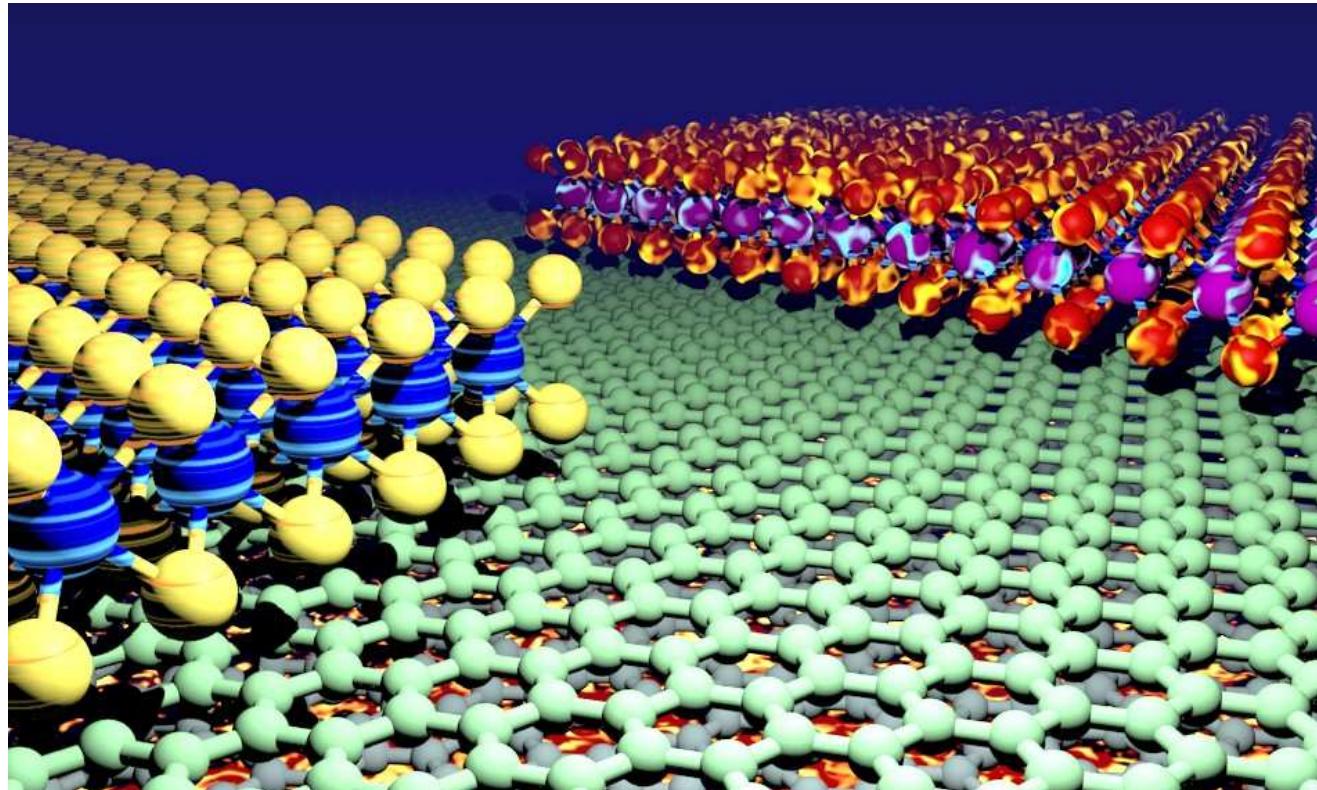


# Lecture 1: An introduction to 2D materials



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

January 7<sup>th</sup> 2023, Tata Institute of Fundamental Research (TIFR), India



# Today's plan

- Families of 2D materials
- An introduction to the theory tools: electronic structure, second quantization and mean-field theory
- The tunability of 2D materials
- An introduction to computational tools

# Schedule for the lecture

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

*You can download the slides and software from*

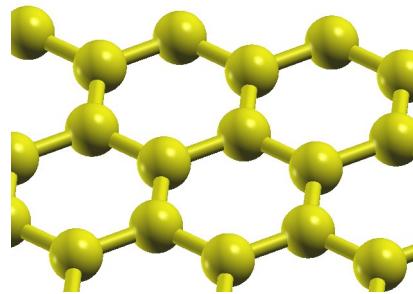


[https://github.com/joselado/emergent\\_phenomena\\_in\\_van\\_der\\_Waals\\_school\\_tifr\\_2023](https://github.com/joselado/emergent_phenomena_in_van_der_Waals_school_tifr_2023)

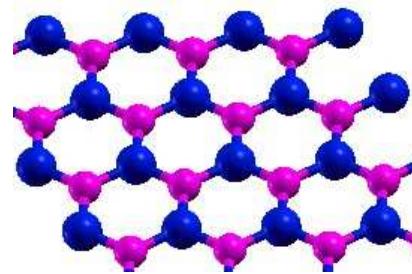
# The world of 2D materials

# The two-dimensional materials world

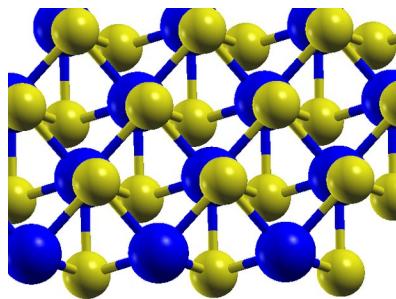
Semimetal  
Graphene



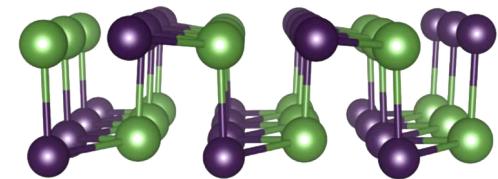
Insulator  
BN



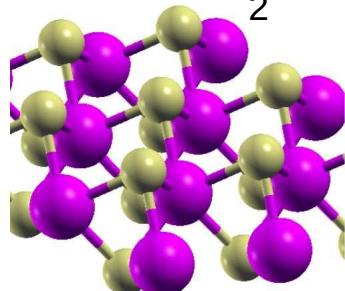
Superconductor  
 $\text{NbSe}_2$



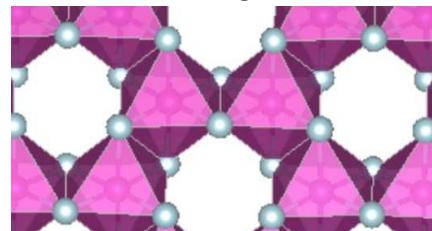
Ferroelectric  
 $\text{SnTe}$



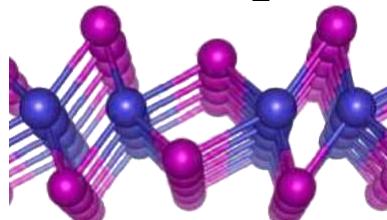
Semiconductor  
 $\text{WSe}_2$



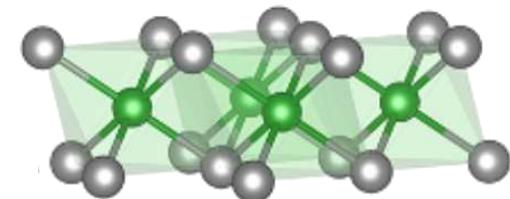
Ferromagnet  
 $\text{CrI}_3$



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

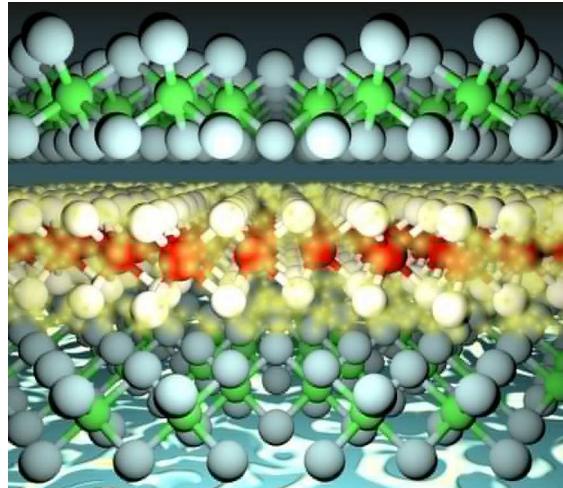


Multiferroic  
 $\text{NiI}_2$

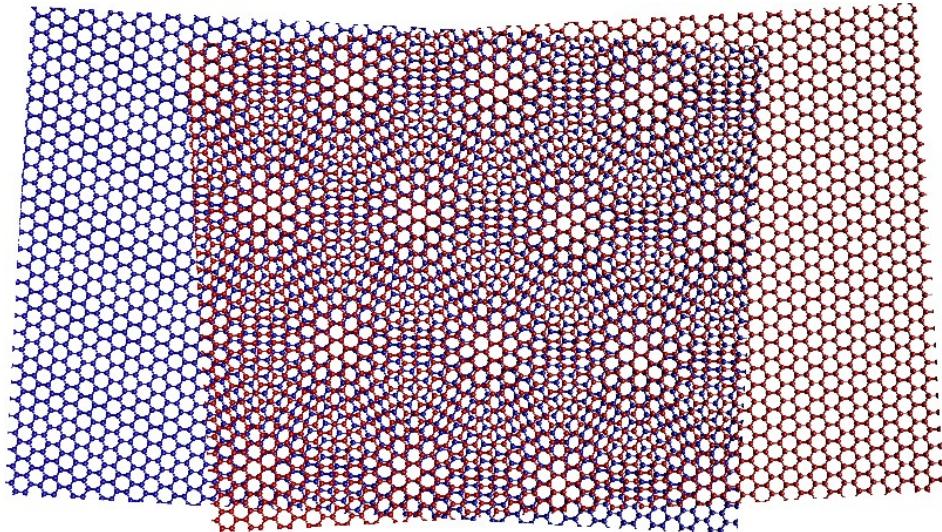


# The flexibility of two-dimensional materials

**They can be stacked**



**They can be rotated**

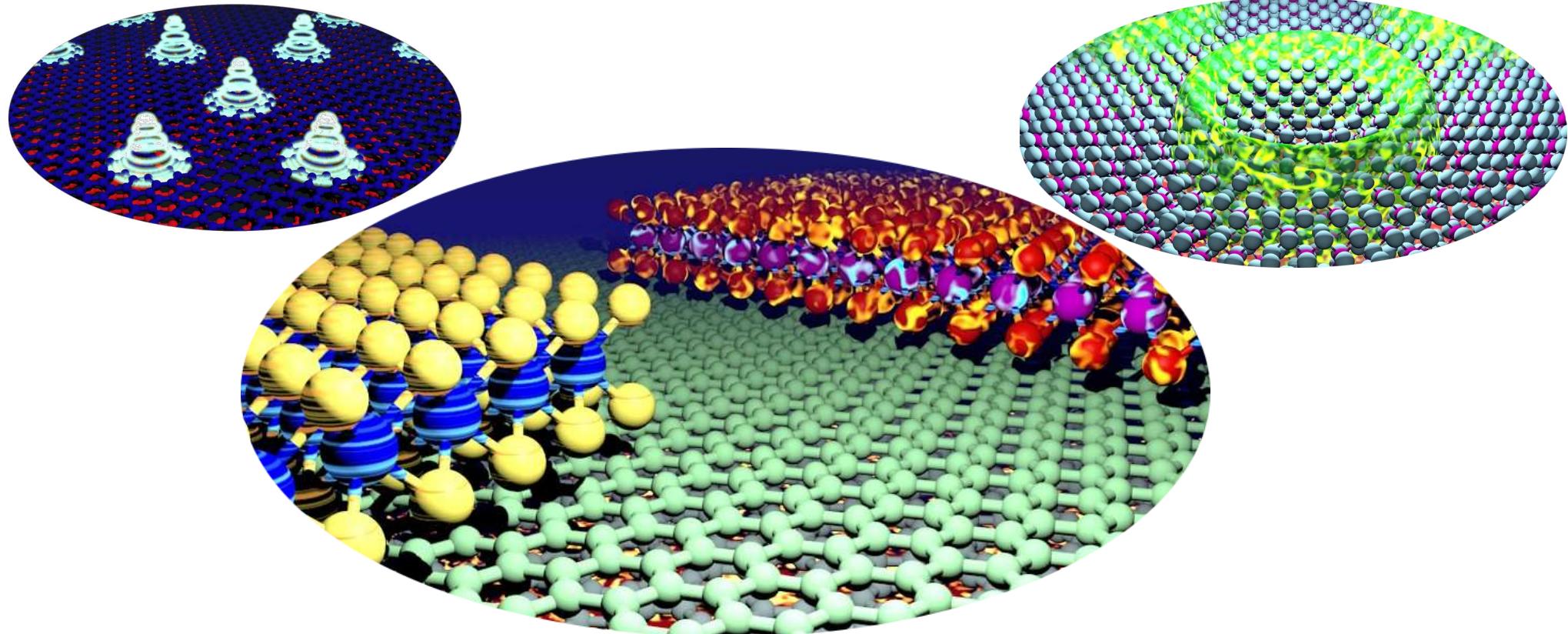


*Nature* 499.7459 419. (2013)

*Science* 361.6403 690-693. (2018)

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

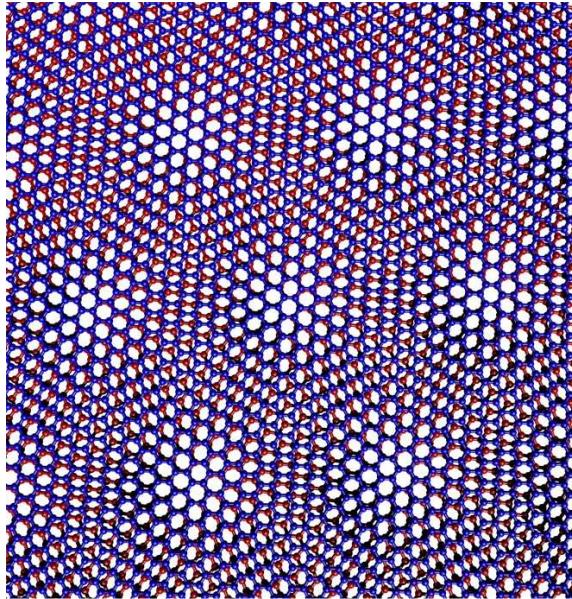
# A new universe in each van der Waals heterostructure



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

# One material, a zoo of electronic phases

## Twisted bilayer graphene

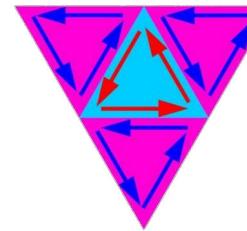


## Superconductivity



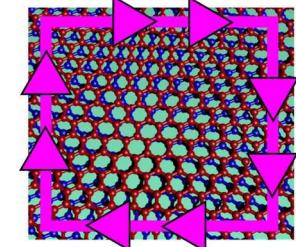
Nature 556, 43–50 (2018)

## Topological networks



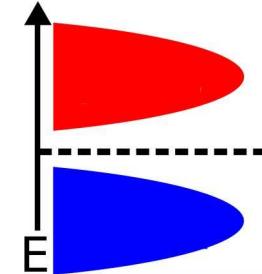
Nano Lett. 18, 11,  
6725-6730 (2018)

