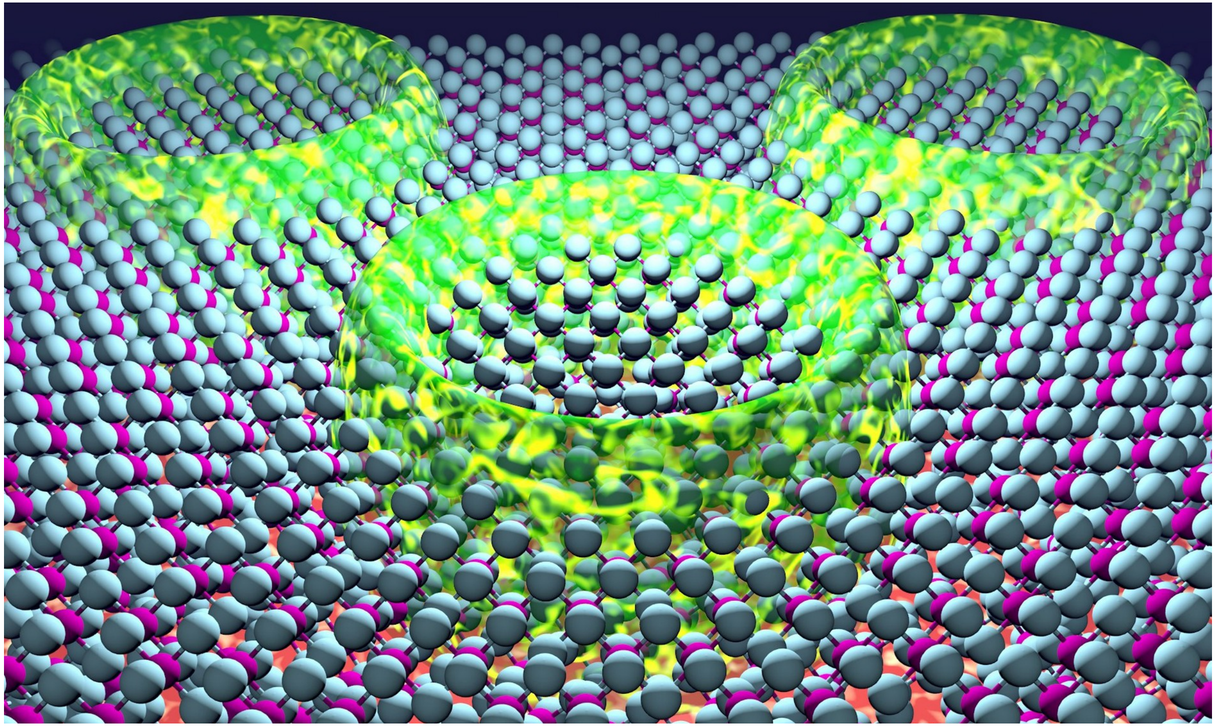
Lecture 3: Moire electronic states and twisted van der Waals heterostructures



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

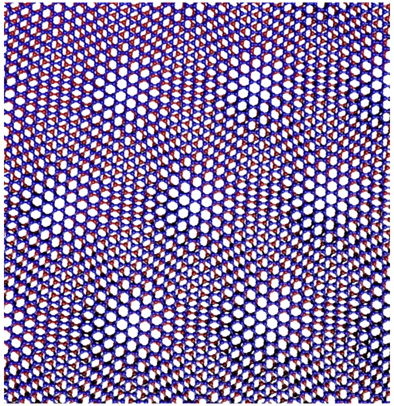
- 30 min lecture
- 5 min break
- 30 min lecture

You can download the slides and software from

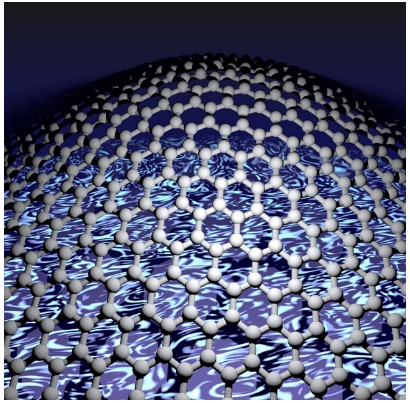
https://github.com/joselado/emergent_phenomena_in_van_der_Waals_school_tifr_2023

Moire materials

Twisted graphene multilayers



Buckled 2D materials

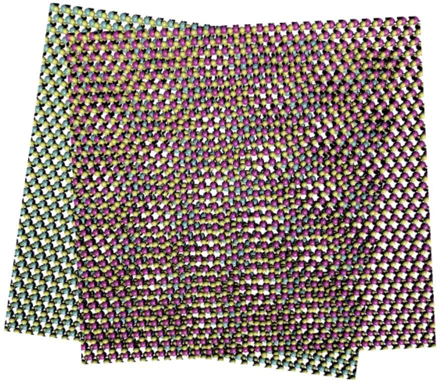


graphene

Moire states in several layers

Moire states in single layer

Twisted TMDCs

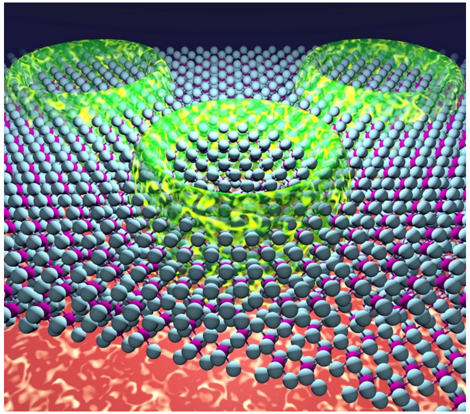


MoS_2, WSe_2

Moire states in single/several layer

Moire in electronic properties

Twisted magnetic 2D materials



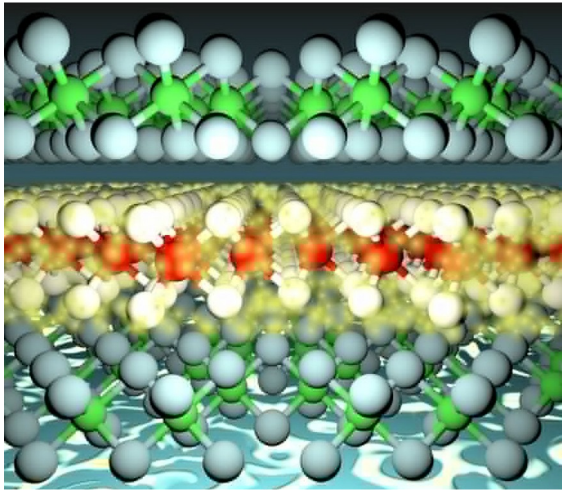
$CrCl_3$, $CrBr_3$

Moire magnetism

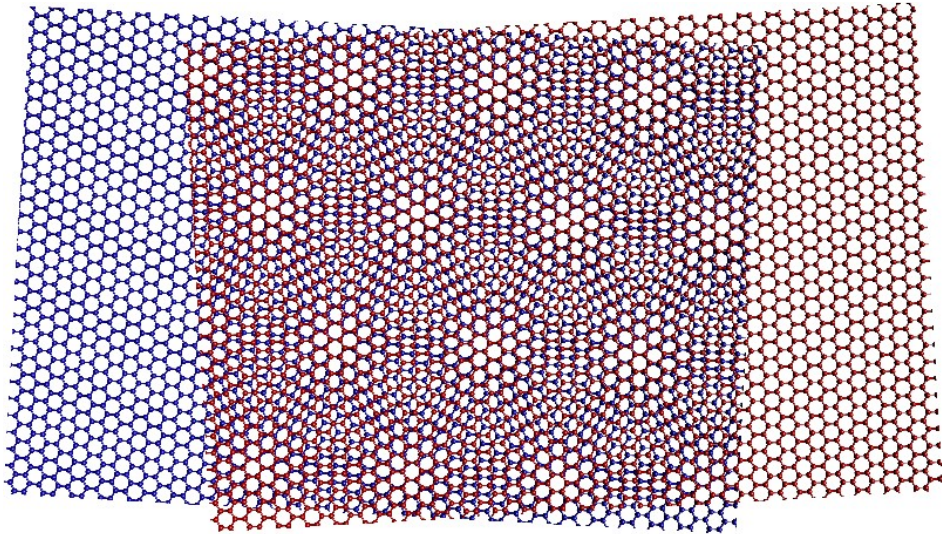
Moire in magnetic properties

How to create moire states with 2D materials

Stacking



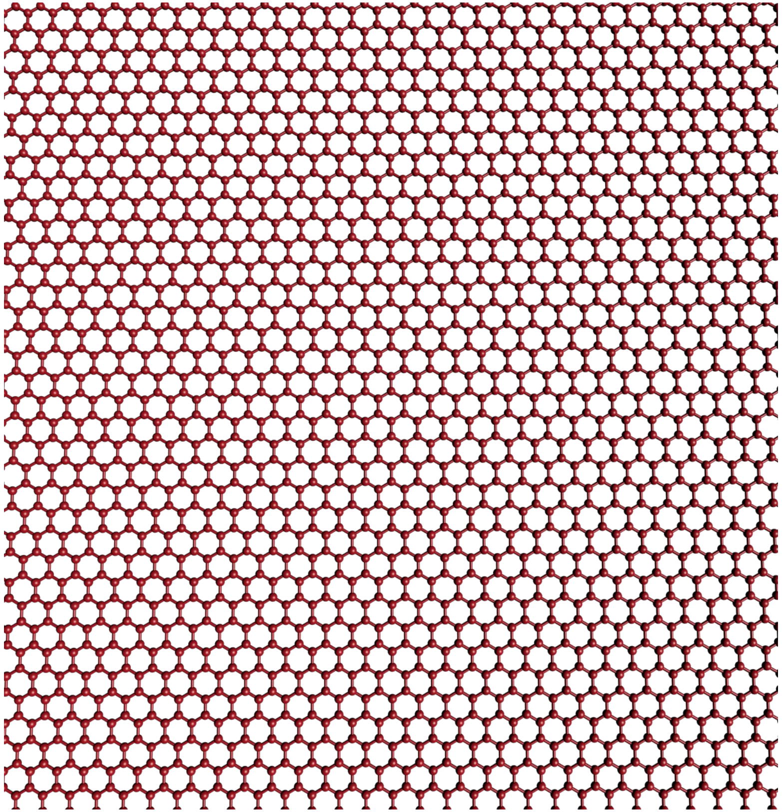
Rotating



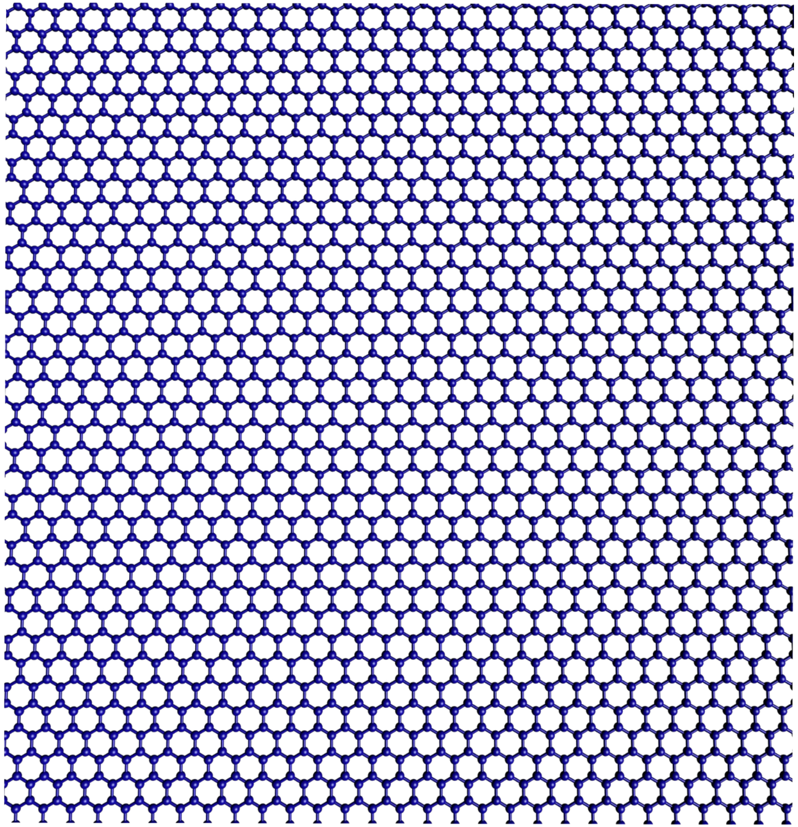
These are unique features of two-dimensional materials

A bilayer van der Waals heterostructure

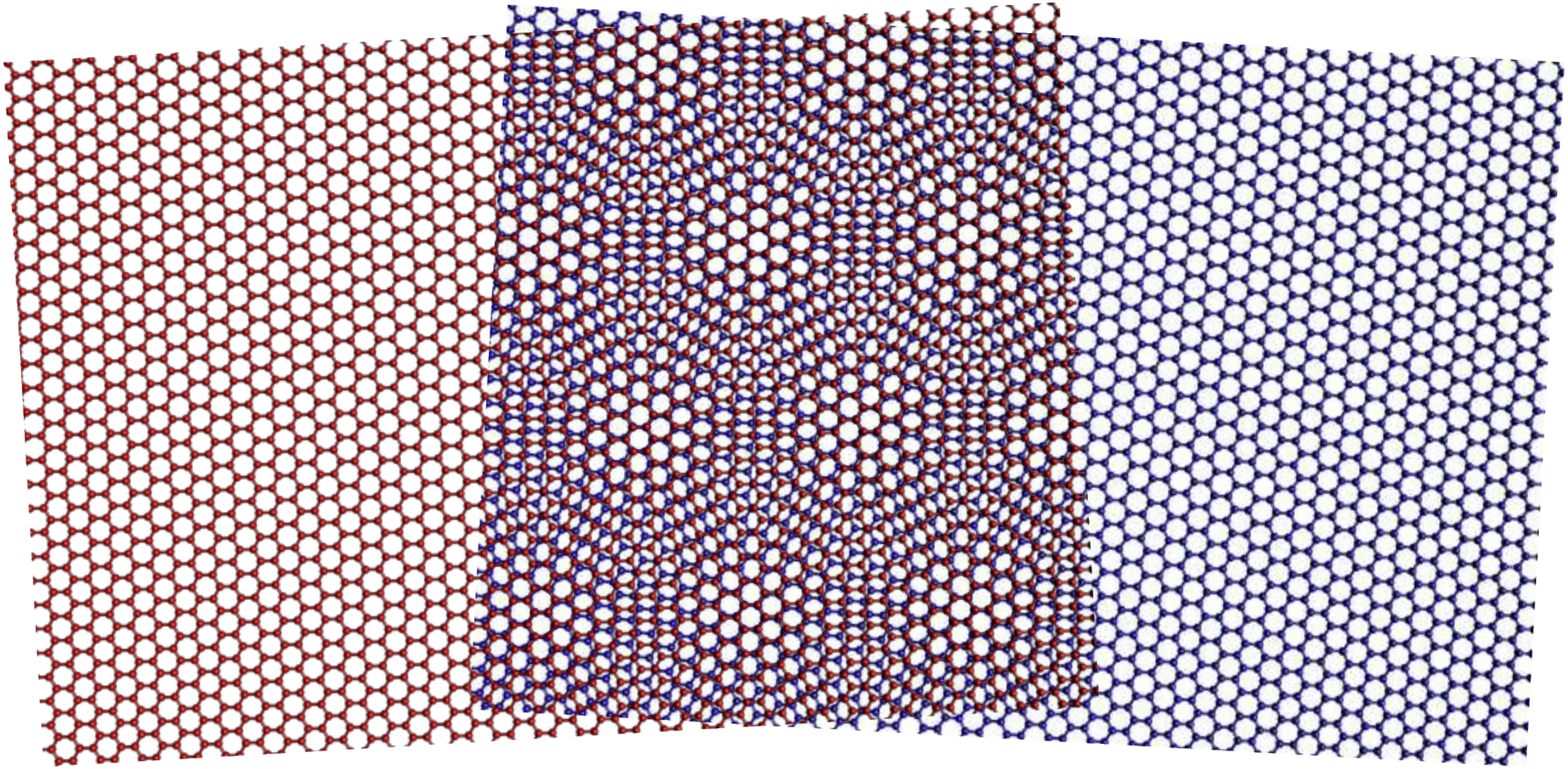
Upper graphene layer



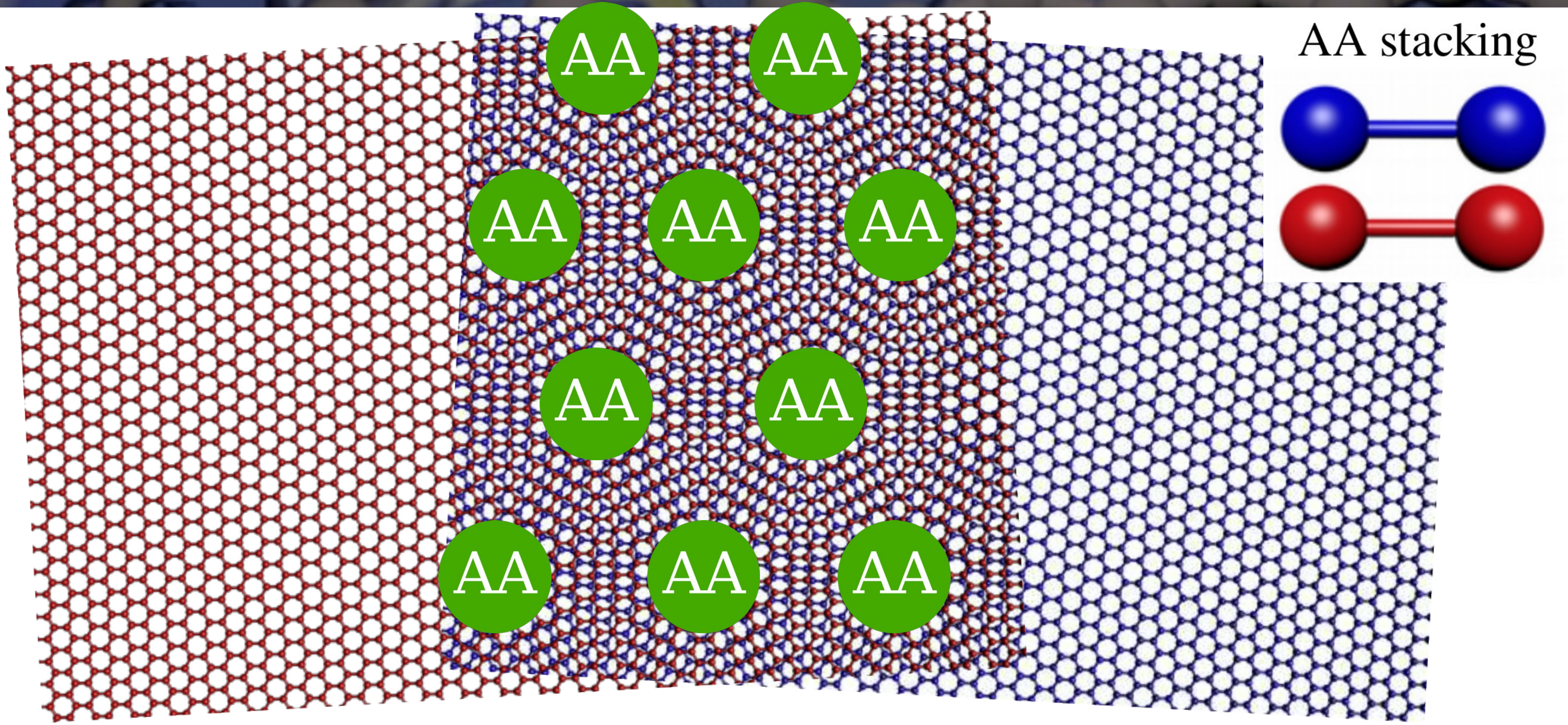
Lower graphene layer



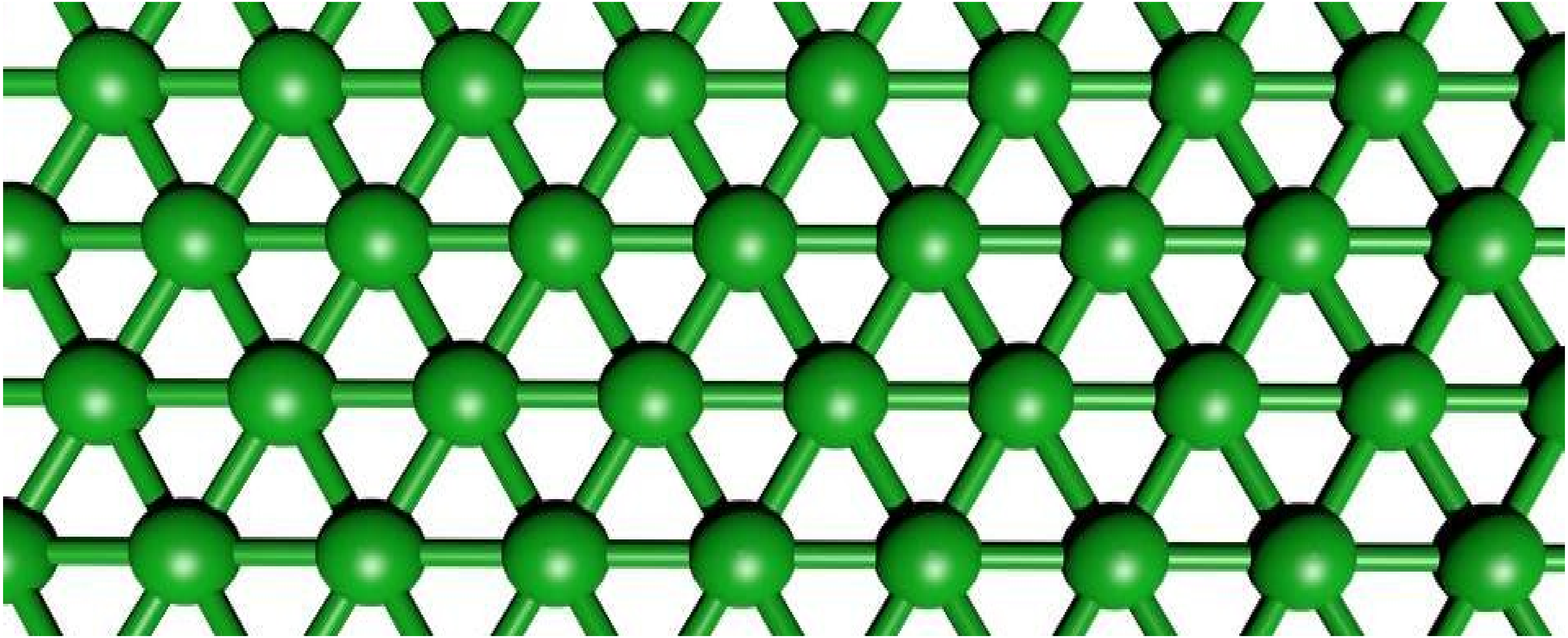
A bilayer van der Waals heterostructure



A bilayer van der Waals heterostructure

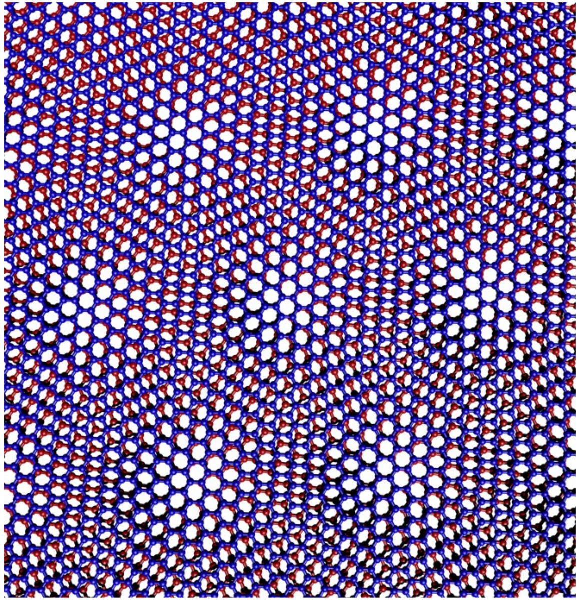


A bilayer van der Waals heterostructure

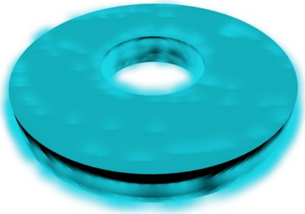


Electronic states in a single moire superlattice

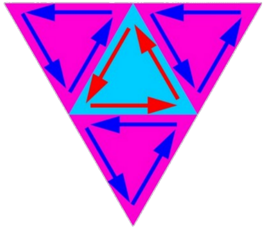
Twisted bilayer graphene



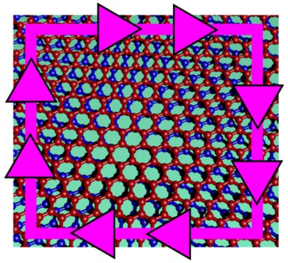
Superconductivity



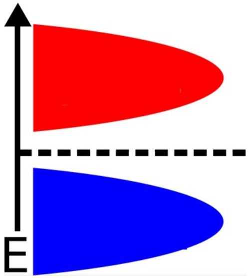
Topological networks



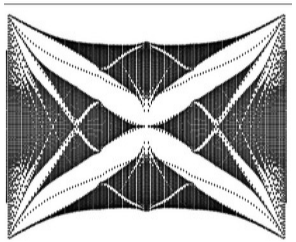
Chern insulators



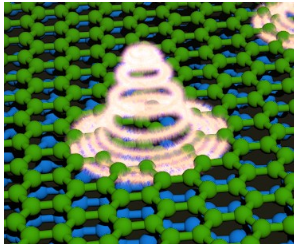
Correlated insulators



Quasicrystalline physics



Fractional Chern insulators

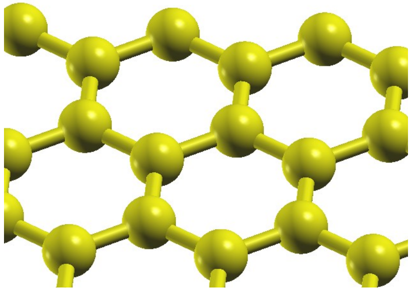


A single twisted van der Waals material realizes a variety of widely different electronic states

