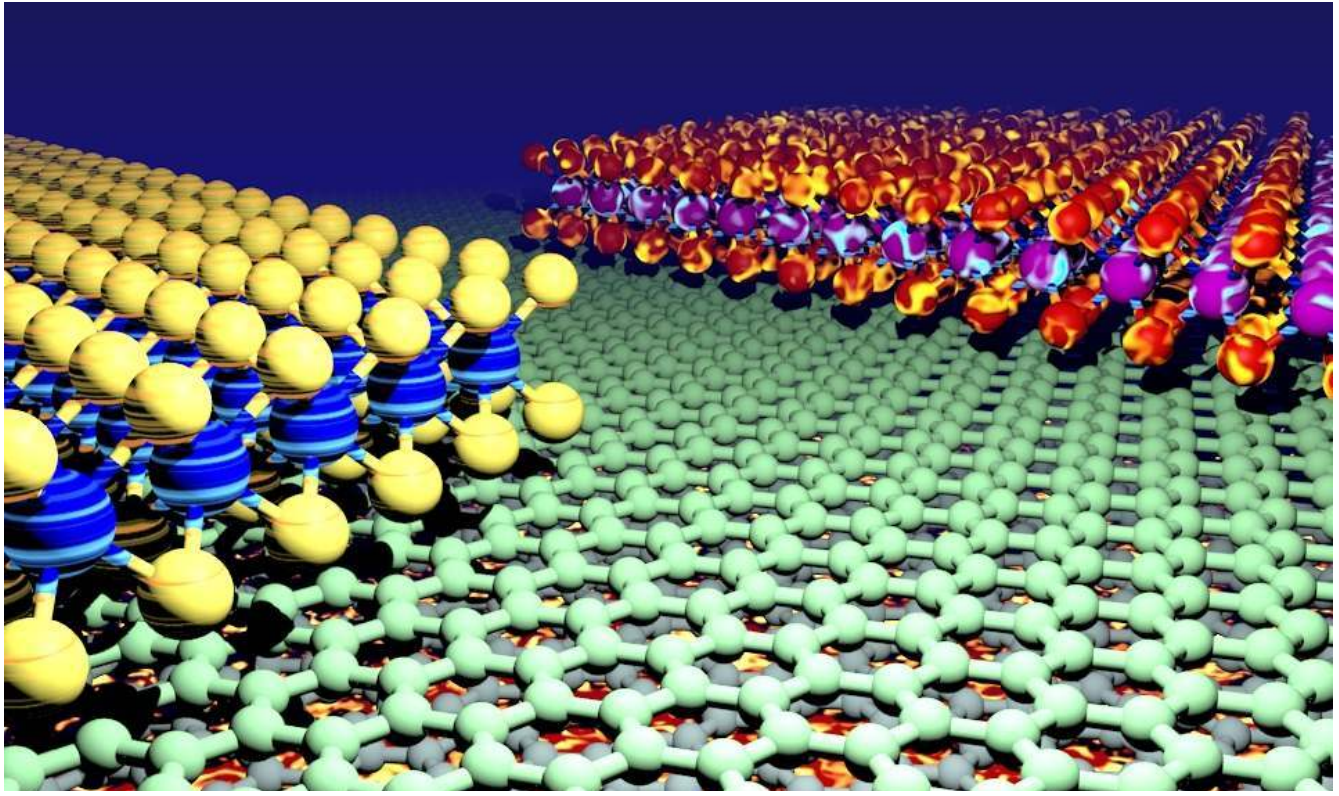
Session 1: Introduction to 2D materials



Jyväskylä Summer School "Emergent Quantum Matter in Artificial Two-dimensional Materials"

Monday, August 8th 2022

Introductions

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Shawulienu Kezilebieke

Jose Lado

University of Jyväskylä

Aalto University

Today's plan

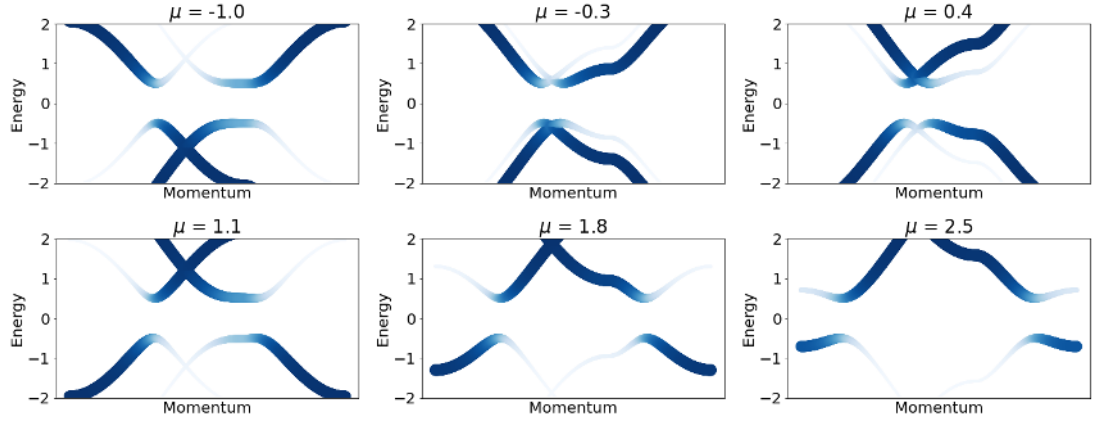
- Welcome and introductions to the summer school
- Introduction to 2D materials
- An introduction to the theory tools: electronic structure, second quantization and mean-field theory
- The tunability of 2D materials
- An introduction to the computational tools

A few practicalities

- Please feel free to interrupt at any point, the more questions the better
- Any questions are greatly welcome
- The lectures are recorded, if you want to remove any questions from the recording let us know

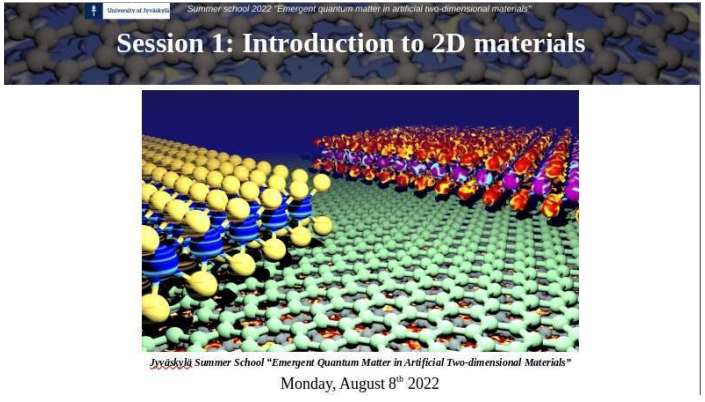
The aim of the summer school

- The main objective is to learn to design 2D materials by experimenting in a “computational lab”
- The lecture slides support the objectives of the exercises sessions



About the lecture slides

- The slides will be publicly available for your reference
- For the hands-on sessions, the slides can be helpful, but they are not necessary to do the exercises



About the lecture notes

- Each session has associated lecture notes, that are made available each day
- The lecture notes are not necessary at all for following the lecture or exercises
- The lecture notes are given as further detailed material, yet you are not required to read them for the summer school
- The lecture notes will be made publicly available

About the hands-on exercise sessions

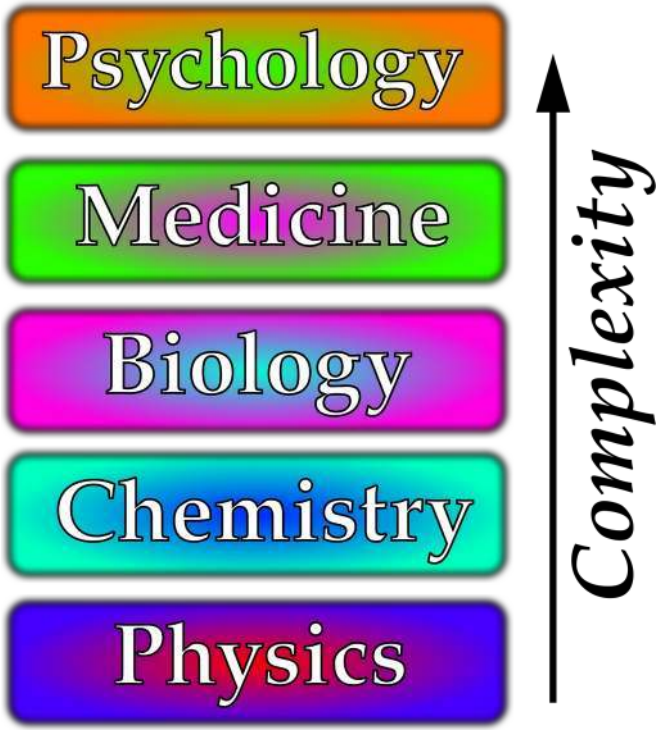
- The exercise sessions are based on hands-on computational exercises with a Python-based library (pyqula)
- You will do the exercises in pairs, and several exercises require you to discuss with each other
- The exercises are organized in Jupyter-notebooks
- You are given examples, and asked to explain what you observe and perform further calculations to answer specific questions
- The exercises demonstrate the concepts discussed during the lectures

Schedule for the lecture

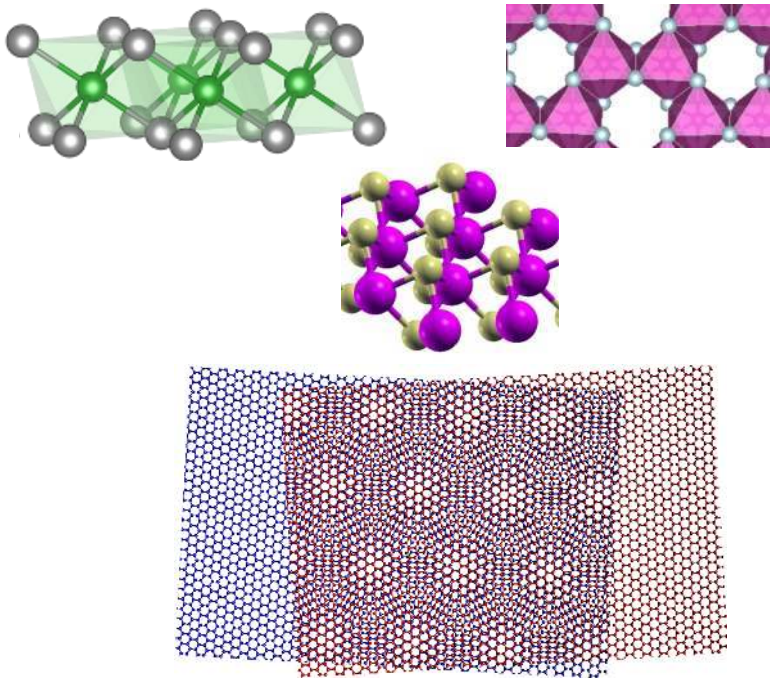
- 40 min lecture
- 15 min break
- 40 min lecture
- 15 min break
- 40 min lecture

The world of 2D materials

Complexity, universality and emergence



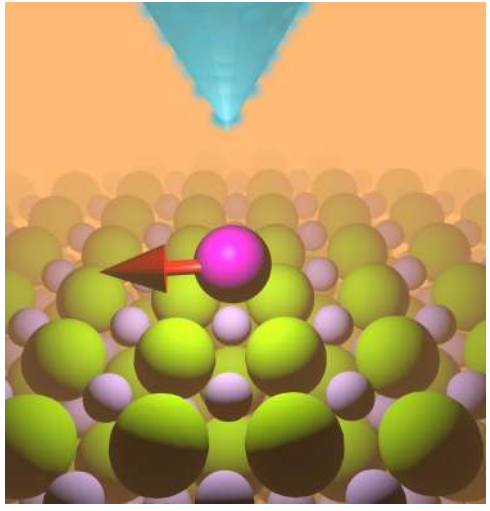
Van der Waals heterotructures



Complex systems allow to have new phenomena that did not exist before

Building quantum matter with artificial materials

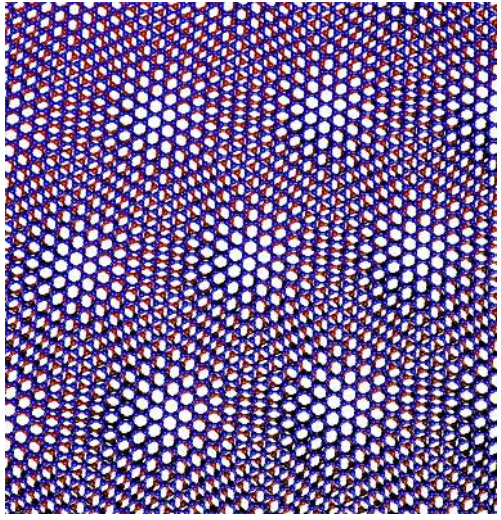
Atomic lattices



a = 0.5 nm

Nature Physics 12 (7), 656 (2016)
Nature Physics 13 (7) 668 (2017)
Science 335 (6065), 196-199 (2012)

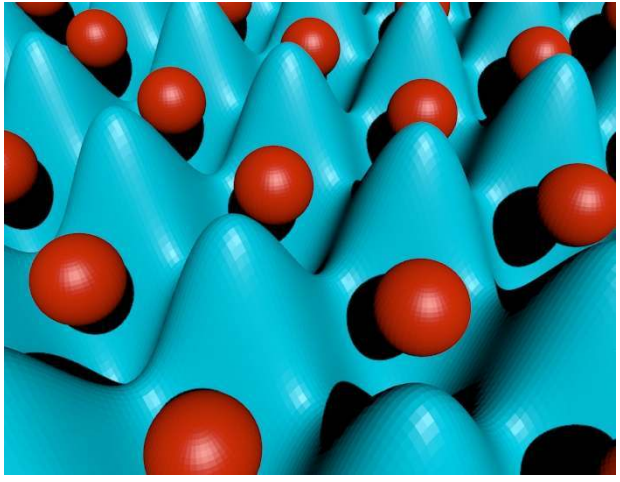
Twisted 2D moire materials



a = 30 nm

Phys. Rev. Lett. 99, 256802 (2007)
Nature Physics 6, 109–113 (2010)
PNAS 108 (30) 12233-12237 (2011)
Nature 556, 80–84 (2018)

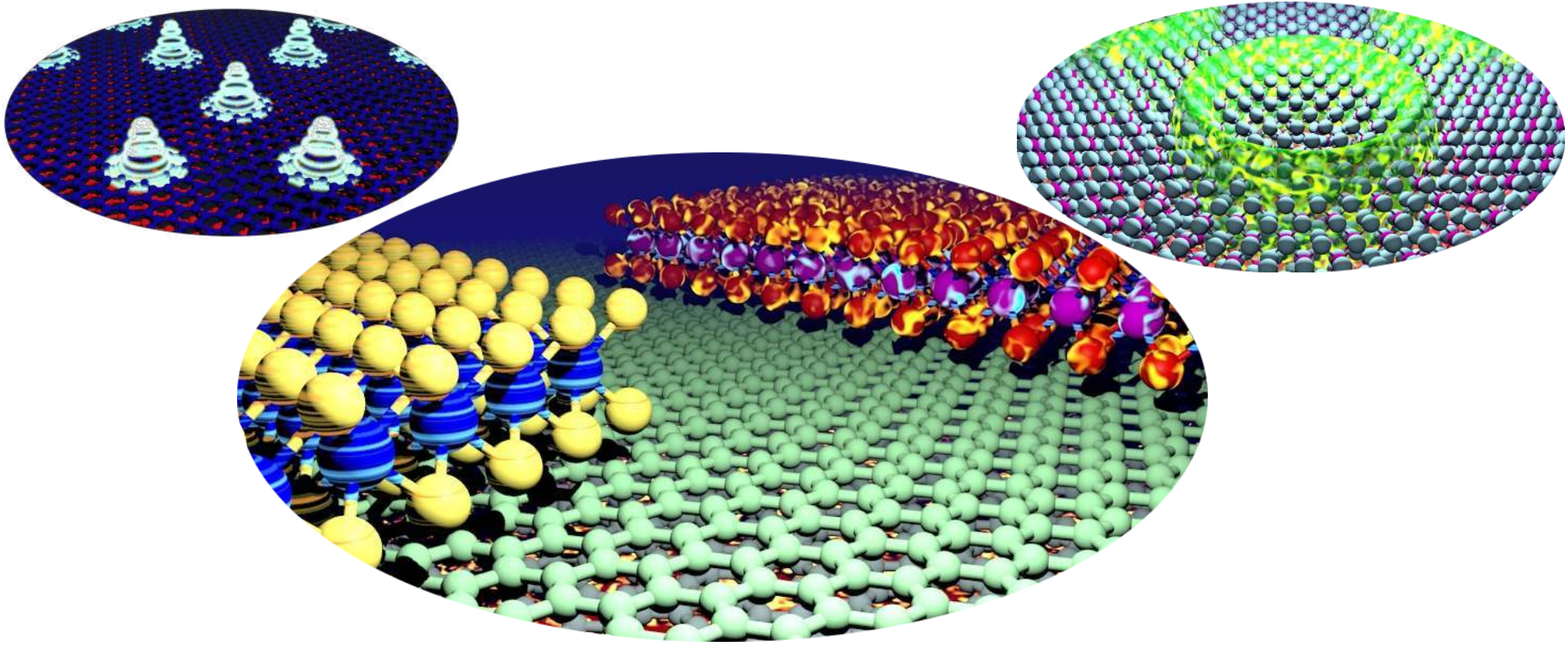
Cold atoms



a = 1000 nm

Nature 545, 462–466 (2017)
Nature 455, 204–207 (2008)
Phys. Rev. Lett. 111, 185307 (2013)

A new universe in each van der Waals heterostructure

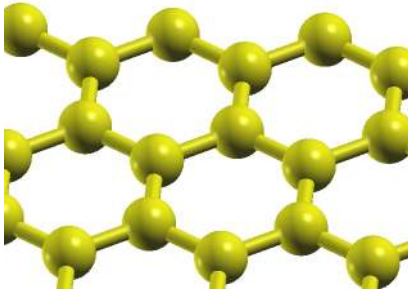


Each van der Waals heterostructure allows creating a whole new universe for electrons

The two-dimensional materials world

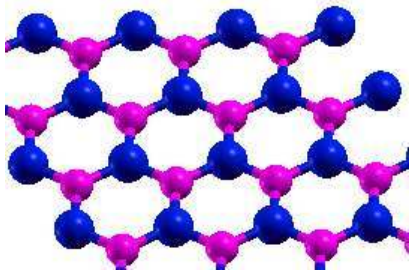
Semimetal

Graphene



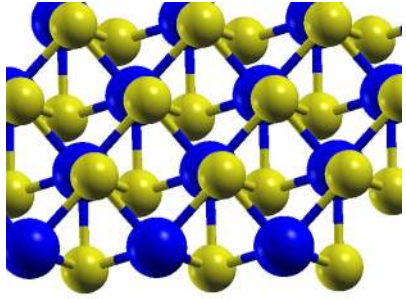
Insulator

BN



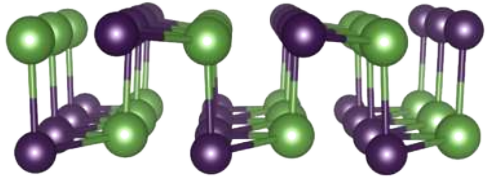
Superconductor

$NbSe_2$



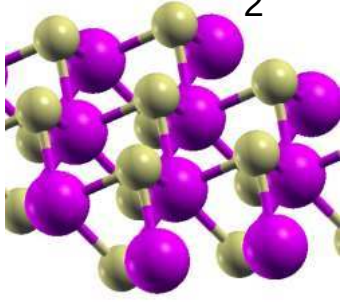
Ferroelectric

SnTe



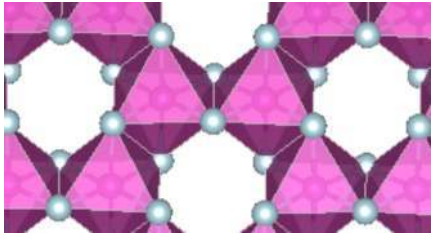
Semiconductor

WSe_2



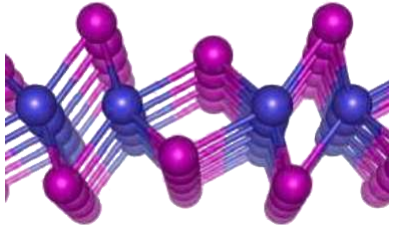
Ferromagnet

CrI_3



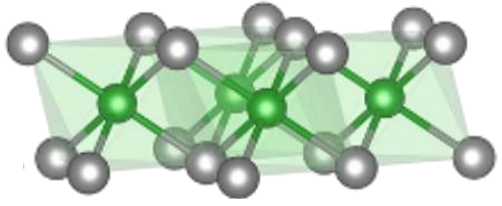
Quantum spin Hall insulator

WTe_2



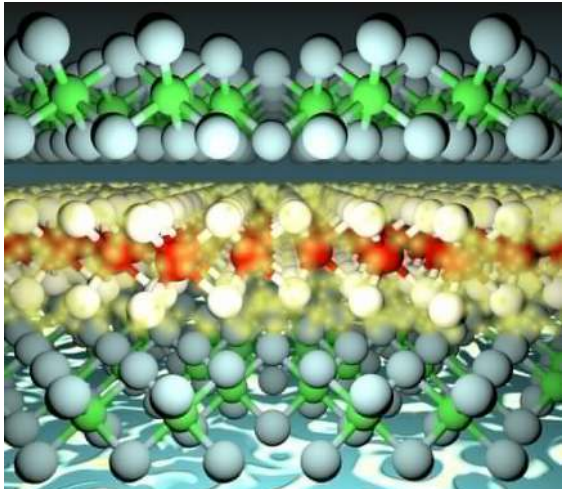
Multiferroic

NiI_2



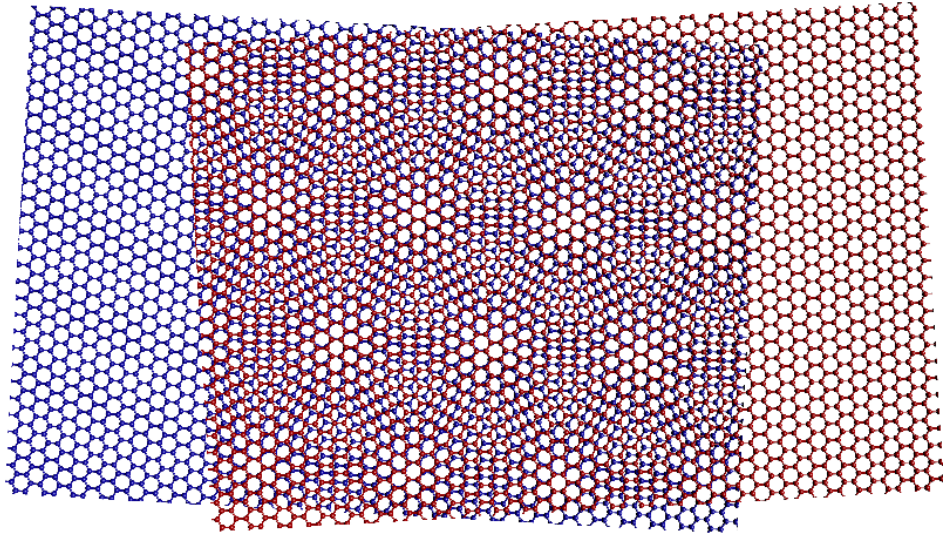
The flexibility of two-dimensional materials

They can be stacked



Nature 499.7459 419. (2013)

They can be rotated

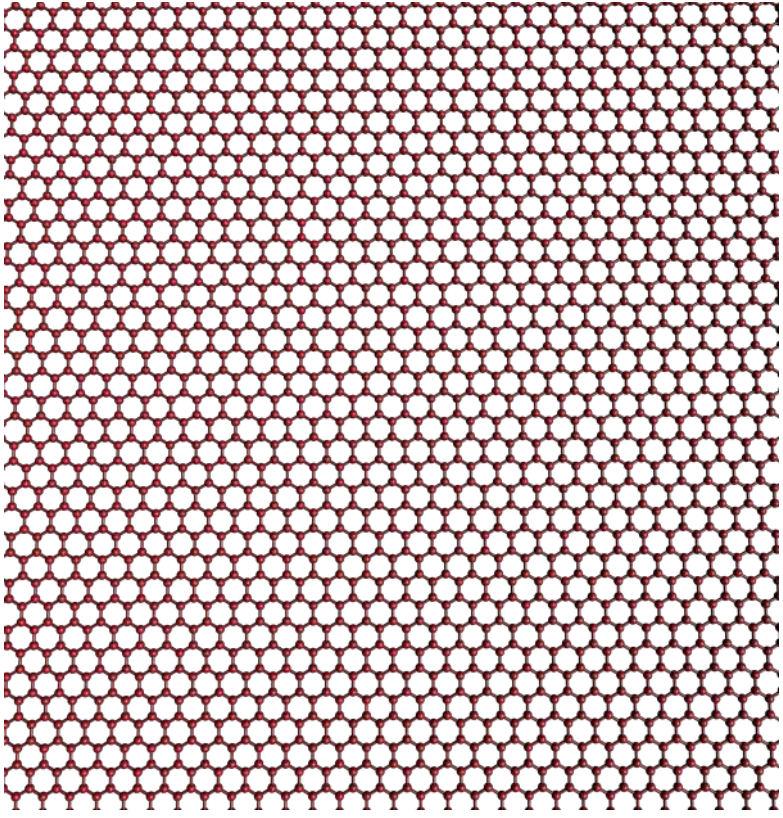


Science 361.6403 690-693. (2018)