## Chern insulators



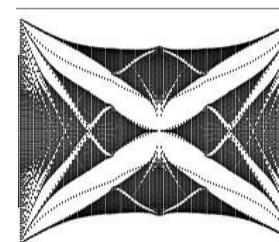
Science 365, 605-608  
(2019)

## Correlated insulators



Nature 556, 80–84  
(2018)

## Quasicrystalline physics



Science 361, 782-786 (2018)

## Fractional Chern insulators



Nature 600, 439–443  
(2021)

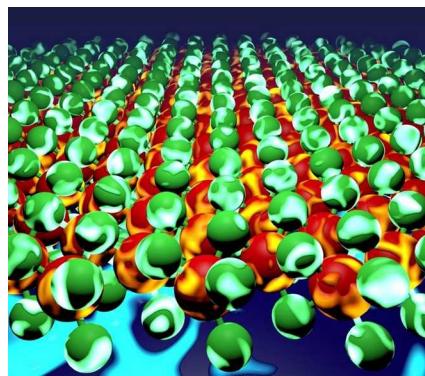
A bilayer of a van der Waals material realizes a variety of widely different electronic states

# Controlling electronic states in van der Waals materials

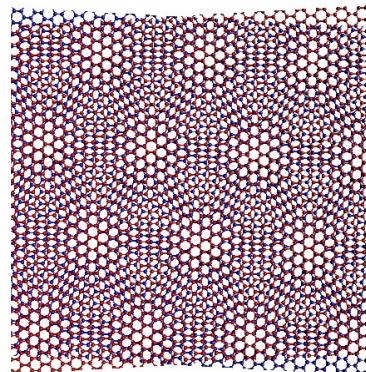
*Of course, we can use the typical knobs of bulk compounds  
(pressure, chemical doping, etc)*

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

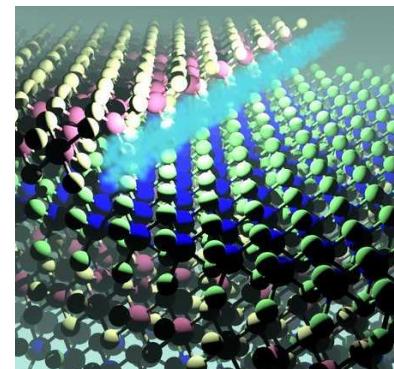
Gating



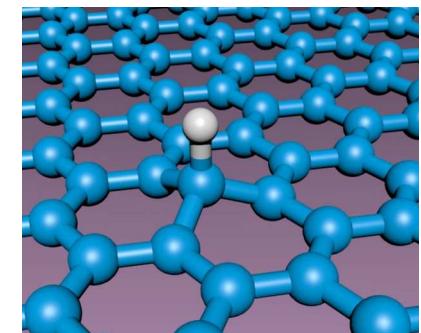
Twist engineering



Materials engineering



Atomic engineering



Science 306, 5696, 666-669 (2004)

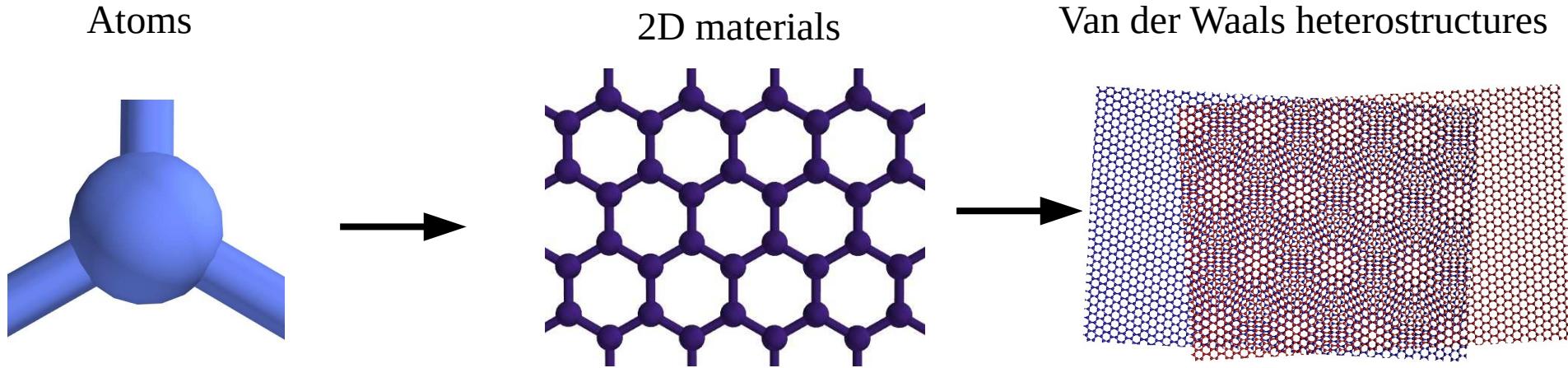
Nat, Rev, Mat, 6, 201–206 (2021)

Nature 499, 419–425 (2013)

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

*Allowing to independently control different features of the electronic structure*

# From atoms to quantum matter



***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

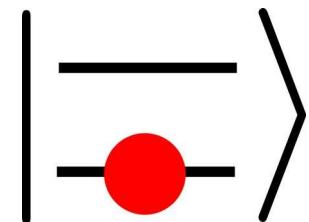
# Two different kinds of quantum mechanical formalism

**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

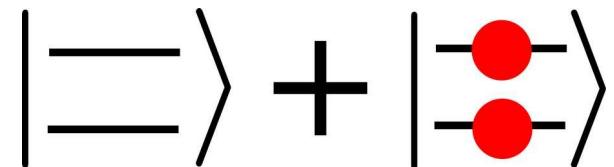


**Systems where the number of particles fluctuates**

Second quantization, description based on a Fock space

Describes superconductors, superfluids, correlated matter

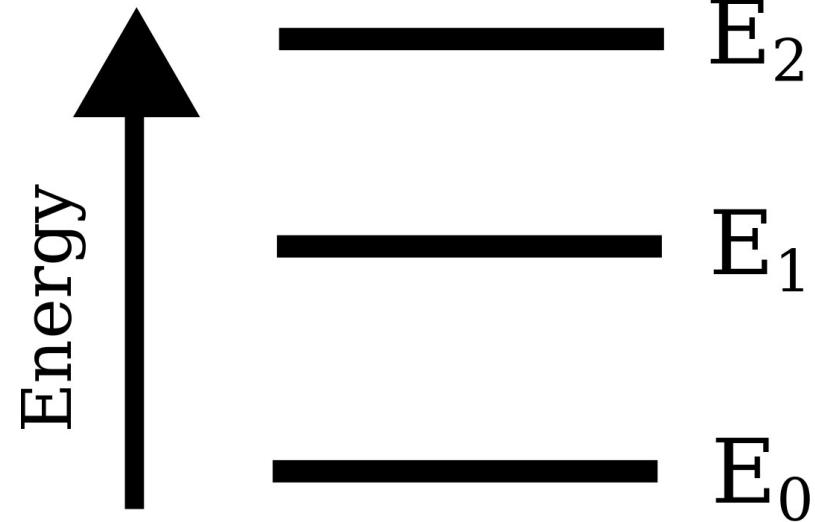
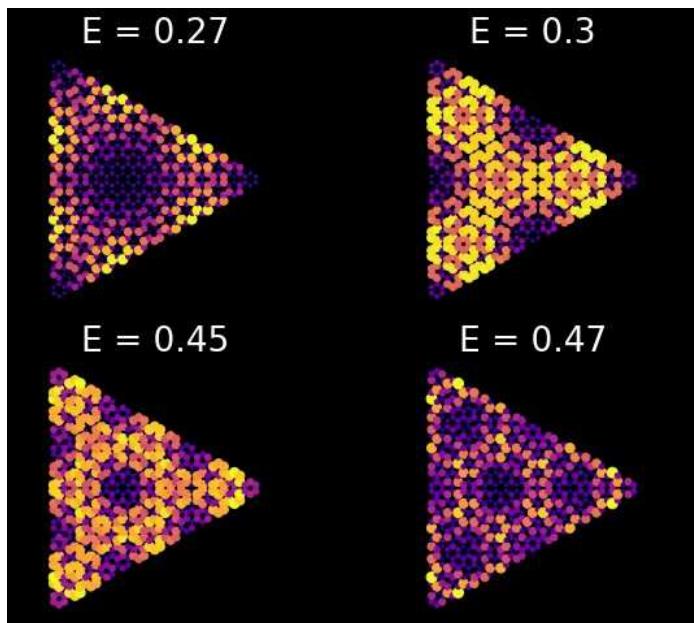
Leads to much exotic phenomena, yet also more challenging



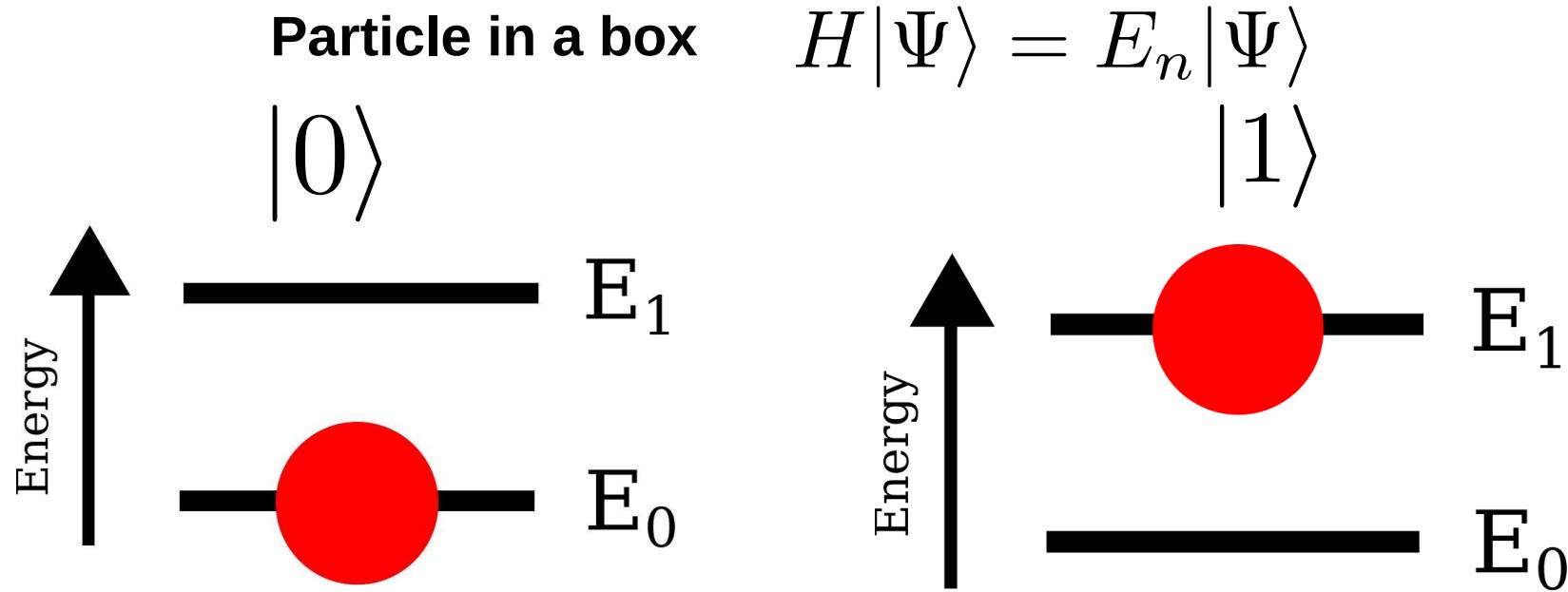
# A reminder of a simple single particle state

Particle in a box

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



# A reminder of a simple single particle state

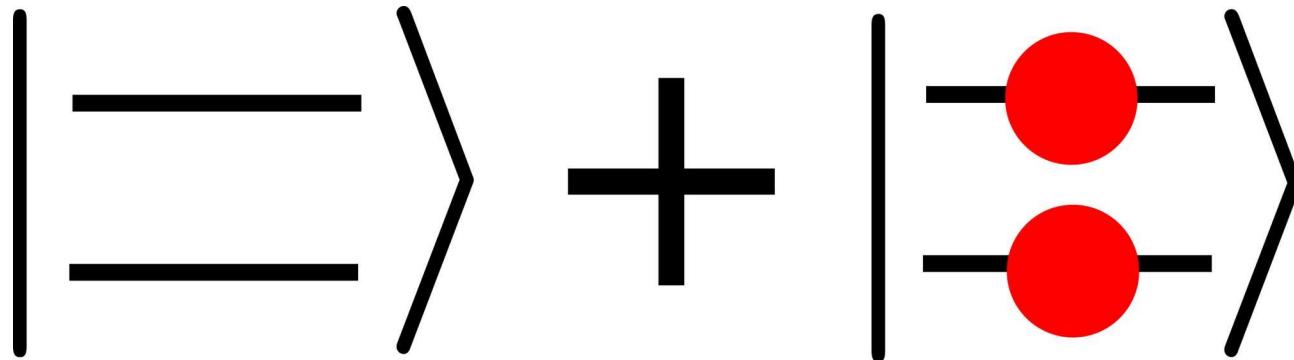


*These two states describe having one particle, in one of the possible energy level*

# 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?**

# 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

$$H = c_0^\dagger c_1 + h.c.$$

# The idea of second quantization

Lets see some examples using the two-levels presented before

$$|\Omega\rangle = \left| \begin{array}{c} \text{---} \\ \text{---} \end{array} \right\rangle$$

The “vacuum” state

$$c_0^\dagger |\Omega\rangle = \left| \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \right\rangle$$

One particle in level #0

$$c_1^\dagger |\Omega\rangle = \left| \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \right\rangle$$

One particle in level #1

$$c_0^\dagger c_1^\dagger |\Omega\rangle = \left| \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \right\rangle$$

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

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

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

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j$$

*Insulators, semiconductors, metals*

Many-body Hamiltonian

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

*Fractional quantum Hall states, superconductors, quantum magnets*

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



# What about interactions?

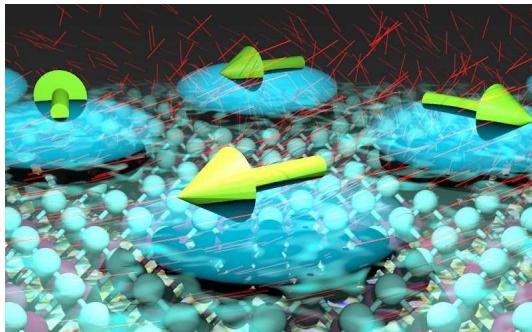
**What happens when we put interactions?**

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

# The role of electronic interactions

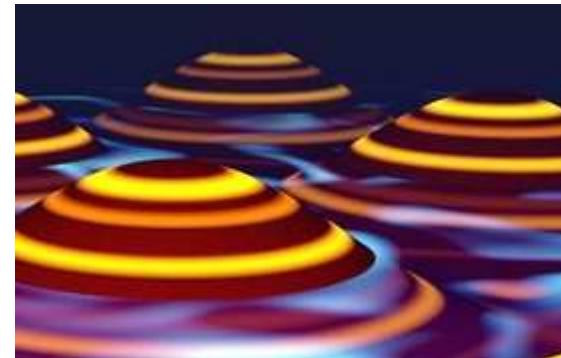
Electronic interactions are responsible for symmetry breaking

