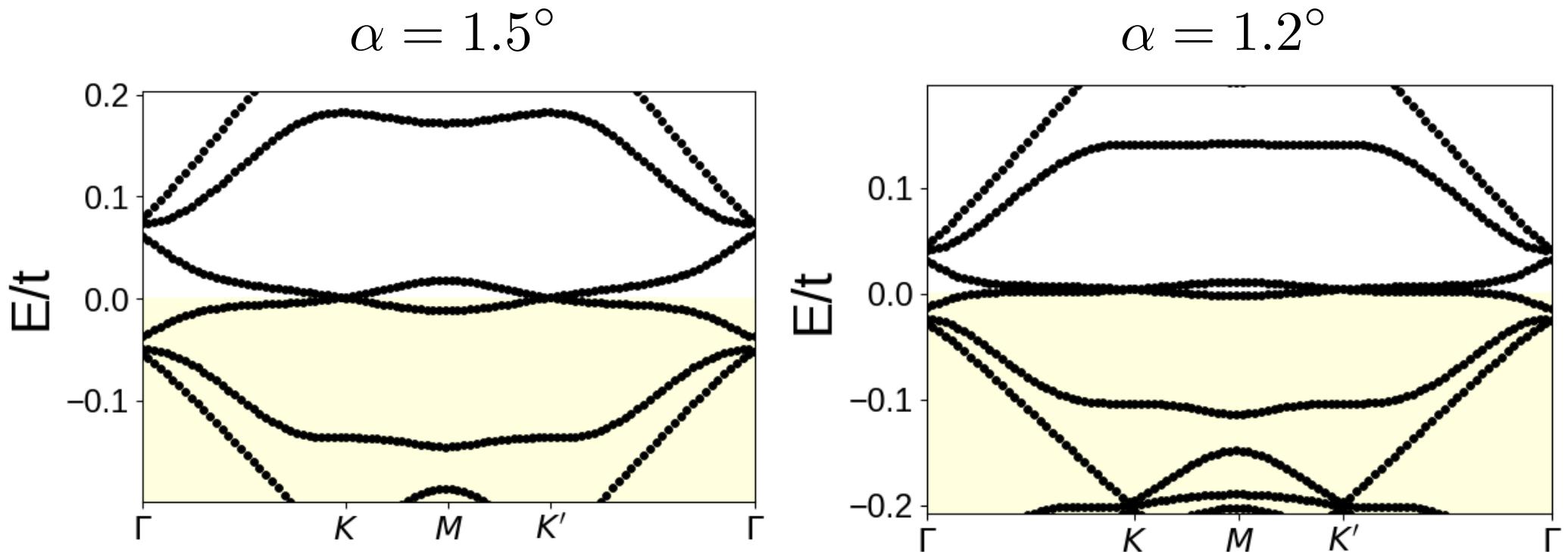


# Band structure of twisted bilayer graphene



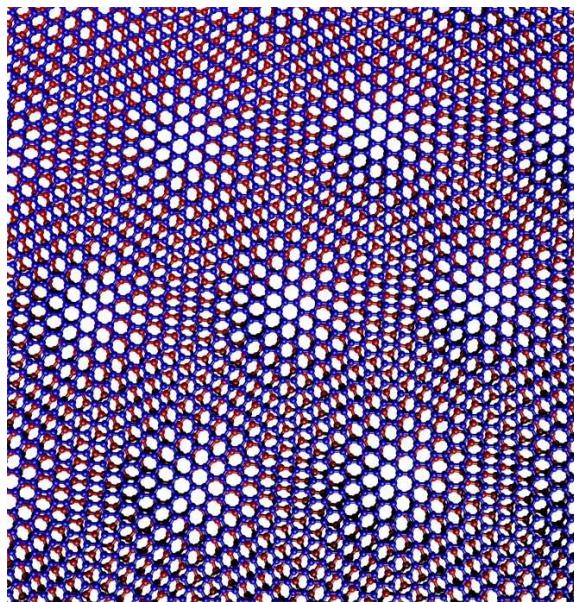
As the angle between layers is decreased, the bands become flatter

# Band structure of twisted bilayer graphene

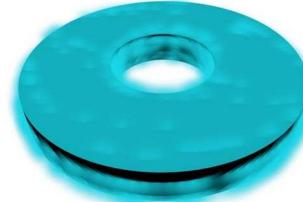


As the rotation angle approached 1 degree, the lowest band becomes flatter

# Correlations in twisted bilayer graphene flat bands

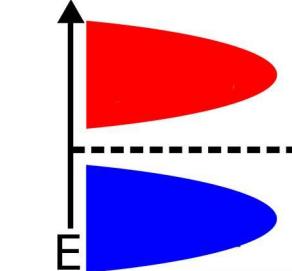


*Superconductivity*



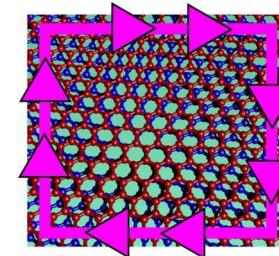
*Nature* 556, 43–50 (2018)

*Correlated insulators*



*Nature* 556, 80–84  
(2018)

*Chern insulators*



*Science* 365, 605–608  
(2019)