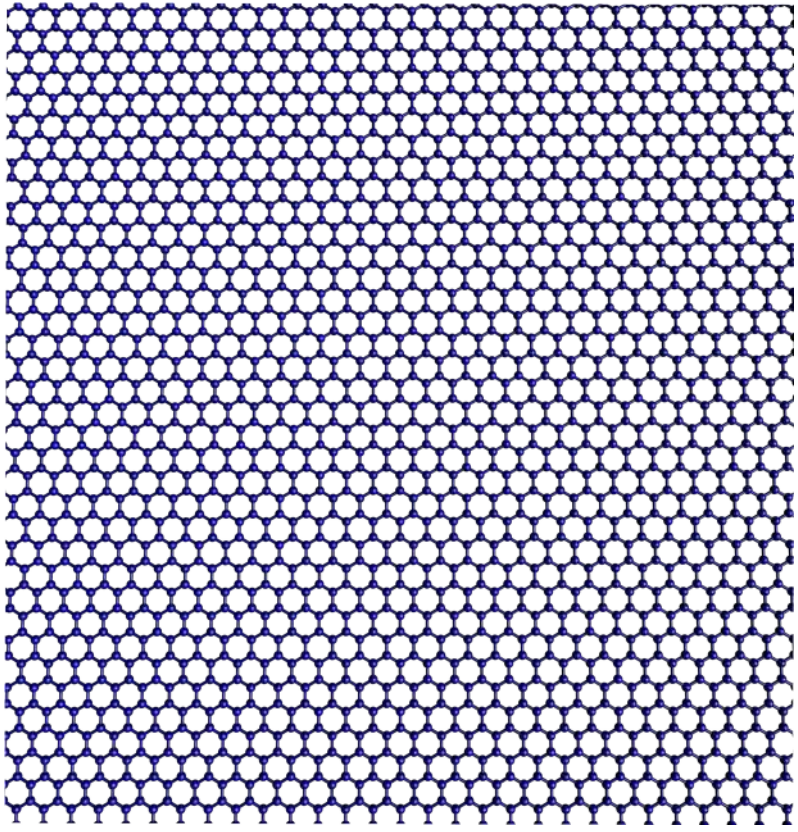
These are unique features of two-dimensional materials

A bilayer van der Waals heterostructure

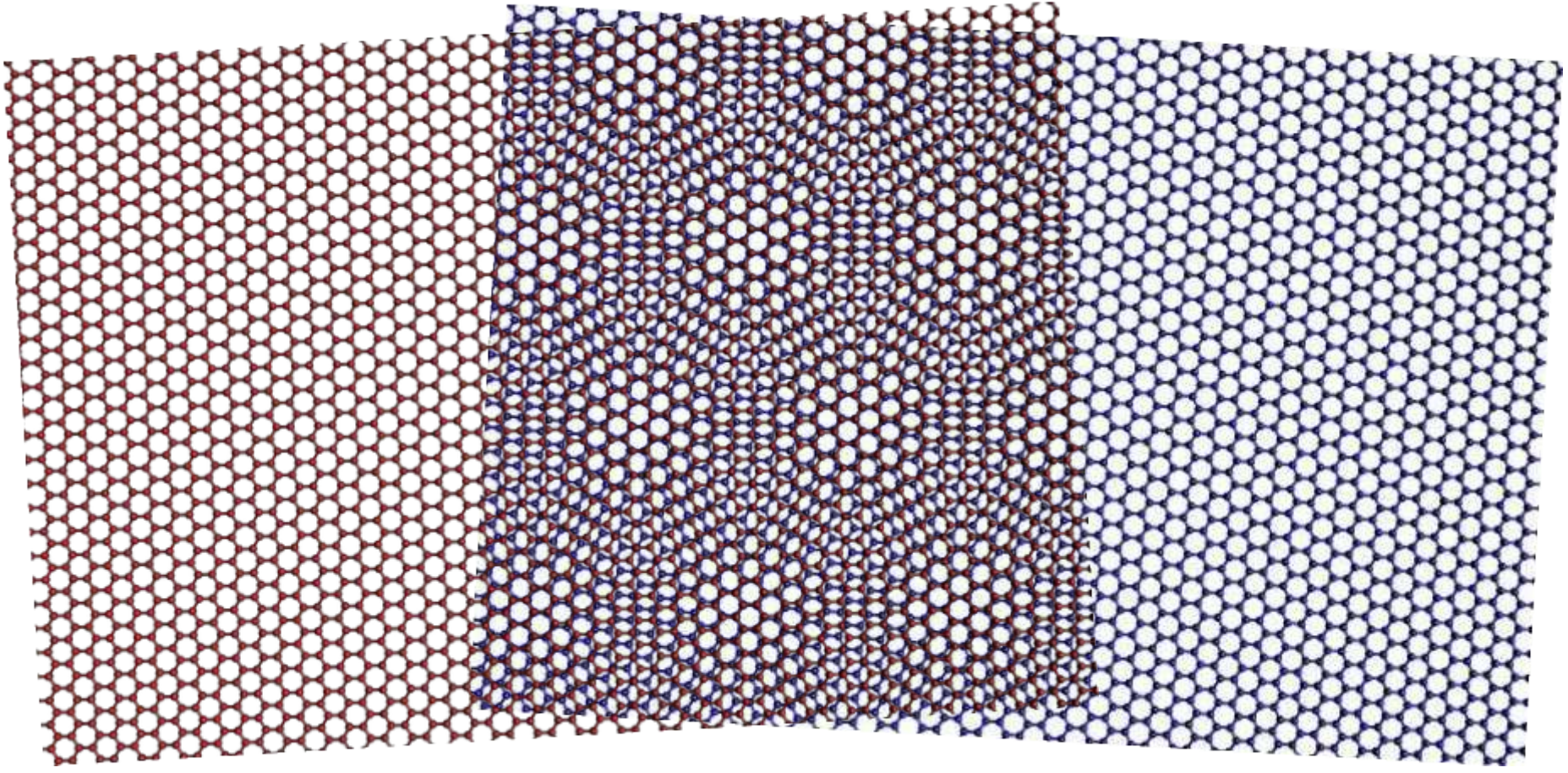
Upper graphene layer



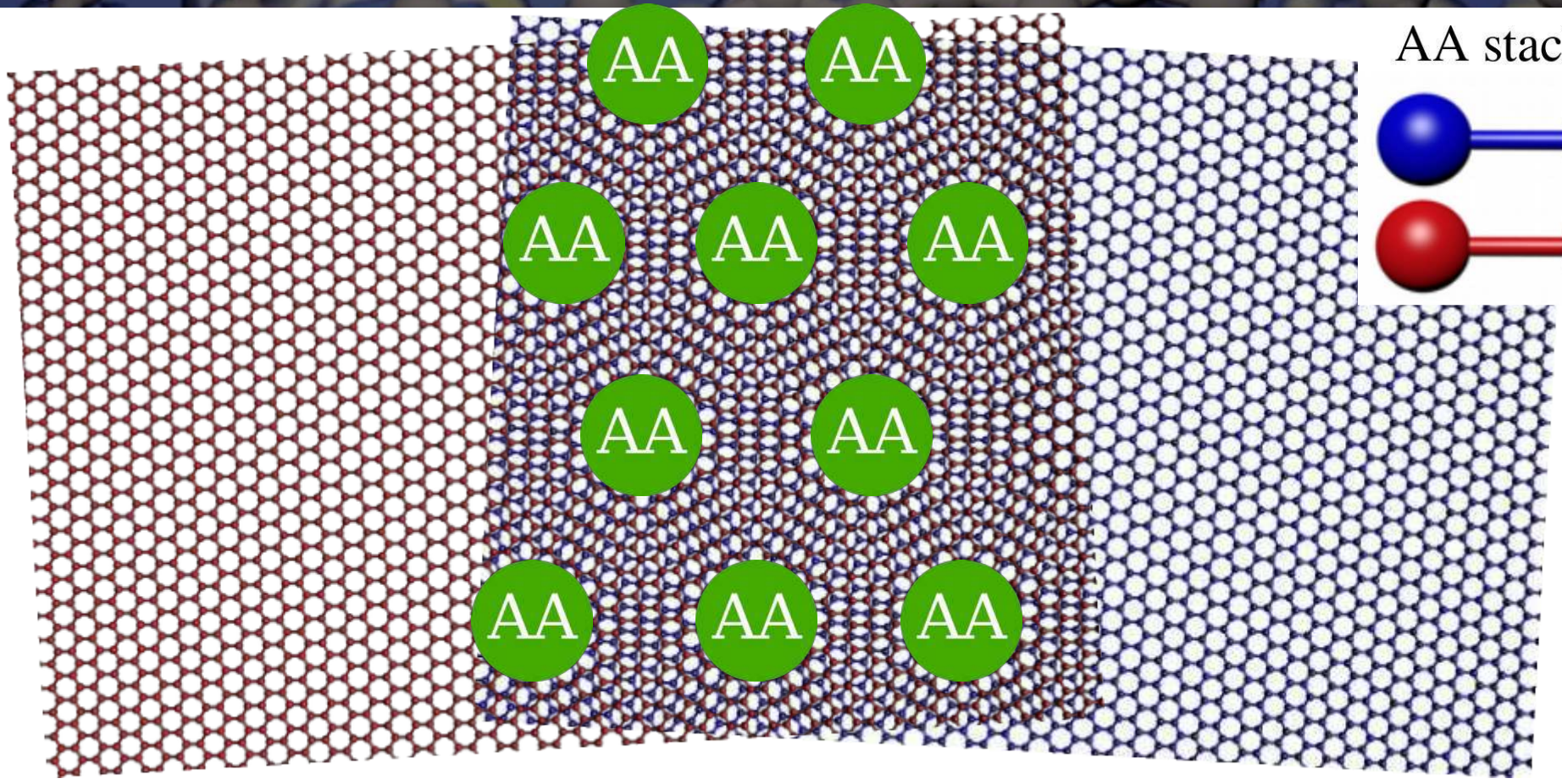
Lower graphene layer



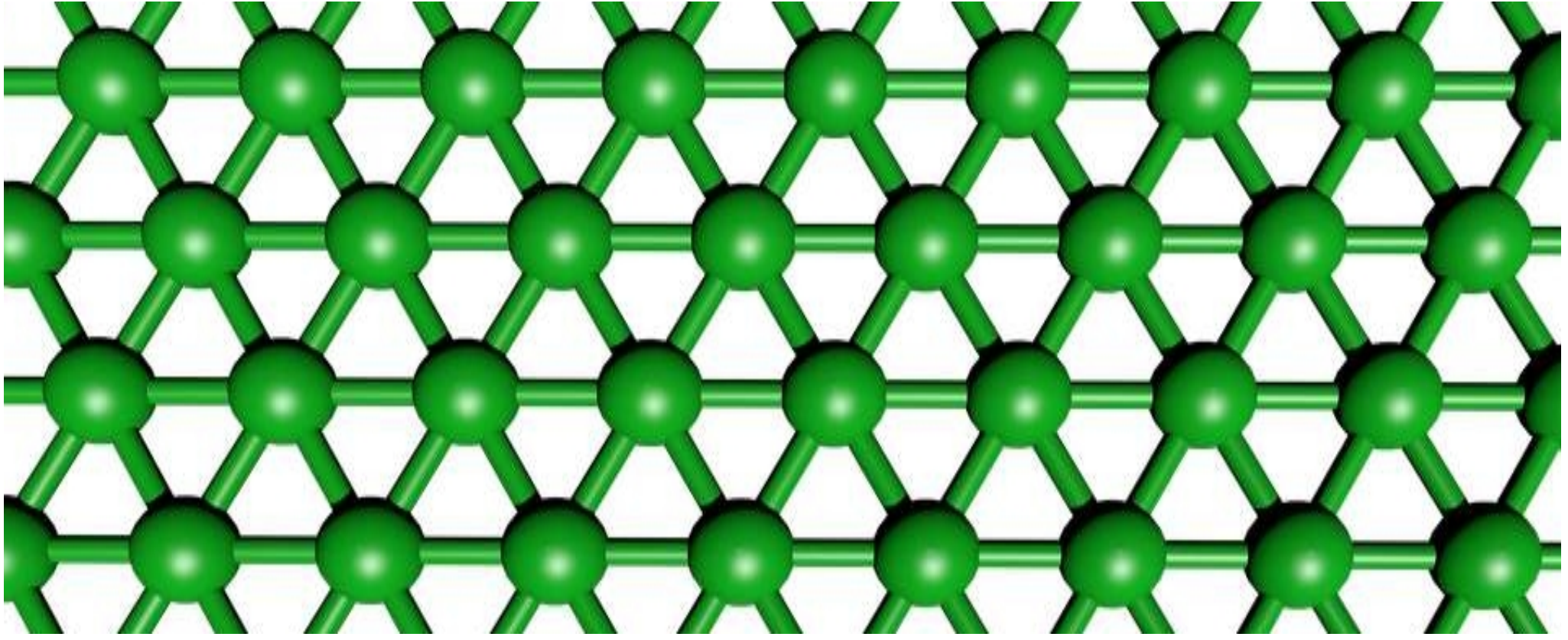
A bilayer van der Waals heterostructure



A bilayer van der Waals heterostructure

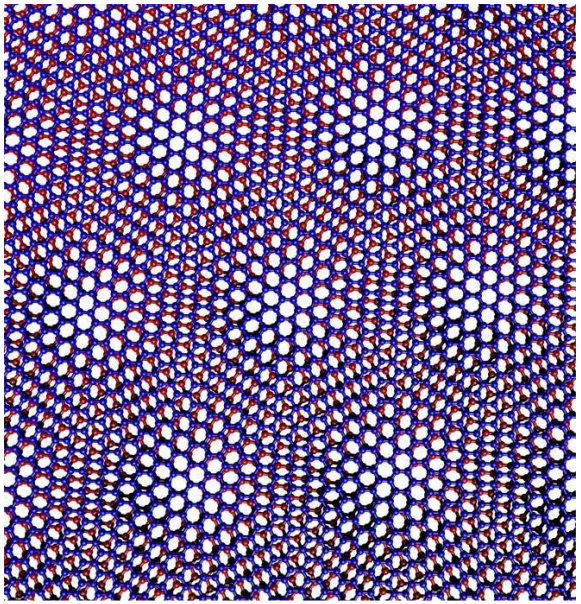


A bilayer van der Waals heterostructure

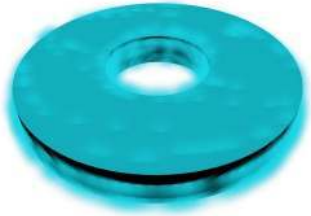


One material, a zoo of electronic phases

Twisted bilayer graphene



Superconductivity

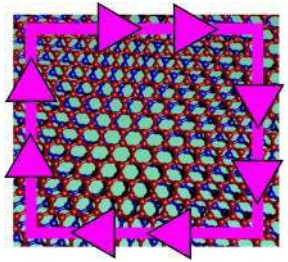


Nature 556, 43–50 (2018)

Topological networks

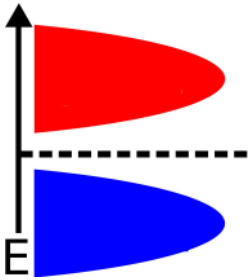
Nano Lett. 18, 11, 6725-6730 (2018)

Chern insulators



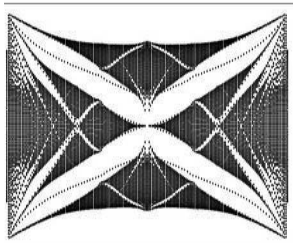
Science 365, 605-608 (2019)

Correlated insulators



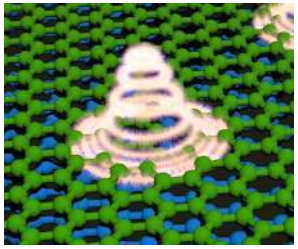
Nature 556, 80–84 (2018)

Quasicrystalline physics



Science 361, 782-786 (2018)

Fractional Chern insulators



Nature 600, 439–443 (2021)

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

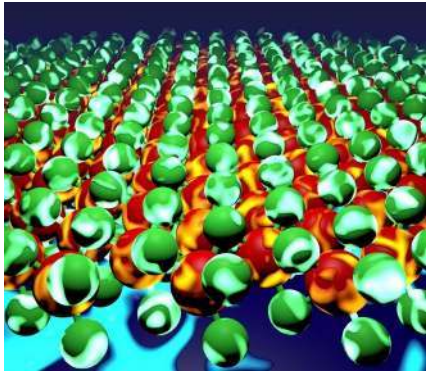
Controlling electronic states in van der Waals materials

Of course, we can use the typical knobs of bulk compounds

(pressure, chemical doping, etc)

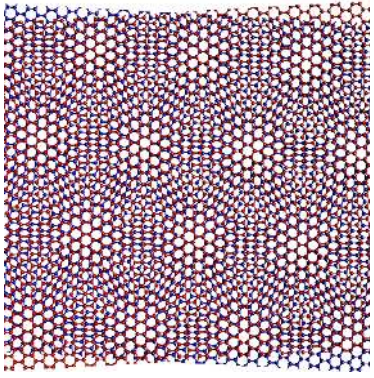
Most importantly, we can exploit the full tunability of van der Waals materials

Gating



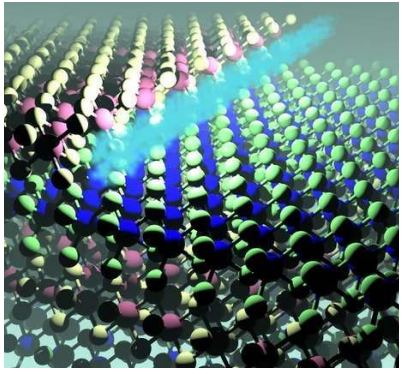
Science 306, 5696, 666-669 (2004)

Twist engineering



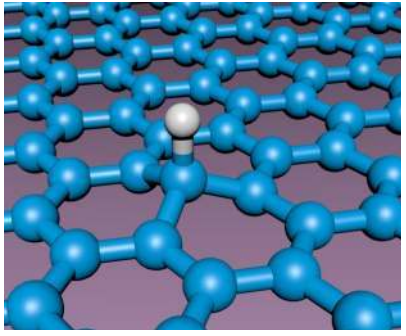
Nat, Rev, Mat, 6, 201–206 (2021)

Materials engineering



Nature 499, 419–425 (2013)

Atomic engineering

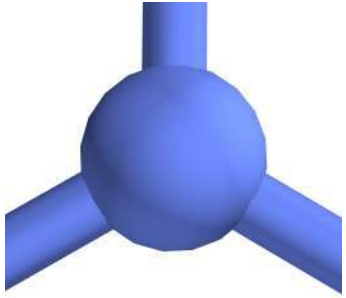


Science, 352(6284), 437-441 (2016)

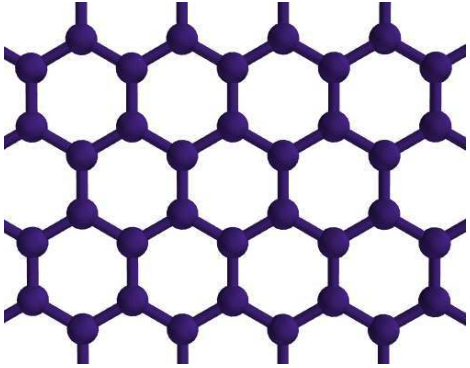
Allowing to independently control different features of the electronic structure

From atoms to quantum matter

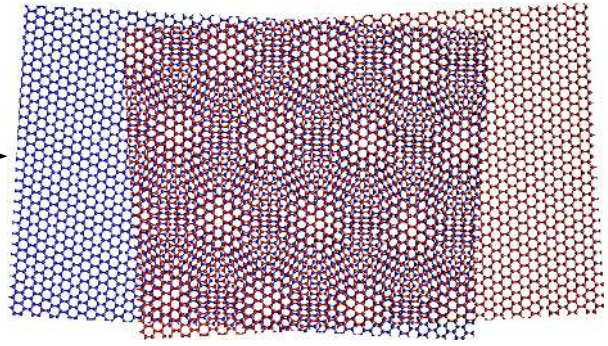
Atoms



2D materials



Van der Waals heterostructures



How do we understand and predict properties as we put more and more atoms together?

A reminder about theory tools: second quantization, electronic structure and mean-field theory

How do we describe quantum matter?

We use quantum mechanics to understand electrons in materials

$$H|\Psi\rangle = -i\partial_t|\Psi\rangle$$

Hamiltonian

Wavefunction of the system

Two main kinds of phenomena can emerge

Single particle phenomena

Many-body phenomena

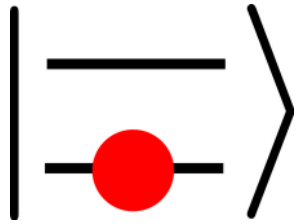
Two different kinds of quantum mechanical formalism

Systems where our number of particles is constant

First quantization, description based on a Hilbert space

Describes metals, semiconductors, insulators

Highly successful and easy formalism

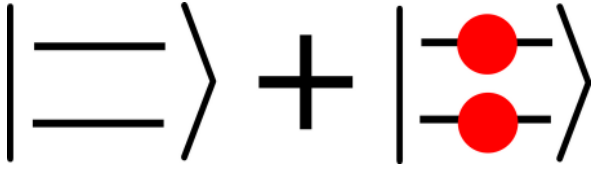


Systems where the number of particles fluctuates

Second quantization, description based on a Fock space

Describes superconductors, superfluids, correlated matter

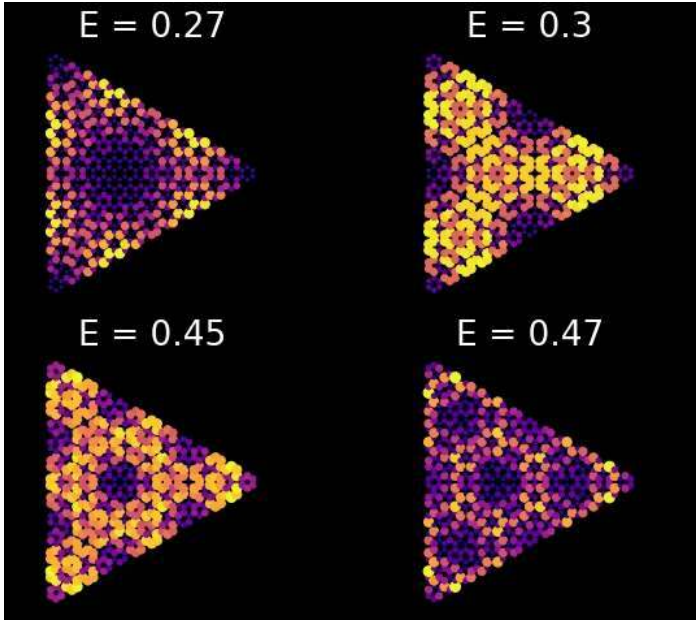
Leads to much exotic phenomena, yet also more challenging