**Broken  
time-reversal symmetry**  
*Classical magnets*



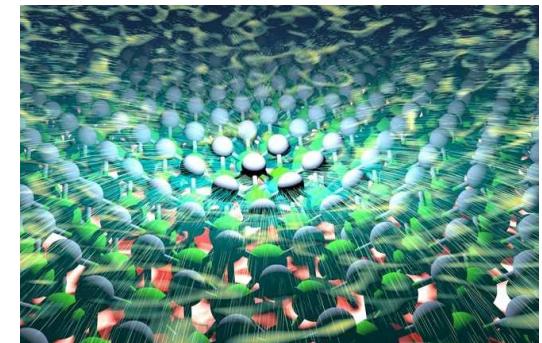
$$\mathbf{M} \rightarrow -\mathbf{M}$$

**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)*

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

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)*

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

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

For  $U < 0$   
i.e. attractive interactions

$\Delta \sim \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle$  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)**

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

**Two fermions  
(exactly solvable)**

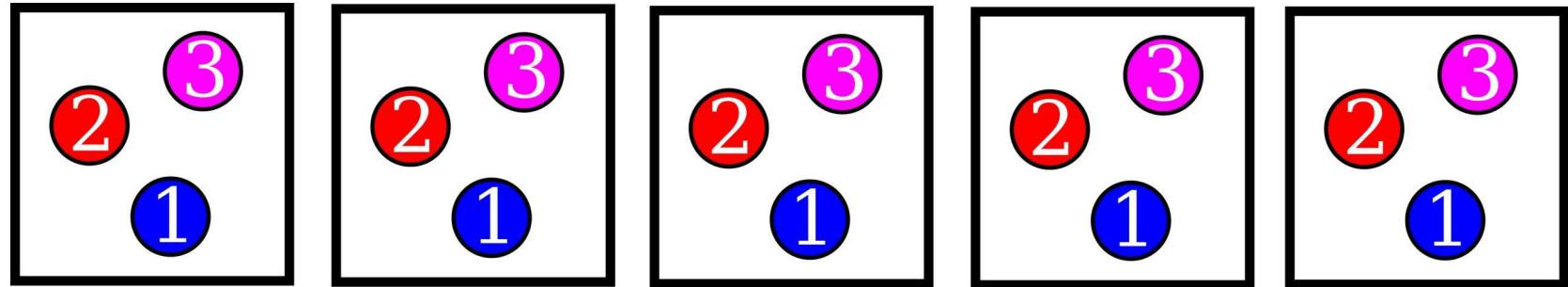
$$U c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \approx M \sigma_{ss'}^z c_{i,s}^\dagger c_{i,s'} + h.c.$$

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

Magnetic order

$$M \sim \langle c_{i\uparrow}^\dagger c_{i\uparrow} \rangle - \langle c_{i\downarrow}^\dagger c_{i\downarrow} \rangle$$

# Electronic band-structures

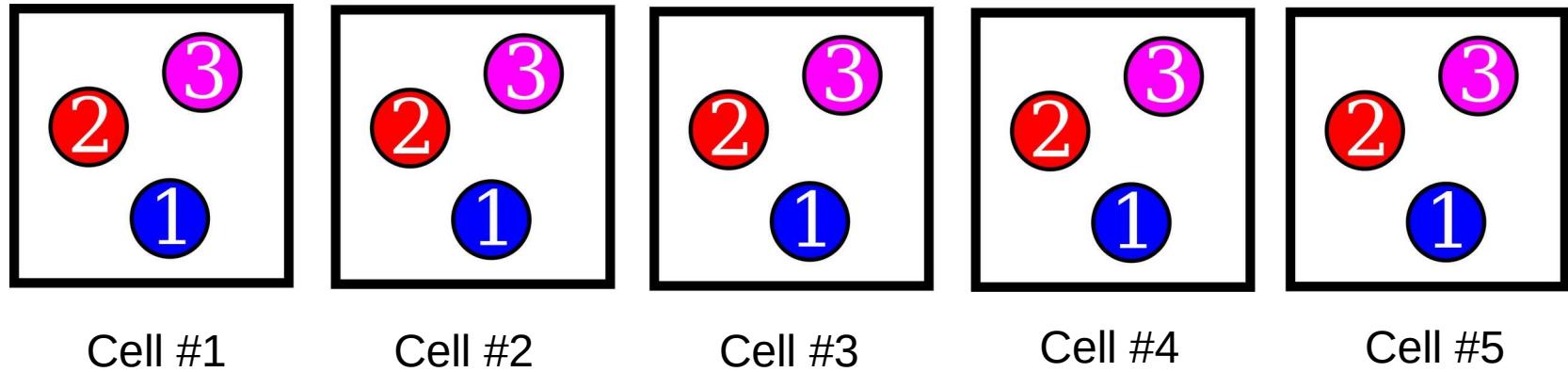


$$c_{\alpha,n}^\dagger$$

index of the orbital in the unit cell

Index of the unit cell

# Electronic band-structures



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

Intra-cell hoppings      Inter-cell hoppings

# Electronic band-structures

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

**Unitary transformation**

$$\Psi_{\phi,\alpha}^\dagger \sim \sum_{n,\beta} e^{i\phi n} U_{\alpha\beta} c_{n,\beta}^\dagger \quad H = \sum_{\phi,\alpha} \epsilon_{\phi,\alpha} \Psi_{\phi,\alpha}^\dagger \Psi_{\phi,\alpha}$$

$\epsilon_{\phi,\alpha}$  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**

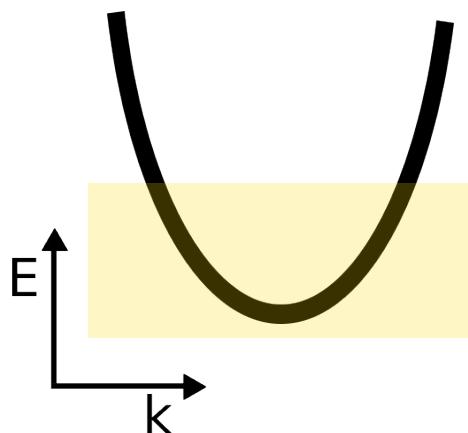
$$\frac{1}{m_{\alpha\beta}} = \frac{\partial^2 \epsilon_{\vec{k}}}{\partial k_\alpha \partial k_\beta}$$

**Fermi surface**

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

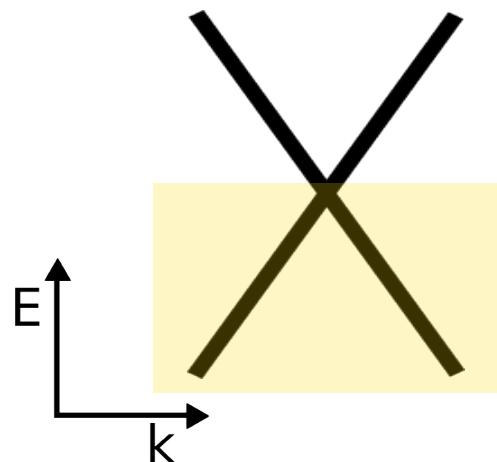
# Three important electronic dispersions

Parabolic bands



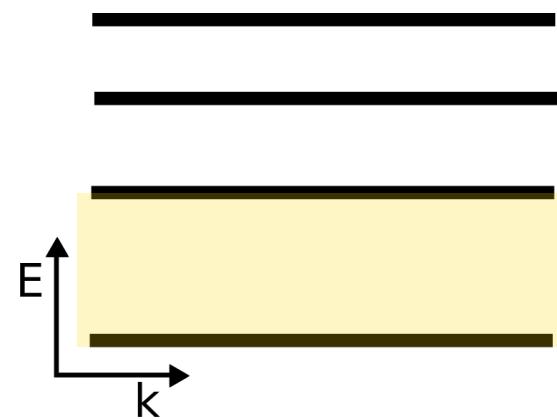
TMDCs  
*Effective free-electrons*

Dirac dispersion



graphene  
*Topology & relativistic physics*

Flat bands



Quantum Hall, moire  
*Topology & correlations*



# Break

5 min break

*(optional) to discuss during the break*

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

$$c_{n,\uparrow}^\dagger c_{n,\downarrow}$$

$$c_{n,\uparrow}^\dagger c_{n+1,\downarrow}$$

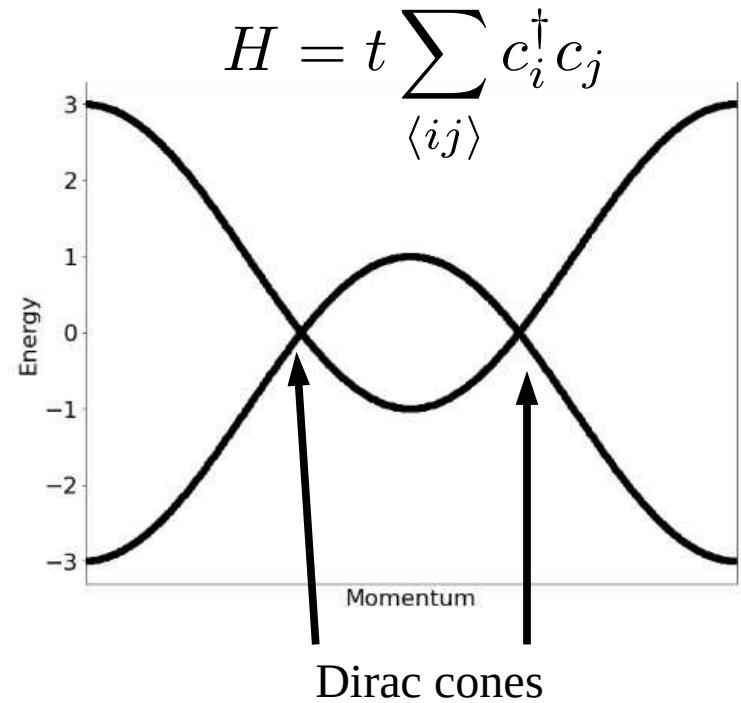
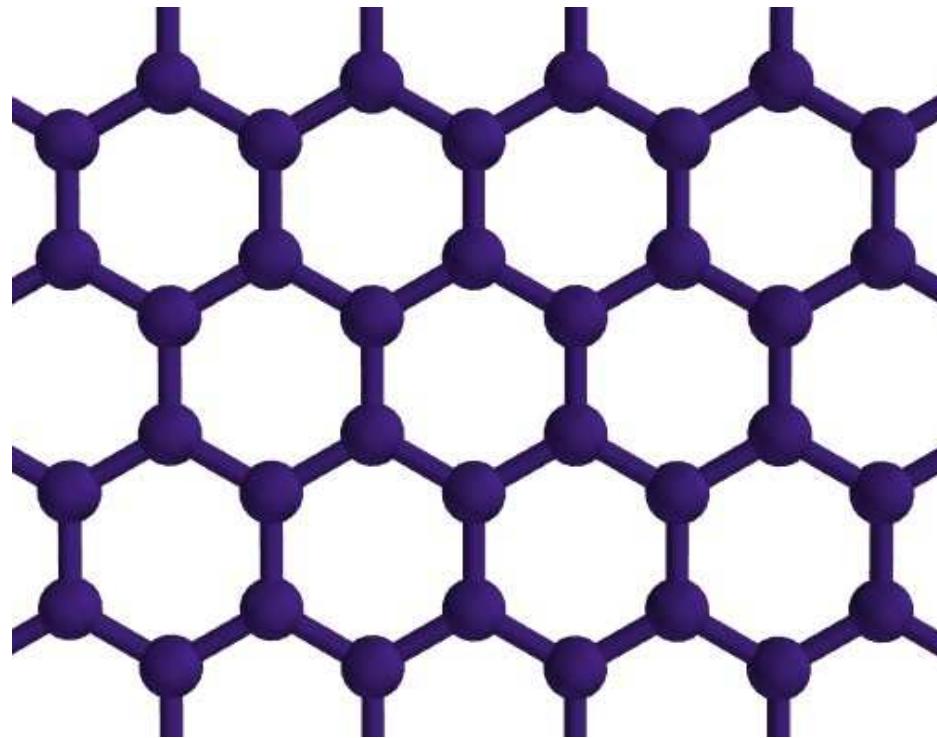
$$c_{n,\uparrow}^\dagger c_{n+1,\uparrow}^\dagger$$

and which symmetries do they break?

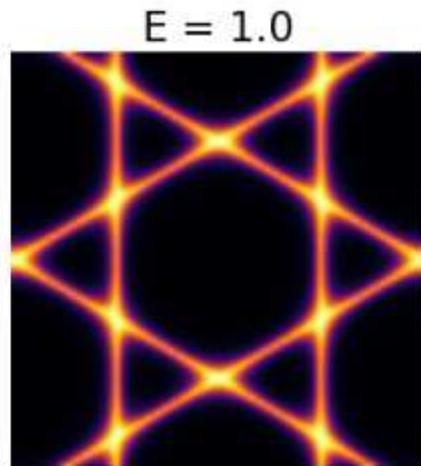
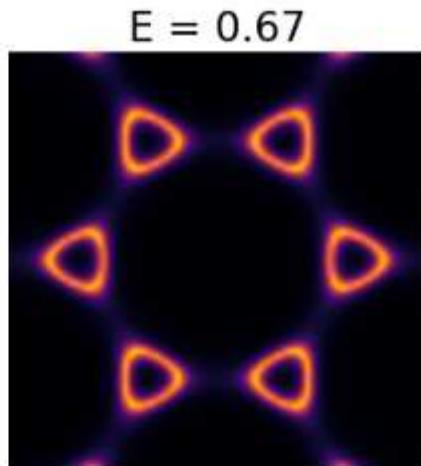
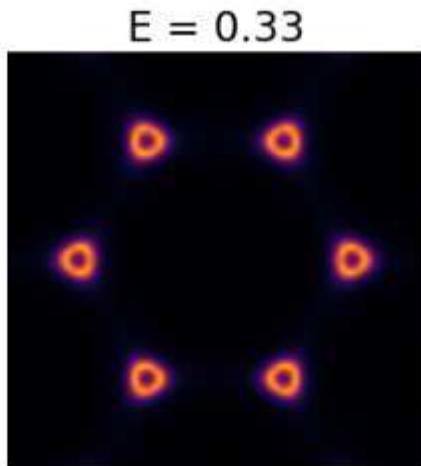
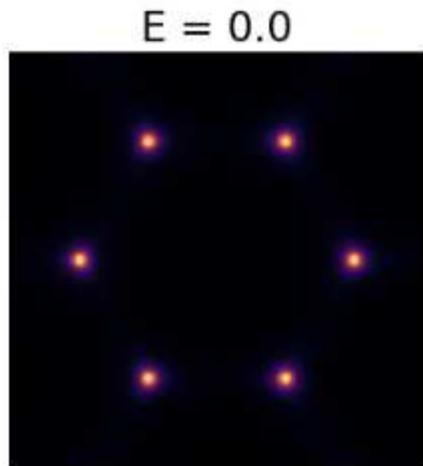
# Graphene and its electronic structure