The building blocks for twisted van der Waals heterostructure

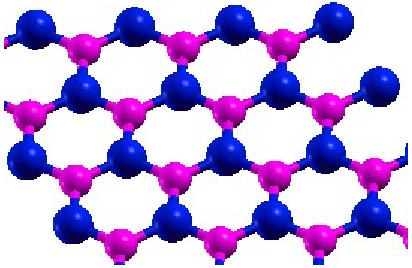
Semimetal

Graphene



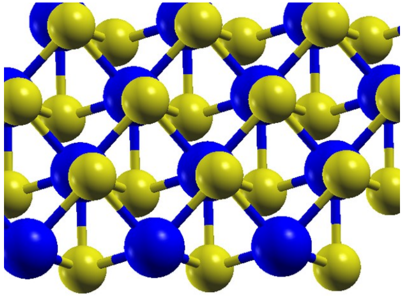
Insulator

BN



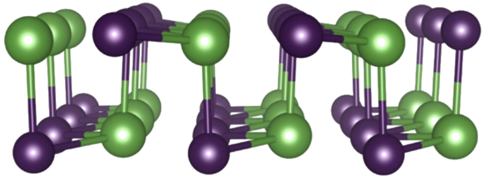
Superconductor

$NbSe_2$



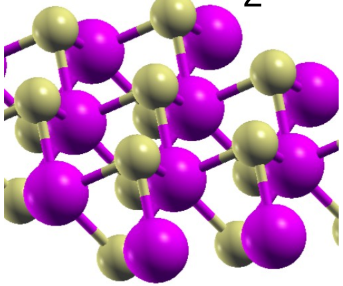
Ferroelectric

SnTe



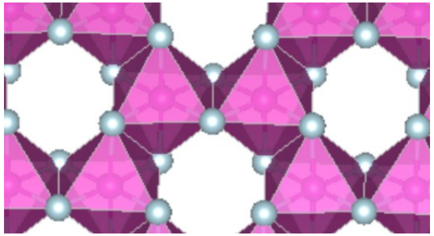
Semiconductor

WSe_2



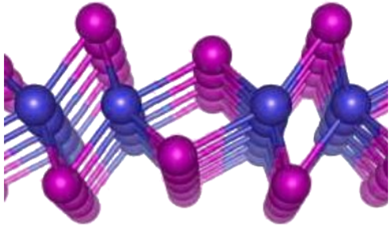
Ferromagnet

CrI_3



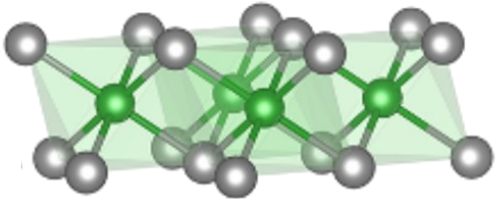
Quantum spin Hall insulator

WTe_2



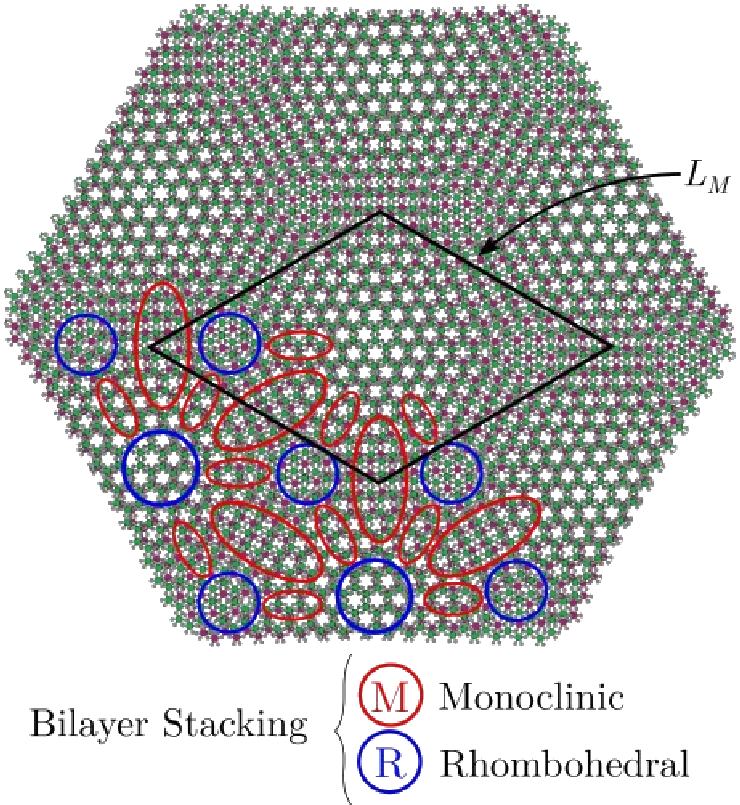
Multiferroic

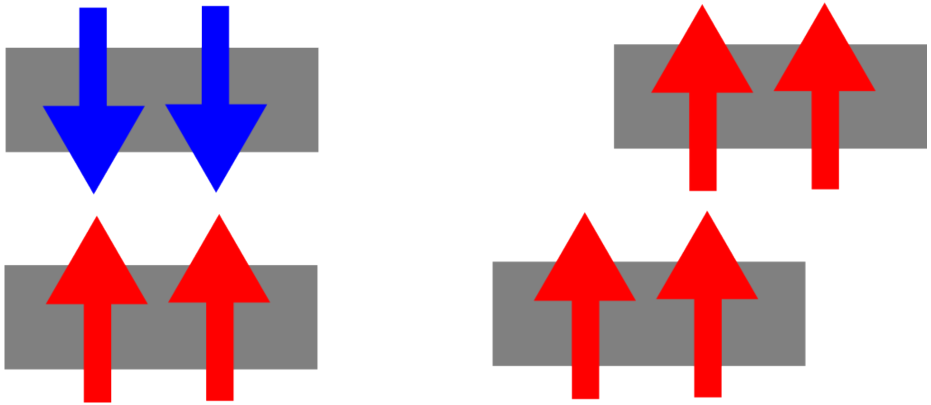
NiI_2



Twisted 2D magnetic materials

$CrCl_3$, $CrBr_3$

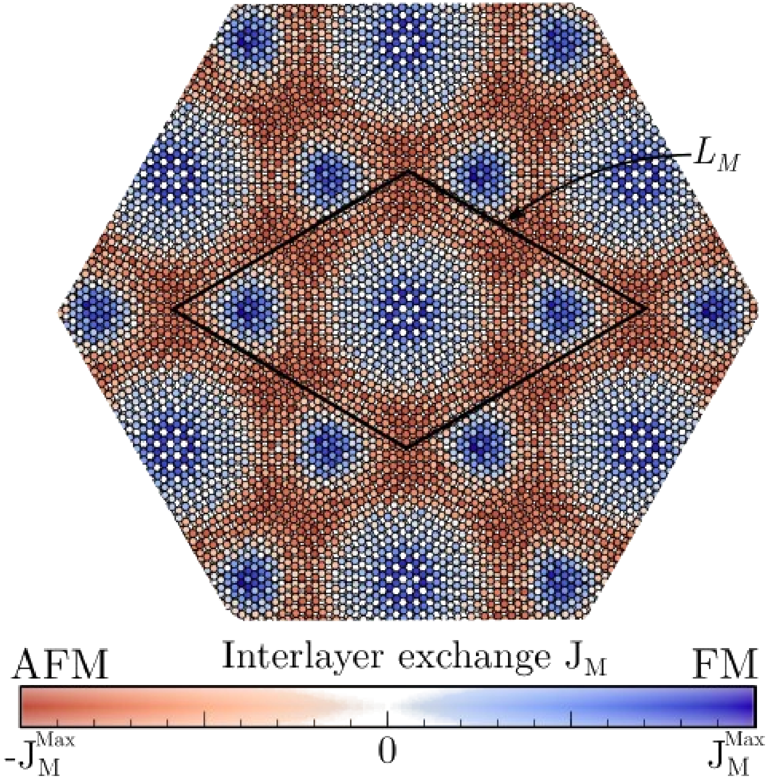


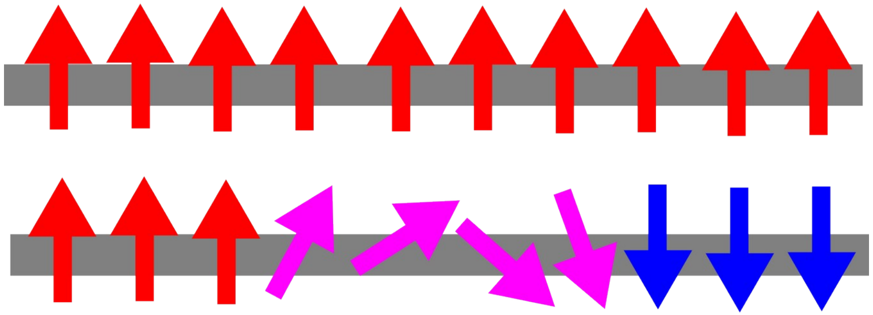


The local stacking determines
the coupling between layers

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

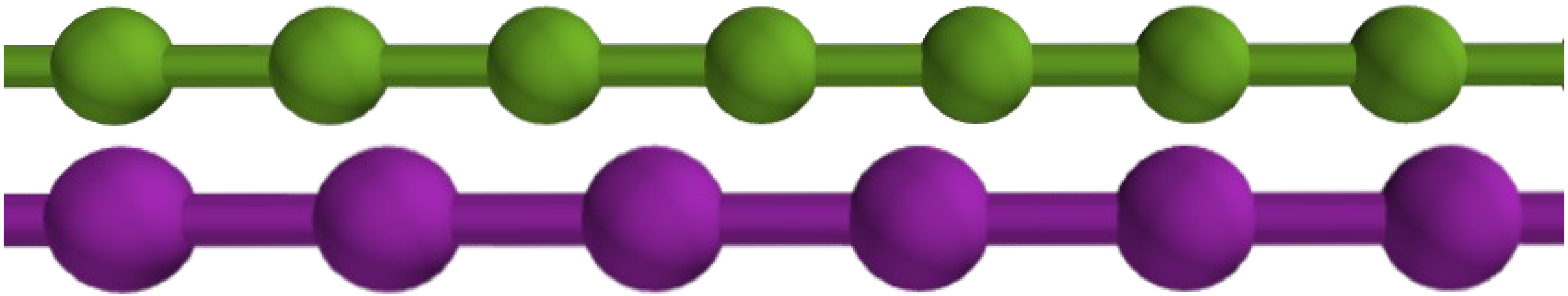
Wavevector of the spin spiral

Spin rotation axis

Superpotentials and quasiperiodicity

A minimal moire potential

Let us now take a one dimensional superlattice



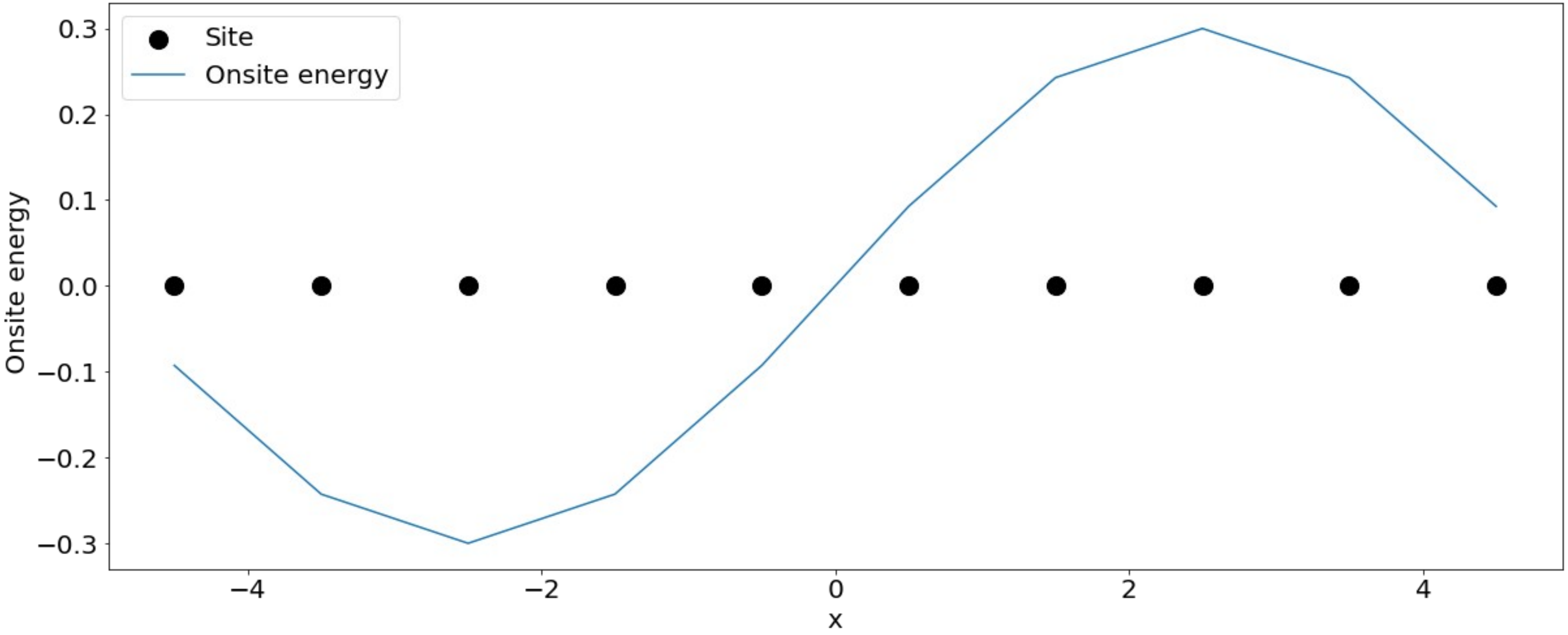
We have now two length scales

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

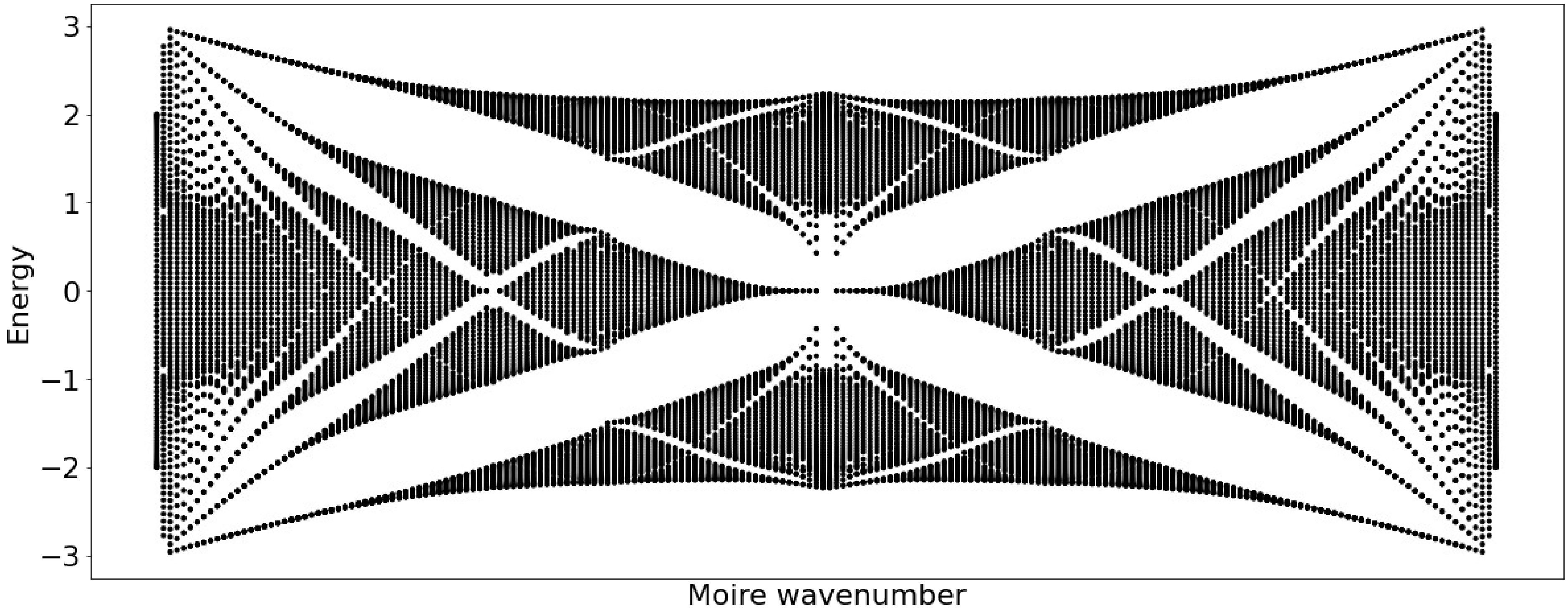
Let us see how the electronic structure gets modified by the superlattice effect

A minimal moire potential

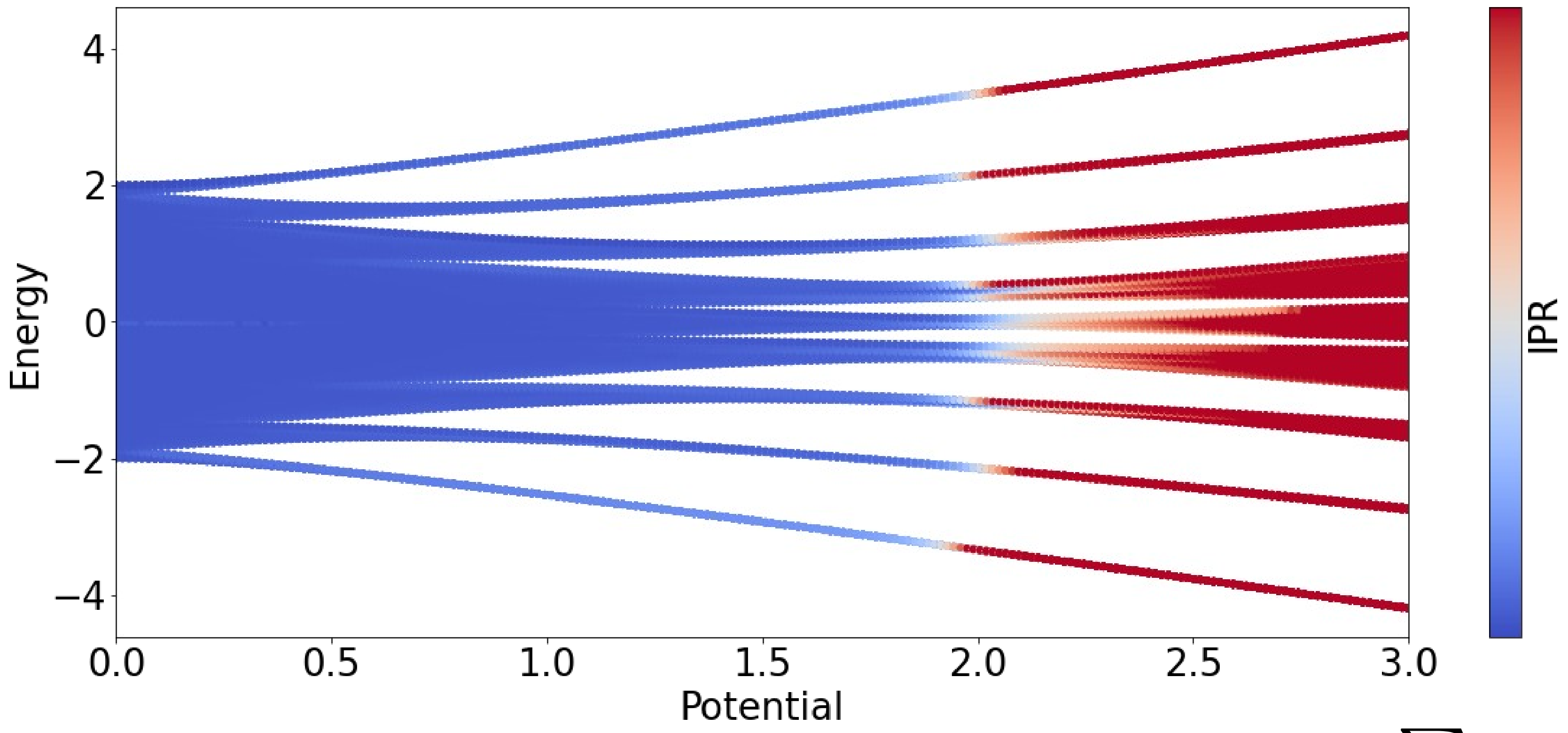
$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + \lambda \sum_n \cos(qn) c_n^\dagger c_n$$



Spectrum as a function of the moire wavevector



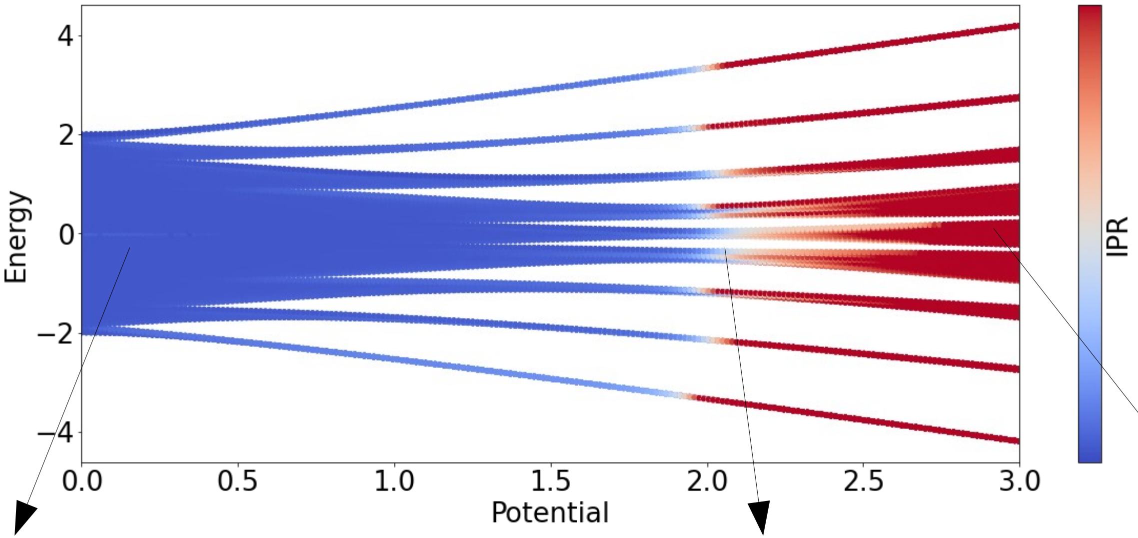
Superpotentials and criticality



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

Moire potentials can give rise to critical wavefunctions

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

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

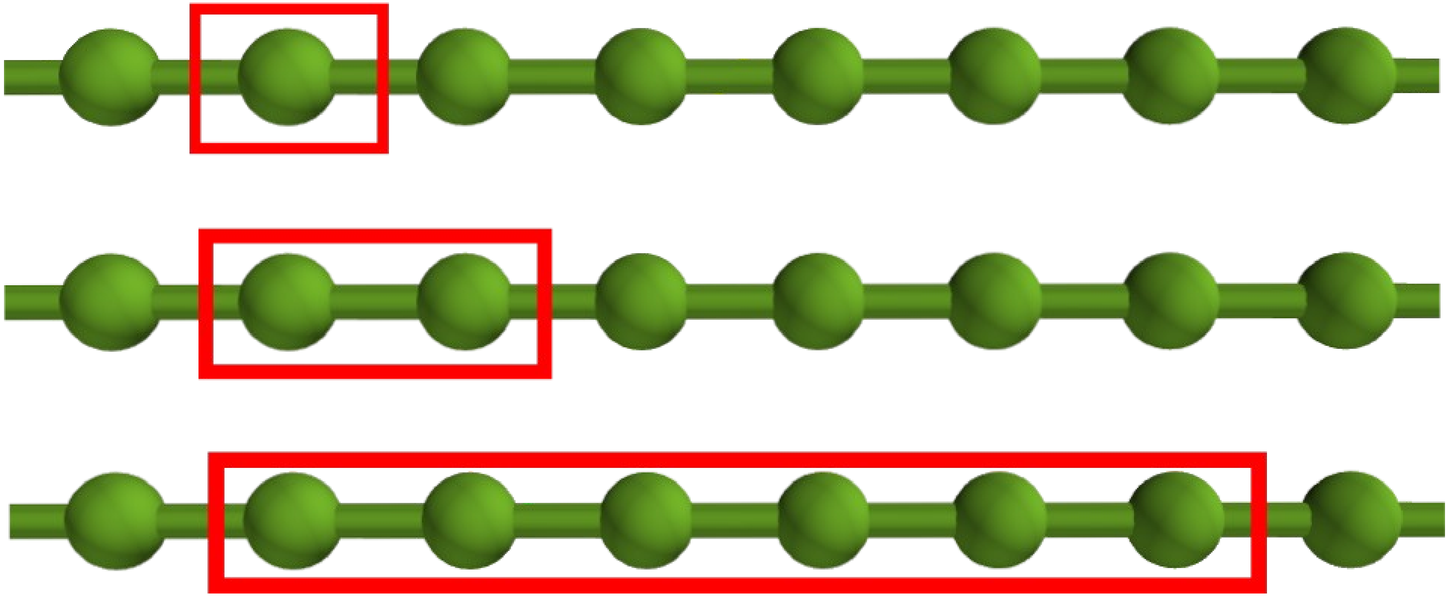
Minibands and band structure unfolding

Supercells and band folding

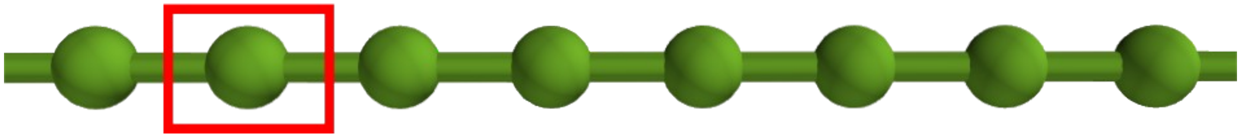
Let us take a 1D chain

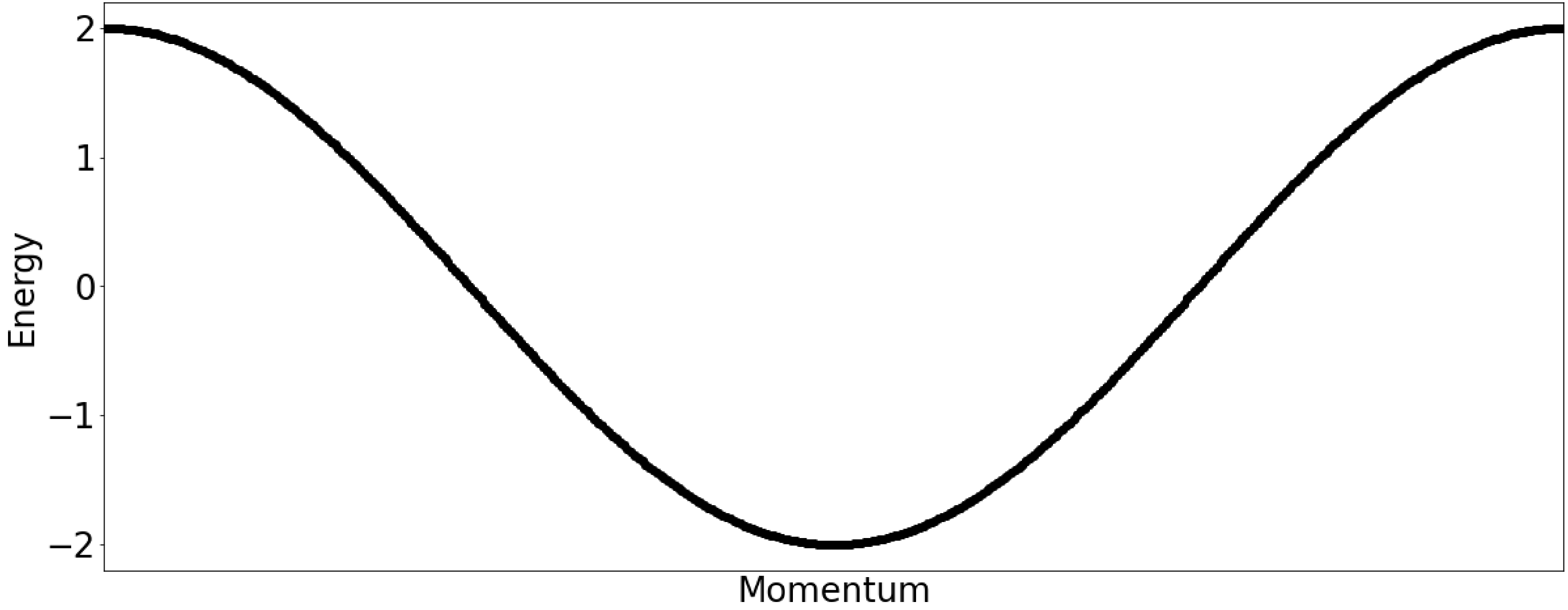
$$H = \sum_n c_n^\dagger c_{n+1} + h.c.$$

