Moire physics and symmetry breaking in magnetically encapsulated van der Waals heterostructures

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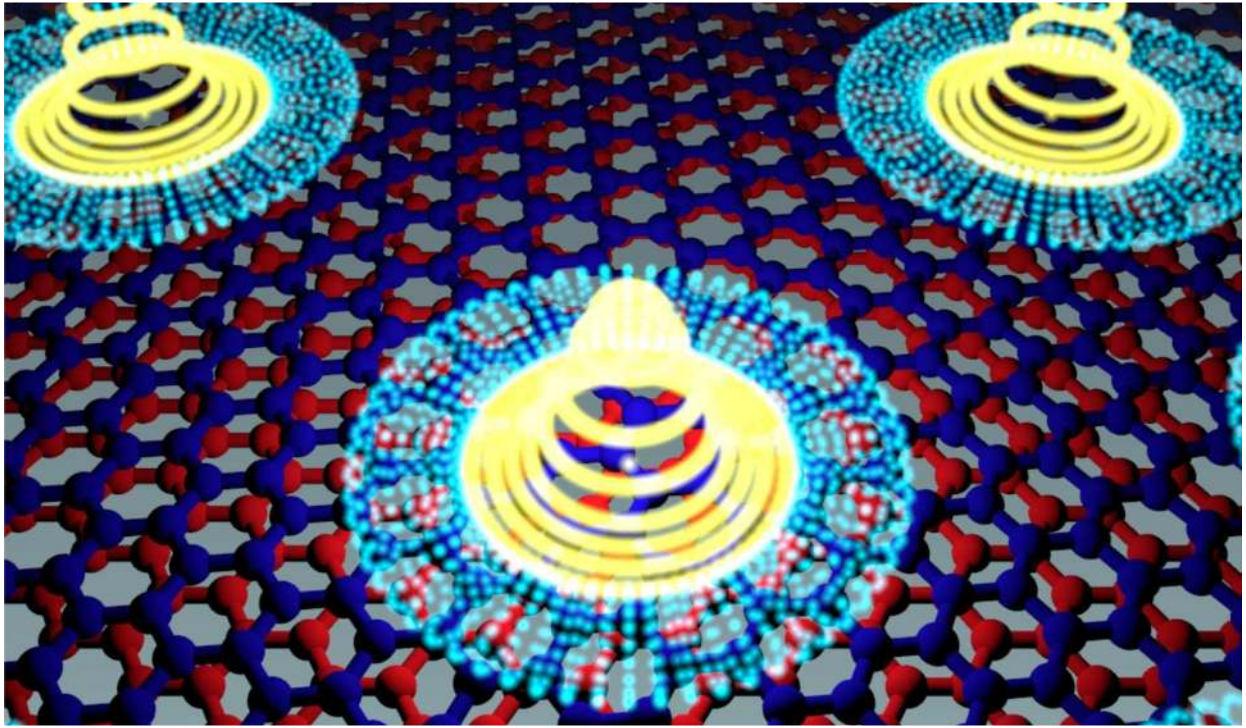


CMD2020GEFES Flat band Moires Mini-colloquia, September 3rd 2020

Exotic physics in quantum materials

Quantum spin liquids

Unconventional superconductivity

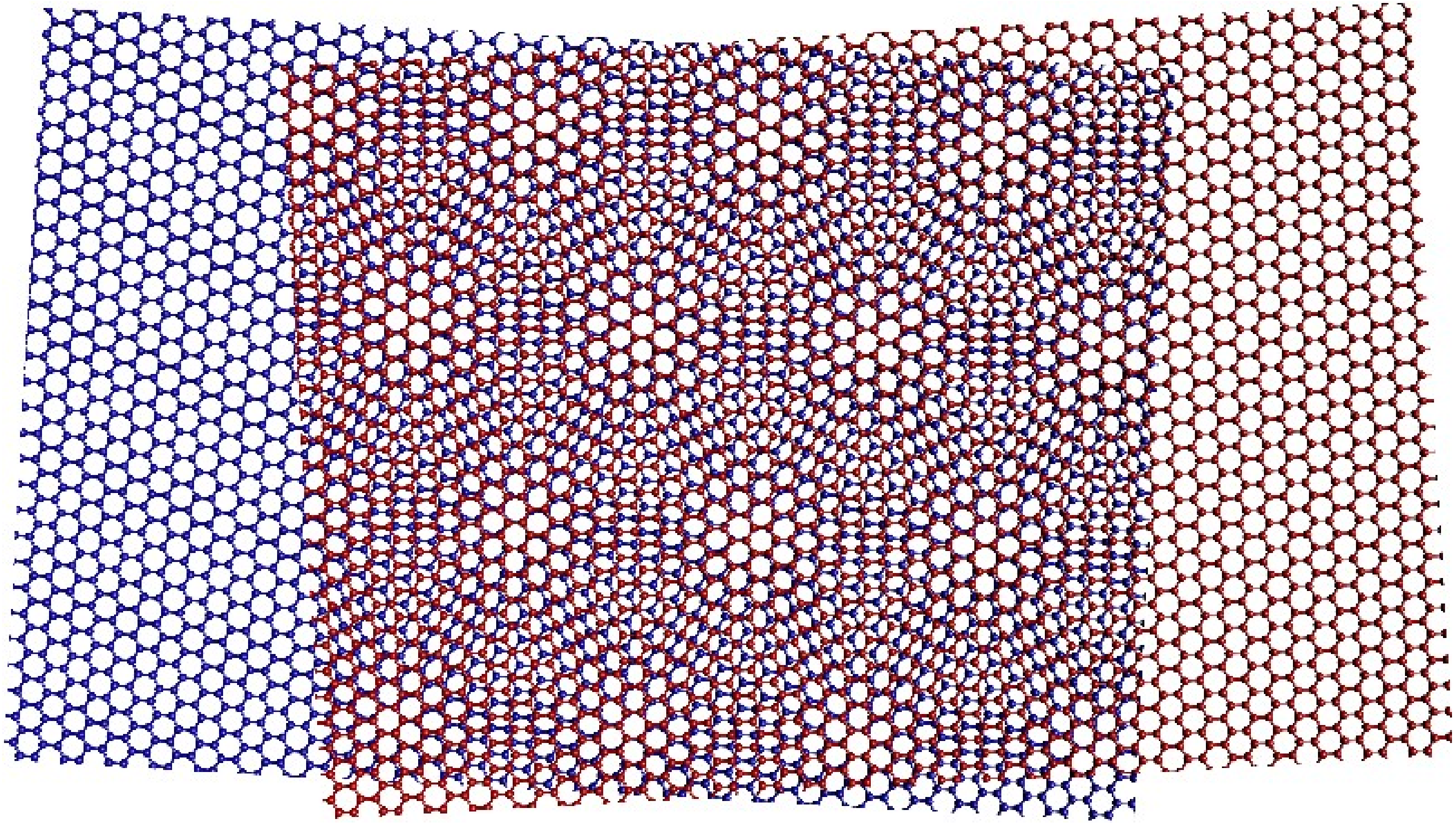
Topological matter

Topological quantum computing

Low consumption electronics

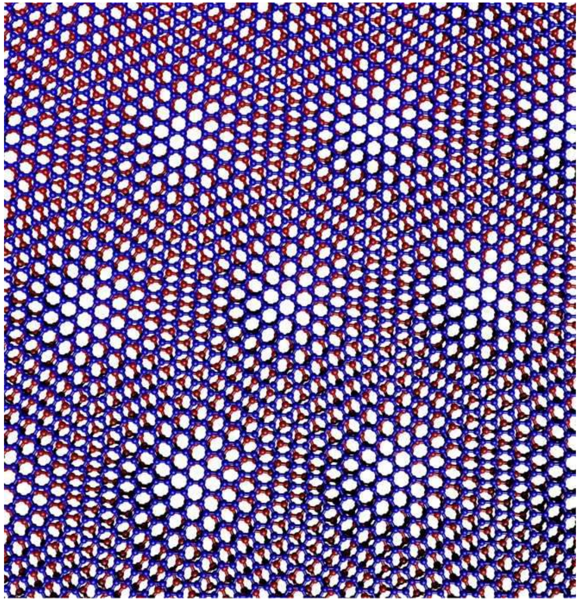
New physics not yet realized in nature (fractional quantum particles)

Twisted 2D materials as a platform for artificial quantum matter

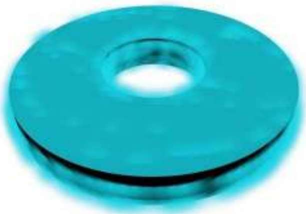


One material, a zoo of electronic phases

Twisted bilayer graphene



Superconductivity

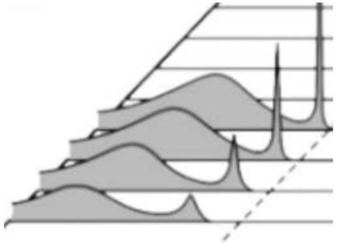


Nature 556, 43–50 (2018)

Topological networks

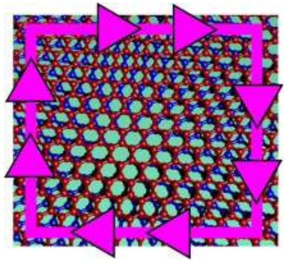
Nano Lett. 18, 11, 6725-6730 (2018)

Strange metals



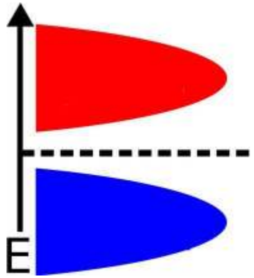
Phys. Rev. Lett. 124, 076801 (2020)

Chern insulators



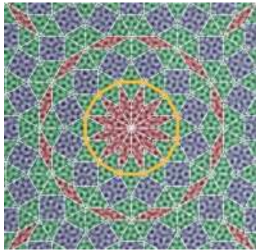
Science 365, 605-608 (2019)

