DFT calculation of Landau levels in 2D crystals: from black phosphorus to dichalcogenides

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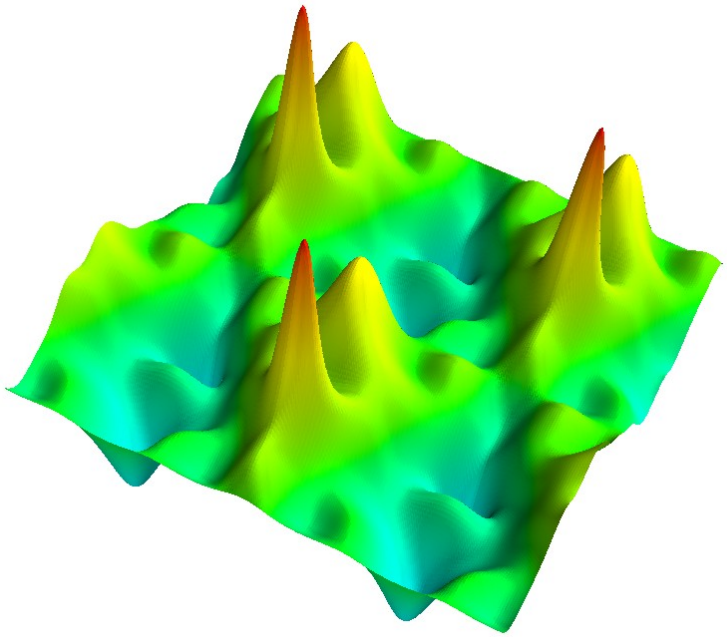
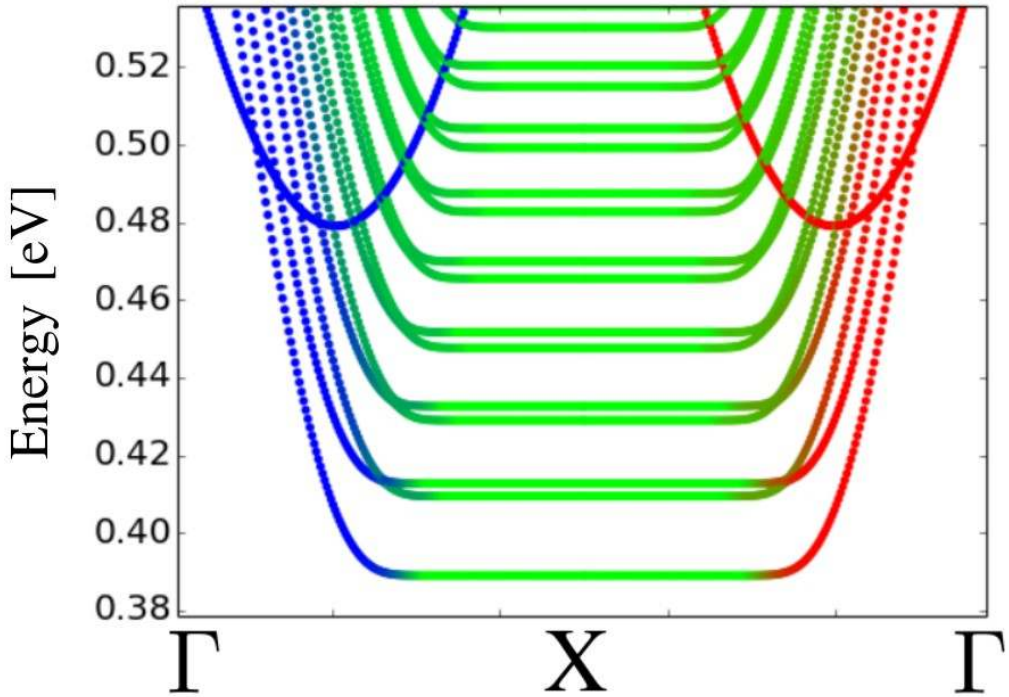
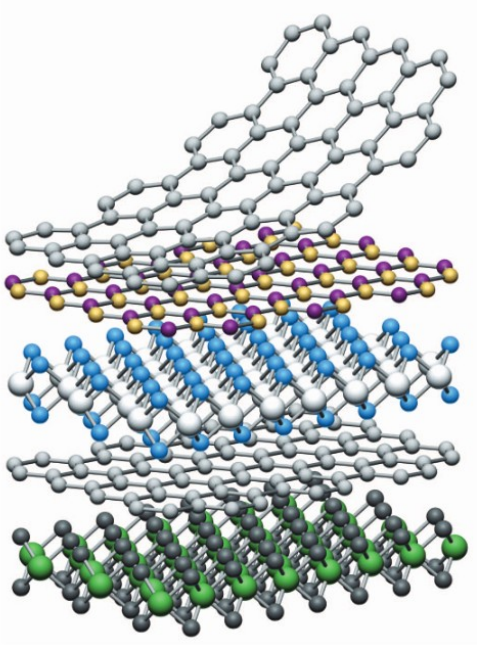


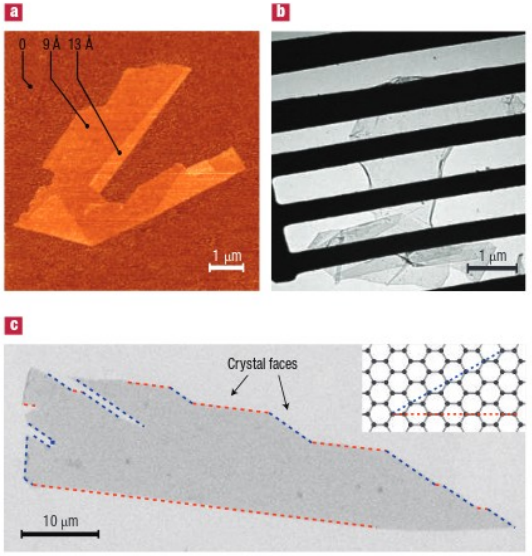


March Meeting Baltimore 2016

The rise of 2d materials



Nature **499**, 419–425 (25 July 2013)



Nature Materials **6**, 183 - 191 (2007)

How to model their electronic properties?

Analytical, tight binding and ab initio

What if no approach works?

The problem:

Quantum Hall effect in an arbitrary material

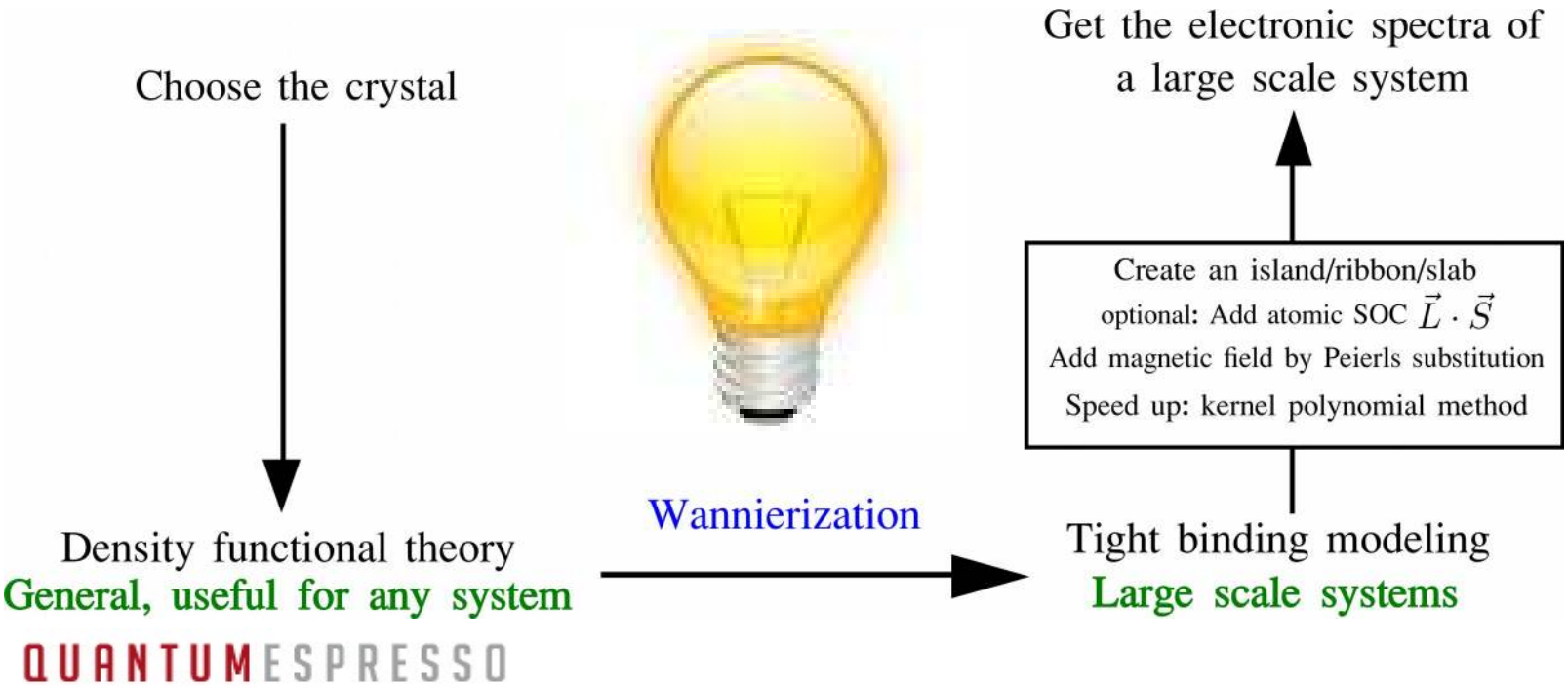
Different approaches fail

- Analytical model
  - **No clue of the analytical k.p Hamiltonian, requires derivation**
- Tight binding
  - **No clue of parameters**
- Density functional theory
  - **Way beyond current computational power**

What do we do when the three of them fail?