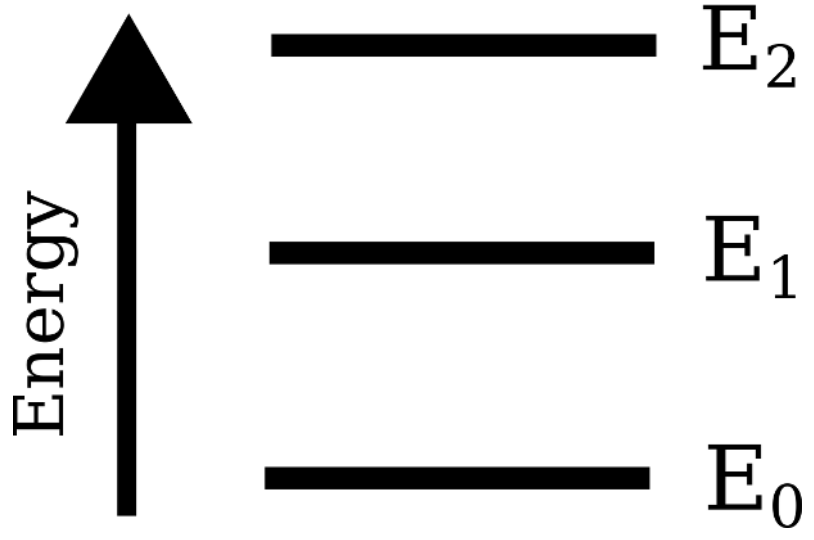


A reminder of a simple single particle state

Particle in a box

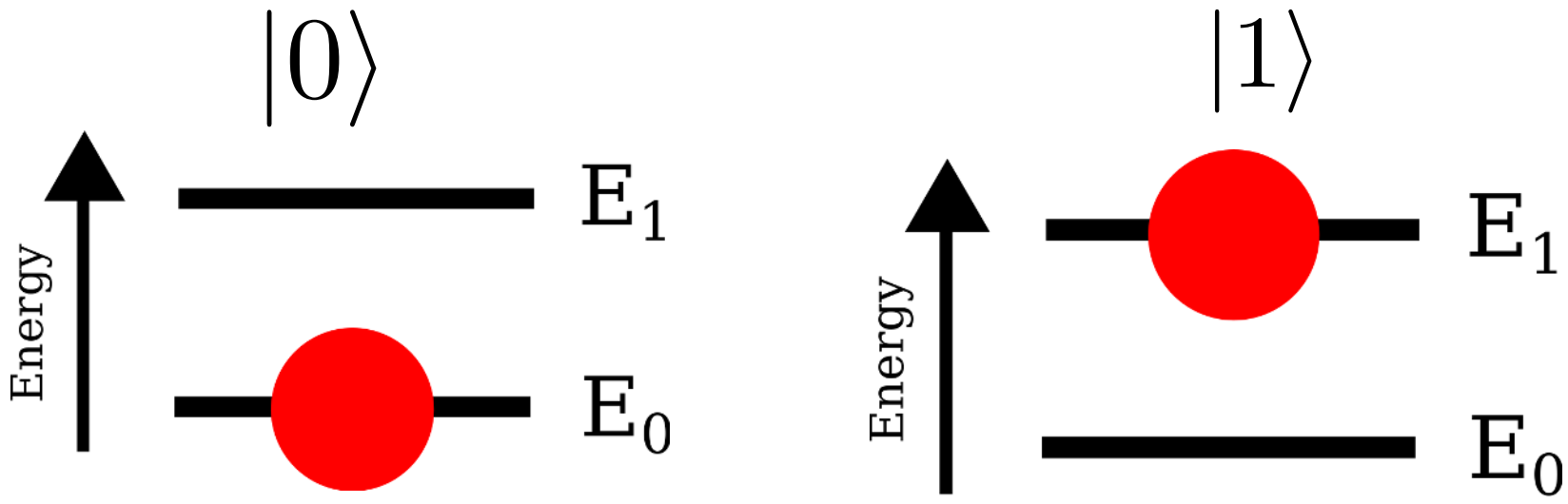
$$H|\Psi\rangle = E_n|\Psi\rangle$$





A reminder of a simple single particle state

Particle in a box $H|\Psi\rangle = E_n|\Psi\rangle$

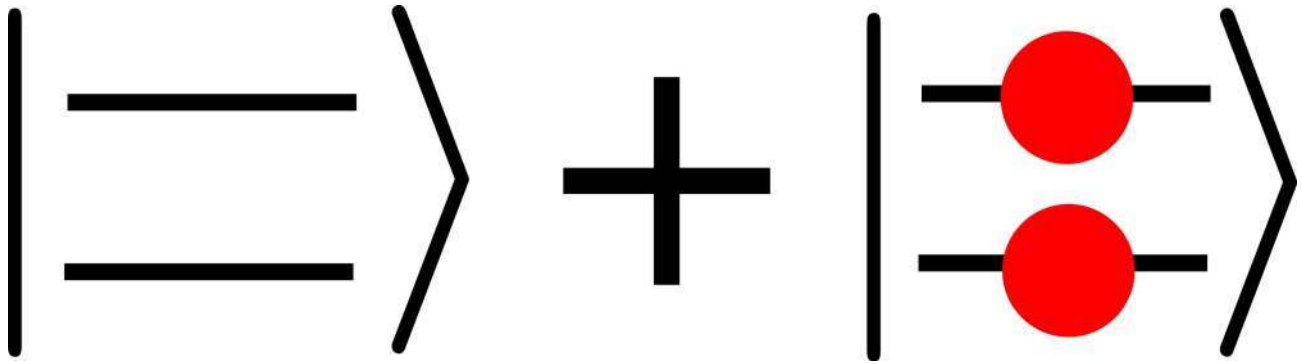


These two states describe having one particle, in one of the possible energy level

From single particle to many body

But what if our state is a combination of states with different numbers of particles?

A state having both 0 particles and 2 particles

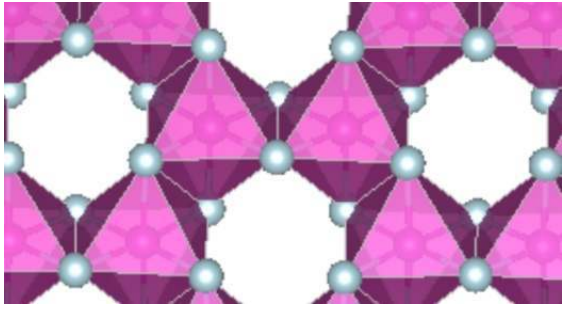


How do we describe states like these?

Non-constant number of particles

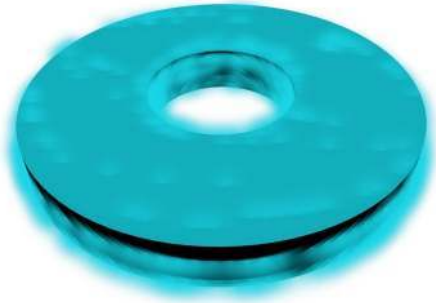
Why is this even relevant to understand materials?

Magnetic ordering of materials depends on processes in which the number of electrons fluctuates



Goodenough-Kanamori rules

The effective description of superconductors does not conserve electron number



Bogoliubov-de Gennes formalism

The idea of second quantization

Define operators that can create or destroy particles

c_i Annihilation operator, destroys a particle in site i

$c_i^\dagger$ Creation operator, creates a particle in site i

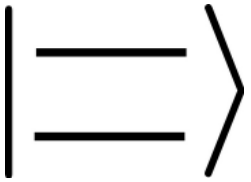
The empty vacuum state $|\Omega\rangle$ is defined as $c_i|\Omega\rangle = 0$

The Hamiltonian is written in terms of creation and annihilation operators

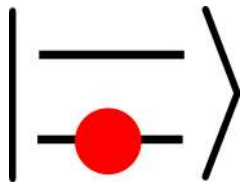
$$\mathrm{H} = \mathrm{c}_0^\dagger c_1 + h.c.$$

The idea of second quantization

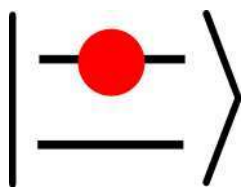
Lets see some examples using the two-levels presented before

$|\Omega\rangle =$ 

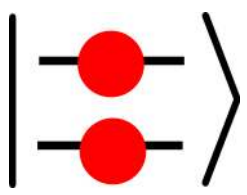
The “vacuum” state

$c_0^\dagger |\Omega\rangle =$ 

One particle in level #0

$c_1^\dagger |\Omega\rangle =$ 

One particle in level #1

$c_0^\dagger c_1^\dagger |\Omega\rangle =$ 

Two particles in level #0 & #1

Fermionic quantum statistics in second quantization

Fermi-Dirac statistics for electrons

→ Wavefunctions are antisymmetric with respect to interchanging labels

→ There can only be 0 or 1 fermion per level

$$\{c_i^\dagger, c_j\} = c_i^\dagger c_j + c_j c_i^\dagger = \delta_{ij} \qquad \{c_i, c_j\} = 0$$

Anti-symmetric wavefunction $c_0^\dagger c_1^\dagger |\Omega\rangle = -c_1^\dagger c_0^\dagger |\Omega\rangle$

At most one fermion per site $c_0^\dagger c_0^\dagger |\Omega\rangle = 0$

Different kinds of Hamiltonians

Single particle Hamiltonians $\mathrm{H} = \sum_{ij} t_{ij} c_i^\dagger c_j$

Insulators, semiconductors, metals

Many-body Hamiltonian $\mathrm{H} = \sum_{ijkl} V_{ijkl} c_i^\dagger c_j c_k^\dagger c_l$

Fractional quantum Hall states, superconductors, quantum magnets

With second quantization, both cases can be treated on the same footing

What about interactions?

What happens when we put interactions?

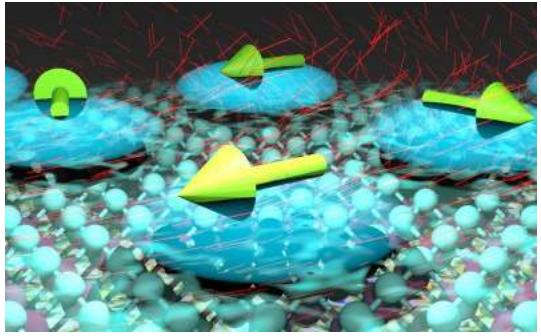
$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} V_{ijkl} c_i^\dagger c_j c_k^\dagger c_l$$

The role of electronic interactions

Electronic interactions are responsible for symmetry breaking

Broken time-reversal symmetry

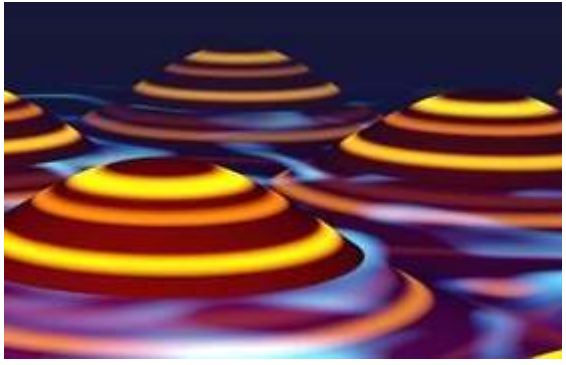
Classical magnets



$$\mathbf{M} \rightarrow -\mathbf{M}$$

Broken crystal symmetry

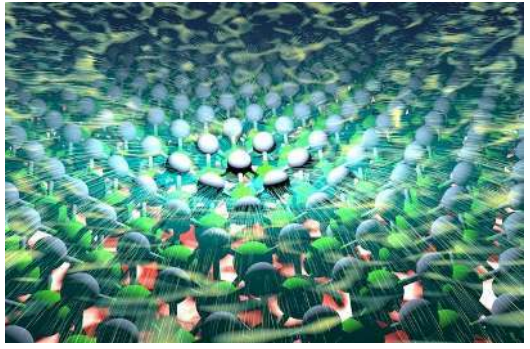
Charge density wave



$$\mathbf{r} \rightarrow \mathbf{r} + \mathbf{R}$$

Broken gauge symmetry

Superconductors



$$\langle c_\uparrow c_\downarrow \rangle \rightarrow e^{i\phi} \langle c_\uparrow c_\downarrow \rangle$$

A simple interacting Hamiltonian

Free Hamiltonian ***Interactions (Hubbard term)***

$$H = \sum_{ij} t_{ij} [c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}] + \sum_i U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

From now on lets consider we have a spin degree of freedom $\uparrow, \downarrow$

What is the ground state of this Hamiltonian?

$U < 0$ Superconductivity

$U > 0$ Magnetism

The mean-field approximation, superconductivity

Mean field: *Approximate four fermions by two fermions times expectation values*

Four fermions (not exactly solvable) ***Two fermions (exactly solvable)***

$$U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \approx U \langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle c_{i\uparrow} c_{i\downarrow} + h.c.$$

$$U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \approx \Delta c_{i\uparrow} c_{i\downarrow} + h.c.$$

For $U < 0$

i.e. attractive interactions

$\Delta \sim \langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle$ is the superconducting order

The mean-field approximation, magnetism

Mean field: *Approximate four fermions by two fermions times expectation values*

Four fermions (not exactly solvable) ***Two fermions (exactly solvable)***

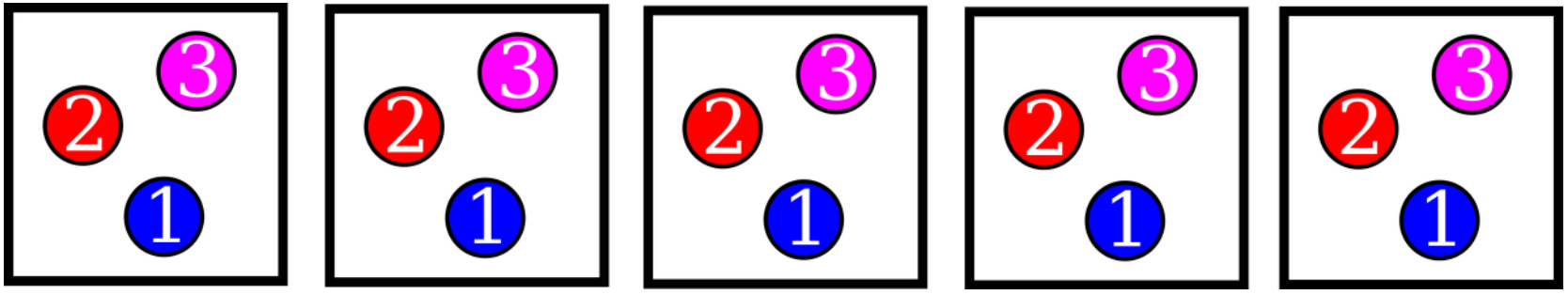
$$U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \approx U \langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle c^\dagger_{i\downarrow} c_{i\downarrow} + ... + h.c.$$

$$U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \approx M \sigma^z_{ss'} c^\dagger_{i,s} c_{i,s'} + h.c.$$

For $U > 0$
i.e. repulsive interactions

Magnetic order
$$M \sim \langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle - \langle c^\dagger_{i\downarrow} c_{i\downarrow} \rangle$$

Electronic band-structures

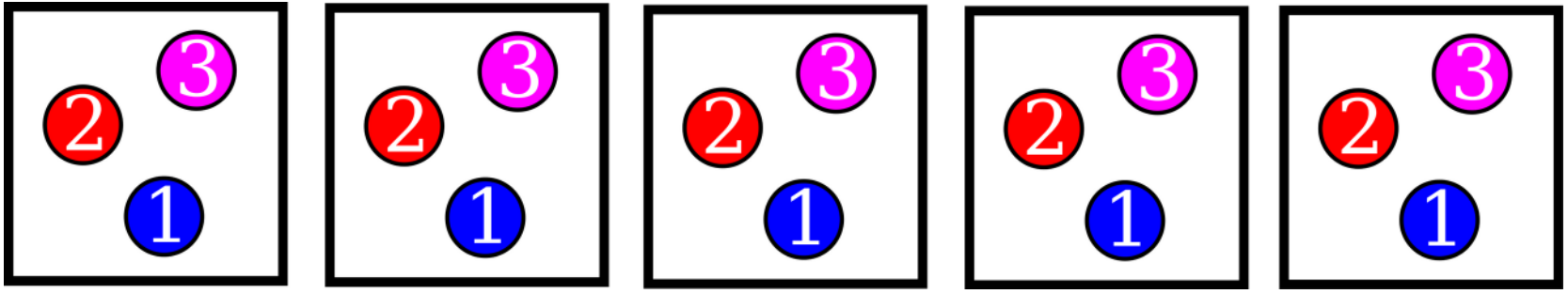


$$c^{\dagger}_{\alpha,n}$$

index of the orbital in the unit cell

Index of the unit cell

Electronic band-structures



$$H = \sum_{n,\alpha,\beta} t_{\alpha\beta} c^{\dagger}_{\alpha,n} c_{\beta,n} + \sum_{n,\alpha,\beta} \gamma_{\alpha\beta} c^{\dagger}_{\alpha,n} c_{\beta,n+1} + h.c.$$

Intra-cell hoppings

Inter-cell hoppings

Electronic band-structures

$$H = \sum_{n,\alpha,\beta} t_{\alpha\beta} c^{\dagger}_{\alpha,n} c_{\beta,n} + \sum_{n,\alpha,\beta} \gamma_{\alpha\beta} c^{\dagger}_{\alpha,n} c_{\beta,n+1} + h.c.$$

Unitary transformation

$$\Psi^{\dagger}_{\phi,\alpha} \sim \sum_{n,\beta} e^{i\phi n} U_{\alpha\beta} c^{\dagger}_{n,\beta} \qquad H = \sum_{\phi,\alpha} \epsilon_{\phi,\alpha} \Psi^{\dagger}_{\phi,\alpha} \Psi_{\phi,\alpha}$$

$\epsilon_{\phi,\alpha}$ **are the eigenvalues of the matrix**

$$h(\phi) = t_{\mu\nu} + \gamma_{\mu\nu} e^{i\phi} + h.c.$$

Properties of the electronic dispersion

From now on, lets work with a specific electronic dispersion $\epsilon_{\vec{k}}$

Density of states $$D(\omega) \sim \int \delta(\omega - \epsilon_{\vec{k}}) d^N \vec{k}$$

Group velocity

$$v_F = \frac{\partial \epsilon_{\vec{k}}}{\partial k_\alpha}$$

Effective mass

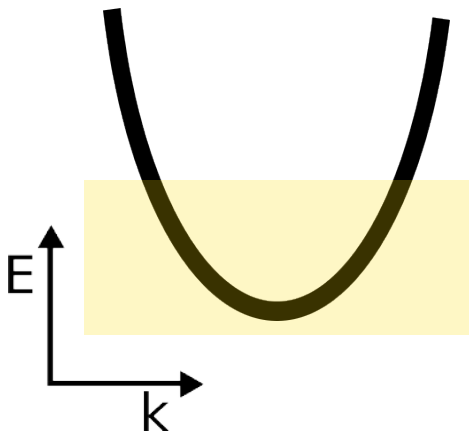
$$\frac{1}{m_{\alpha\beta}} = \frac{\partial^2 \epsilon_{\vec{k}}}{\partial k_\alpha \partial k_\beta}$$

Fermi surface

$$\{\vec{k}\} \text{ with } \epsilon_{\vec{k}} = \epsilon_F$$

Three important electronic dispersions

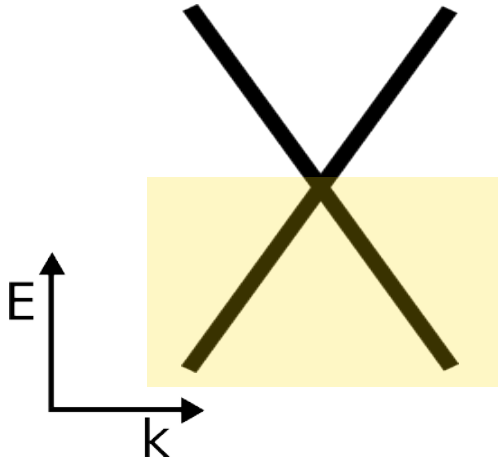
Parabolic bands



TMDCs

Effective free-electrons

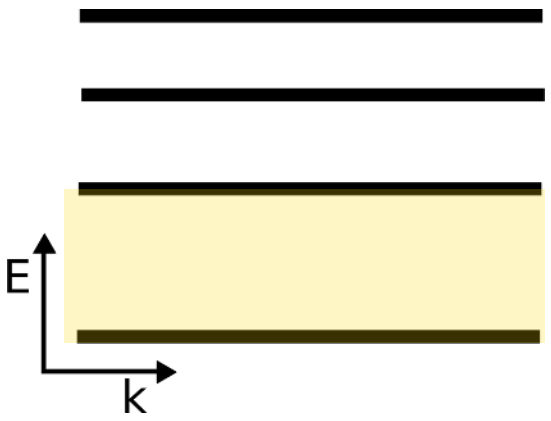
Dirac dispersion



graphene

Topology & relativistic physics

Flat bands



Quantum Hall, moire

Topology & correlations

Break

10-15 min break

(optional) to discuss during the break

What is the physical meaning of these terms in the Hamiltonian?

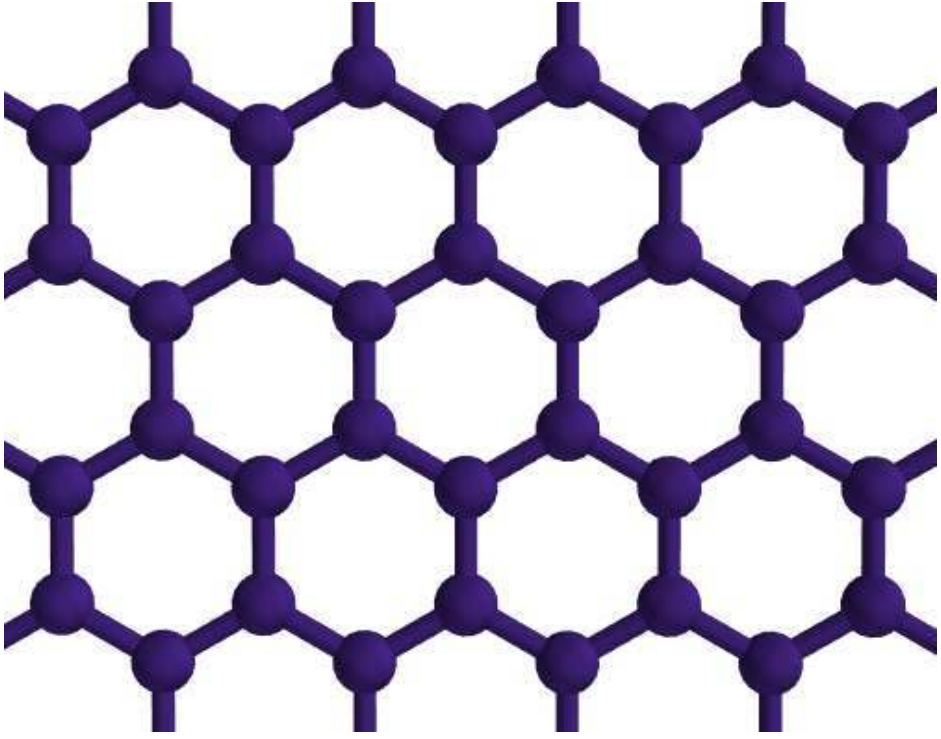
$$c^\dagger_{n,\uparrow} c_{n,\downarrow} \qquad c^\dagger_{n,\uparrow} c_{n+1,\downarrow} \qquad c^\dagger_{n,\uparrow} c^\dagger_{n+1,\uparrow}$$

and which symmetries do they break?

