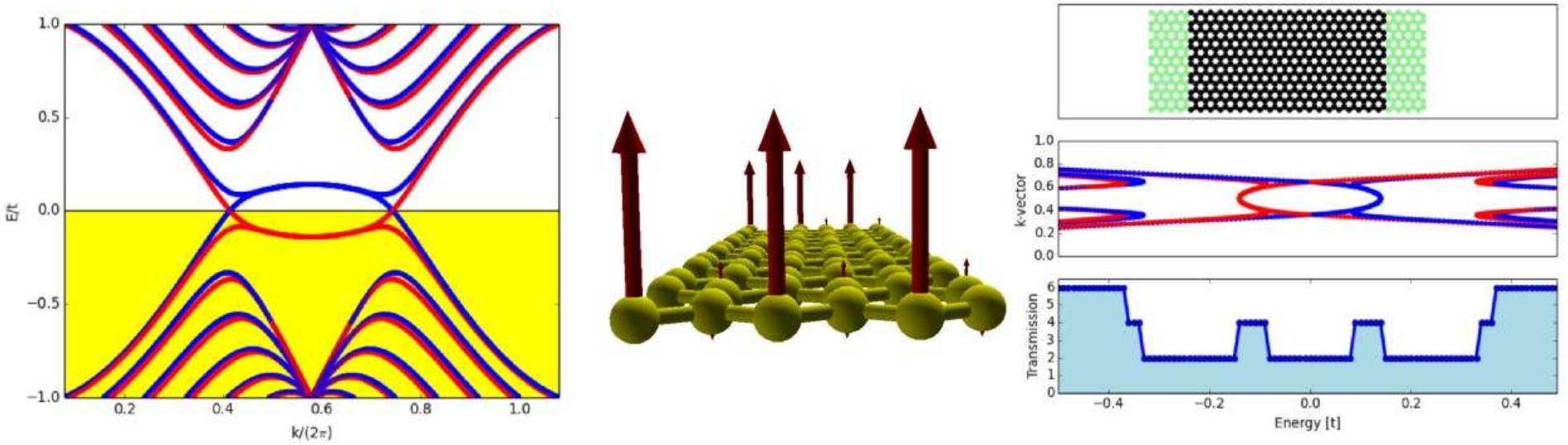
User friendly tight binding

Landauer@non-collinear mean field calculations

Jose Lado and Joaquin Fernandez Rossier

International Nanotechnology Laboratory (INL), Braga, Portugal

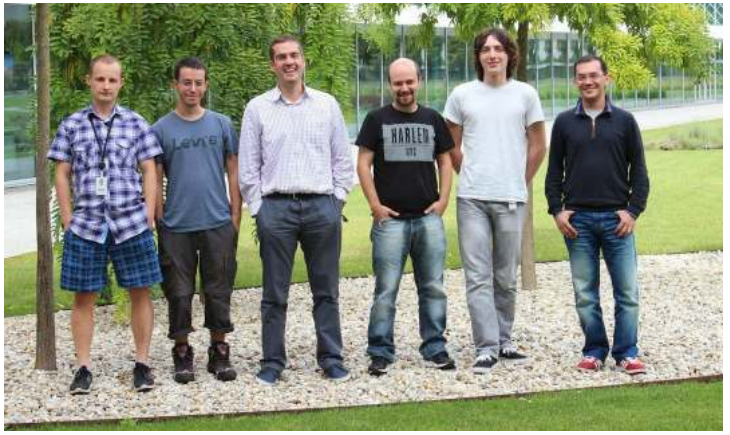


ICCP-9, Singapore Friday 9 January

The team

Theory group at INL, Braga, Portugal

Jose Lado



Joaquin Rossier

Most cited papers

The top 100 papers

***Nature* explores the most-cited research of all time.**

Richard Van Noorden, Brendan Maher & Regina Nuzzo

29 October 2014

12 papers on density functional theory (DFT)

In the first 10, two in physics, both in DFT

Most of them are synthesis and computational methods

Motivation

- Numerical calculations are a **key tool** in understanding physical phenomena
- Numerical codes are usually **not intuitive for non-experts** in computation
- Undesired **gap inside a community** which works in the same problem

We want to close this GAP

Our goal

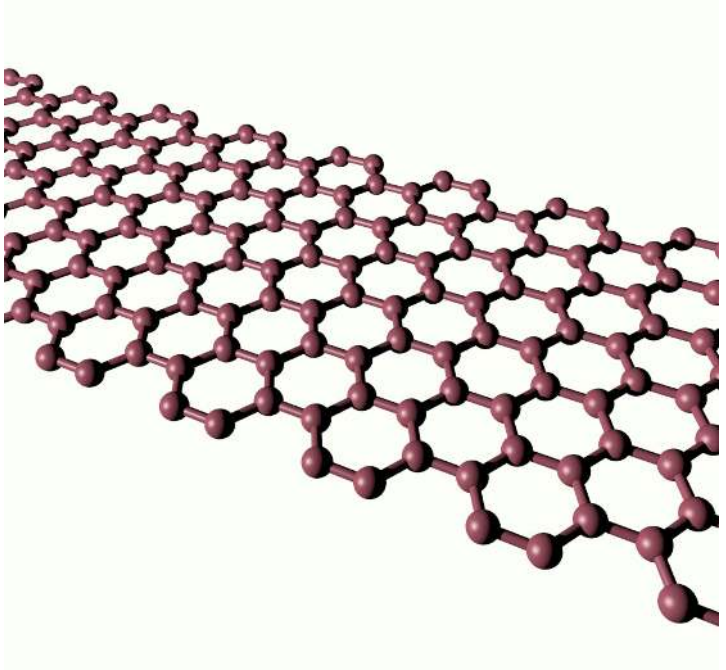
We want a **tool** that allows to calculate electronic properties in **graphene-like systems**

- We want it **SIMPLE**
- We want it **FAST**
- We want it **INTERACTIVE**
- We want it **FREE**

What can we do?

We have implemented

- Honeycomb in ribbon geometry
- Magnetic fields, AB imbalance, spin-orbit coupling
- Local interactions



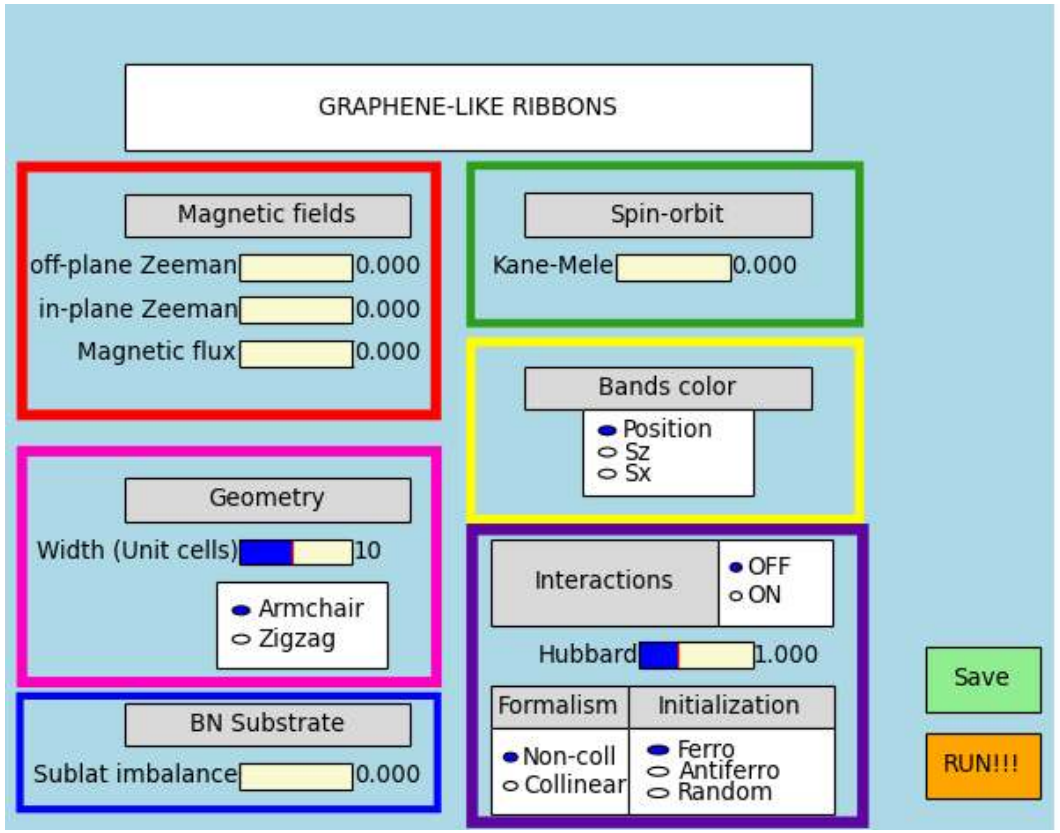
to calculate

→ **Band structure**
→ **Magnetic structure**
→ **Two terminal transport**

in these systems

→ Graphene, silicene, germanene
→ Metal organic frameworks
→ Oxide multilayers
→ Hydrogenated bismuth