The solution: start with DFT, end up in tight binding

Ab initio → **Tight binding**



Wannier90 open source package

Comput. Phys. Commun. 178, 685 (2008)

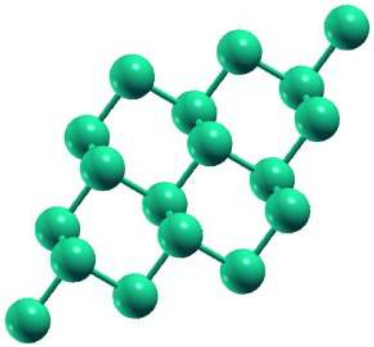
What can we calculate?

With the tight binding model, we can study:

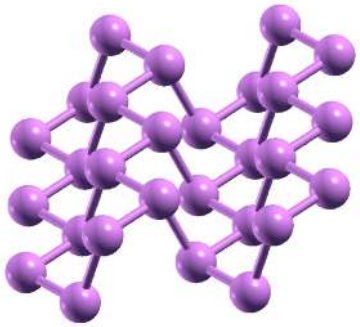
- Quantum Hall effect
- Large scale systems

Applying the general technique to new 2D materials

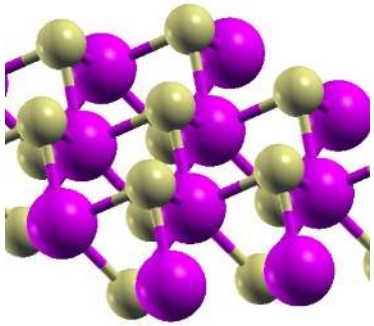
Topological insulator
Bi (111)