*Fractional Chern insulators*

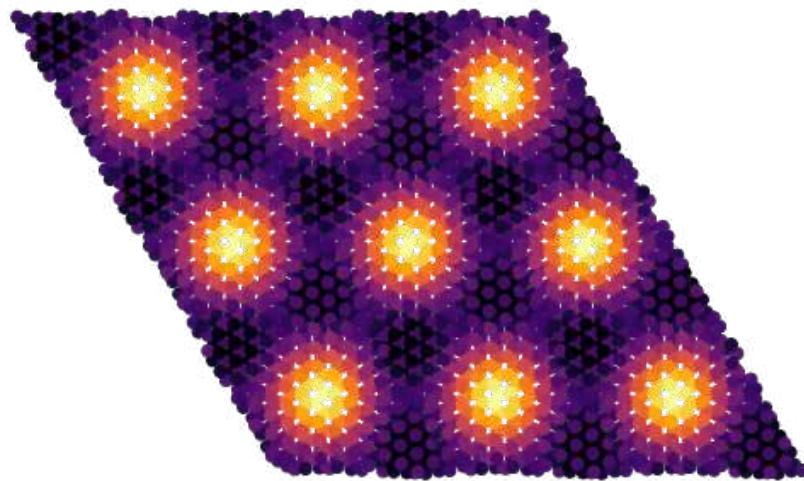


*Nature* 600, 439–443  
(2021)

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

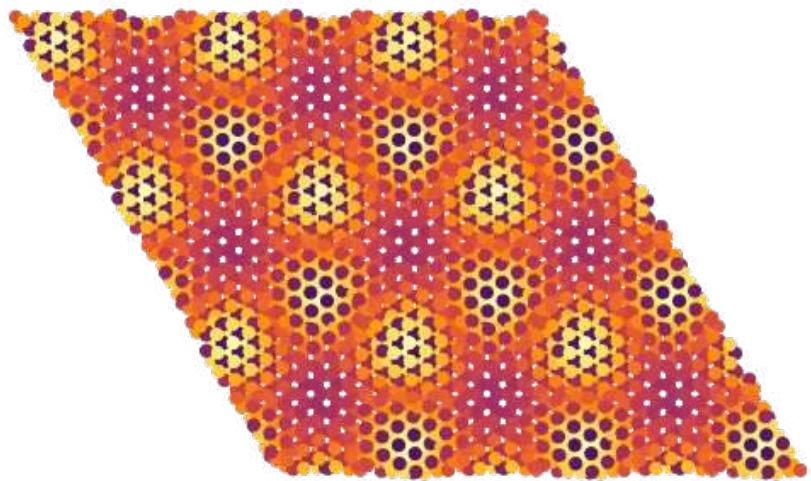
# Distribution of states in the twisted graphene bilayer

$E = 0.0$



*Triangular*

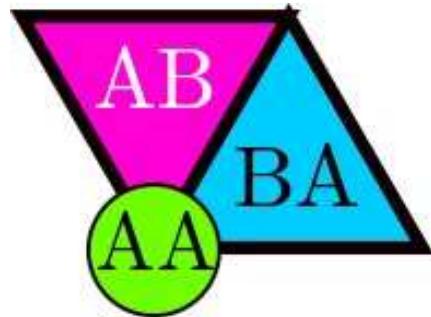
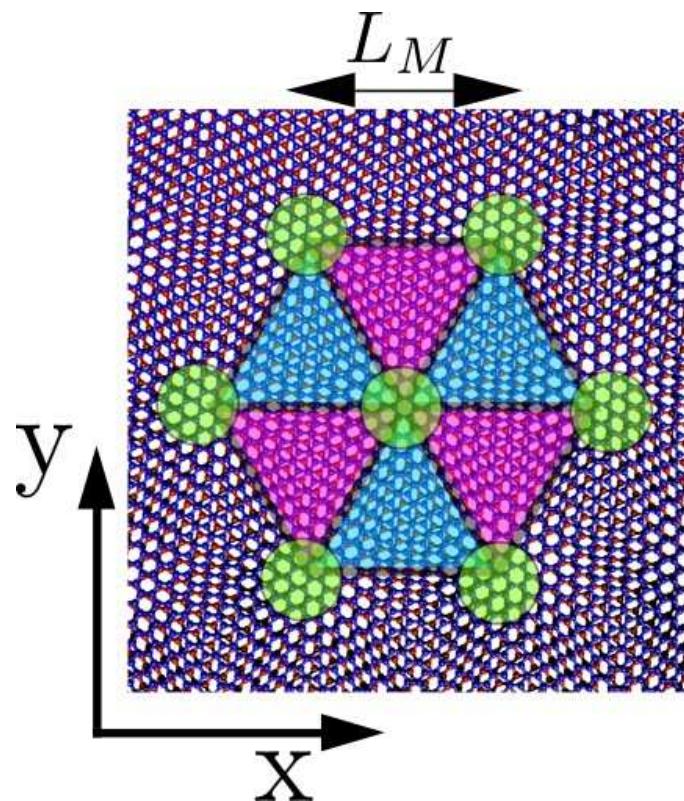
$E = 0.25$