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

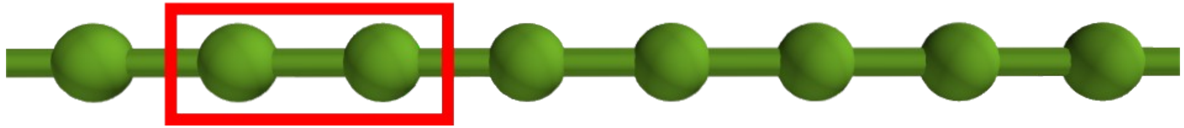


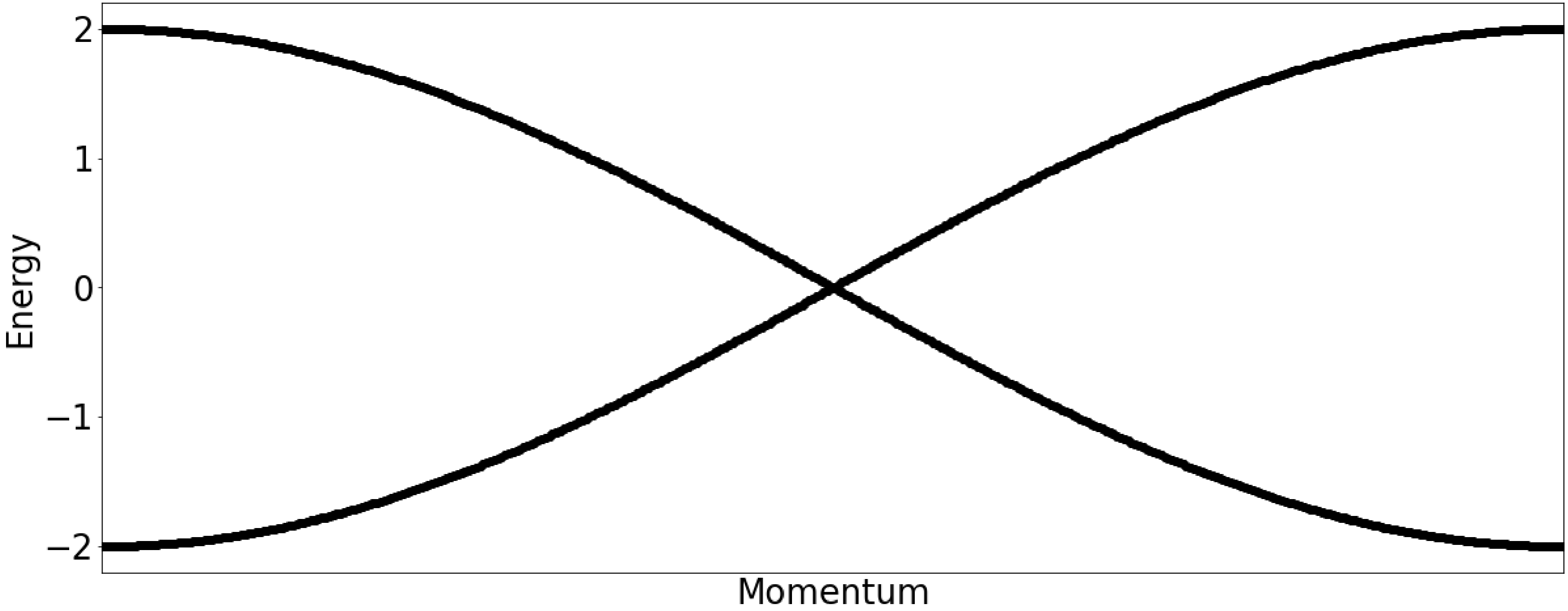
Supercells and band folding



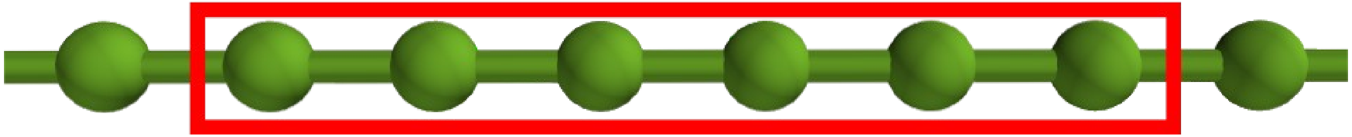


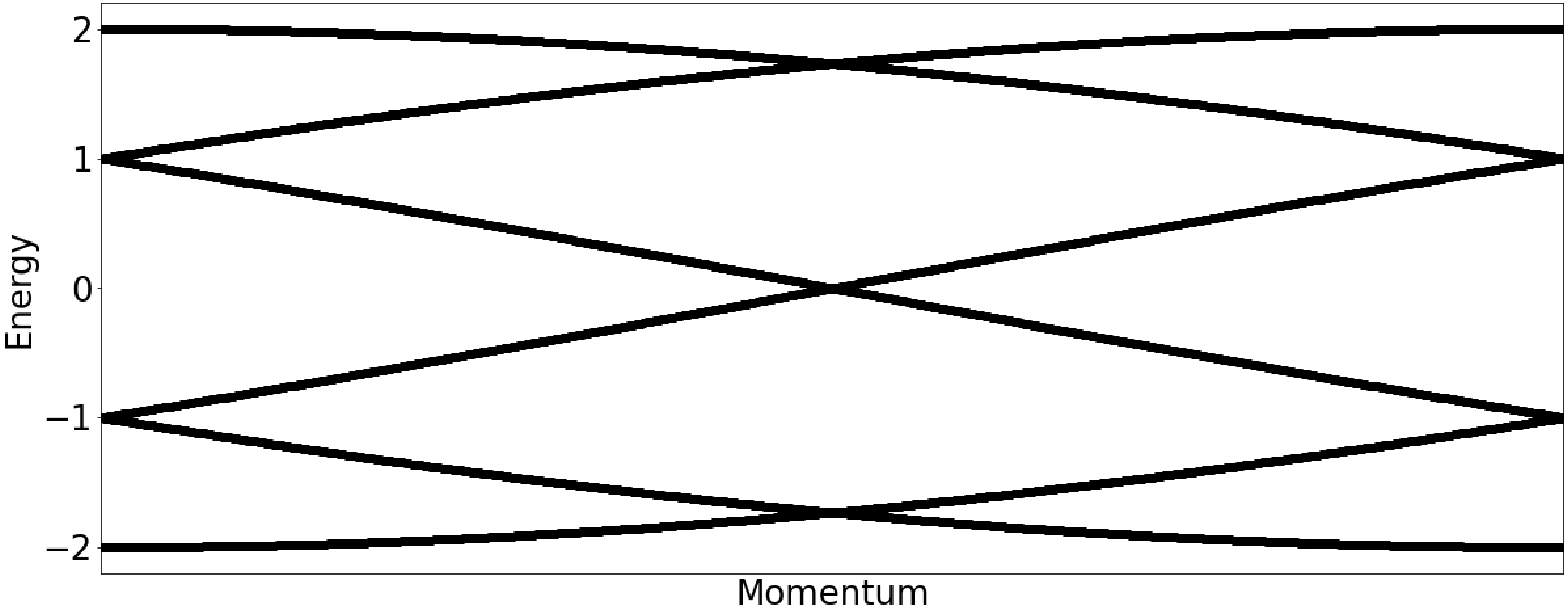
Supercells and band folding



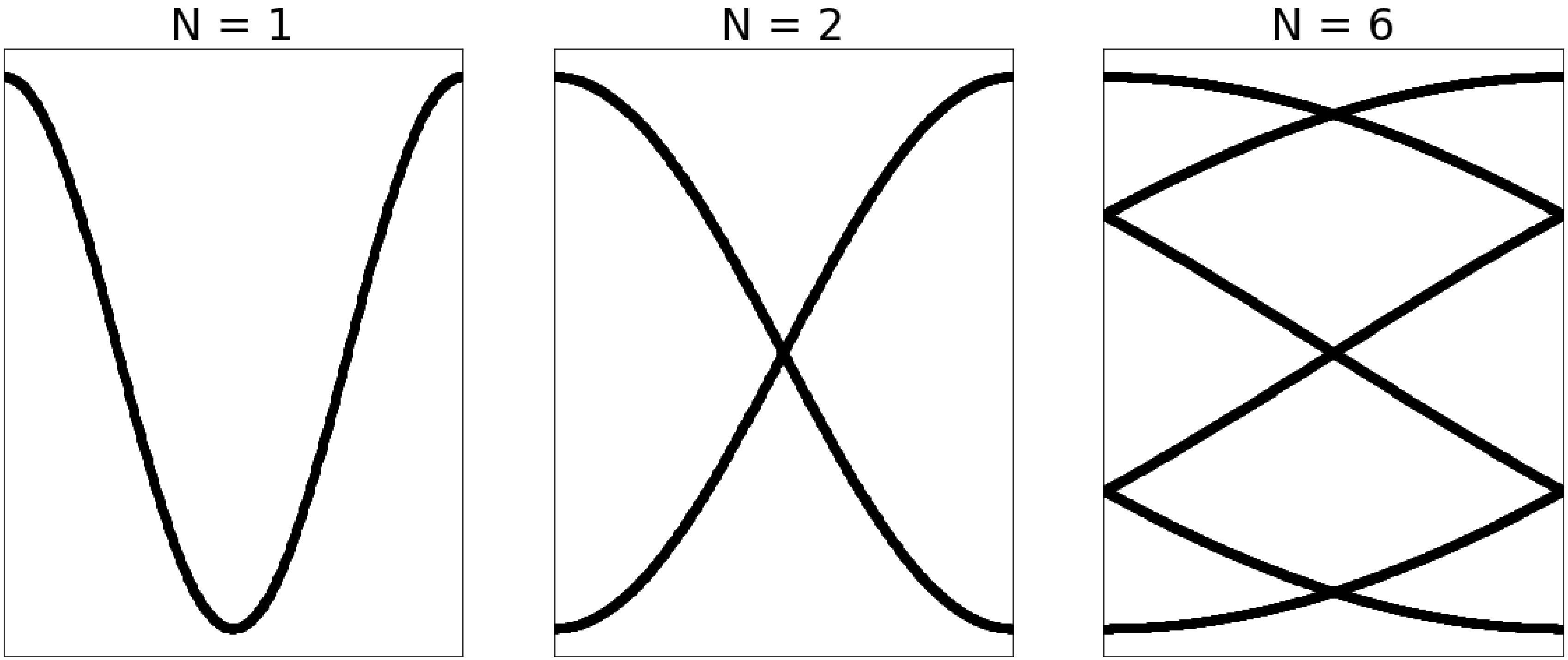


Supercells and band folding



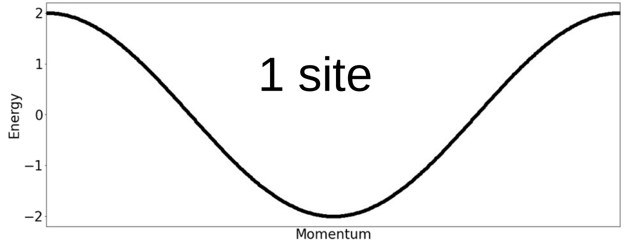


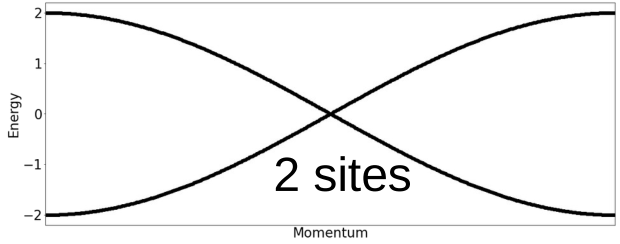
Supercells and band folding

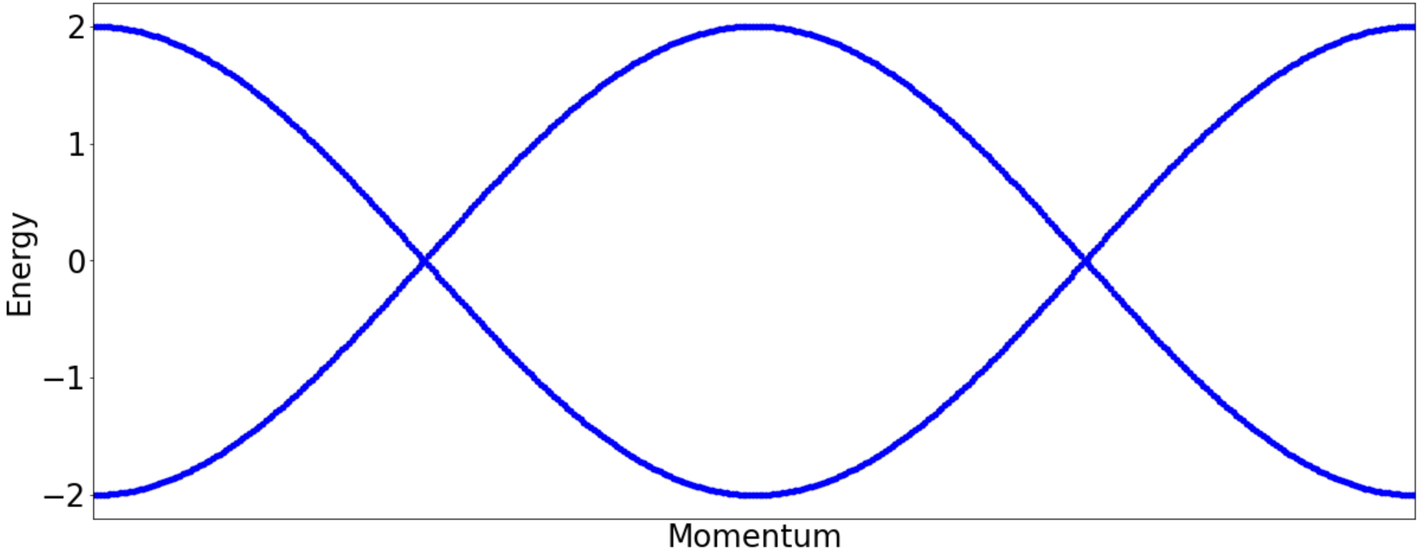


All these electronic structures represent the same physical system, but how do we see that?

Supercells and band folding

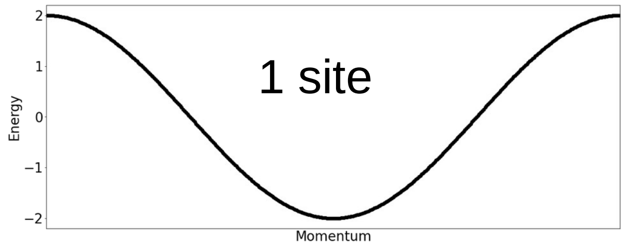


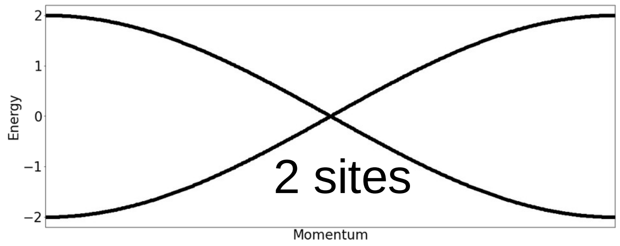


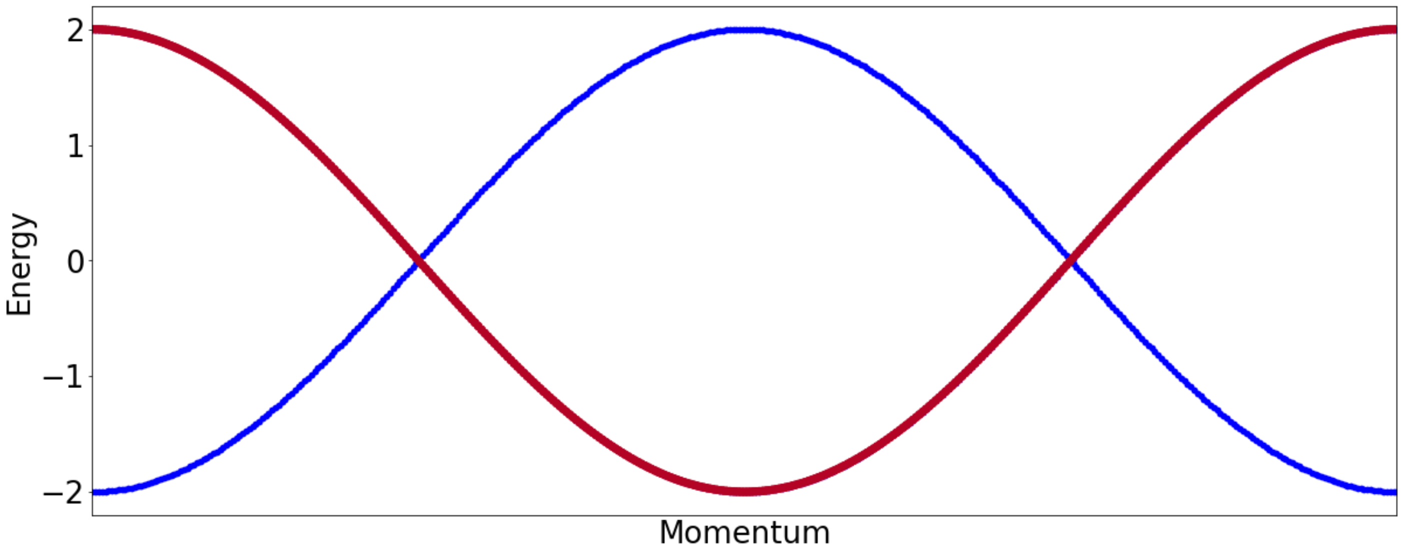


Repeating the electronic structure recovers the original electronic dispersion

Supercells and band folding

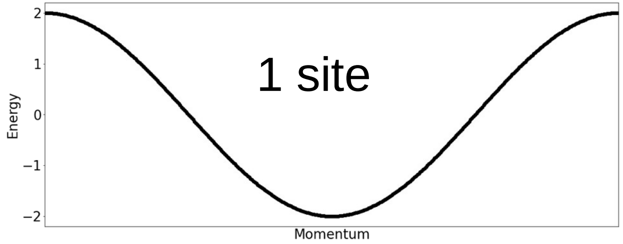


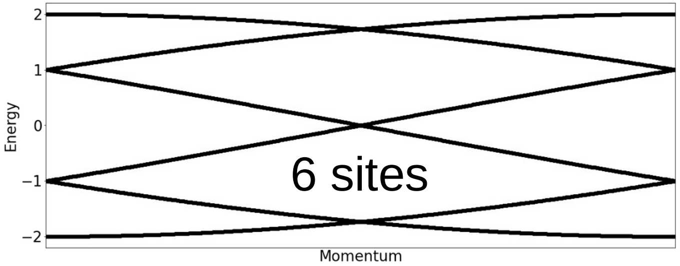


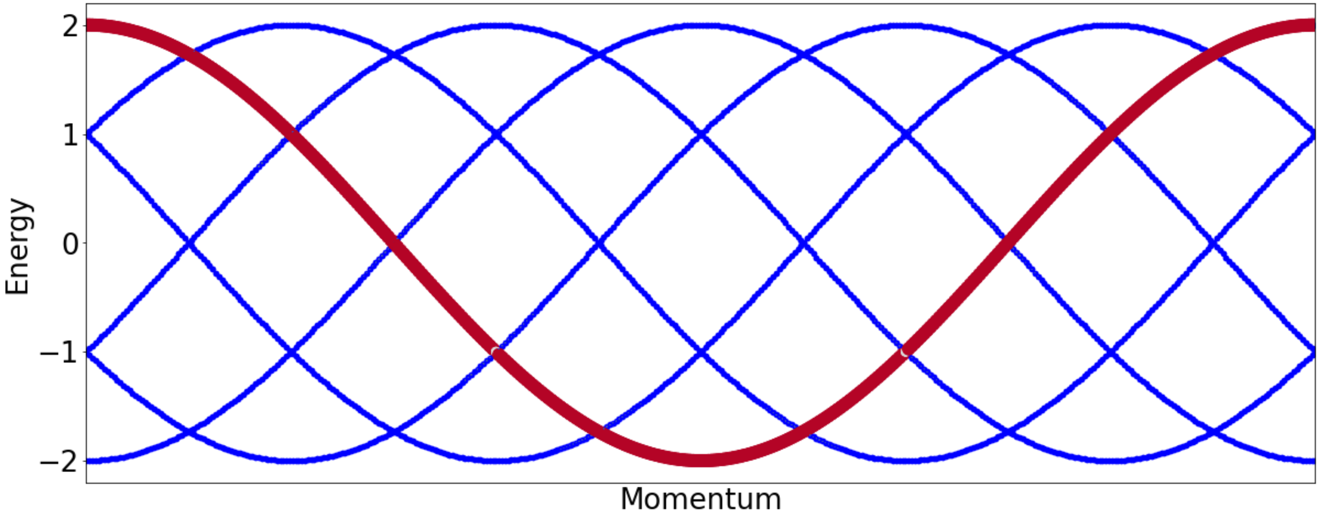


Repeating the electronic structure recovers the original electronic dispersion

Supercells and band folding



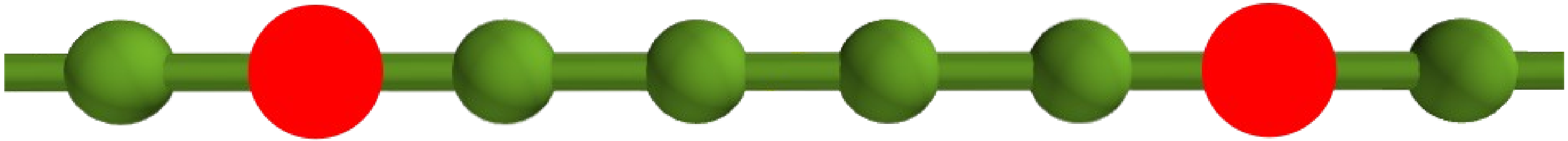




Repeating the electronic structure recovers the original electronic dispersion

Unfolding and anticrossings in superlattices

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

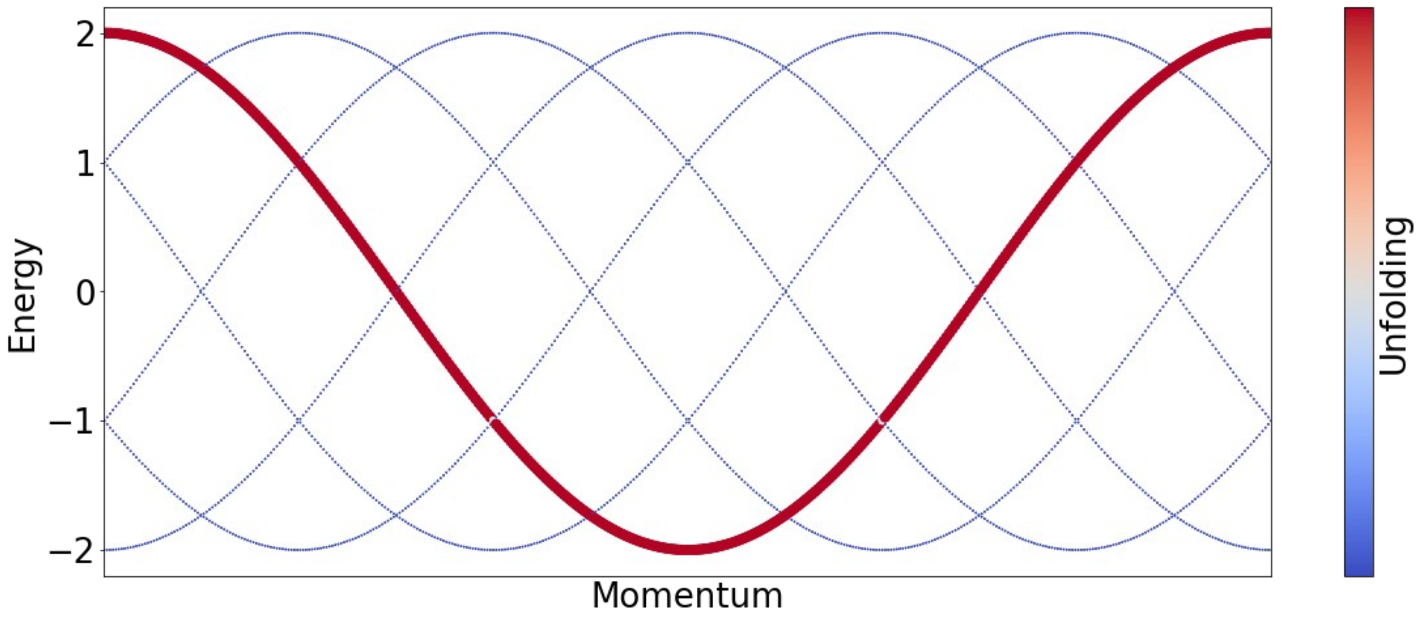


$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V_0 \sum_\alpha c_n^\dagger c_n \qquad \alpha \equiv 0 \pmod 6$$

Unfolding and anticrossings in superlattices

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

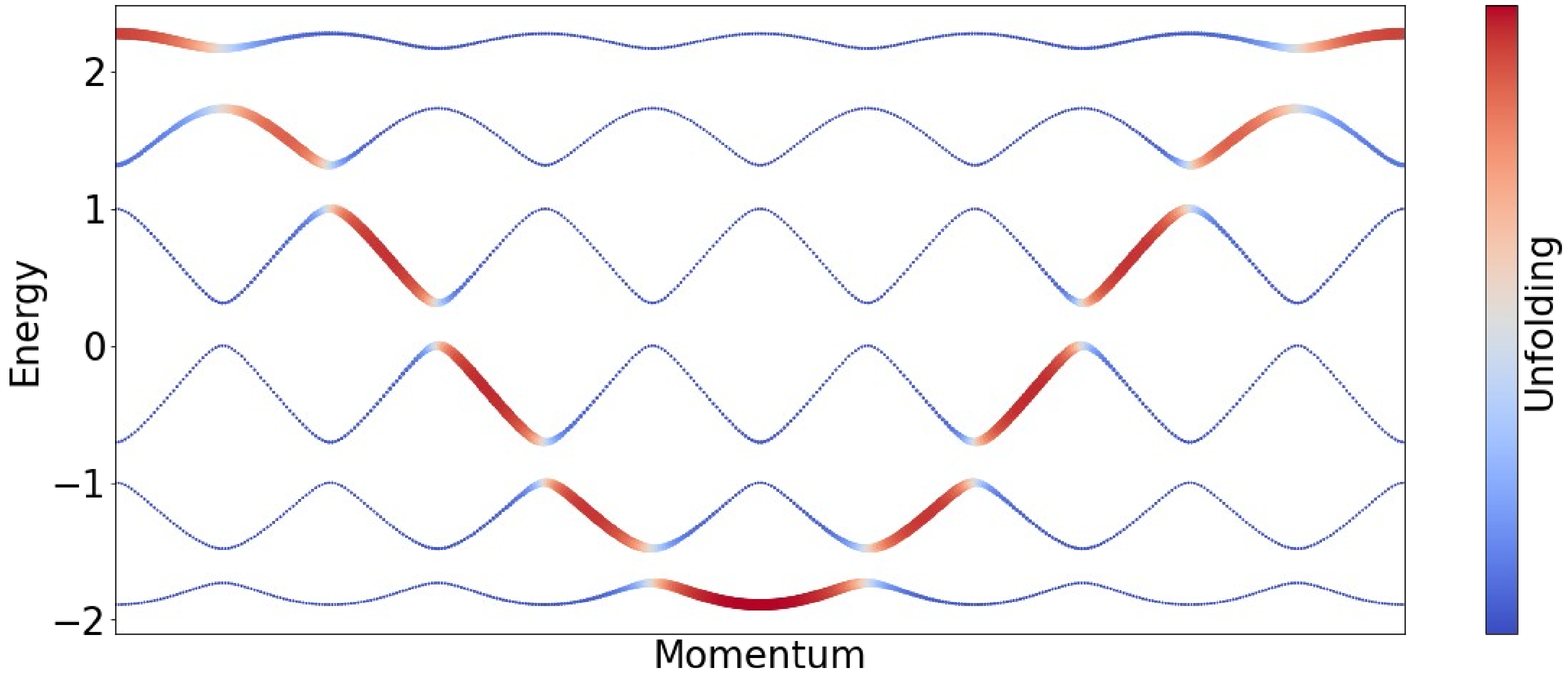
$$V_0 = 0$$



Electronic structure unfolding

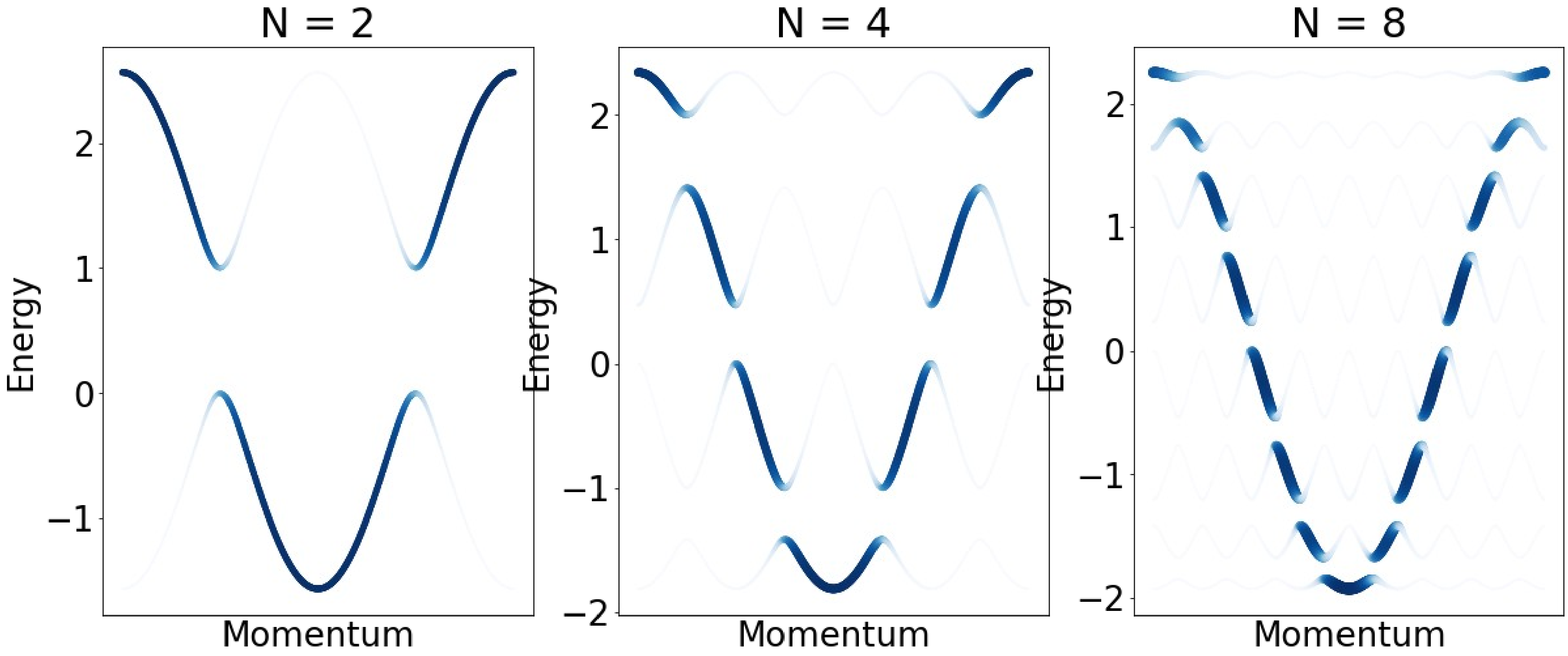
$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V_0 \sum_\alpha c_n^\dagger c_n$$

$$V_0 \neq 0$$



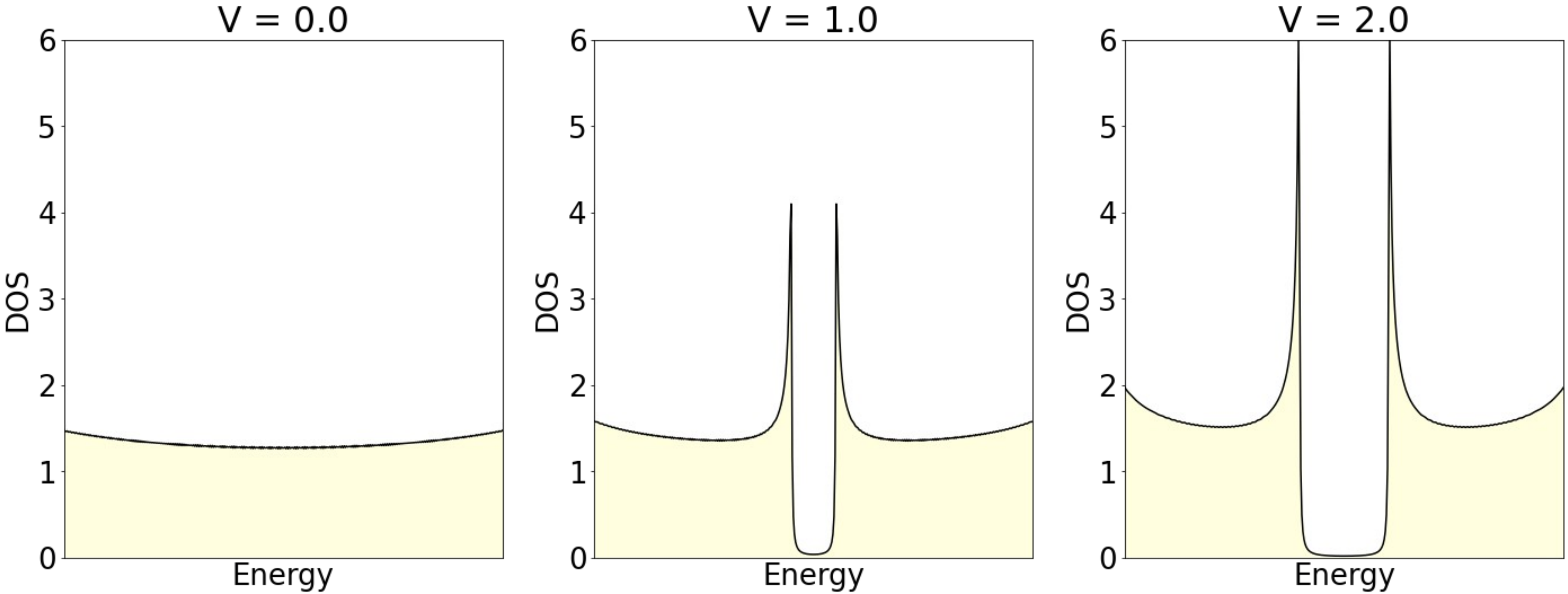
Anticrossing between the bands appear due to the superlattice potential