2D semiconductor
black phosporus

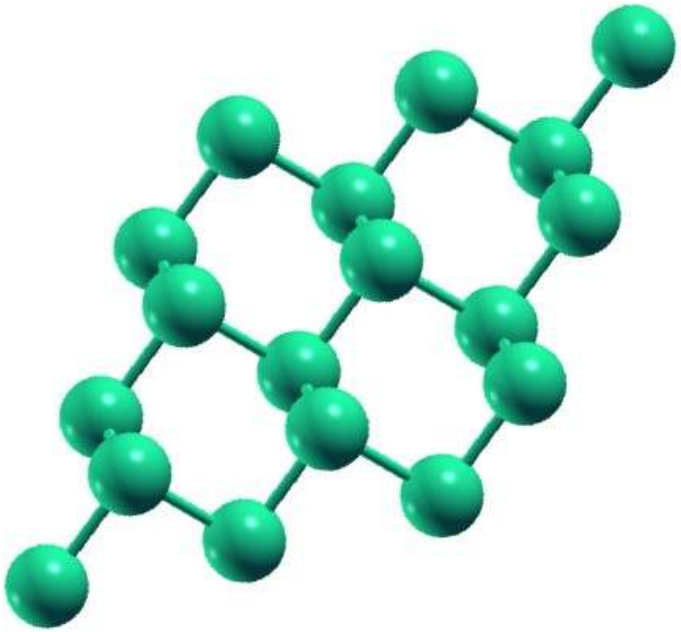


Gapped Dirac material
WSe_2, MoS_2

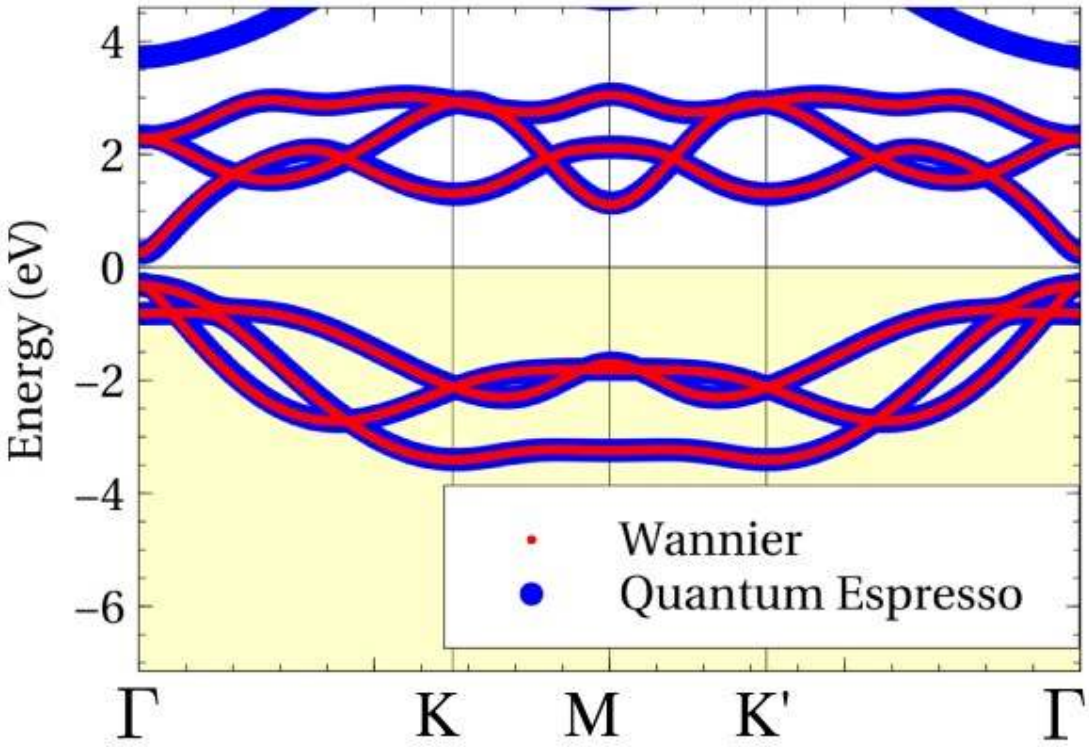


Bismuth 111

Buckled honeycomb structure



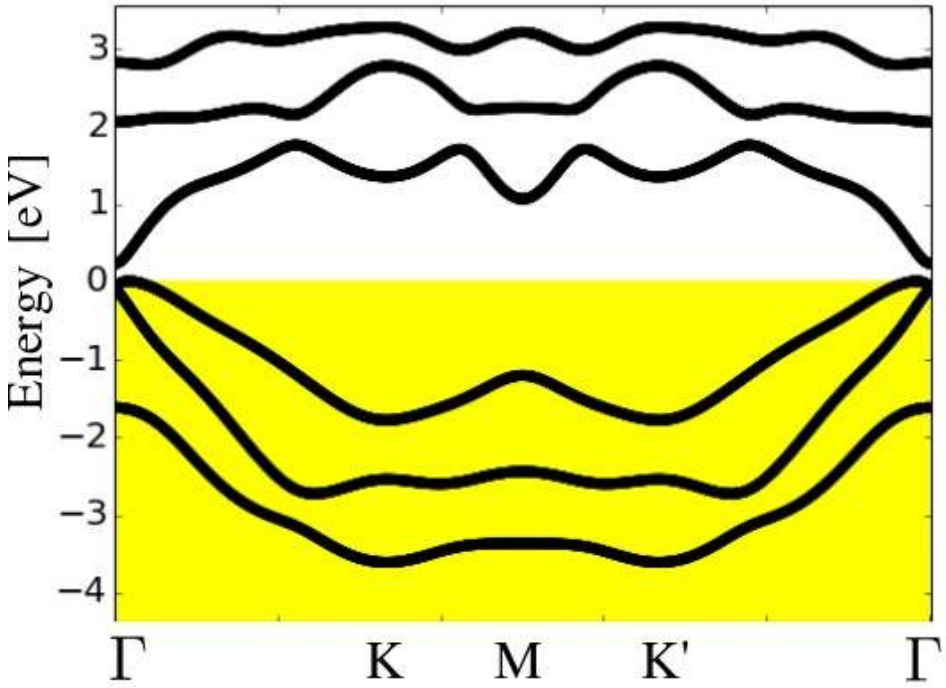
Band structure without SOC



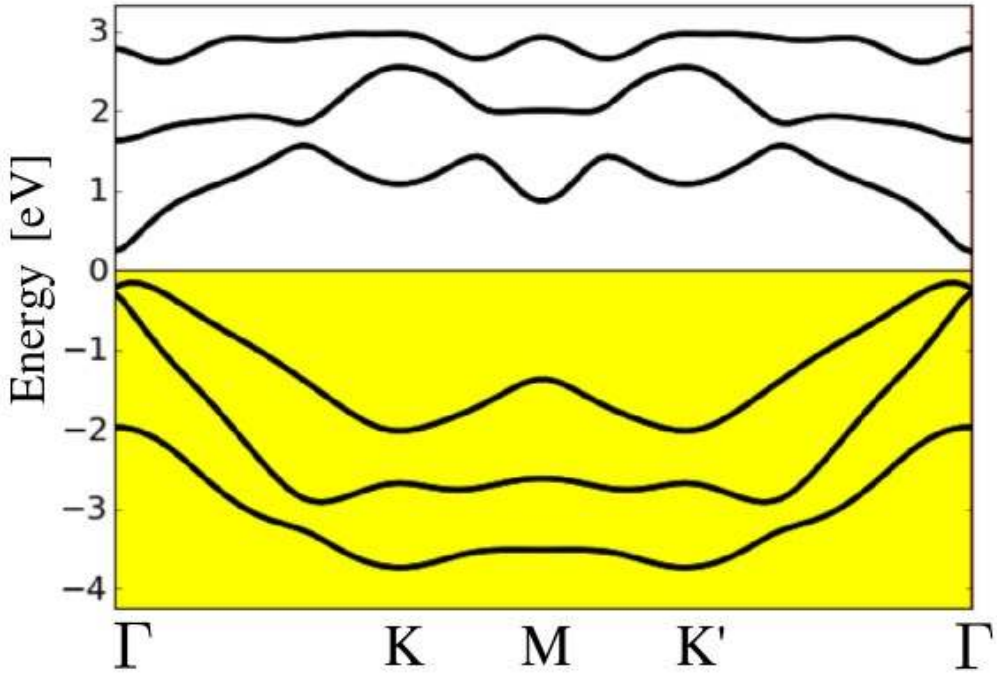
Wannier band structure with p-like states matches DFT

Bismuth 111 with spin-orbit coupling

Wannier + atomic SOC



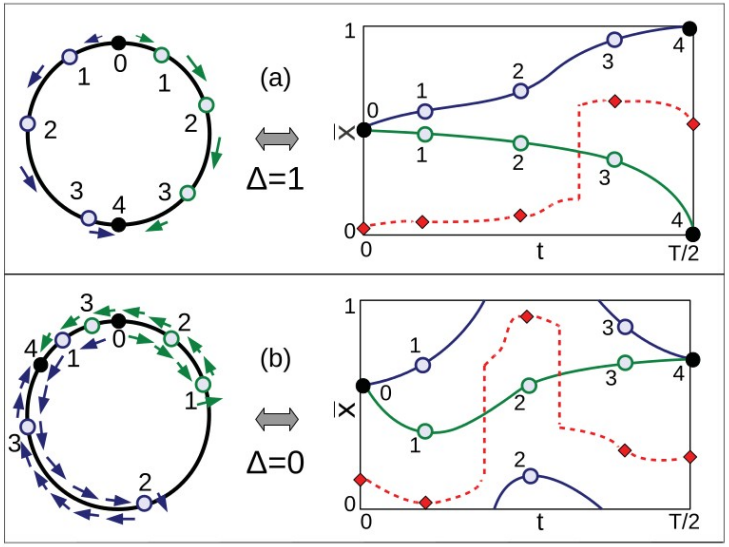
All electron DFT with SOC



Wannier + atomic SOC agrees with fully relativistic DFT

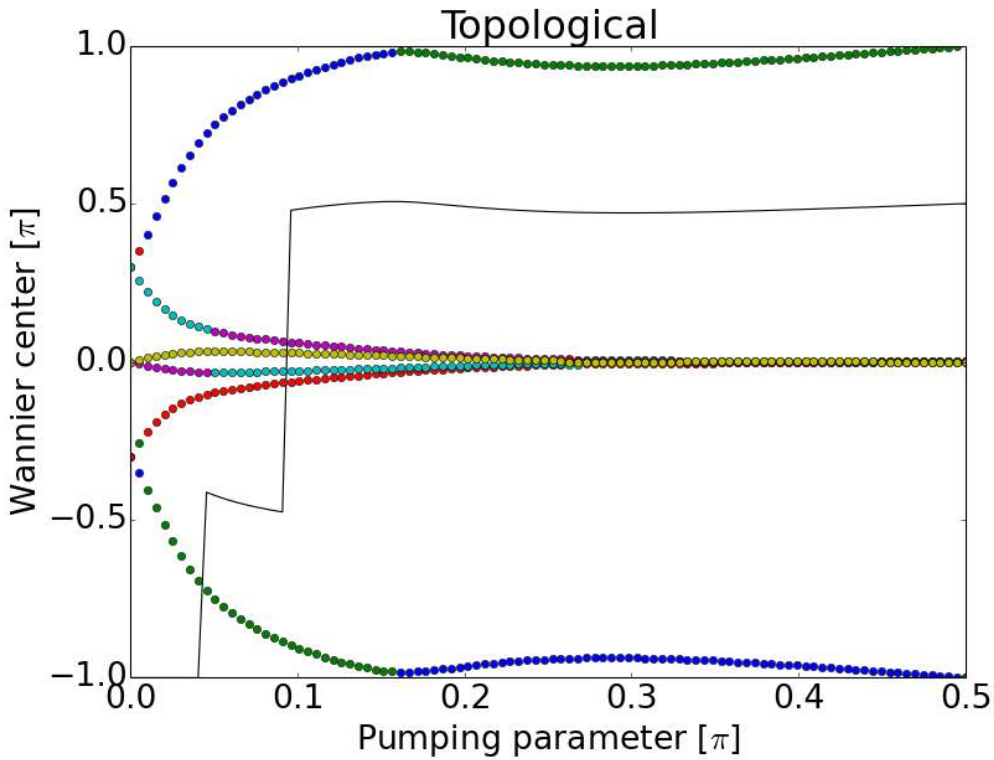
Tracking Wannier centers in Bi (111)

Follow flow of Wannier centers
in half Brillouin zone



Phys. Rev. B 83, 235401 (2011)