# Electronic structure of monolayer graphene

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

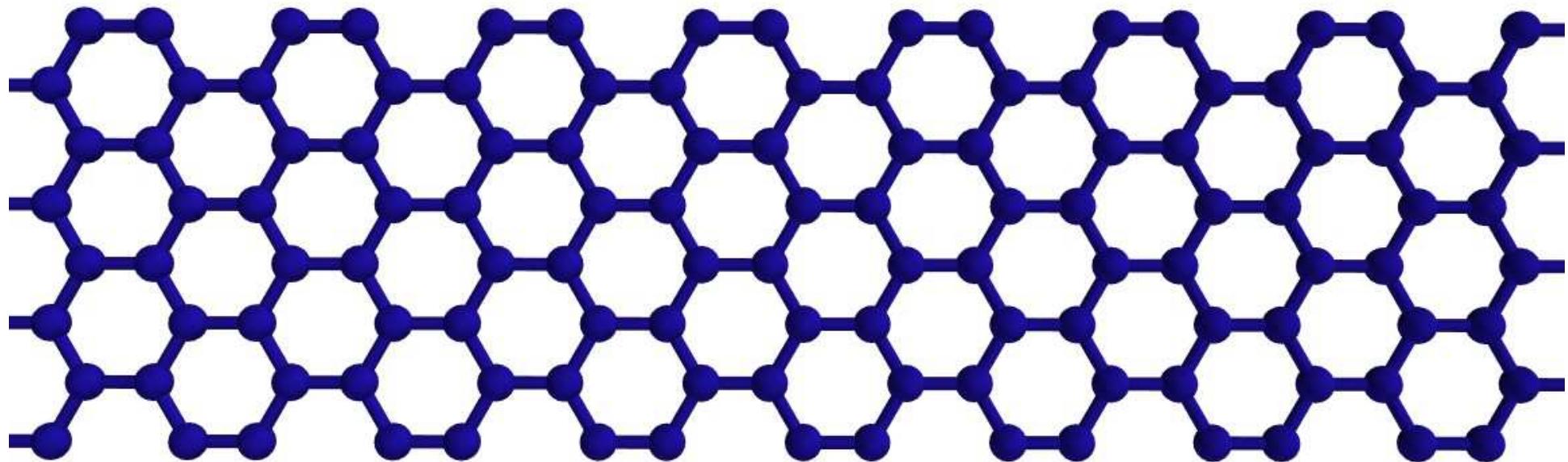


# Fermi surface of graphene



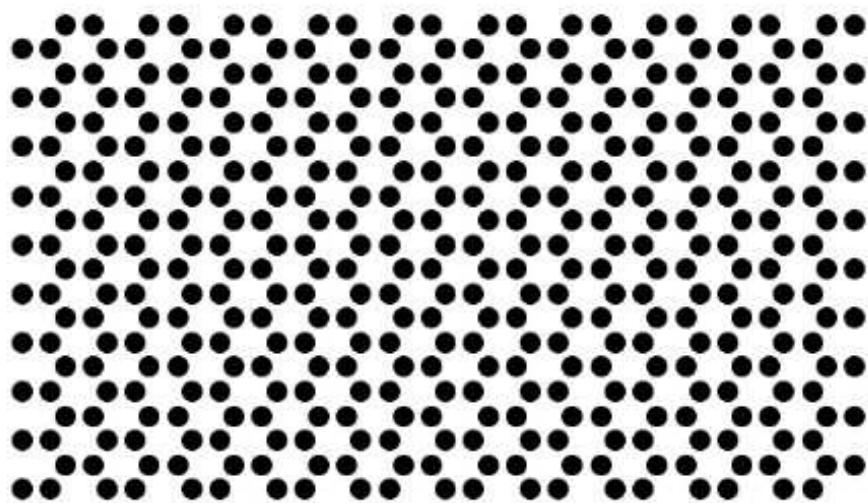
# Confining two-dimensional materials, graphene nanoribbons

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



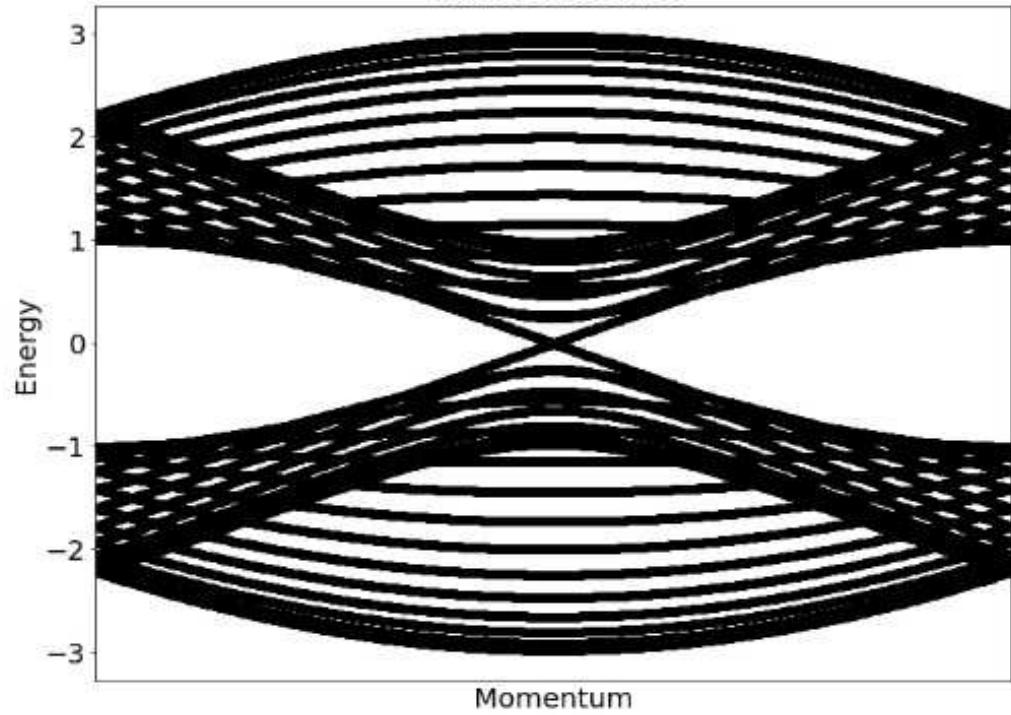
# Graphene nanoribbons

Structure



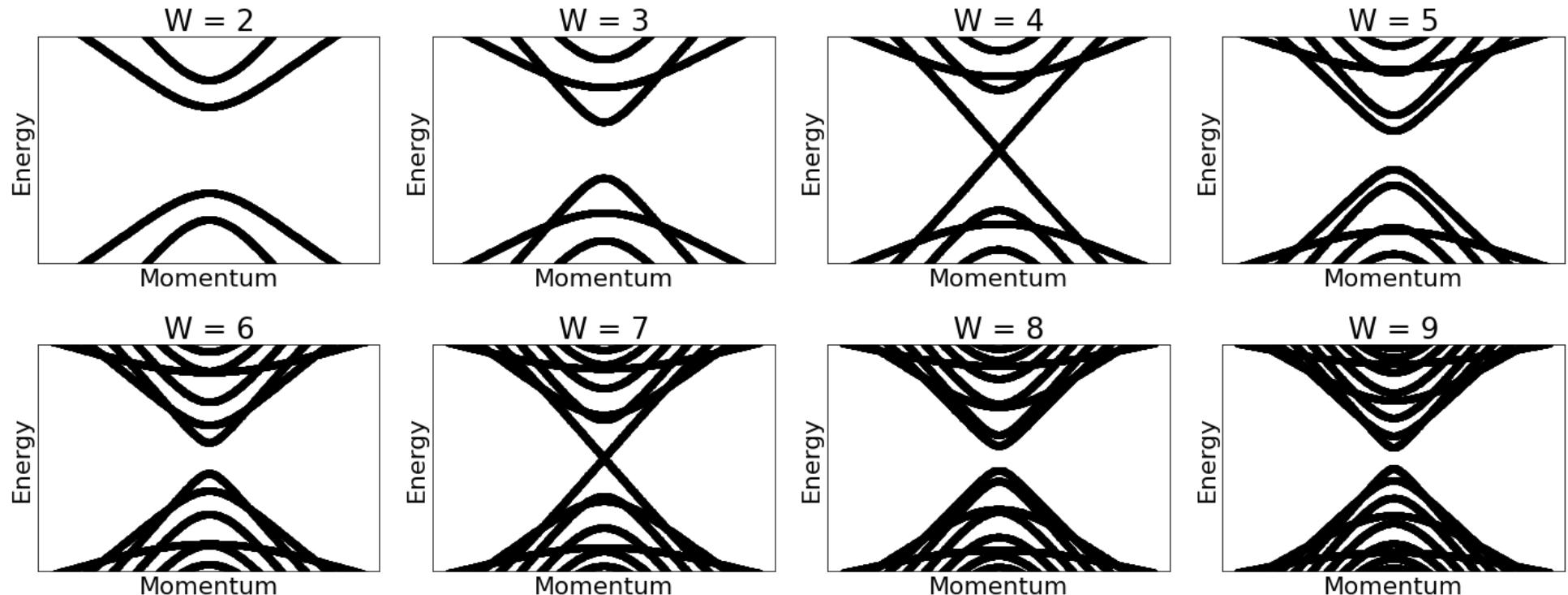
$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j$$

Band structure



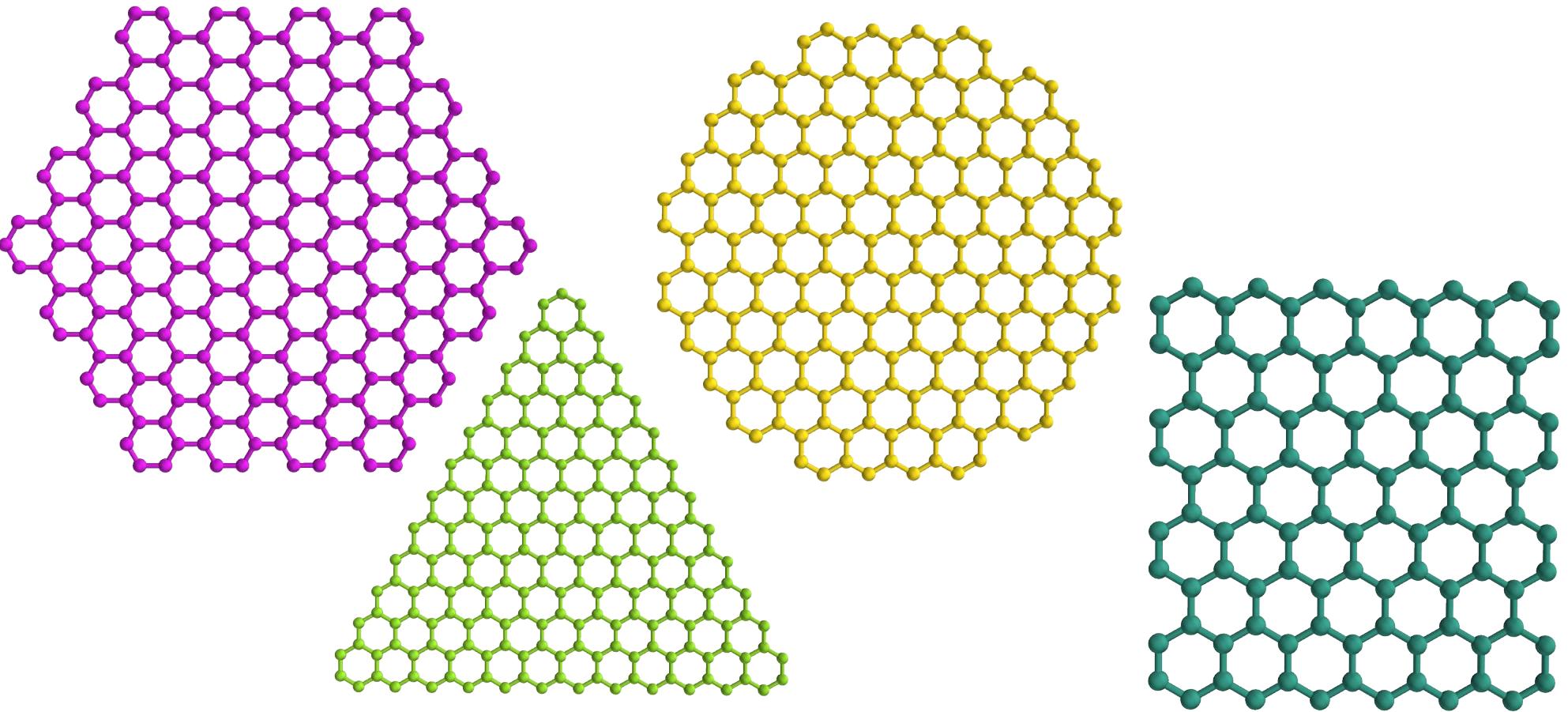
# Electronic structure of graphene armchair nanoribbons

The width of a graphene nanoribbon drastically controls its electronic properties

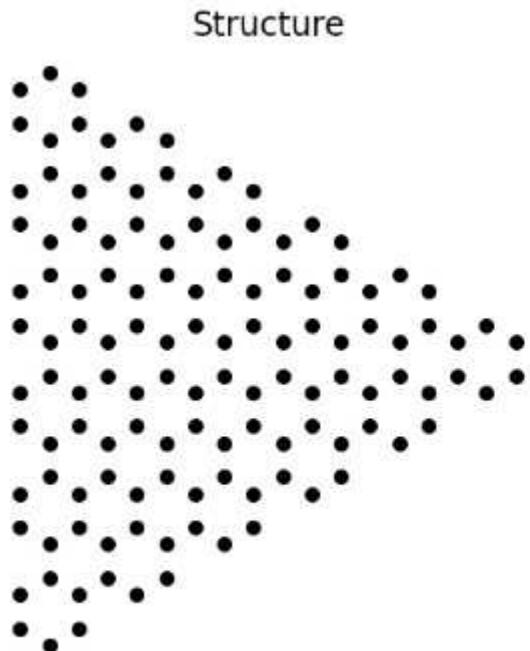


# Quantum dots of 2D materials

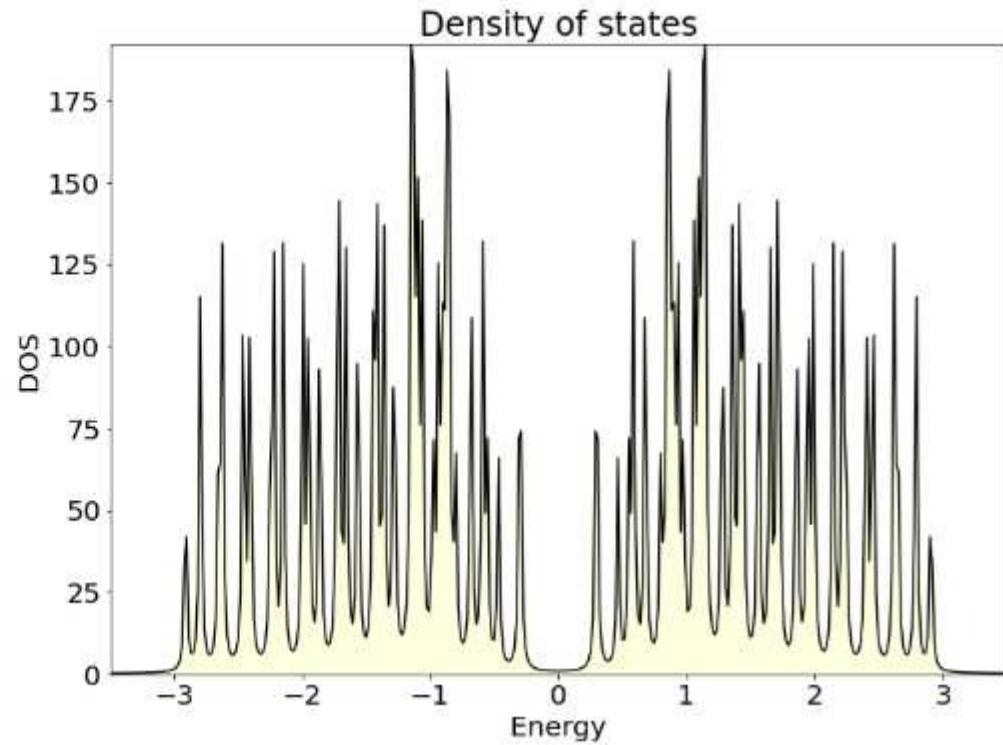
# Graphene quantum dots



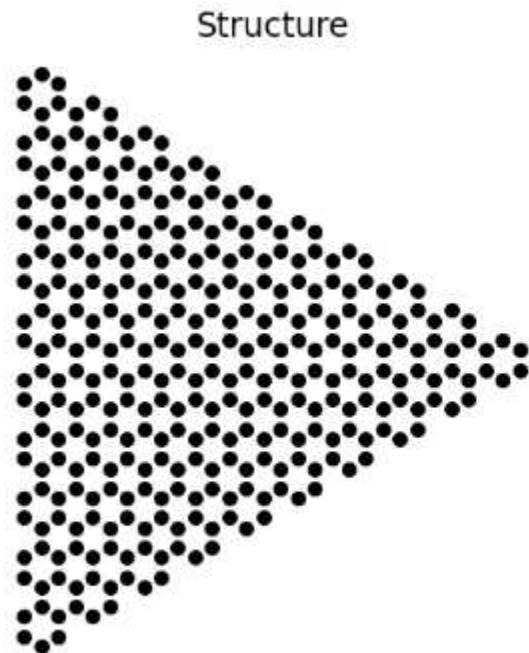
# Electronic structure of graphene armchair nanoislands