Electronic structure unfolding



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

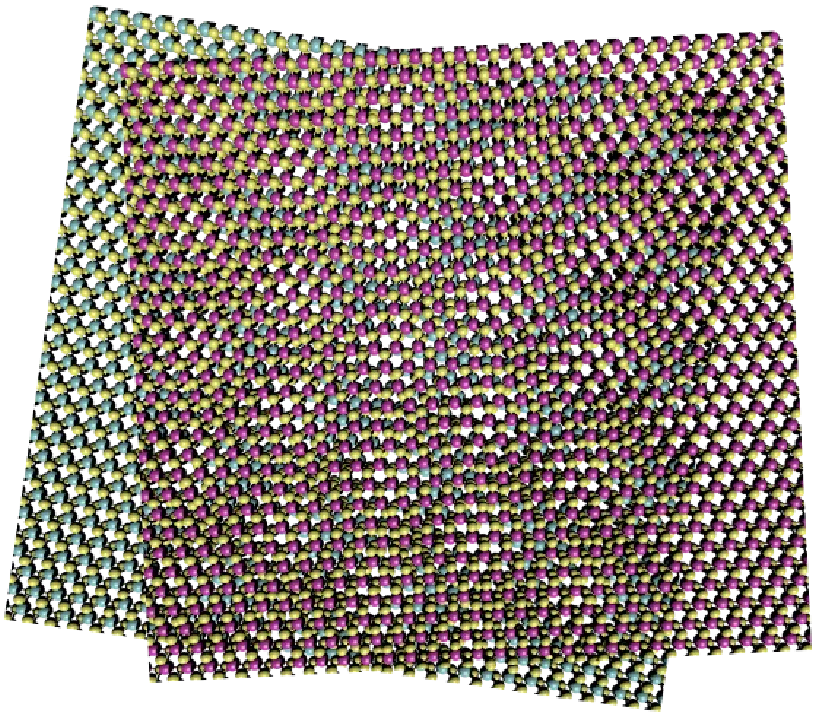
Moire electronic structure

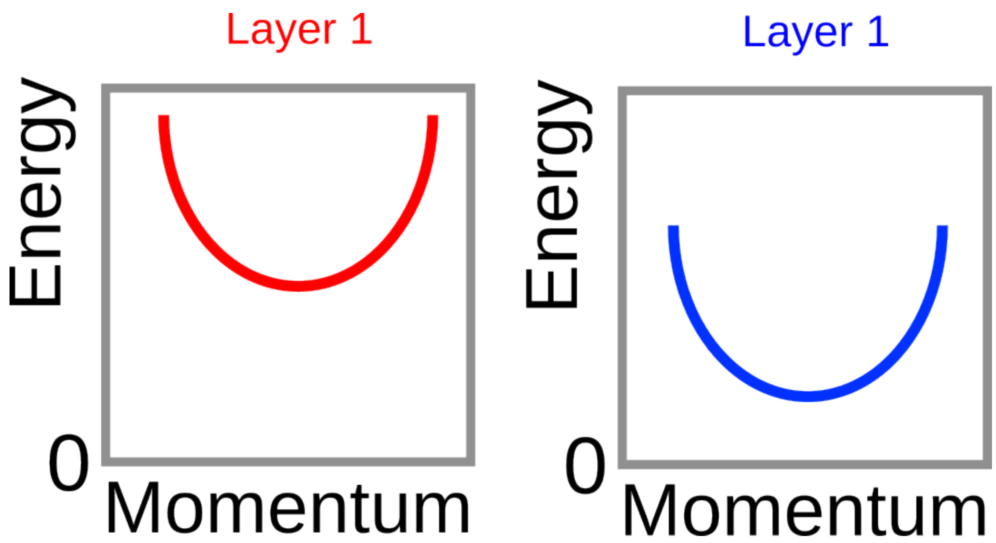


As the strength of the miore potential increases, the density of states gets enhanced

Moire in twisted TMDC

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

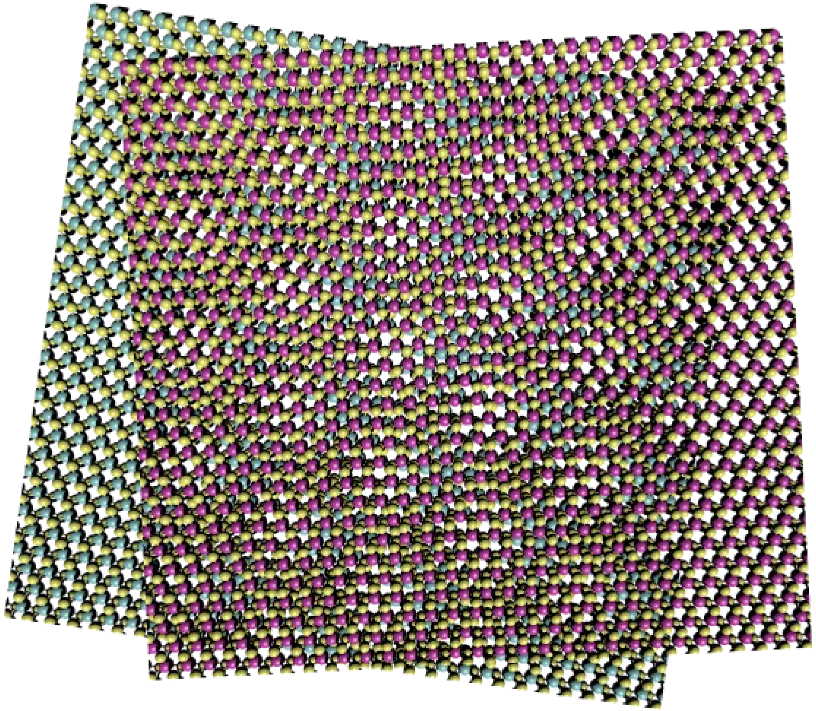


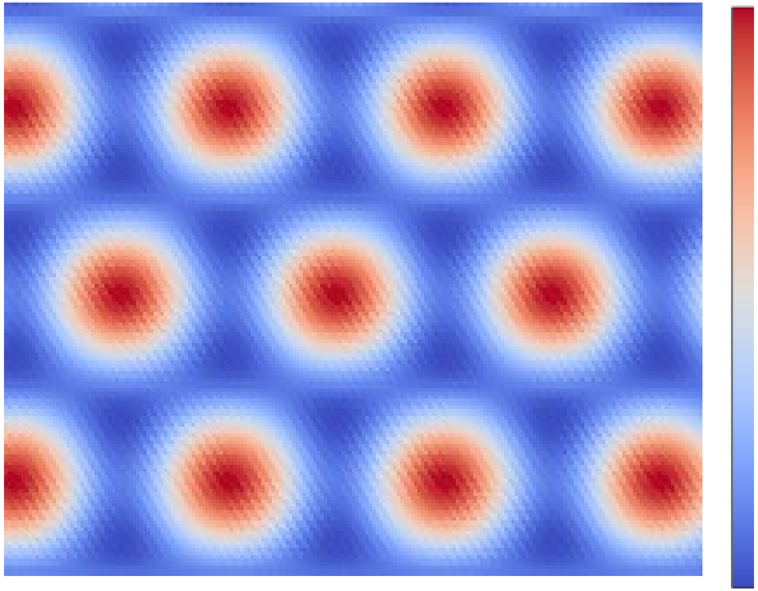


Moire in twisted TMDC

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

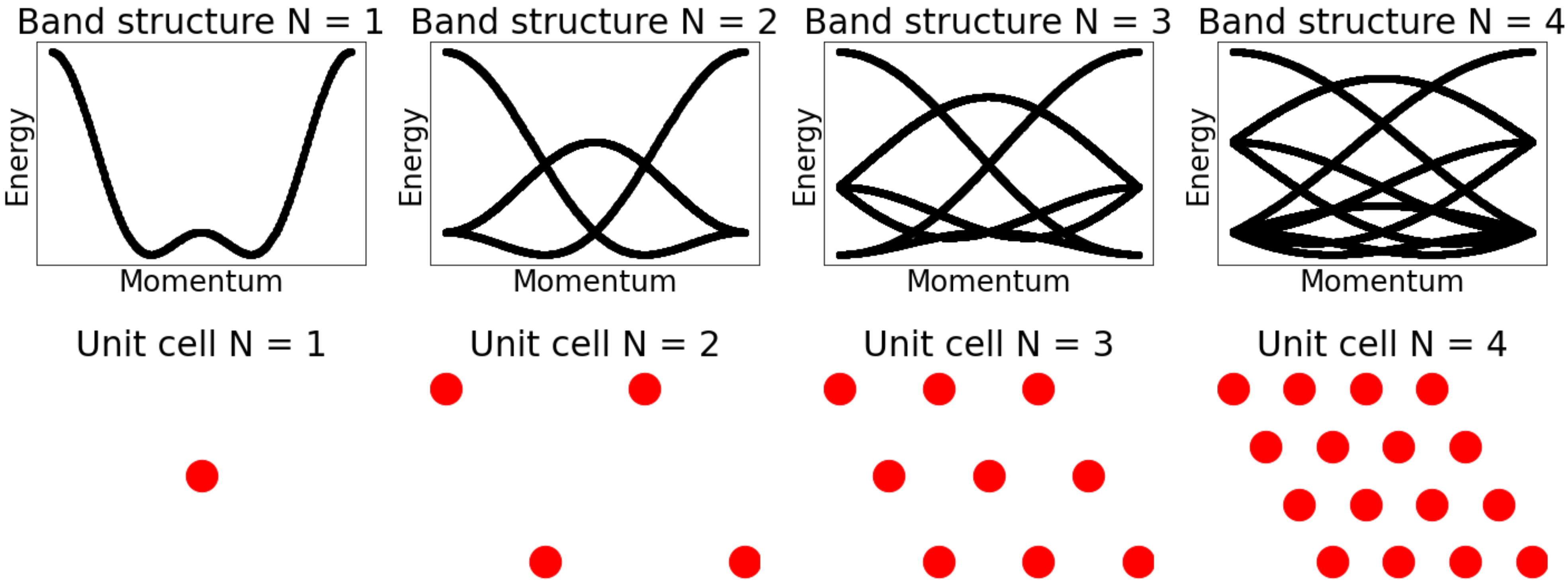
$$H = \sum_{ij} c_i^\dagger c_j + h.c. + \sum_n V(\mathbf{r}_n) c_n^\dagger c_n$$





$V(\mathbf{r})$

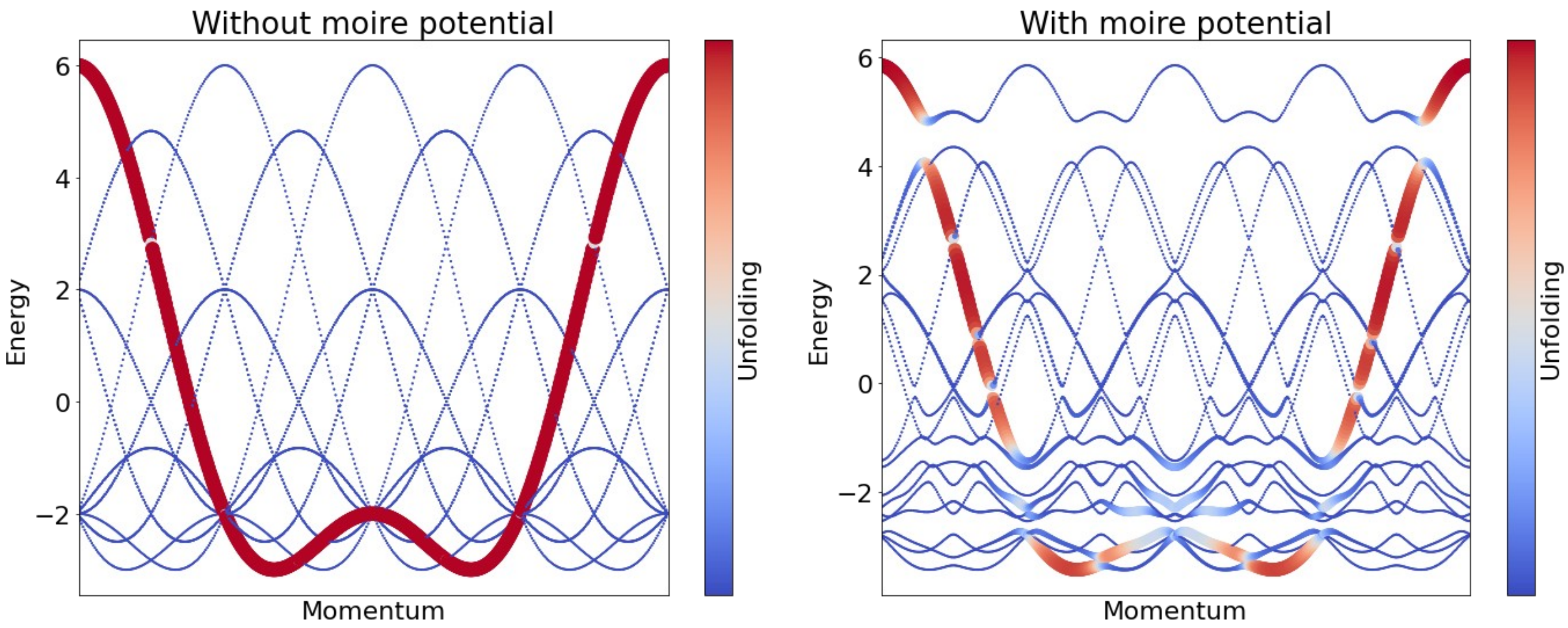
Band structure folding in 2D superlattices



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

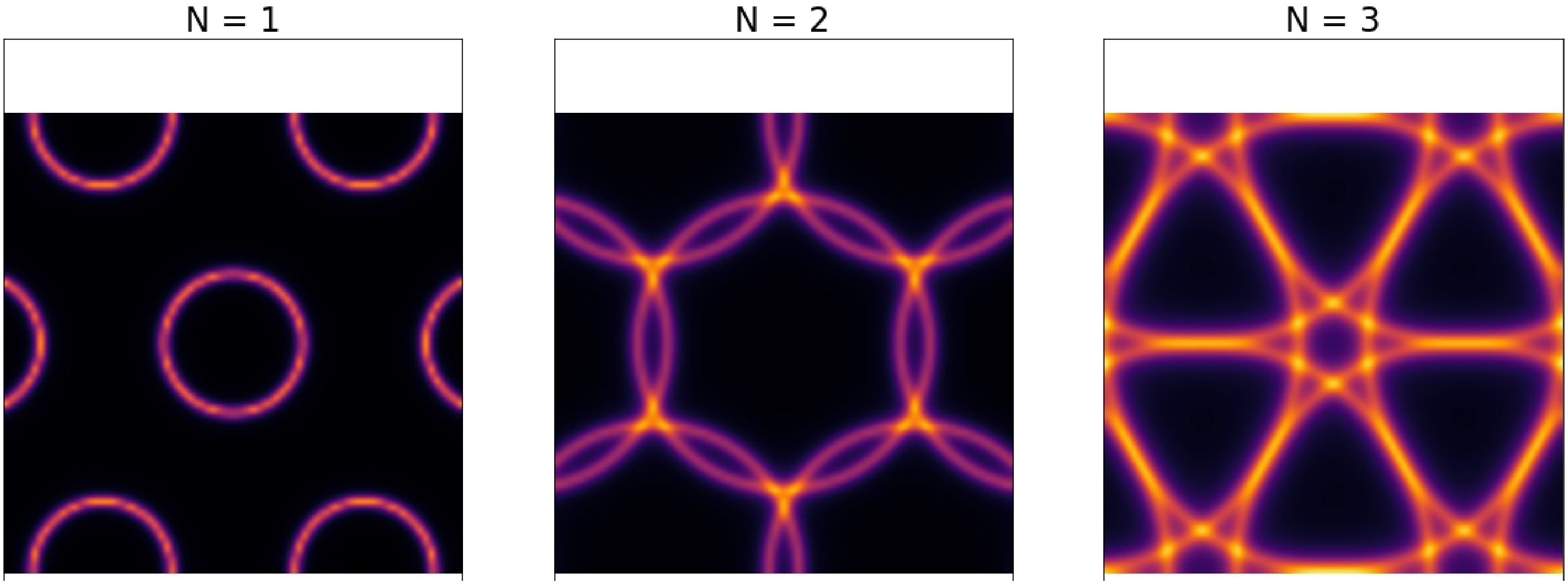
Band structure folding in 2D superlattices

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



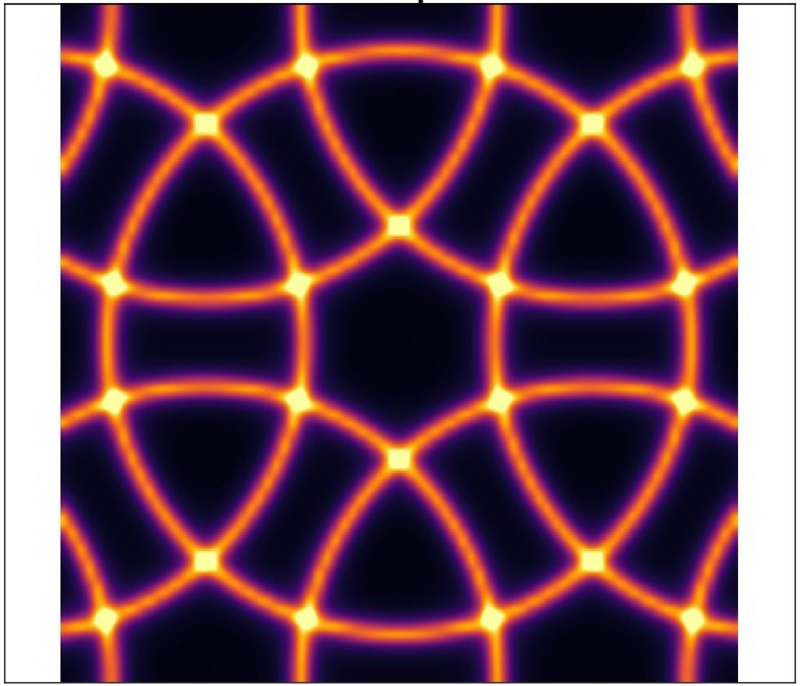
Fermi surface folding in superlattices

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

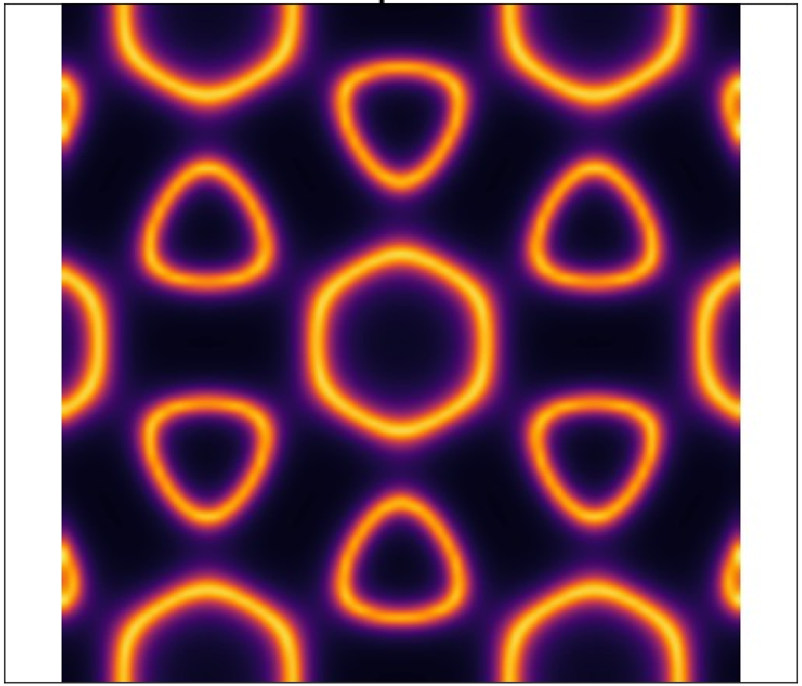


Fermi surface folding in superlattices

Without superlattice

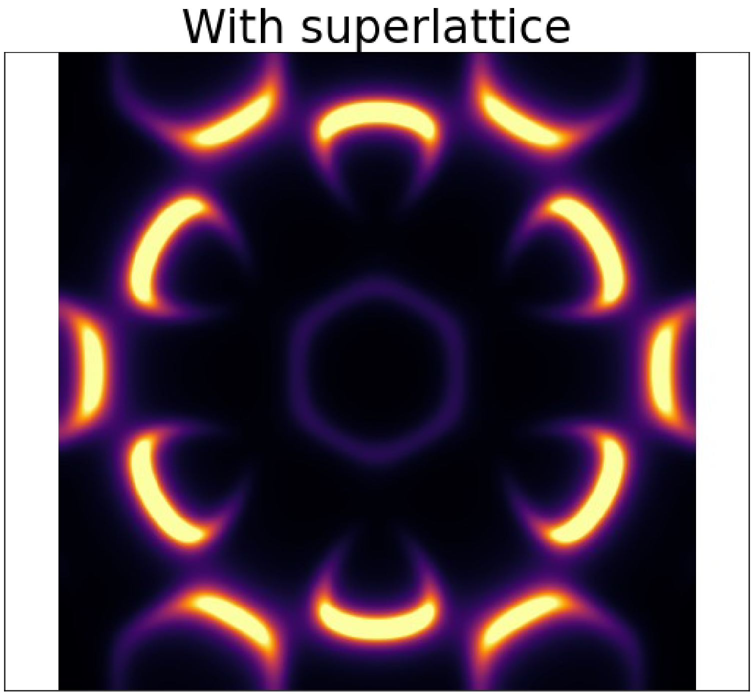


With superlattice



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

Fermi surface unfolding in superlattices



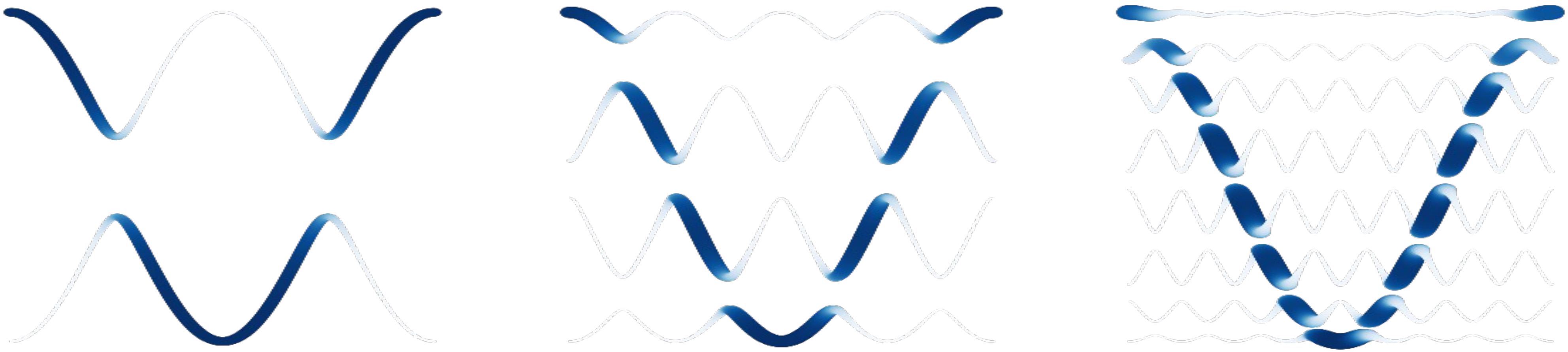
Superlattices fragment the original Fermi surface when unfolded to the original unit cell

Break

5 min break

(optional) to discuss during the break

Which band structure has more van Hove singularities?