Evolution of Wannier centers



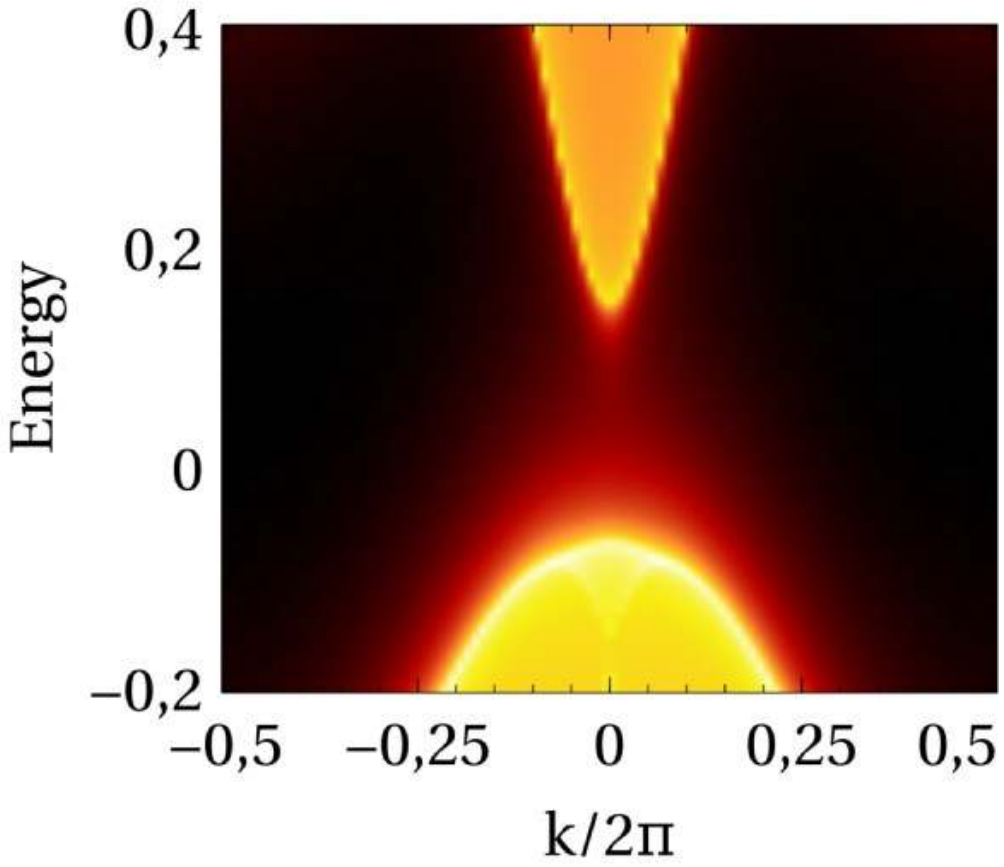
Black line cuts odd number of times

System is topological

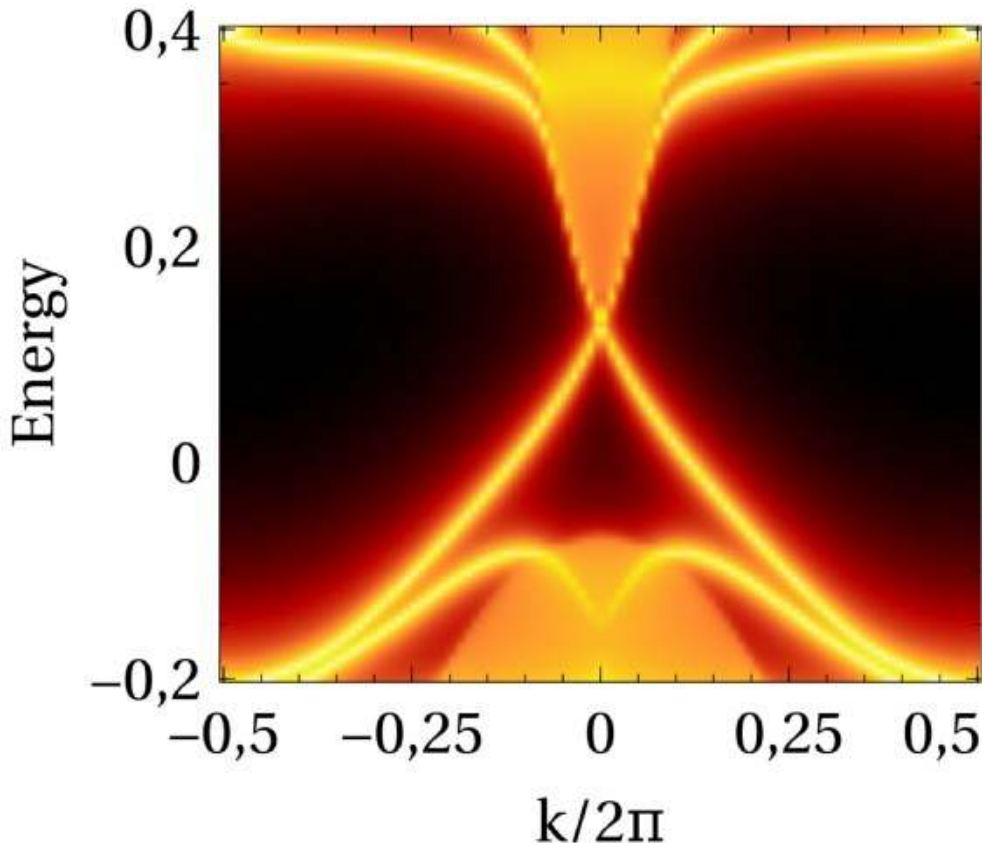
k-resolved spectral DOS Bi(111)

Gapless surface states and gapped bulk spectrum

Bulk k-resolved DOS



Surface k-resolved DOS

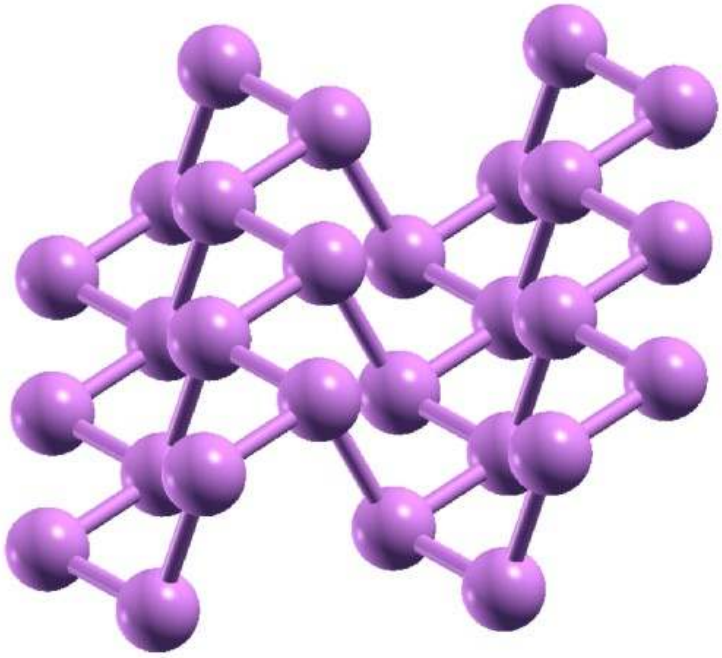


Non trivial topology

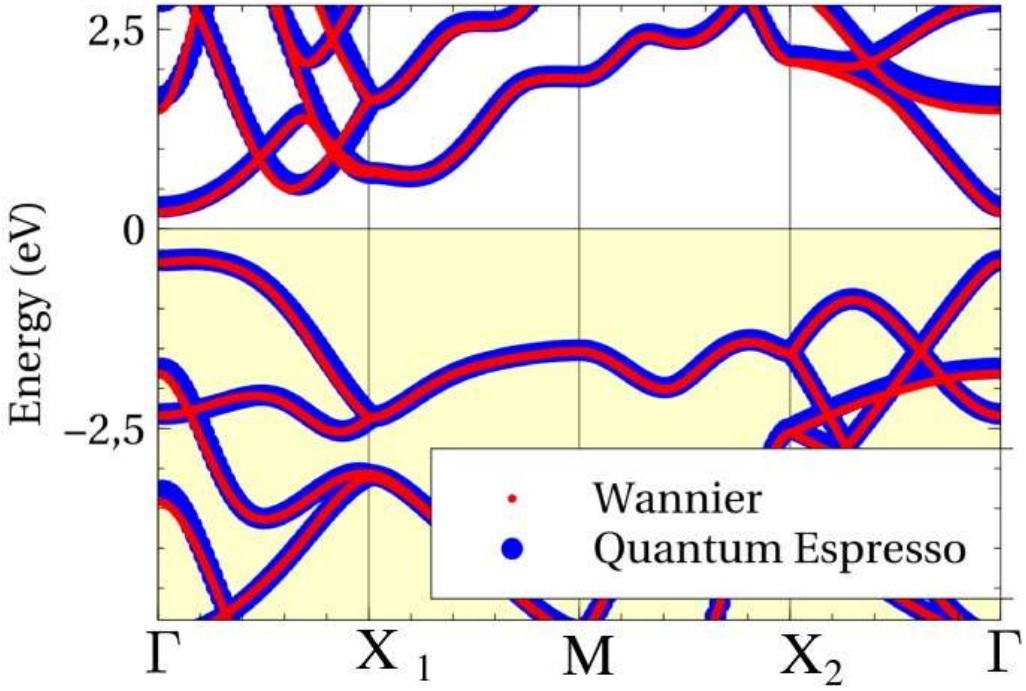
Phys. Rev. Lett. 107, 166801 (2011)