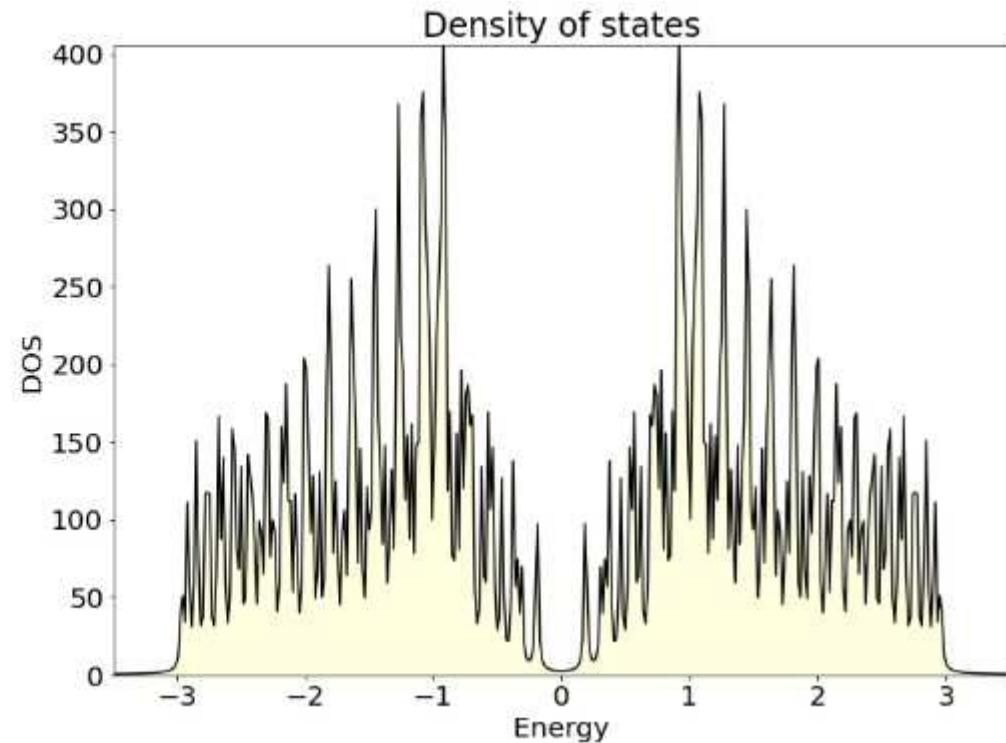
$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j$$



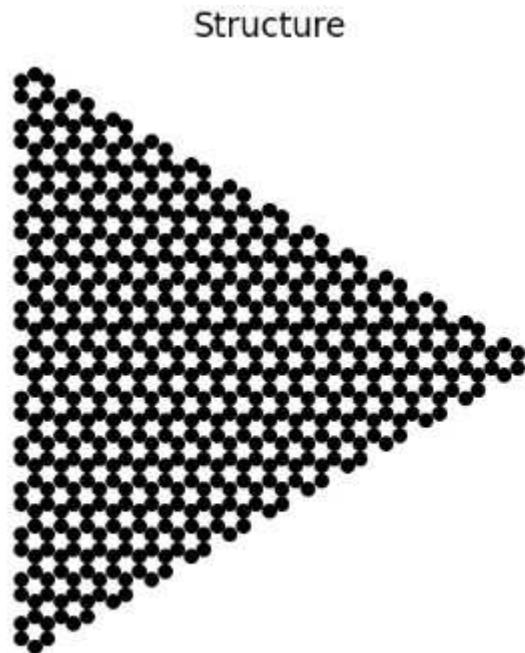
# Electronic structure of graphene armchair nanoislands



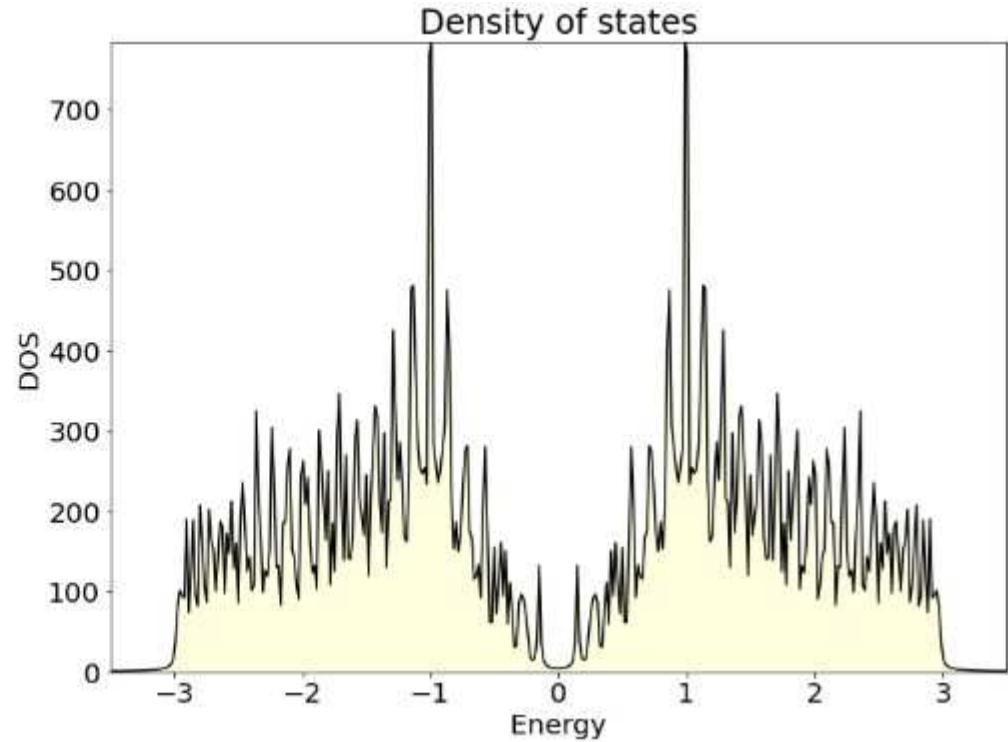
$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j$$