Parts of the main interface



Magnetic fields

Geometry of the system

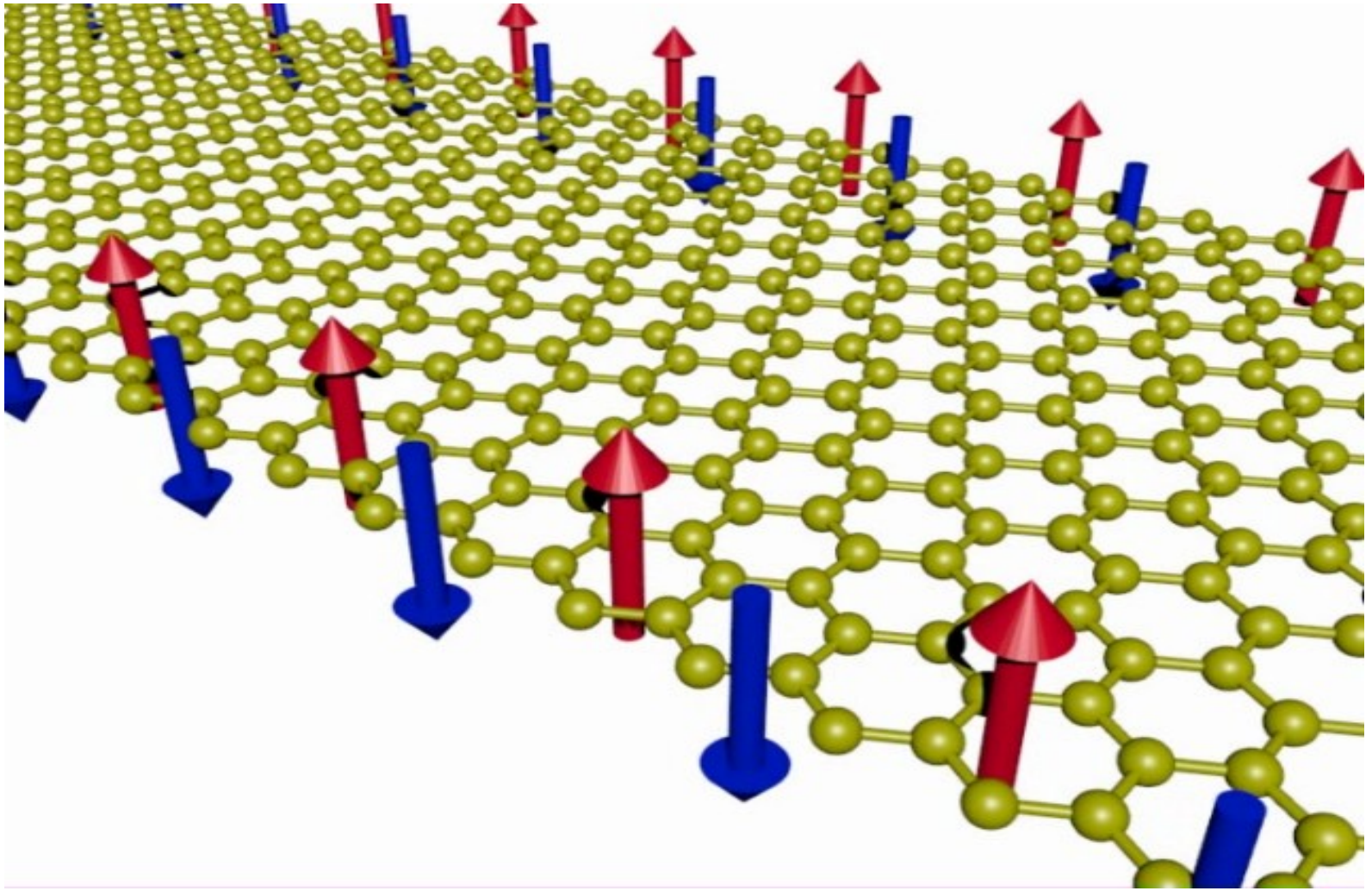
Sublattice imbalance

Spin orbit coupling

Color code of the bands

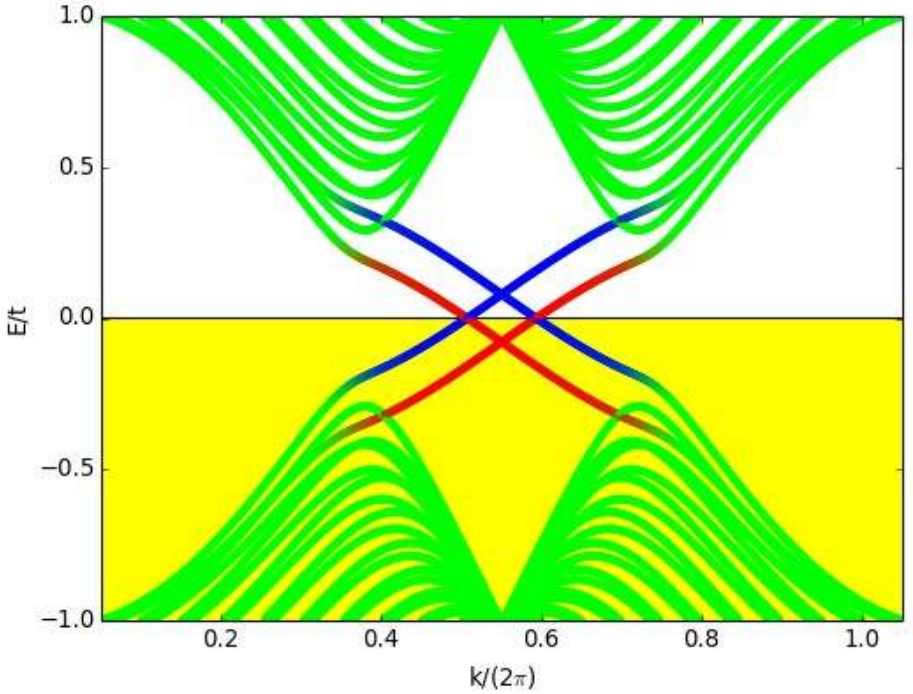
Local coulomb interactions

$$H = H_{NN}(\phi_z) + H_{AB} + H_{Zeeman} + H_{KM} + H_{Hubbard}$$



SOC and AB imbalance, topological

Location

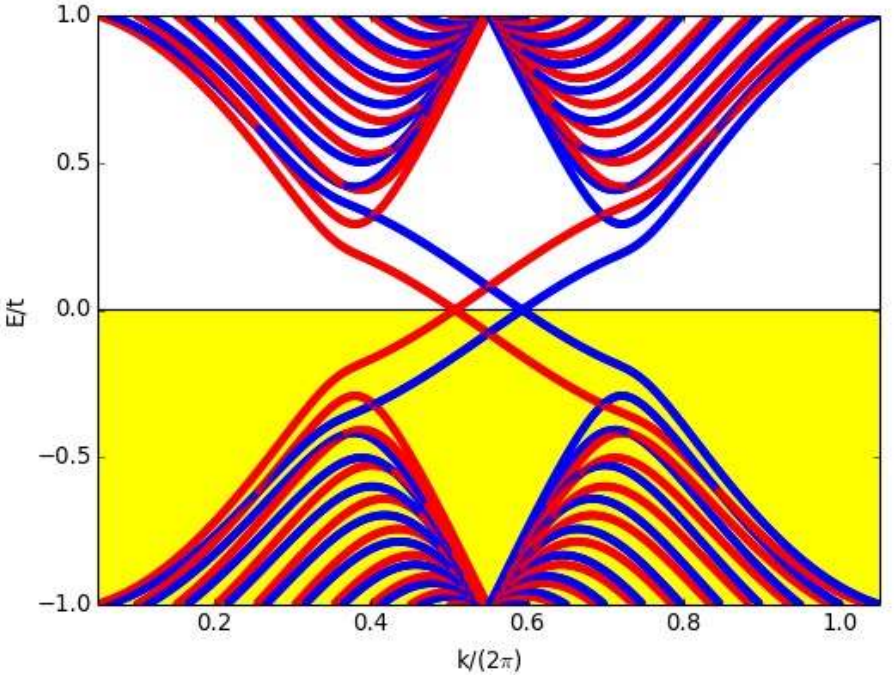


Bulk of the ribbon