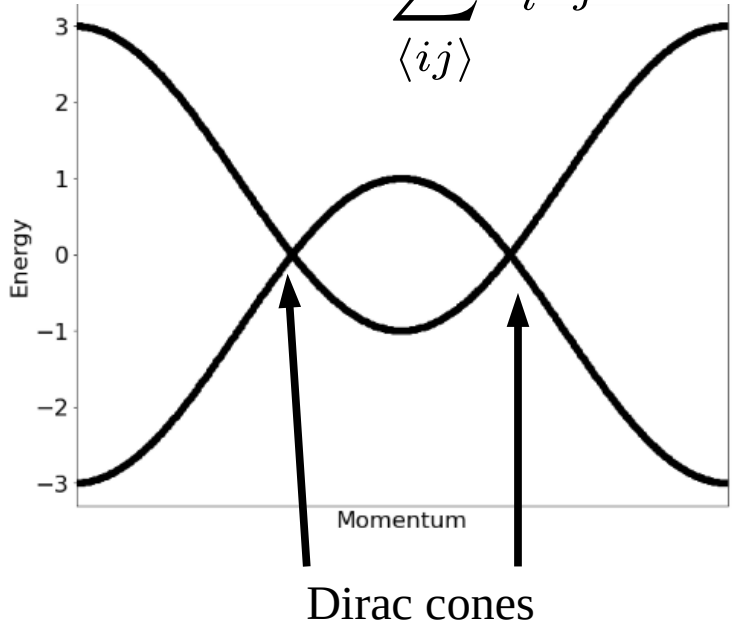
Graphene and its electronic structure

Electronic structure of monolayer graphene

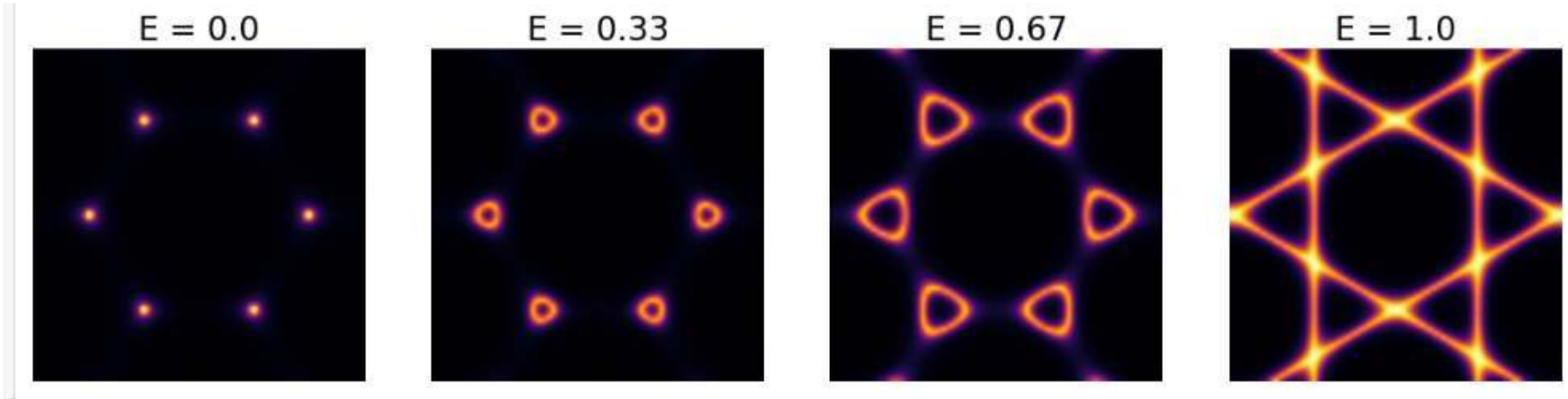
The electronic structure of graphene is captured by a single orbital model in the honeycomb lattice



$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j$$

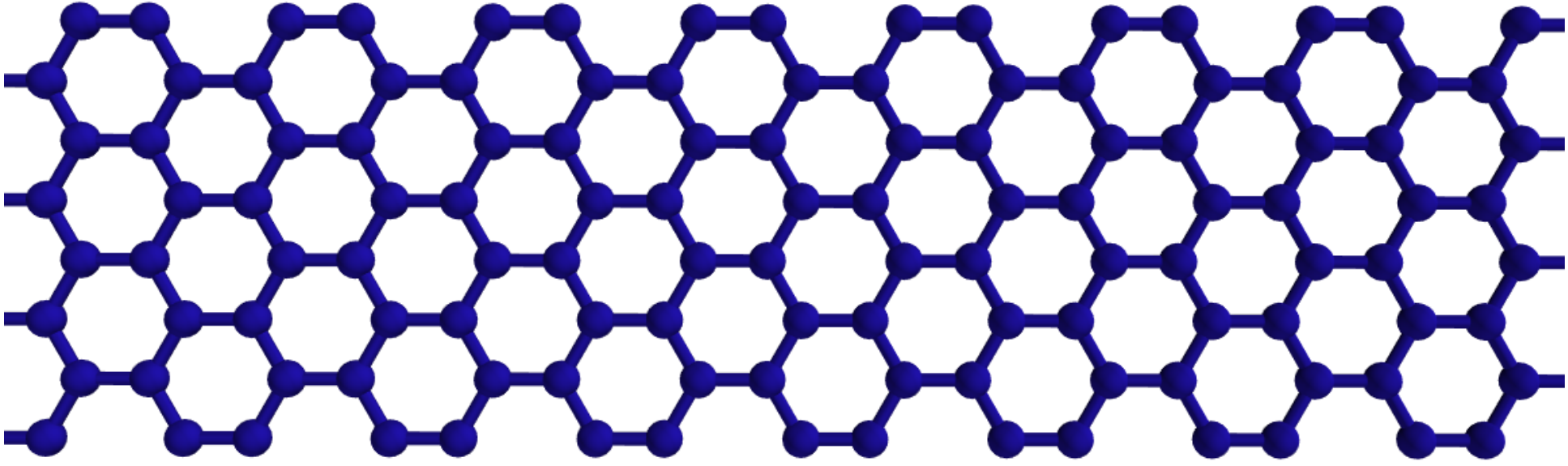


Fermi surface of graphene



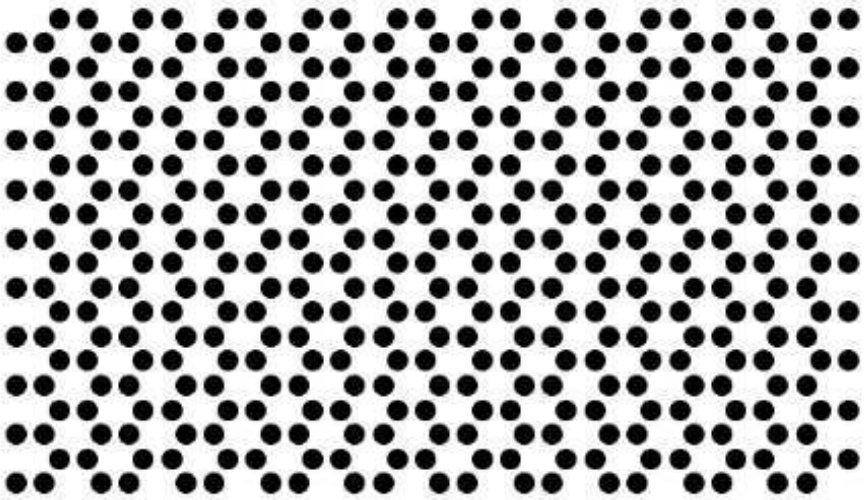
Confining two-dimensional materials, graphene nanoribbons

Let us see what happens to the electronic structure when we reduce the dimensionality



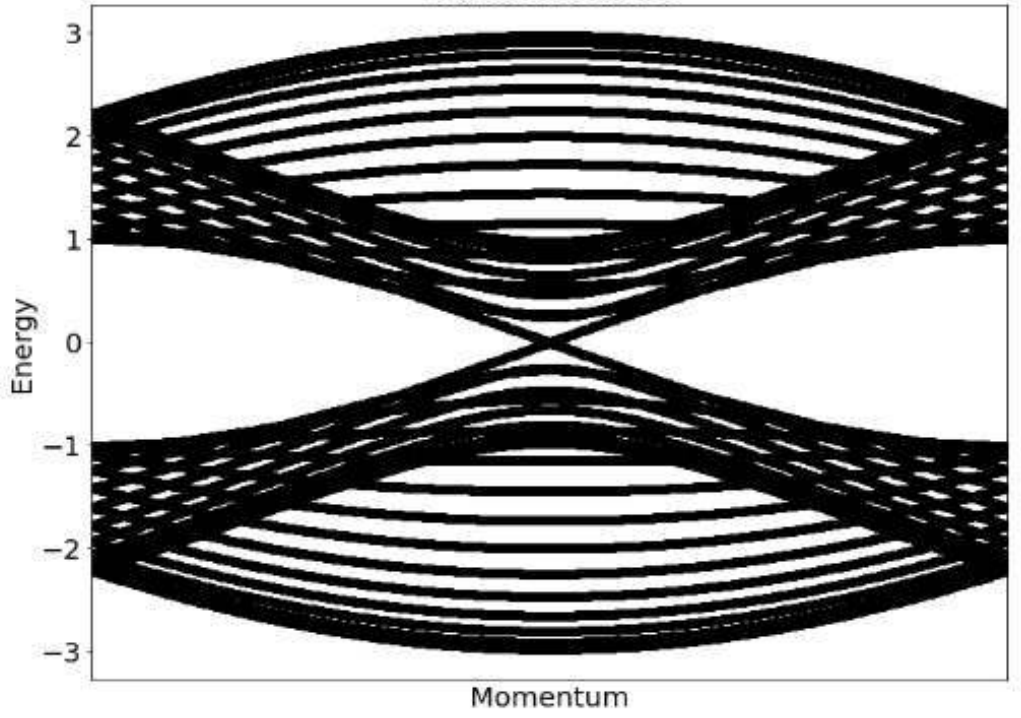
Graphene nanoribbons

Structure



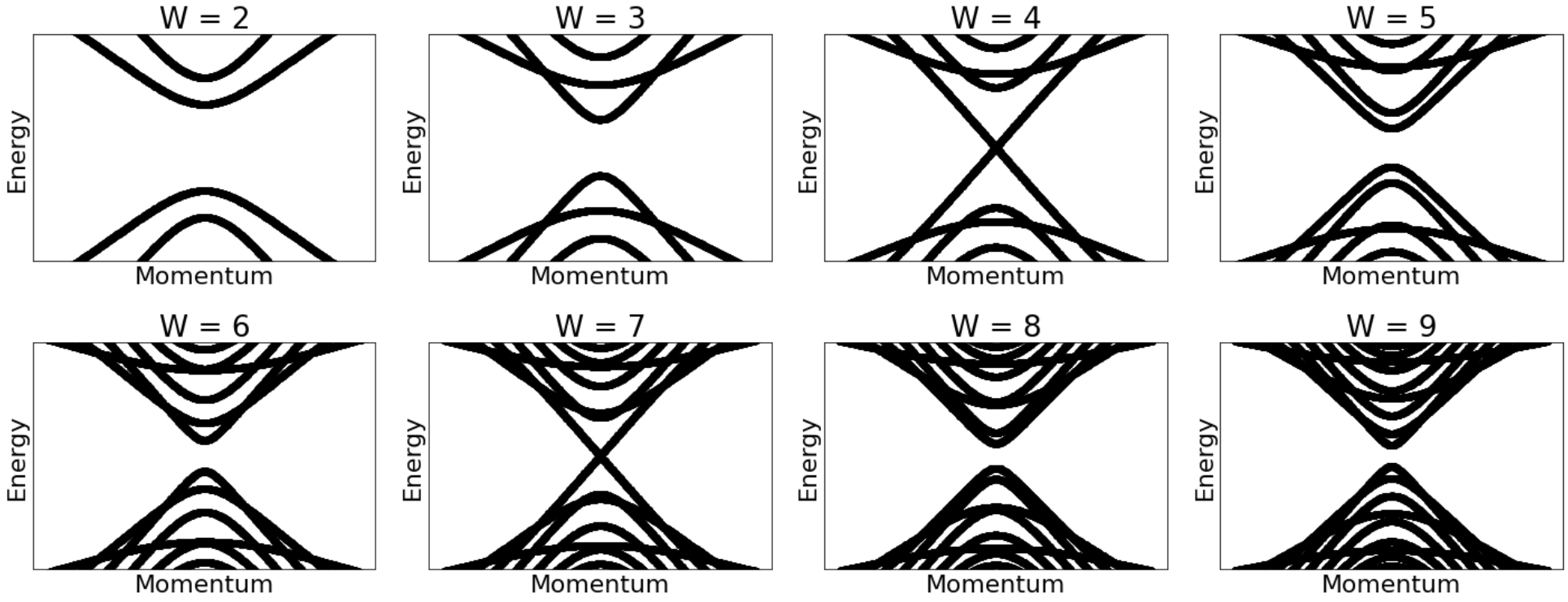
$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j$$

Band structure



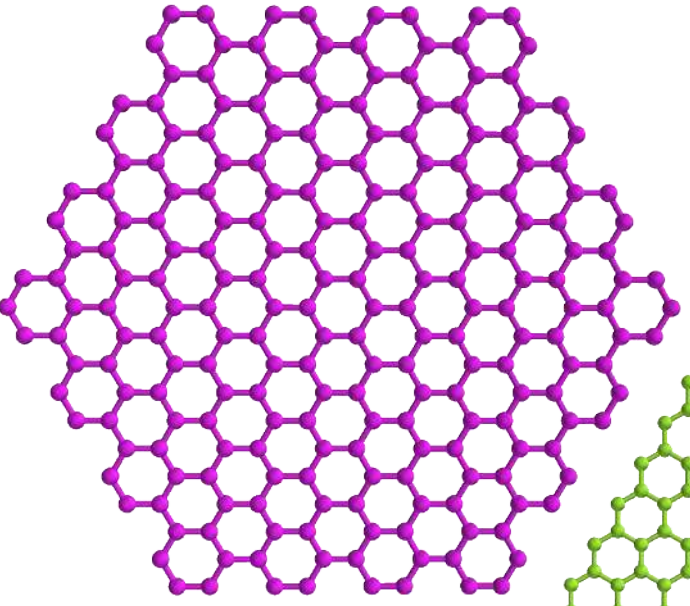
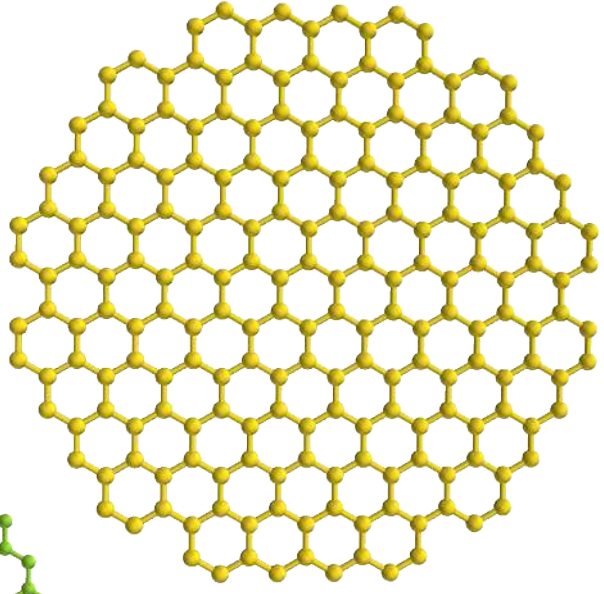
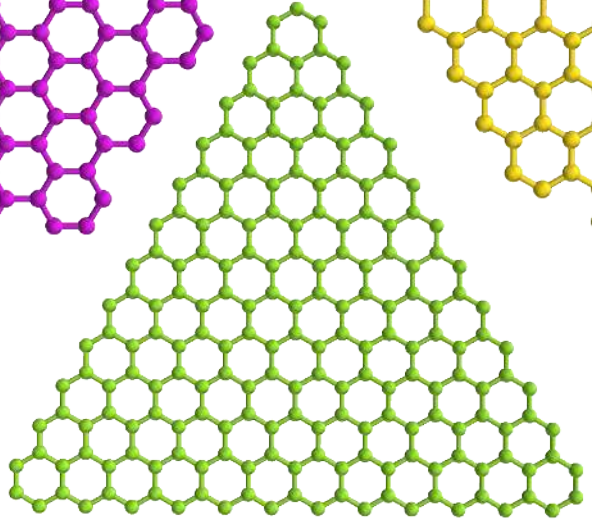
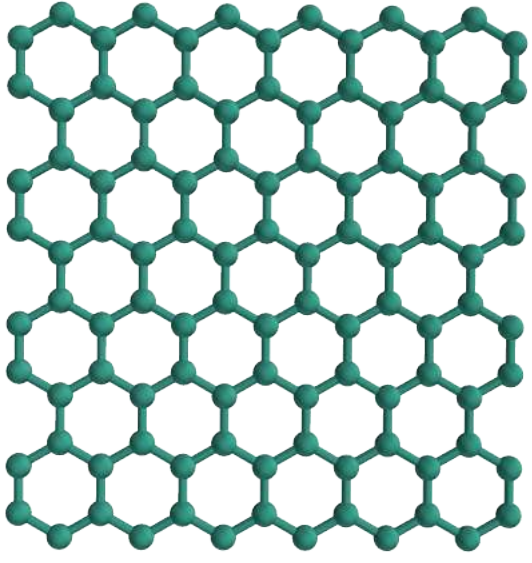
Electronic structure of graphene armchair nanoribbons

The width of a graphene nanoribbon drastically controls its electronic properties

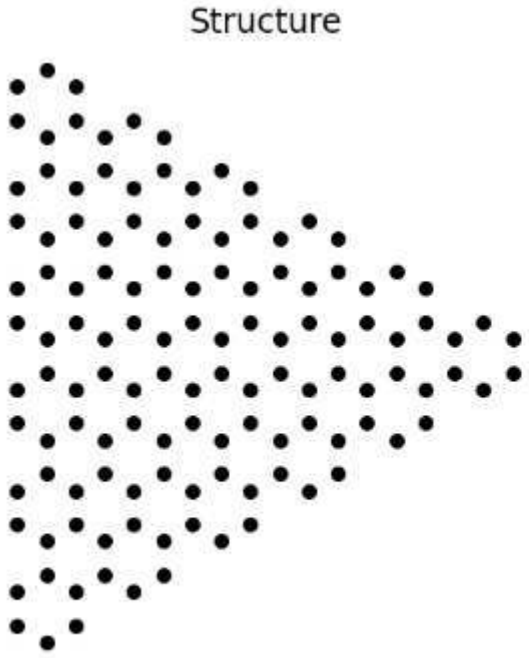


Quantum dots of 2D materials

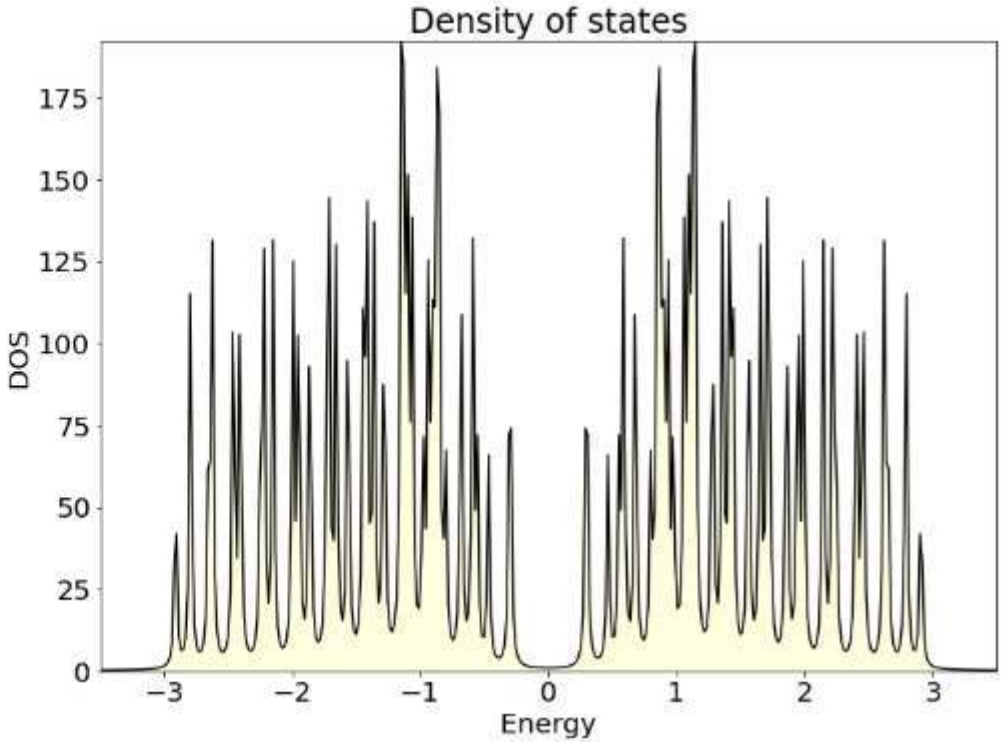
Graphene quantum dots

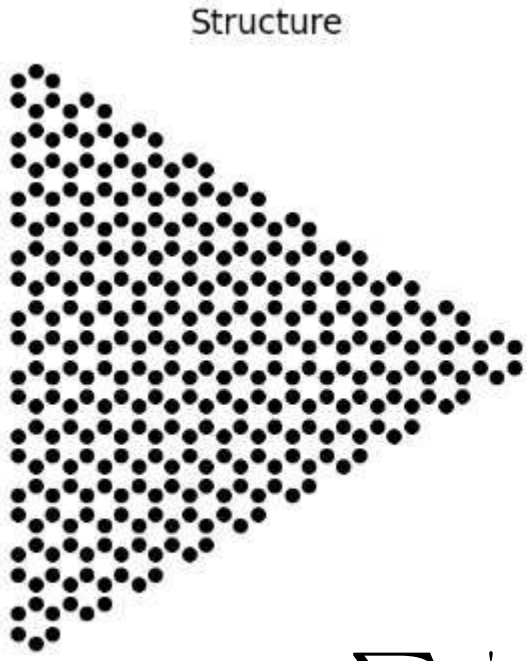
Electronic structure of graphene armchair nanoislands



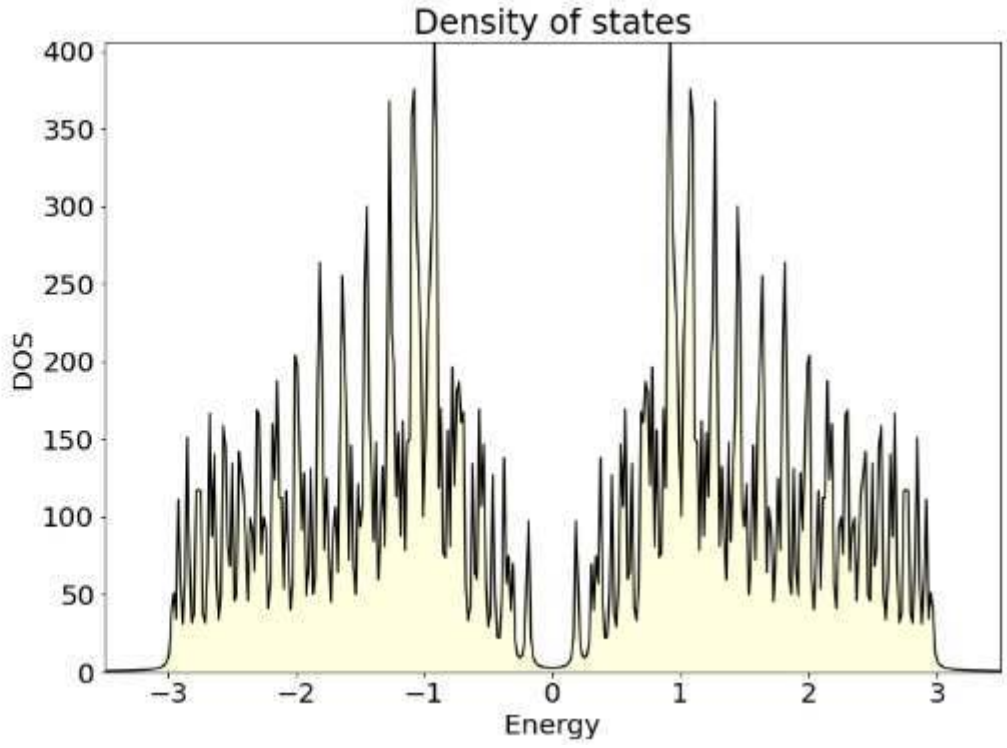
$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j$$



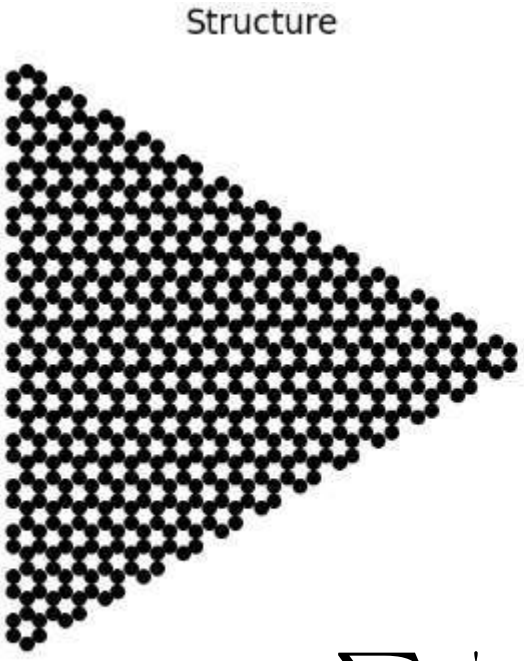
Electronic structure of graphene armchair nanoislands



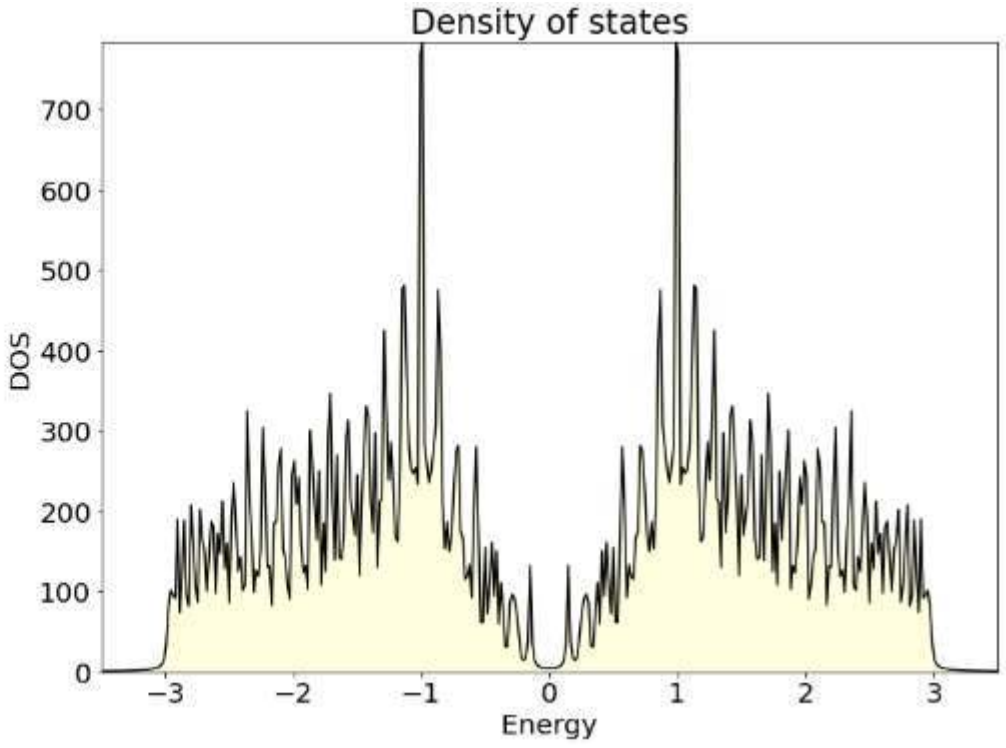
$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j$$