2D semiconductor: black phosphorus

Distorted hexagonal lattice

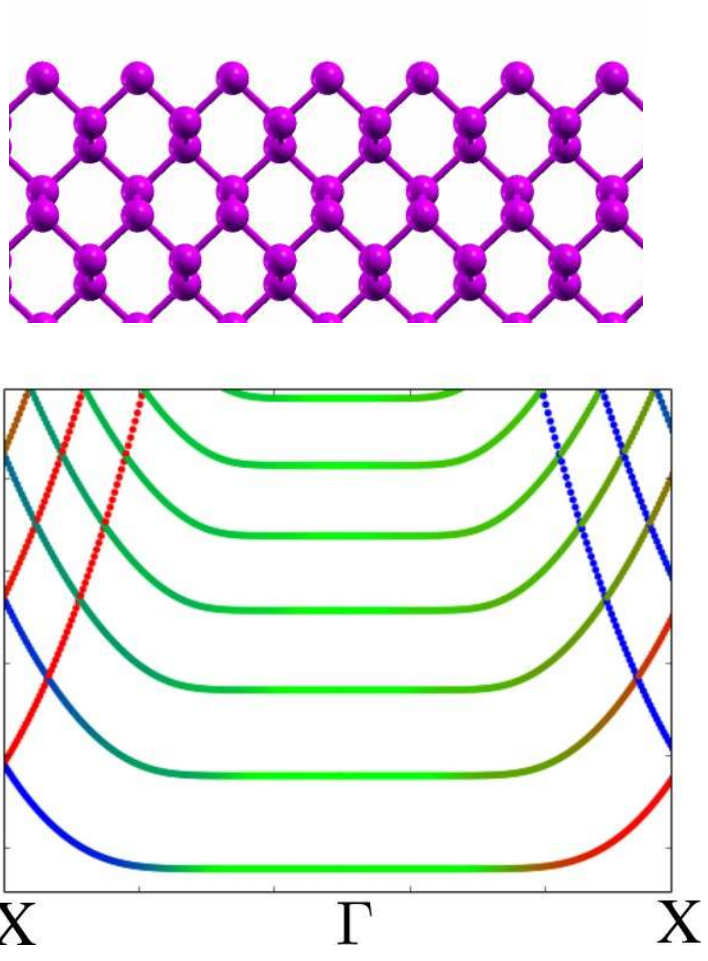


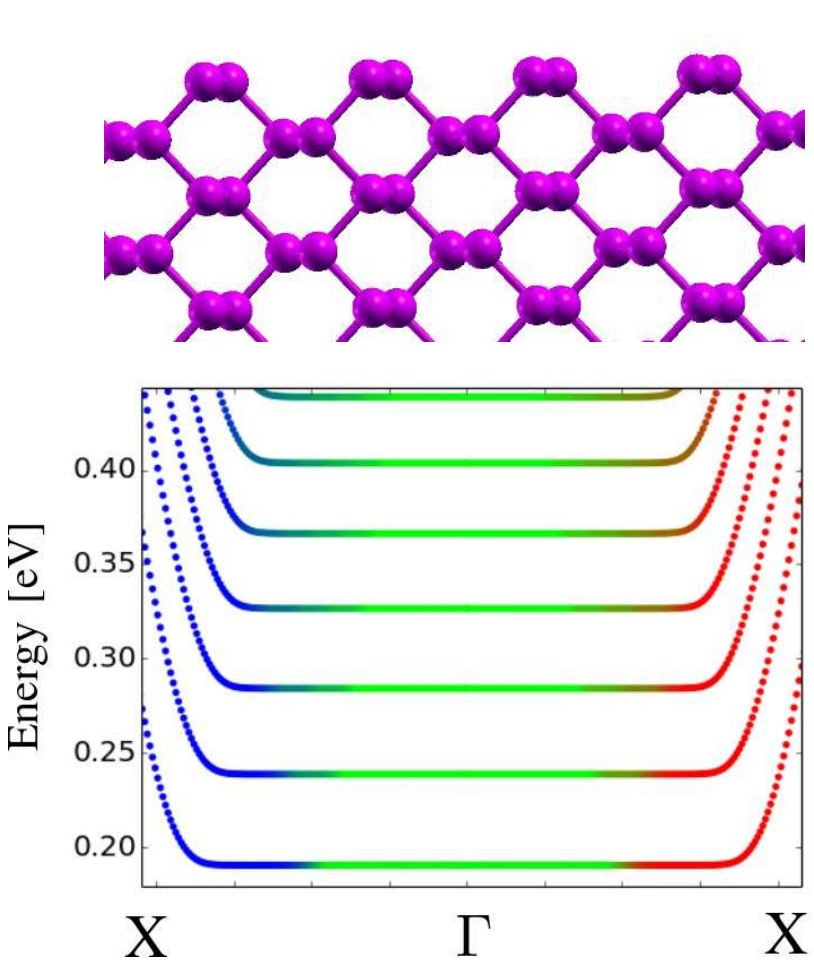
2D band-structure



Band structure is well captured with Wannier

Quantum Hall effect in black phosphorus



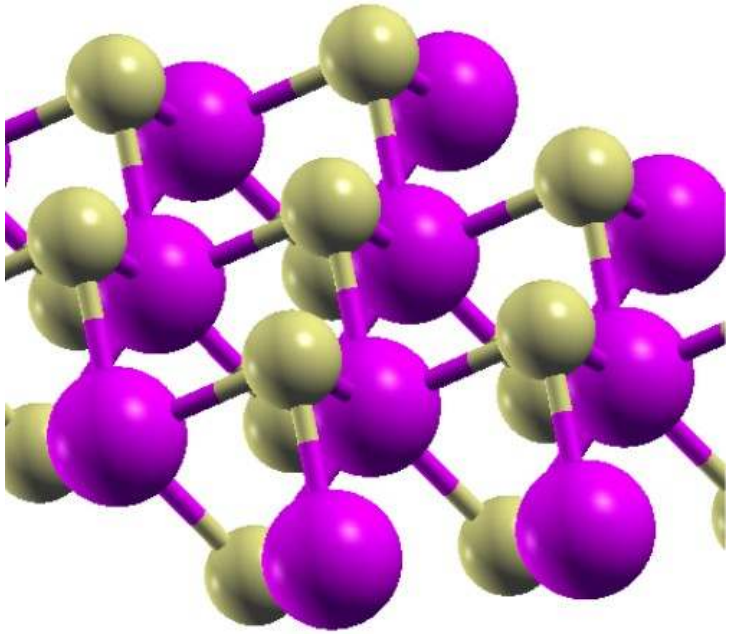


Phys. Rev. B 92, 075437 (2015)
arXiv:1504.07155 (2015)