Right edge state

Left edge state

Spin along z

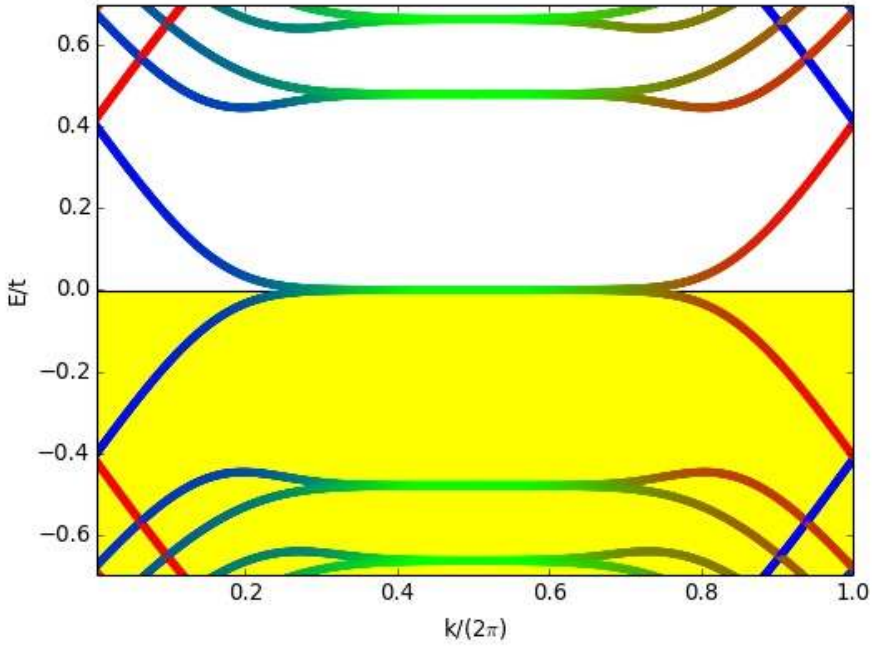


Spin up

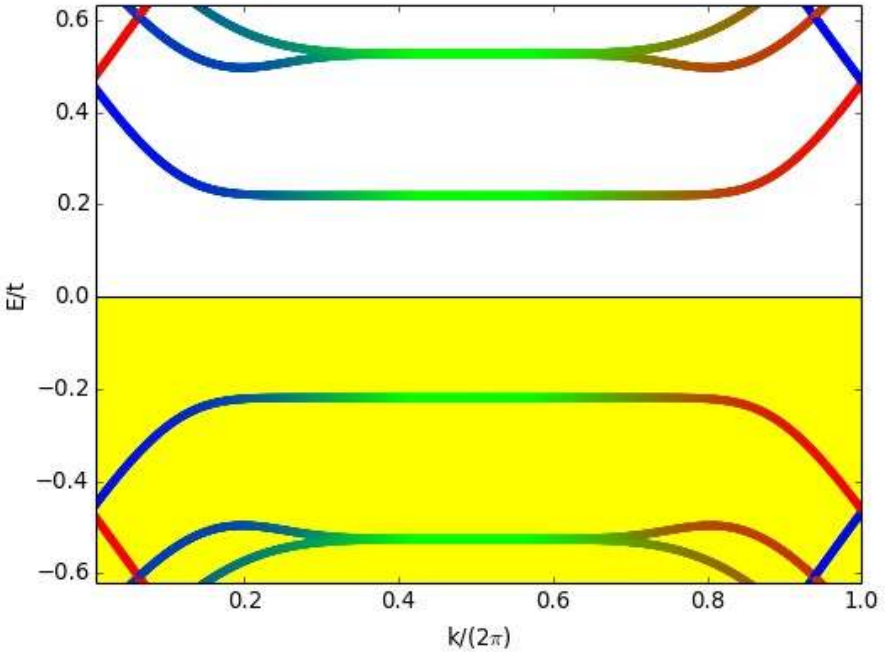
Spin down

Quantum Hall effect

Without AB imbalance



With AB imbalance

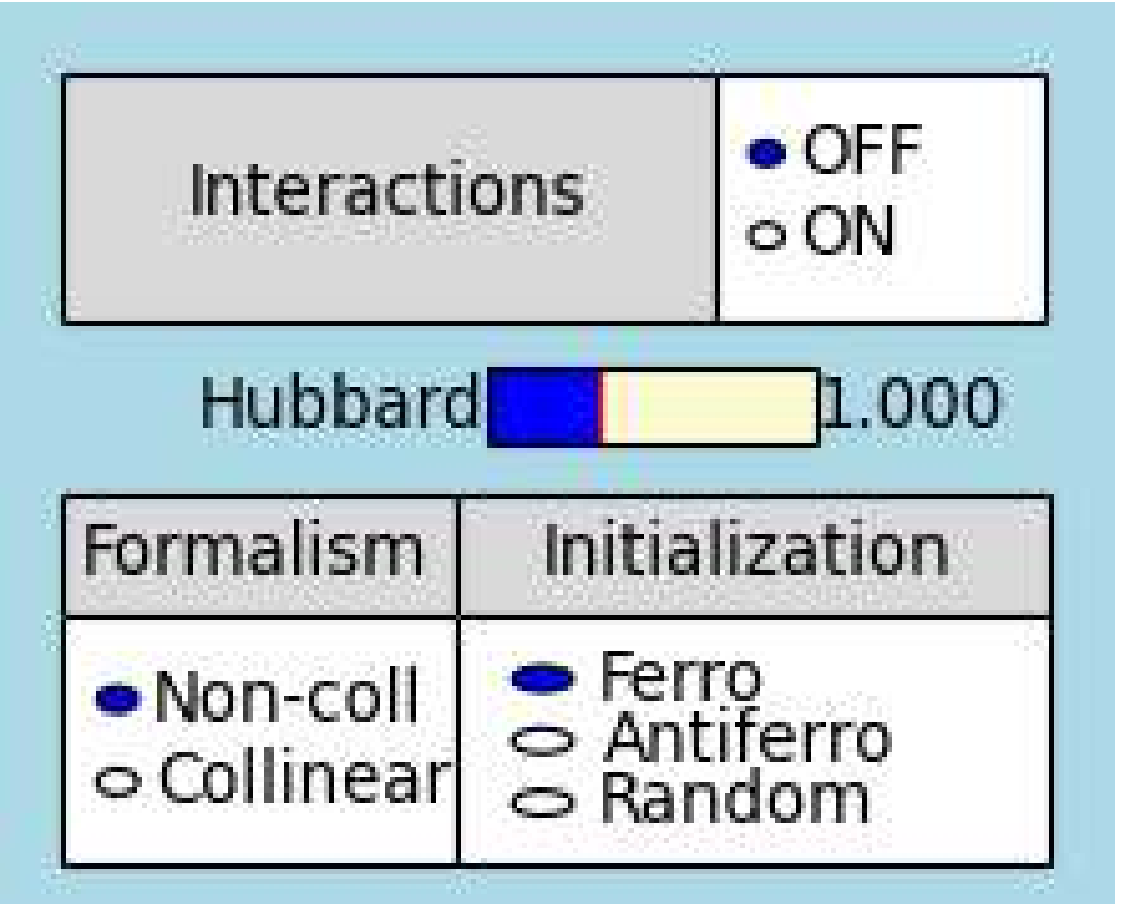


Landau level

Right edge state

Left edge state

Turning on interactions

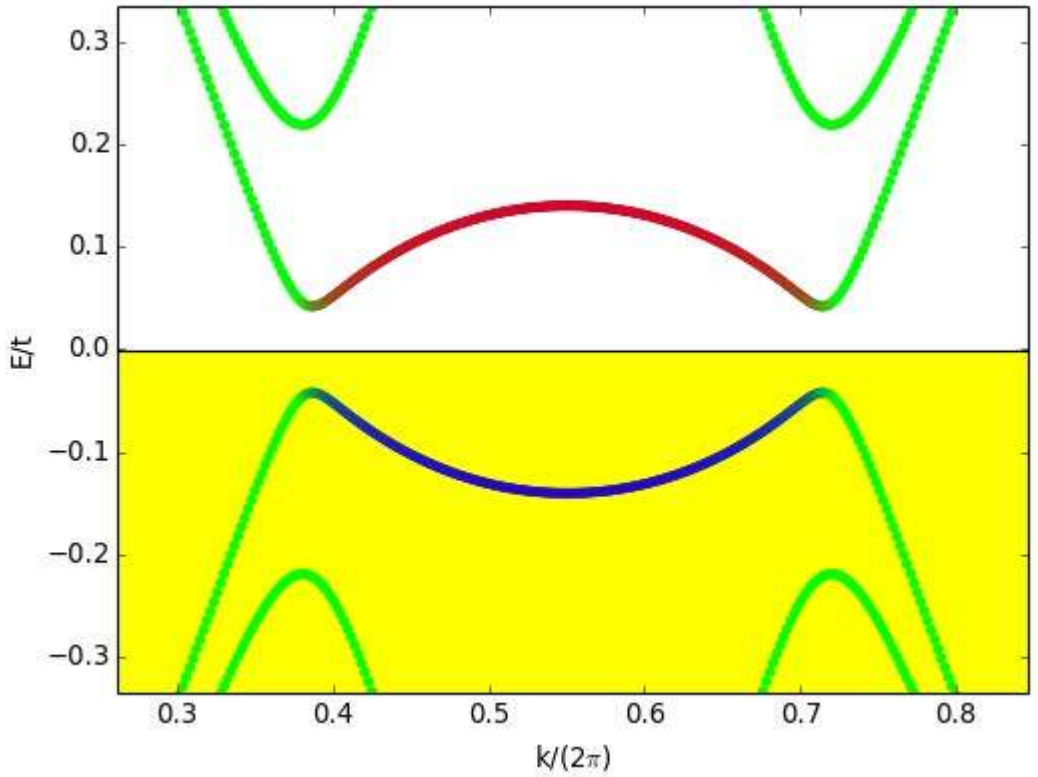


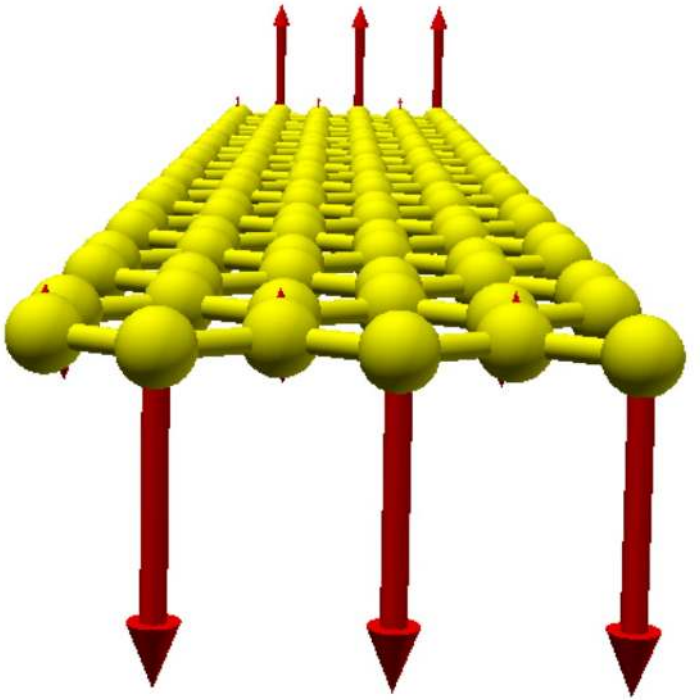