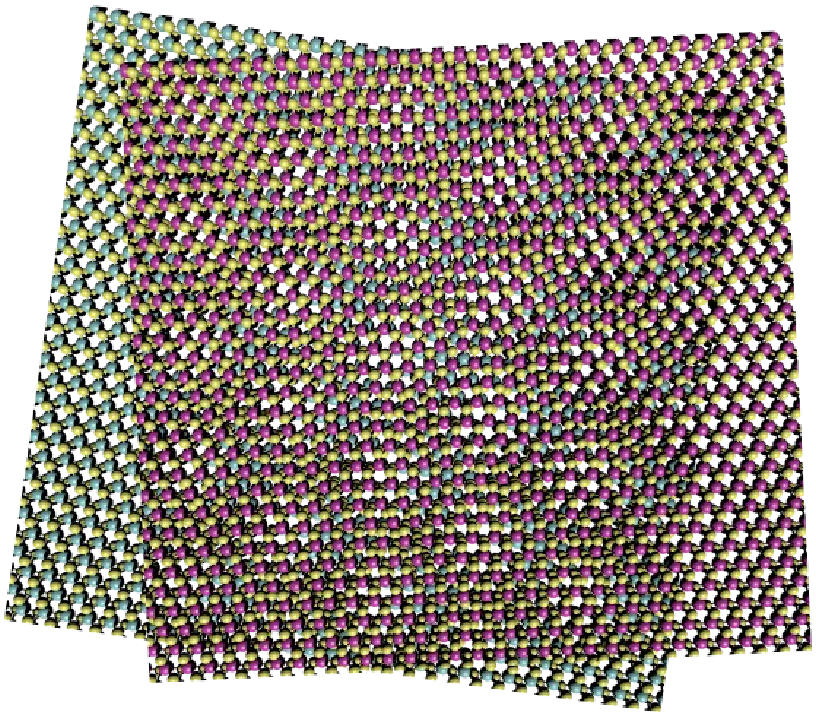


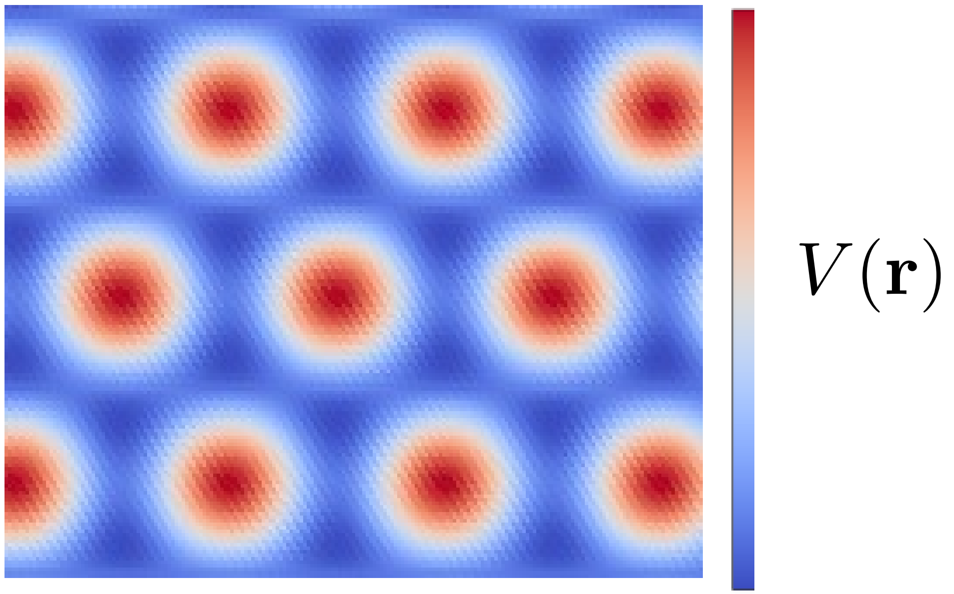
Moire-driven correlated states

Moire in twisted TMDC

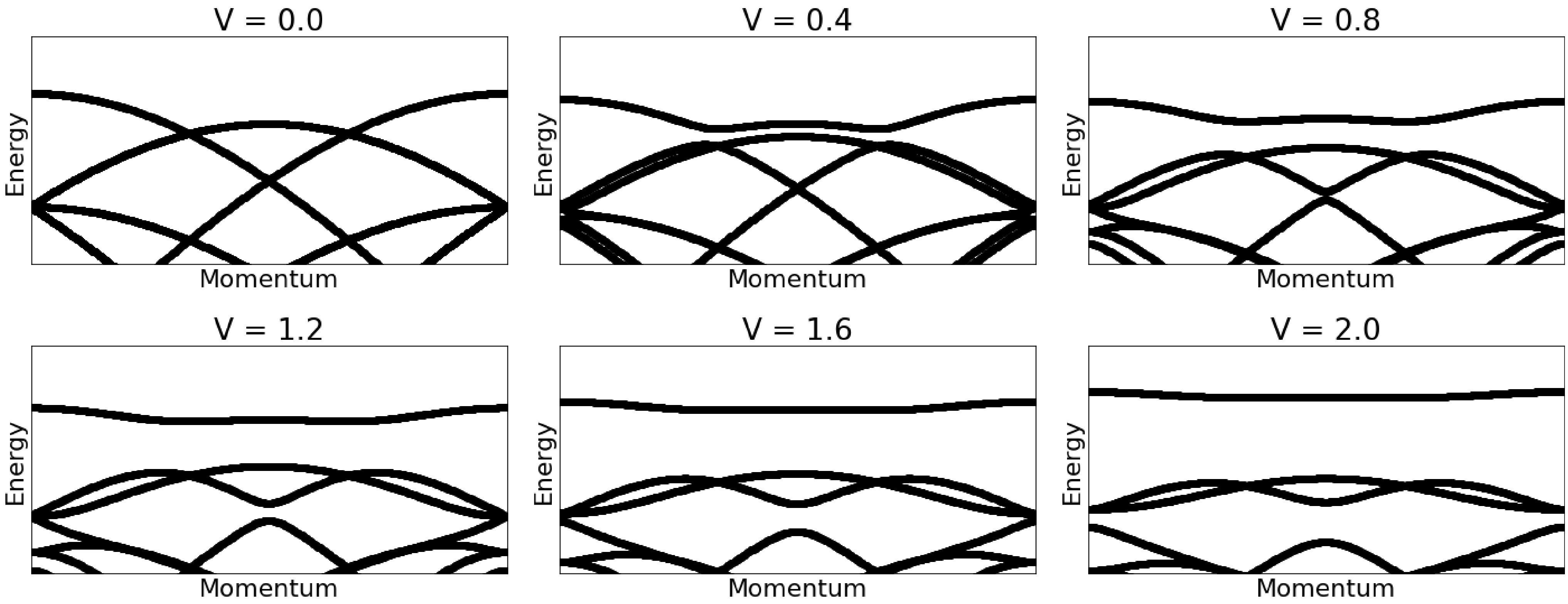
In twisted TMDC heterobilayers, the moire modulates the band off set of one layer

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



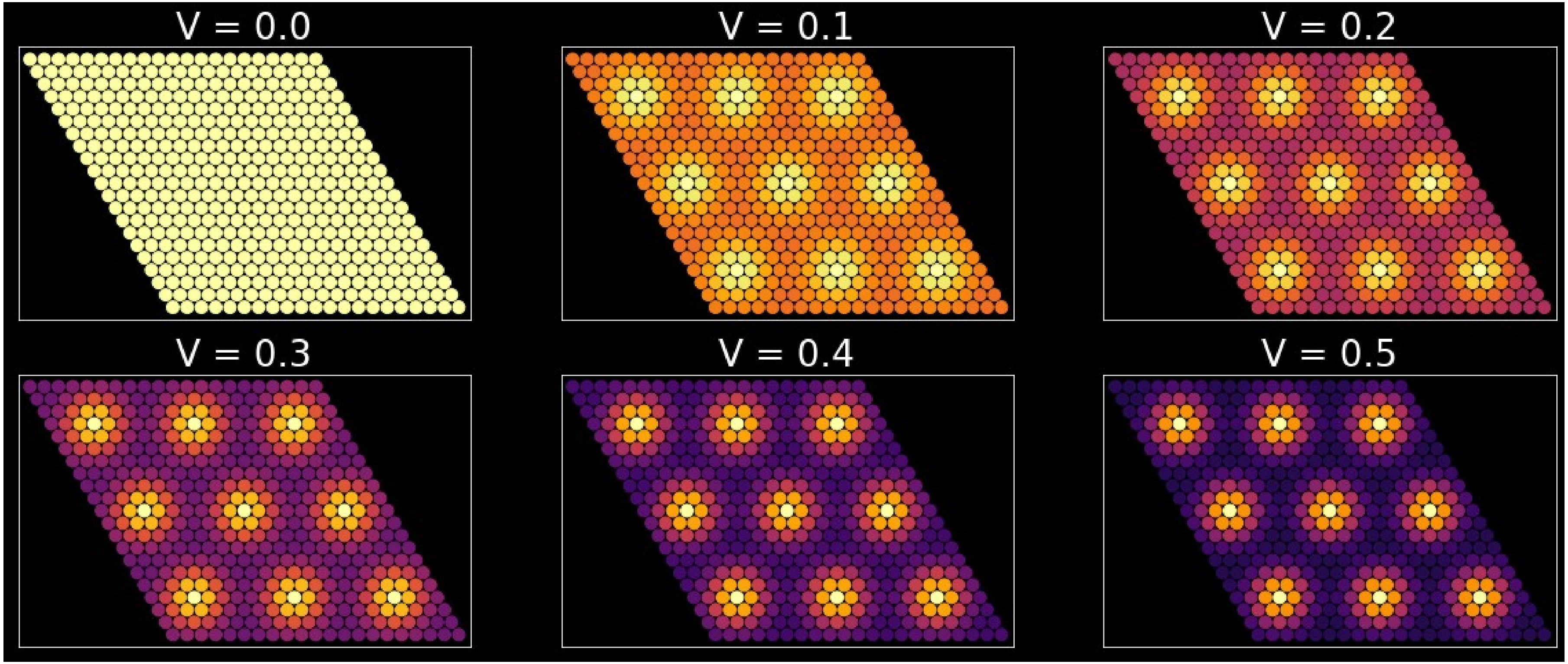


Band flattening by a moire

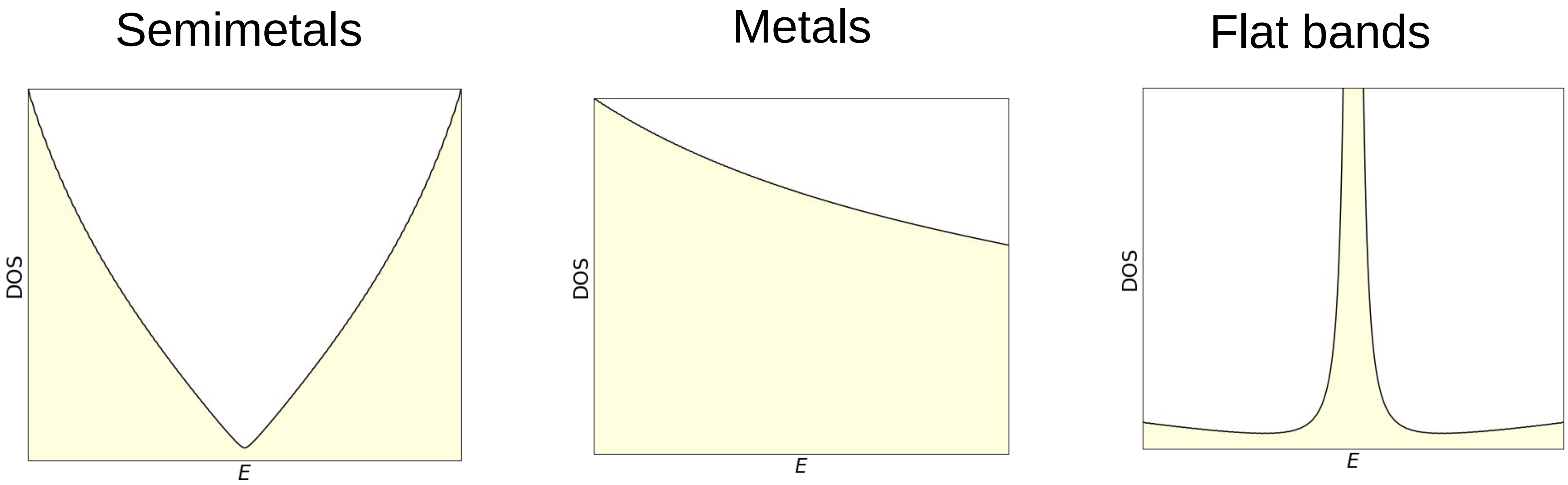


As the strength of a modulation is increased, flat bands appear

Emergence of moire states



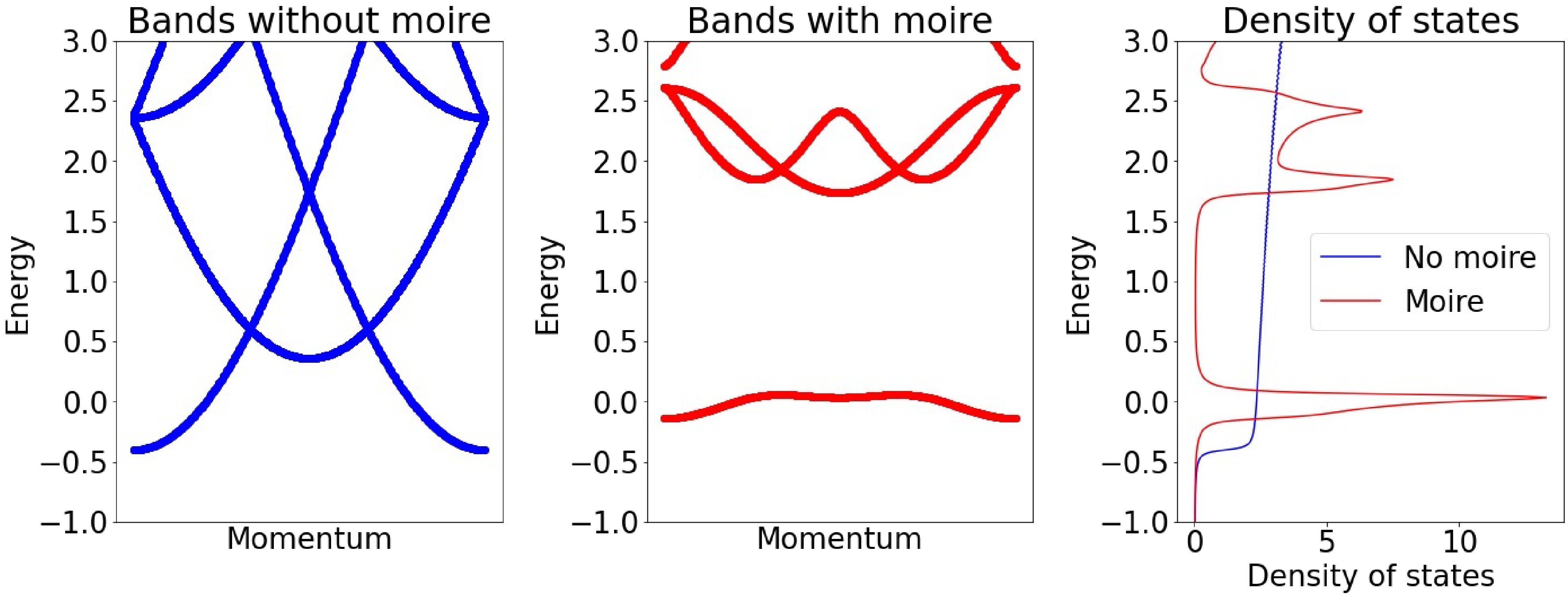
Controlling the electronic spectra with the moire angle



Moire/twist angle

Moire potentials allow driving systems to the correlated limit $U_C \sim \frac{1}{D(E_F)}$

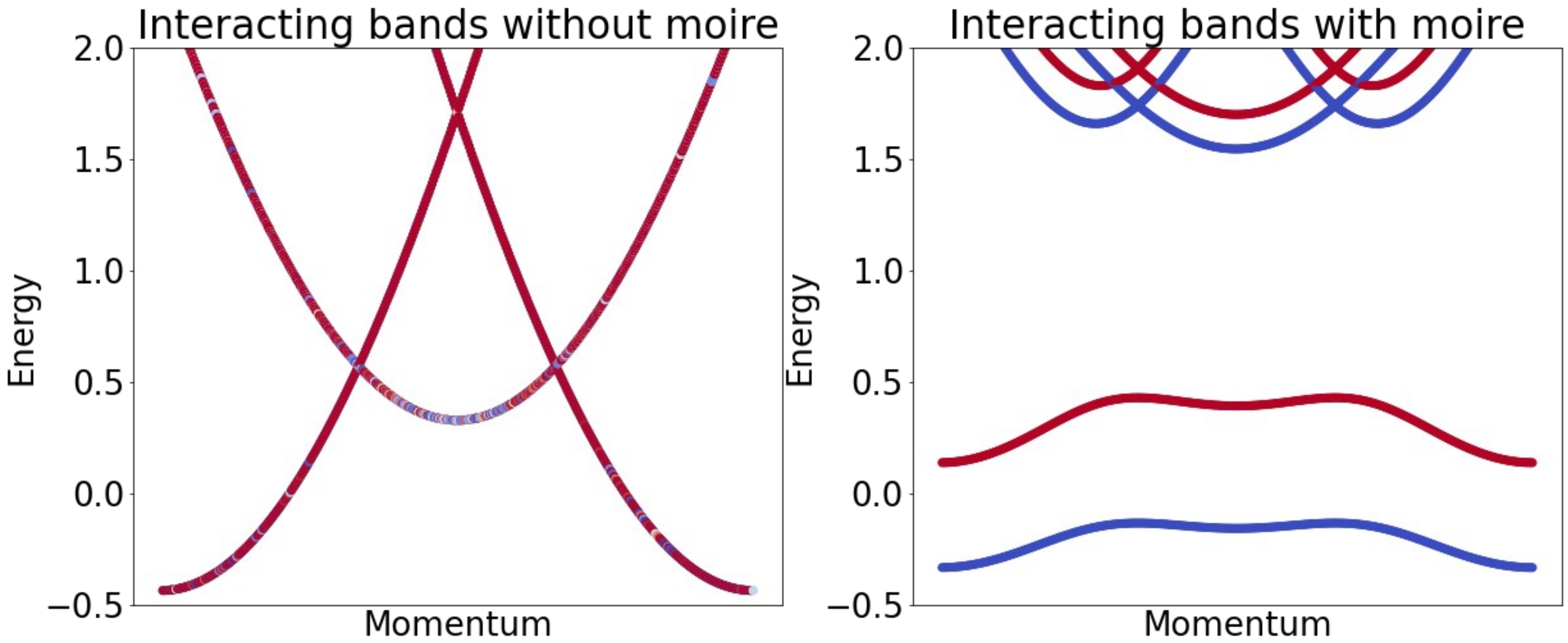
Moire-enhanced DOS



The moire potential gives rise to an enhanced DOS

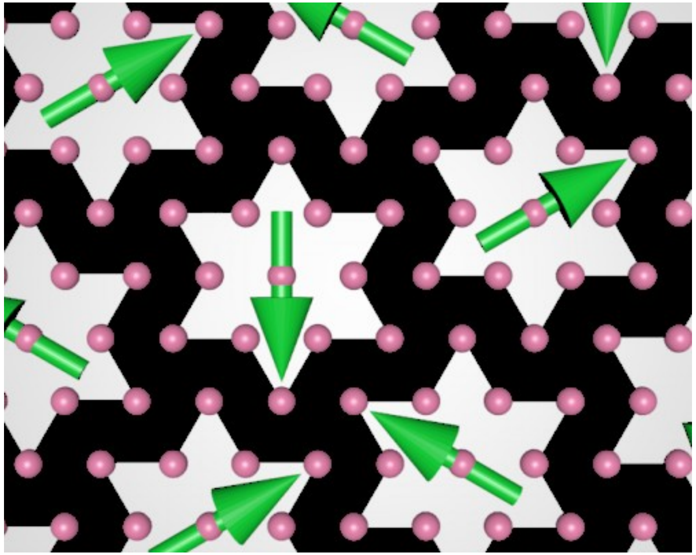
Interactions in the absence and presence of a moire

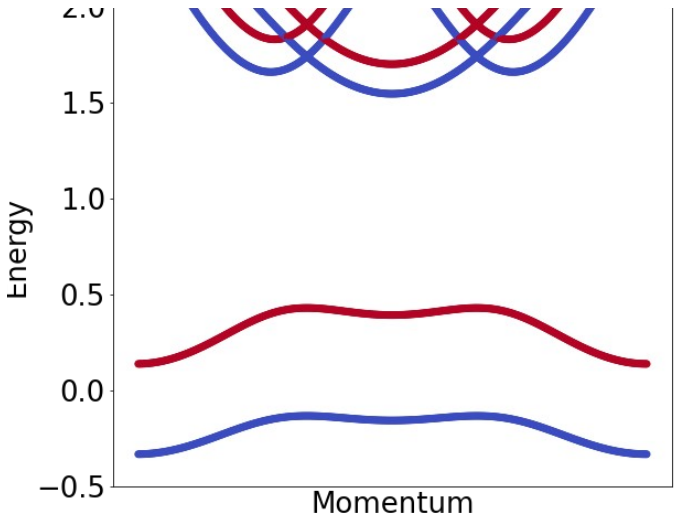
$$H = \sum_{ij,s} t_{ij} c^\dagger_{i,s} c_{j,s} + \sum_i U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} + h.c.$$



Correlated state in 1T-TaS_2 from miniband formation

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





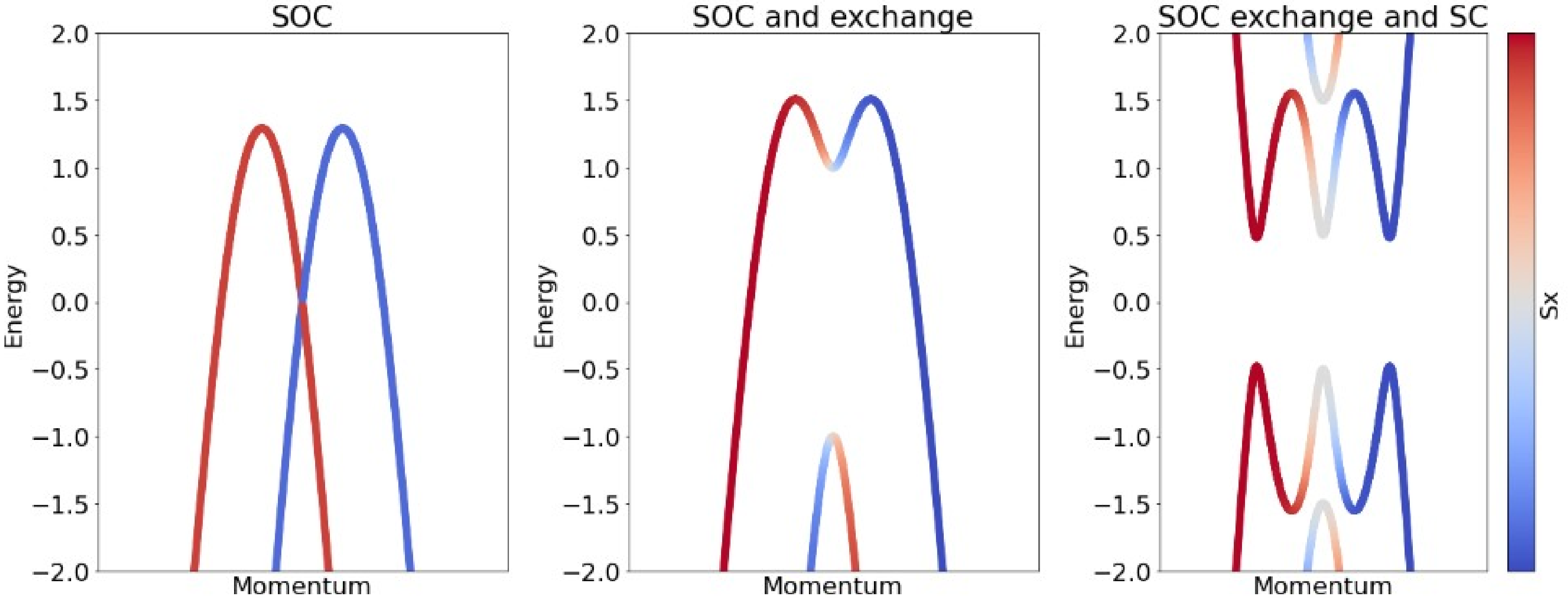
A charge density wave distortion acts as a superlattice modulation

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

Moire-driven topological states

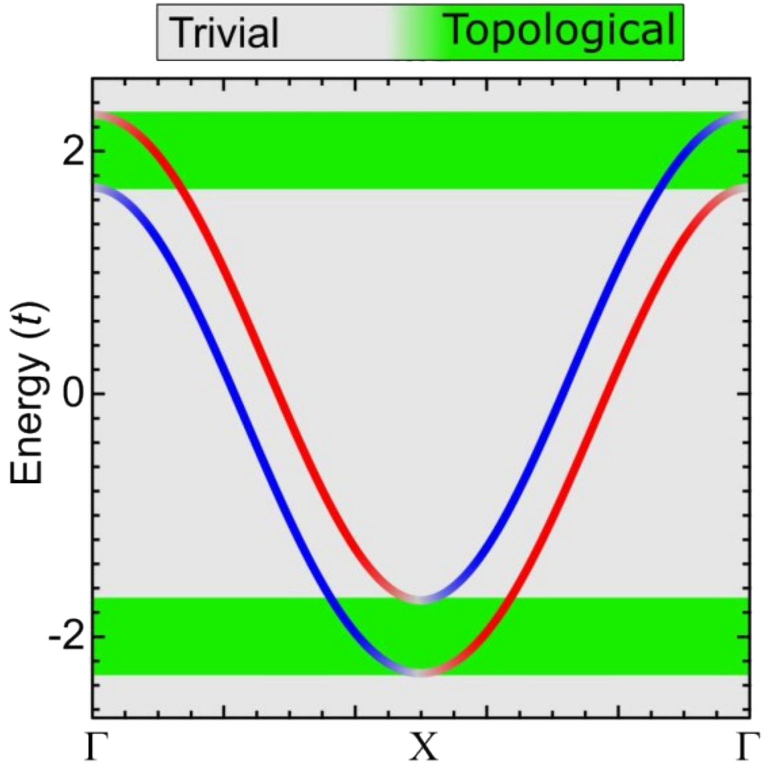
Artificial topological superconductivity

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



$$H = H_0 + H_J + H_R$$

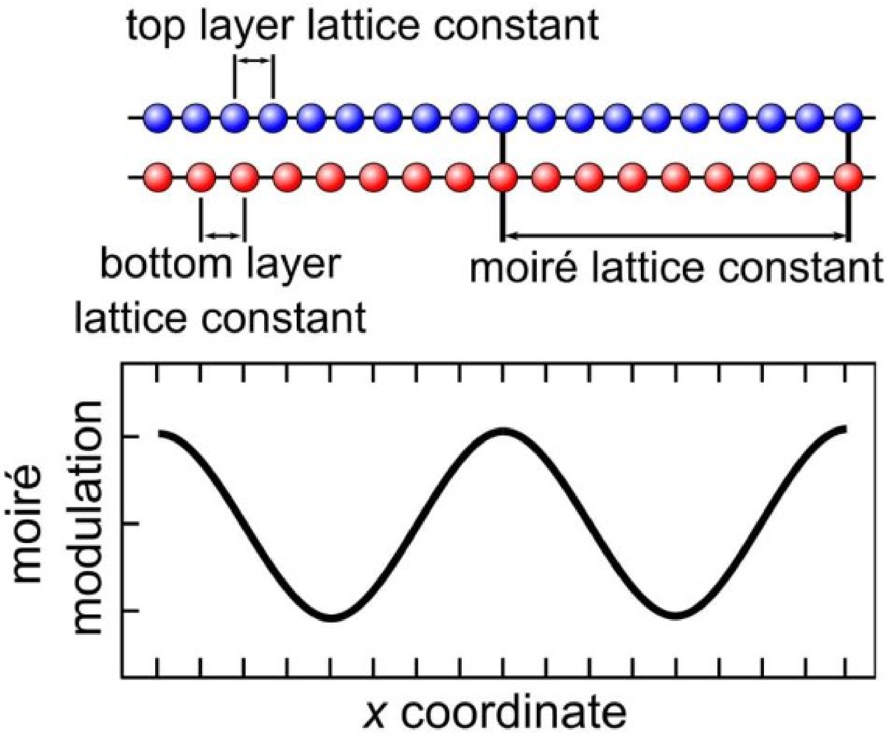
Kinetic energy

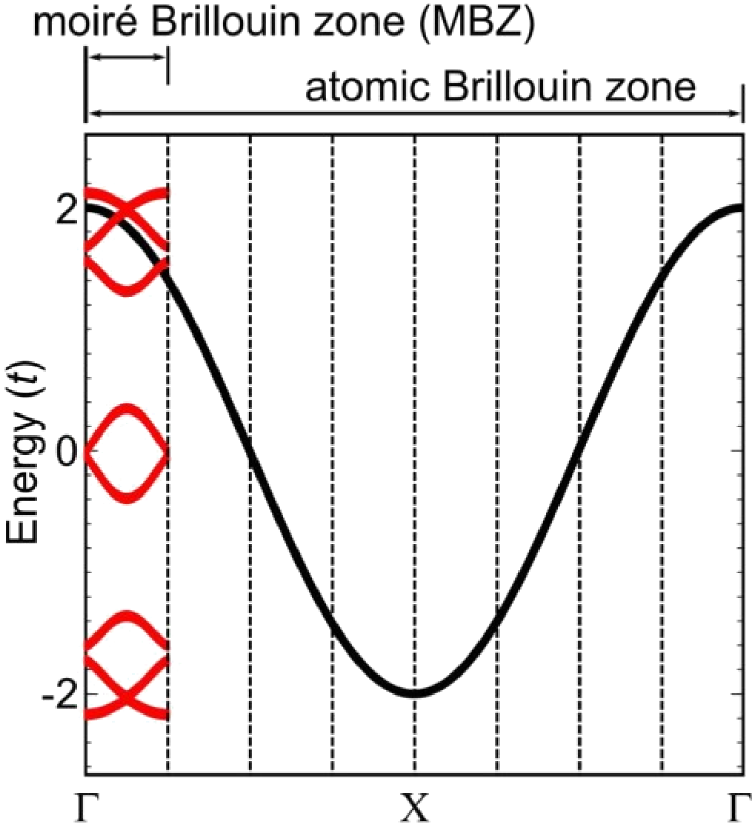
Exchange field

Rashba spin-orbit coupling

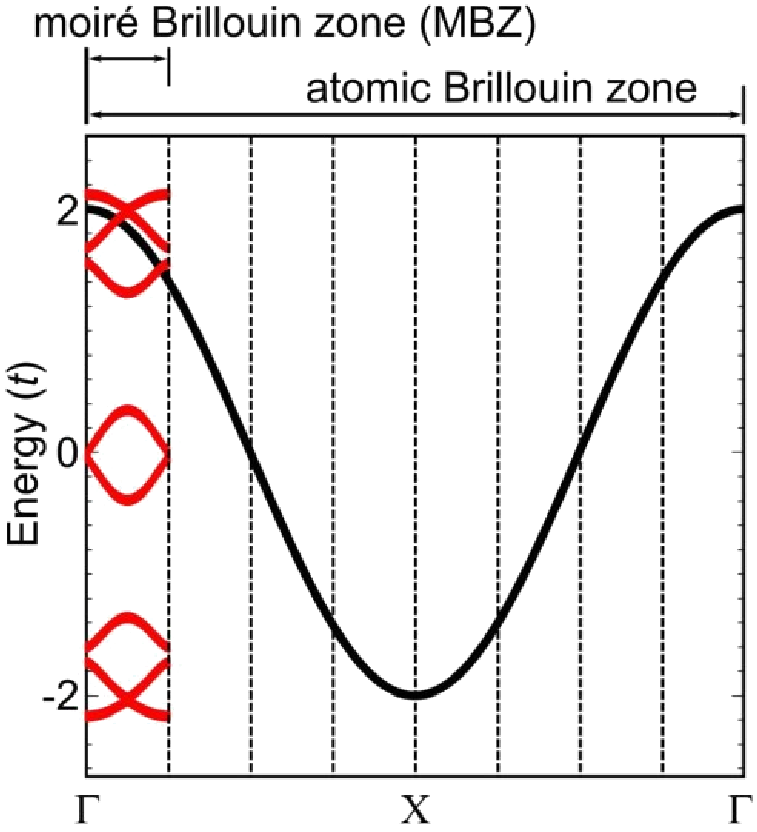
When switching on an s-wave pairing,
green regions lead to topological superconductivity