Electronic structure of graphene armchair nanoislands

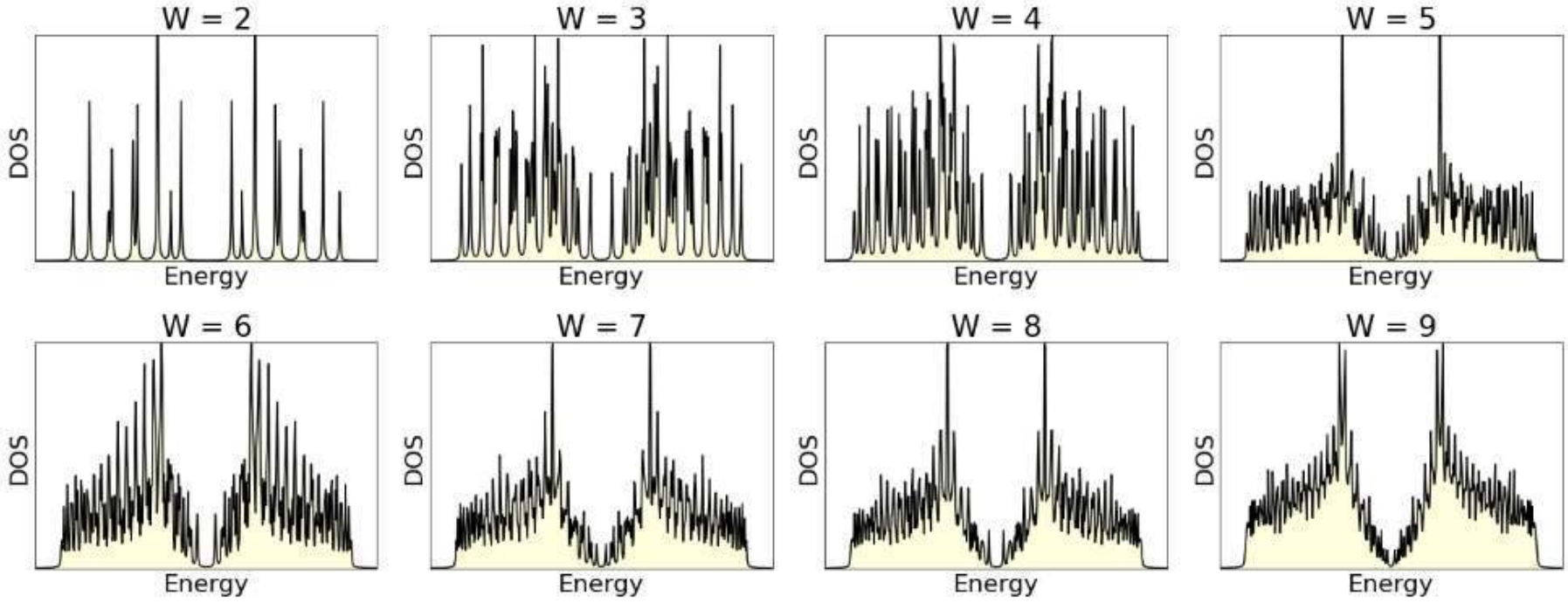


$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j$$

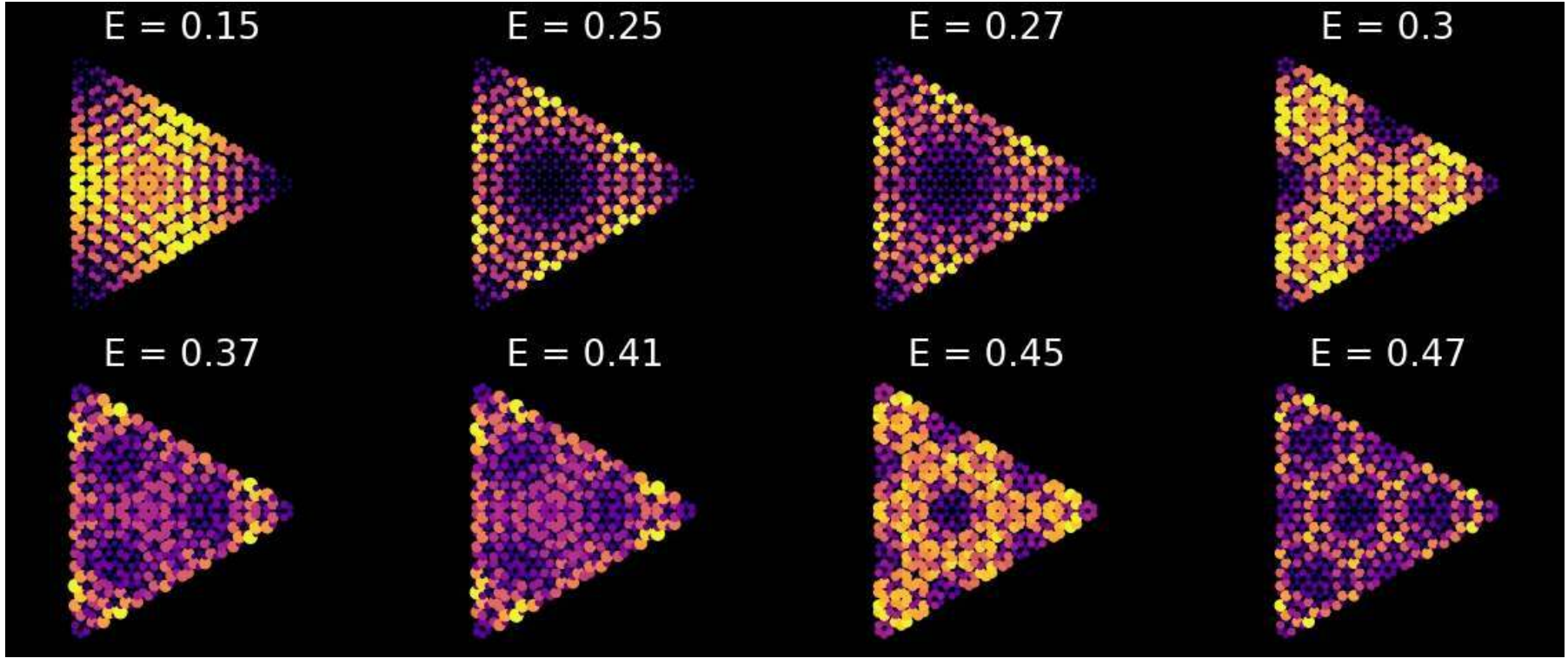


Graphene islands of different widths

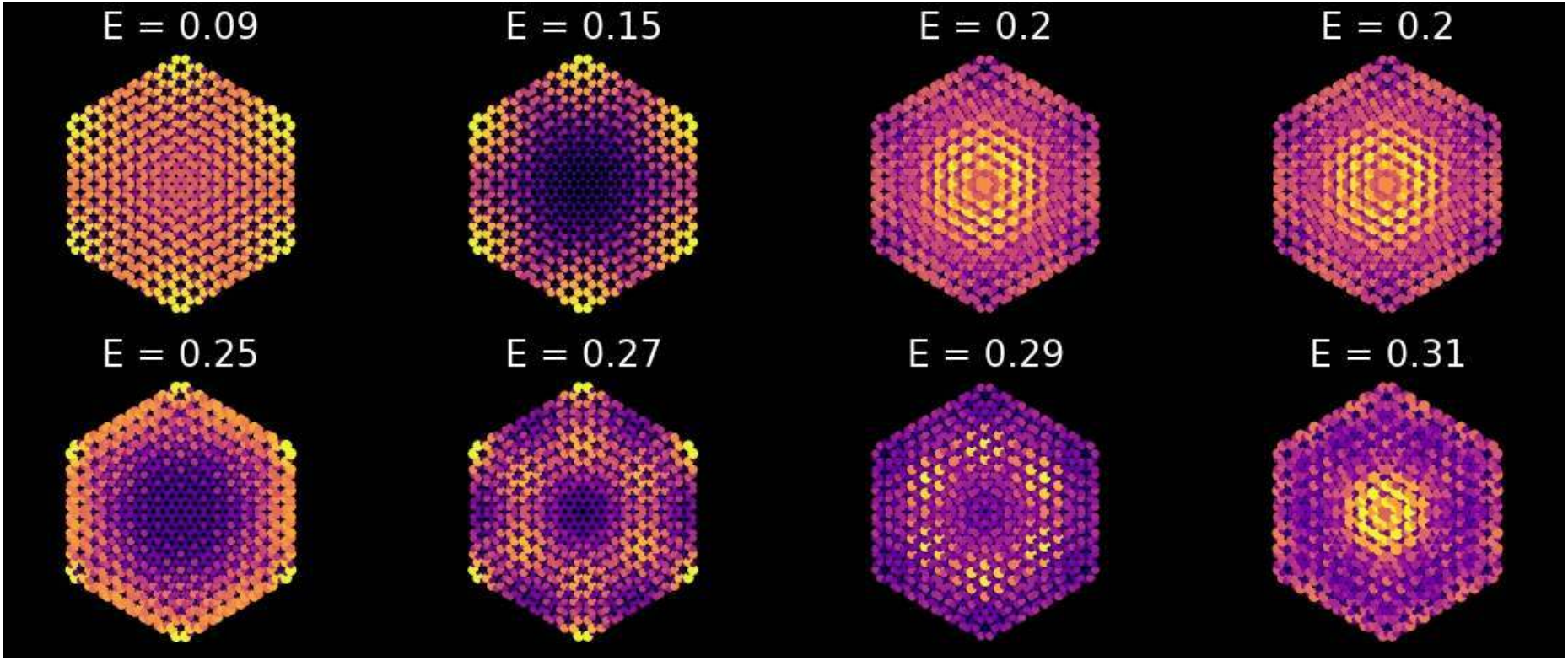
As the island becomes bigger, the spectrum of graphene is recovered



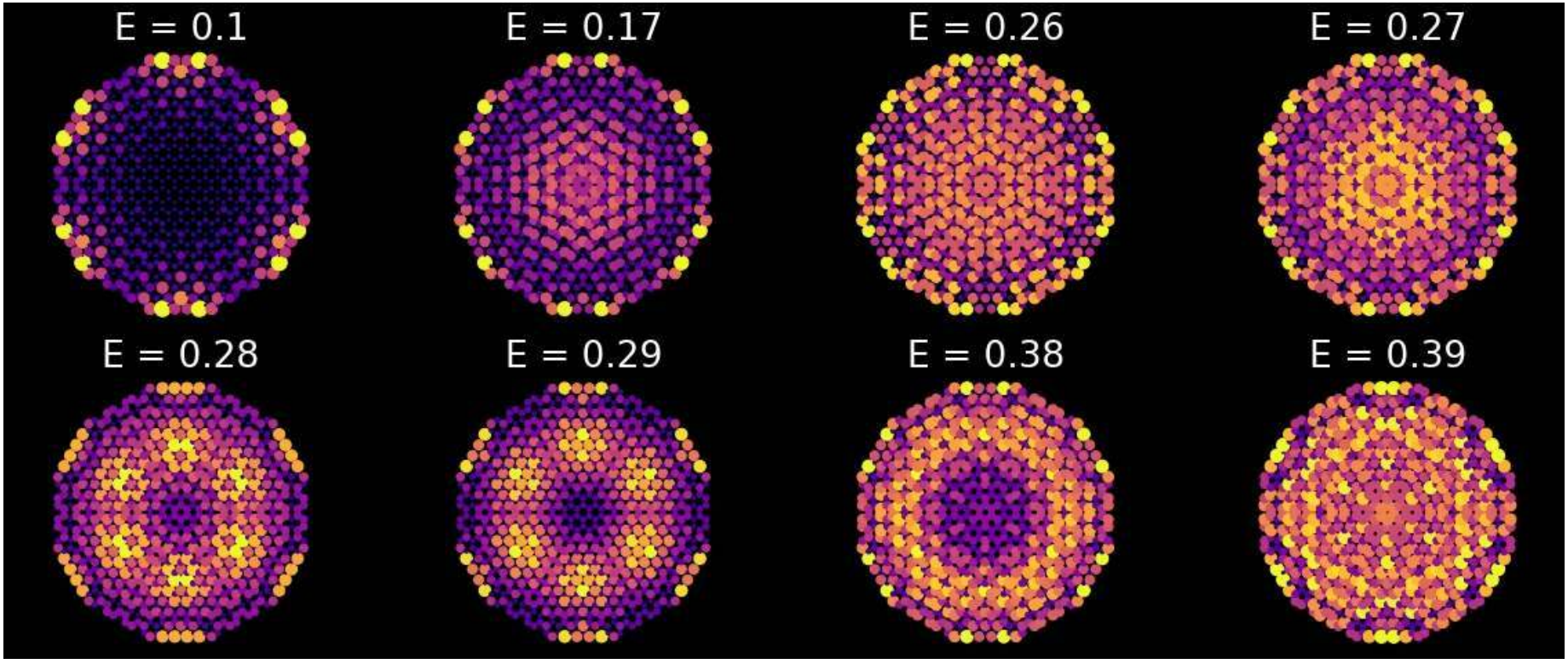
Confined modes in graphene islands



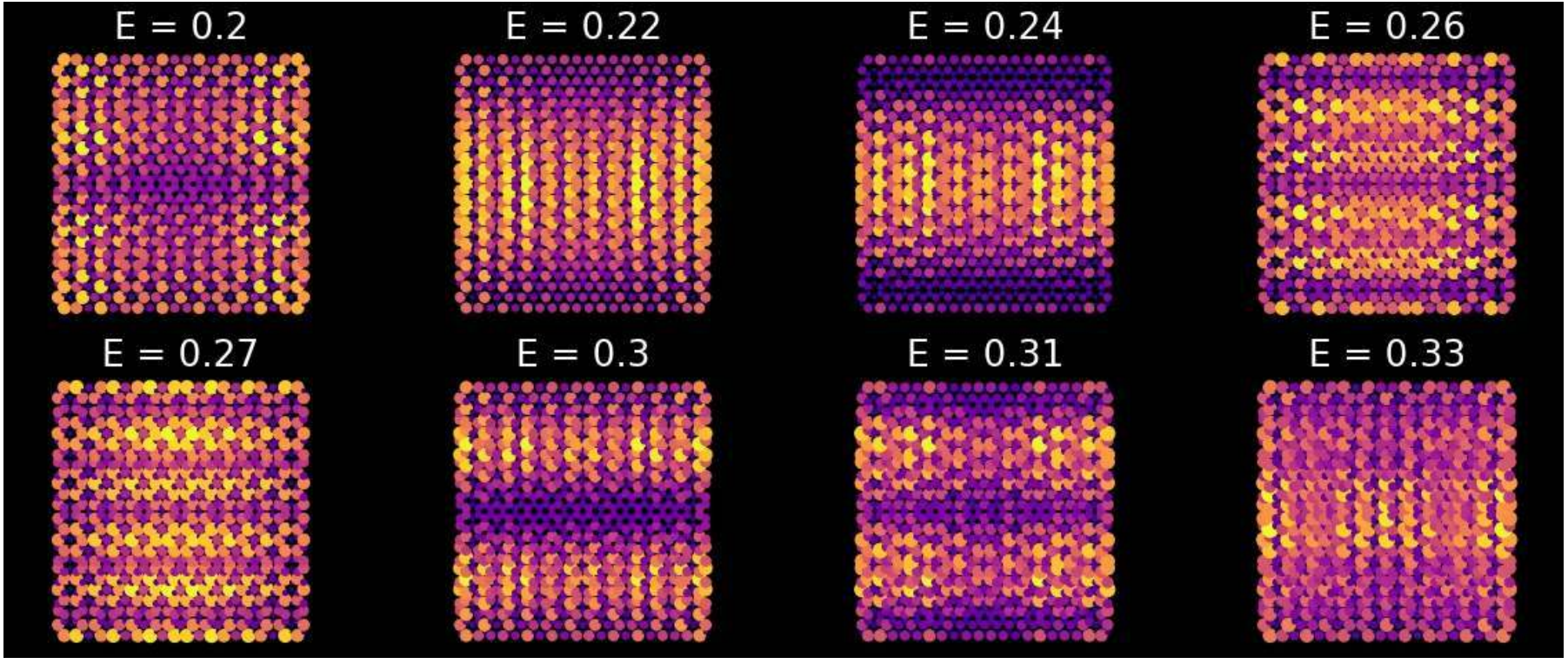
Confined modes in graphene islands



Confined modes in graphene islands



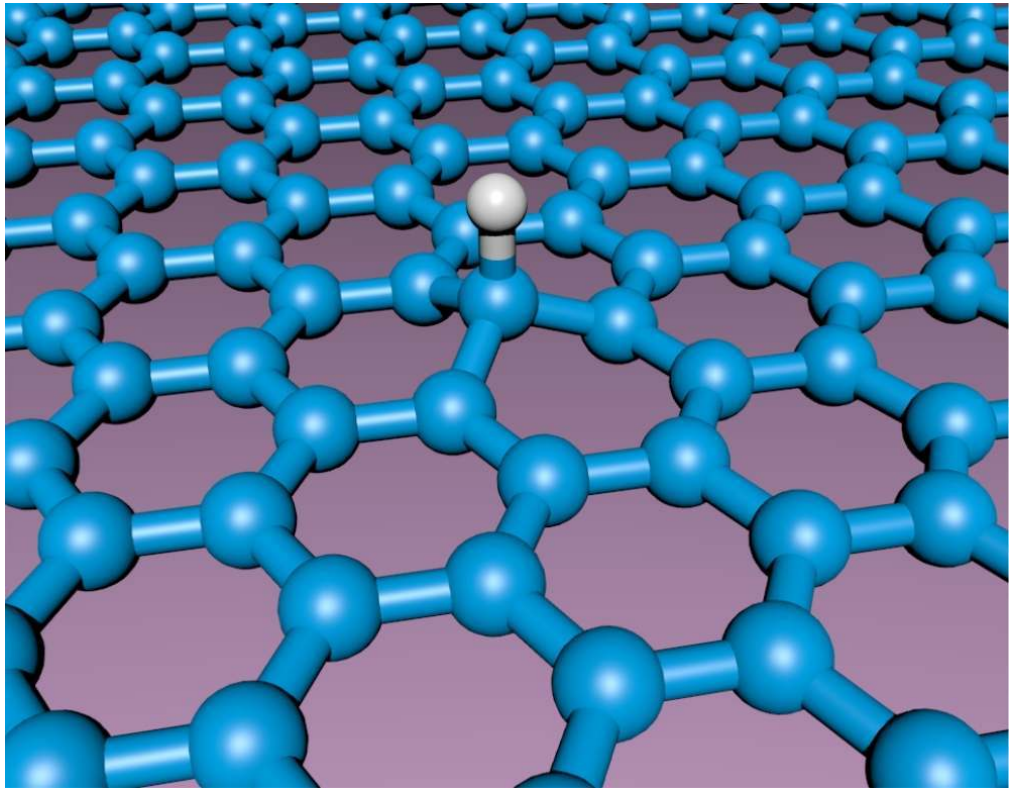
Confined modes in graphene islands



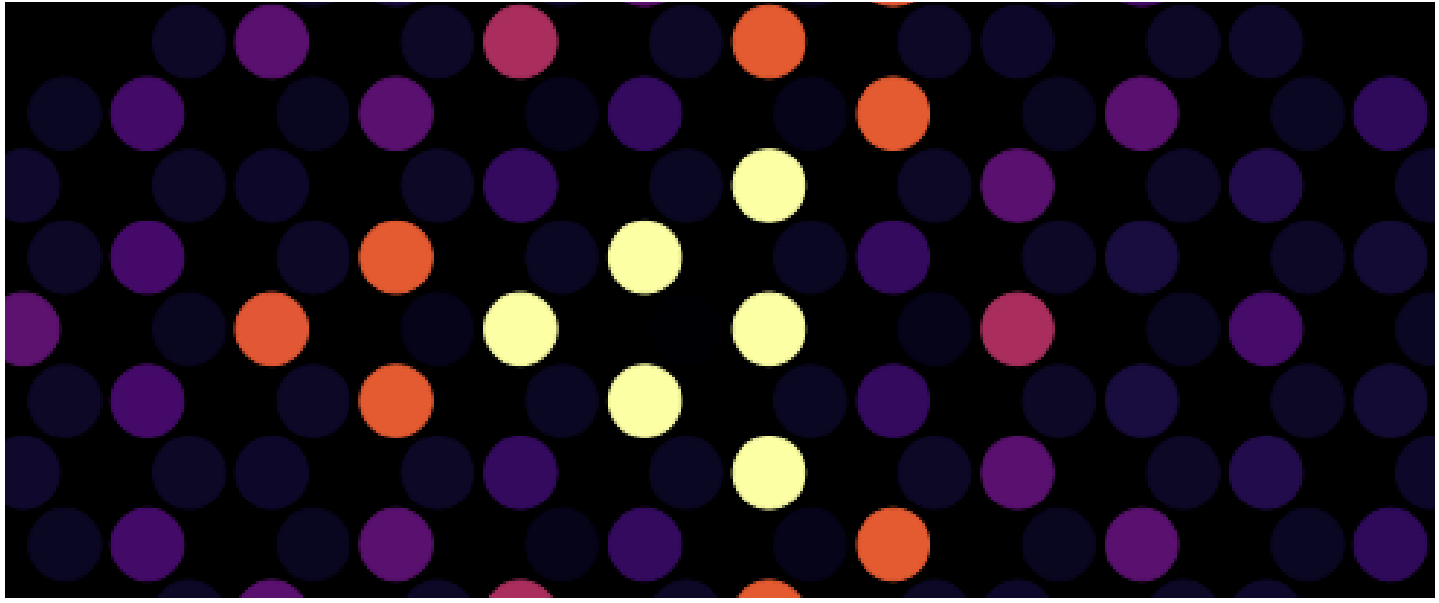
Defects in 2D materials

Impurities in monolayer graphene

Hydrogen adsorption in graphene



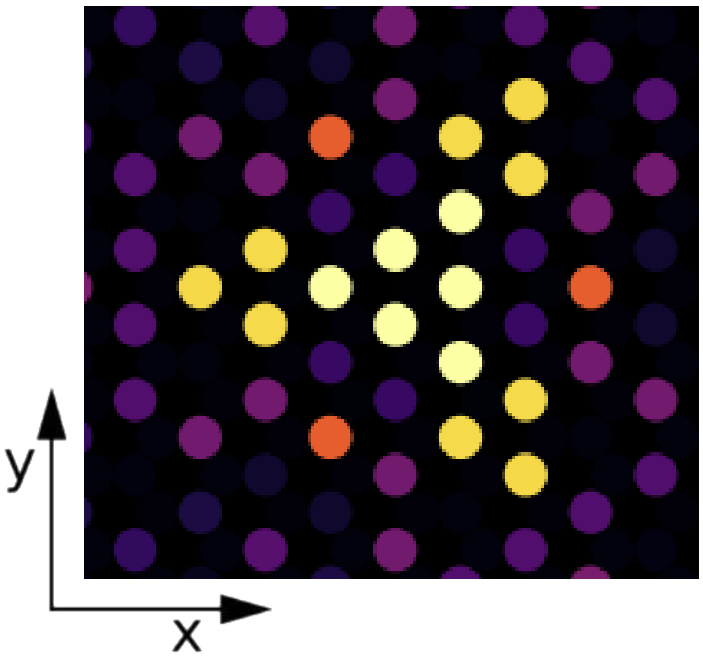
Individual hydrogen atoms in graphene



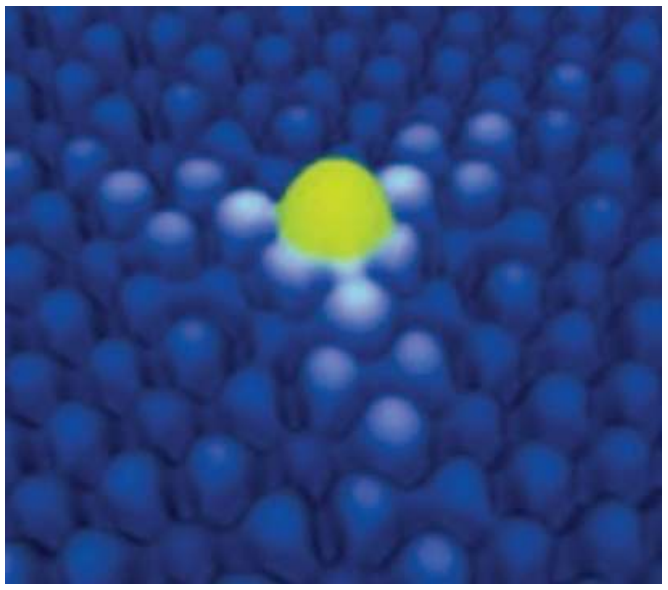
$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j$$