Correlated insulators



Nature 556, 80–84 (2018)

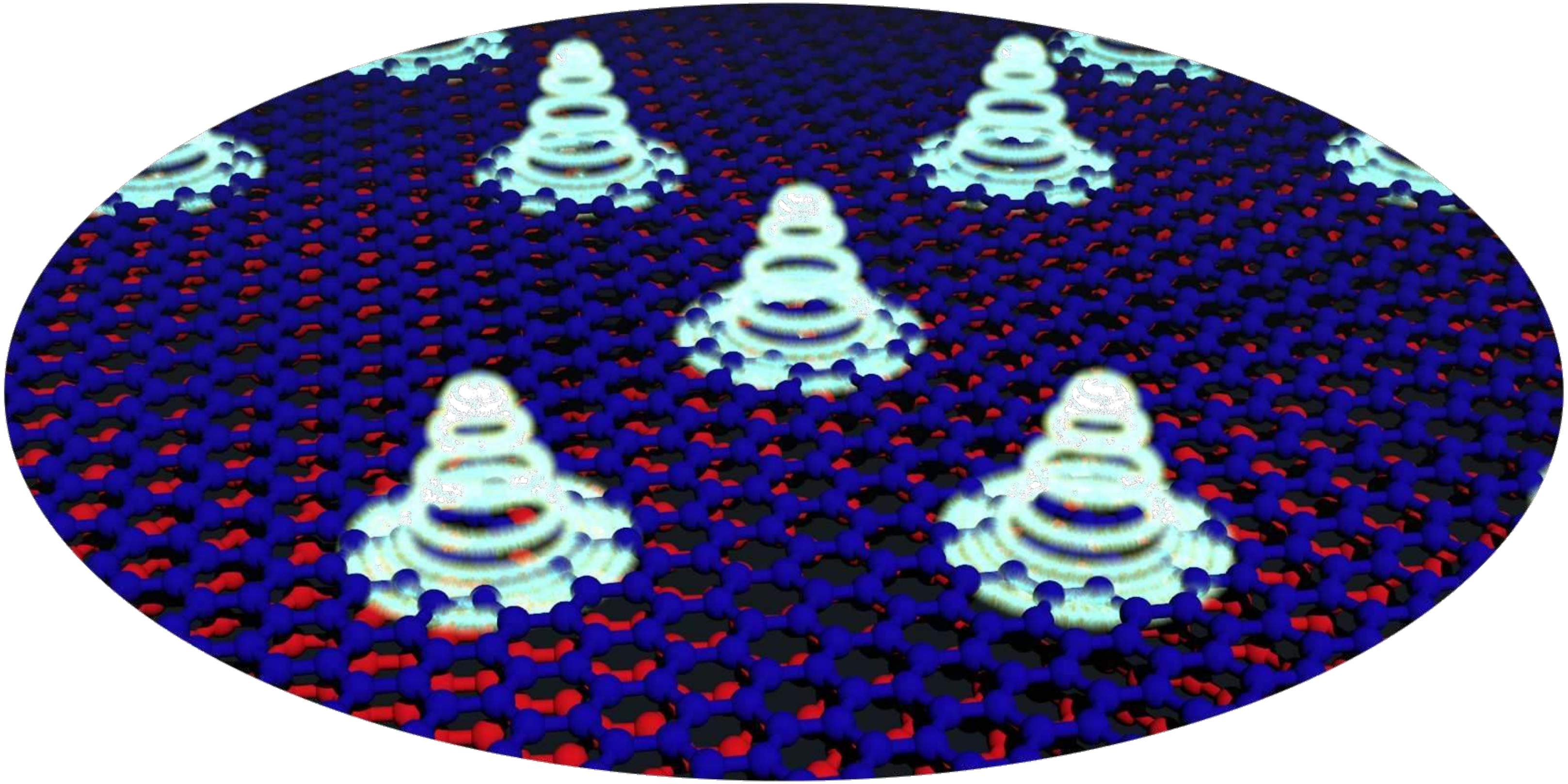
Quasicrystalline physics



Science 361 782-786 (2018)

Twisted graphene multilayers provide a powerful platform for emergent phenomena

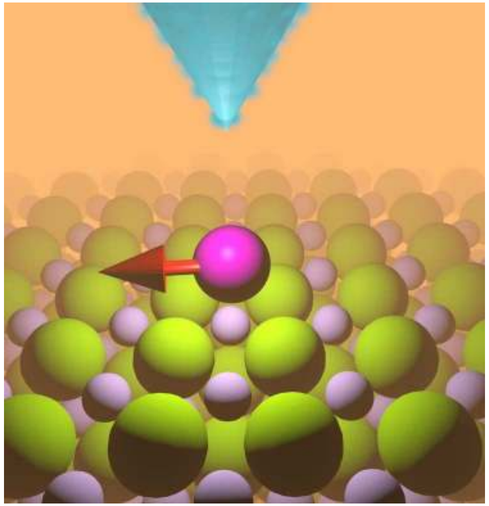
A new universe in each new twisted material



Each twisted material is a new universe for electrons, with laws that change from twist to twist

Building quantum matter with artificial lattices

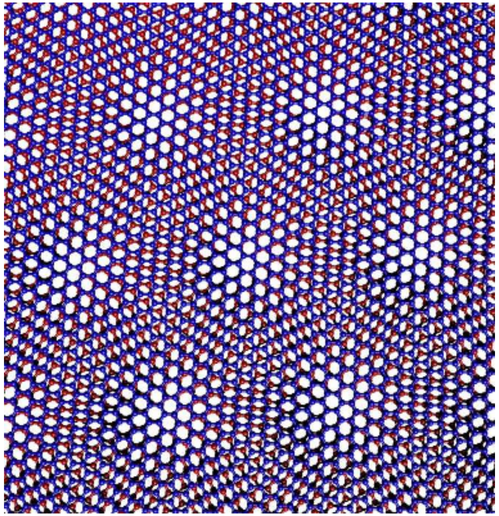
Atomic lattices



a = 0.5 nm

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

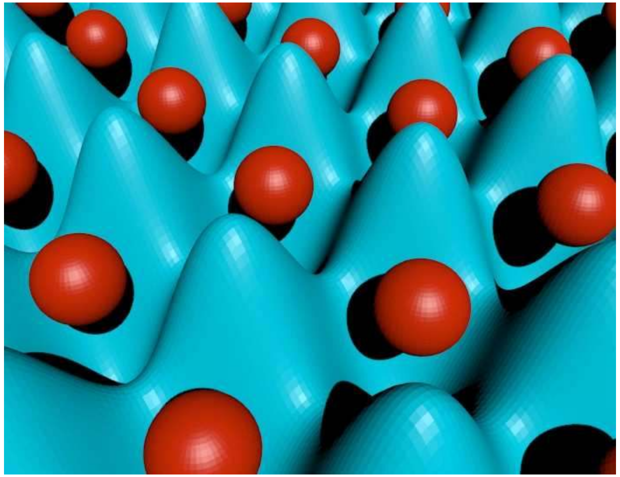
Twisted 2D moire materials



a = 30 nm

Nature 556, 80–84 (2018)
Science 363 (6431) 1059-1064. (2019)

Cold atoms



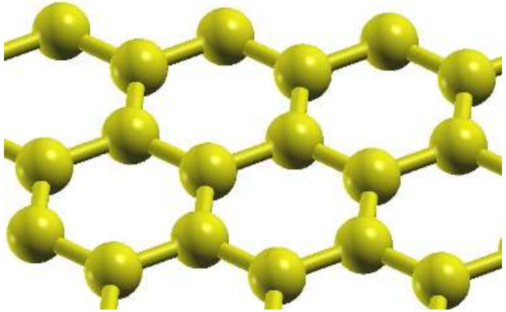
a = 1000 nm

Nature 545.7655 (2017)
Nature 455.7210 (2008)
Phys. Rev. Lett. 111, 185307 (2013)