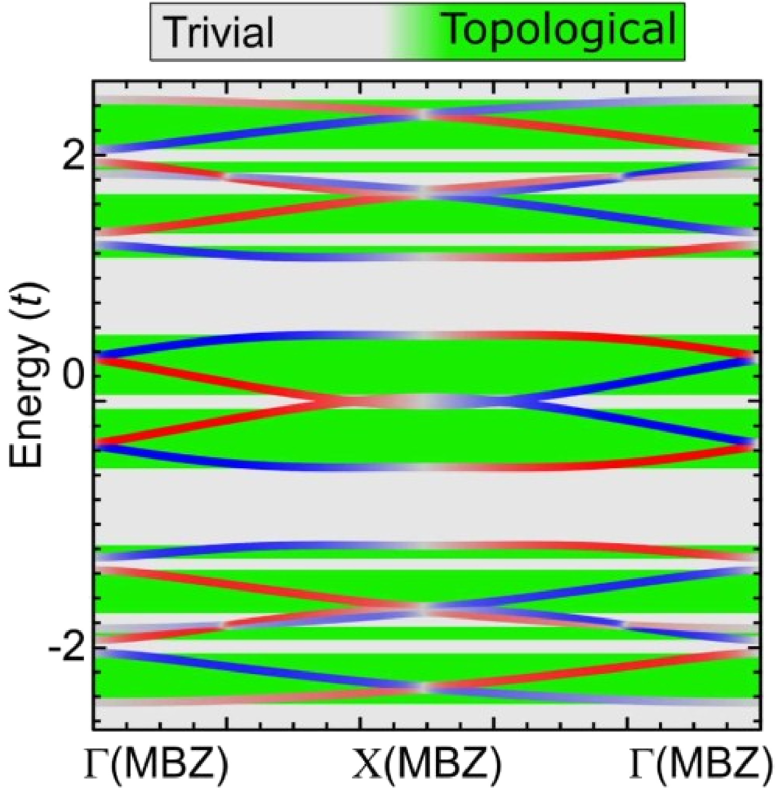
Artificial moire topological superconductor





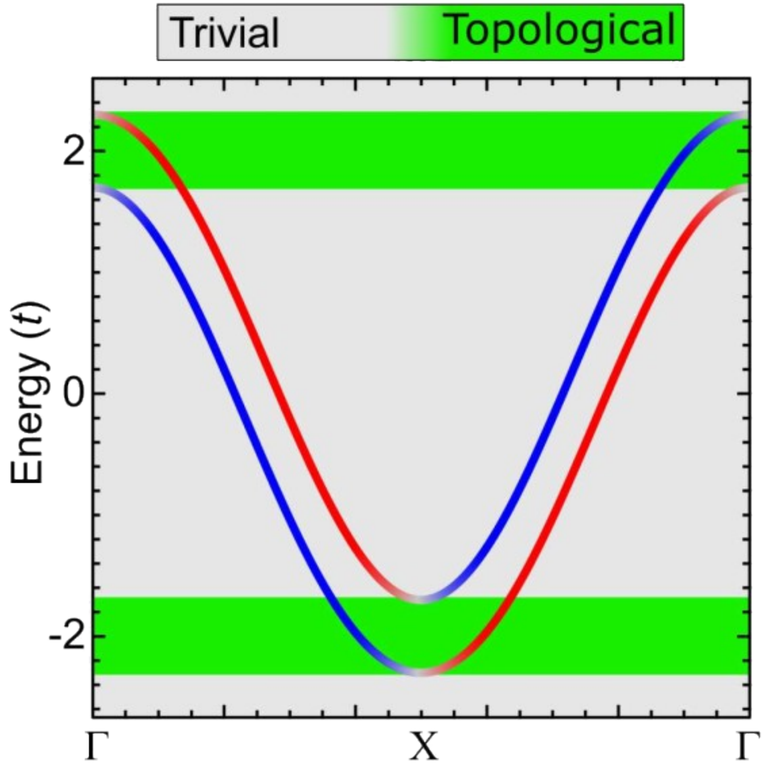
Artificial moire topological superconductor



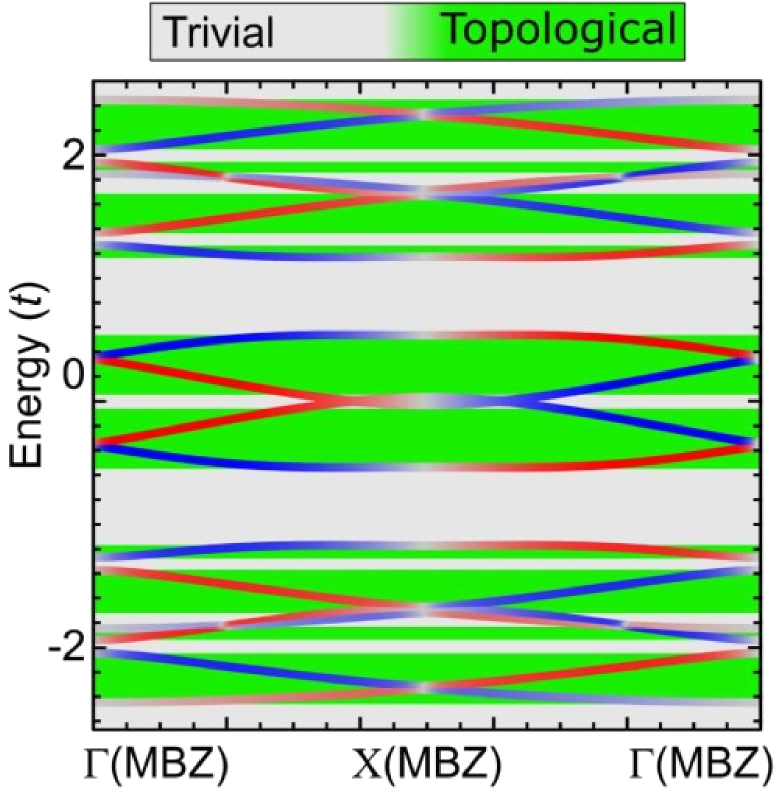


Artificial moire topological superconductor

Without moire

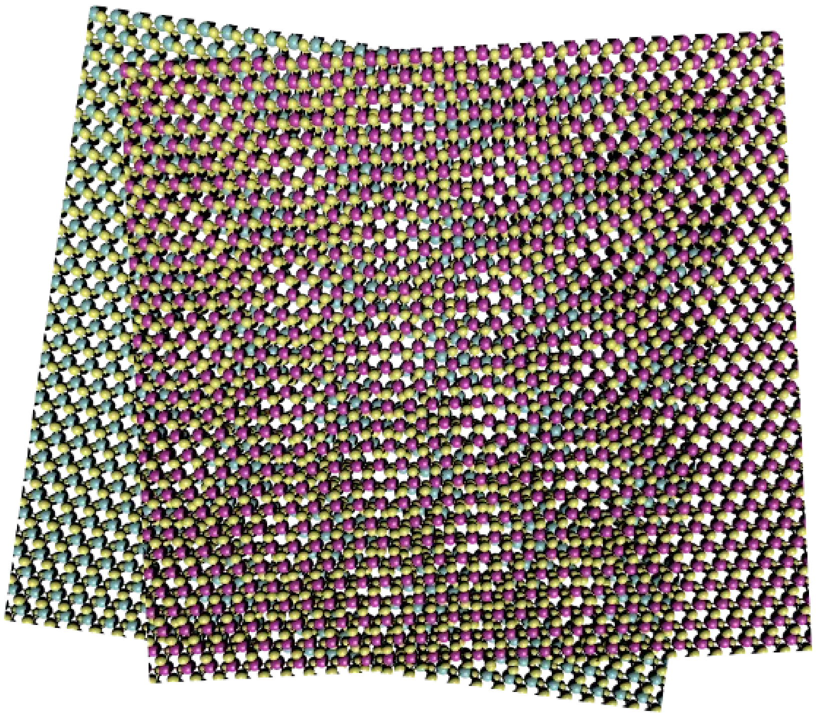


With moire



Moire driven gaps in the band structure

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



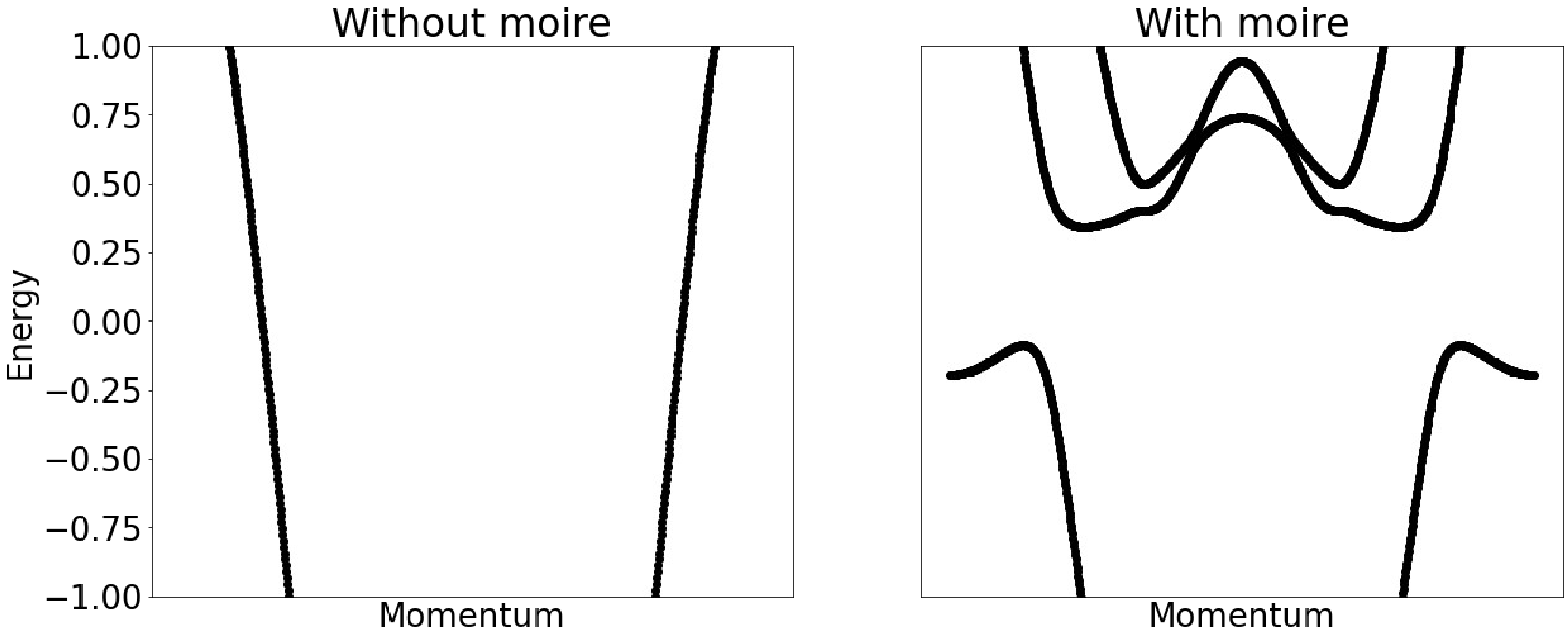
$$H = H_0 + H_J + H_R$$

Kinetic energy

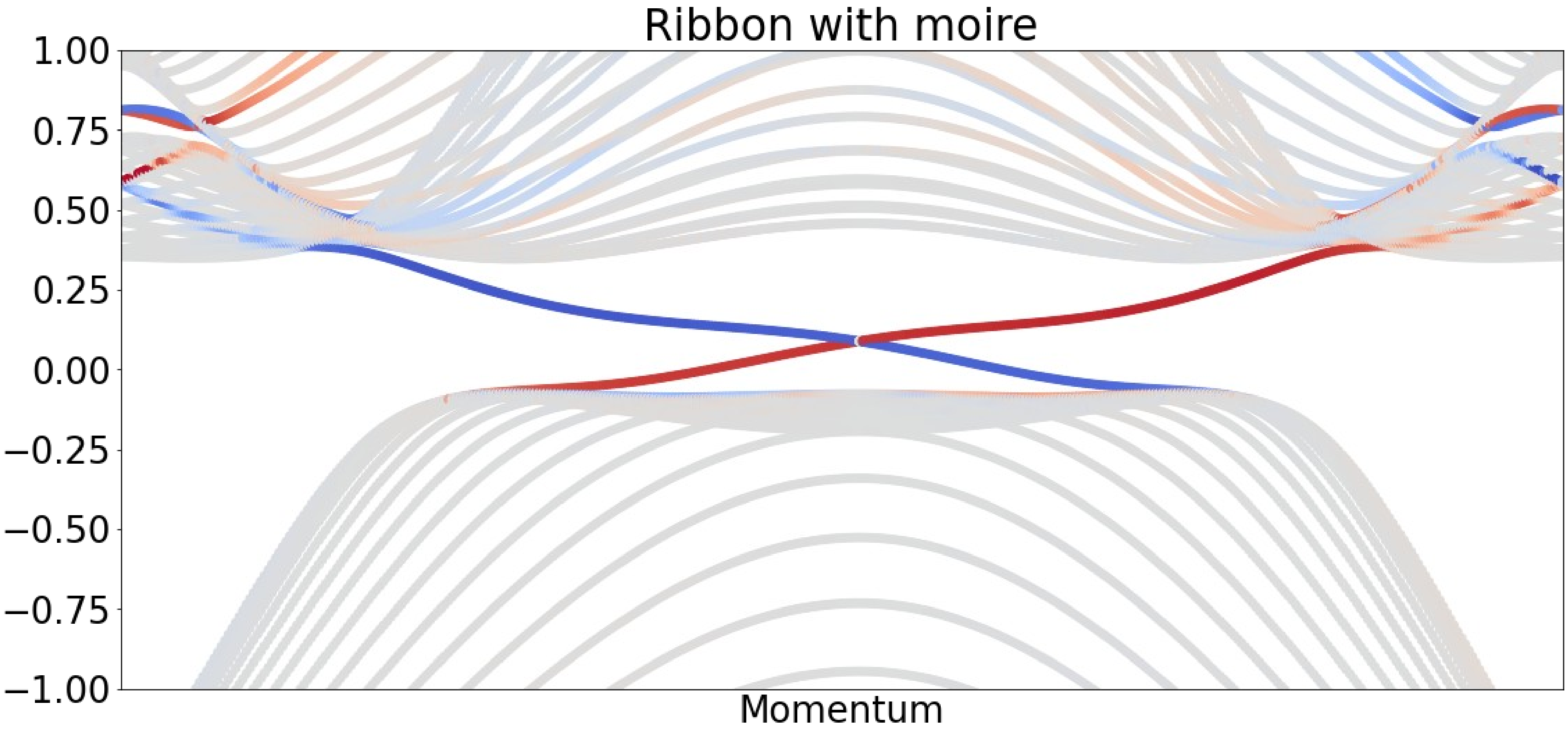
Exchange field

Rashba spin-orbit coupling

Moire driven gaps in the band structure



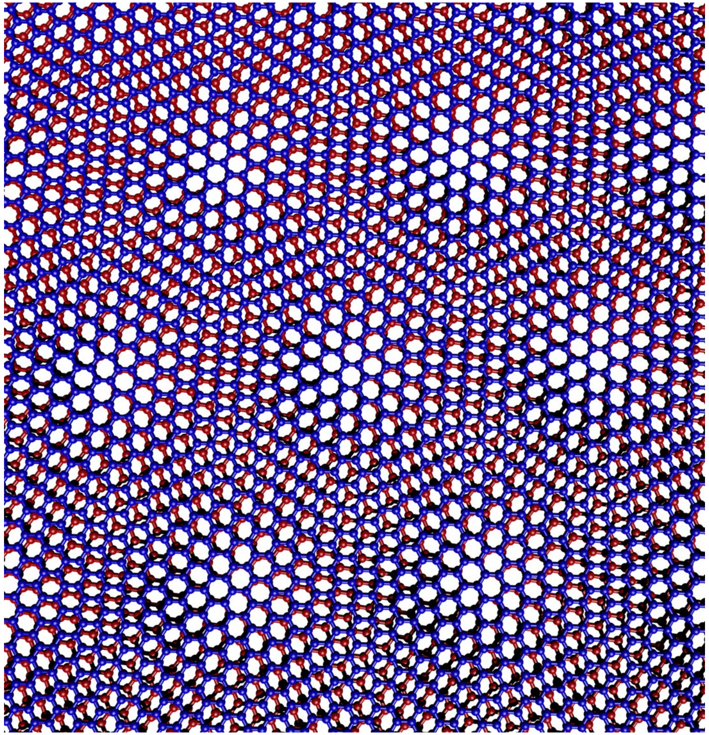
Moire driven gaps in the band structure

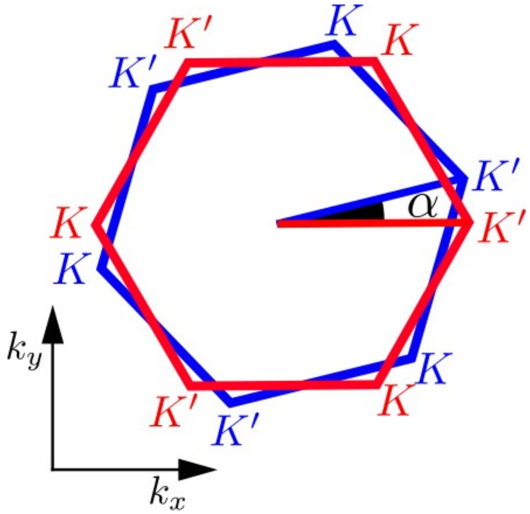


Chiral states appear in a ribbon driven by the moire

Electronic structure of twisted graphene multilayers

Twisted bilayer graphene



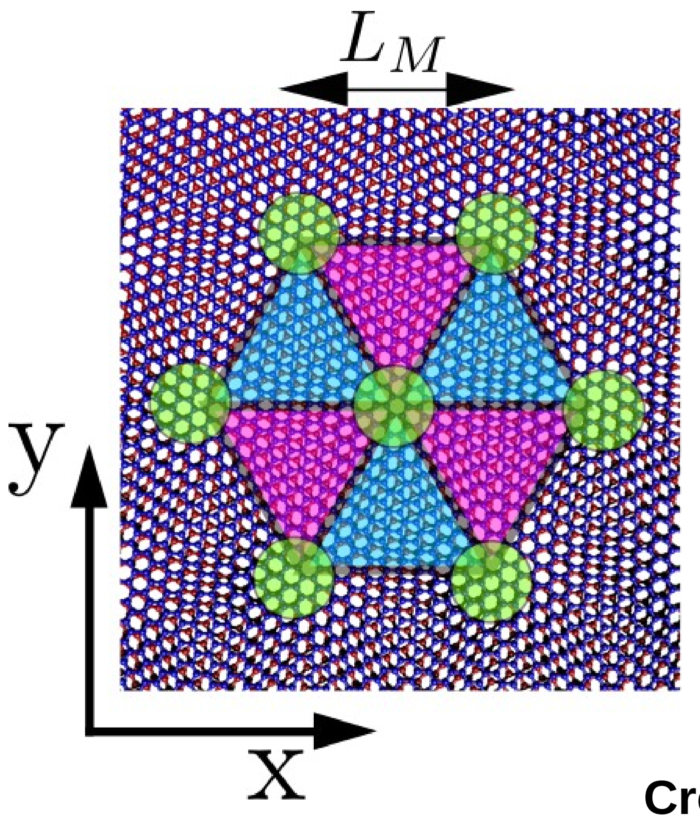


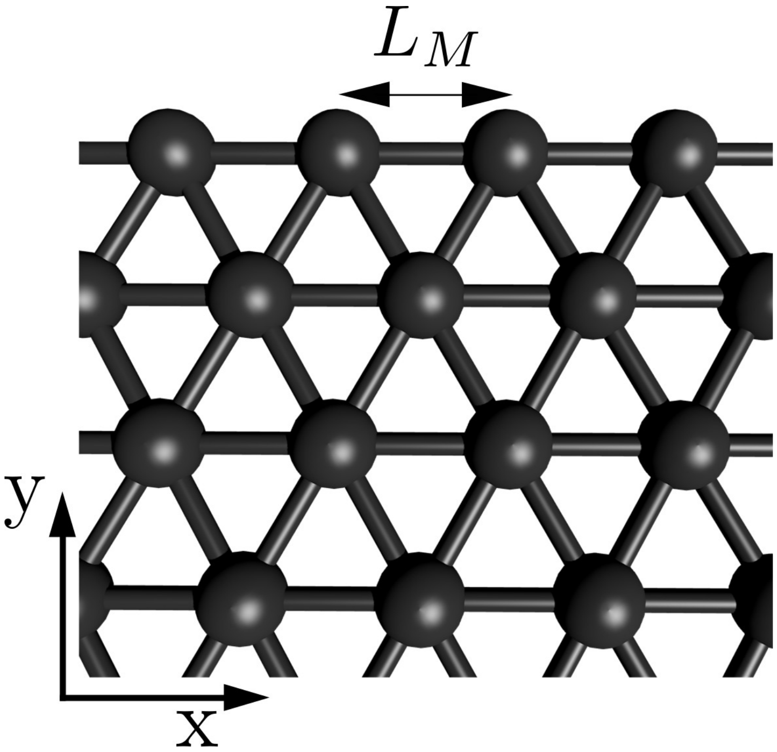
Additional parameters in the system

Angle between the layers α

Bias between the layers U

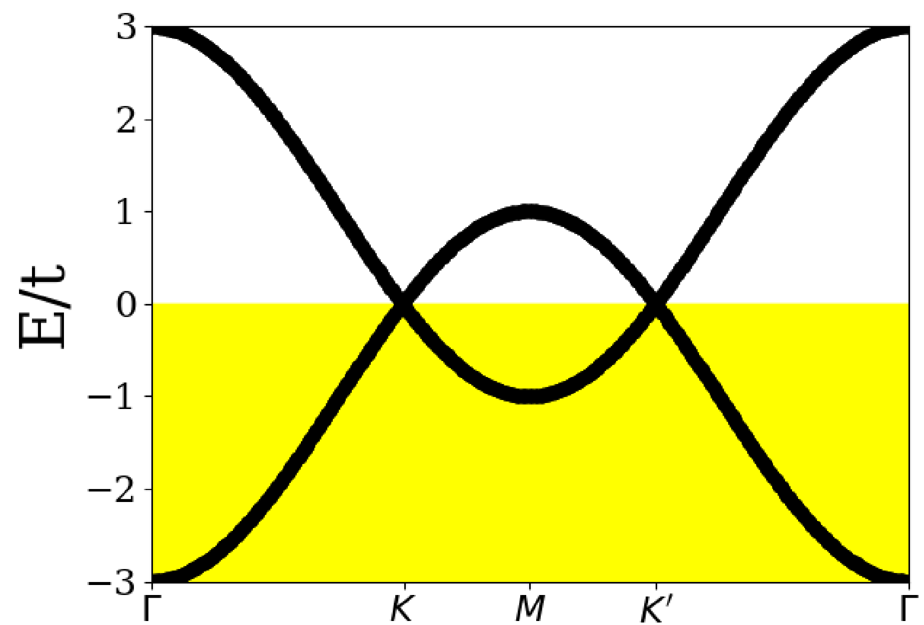
A new length scale: the moire length

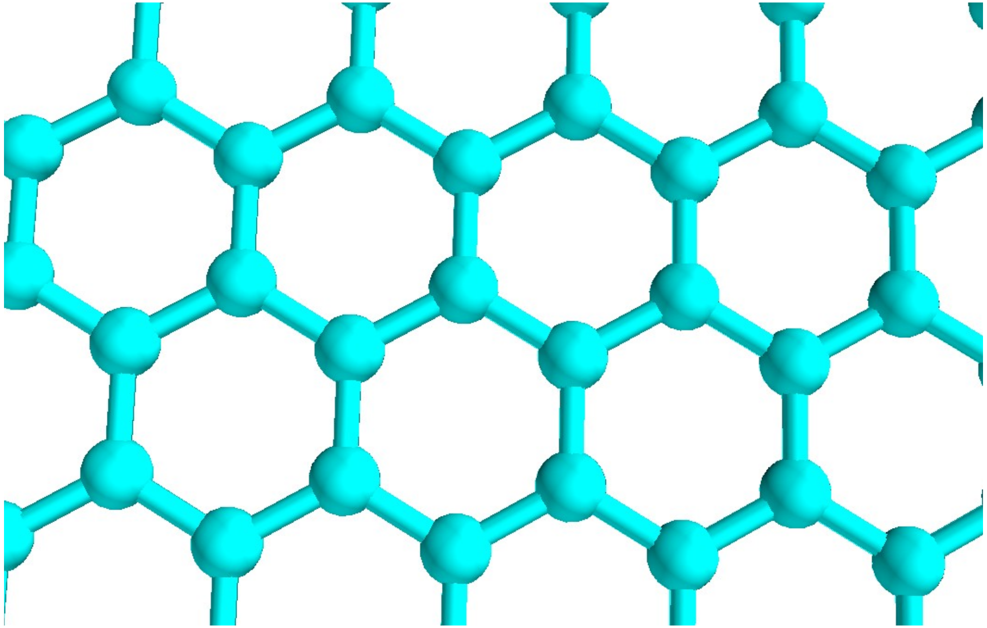




Creating effective lattices with tunable lattice constants

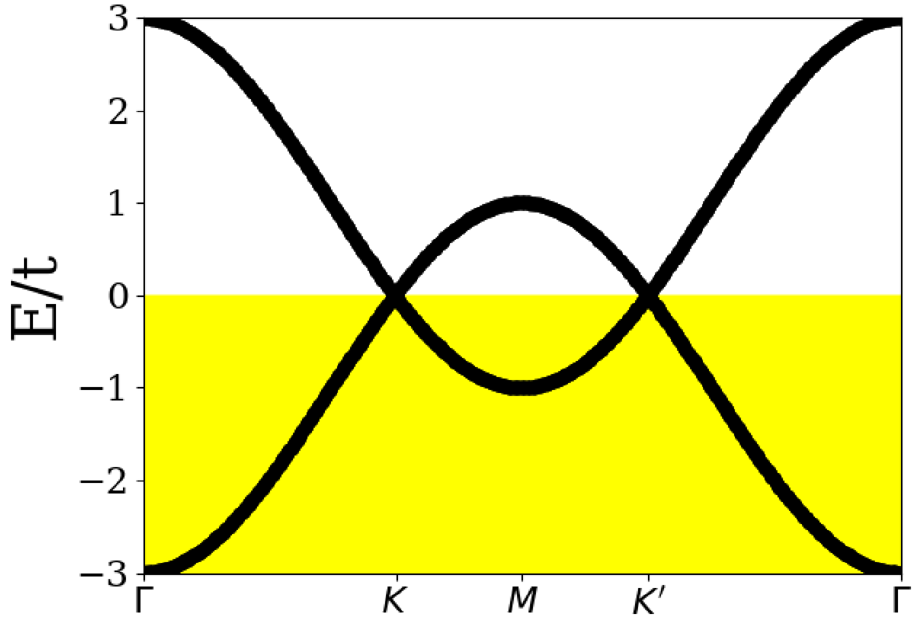
Structure of graphene





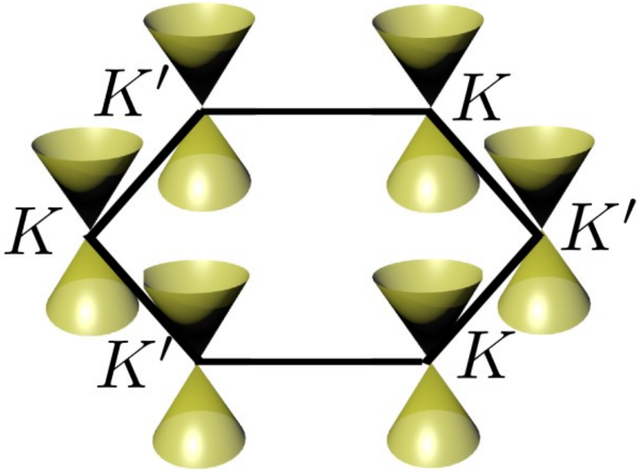
Minimal model: Single orbital in a honeycomb lattice