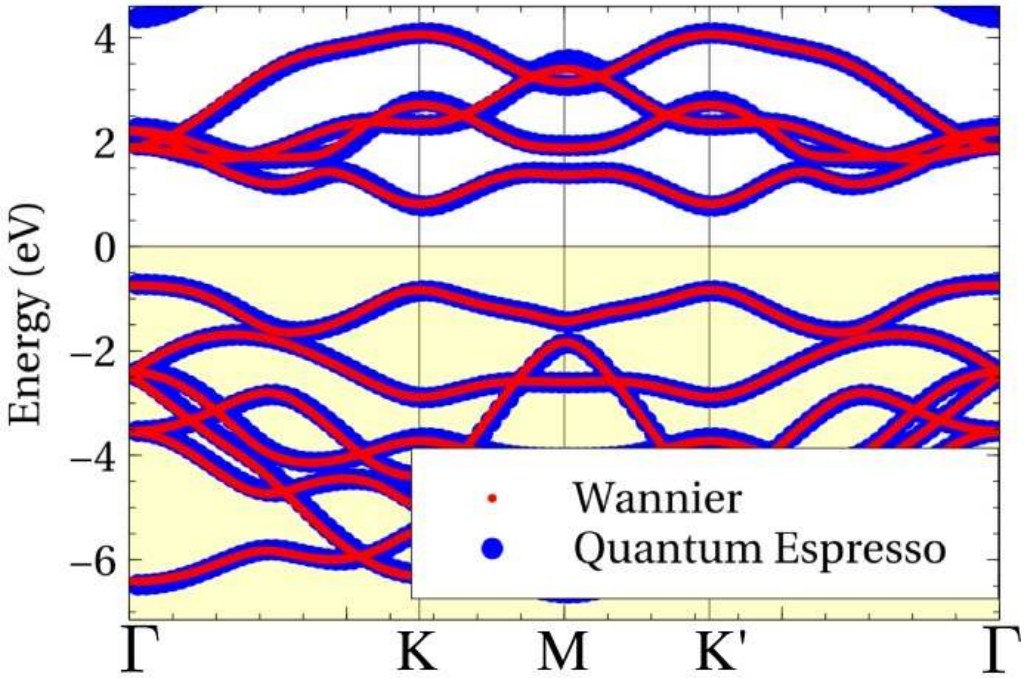
Landau spectrum in black phosphorus

Gapped Dirac material: MoS_2

Hexagonal-like structure

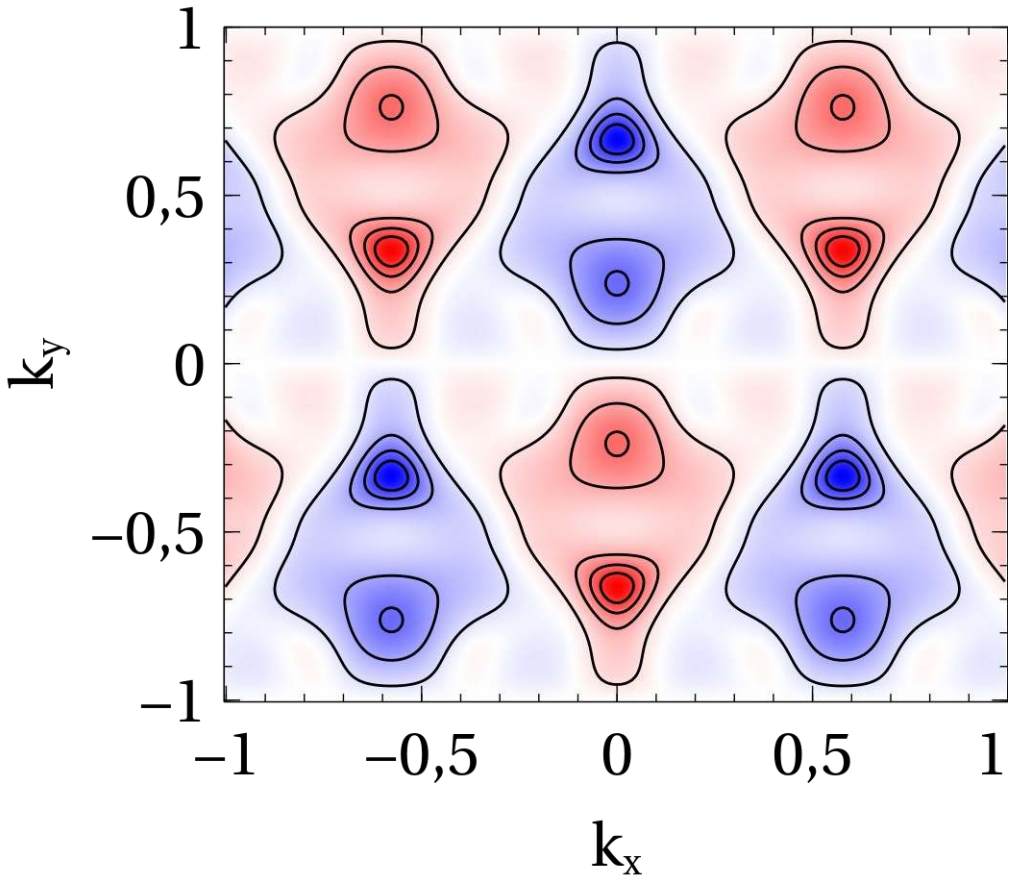


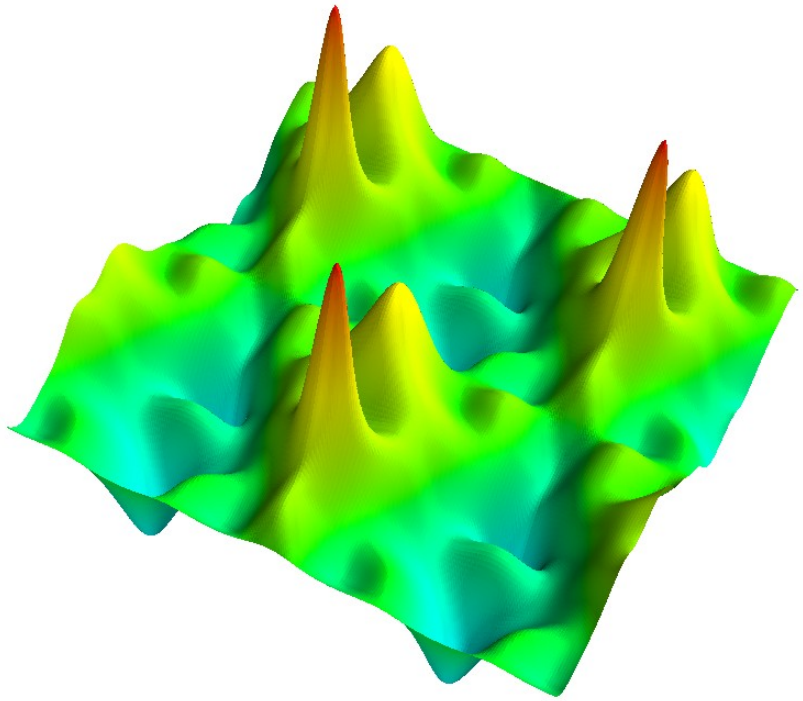
Bulk band structure



Band structure well captured with Mo d-like and S p-like Wannier states

Berry curvature in MoS_2

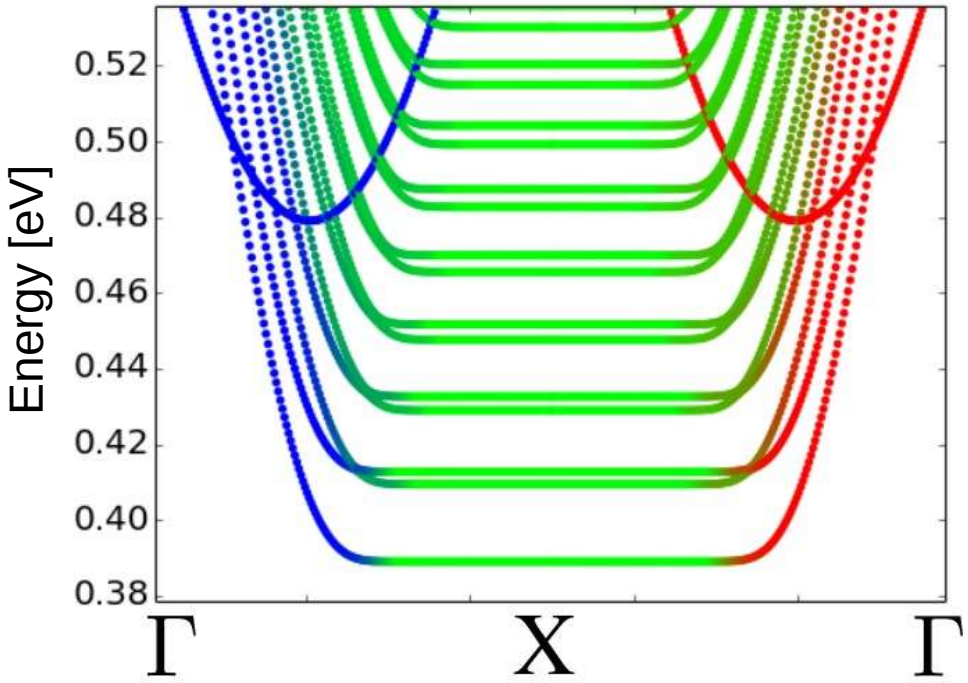




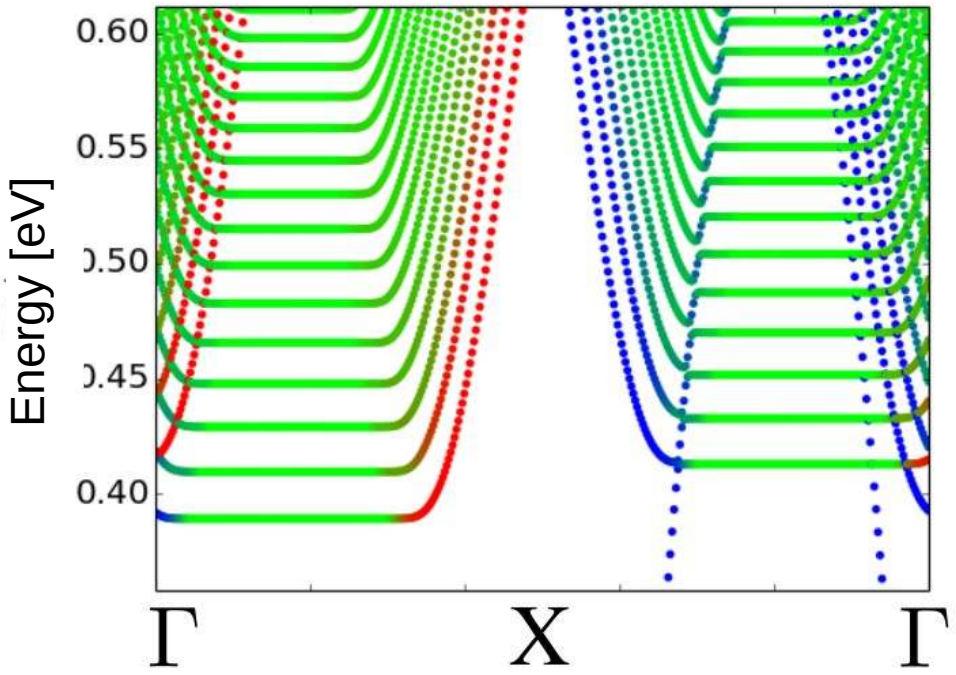
Tight binding from Wannier allows to calculate Berry curvature effects