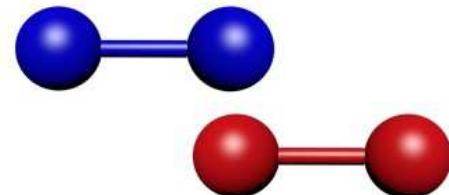
*Hexagonal*

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

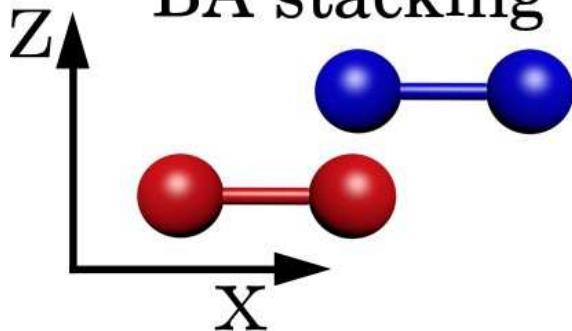
# Stacking of twisted bilayer graphene



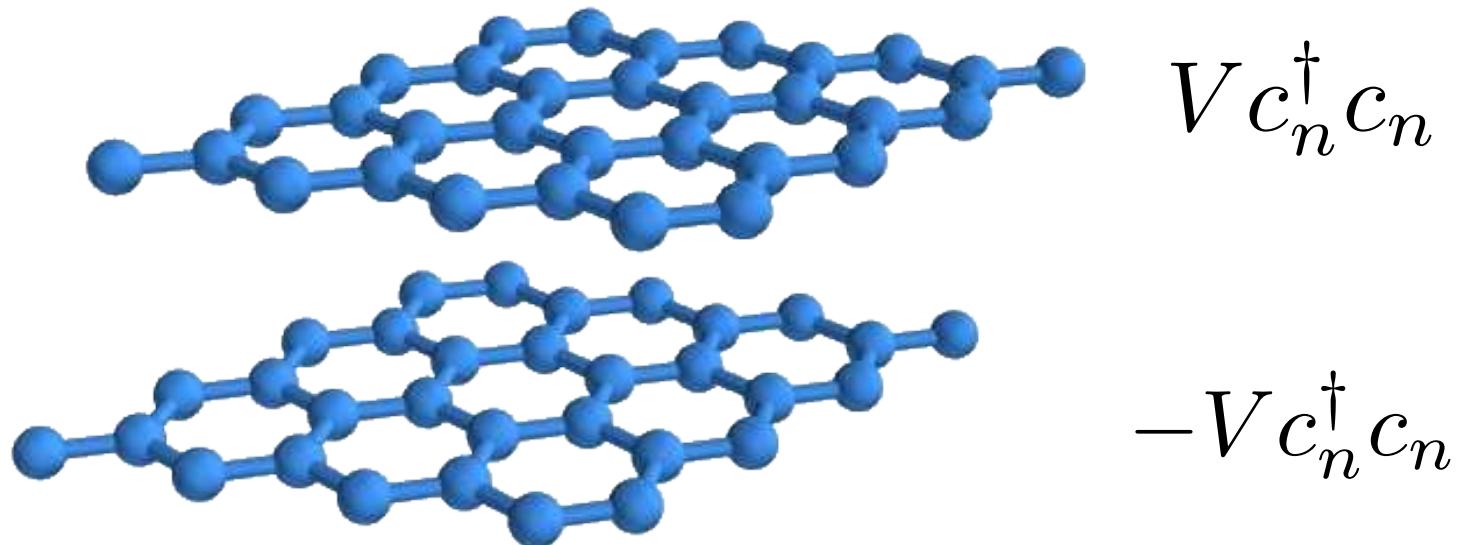
AB stacking