$$H_{Hubbard} = U \sum_{i,s} c^{\dagger}_{i,\uparrow} c_{i,\uparrow} c^{\dagger}_{i,\downarrow} c_{i,\downarrow}$$

Variational mean field wave function

$$|\Omega\rangle = \prod_i \left(u_i c^{\dagger}_{i\uparrow} + v_i c^{\dagger}_{i\downarrow} \right) |0\rangle$$

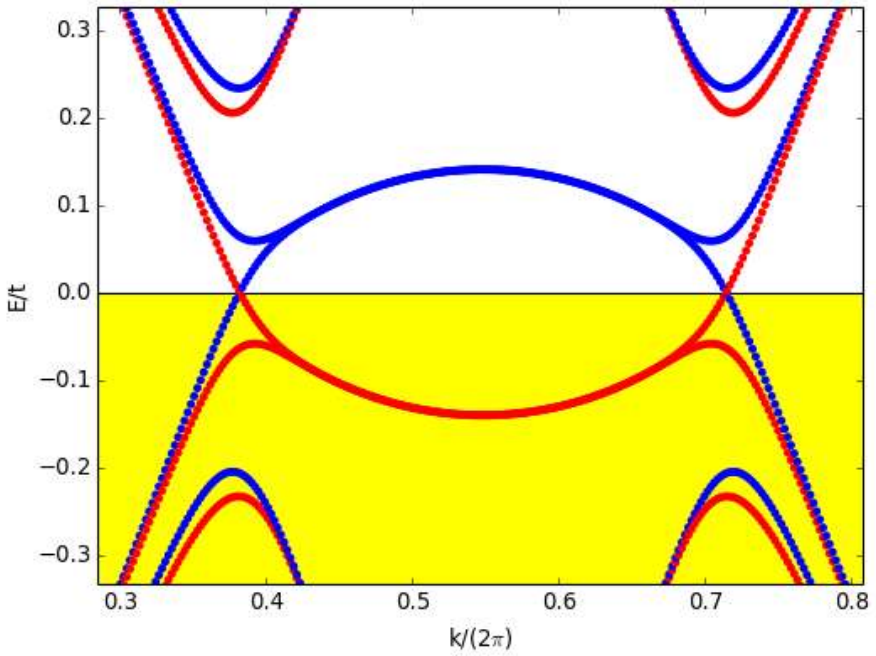
Ferromagnetism in zigzag

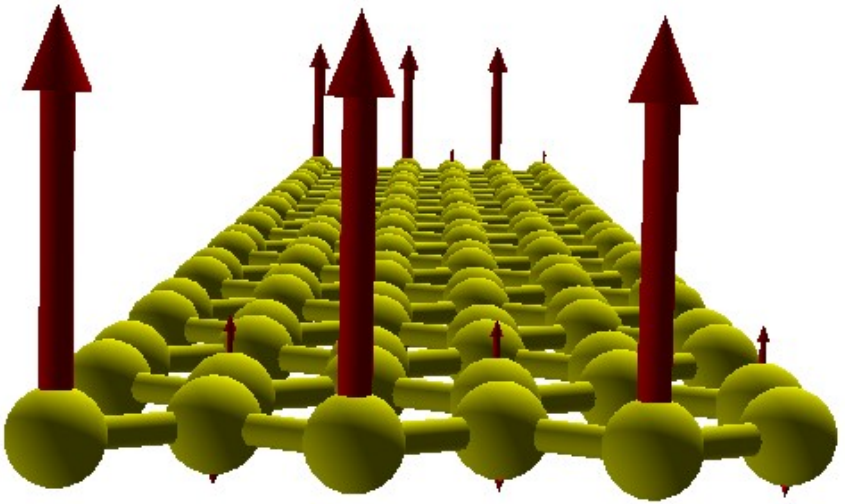




True GS configuration (edge antiferro)