The two-dimensional materials world

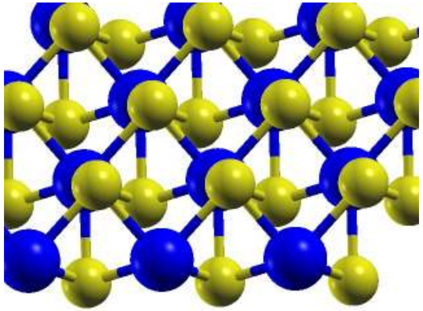
Semimetal

Graphene



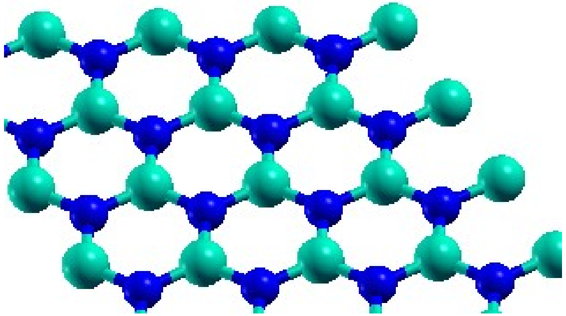
Superconductor

$NbSe_2$



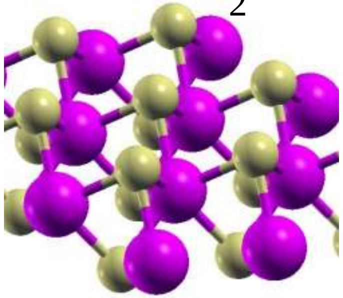
Insulator

BN



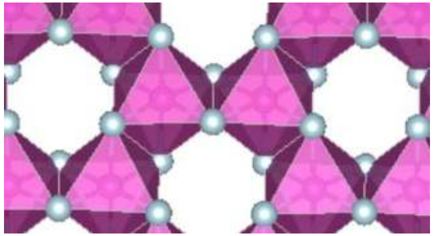
Semiconductor

WSe_2



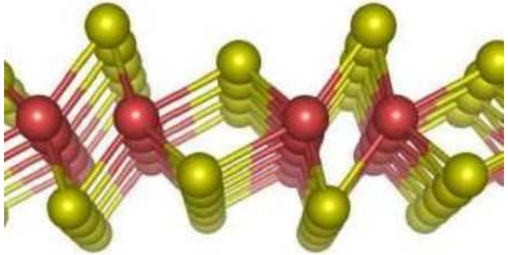
Ferromagnet

CrI_3



Quantum spin Hall insulator

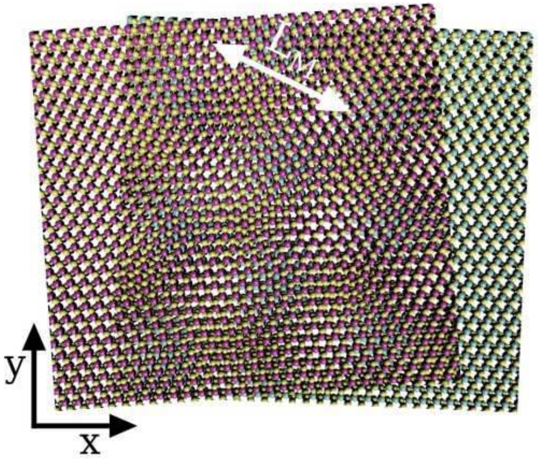
WTe_2



The generality of correlated physics in twisted 2D materials

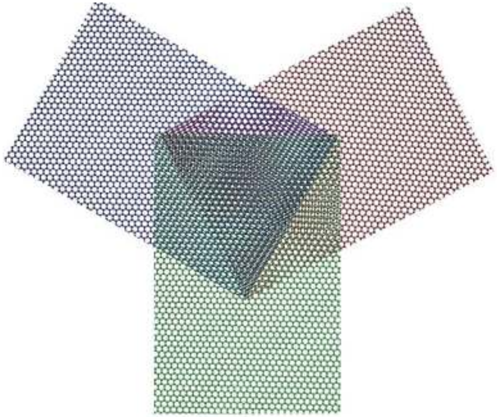
Superconductivity & Correlated behavior found also in

Twisted dichalcogenides



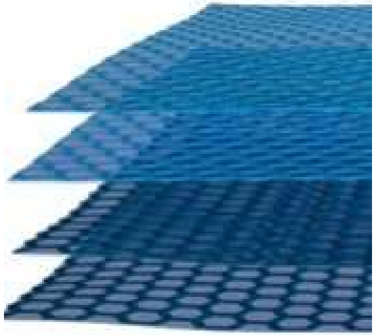
Nature 579, 359–363 (2020)

Twisted graphene trilayers



arXiv:1912.03375 (2019)

Twisted graphene tetralayers

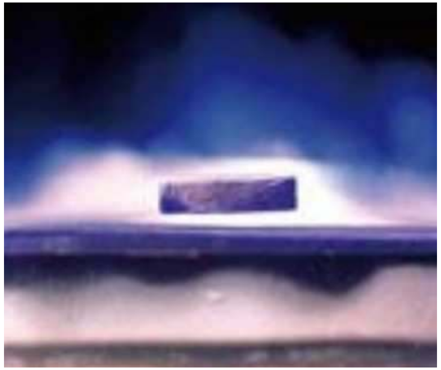


Nature 583, 221–225 (2020)

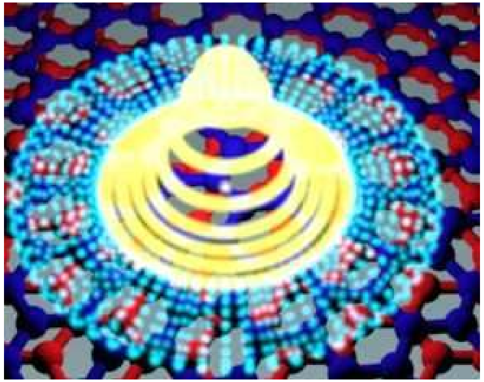
<u>**Some of new physics observed were only realized before in rare, heavy or even toxic compounds**</u>

The opportunities of twisted van der Waals materials

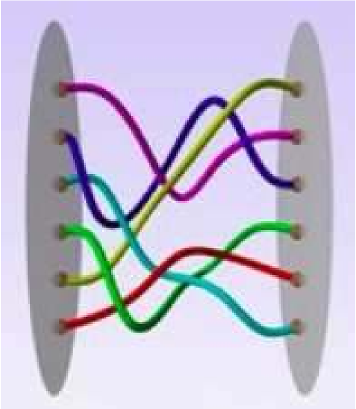
"Unveil" the nature of high T_C superconductivity (?)



Controllable exotic quantum matter (?)



A platform for topological quantum computing (?)



Explore exotic physics with a degree of control unprecedented in any other material

→ *Control of single particle and many-body interactions*
→ *Explore physics that only appear in rare or toxic compounds*

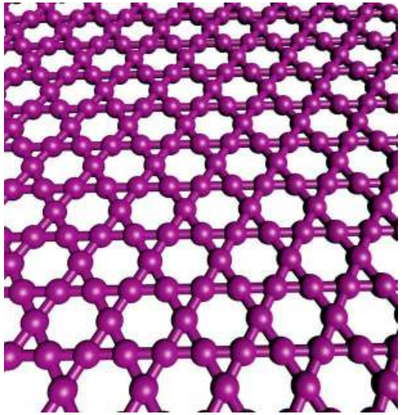
Designing quantum matter in twisted materials

The strength of electronic correlations

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

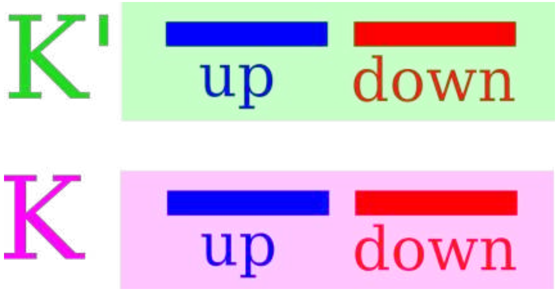
Twist angle control

The details of the electronic dispersion



Interlayer bias

The local quantum degrees of freedom

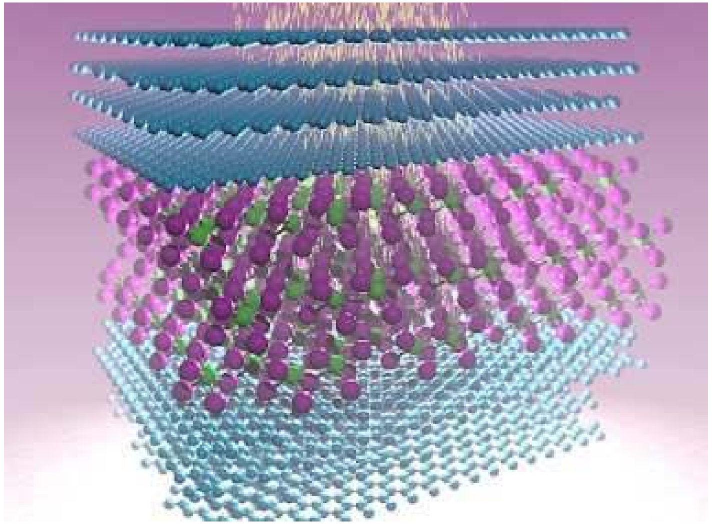


<u>Magnetic encapsulation</u>

Goal: control local degrees of freedom via magnetic encapsulation a twisted material

Van der Waals spinorbitronics

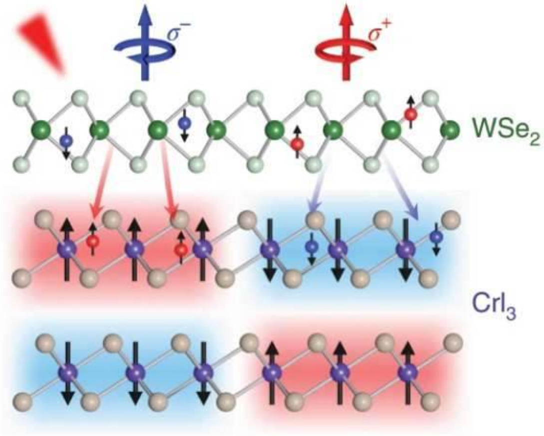
Graphene/CrI_3 heterostructures



Giant magnetoresistance

Science 360 (6394), 1218-1222 (2018)

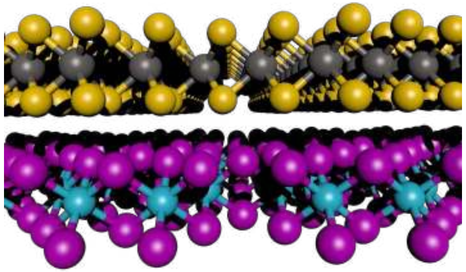
$MoSe_2$/CrI_3 heterostructures



Exchange proximity from magneto-optics

Nature Nanotechnology 15, 187–191 (2020)

$NbSe_2$/$CrBr_3$ heterostructures

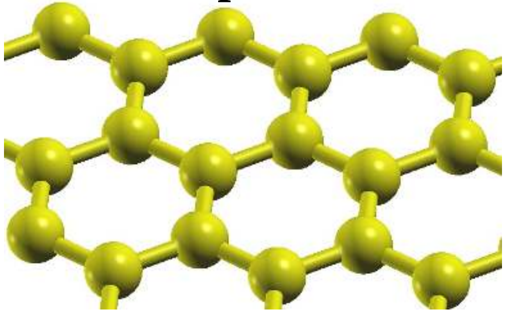


Topological superconductivity

arXiv:2002.02141 (2020)