BA stacking



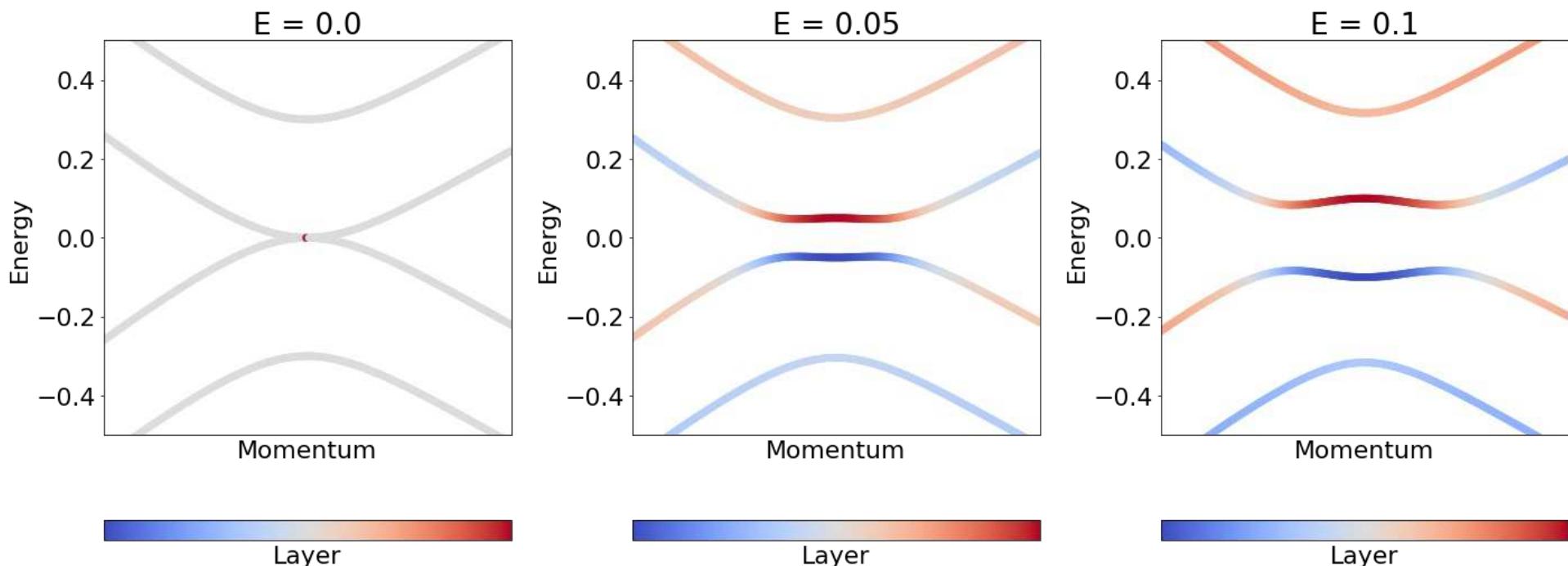
# Bias in AB bilayer graphene



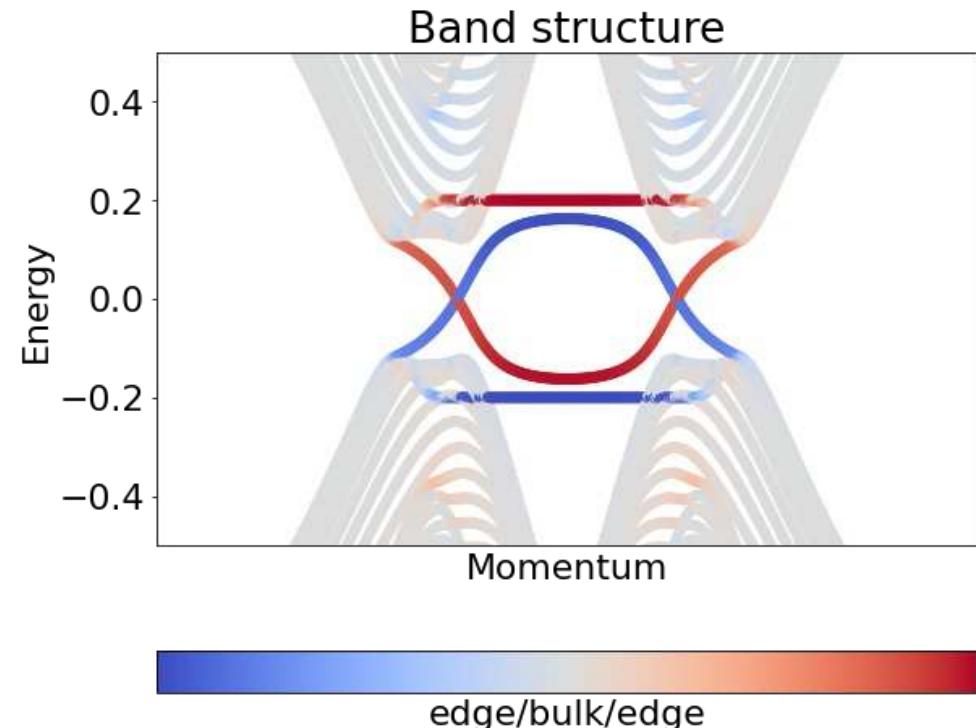
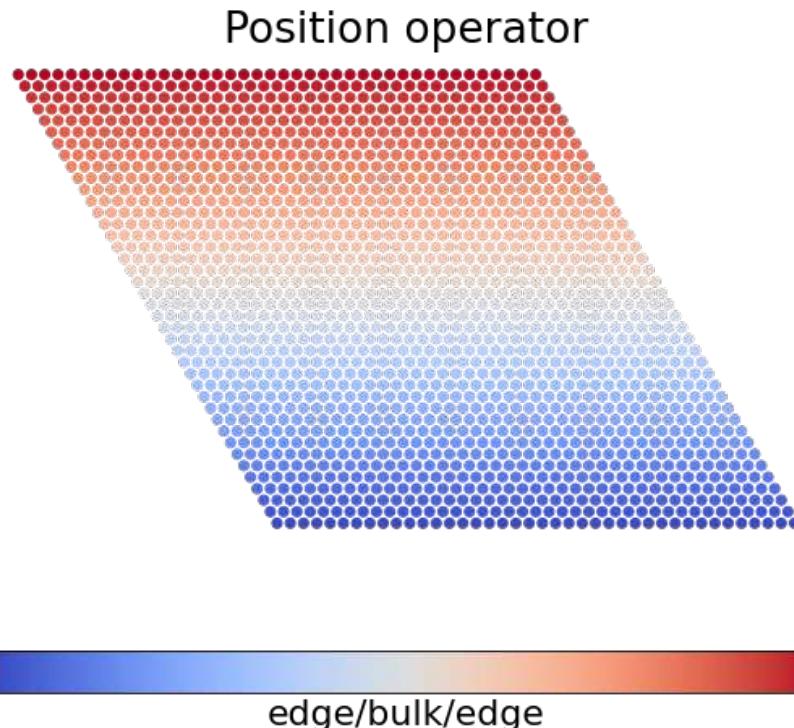
Let us look at the impact of a bias in an aligned graphene bilayer