Ferromagnetism in zigzag



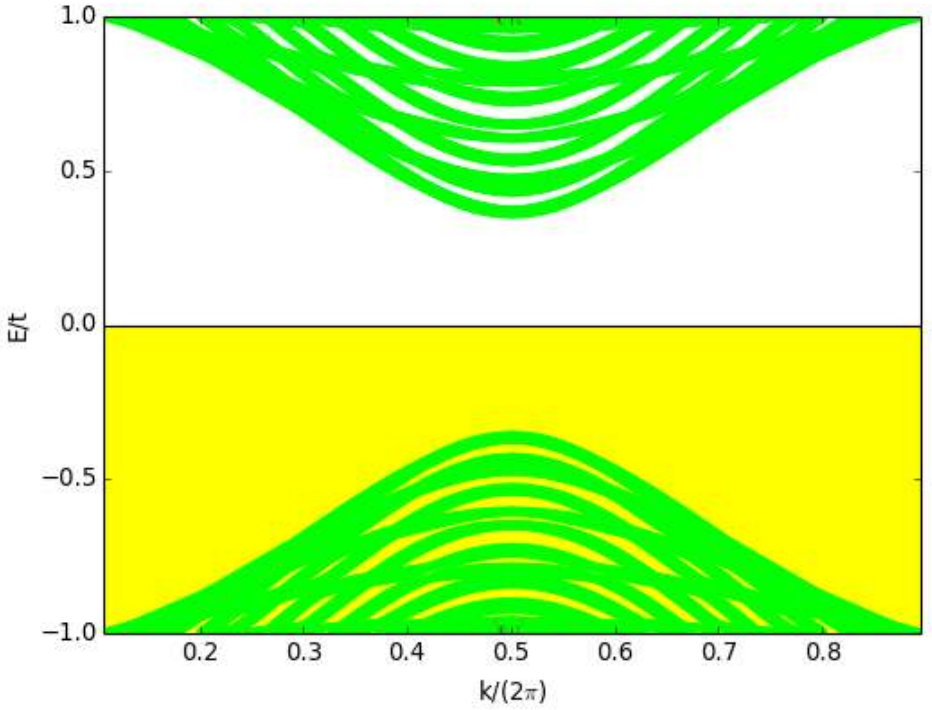


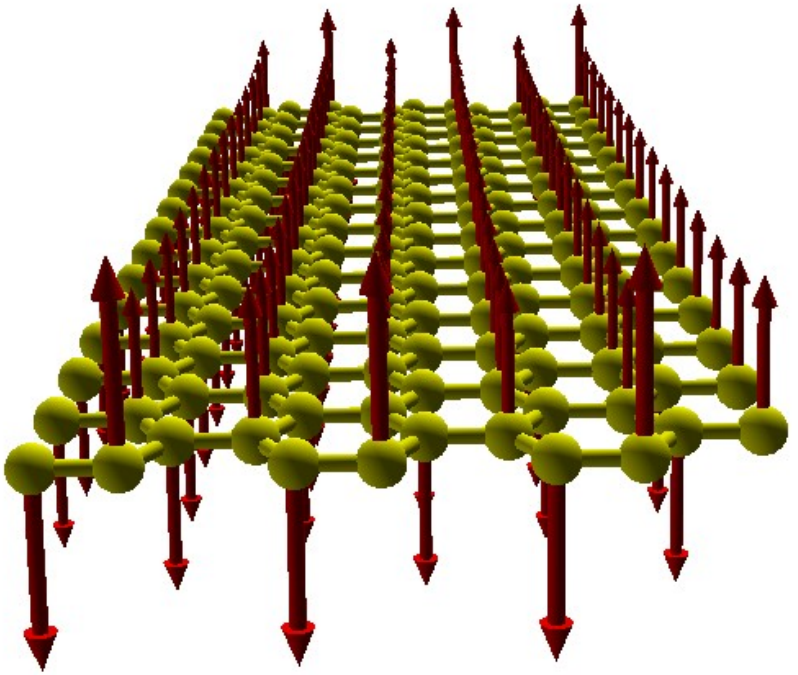
Spin up

Spin down

Antiferromagnetic bulk transition

For U > 2.2t



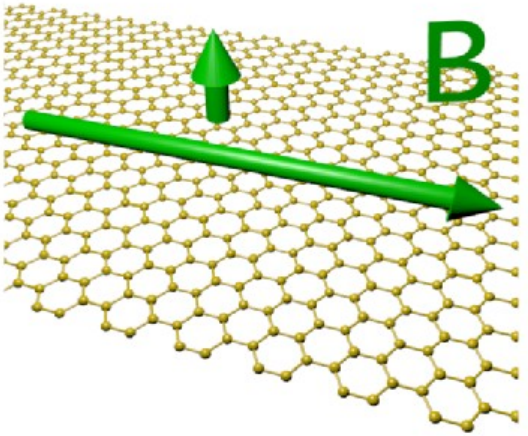


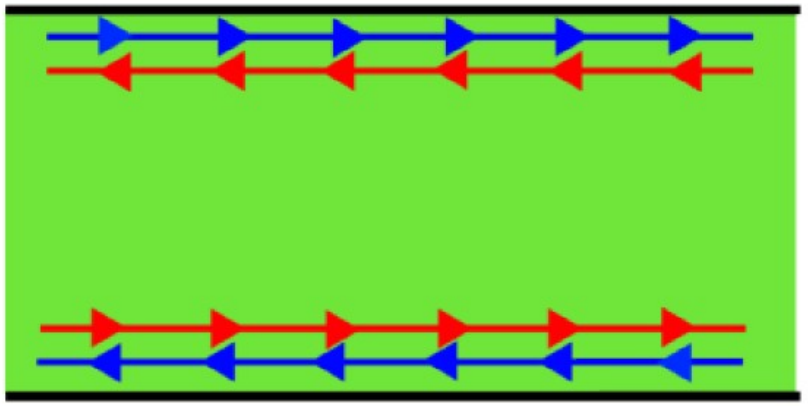
Quantum Spin Hall in graphene

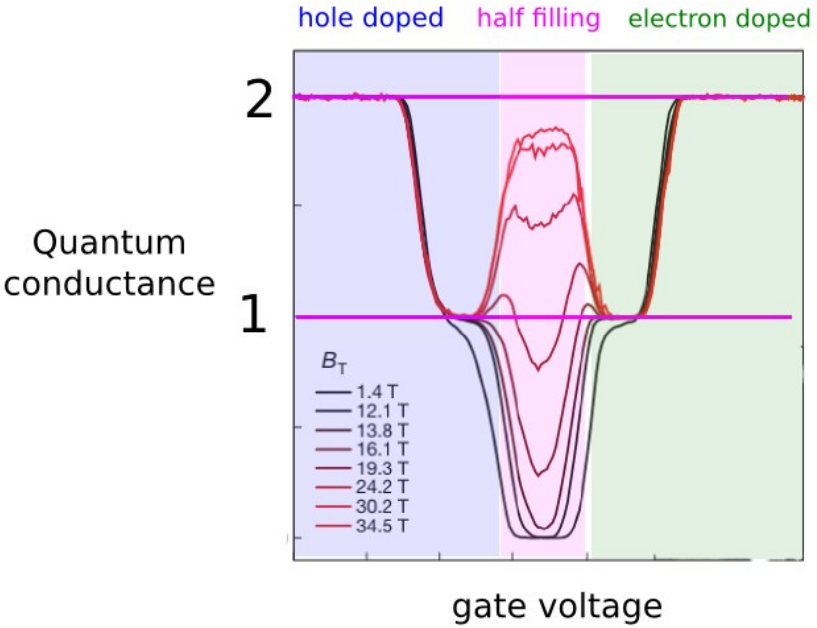
nature

Tunable symmetry breaking and helical edge transport in a graphene quantum spin Hall state

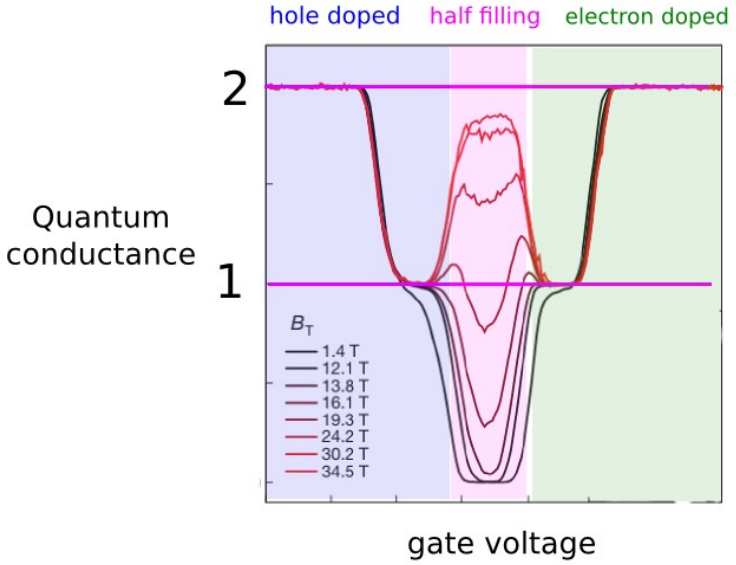
A. F. Young, J. D. Sanchez-Yamagishi, B. Hunt, S. H. Choi, K. Watanabe, T. Taniguchi, R. C. Ashoori & P. Jarillo-Herrero