# Electronic structure of graphene armchair nanoislands

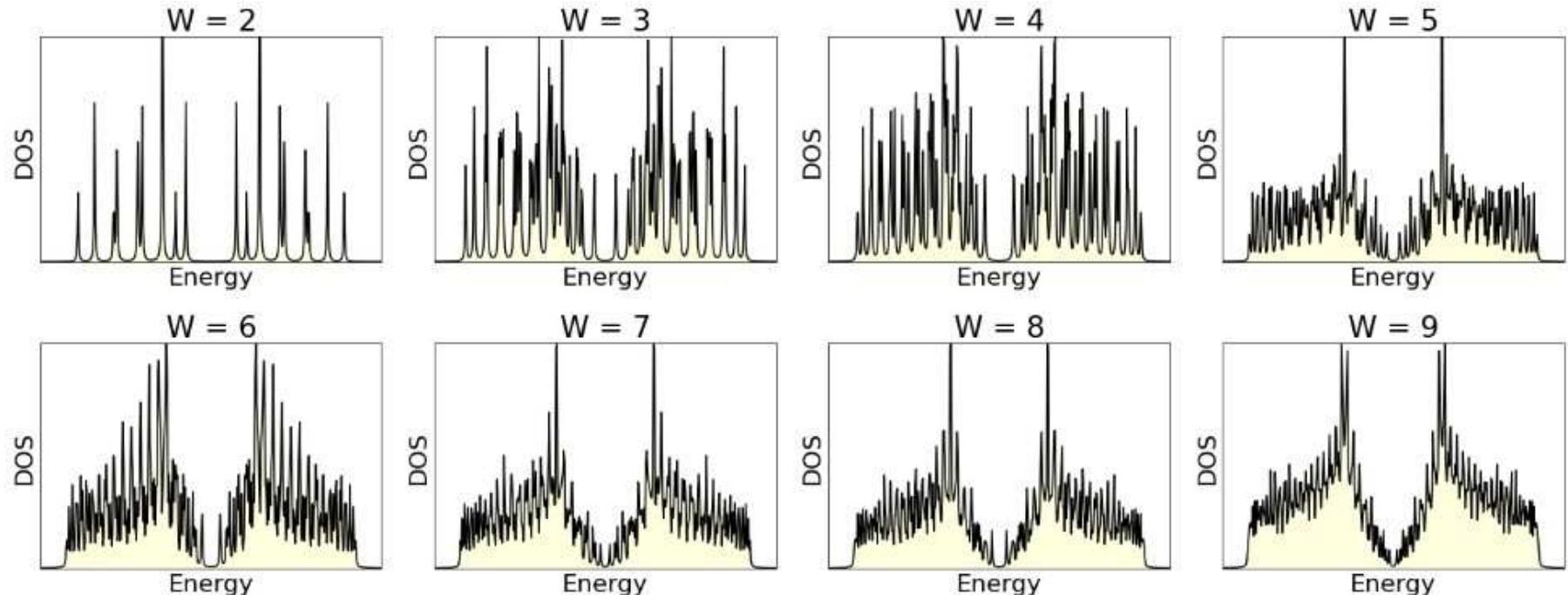


$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j$$

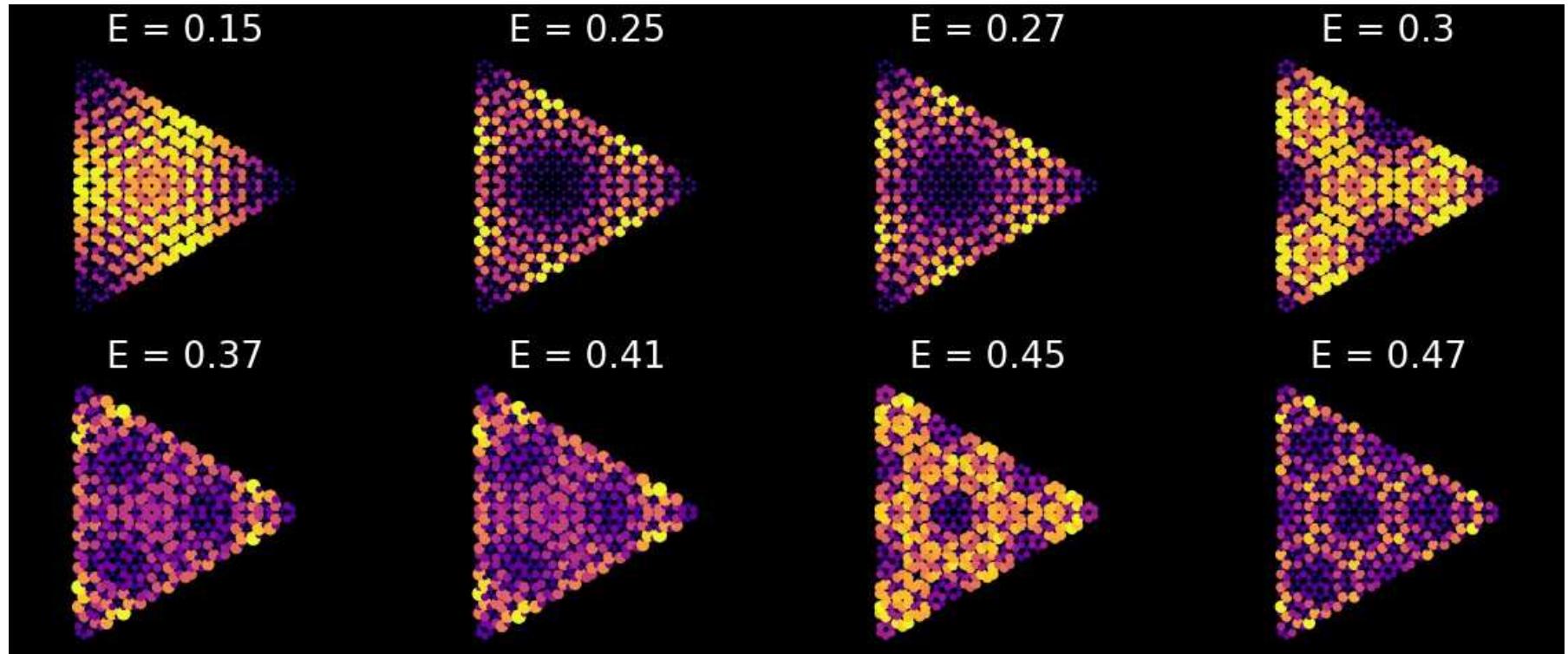


# Graphene islands of different widths

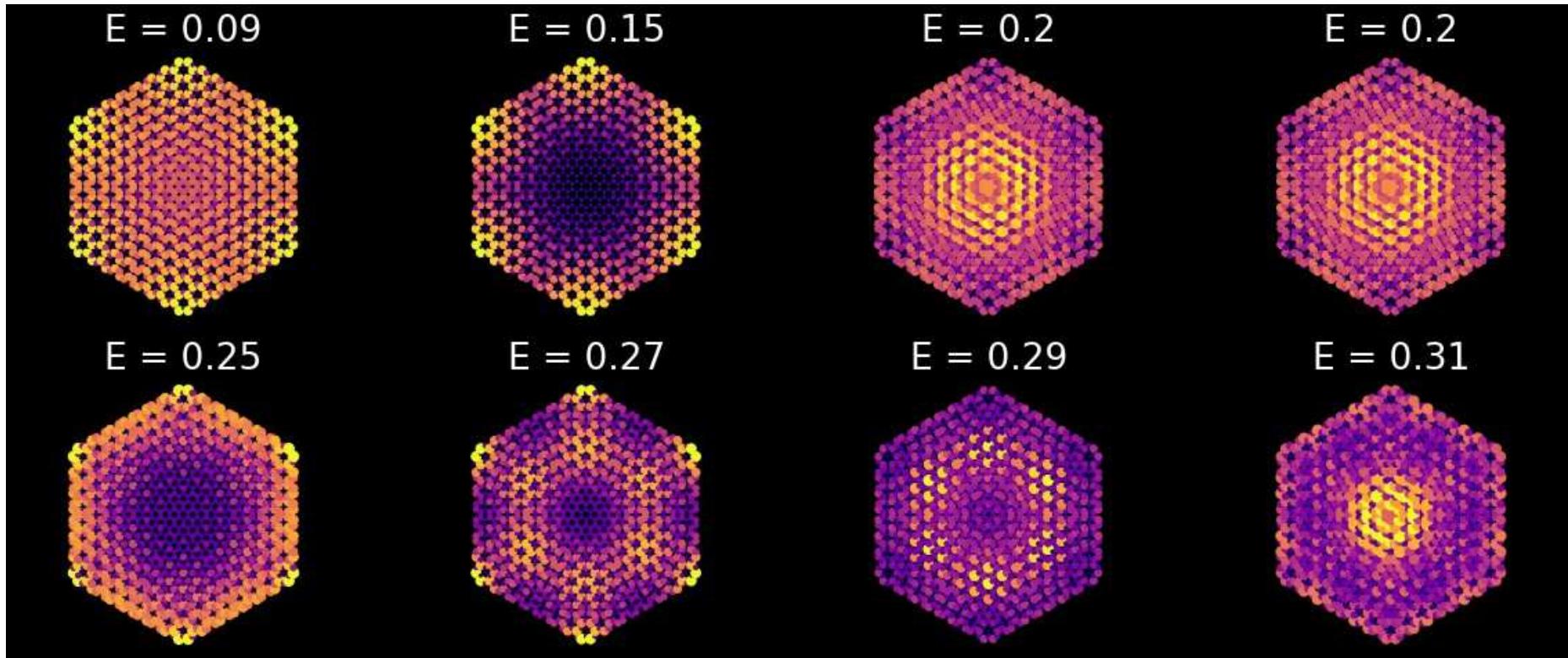
As the island becomes bigger, the spectrum of graphene is recovered



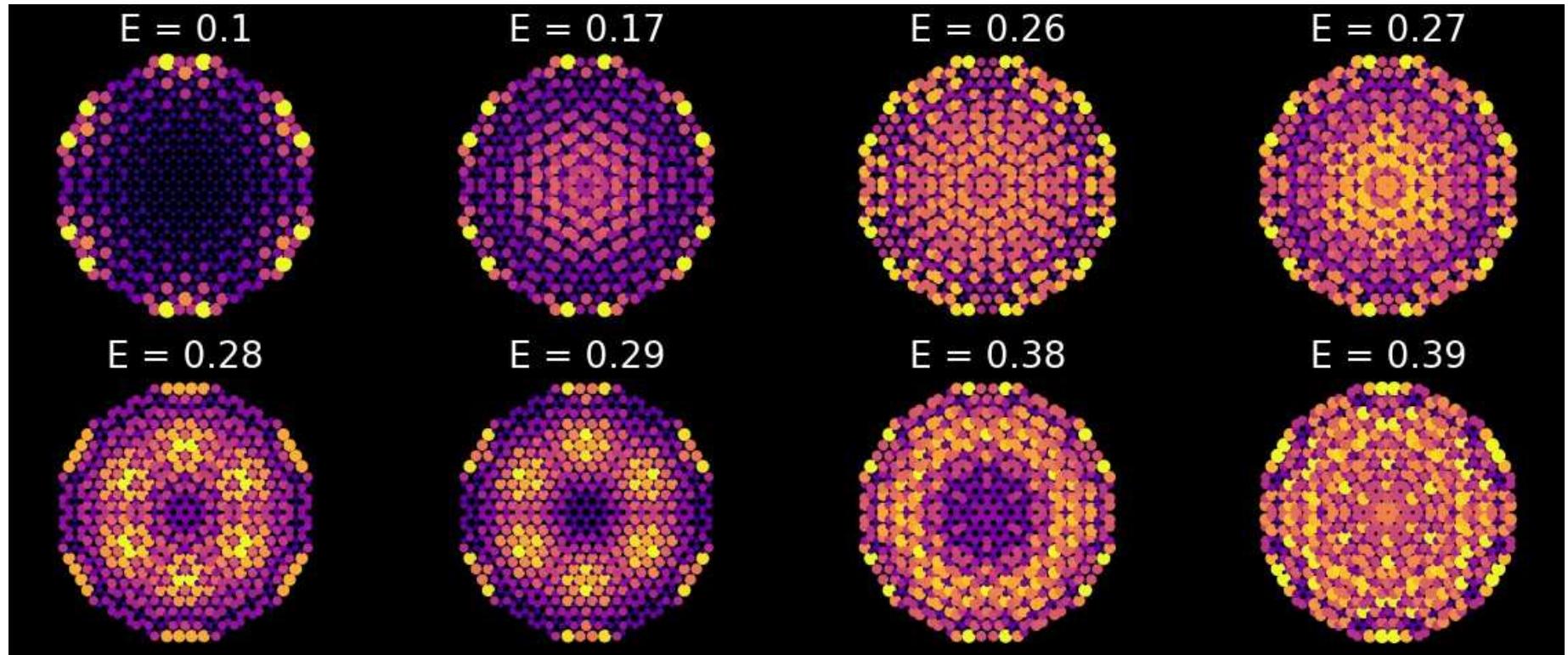
# Confined modes in graphene islands



# Confined modes in graphene islands



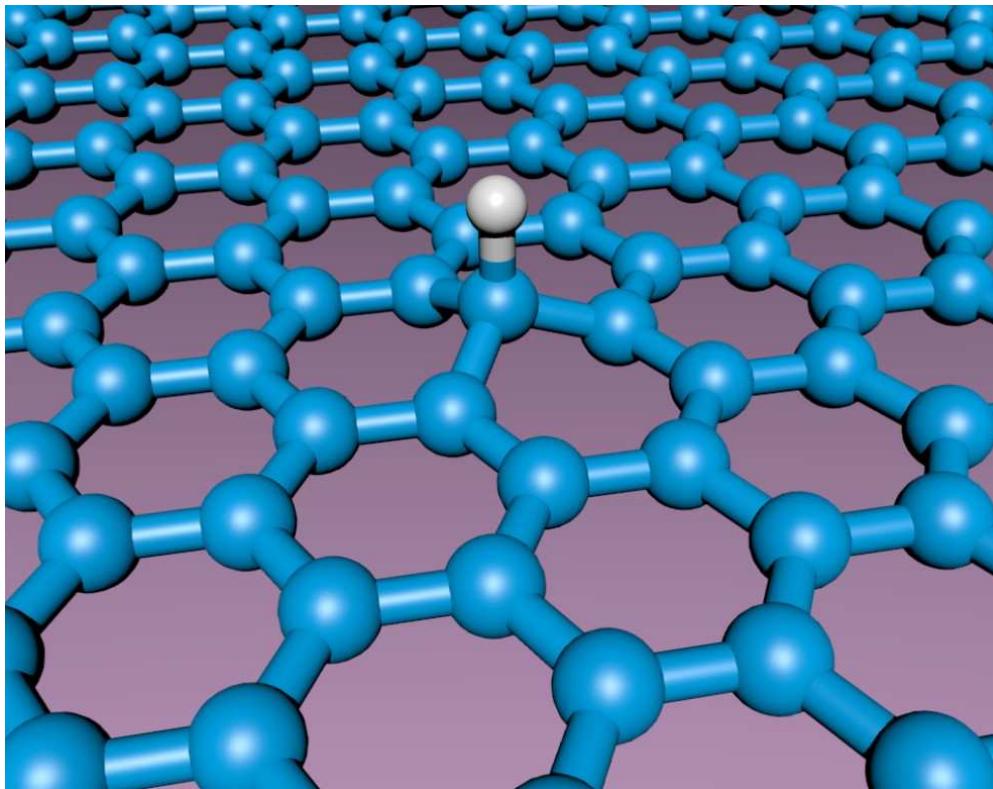
# Confined modes in graphene islands



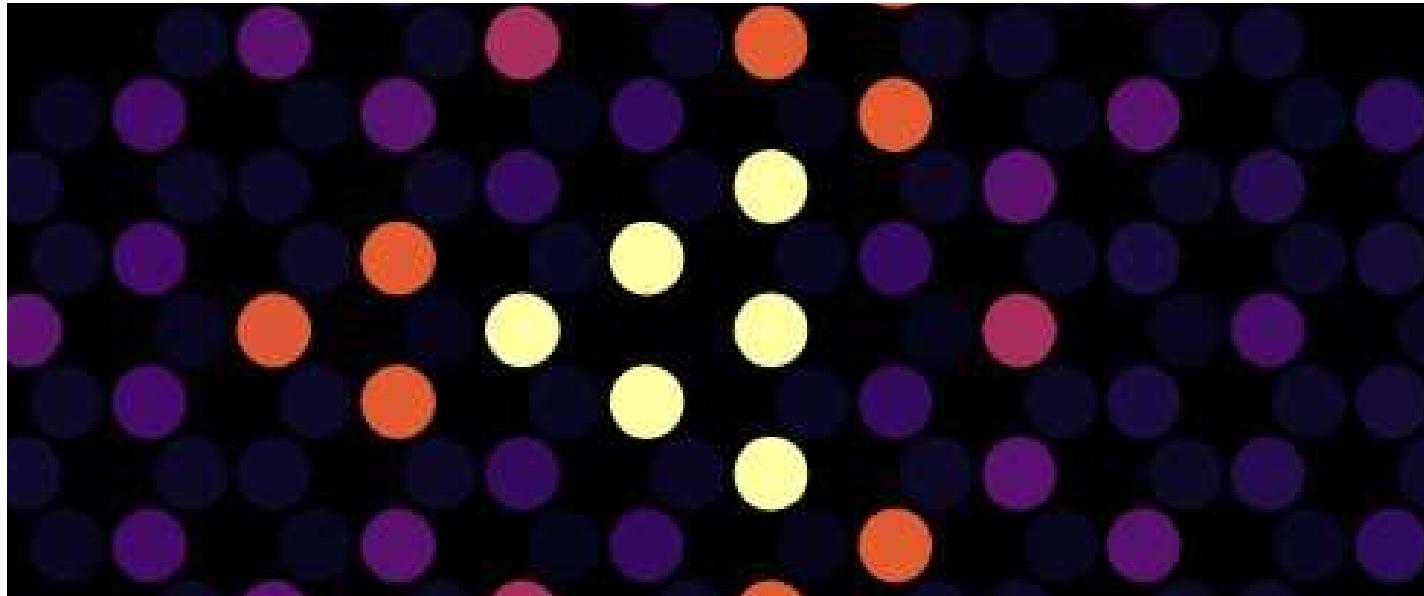
# Defects in 2D materials

# Impurities in monolayer graphene

Hydrogen adsorption in graphene



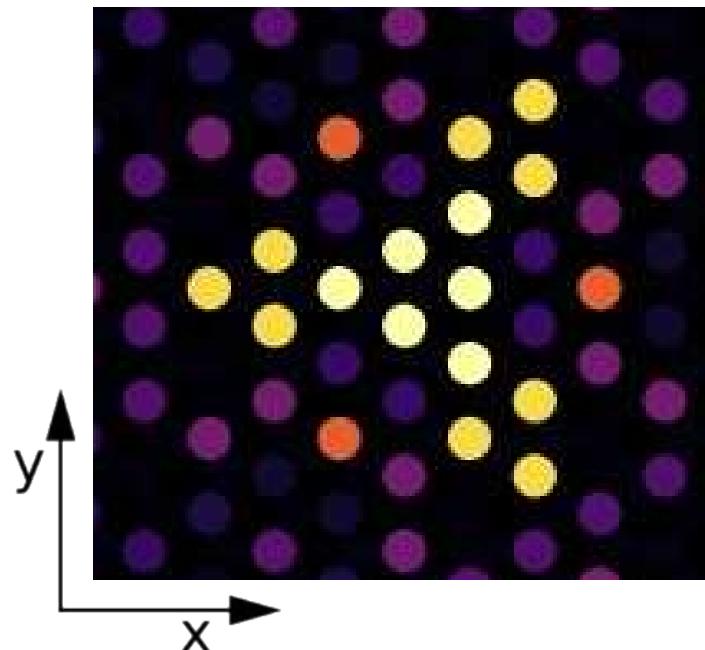
# Individual hydrogen atoms in graphene



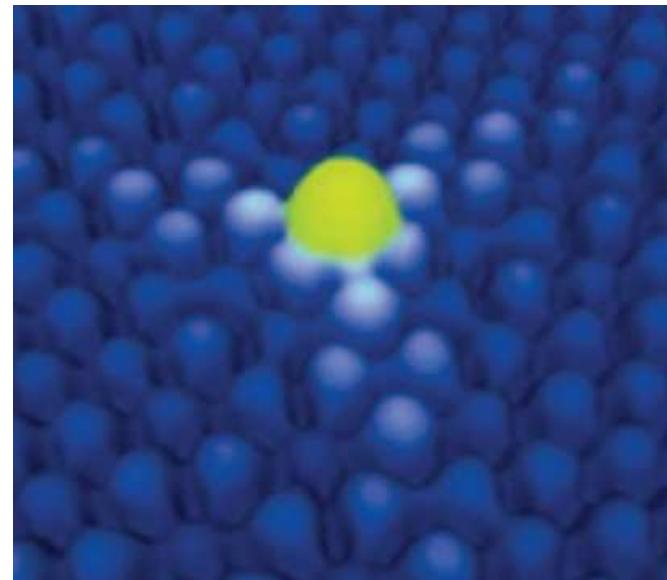
$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j$$