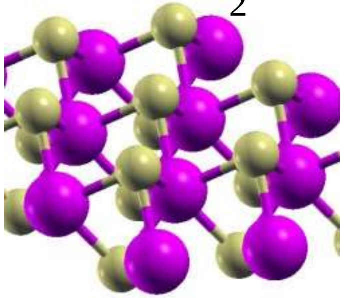
Designing quantum matter in magnetically encapsulated twisted materials

Graphene



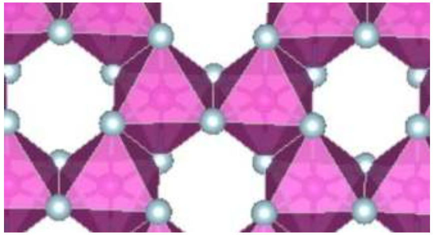
Semiconductor

WSe_2



Ferromagnet

$CrBr_3$ & CrI_3



Ingredients: Twist + exchange proximity + spin-orbit coupling + interactions

Behind the scenes

Flavor-controllable correlations in $CrBr_3$/twisted $(WSe_2)_2$/$CrBr_3$

David Soriano

arXiv:2006.09953

Valley-mixing correlations in CrI_3/twisted BG/CrI_3

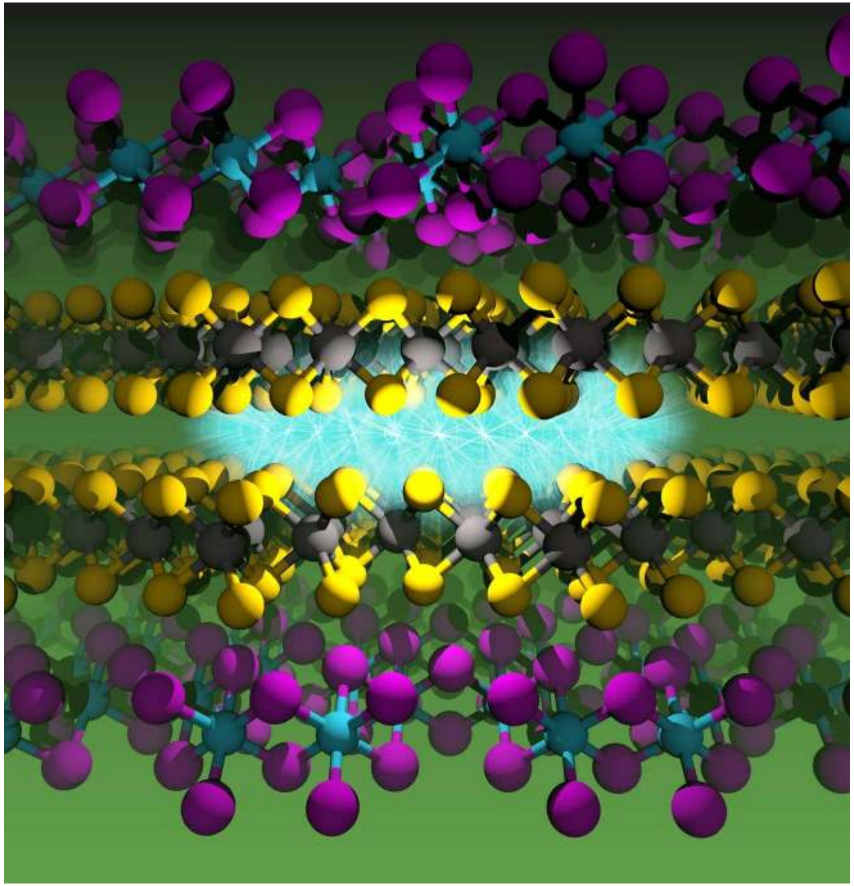
Tobias Wolf

Gianni Blatter

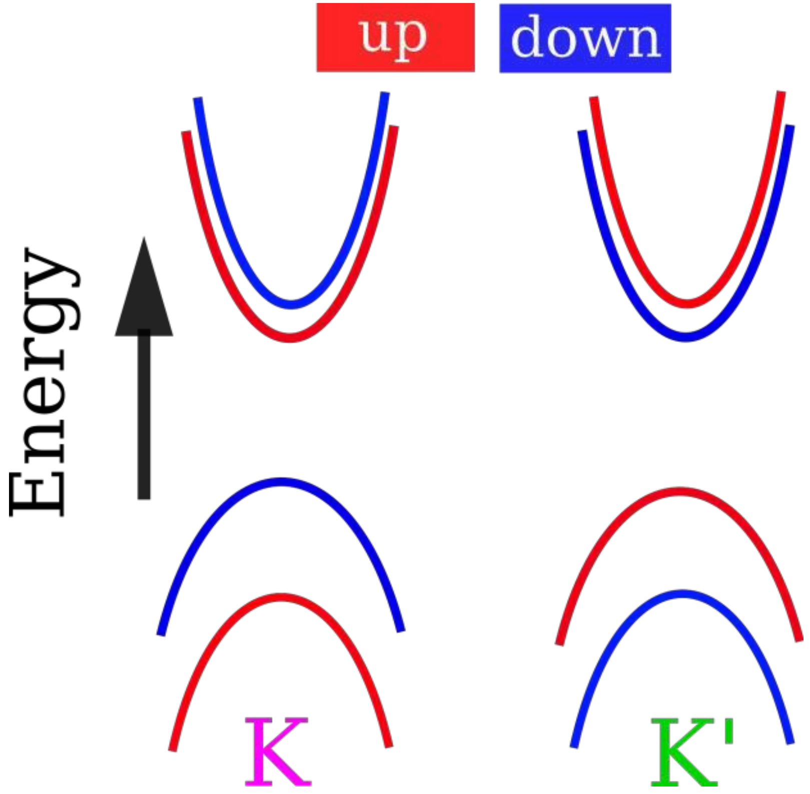
Oded Zilberberg

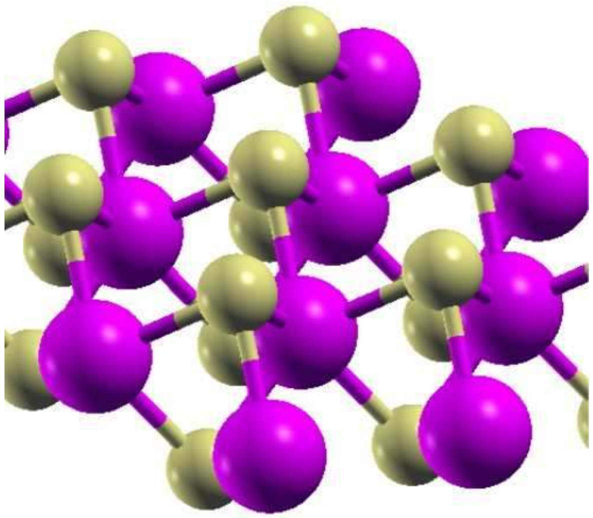
arXiv:2008.06441

Controlling flavor instabilities in twisted transition metal dichalcogenides



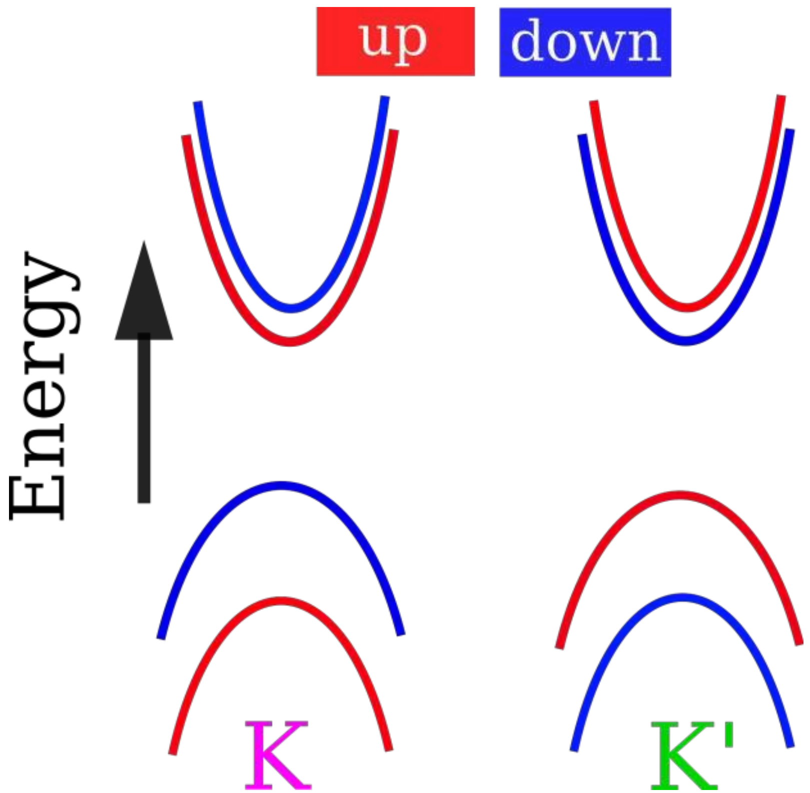
Electronic structure of WSe_2

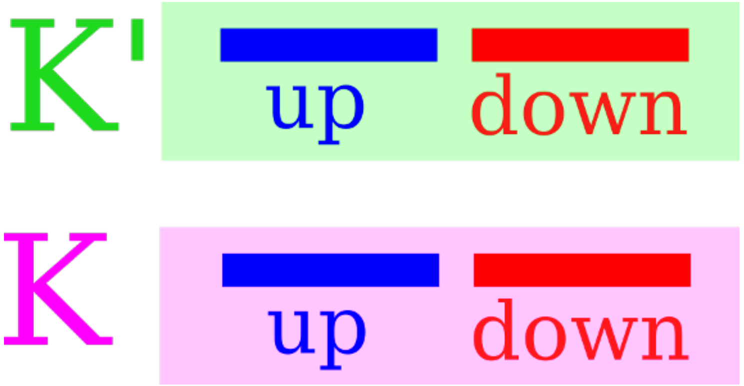