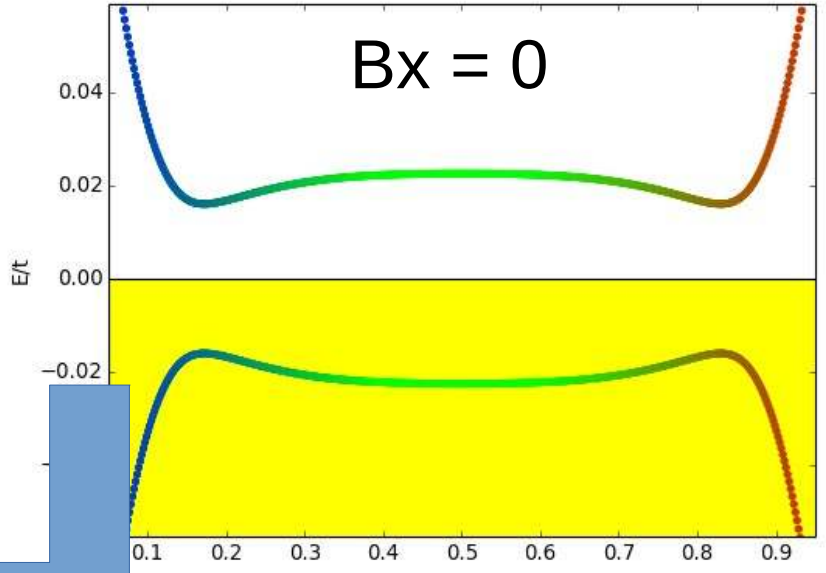


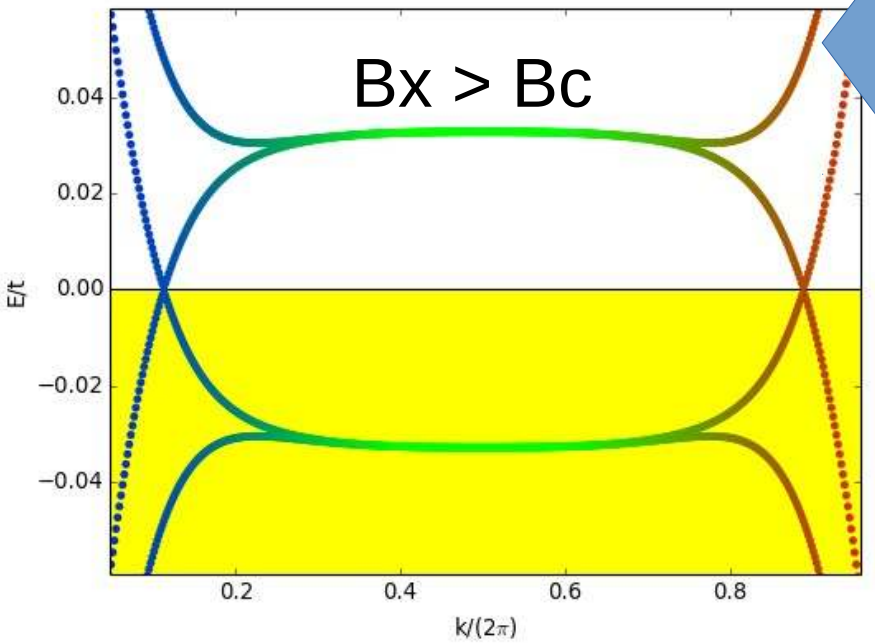


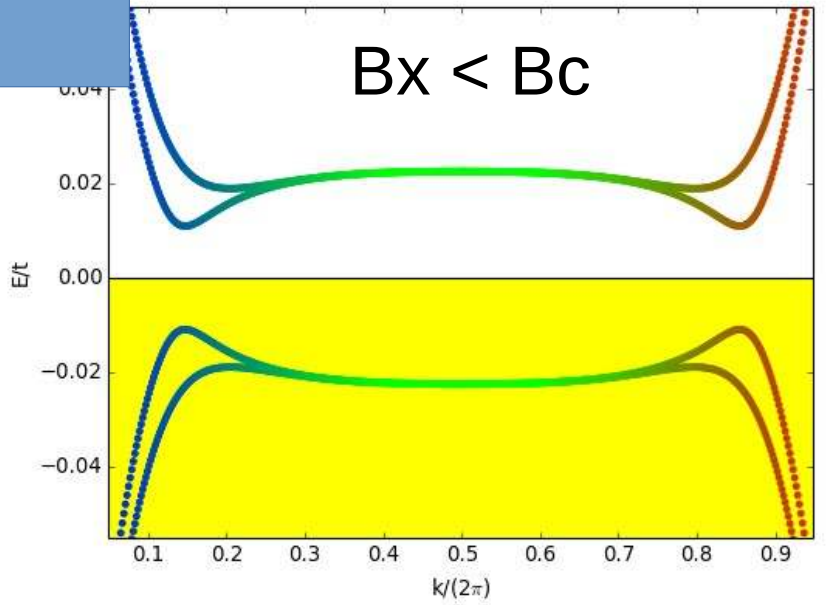


Increasing in-plane magnetic field



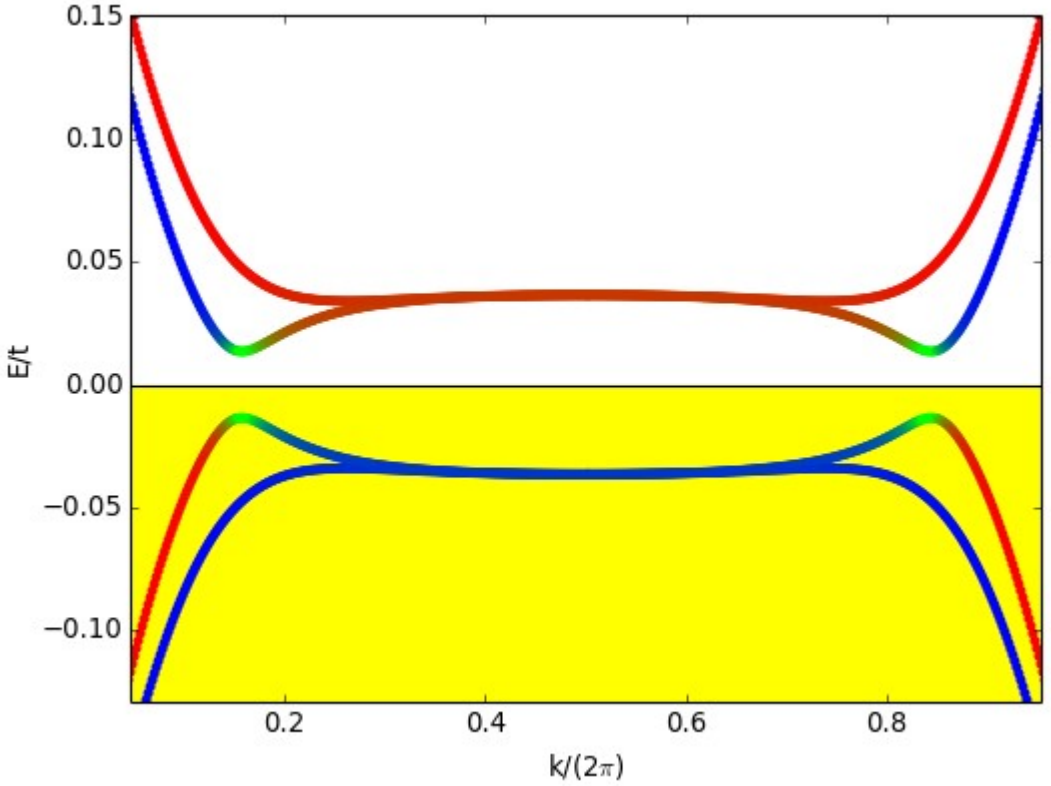