# The electronic structure of bilayer graphene

Graphene bilayers open a gap when an interlayer bias is applied

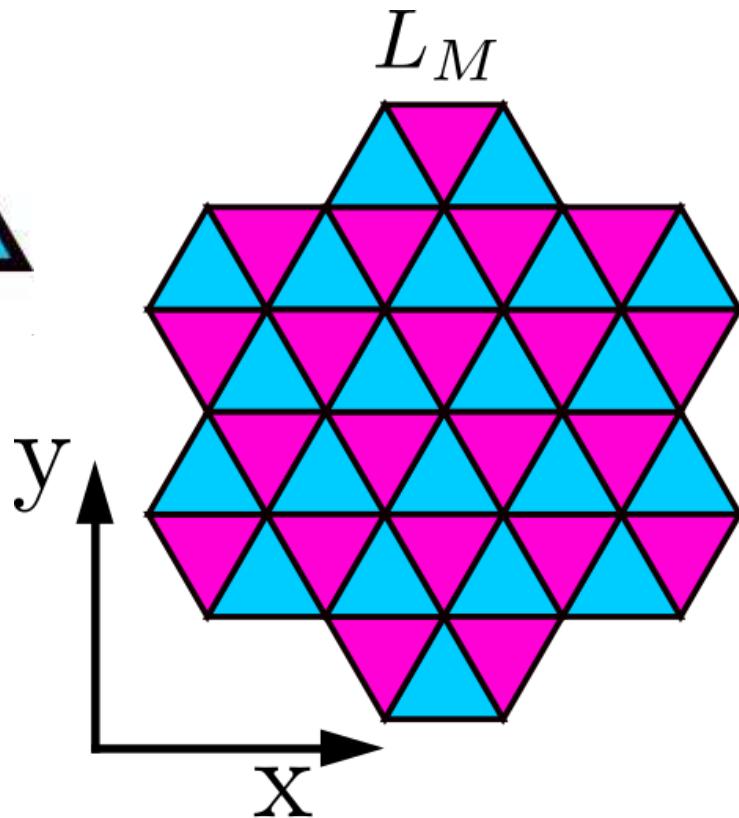
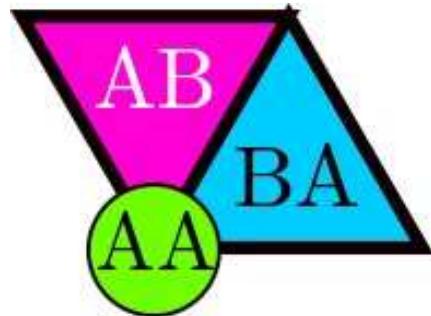
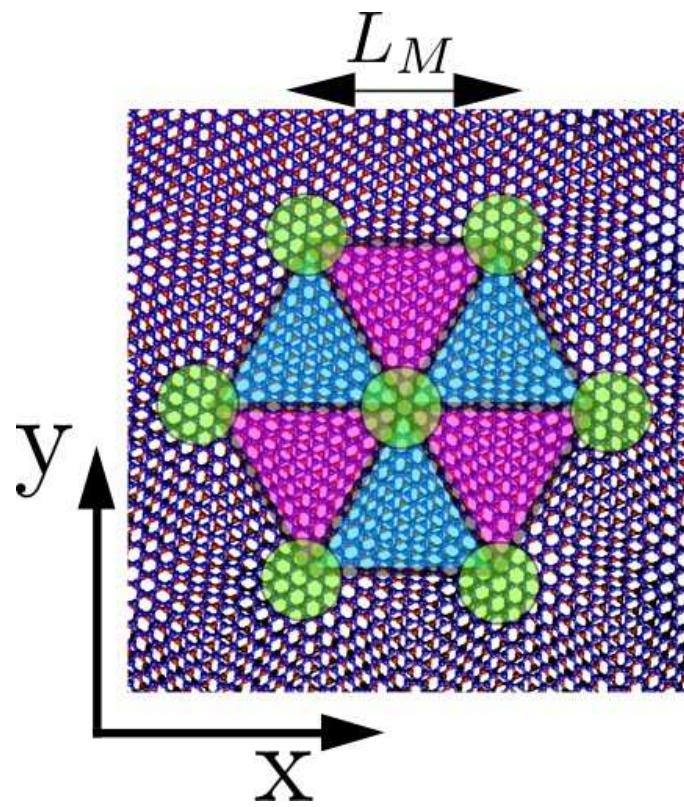