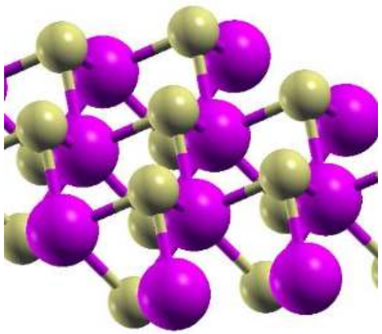


In the following lets assume we have WSe_2

Degrees of freedom a monolayer dichalcogenide

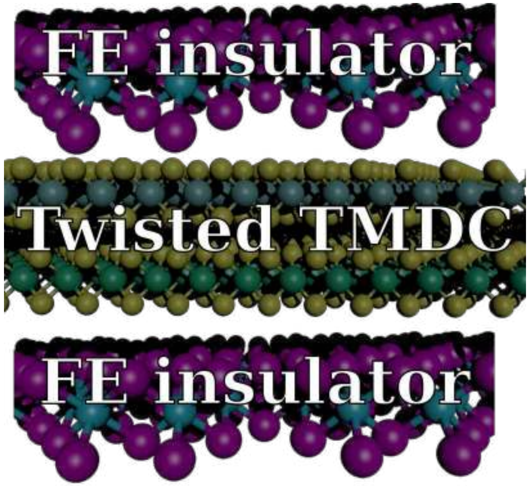




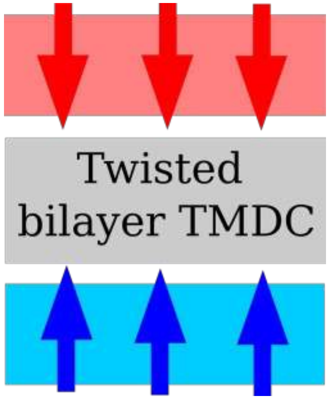


Magnetically encapsulated TMDC heterostructure

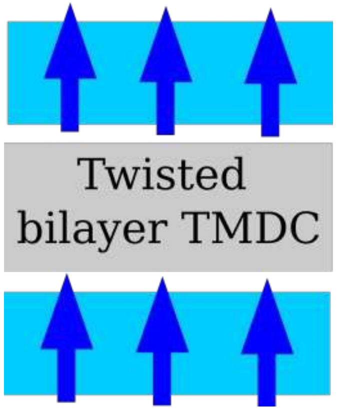
Structure



Antiferromagnetic configuration



Ferromagnetic configuration



Hamiltonian of the heterostructure

$$H = H_0 + H_{SOC} + H_J$$

Kinetic energy

Spin-orbit coupling

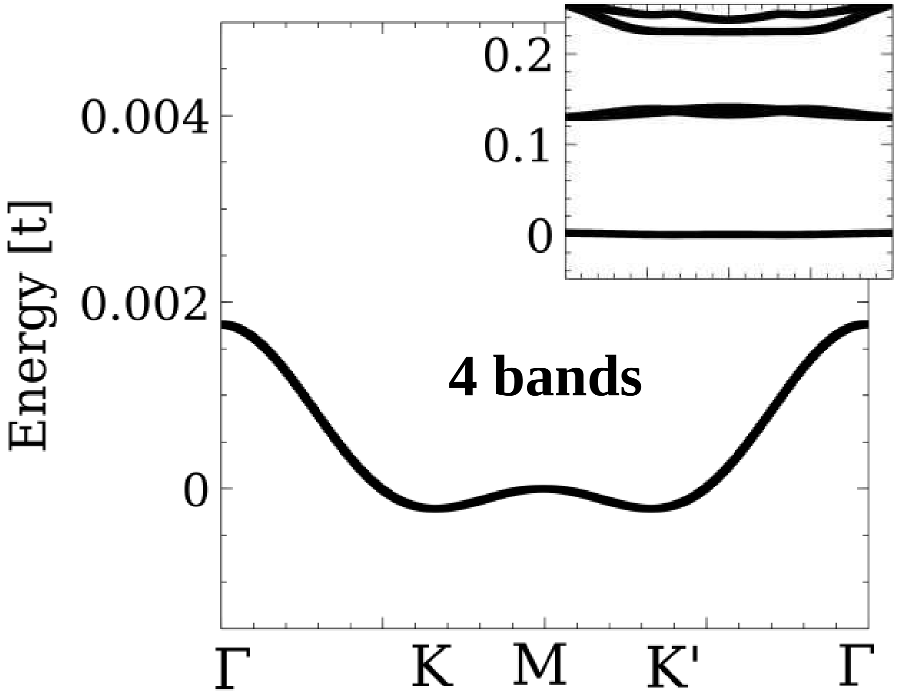
Exchange proximity

$CrBr_3$/twisted $(WSe_2)_2$/$CrBr_3$

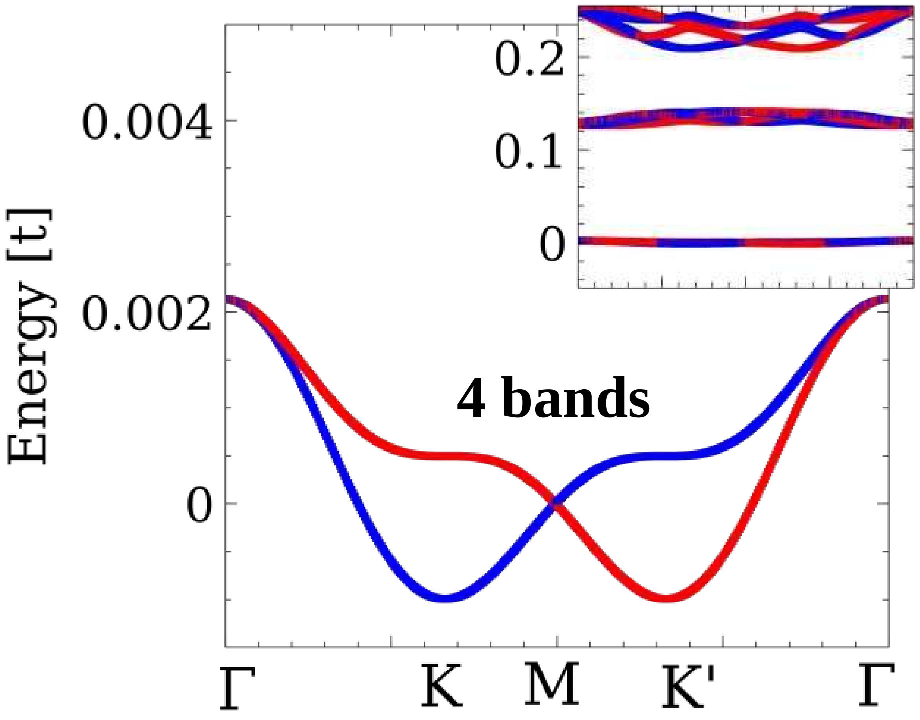
$$\alpha \approx 1.5^\circ - 2^\circ$$

In the absence of exchange proximity effect

Without SOC



With SOC

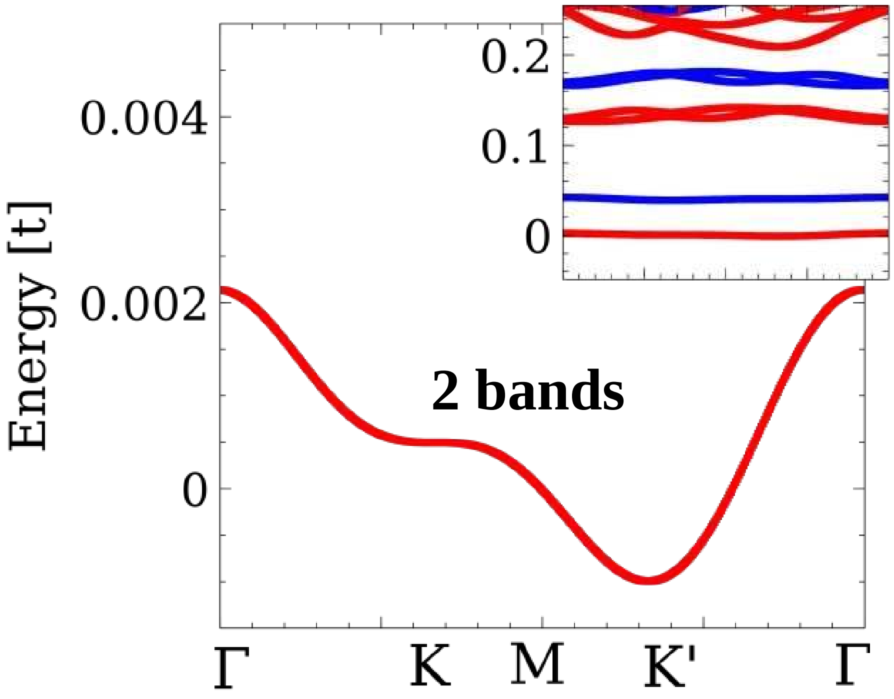


Phys. Rev. Lett. 121, 266401 (2018)