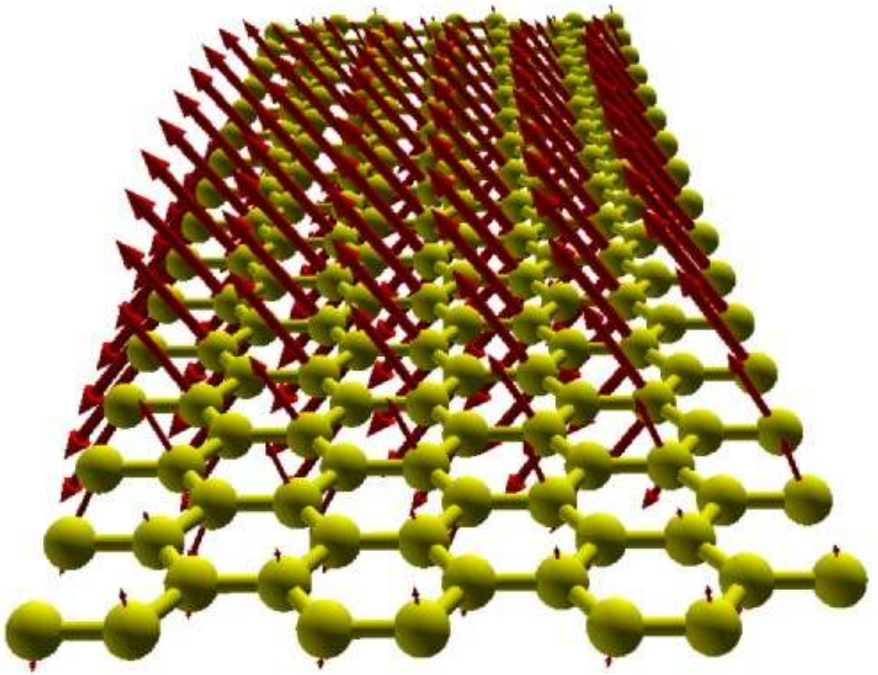


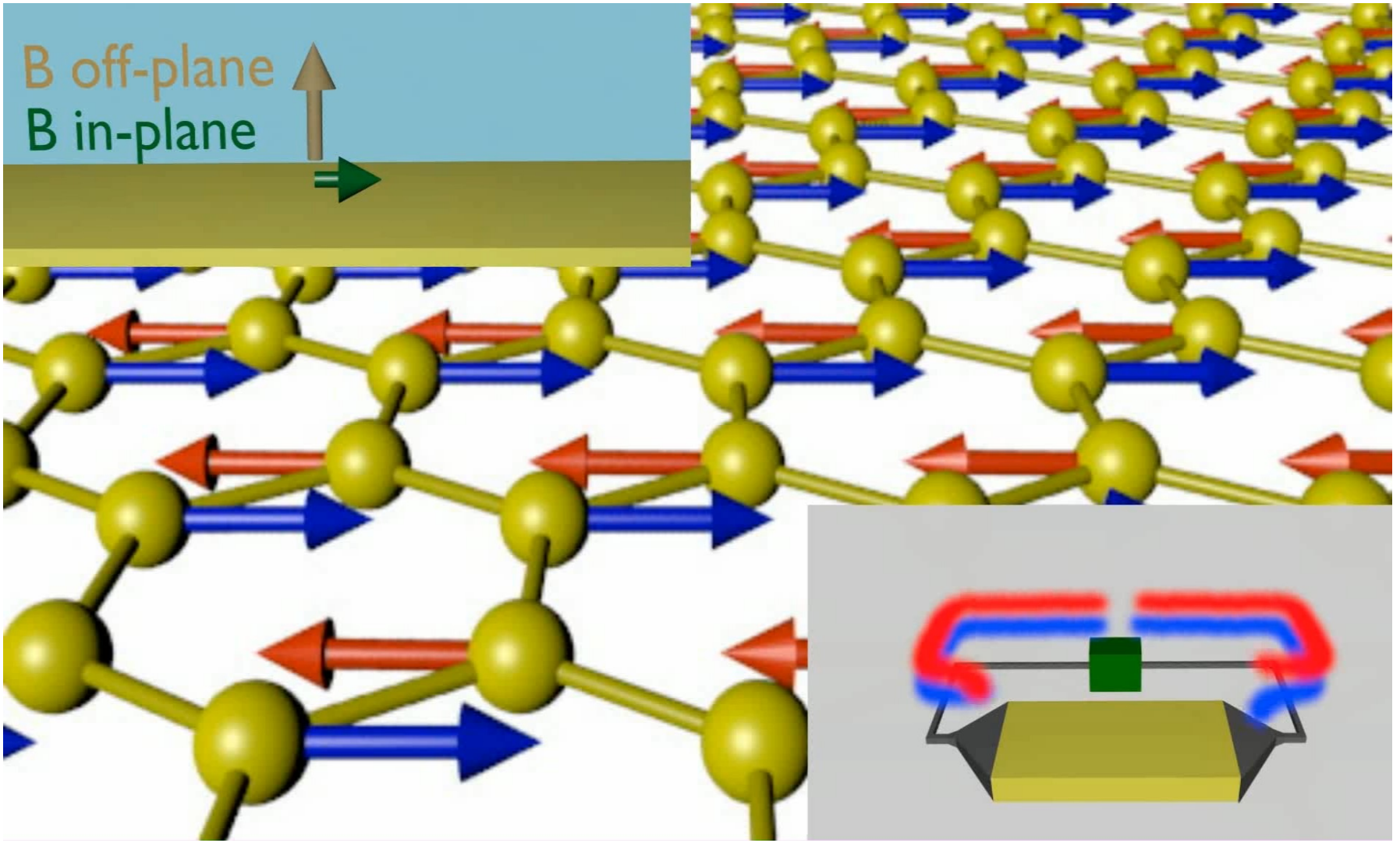


Canted Quantum Hall magnetism

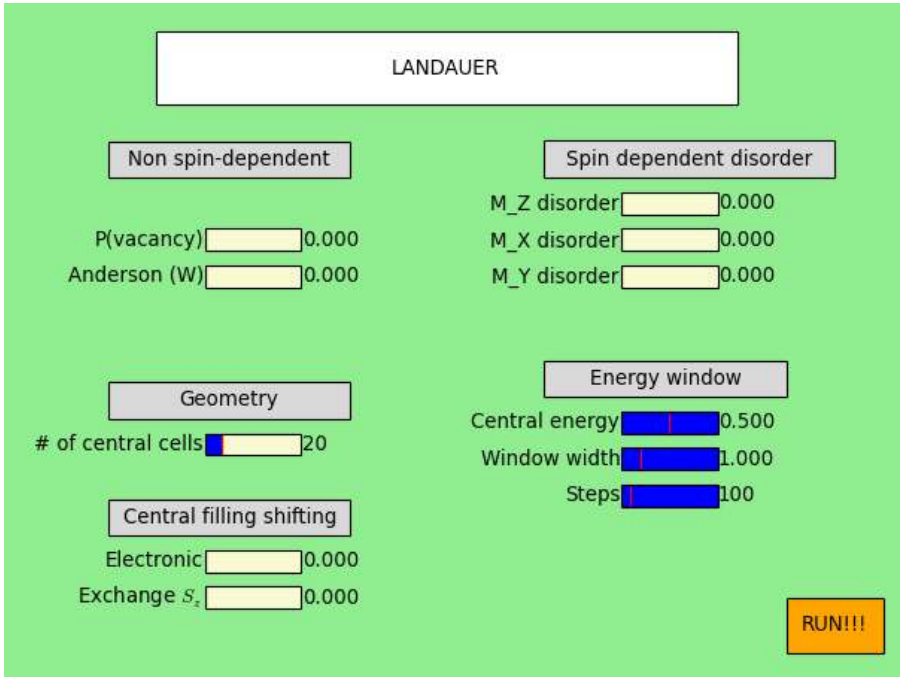
Quantum Hall regime with in-plane Zeeman field