# Biased bilayer graphene, pseudo-helical states

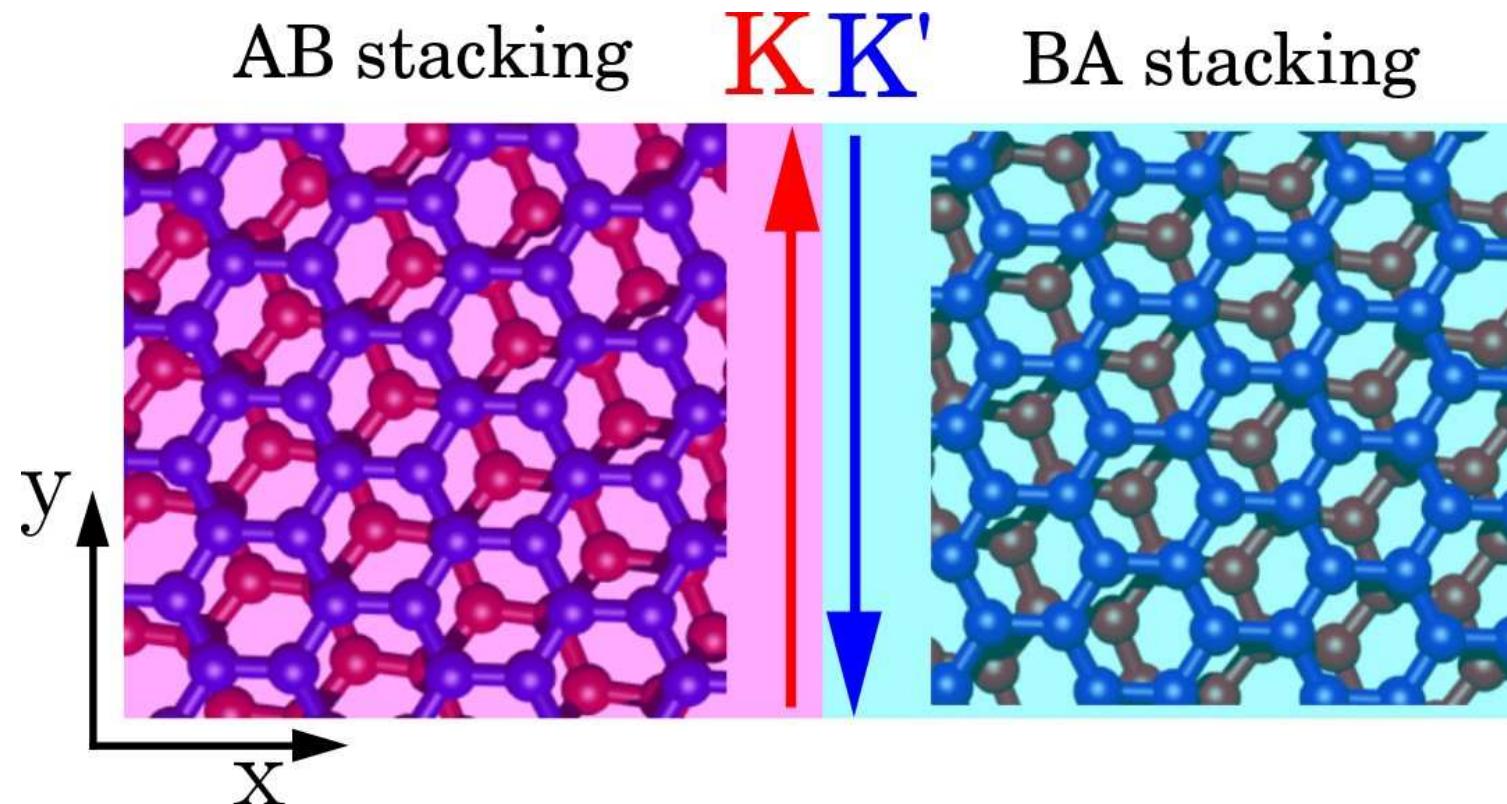


Edge states appear in the presence of a bias between layers

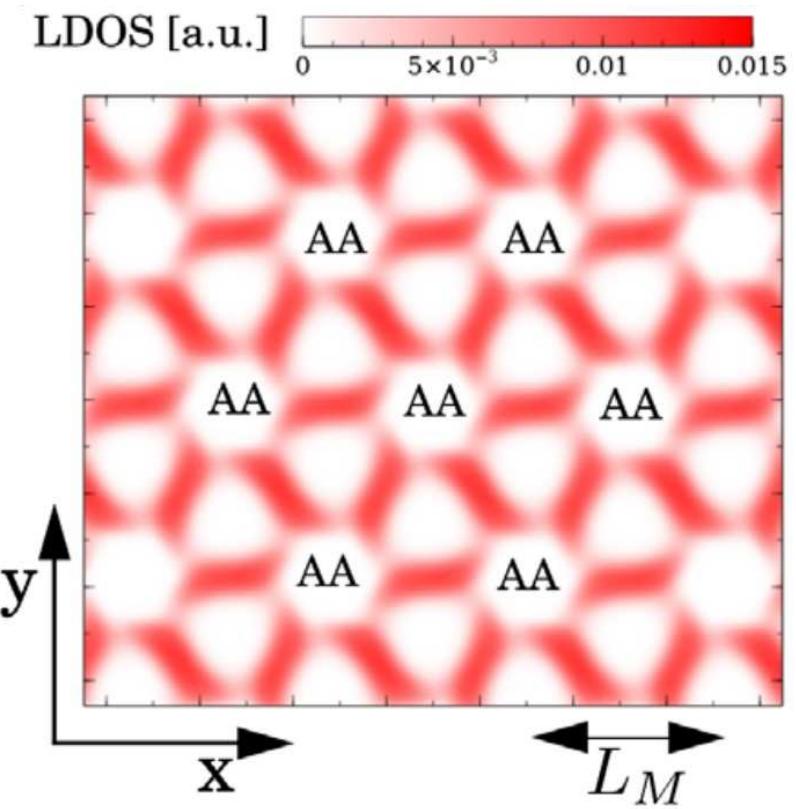
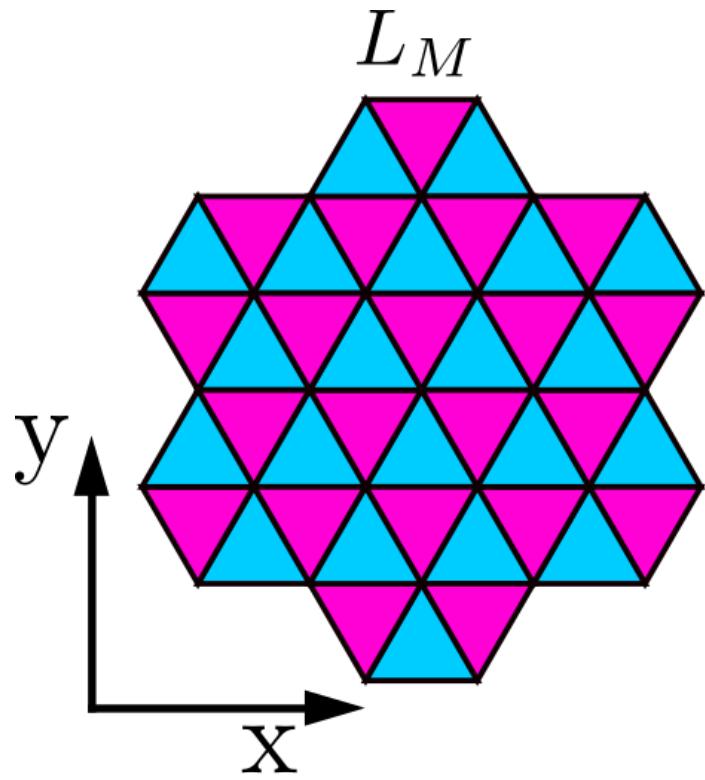
# Stacking of twisted bilayer graphene