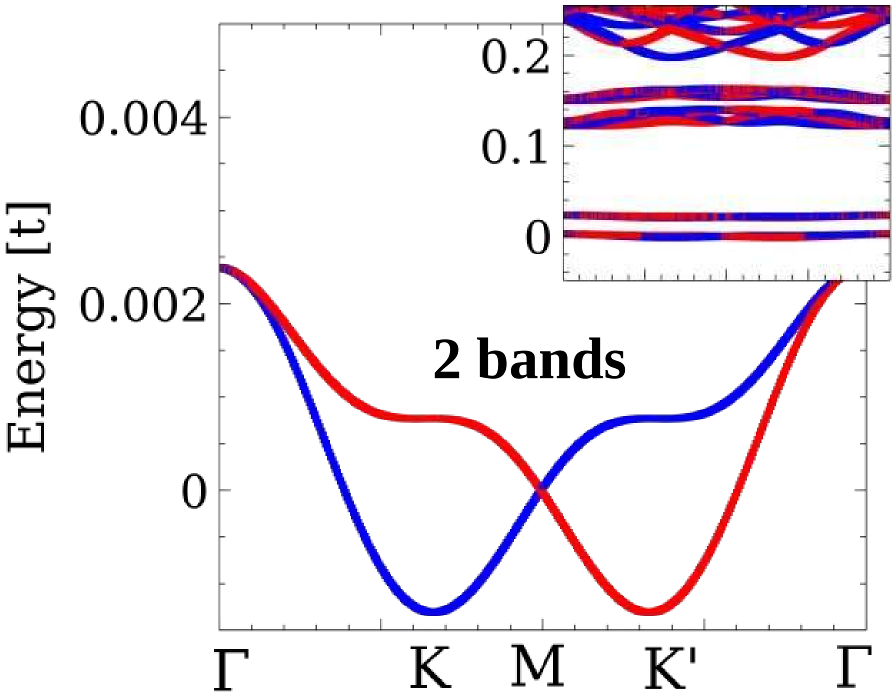
Low energy described by a 4-band model

With exchange proximity effect

Ferromagnetic configuration

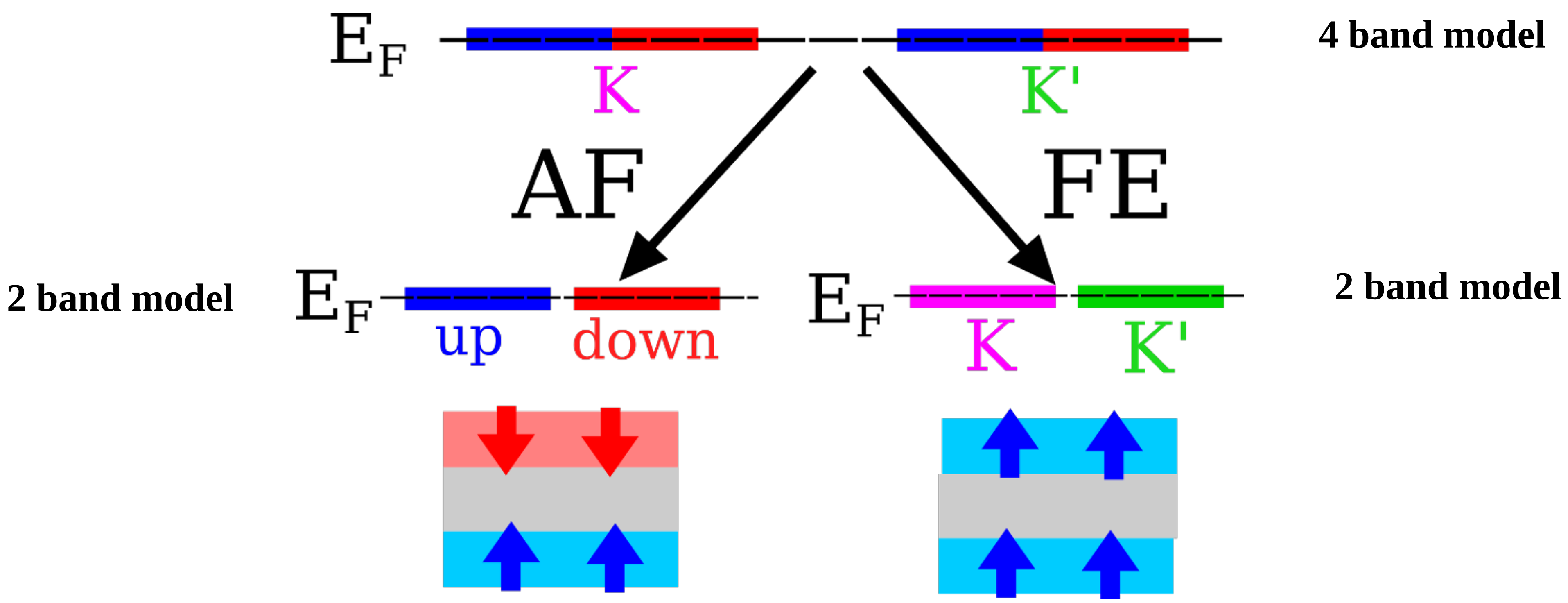


Antiferromagnetic configuration



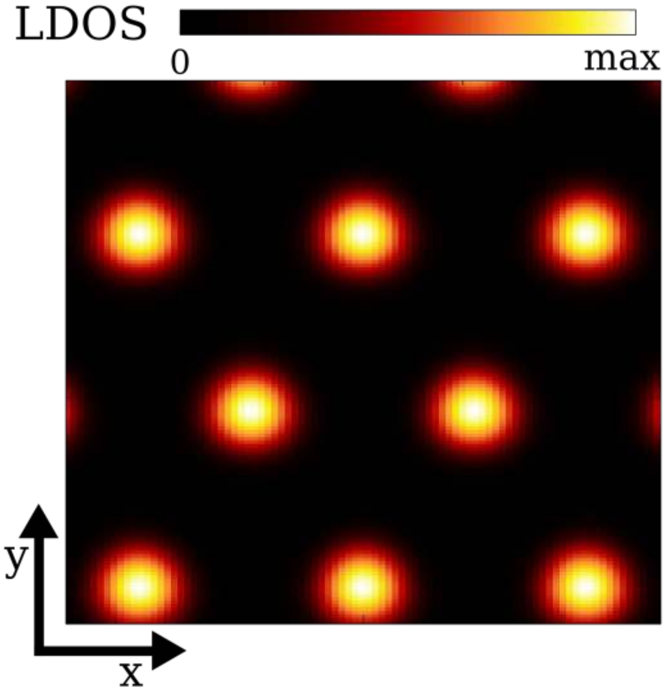
Low energy described by a 2-band model

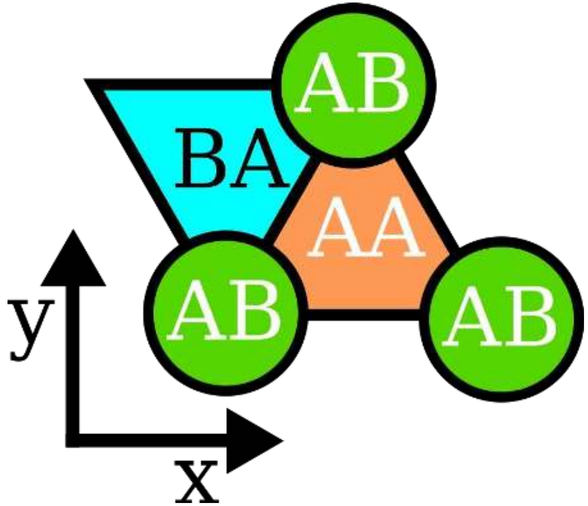
Controlling the low energy sector via exchange bias