Quantum Hall in MoS_2

Armchair edge



Zigzag edge



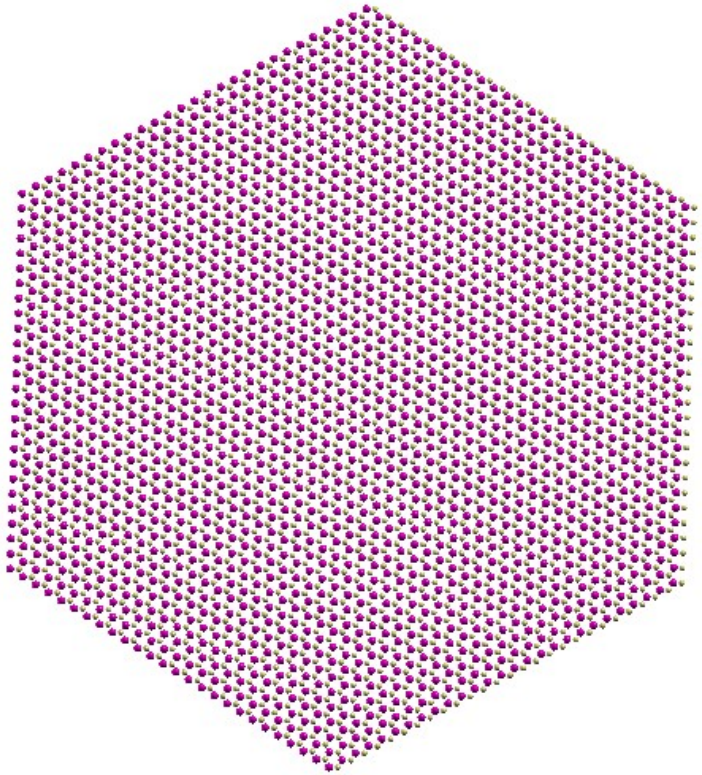
Anomalous Landau level spectra, valley dependent splitting

Phys. Rev. B 90, 045427 (2014)
Phys. Rev. B 91, 075433 (2015)

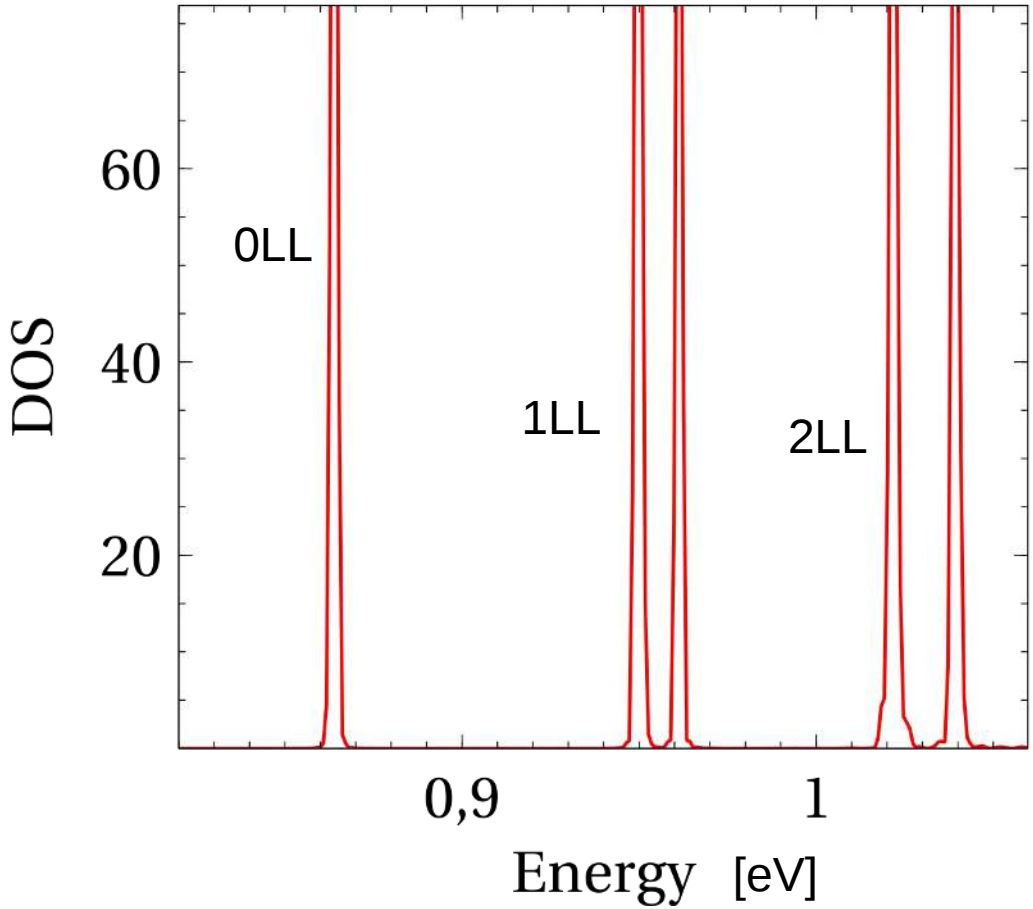
(ignoring SOC in conduction)