# Single impurity in monolayer graphene

Local density of states



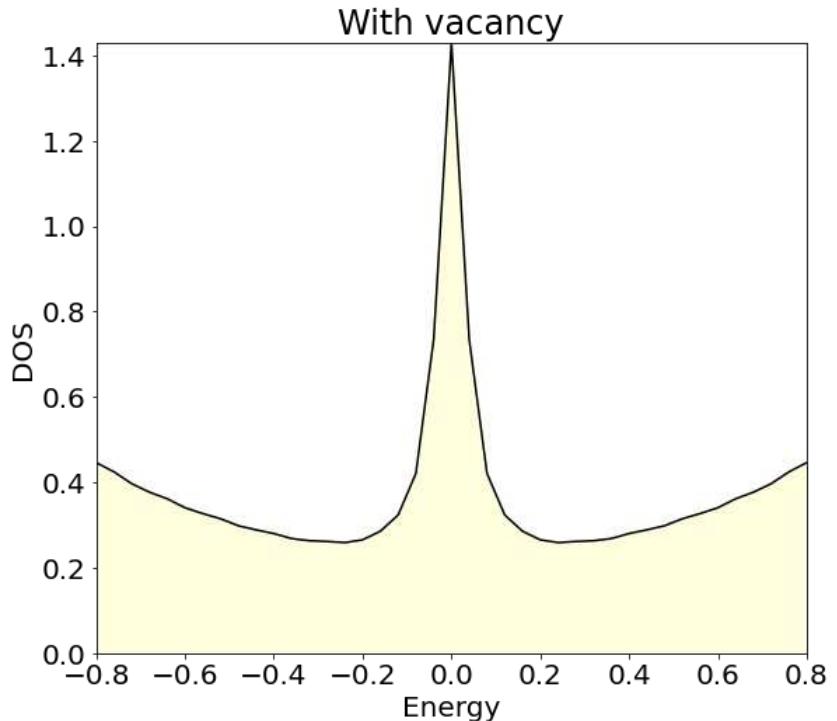
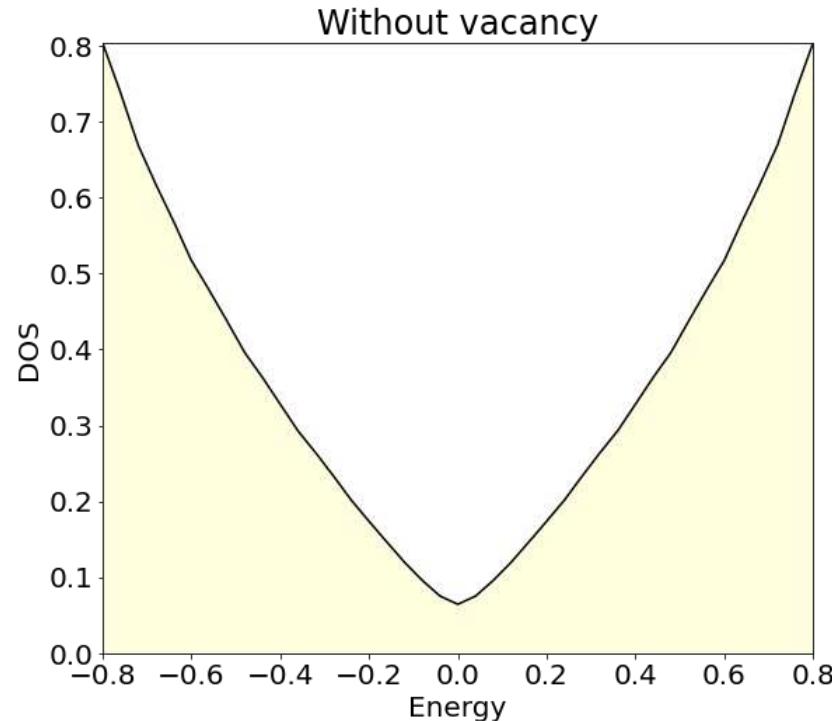
Experimental local density of states



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

Hydrogen atoms create zero modes in graphene

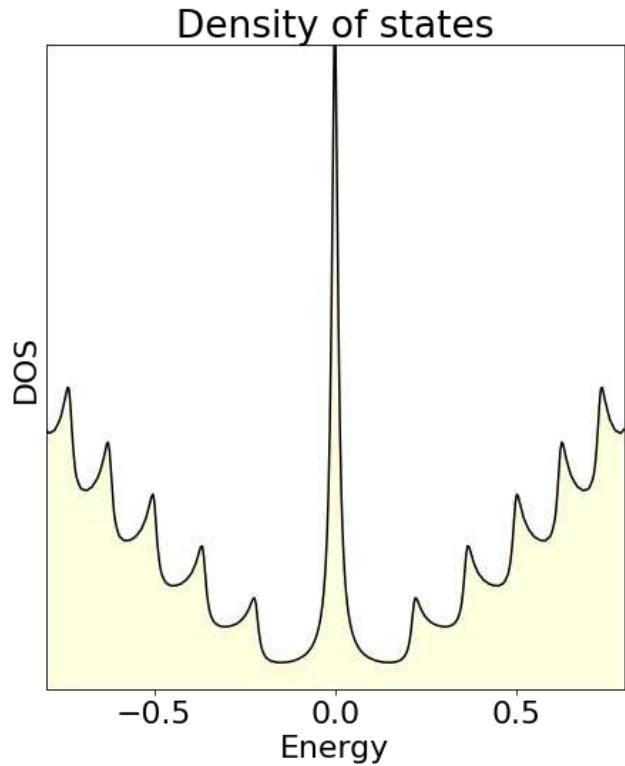
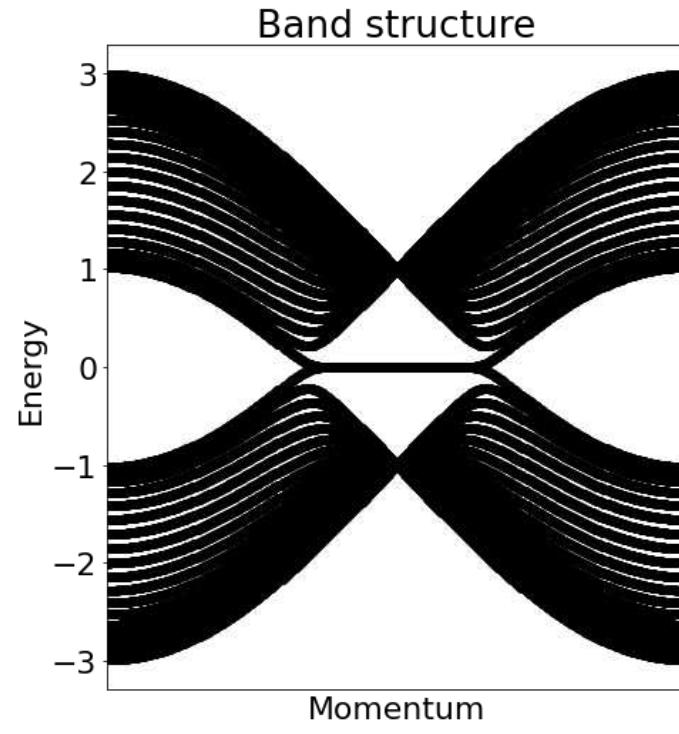
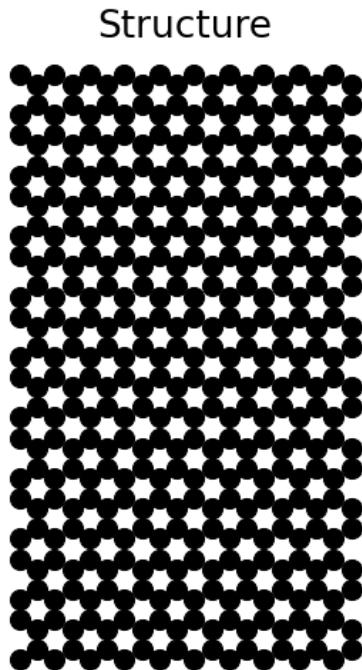
# Individual hydrogen atoms in graphene



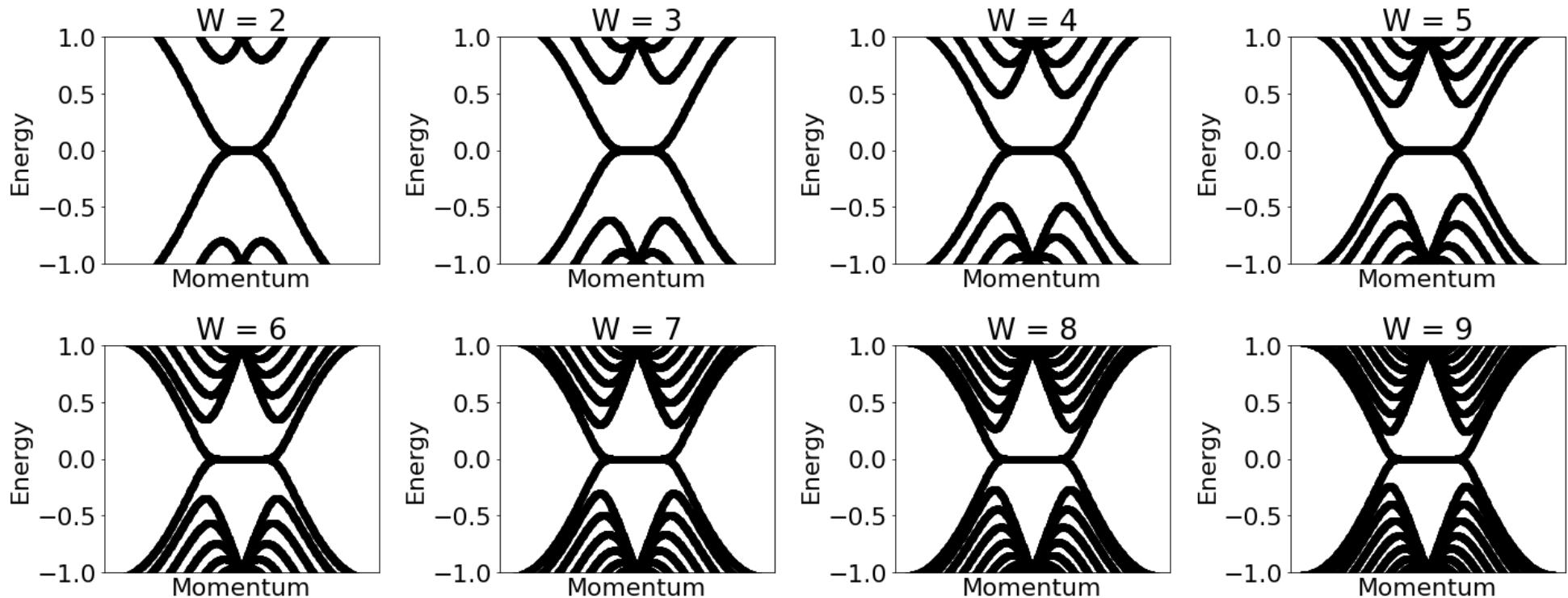
A vacancy in graphene gives rise to resonant zero modes

# Electronic instabilities in 2D materials

# Flat bands in graphene nanoribbons

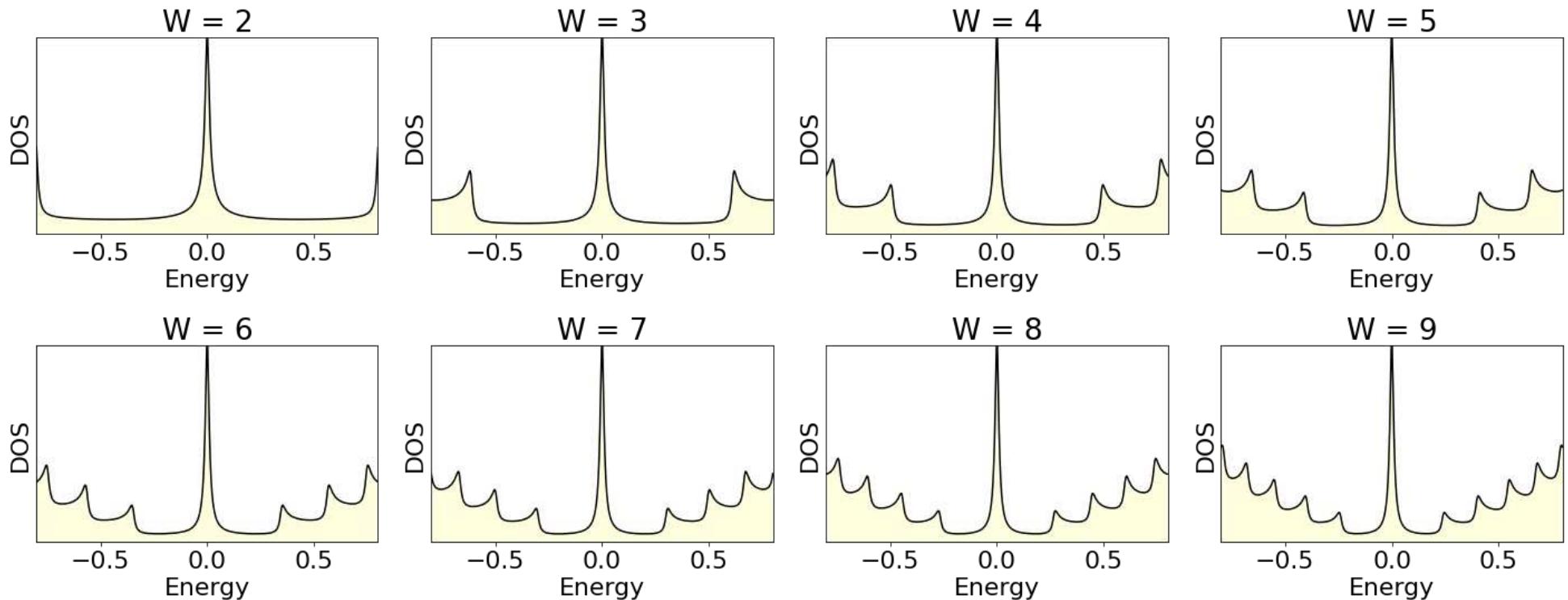


# Electronic structure of zigzag graphene nanoribbons



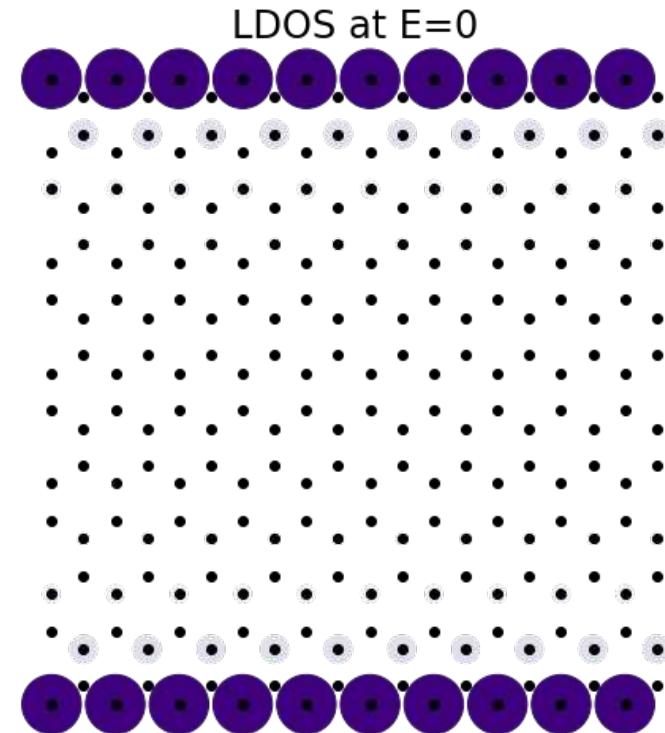
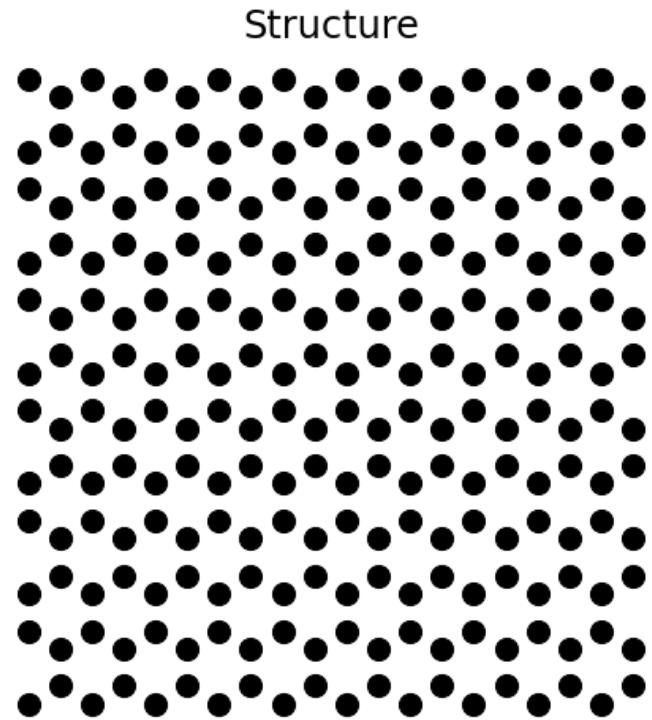
Flat bands appear in graphene zigzag nanoribbon of any width