The magnetic encapsulation controls the nature of the low energy degeneracy

Localization of the low energy modes

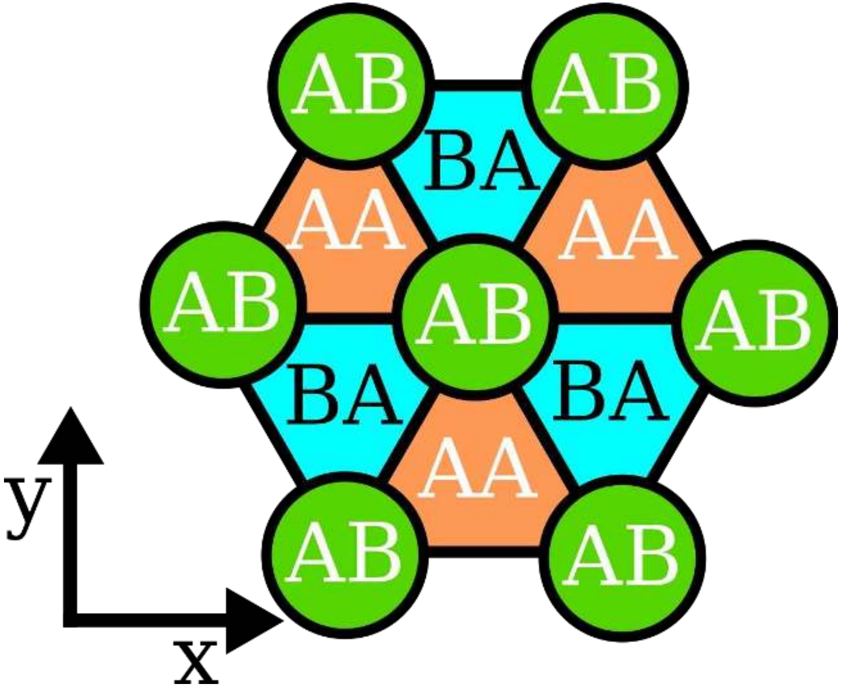


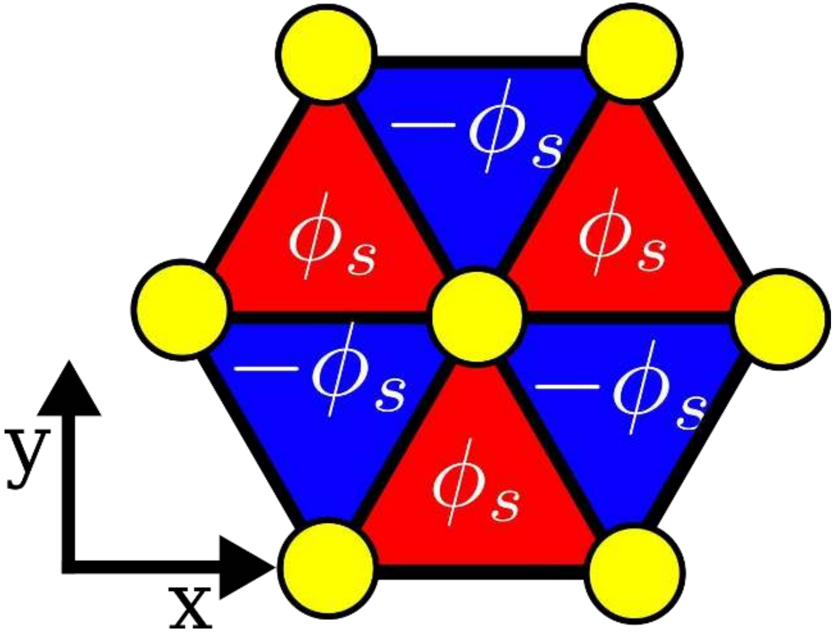


arXiv:2005.13879
arXiv:2006.09953

Low-energy modes are localized in regions with AB stacking

Low energy triangular flux model



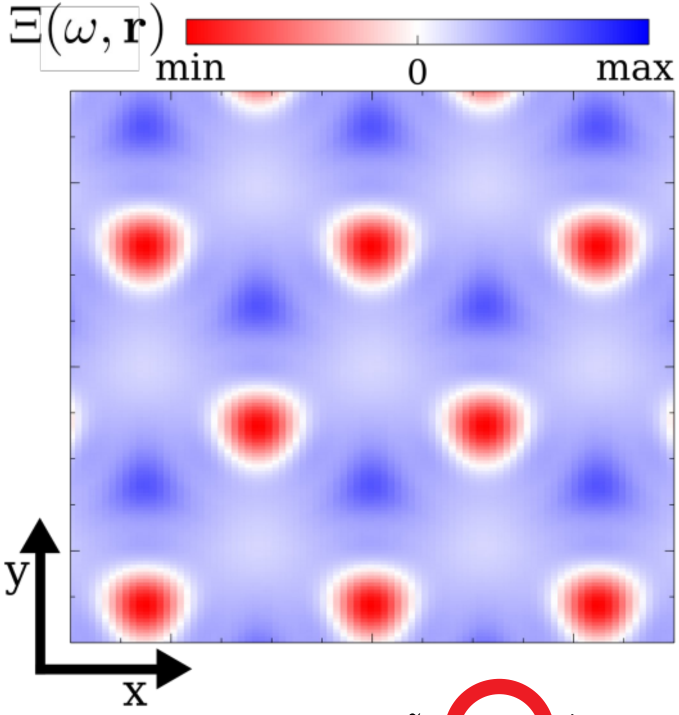


Flux model in a triangular lattice

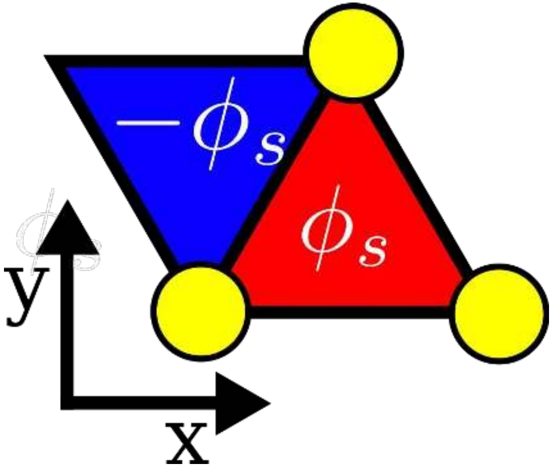
$$H = \sum_{\langle ij \rangle, s, s'} e^{i\sigma^z_{s,s'}\phi_{ij}} d^\dagger_{i,s} d_{j,s'}$$

Real-space topological flux

The real space density of artificial spin-valley gauge field



$$H = \sum_{\langle ij\rangle,s,s'} e^{i\sigma^z_{s,s'}\phi_{ij}} d^\dagger_{i,s} d_{j,s'}$$



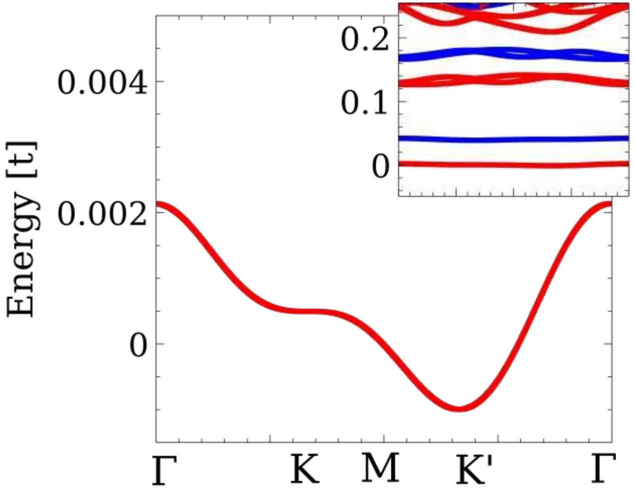
The valley-spin Chern number is defined as

$$\mathcal{C} = \int_{-\infty}^{0} d\omega \int d^2\mathbf{r}\,\Xi(\mathbf{r},\omega)$$

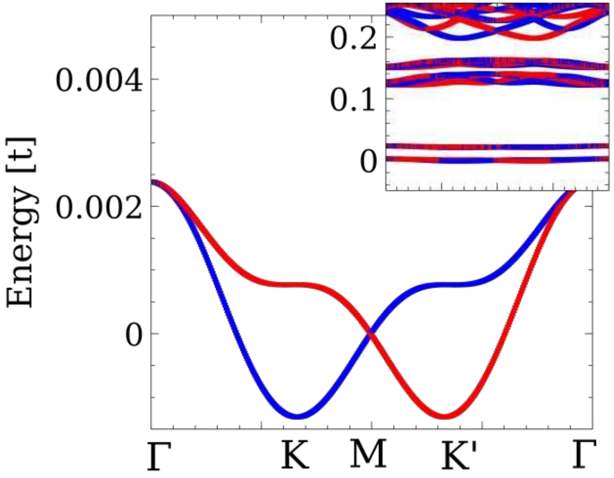
$$\mathcal{C} = (\mathcal{C}_{\uparrow,K} - \mathcal{C}_{\downarrow,K}) - (\mathcal{C}_{\uparrow,K'} - \mathcal{C}_{\downarrow,K'})$$

The impact of interactions

FE configuration



AF configuration



Free Hamiltonian

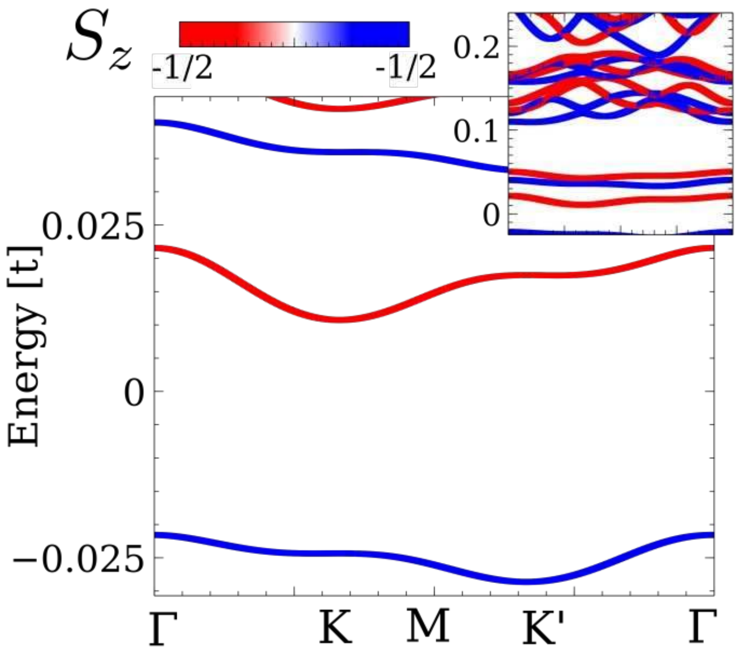
Electronic interactions

$$H = H_0 + H_{int}$$

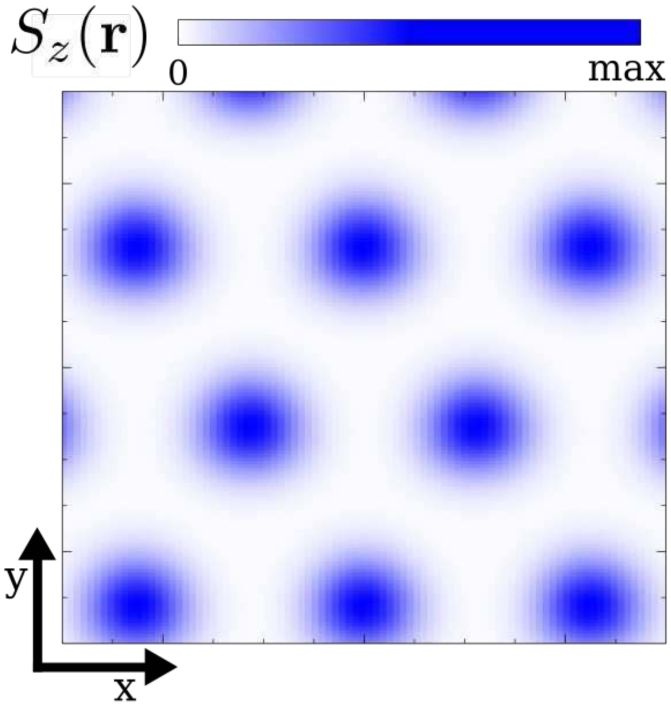
What is the effect of interactions at half filling?