Quantum Hall in MoS_2 flake

Hexagonal MoS_2 flake



DOS in the center of the flake

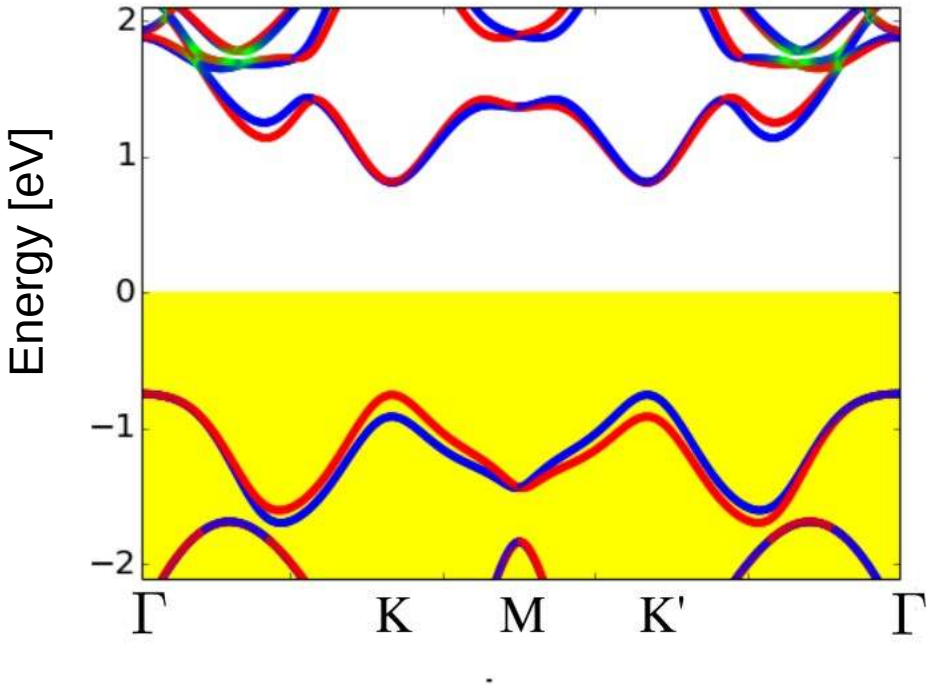


Landau levels in the bulk of quantum Hall MoS_2 flake

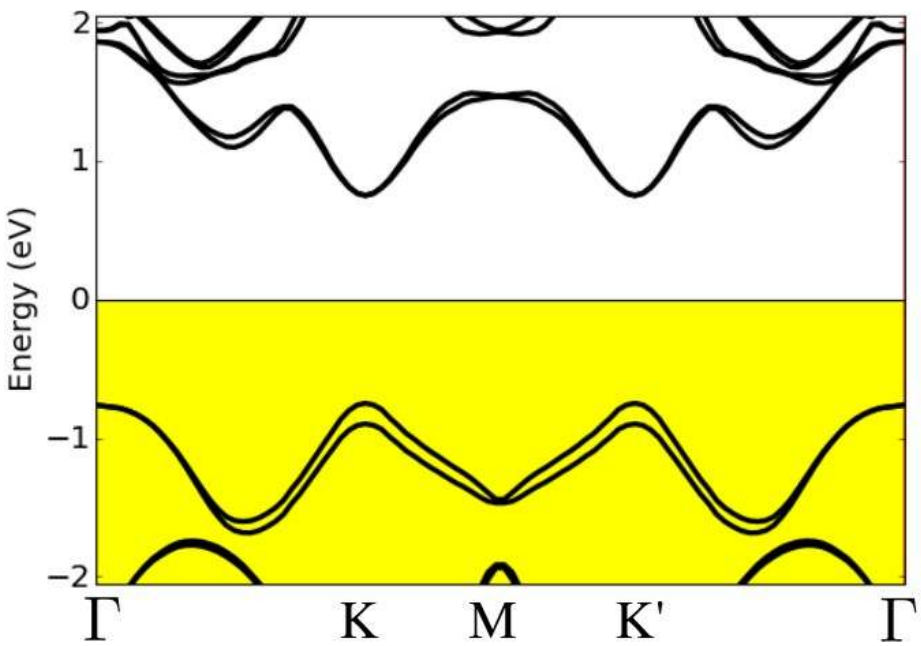
Relativistic effects in MoS_2

Spin orbit coupling can be included in the Wannier Hamiltonian

Wannier + atomic SOC



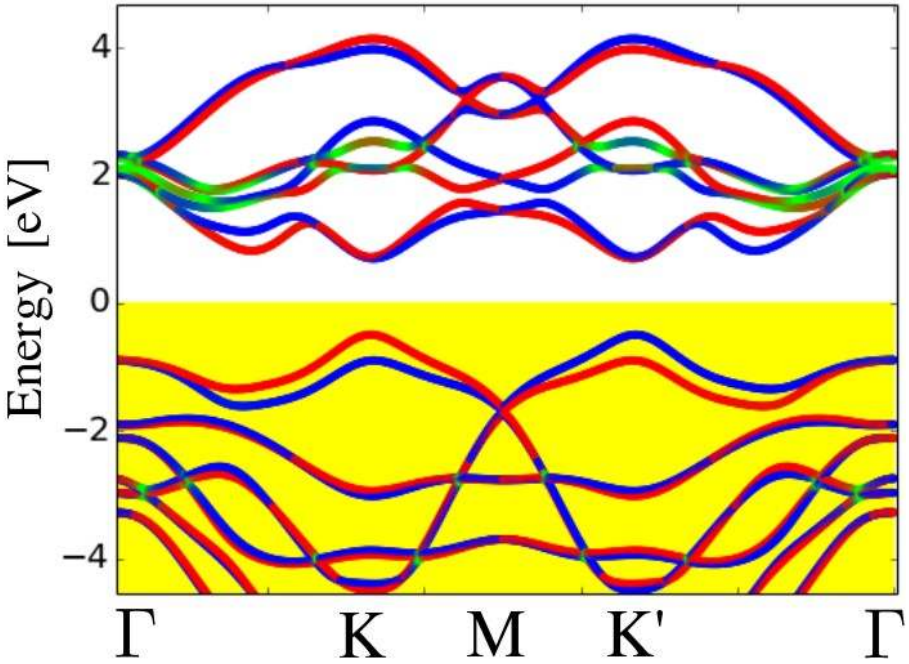
All-electron Elk with SOC



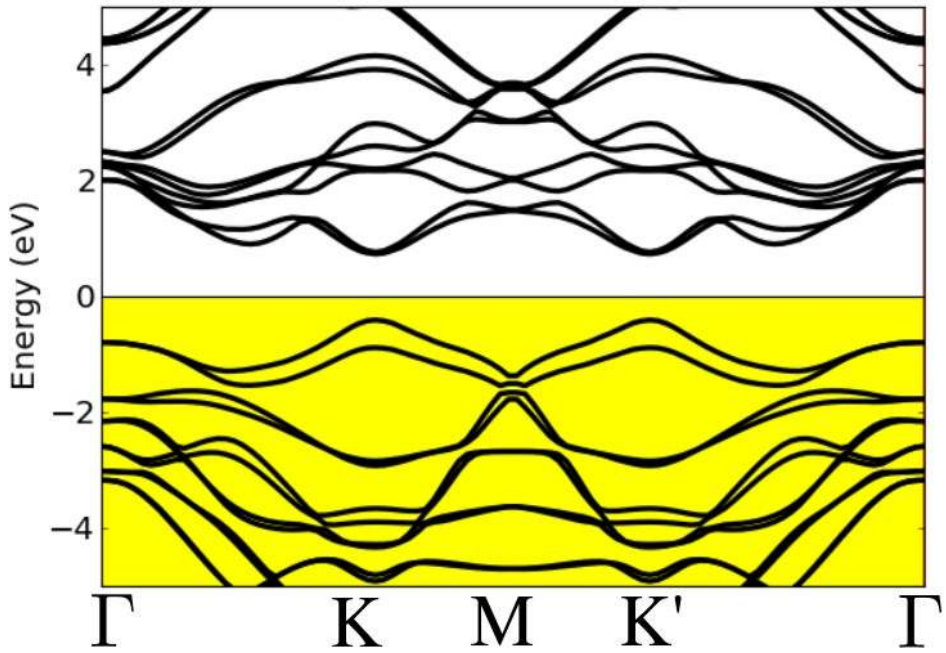
Wannier + atomic SOC captures valley dependent spin splitting

WSe_2 with spin-orbit coupling

Wannier + atomic SOC



Ab initio (Elk)

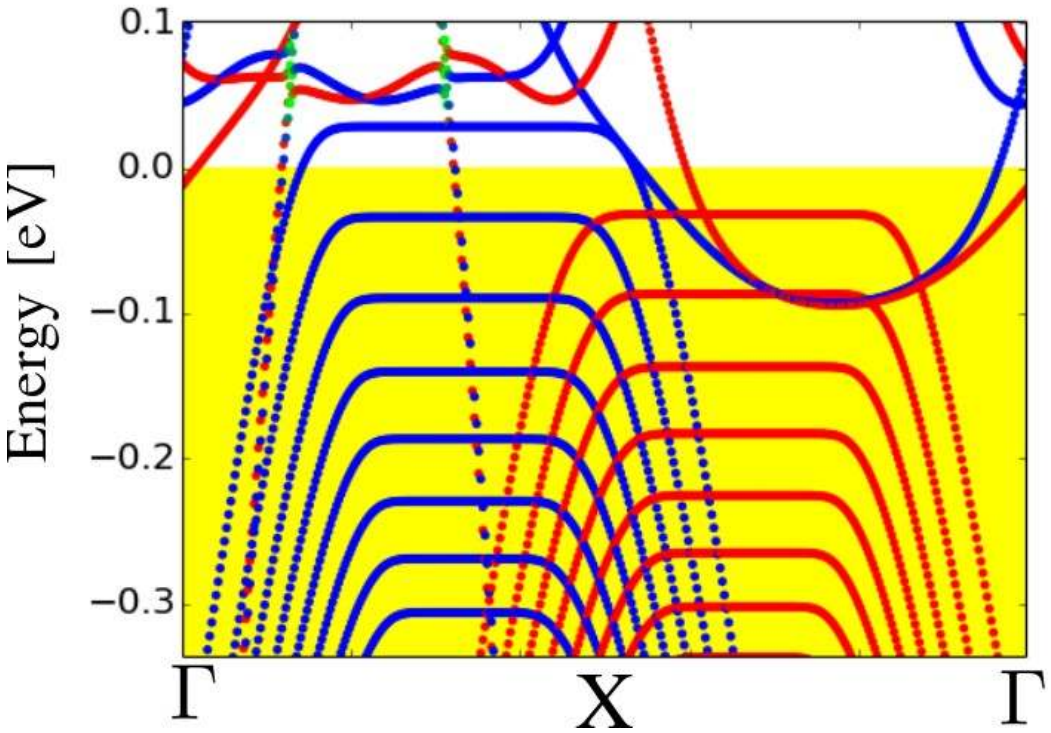


Wannierization can be also applied to other dichalcogenides

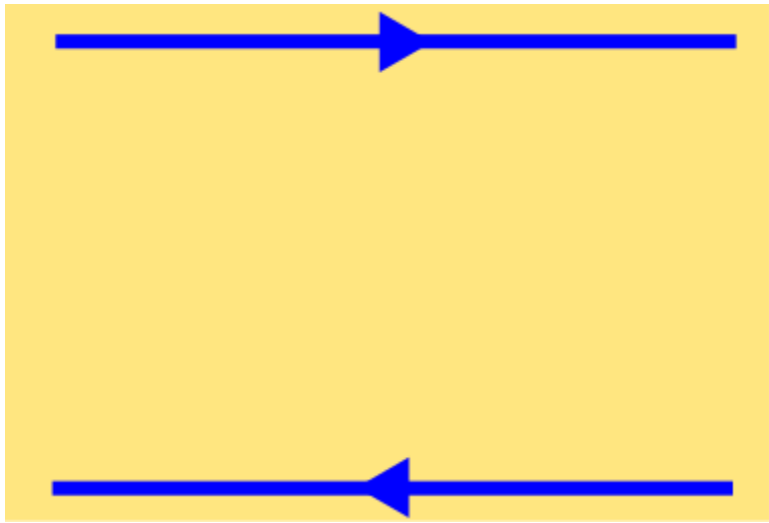
Quantum Hall in WSe_2 (SOC)

Quantum Hall bar (zigzag)

red spin up, blue spin down



Sketch of edge states



Spin polarized Quantum Hall without electronic interactions

Pros and cons of the whole method

- **Pros**
  - Any material (single particle picture)
  - Large scale systems: ribbons, islands, slabs...
  - Allows to control SOC, magnetic field, defects, interfaces...
- **Cons**
  - Ignores structural/surface/electronic reconstruction
  - Inherits all the problems of DFT

Summary

- Wannierization allows to systematically get tight binding models for 2D materials, that can be used as starting point to study further electronic properties

Thank you!!

We acknowledge financial support from

Spinograph
Spintronics in Graphene