# Interfacial modes in biased TBG

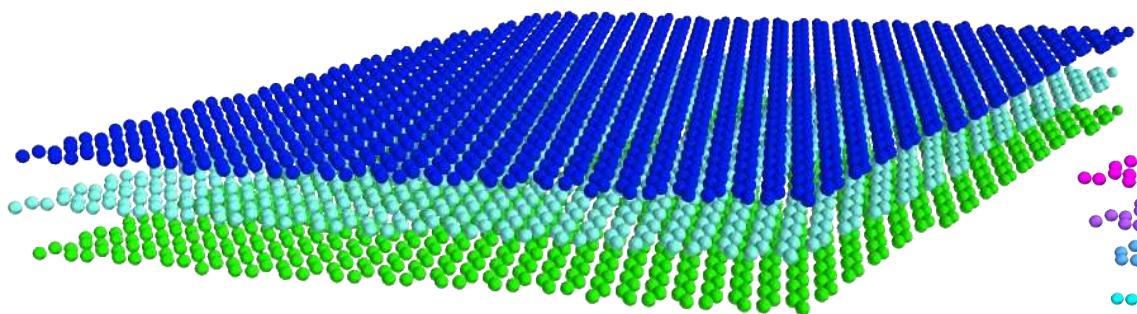


# Helical networks in TBG

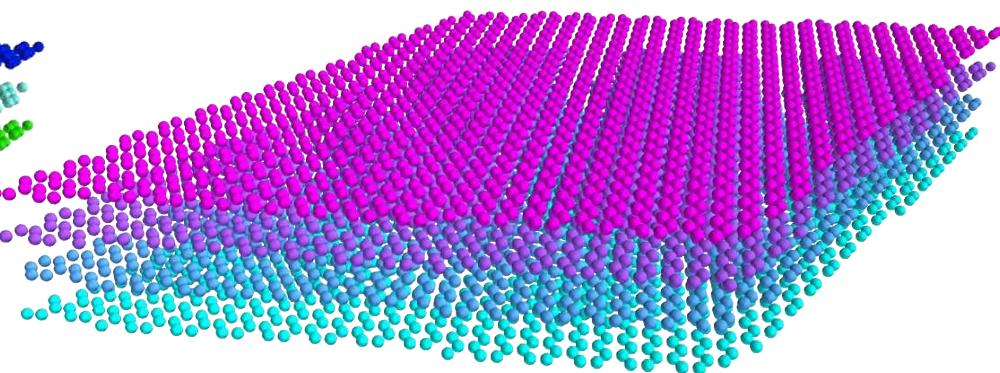


# Other twisted graphene multilayers

Twisted graphene trilayer

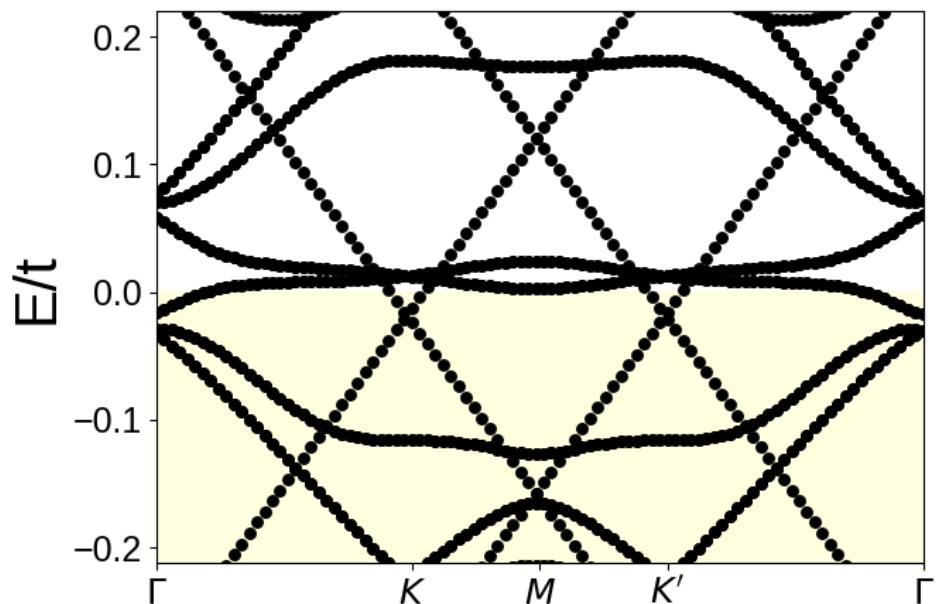


Twisted graphene double bilayer

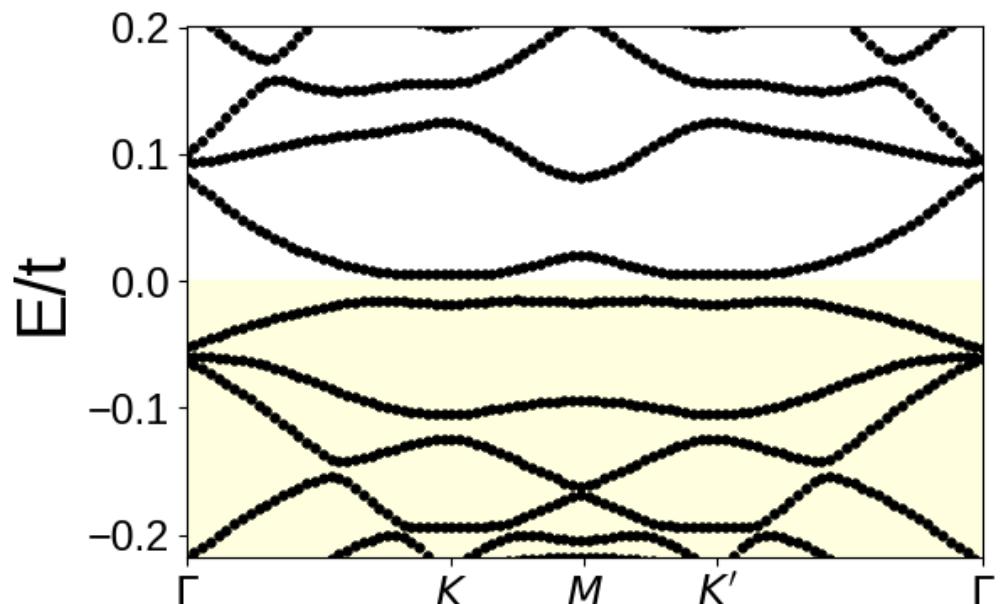


# Other twisted graphene multilayers

Twisted graphene trilayer



Twisted graphene double bilayer



Flat and dispersive moire bands appear in generic twisted graphene multilayers

# For the exercise session this afternoon

Download the Jupyter-notebook from

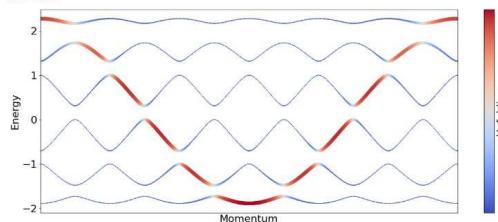
[https://github.com/joselado/emergent\\_phenomena\\_in\\_van\\_der\\_Waals\\_school\\_tifr\\_2023](https://github.com/joselado/emergent_phenomena_in_van_der_Waals_school_tifr_2023)

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
b = g.get_bands()
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 = g.get_r(0) # get the position of the first site
fpot = lambda r: 1.0*((r-r0).dot(r-r0)<=2) # impurity in site r0
# fpot is pythonic and readable ; fpot is a potential; import(r0,v=1.) # this is equivalent

h.add_potential(fpot) # now add the impurity potential
kpath = g.get_kpath() # a complete k path in the original Brillouin zone, just by extending the reciprocal vectors
(k,e,c) = h.get_bandstructure("unfold",kpath=kpath) # compute band structure
plt.figure(figsize=(10,5)); plt.xlabel("Momentum"); plt.ylabel("Energy"); plt.xticks([]); plt.yticks([-2,-1,0,1,2])
plt.colorbar(label="Unfolding")
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