# Electronic structure of zigzag graphene nanoribbons



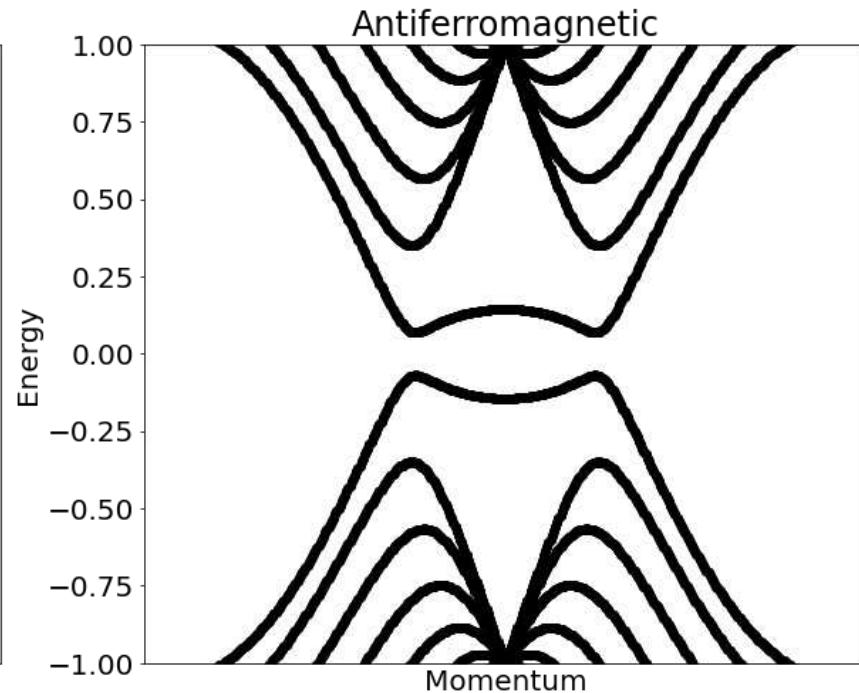
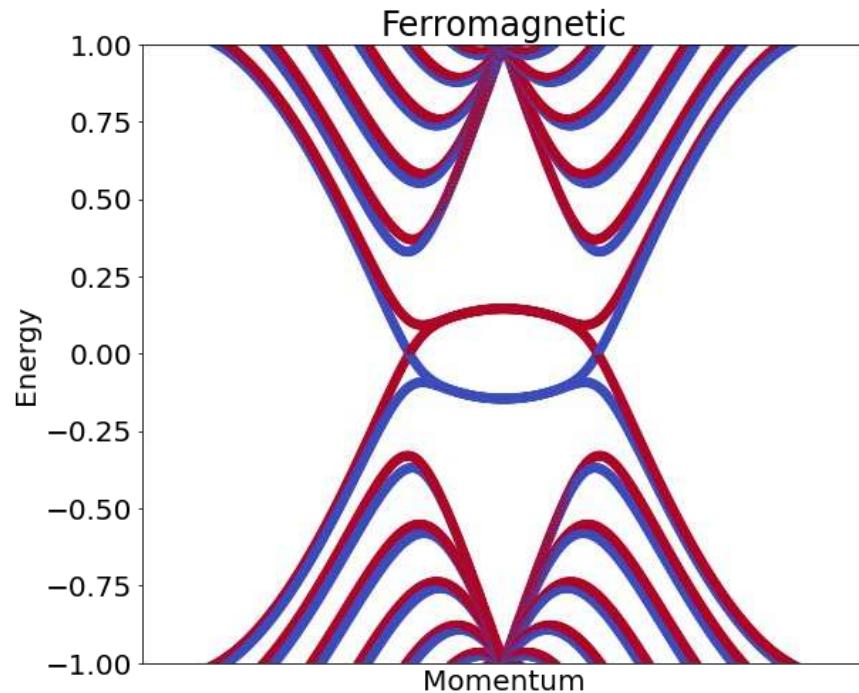
A divergent density of states appears in zigzag nanoribbon of any width

# Electronic structure of graphene zigzag ribbons



# Electronic interactions in graphene nanoribbons

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



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

# Hands-on

# 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

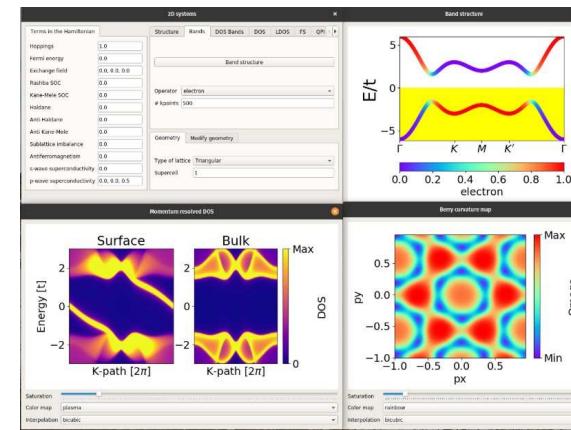
## pyqula (library based)

```
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>

# 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..

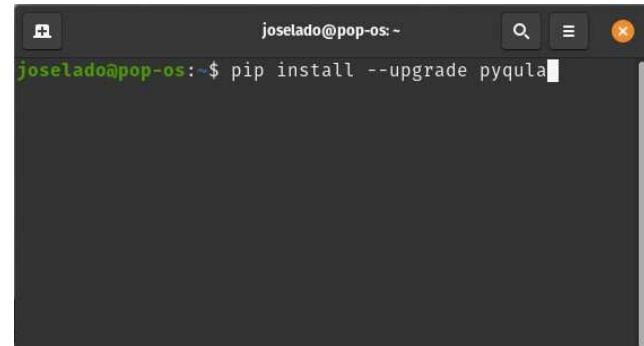
## Compute the different observables of the system

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

# Installation

*With pip (from the command line)*

pip install --upgrade pyqula



A screenshot of a terminal window titled 'joselado@pop-os: ~'. The command 'pip install --upgrade pyqula' is visible in the terminal window.

\*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

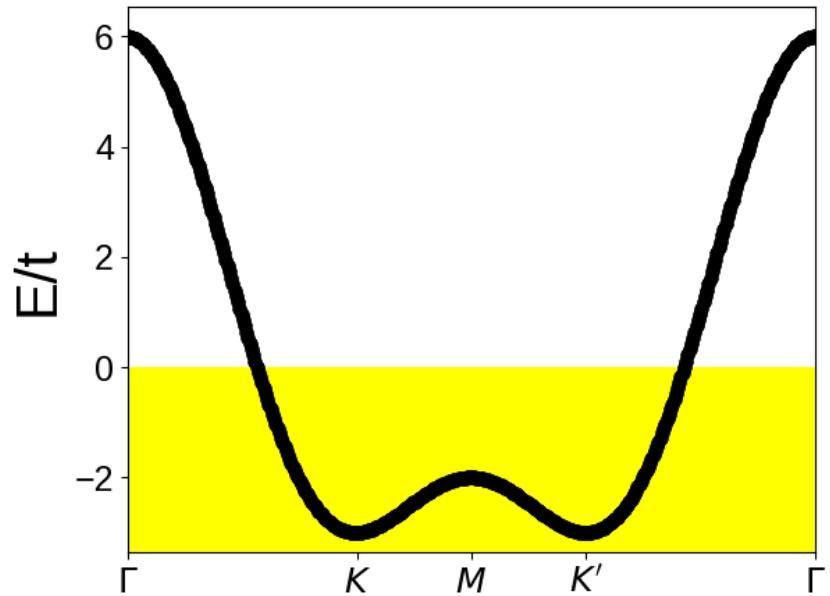
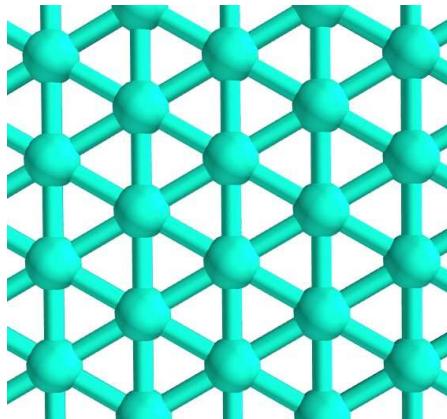
---

- 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

# First neighbor Hamiltonian in a triangular lattice

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

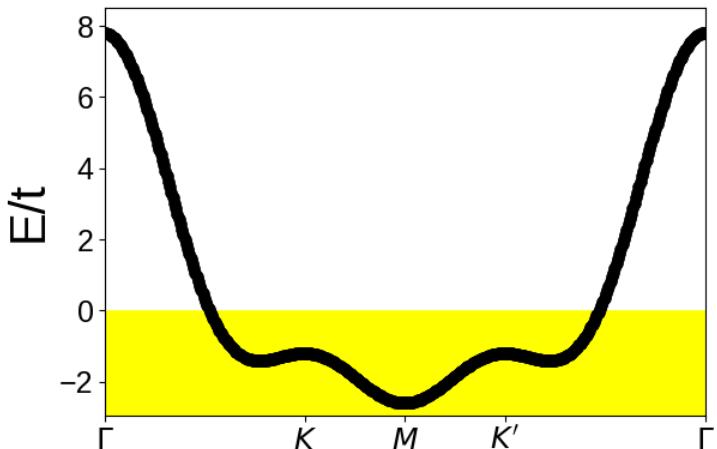
```
from pyqula import geometry
g = geometry.triangular_lattice() # get the geometry object
h = g.get_hamiltonian() # get the Hamiltonian object
(k,e) = h.get_bands() # compute the band structure
```



# First and second neighbor Hamiltonian in a triangular lattice

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

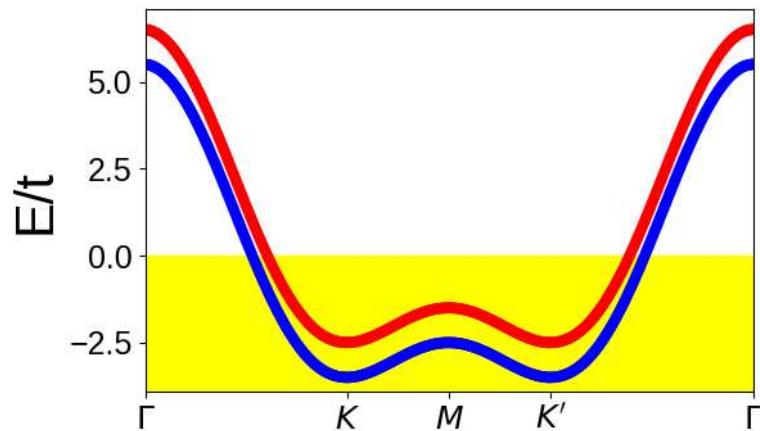
```
from pyqula import geometry
g = geometry.triangular_lattice() # get the geometry object
h = g.get_hamiltonian(tij=[1.0,0.3]) # get the Hamiltonian object
(k,e) = h.get_bands() # compute the band structure
```



# Triangular lattice with an exchange field

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

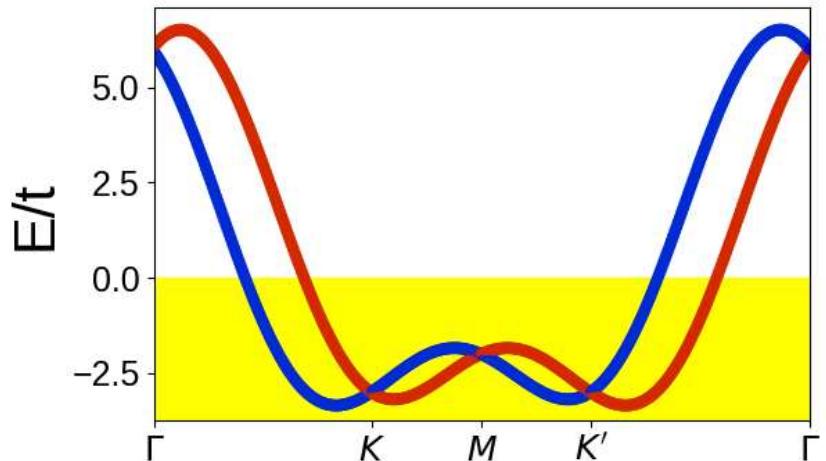
```
from pyqula import geometry
g = geometry.triangular_lattice() # get the geometry object
h = g.get_hamiltonian() # get the Hamiltonian object
h.add_exchange([0.,0.,0.5]) # add exchange field
(k,e,c) = h.get_bands(operator="sz") # compute the band structure
```



# Triangular lattice with Rashba spin-orbit coupling

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

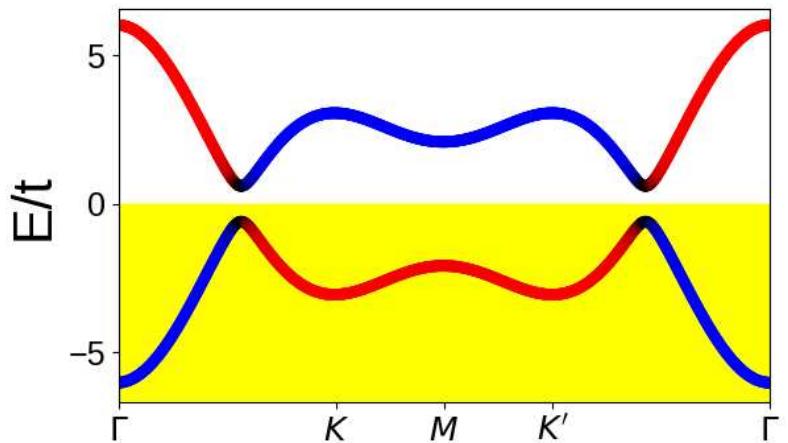
```
from pyqula import geometry
g = geometry.triangular_lattice() # get the geometry object
h = g.get_hamiltonian() # get the Hamiltonian object
h.add_rashba(0.6) # add Rashba SOC
(k,e,c) = h.get_bands(operator="sx") # compute the band structure
```



# Triangular lattice with superconductivity

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

```
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
```



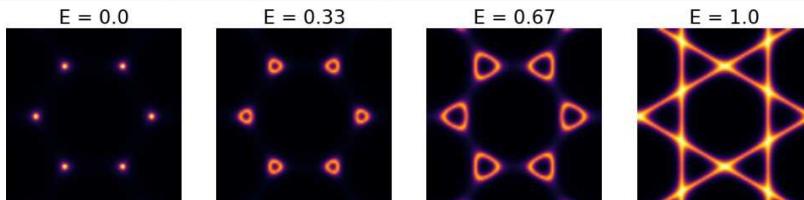
# (Optional) exercise sessions

Download Jupyter-notebook from

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

*You will see examples with the code*

```
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 knet
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?