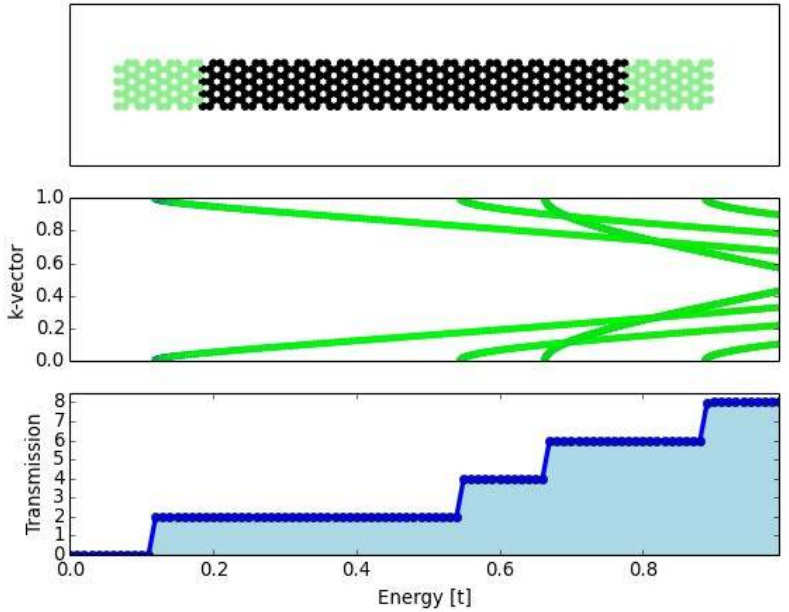





B off-plane
B in-plane

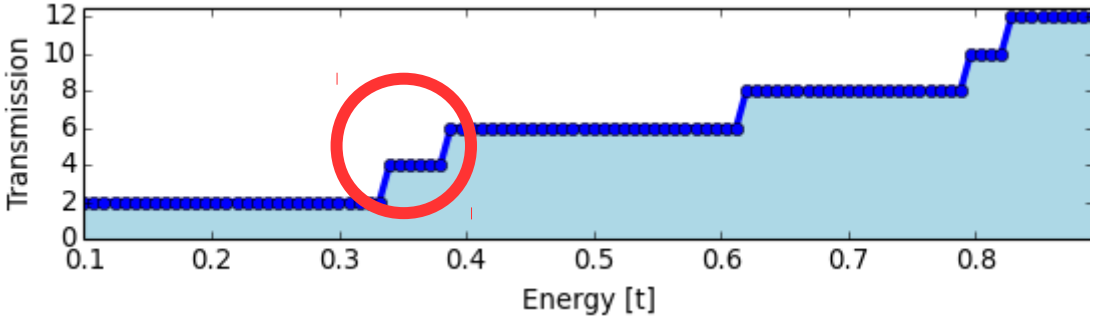
The transport interface

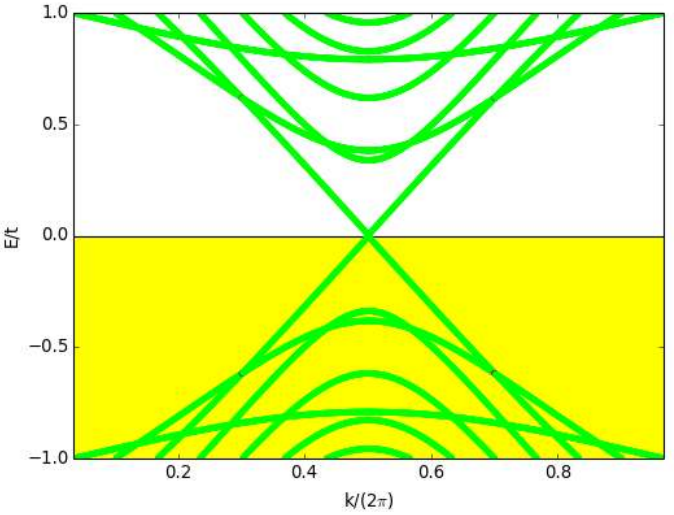


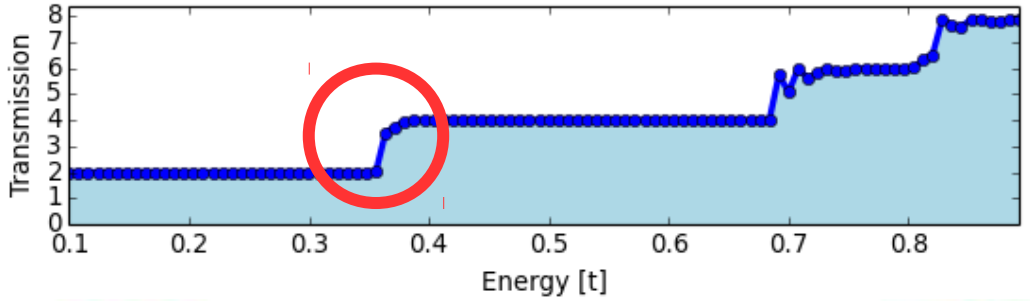


Transport in armchair ribbon

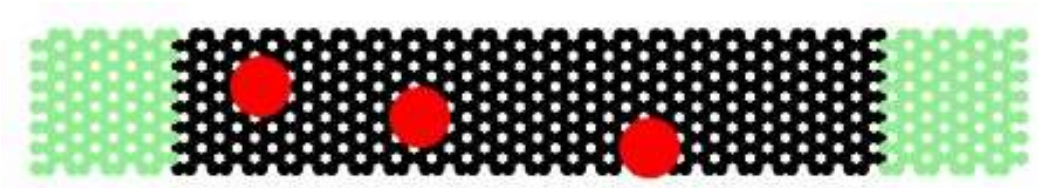
Perfect





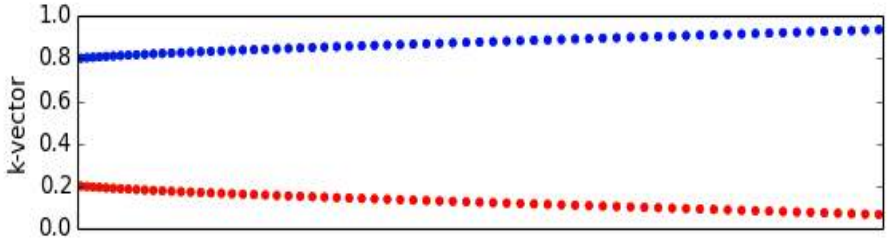


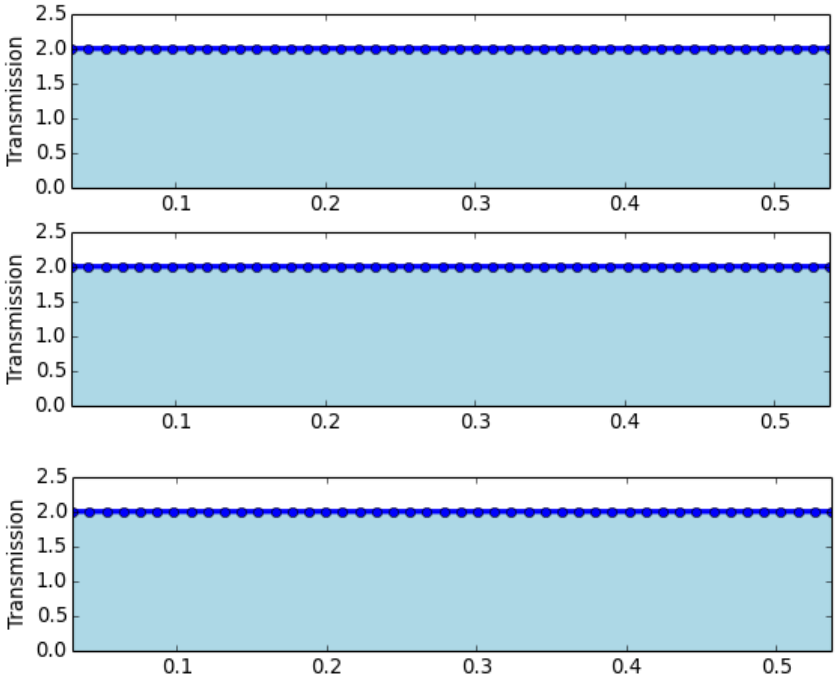
With vacancies

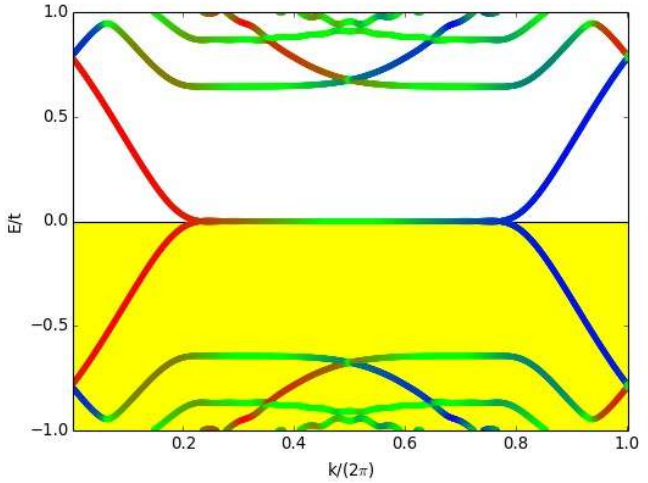


Transport in Quantum Hall

Bandstructure







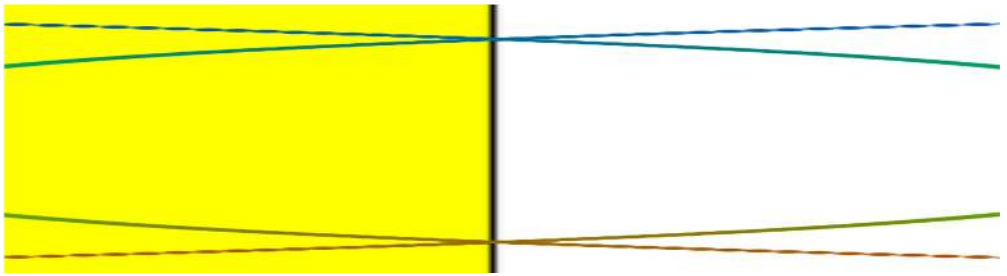
With vacancies

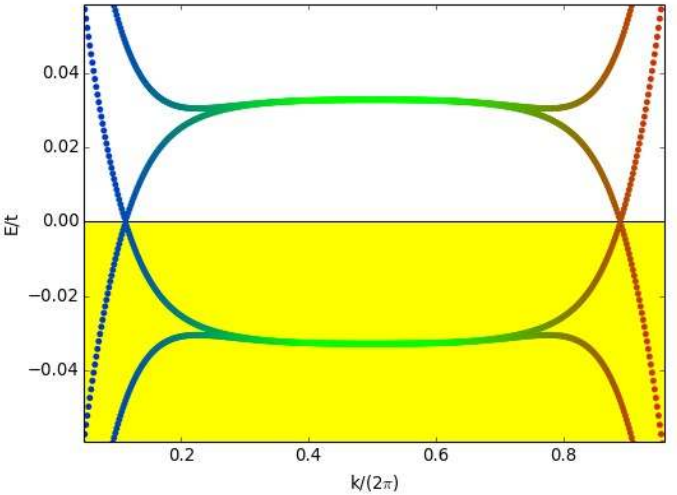
With Anderson disorder

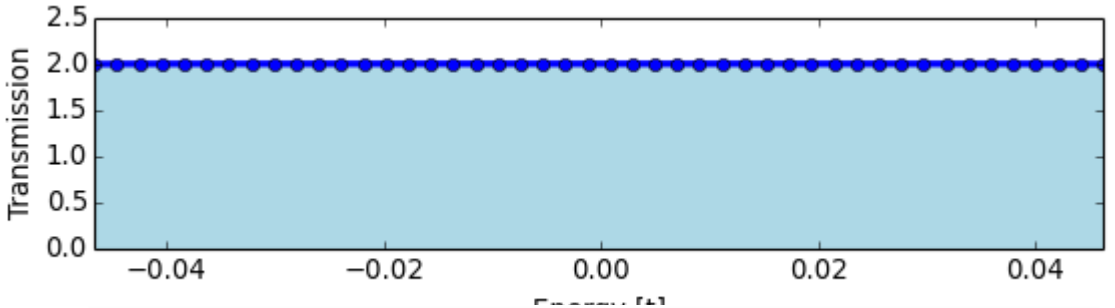
With magnetic Anderson

Transport in Quantum Spin Hall

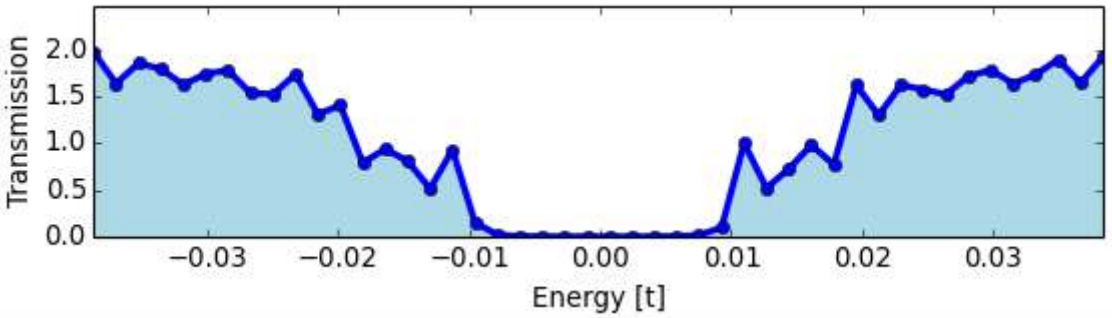
Bandstructure







Anderson disorder



Magnetic Anderson

Take home

- **On the fly** quantum transport calculations over selfconsistent magnetic solutions

https://sourceforge.net/projects/graphenelikeribbons

Funded by

Spinograph
Spintronics in Graphene

Thank you!!!!