The electronic structure of graphene

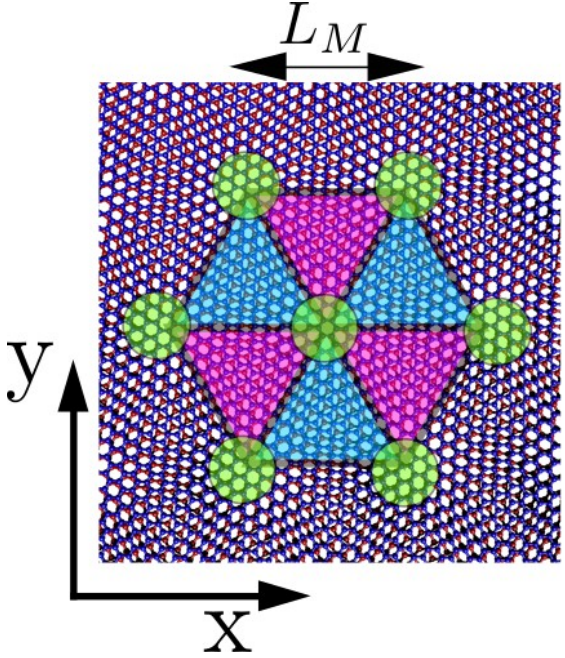


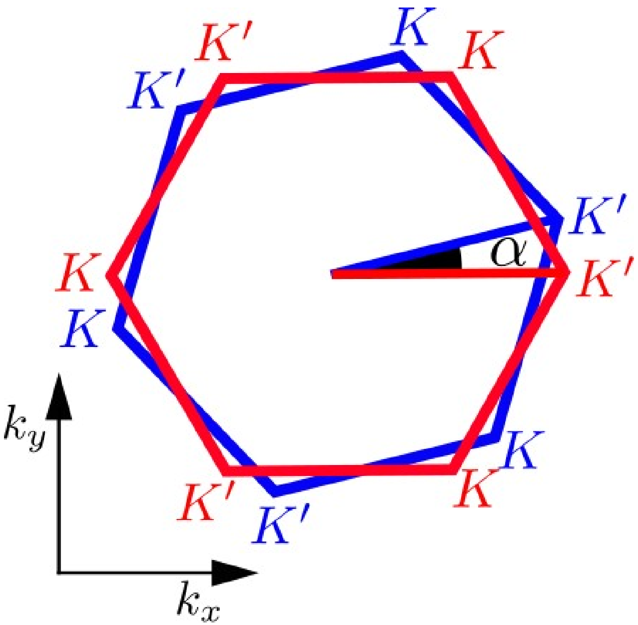
$$H = \begin{pmatrix} 0 & p_x \pm i p_y \\ p_x \mp i p_y & 0 \end{pmatrix}$$

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



Real and reciprocal space in twisted bilayer graphene



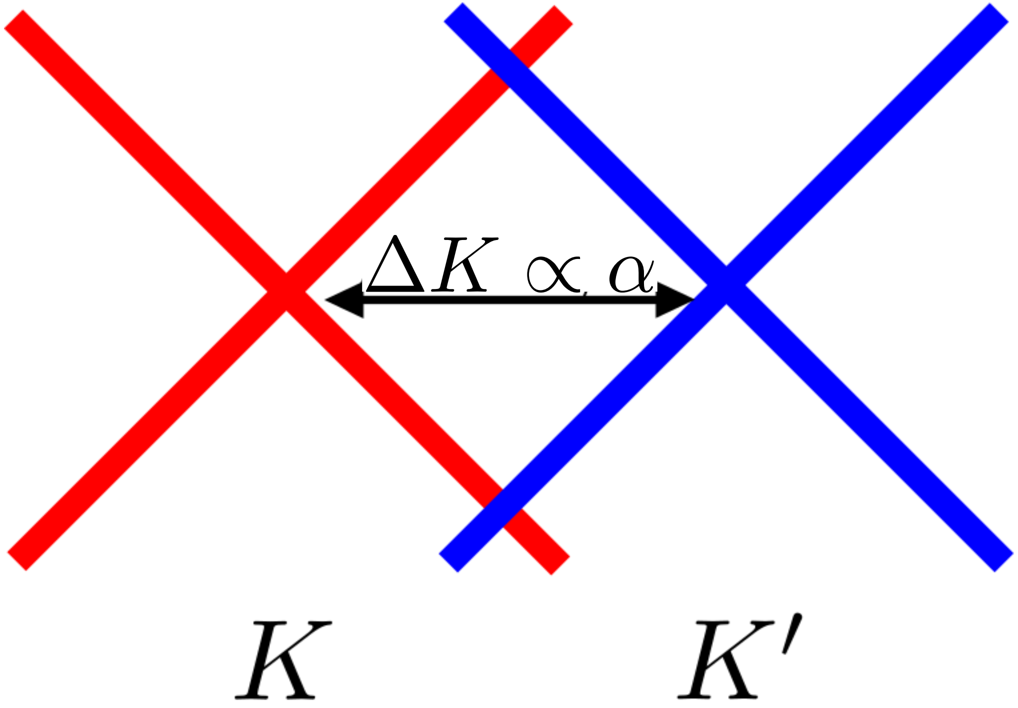


Intralayer   Interlayer   Bias

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

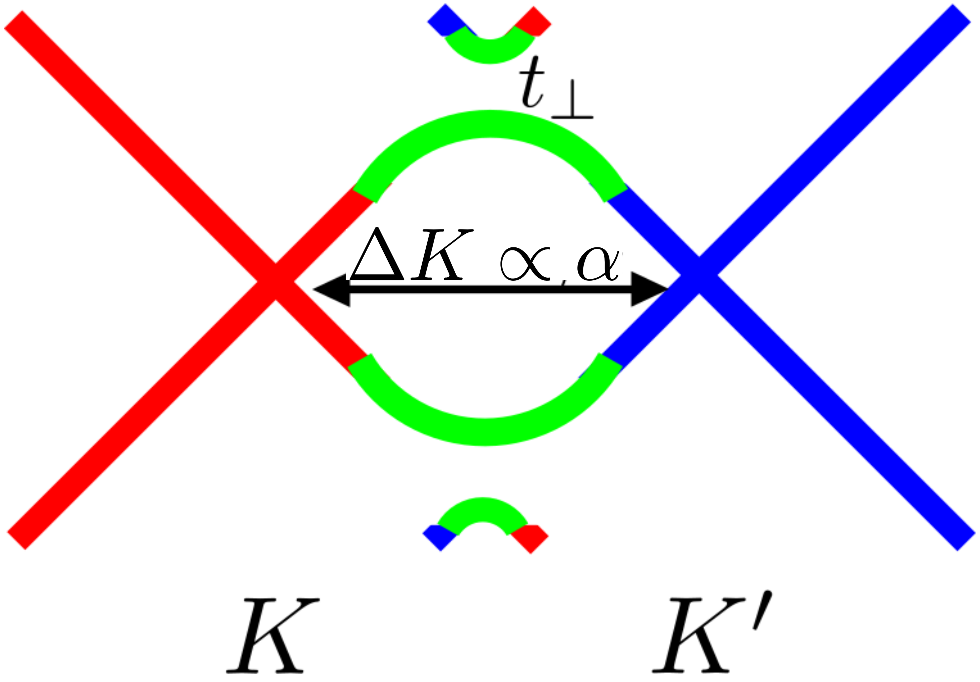
Velocity renormalization at large angle

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



Velocity renormalization at large angle

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

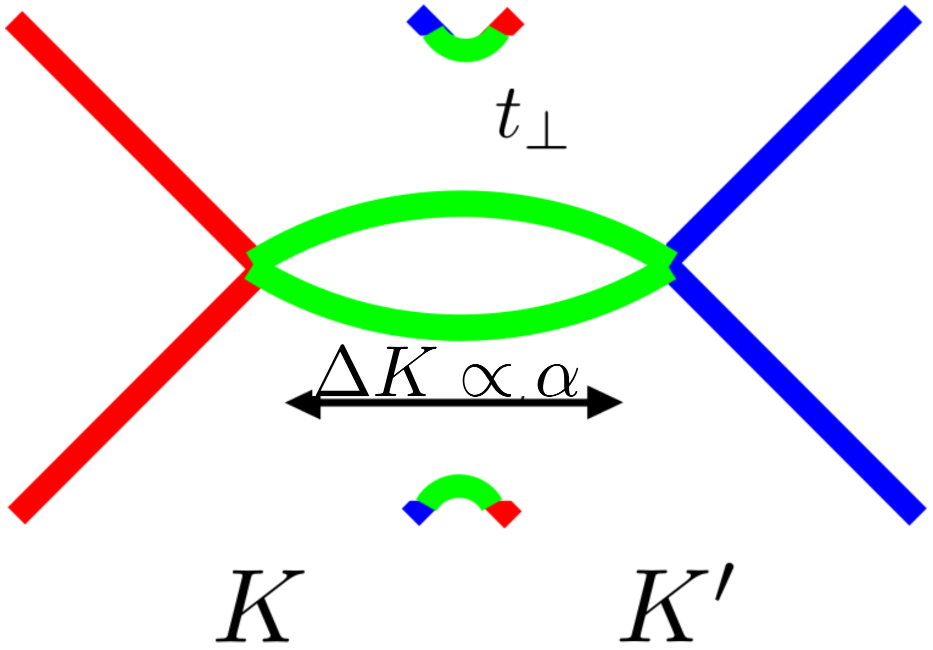


Relevant ratio

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

Velocity renormalization at large angle

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

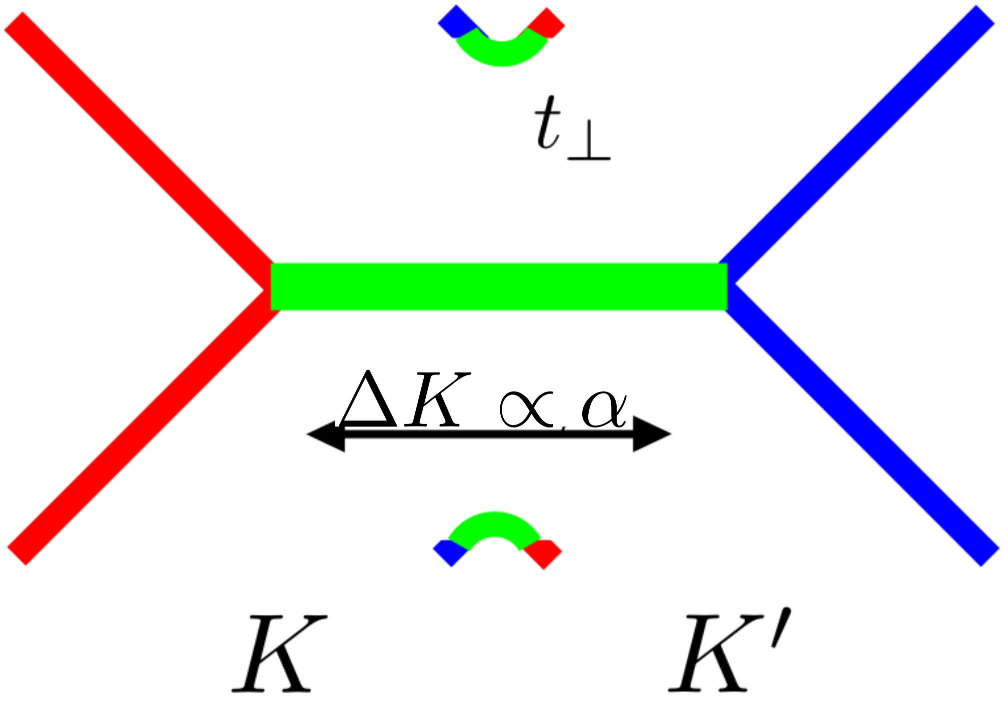


Relevant ratio

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

Velocity renormalization

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

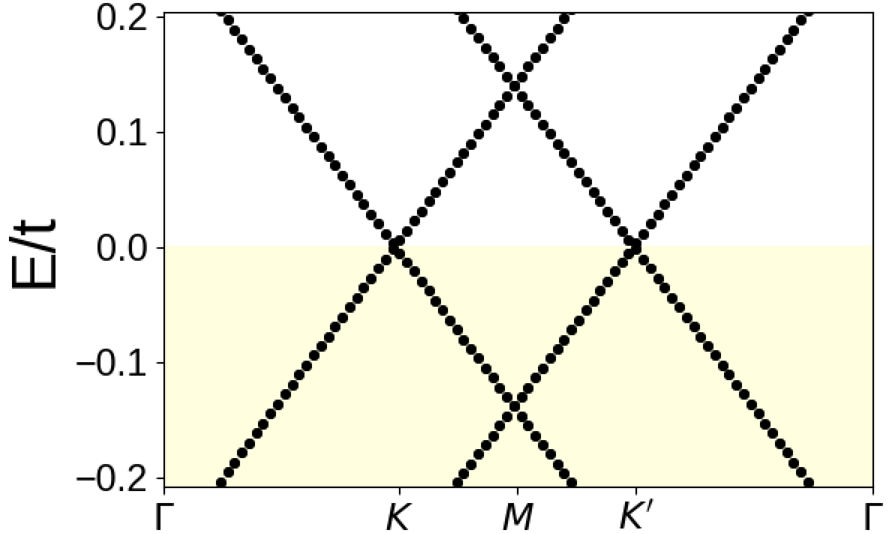


Relevant ratio

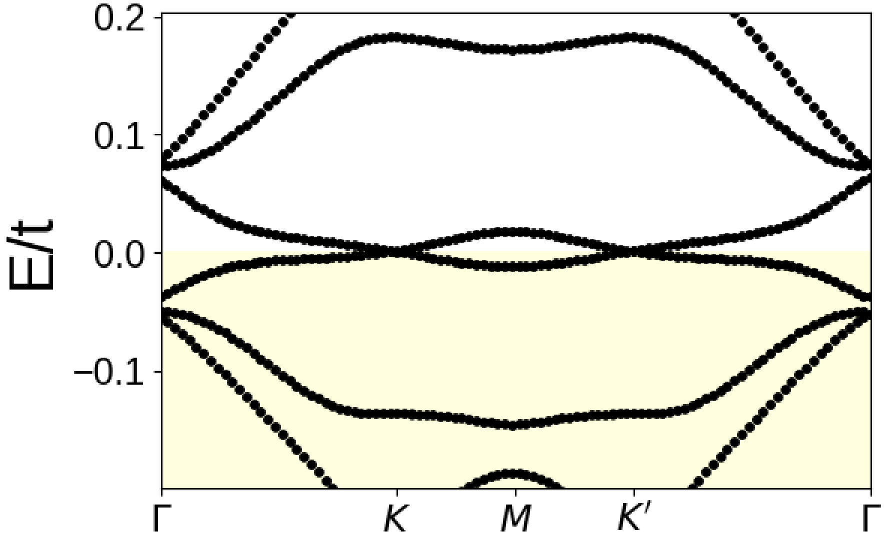
$$\frac{t_\perp}{\alpha}$$

Band structure of twisted bilayer graphene

Decoupled

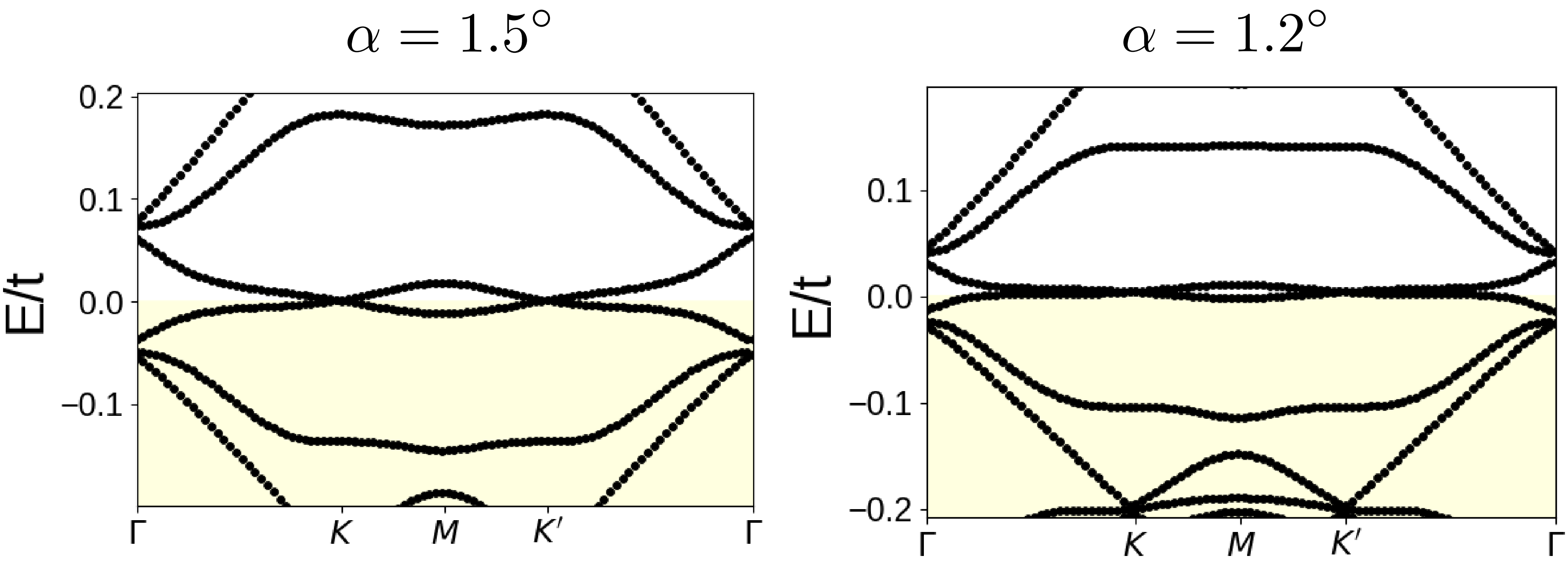


$\alpha = 1.5^\circ$



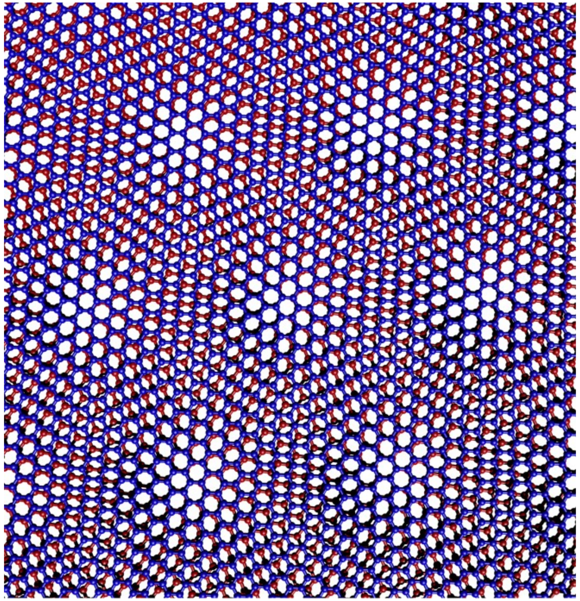
As the angle between layers in decreased, the bands become flatter

Band structure of twisted bilayer graphene

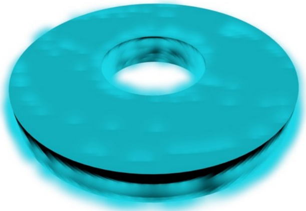


As the rotation angle approached 1 degree, the lowest band becomes flatter

Correlations in twisted bilayer graphene flat bands

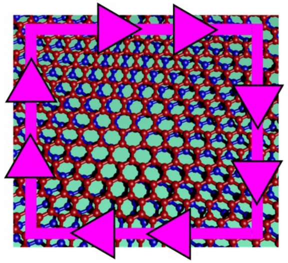


Superconductivity



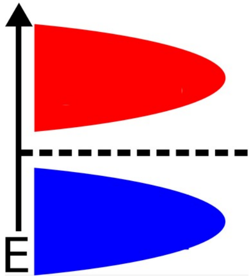
Nature 556, 43–50 (2018)

Chern insulators



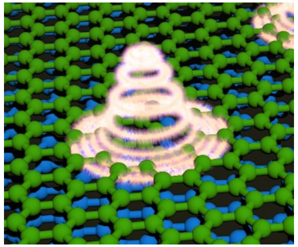
Science 365, 605-608 (2019)

Correlated insulators



Nature 556, 80–84 (2018)

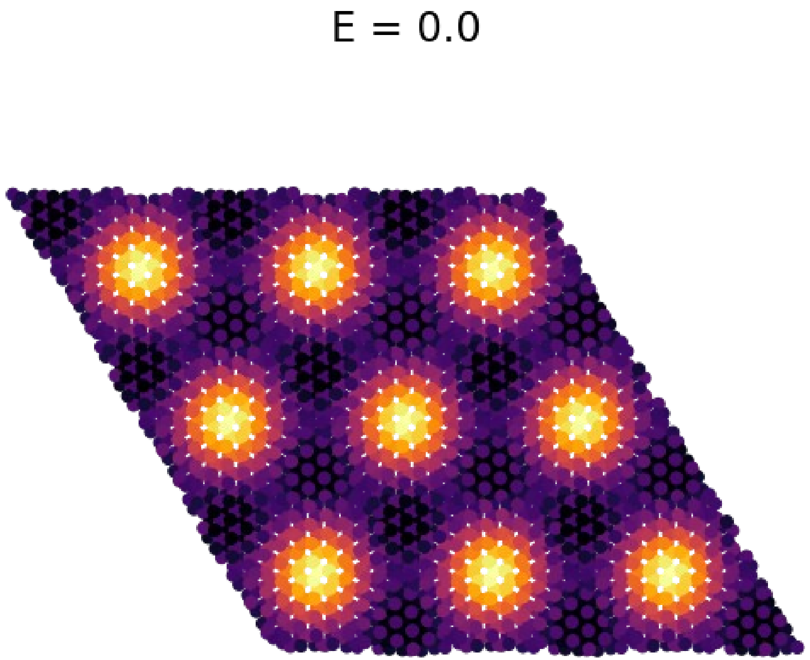
Fractional Chern insulators



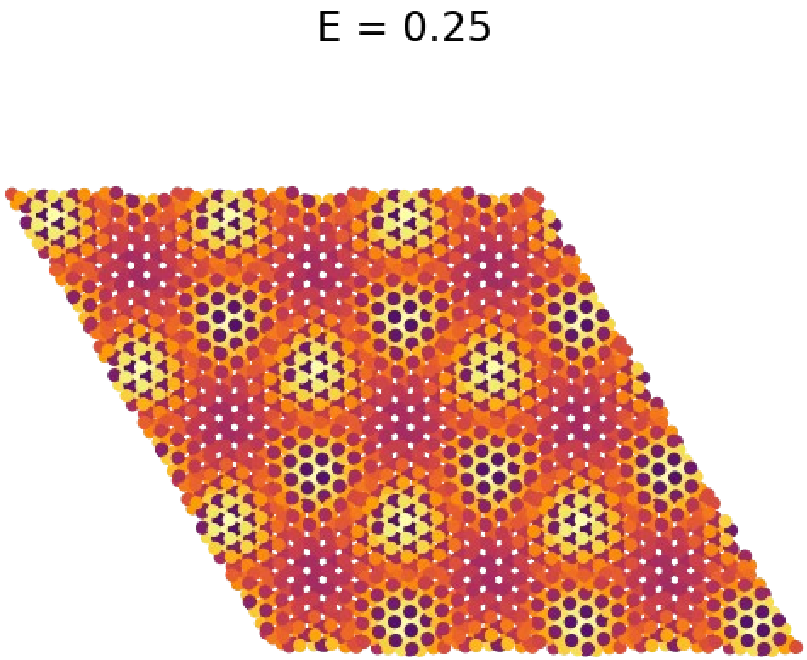
Nature 600, 439–443 (2021)