Single impurity in monolayer graphene

Local density of states



Experimental local density of states



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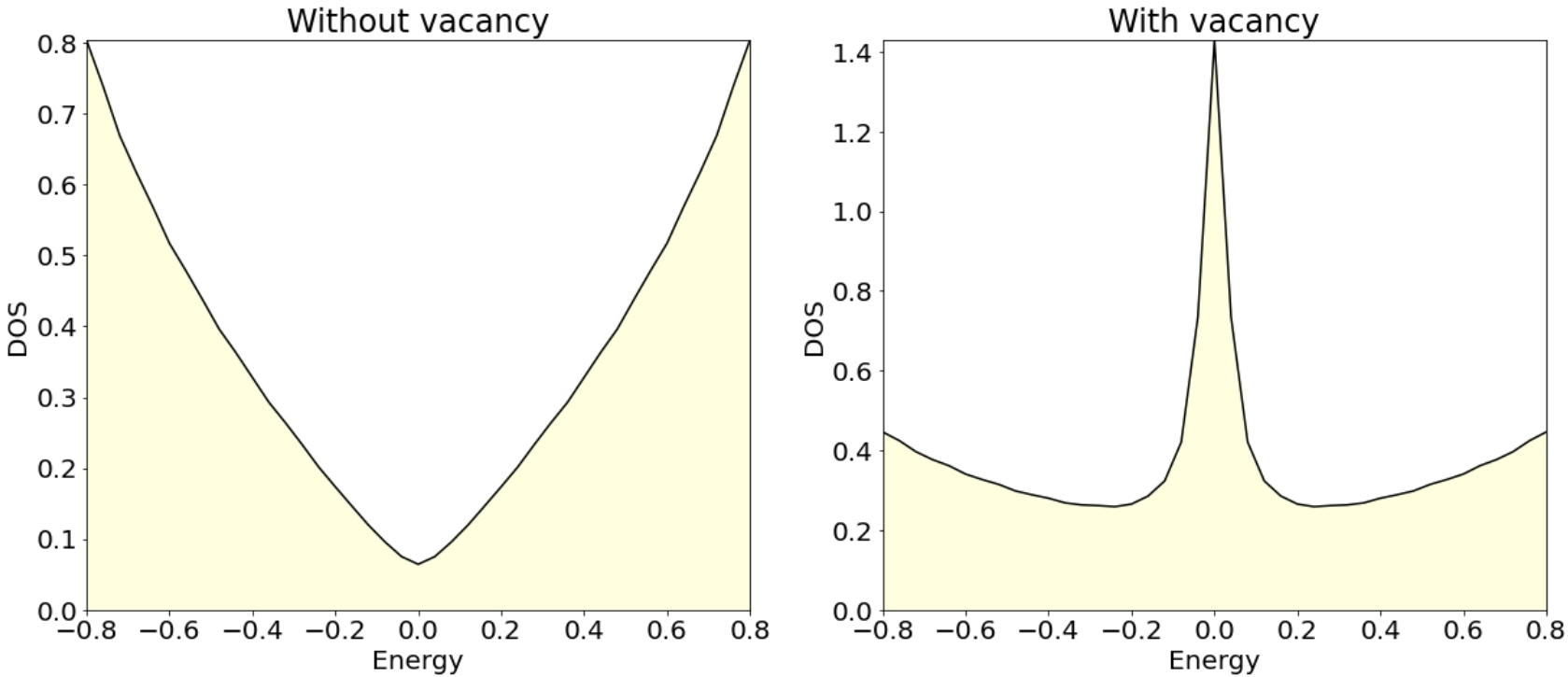
Hydrogen atoms create zero modes in graphene

Individual hydrogen atoms in graphene

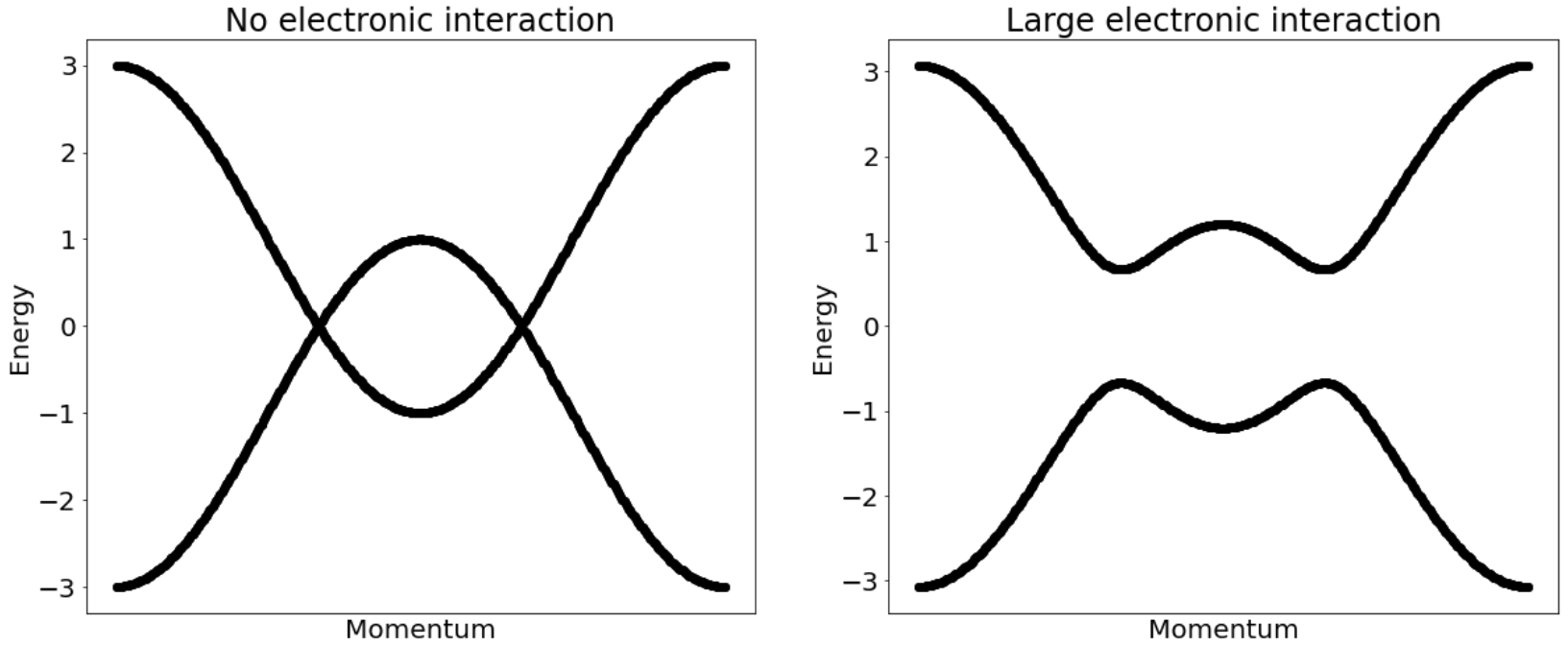


A vacancy in graphene gives rise to resonant zero modes

Electronic instabilities in 2D materials

Electronic interactions

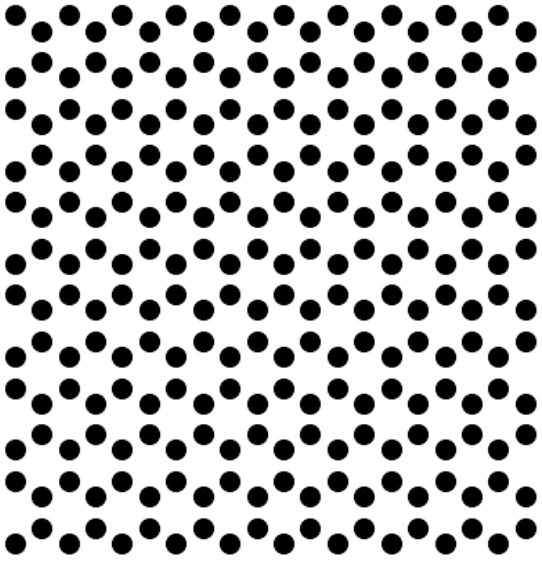
Large electronic interactions lead to gap opening in the electronic structure



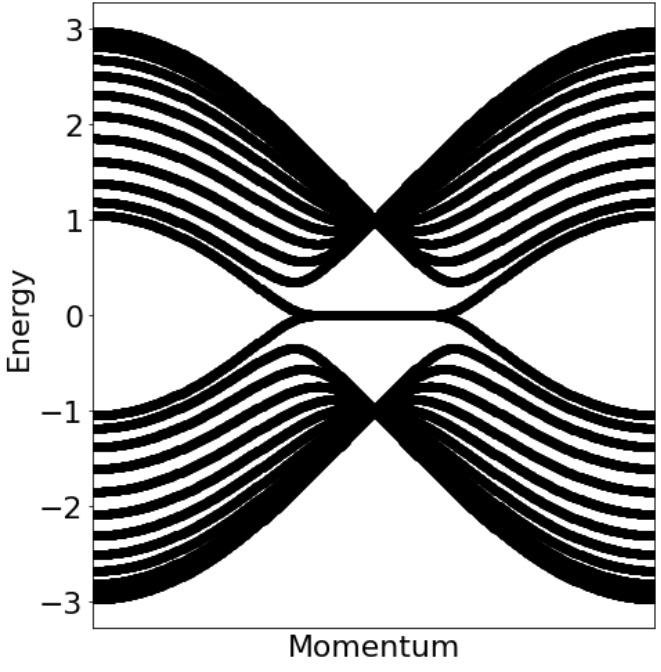
But by solely looking at the electronic spectrum it is hard to know the nature of the gap opening

Flat bands in graphene nanoribbons

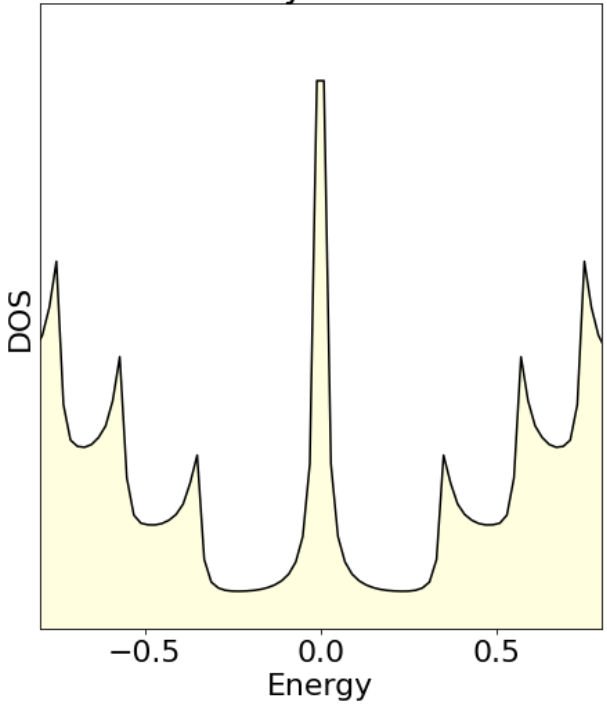
Structure



Band structure

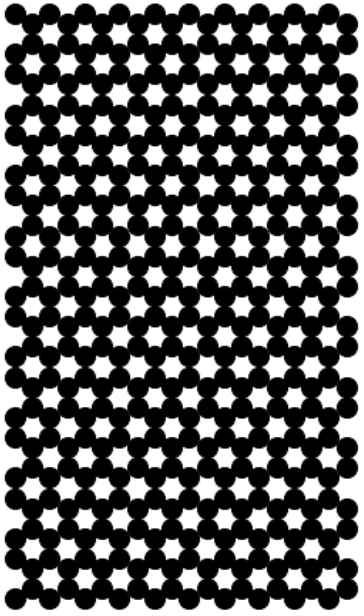


Density of states

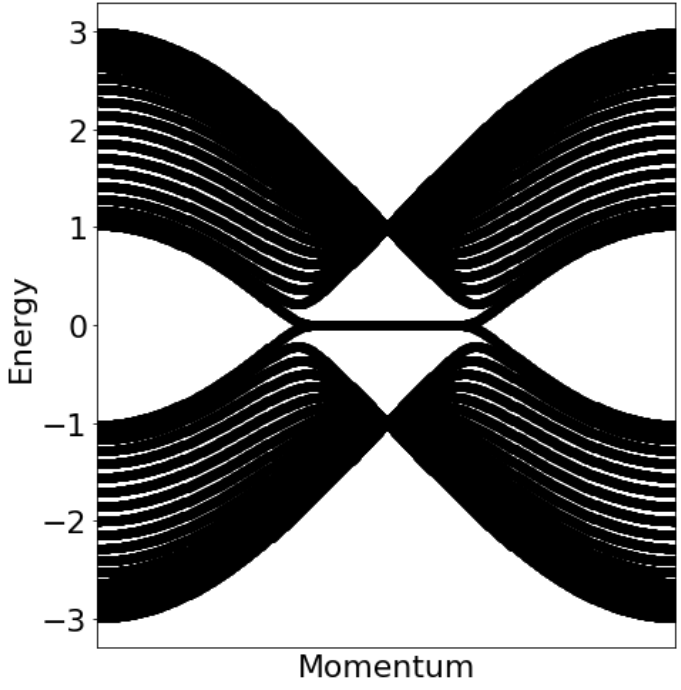


Flat bands in graphene nanoribbons

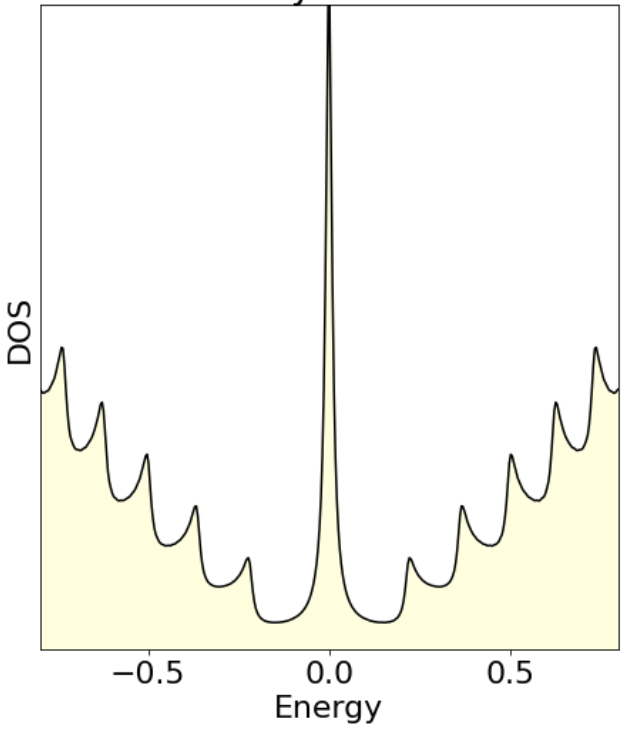
Structure



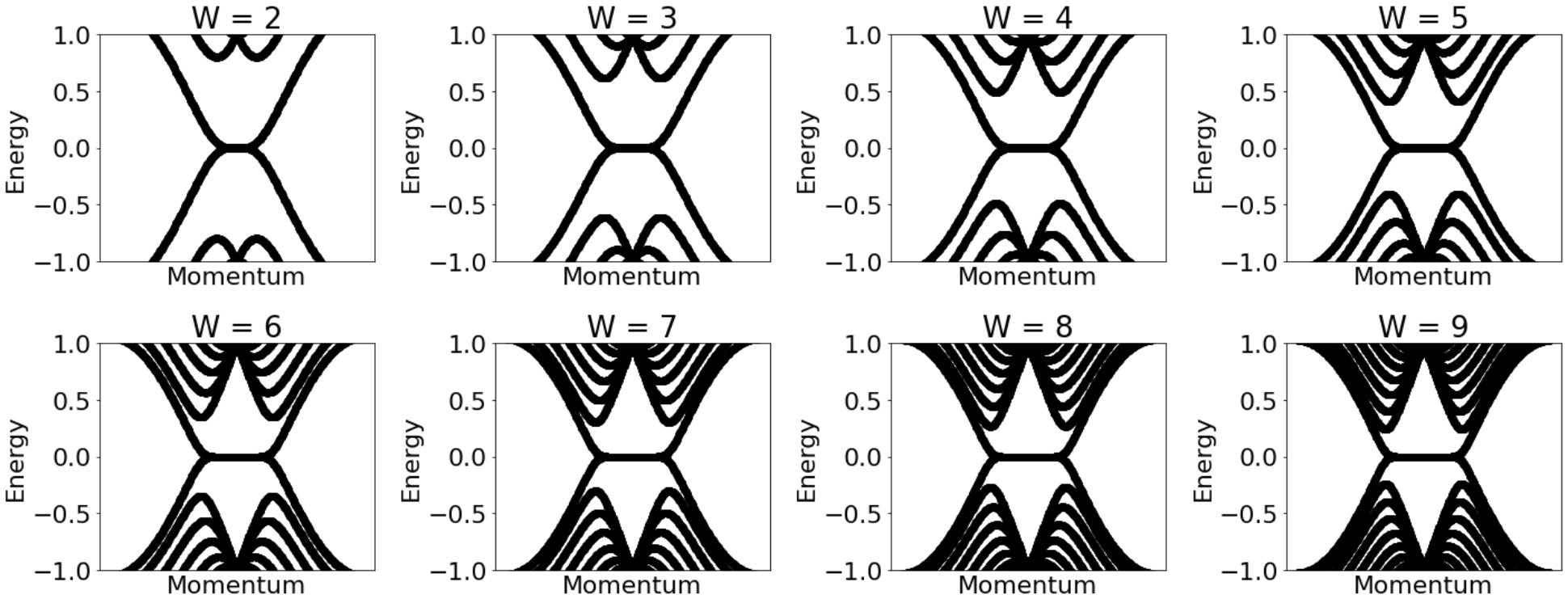
Band structure



Density of states

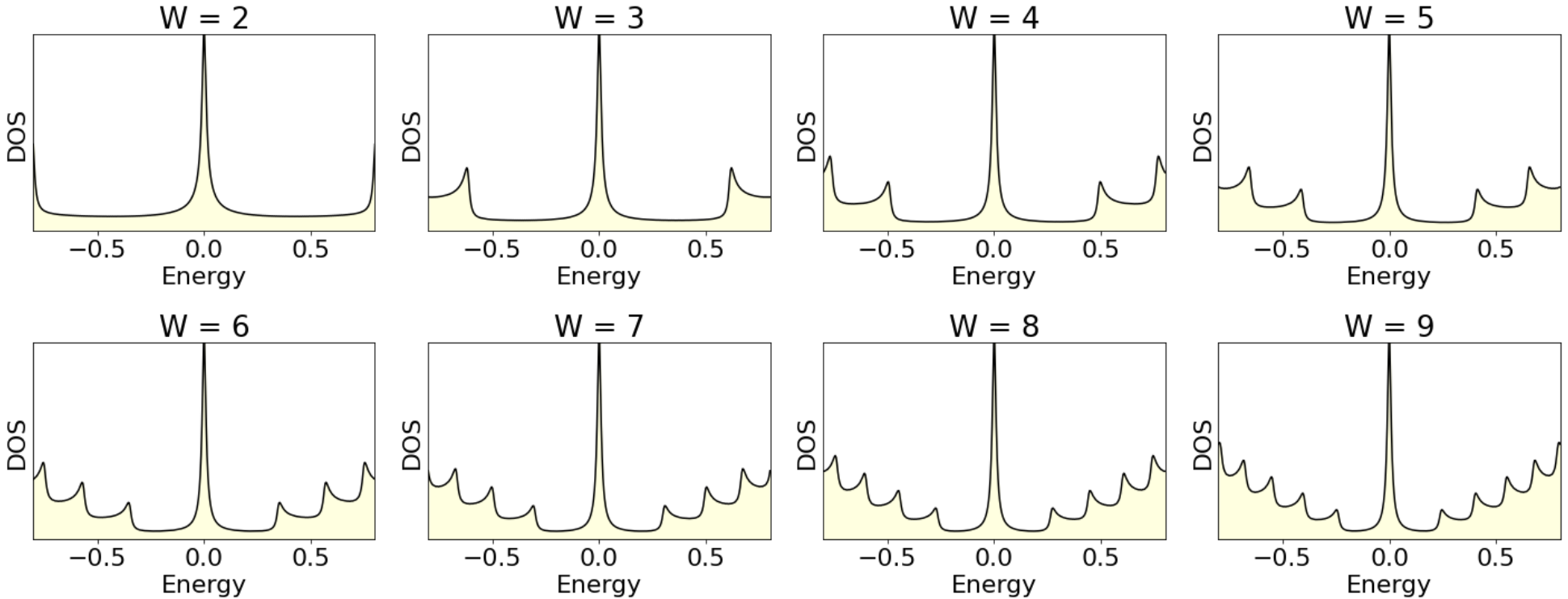


Electronic structure of zigzag graphene nanoribbons



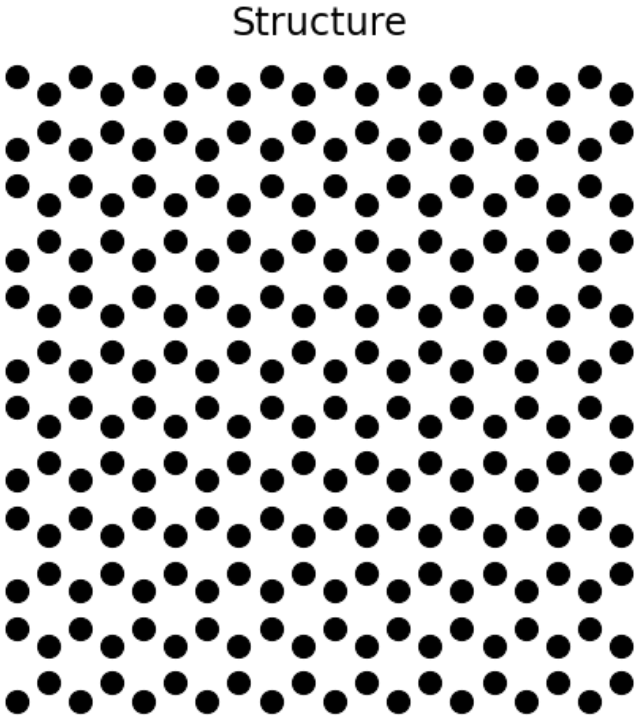
Flat bands appear in graphene zigzag nanoribbon of any width

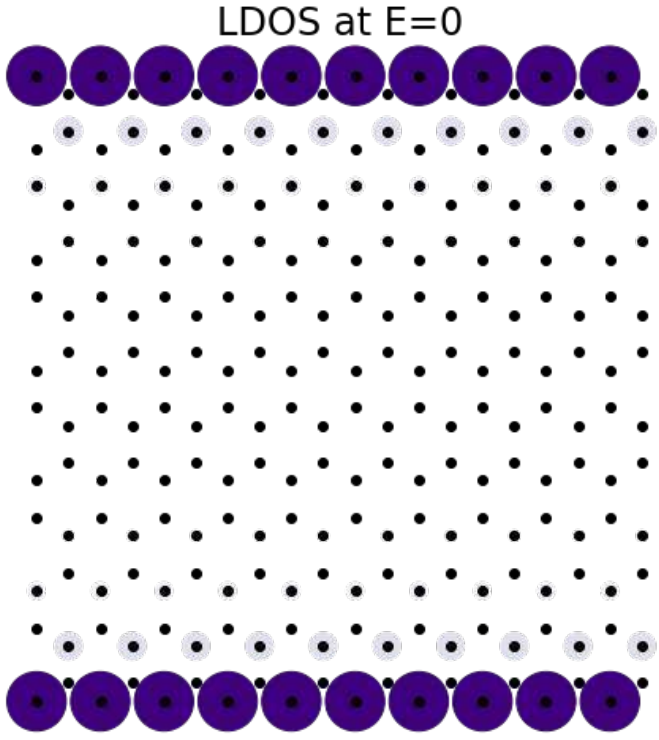
Electronic structure of zigzag graphene nanoribbons



A divergent density of states appears in zigzag nanoribbon of any width

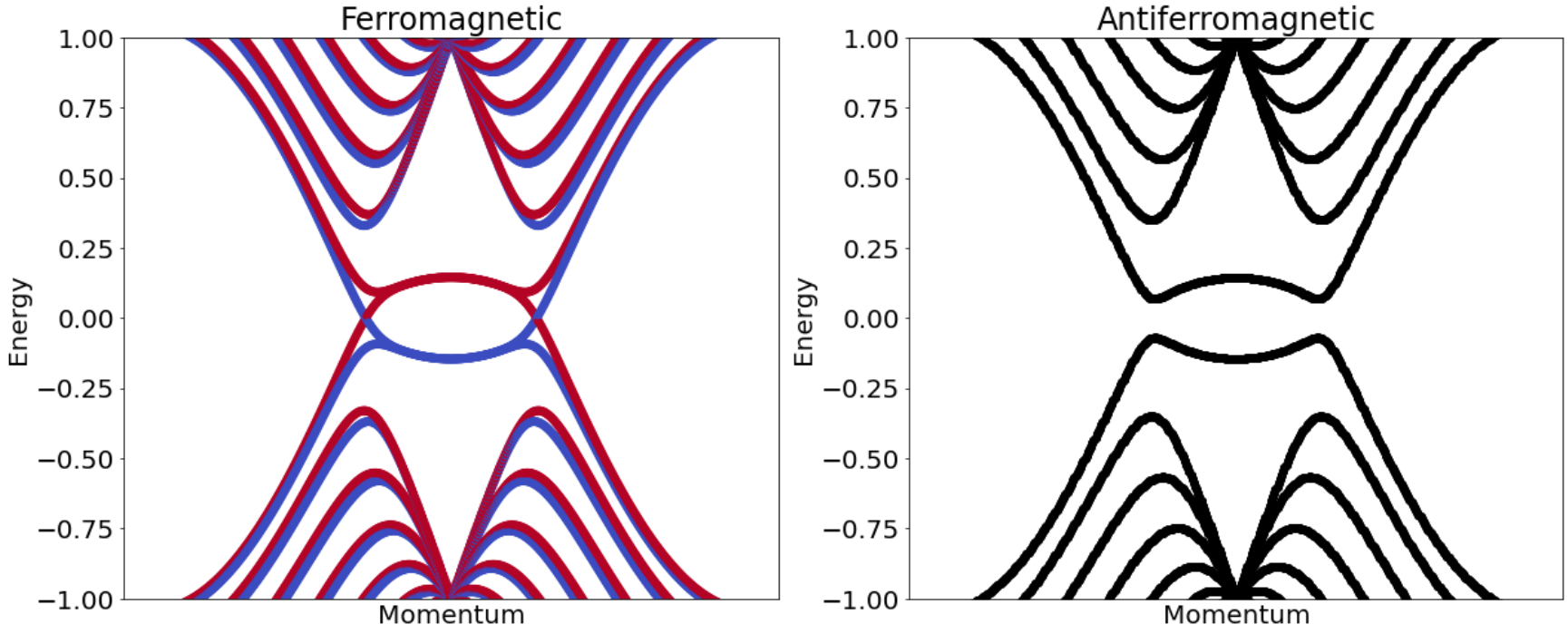
Electronic structure of graphene zigzag ribbons





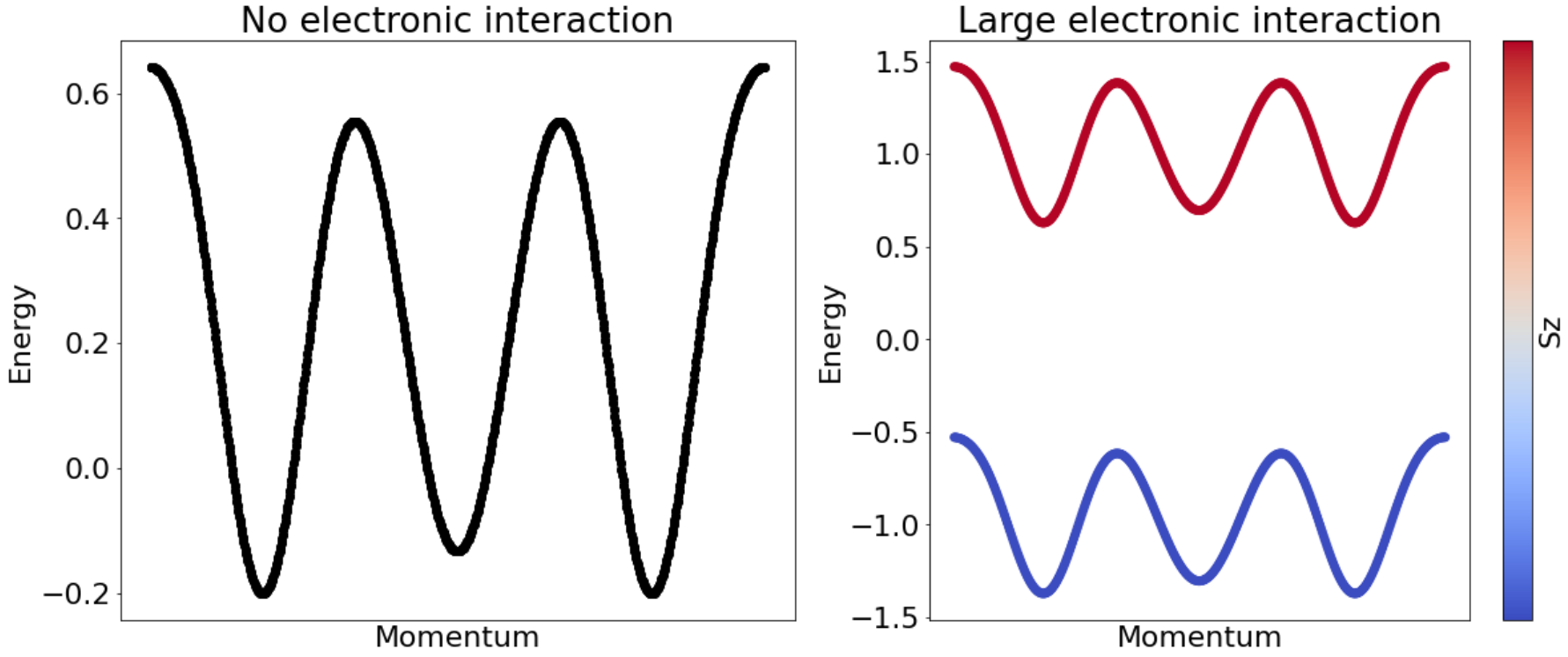
Electronic interactions in graphene nanoribbons

Depending on the selfconsistent solution, the electronic structure can radically change



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

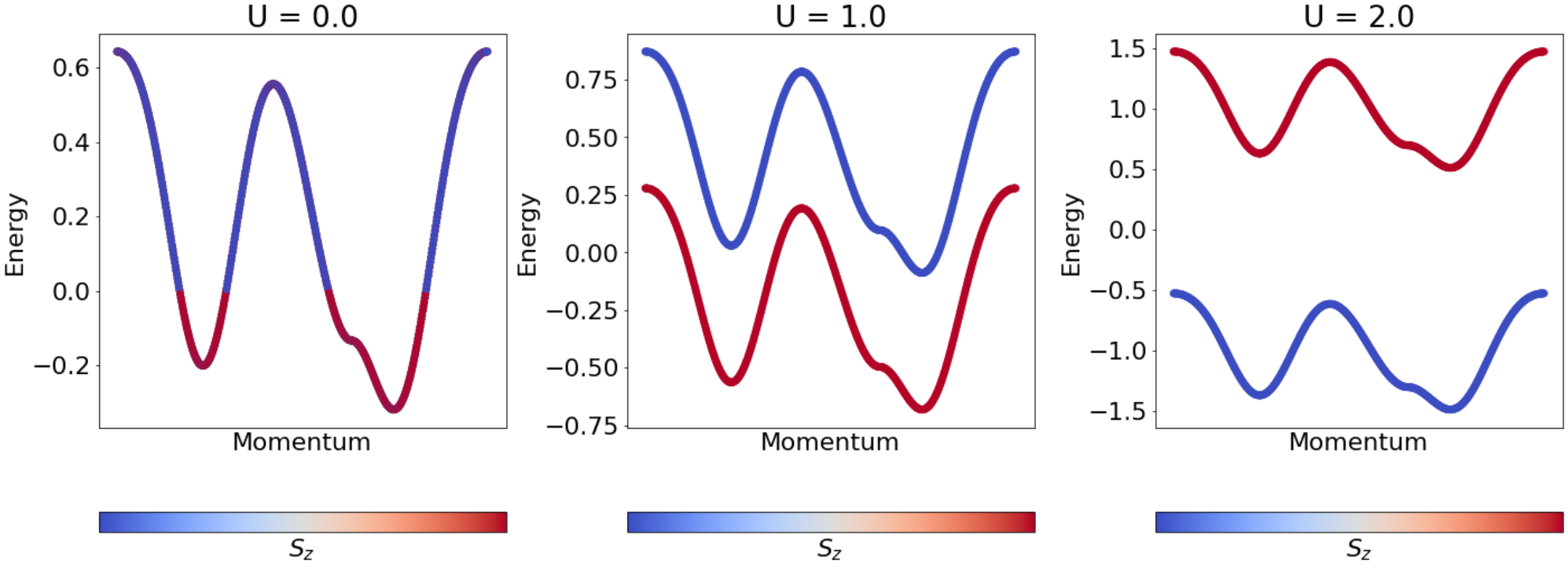
Interaction-driven ferromagnetism



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

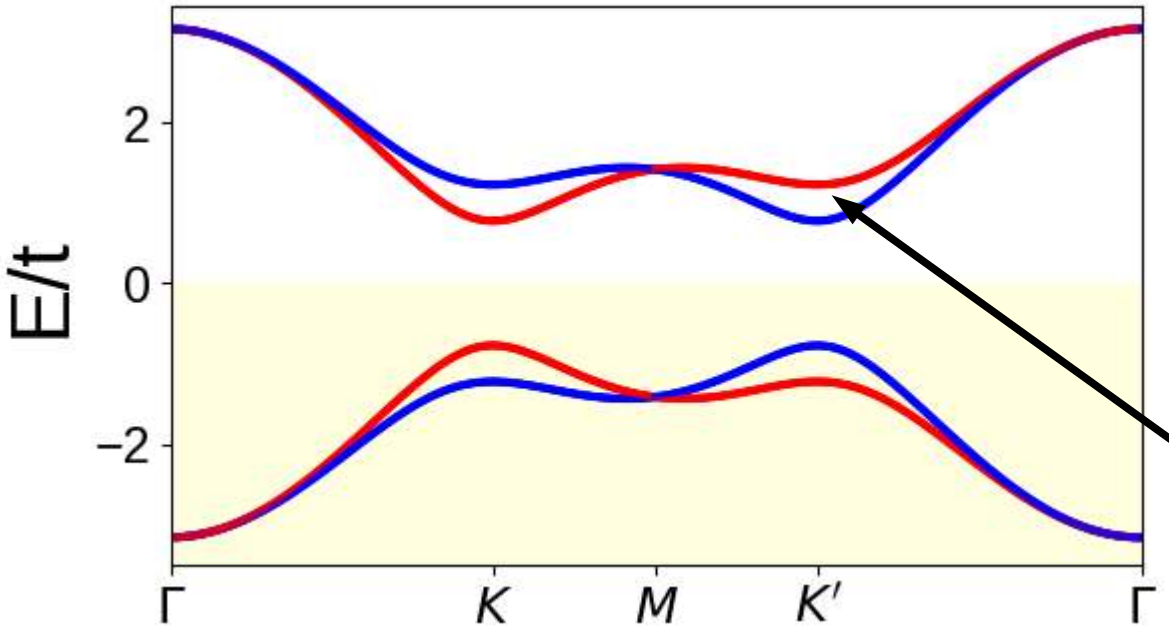
Interaction-driven ferromagnetism

As we ramp up interactions, a correlated state appears

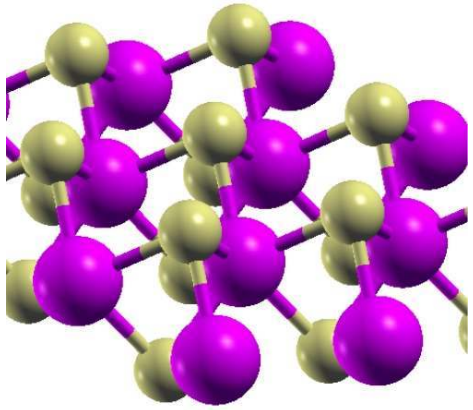


Proximity effects in TMDC-based van der Waals heterostructures

The electronic structure of semiconducting TMDC



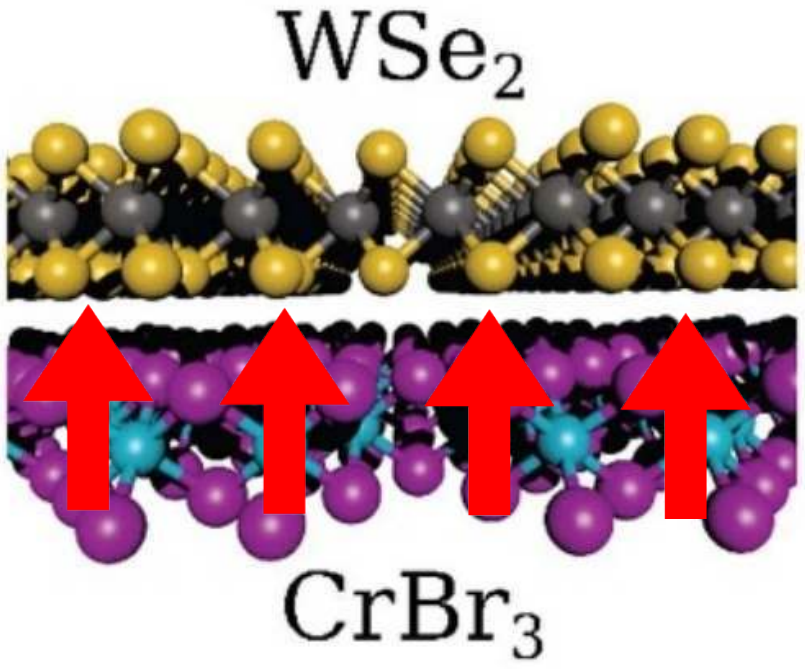
MoS_2, WSe_2,

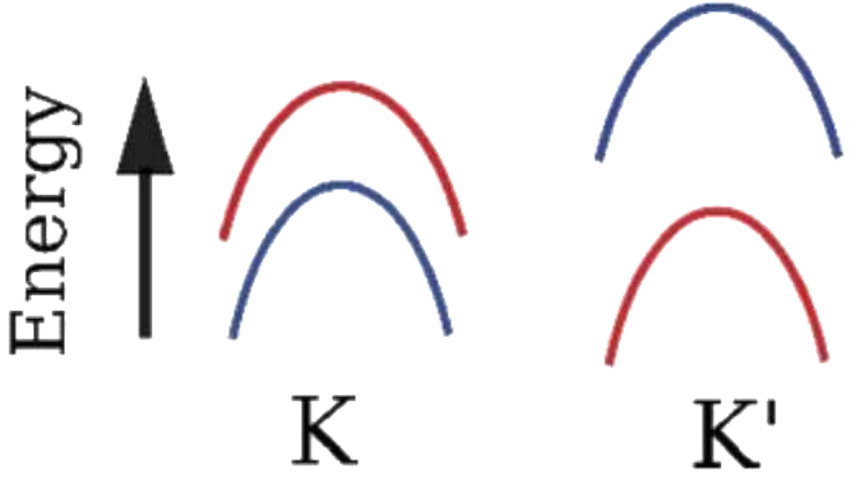


Non-centrosymmetric spin-orbit coupling

Semiconducting TMDC show a strong spin-valley coupling

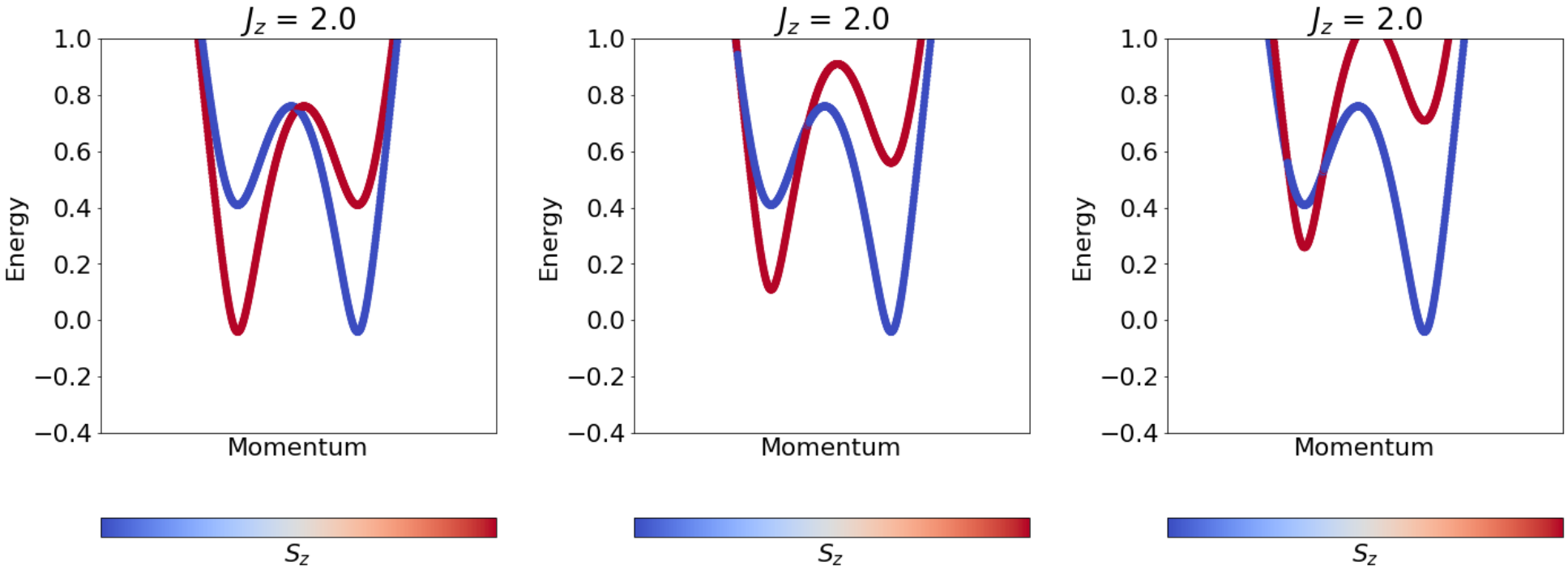
Proximity effects between a TMDC and an out-of-plane 2D ferromagnet





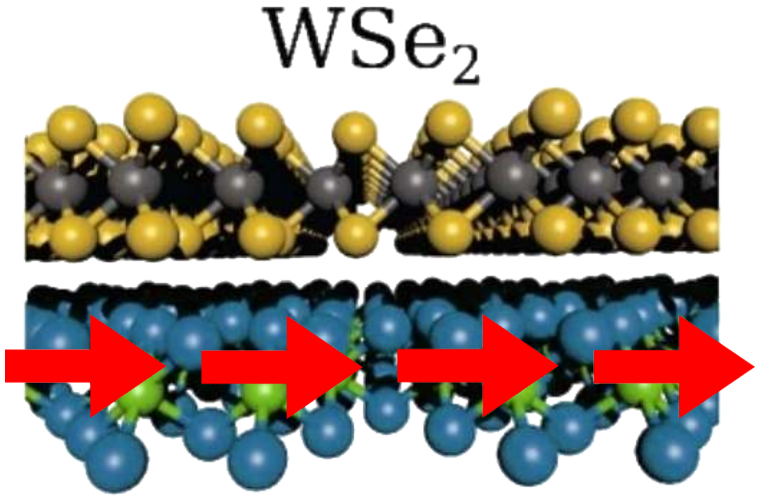
An exchange coupling leads to a valley-dependent splitting

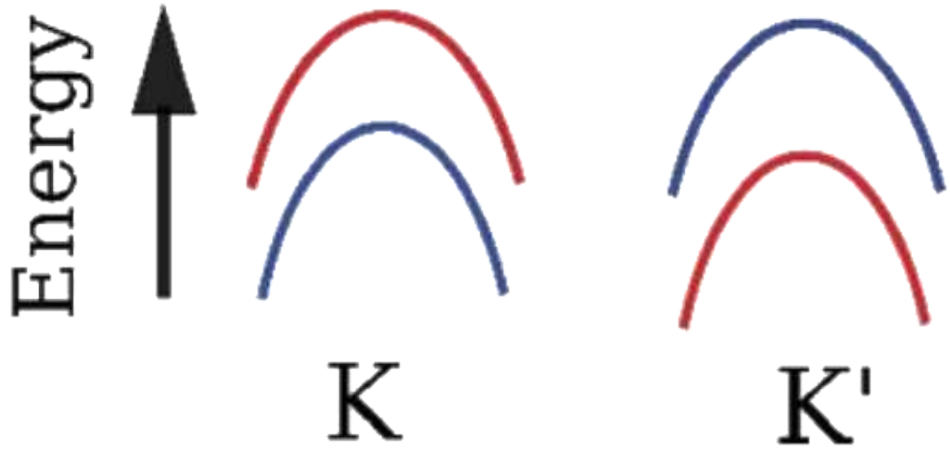
Proximity effects between a TMDC and an out-of-plane 2D ferromagnet



A valley-dependent splitting appears due to valley-momentum locking of TMDC

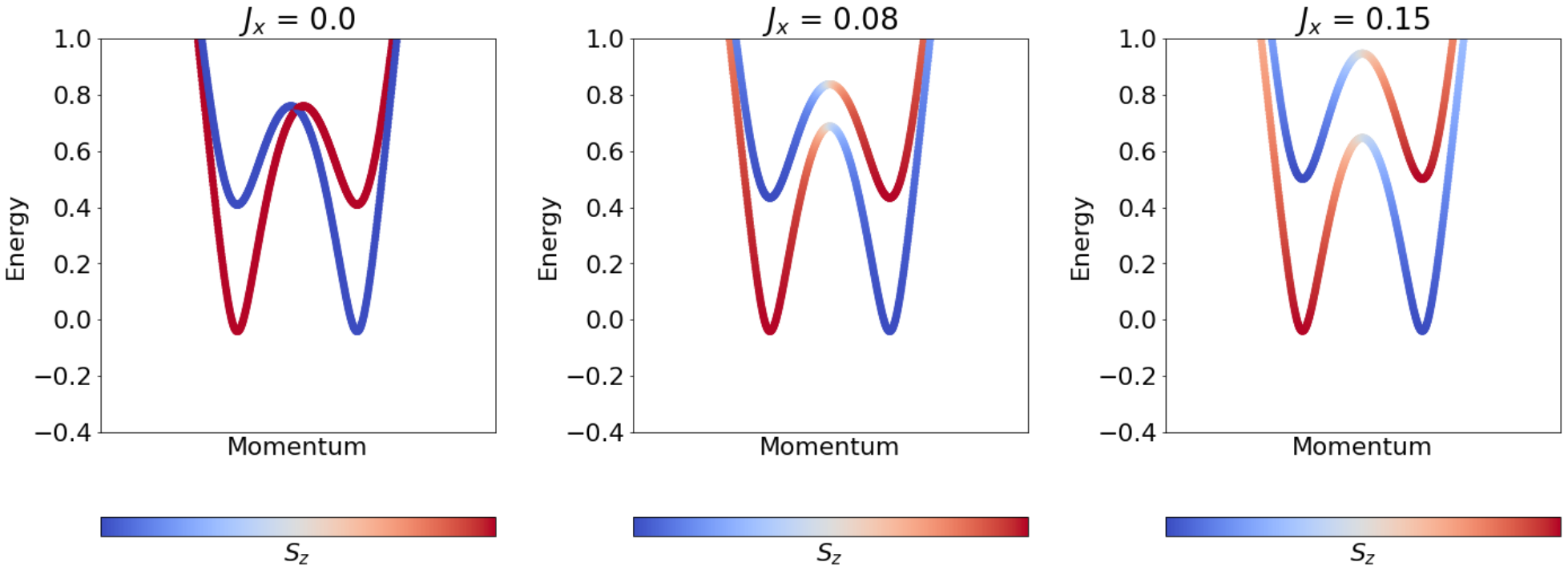
Proximity effects between a TMDC and an in-plane 2D ferromagnet





An exchange coupling leads to a valley-dependent splitting

Proximity effects between a TMDC and an in-plane 2D ferromagnet



No valley-dependent splitting appears for an in-plane ferromagnet

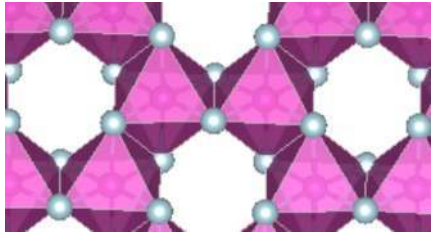
Break

10-15 min break

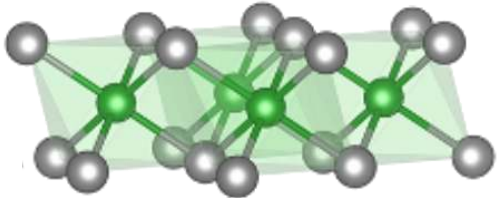
(optional) to discuss during the break

Which symmetries breaks the electronic order of these 2D materials?