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

Distribution of states in the twisted graphene bilayer



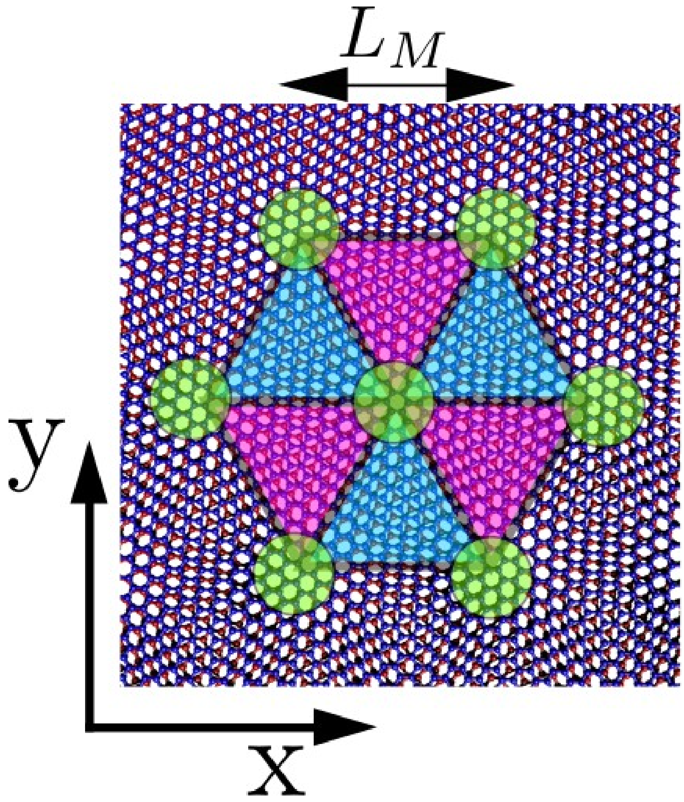
Triangular

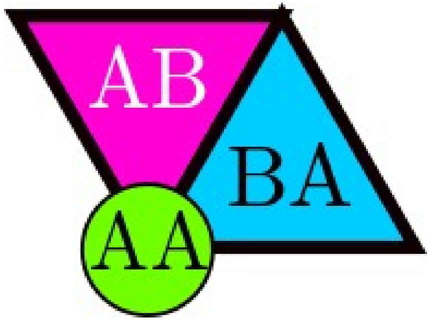


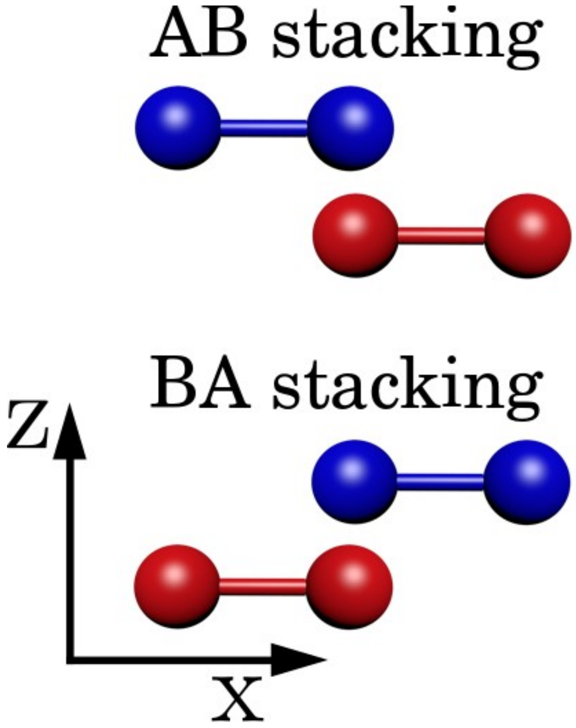
Hexagonal

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

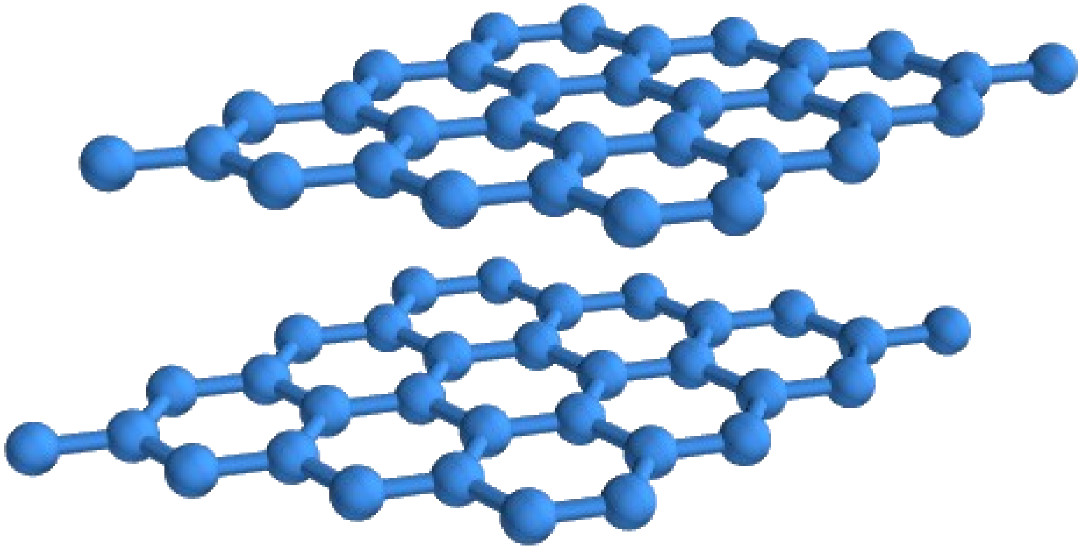
Stacking of twisted bilayer graphene







Bias in AB bilayer graphene



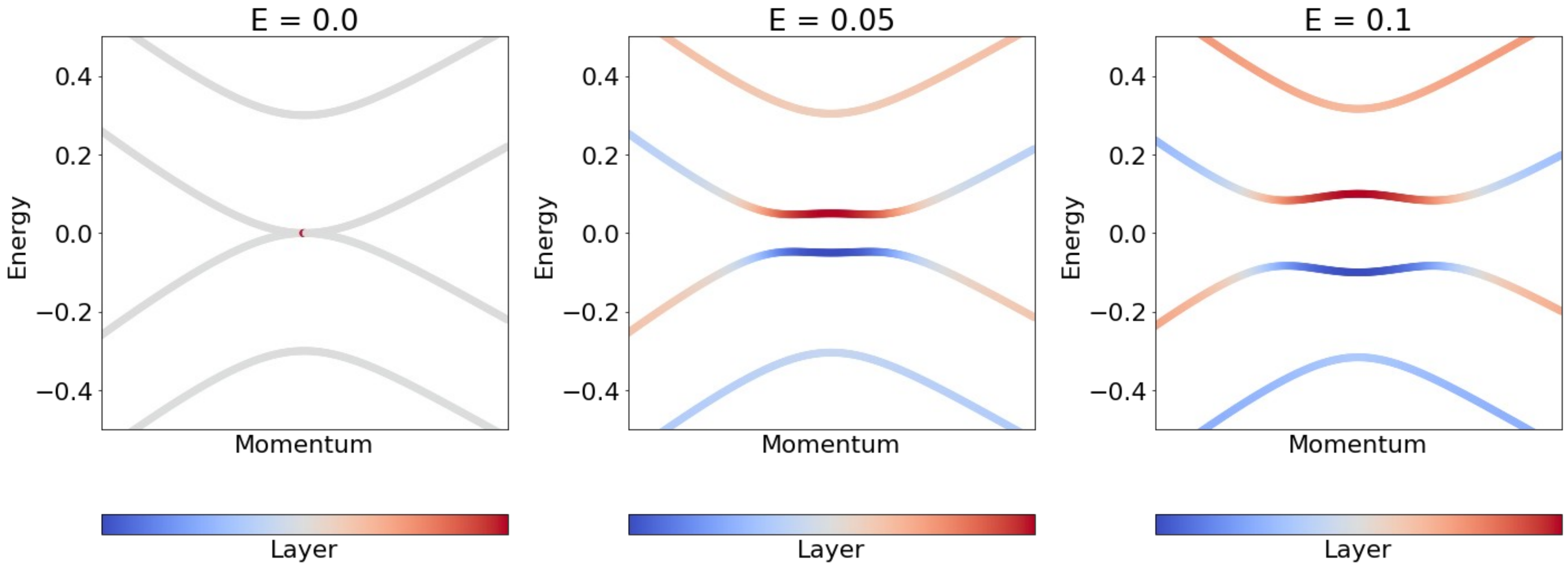
$$V c_n^\dagger c_n$$

$$-V c_n^\dagger c_n$$

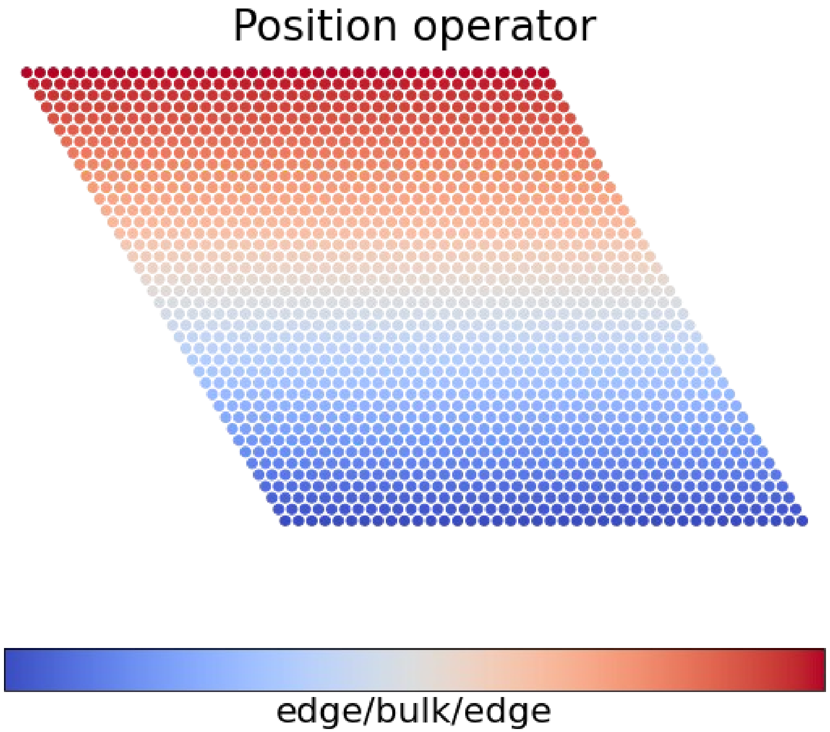
Let us look at the impact of a bias in an aligned graphene bilayer

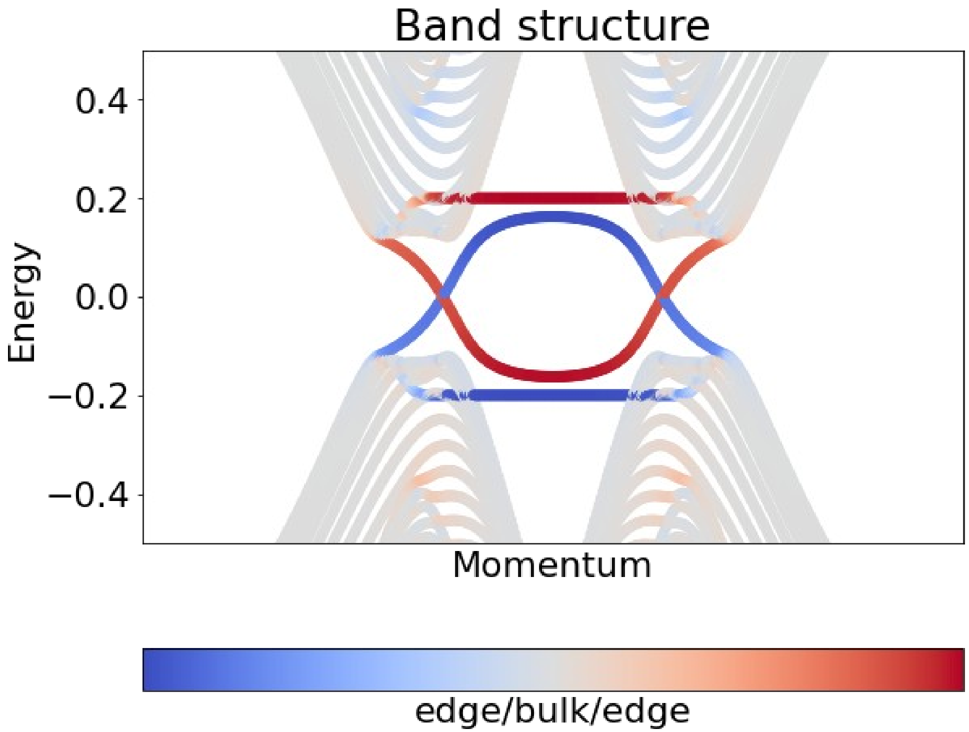
The electronic structure of bilayer graphene

Graphene bilayers open a gap when an interlayer bias is applied



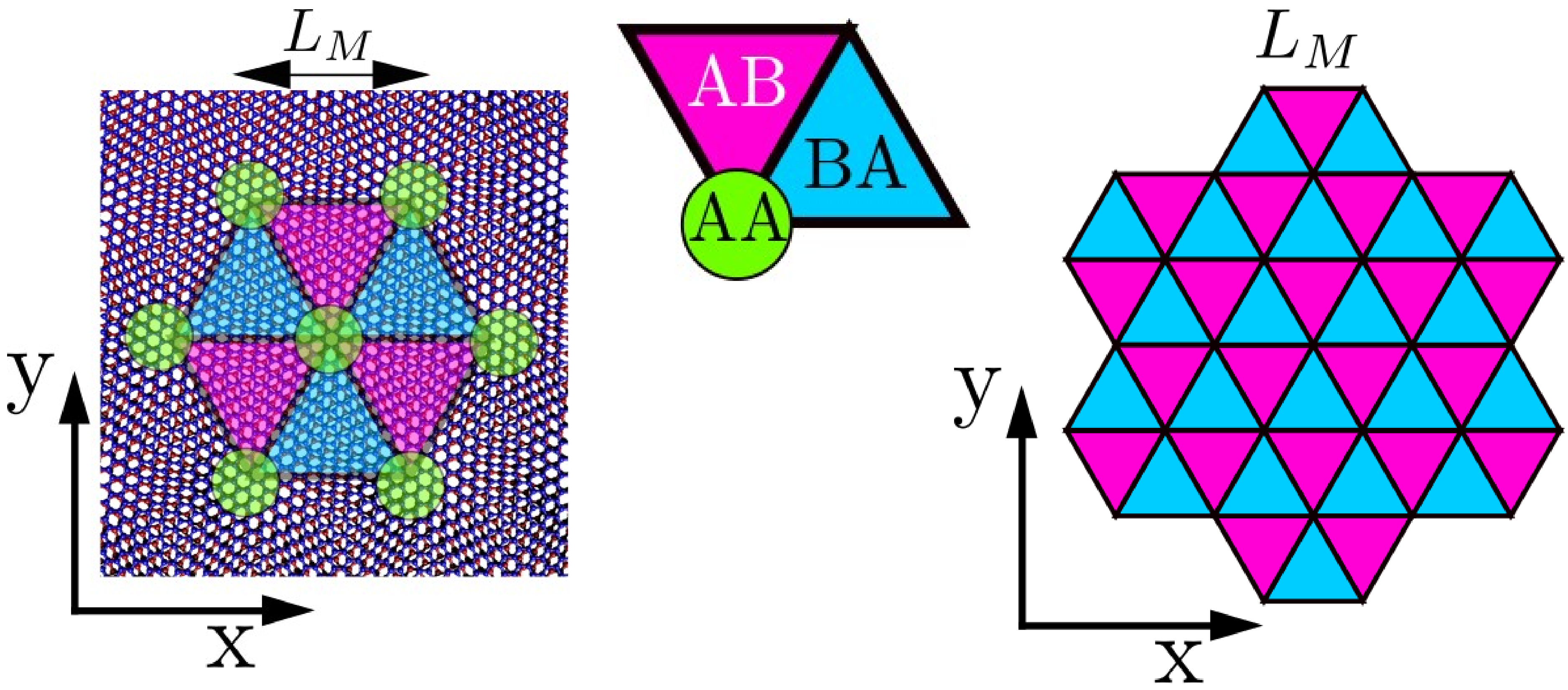
Biased bilayer graphene, pseudo-helical states



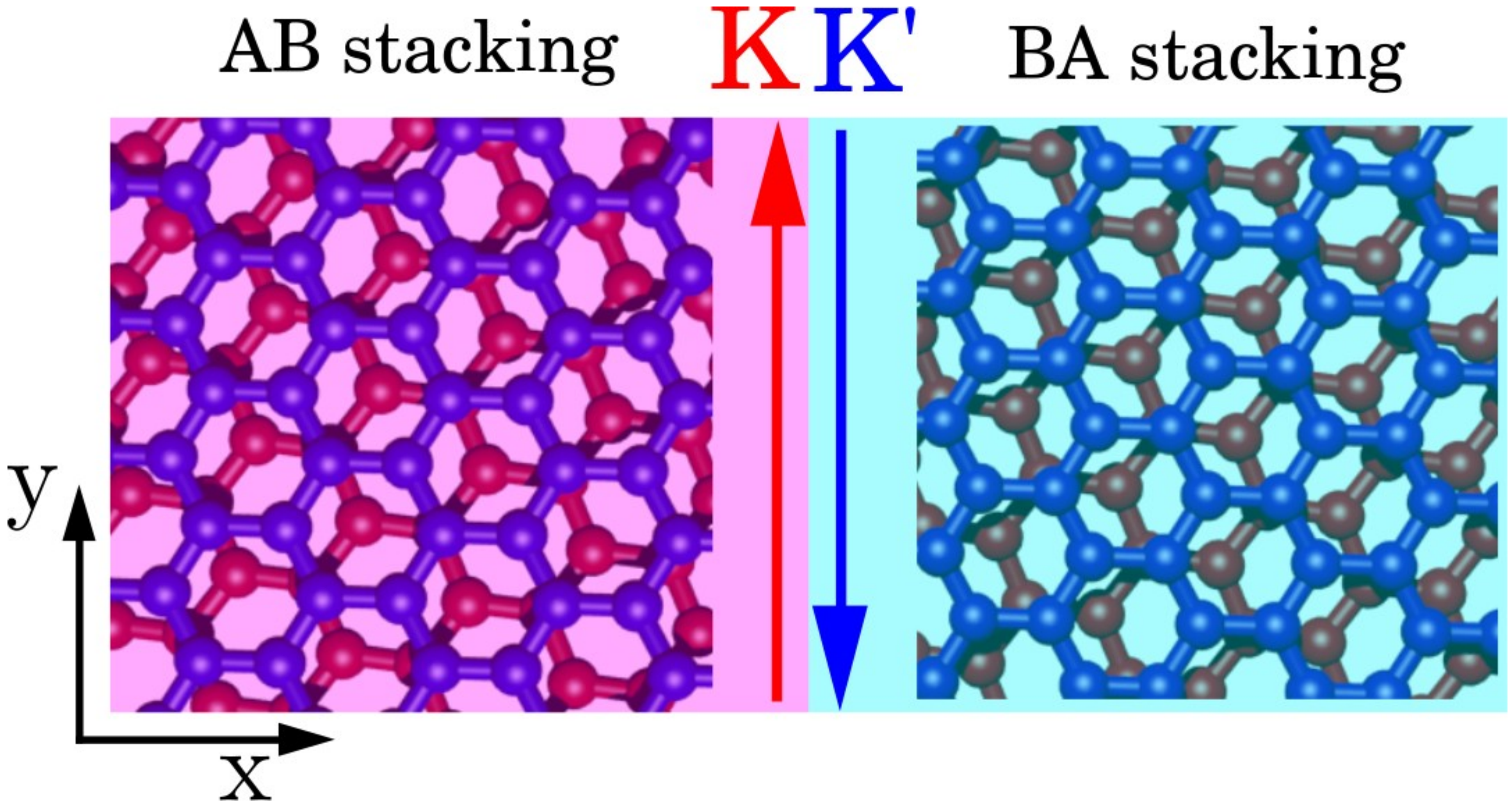


Edge states appear in the presence of a bias between layers

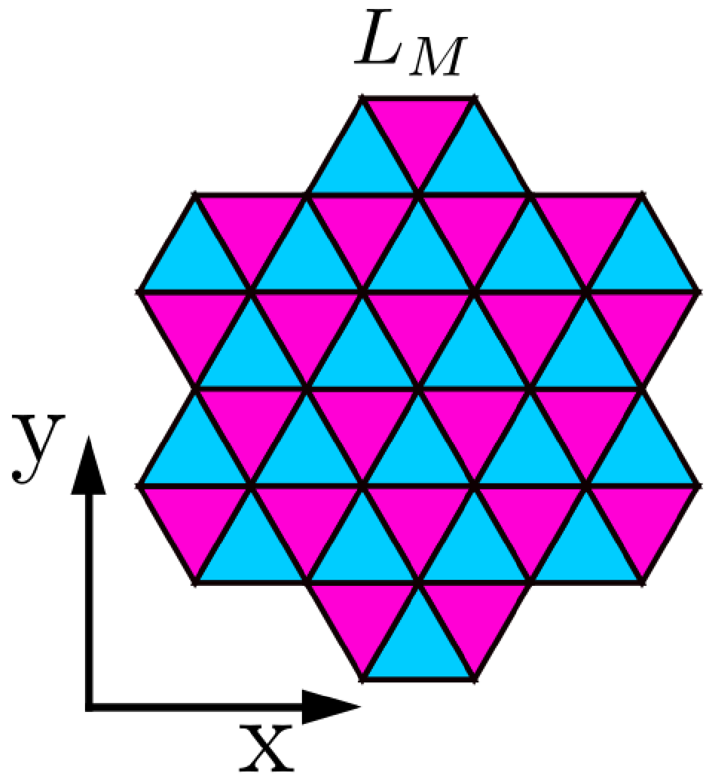
Stacking of twisted bilayer graphene

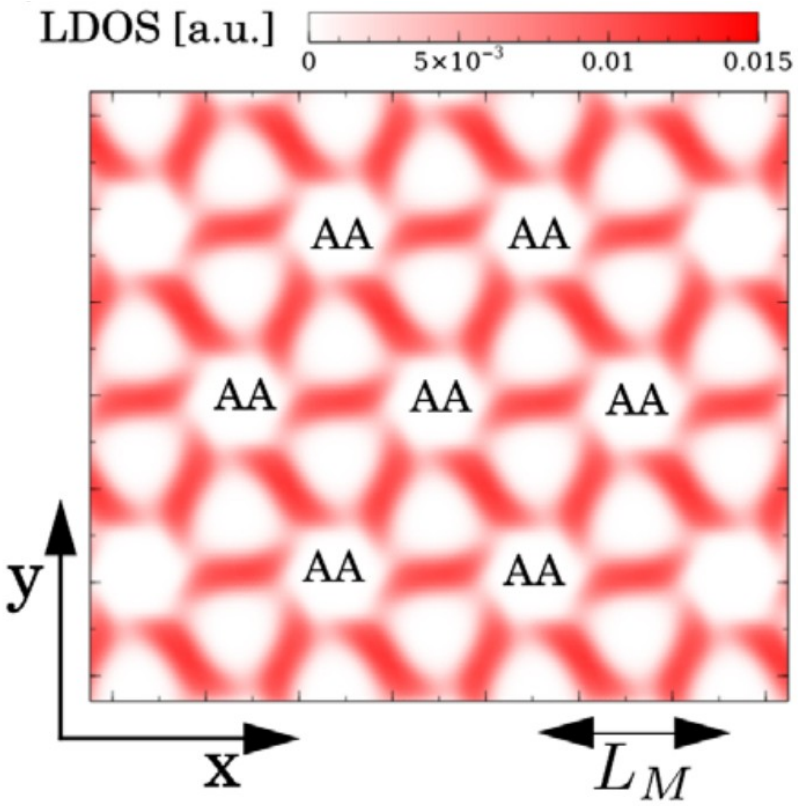


Interfacial modes in biased TBG



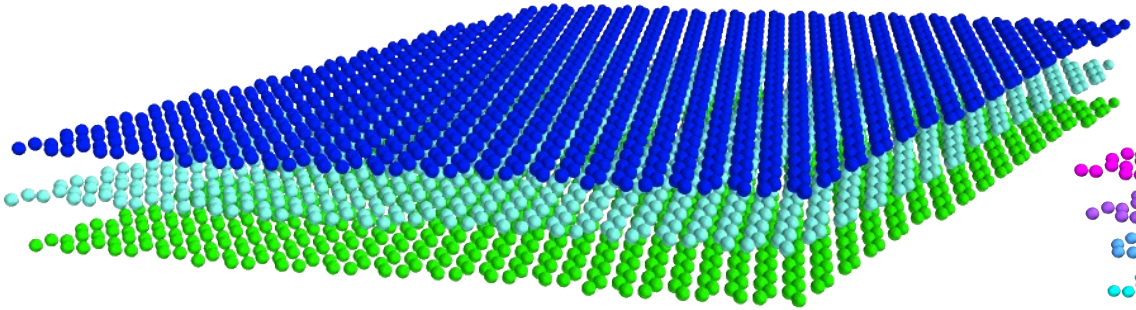
Helical networks in TBG



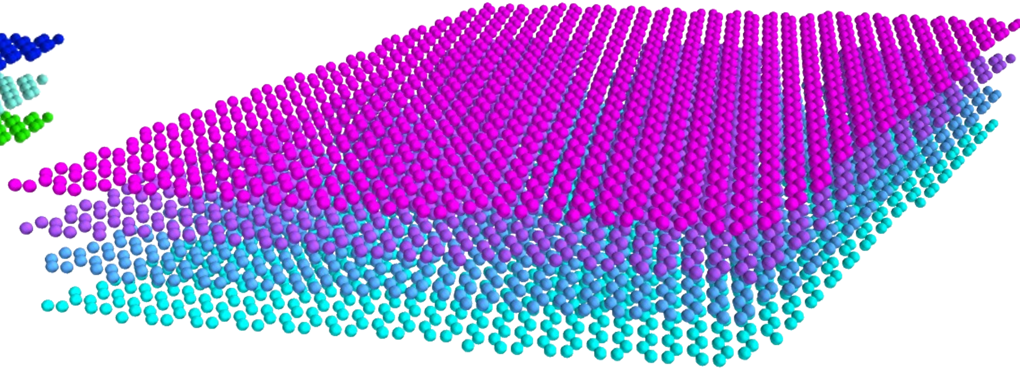


Other twisted graphene multilayers

Twisted graphene trilayer

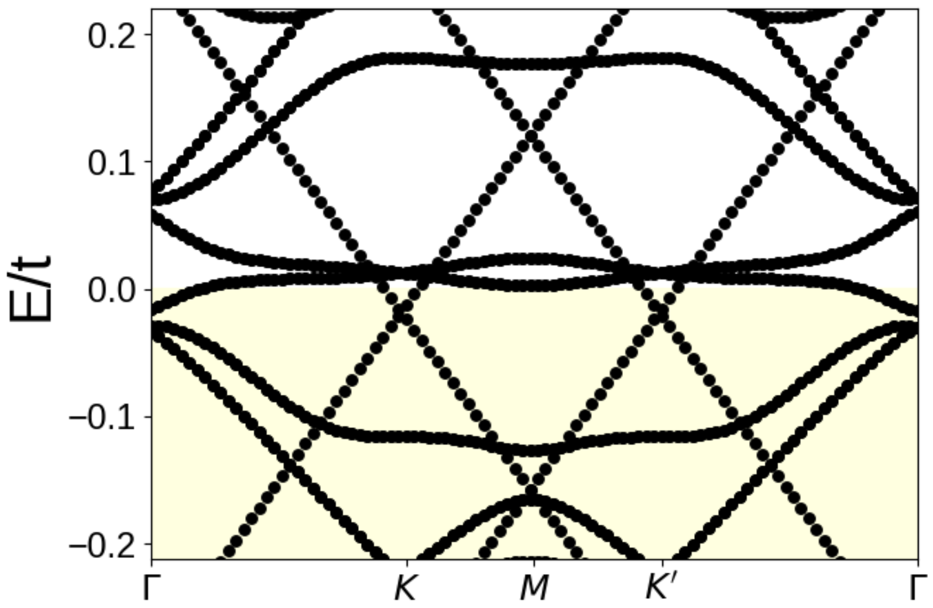


Twisted graphene double bilayer

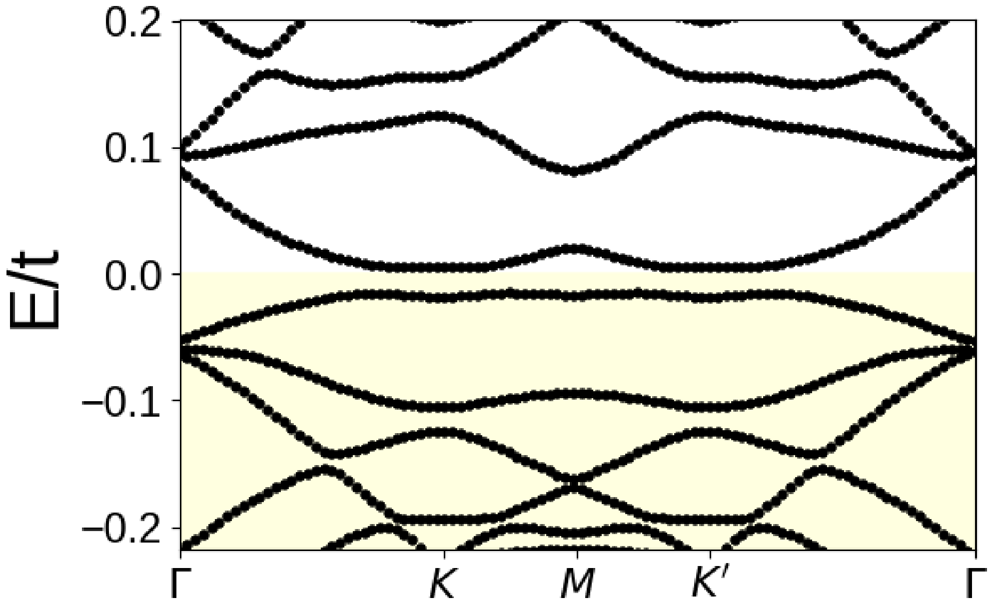


Other twisted graphene multilayers

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

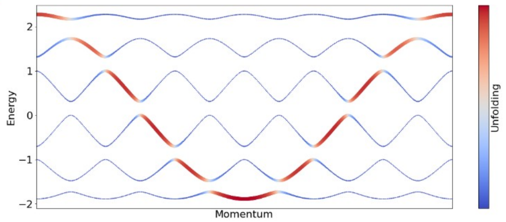
You will see examples with the code

In [17]:
```
# let us now add an impurity in the previous supercell, and see how it leads to anticrossings in the bands
from pyqula import geometry
g = geometry.chain() # generate chain
N = 6 # size of the supercell
g = g.get_supercell(N,store_primal=True) # generate a supercell, store_primal is required for unfolding
h = g.get_hamiltonian() # and generate the Hamiltonian

# let us define a potential for an impurity
r0 = g.r[0] # location of the impurity
fpot = lambda r: 1.*(((r-r0).dot(r-r0))<1e-2) # impurity in site r0
# from pyqula import potentials ; fpot = potentials.impurity(r0,v=1.) # this is equivalent

h.add_onsite(fpot) # and add the impurity potential
kpath = g.get_kpath()*N # compute in the original Brillouin zone, just by extending the reciprocal vectors
(k,e,c) = h.get_bands(operator="unfold",kpath=kpath) # compute band structure
plt.scatter(k,e,c=c,s=c*8+.5) ; plt.xlabel("Momentum") ; plt.ylabel("Energy") ; plt.xticks([]) # plot
plt.colorbar(label="Unfolding",ticks=[])
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