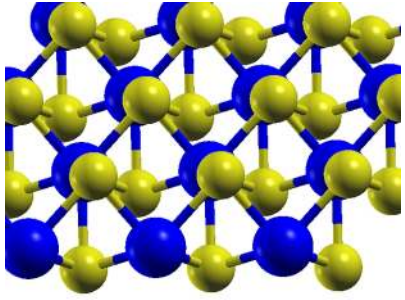
CrI_3



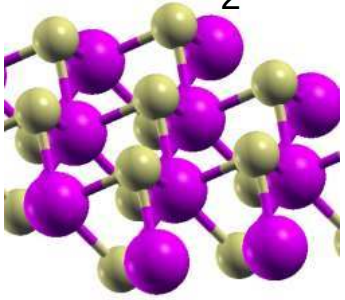
NiI_2



$NbSe_2$



WSe_2



Warming up for the exercise sessions

Pyqula for the exercise sessions

- High level user friendly library for Python to solve tight-binding models
- Focus on:
  - Easy to use
  - Performing complex calculations with minimal effort
  - Full compatibility of different calculation modes

About the library

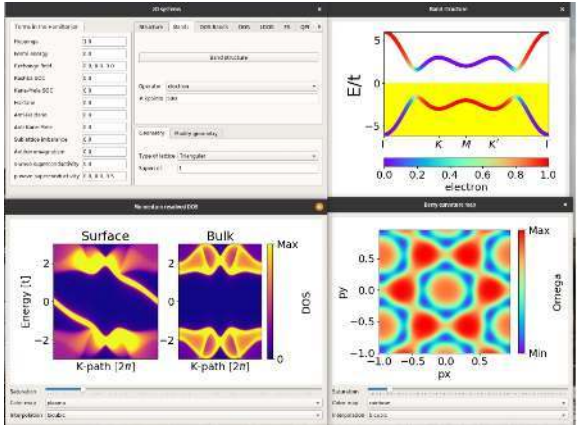
pyqula (for all the sessions)

```
from pyqula import geometry
g = geometry.honeycomb_lattice()
h = g.get_hamiltonian()
h.add_rashba(0.2) # Rashba spin-orbit coupling
h.add_zeeman([0.,0.,0.6]) # Zeeman field
from pyqula import topology
(kx,ky,omega) = h.get_berry_curvature() # compute Berry curvature
c = h.get_chern() # compute the Chern number
```

- Python library
- Ideal for complex models/calculations
- For writing in Python

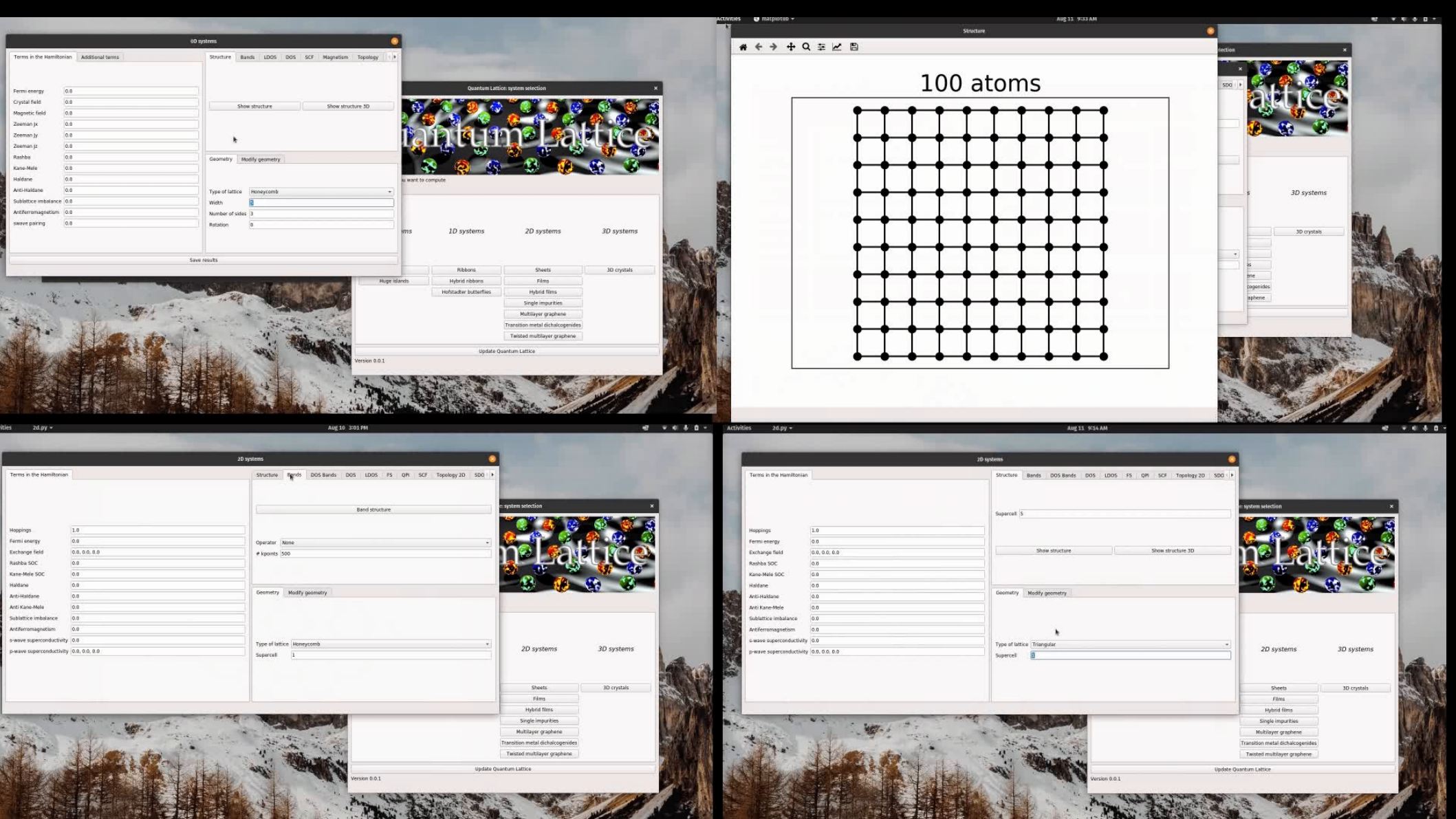
https://github.com/joselado/pyqula

Quantum-lattice (built on top of pyqula)



- User-friendly interface for tight binding models
- Ideal for simple models and quick checks
- Fully interface-based, no scripting

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


0D systems
Terms in the Hamiltonian
Additional terms
Fermi energy
Crystal field
Magnetic field
Zeeman jx
Zeeman jy
Zeeman jz
Rashba
Kane-Mele
Haldane
Anti-Haldane
Sublattice imbalance
Antiferromagnetism
swave pairing
Structure
Bands
LDOS
DOS
SCF
Magnetism
Topology
Show structure
Show structure 3D
Geometry
Modify geometry
Type of lattice
Honeycomb
Width
Number of sides
Rotation
Save results
Quantum Lattice: system selection
1D systems
2D systems
3D systems
Ribbons
Sheets
3D crystals
Huge islands
Hybrid ribbons
Films
Hofstadter butterflies
Hybrid films
Single impurities
Multilayer graphene
Transition metal dichalcogenides
Twisted multilayer graphene
Update Quantum Lattice
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Structure
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3D systems
3D crystals
2d.py
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2D systems
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Exchange field
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Kane-Mele SOC
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Anti Kane-Mele
Sublattice imbalance
Antiferromagnetism
s-wave superconductivity
p-wave superconductivity
Structure
Bands
DOS Bands
DOS
LDOS
FS
QPI
SCF
Topology 2D
SDO
Band structure
Operator
None
kpoints
500
Geometry
Modify geometry
Type of lattice
Honeycomb
Supercell
2D systems
3D systems
Sheets
Films
Hybrid films
Single impurities
Multilayer graphene
Transition metal dichalcogenides
Twisted multilayer graphene
Update Quantum Lattice
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Activities
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Terms in the Hamiltonian
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Show structure 3D
Geometry
Modify geometry
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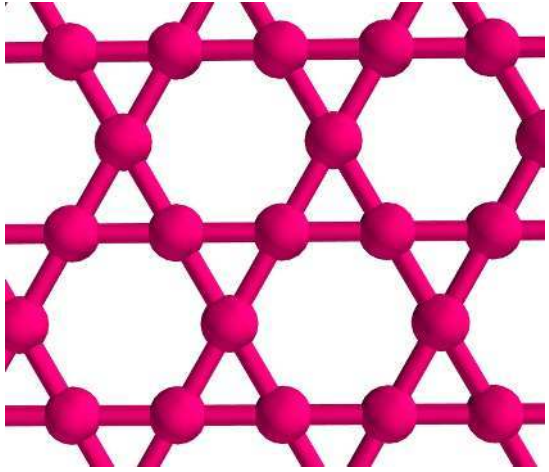
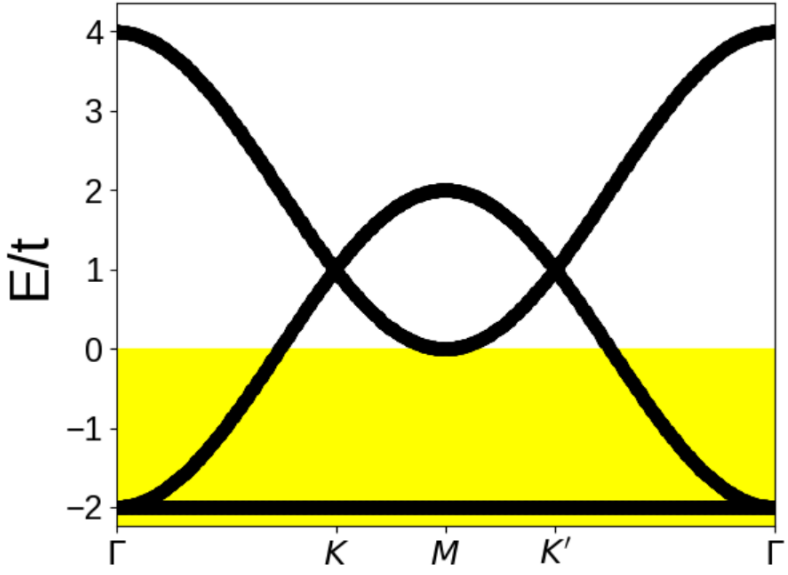
Triangular
Supercell
2D systems
3D systems
Sheets
Films
Hybrid films
Single impurities
Multilayer graphene
Transition metal dichalcogenides
Twisted multilayer graphene
Update Quantum Lattice
Version 0.0.1

A minimal example: Band structure of a Kagome lattice

```
from pyqula import geometry
g = geometry.kagome_lattice() # get the geometry object
h = g.get_hamiltonian() # get the Hamiltonian object
(k,e) = h.get_bands() # compute the band structure
```





Hamiltonians

Real-space tight binding Hamiltonians

$$H_0 = \sum_{i,j,s,s'} t_{i,j}^{s,s'} c_{i,s}^{\dagger} c_{j,s'} + \sum_{i,j,s,s'} \Delta_{i,j}^{s,s'} c_{i,s}^{\dagger} c_{j,s'}^{\dagger} + h.c.$$

With electronic interactions

$$H_{int} = \sum_{i,j,s,s'} V_{i,j} \sum_{s} c_{i,s}^{\dagger} c_{i,s} \sum_{s'} c_{j,s'}^{\dagger} c_{j,s'}$$

Workflow of the library

Create the geometry of the model

Dimensionality, supercell, vacancies, etc...

```
from pyqula import geometry
g = geometry.kagome_lattice() # get the geometry object
h = g.get_hamiltonian() # get the Hamiltonian object
(k,e) = h.get_bands() # compute the band structure
```

Include the different terms in the Hamiltonian

Kinetic energy, spin-orbit coupling, magnetism, superconductivity, interactions, etc..

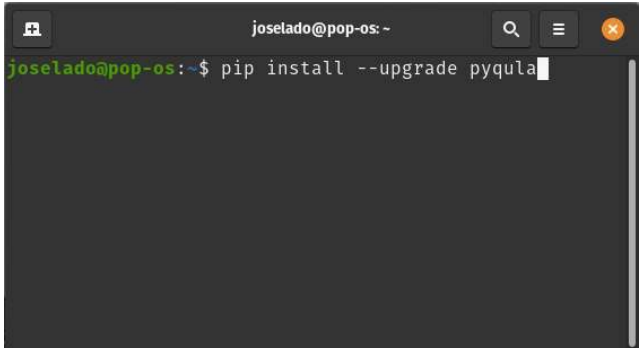
Compute the different observables of the system

Band structure, spectral functions, local DOS, topological invariants, expectation values, etc...

Installation

With pip (from the command line)

pip install --upgrade pyqula



*You can also download the whole source from

https://github.com/joselado/pyqula

Capabilities

Single particle Hamiltonians

- Spinless, spinful and Nambu basis for orbitals
- Full non-collinear electron and Nambu formalism
- Include magnetism, spin-orbit coupling and superconductivity
- Band structures with state-resolved expectation values
- Momentum-resolved spectral functions
- Local and full operator-resolved density of states
- 0d, 1d, 2d and 3d tight binding models
- Electronic structure unfolding in supercells

Capabilities

Interacting mean-field Hamiltonians

- Selfconsistent mean-field calculations with local/non-local interactions
- Both collinear and non-collinear formalism
- Anomalous mean-field for non-collinear superconductors
- Full selfconsistency with all Wick terms for non-collinear superconductors
- Constrained and unconstrained mean-field calculations
- Automatic identification of order parameters for symmetry broken states
- Hermitian and non-Hermitian mean-field calculations

Capabilities

Topological characterization

- Berry phases, Berry curvatures, Chern numbers and Z2 invariants
- Operator-resolved Chern numbers and Berry density
- Frequency resolved topological density
- Spatially resolved topological flux
- Real-space Chern density for amorphous systems
- Wilson loop and Green's function formalism

Capabilities

Spectral functions

- Spectral functions in infinite geometries
- Surface spectral functions for semi-infinite systems
- Interfacial spectral function in semi-infinite junctions
- Single impurities in infinite systems
- Operator-resolved spectral functions
- Green's function renormalization algorithm

Capabilities

Chebyshev kernel polynomial based-algorithms

- Local and full spectral functions
- Non-local correlators and Green's functions
- Locally resolved expectation values
- Operator resolved spectral functions
- Reaching system sizes up to 10000000 atoms on a single-core laptop

Capabilities

Quantum transport

- Metal-metal transport
- Metal-superconductor transport
- Fully non-collinear Nambu basis
- Non-equilibrium Green's function formalism
- Operator-resolved transport
- Differential decay rate
- Tunneling and contact scanning probe spectroscopy

Three technical notes

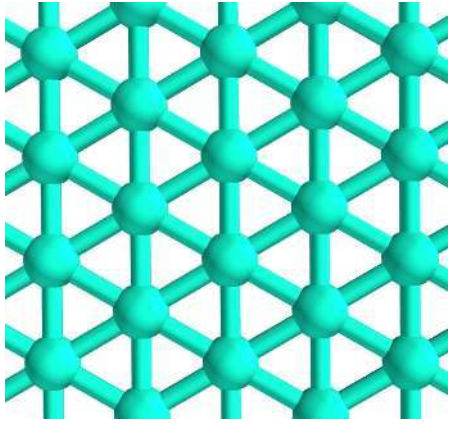
- Object oriented library
  - Geometries, Hamiltonians, Operators, etc are objects with internal structure, methods and built-in algebra
- Performance
  - Computationally intensive parts written in high-performance just-in-time compiled Numba
- Parallelization
  - Multicore shared memory parallelization

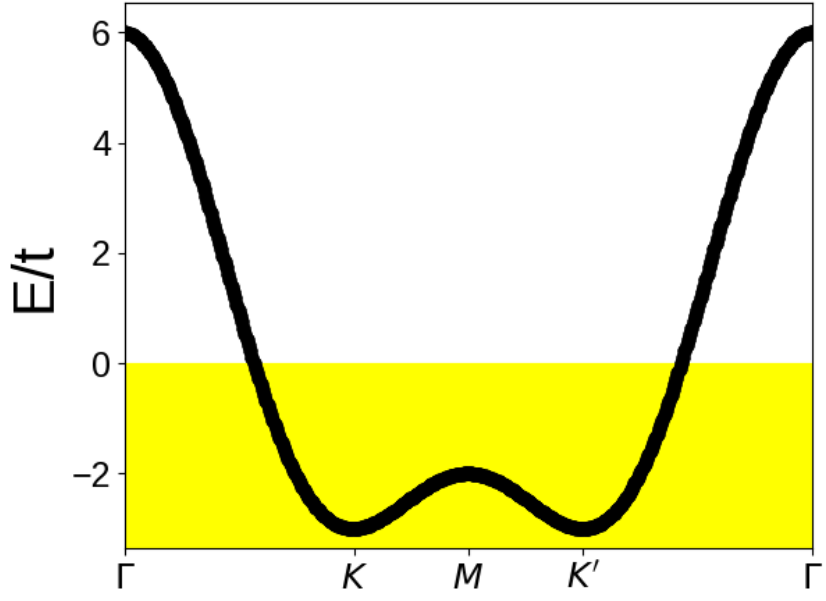
A few minimal examples with pyqula

First neighbor Hamiltonian in a triangular lattice

$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j$$

```
from pyqula import geometry
g = geometry.triangular_lattice() # get the geometry object
h = g.get_hamiltonian() # get the Hamiltonian object
(k,e) = h.get_bands() # compute the band structure
```

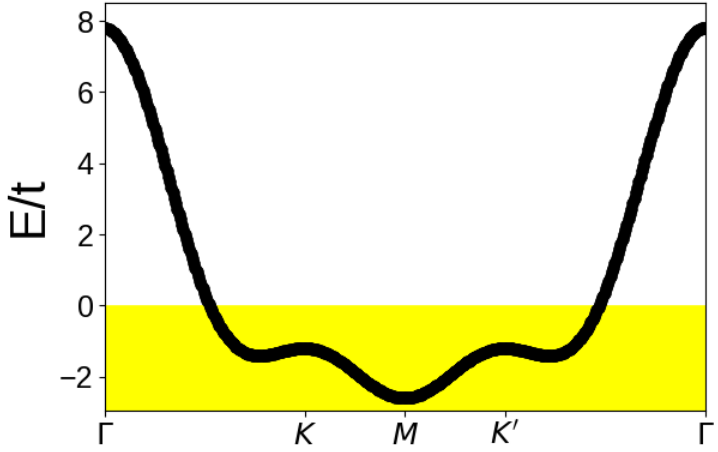




First and second neighbor Hamiltonian in a triangular lattice

$$H = t_1 \sum_{\langle ij \rangle} c_i^\dagger c_j + t_2 \sum_{\langle\langle ij \rangle\rangle} c_i^\dagger c_j$$

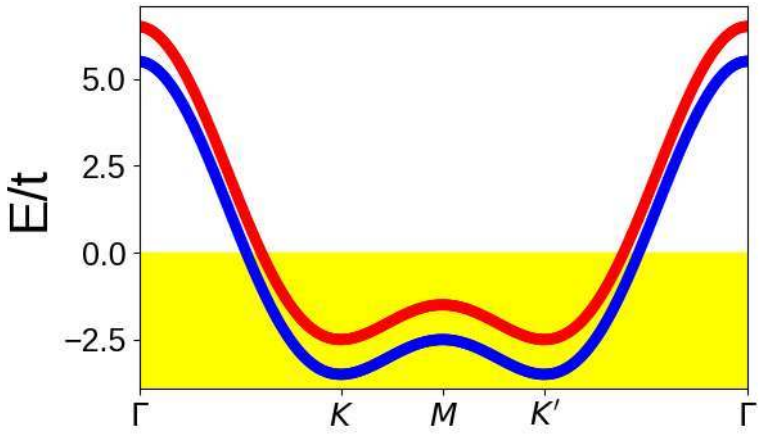
```
from pyqula import geometry
g = geometry.triangular_lattice() # get the geometry object
h = g.get_hamiltonian(tij=[1.0,0.3]) # get the Hamiltonian object
(k,e) = h.get_bands() # compute the band structure
```



Triangular lattice with an exchange field

$$H = t \sum_{\langle ij \rangle} c^{\dagger}_{i,s} c_{j,s} + B_z \sum_{i} \sigma_z^{s,s'} c^{\dagger}_{i,s} c_{j,s}$$

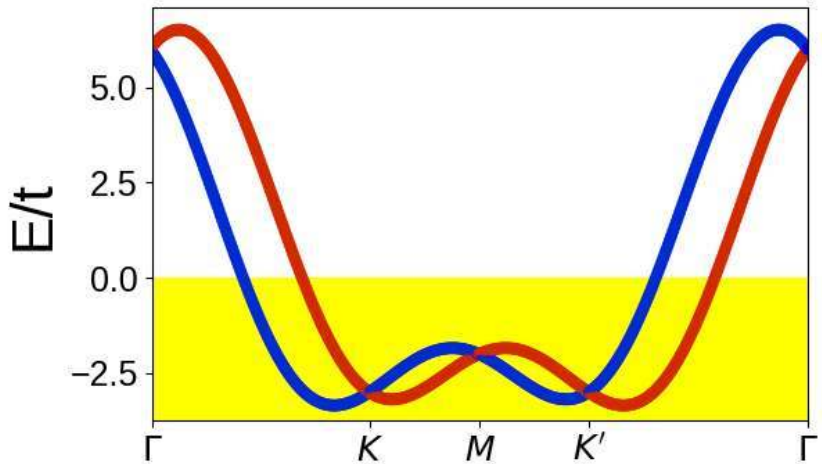
```
from pyqula import geometry
g = geometry.triangular_lattice() # get the geometry object
h = g.get_hamiltonian() # get the Hamiltonian object
h.add_exchange([0.,0.,0.5]) # add exchange field
(k,e,c) = h.get_bands(operator="sz") # compute the band structure
```



Triangular lattice with Rashba spin-orbit coupling

$$H = t\sum_{\langle ij\rangle} c^{\dagger}_{i,s}c_{j,s} + i\lambda_R \sum_{\langle ij\rangle}[(\mathbf{r}_i - \mathbf{r}_j)\times\sigma^{s,s'}]\cdot\hat{z}c^{\dagger}_{i,s}c_{j,s}$$

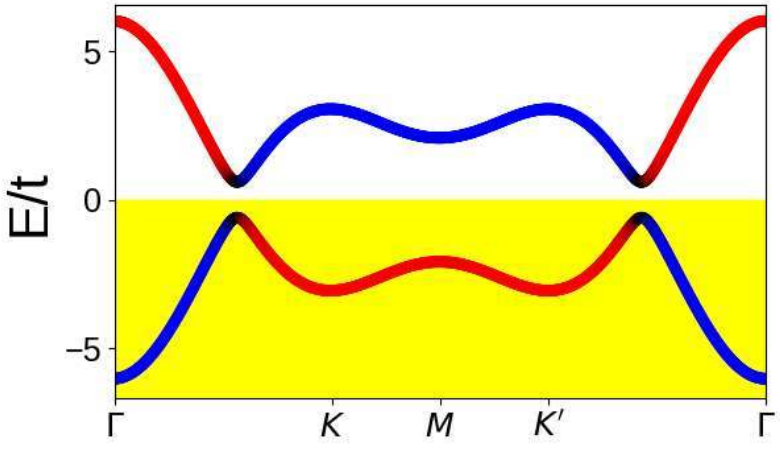
```
from pyqula import geometry
g = geometry.triangular_lattice() # get the geometry object
h = g.get_hamiltonian() # get the Hamiltonian object
h.add_rashba(0.6) # add Rashba SOC
(k,e,c) = h.get_bands(operator="sx") # compute the band structure
```



Triangular lattice with superconductivity

$$H = t \sum_{\langle ij \rangle} c^\dagger_{i,s} c_{j,s} + \Delta \sum_i c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} + h.c.$$

```
from pyqula import geometry
g = geometry.triangular_lattice() # get the geometry object
h = g.get_hamiltonian() # get the Hamiltonian object
h.add_swave(0.6) # add superconductivity
(k,e,c) = h.get_bands(operator="electron") # compute the band structure
```



For the exercise session this afternoon

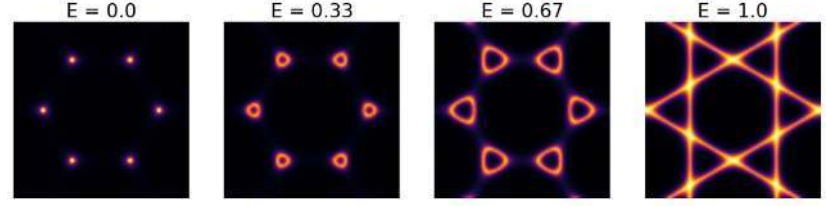
Download the Jupyter-notebook from

https://github.com/joselado/jyvaskyla_summer_school_2022/blob/main/sessions/session1.ipynb

The tasks during the exercise sessions

You will see examples with the code

```
from pyqula import geometry
g = geometry.honeycomb_lattice() # generate a honeycomb lattice
h = g.get_hamiltonian() # generate the Hamiltonian
delta = 0.1 ; nk = 80 # smearing and kmesh
energies = np.linspace(0.,1.,4) # energies
ip = 1 # counter for the plot
for e in energies:
    (x,y,d) = h.get_fermi_surface(e=e,delta=delta,nk=nk) # compute Fermi surface
    plt.subplot(1,len(energies),ip) ; ip += 1 # set subplot
    d2d = d.reshape((nk,nk)) ; plt.imshow(d2d,vmin=0.,vmax=2./delta,cmap="inferno",interpolation="bicubic")
    plt.title("E = "+str(np.round(e,2))) ; plt.axis("off")
```



You have to modify them, and answer questions

Exercise

- Identify at which energy the van Hove singularity appears
- Compute the Fermi surface at higher energies. How many pockets do you have after you pass the van Hove singularity?