Impact of interactions in the AF configuration

Band structure



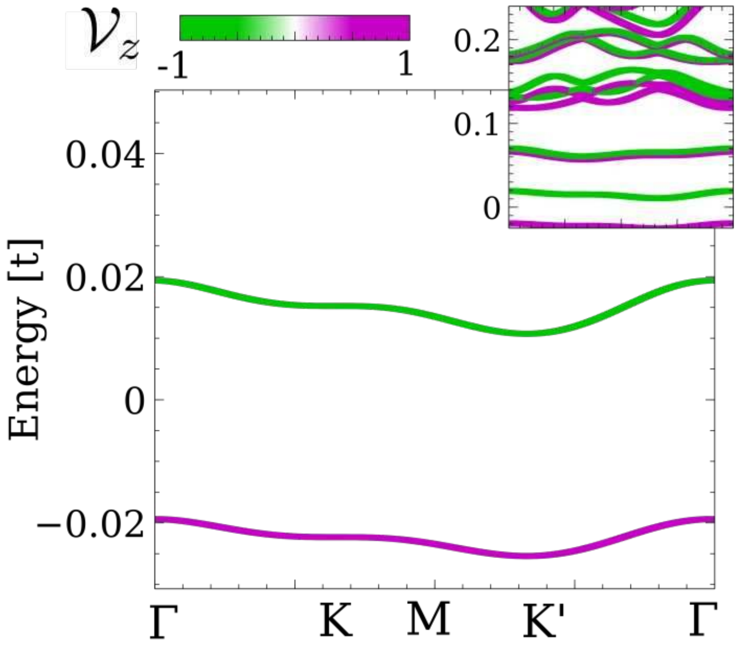
Spin density



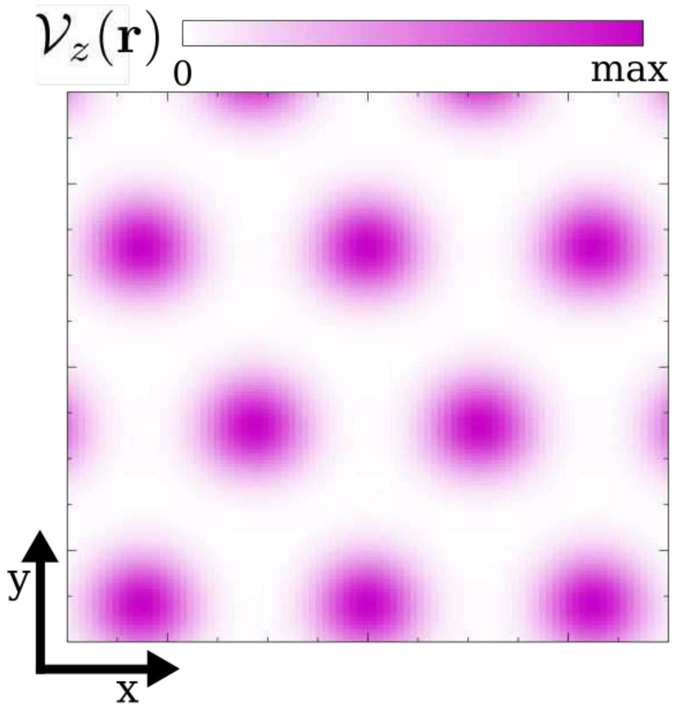
Interaction-induced spin-symmetry breaking

Impact of interactions in the FE configuration

Band structure

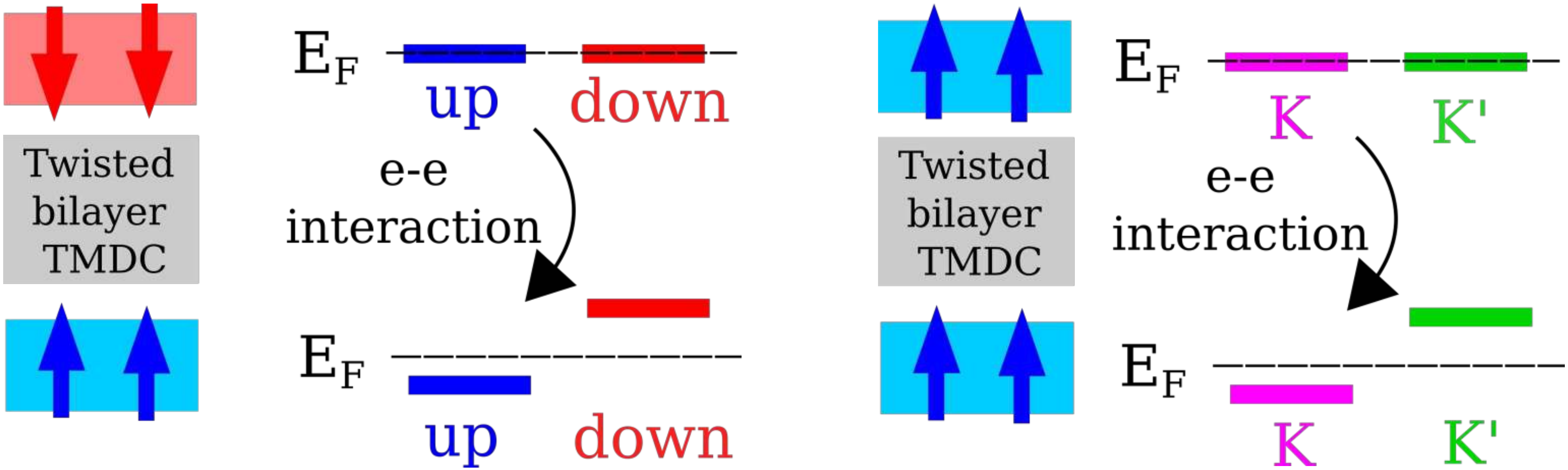


Valley density



Interaction-induced valley-symmetry breaking

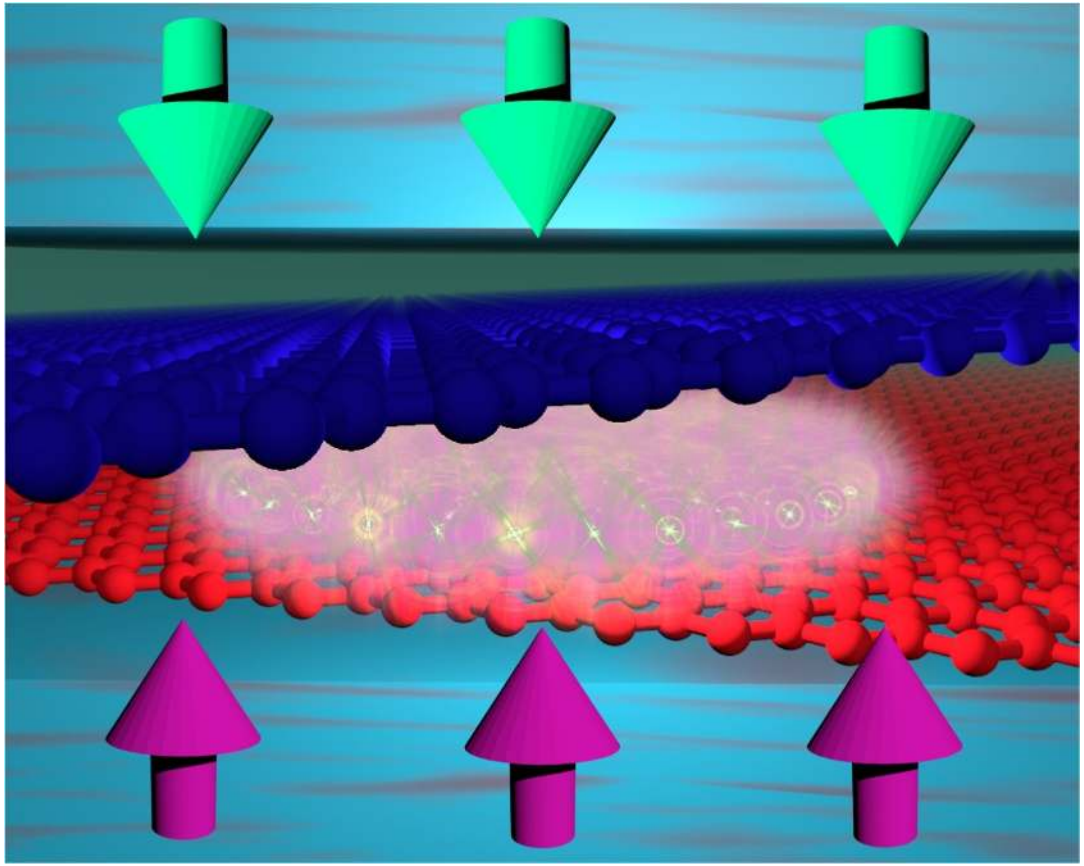
Controlling valley-symmetry breaking with exchange bias



Interaction-induced spin-symmetry breaking

Interaction-induced valley-symmetry breaking

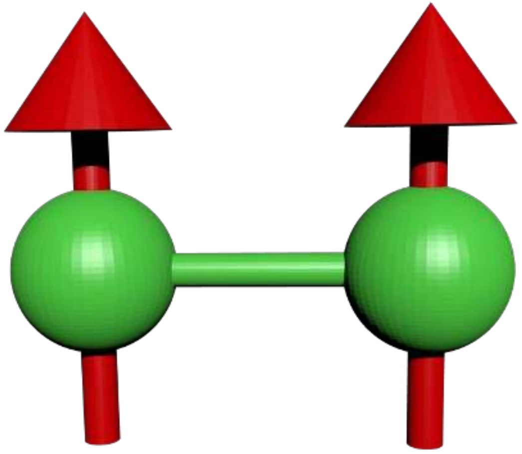
Valley-mixing correlations in magnetically encapsulated tBG



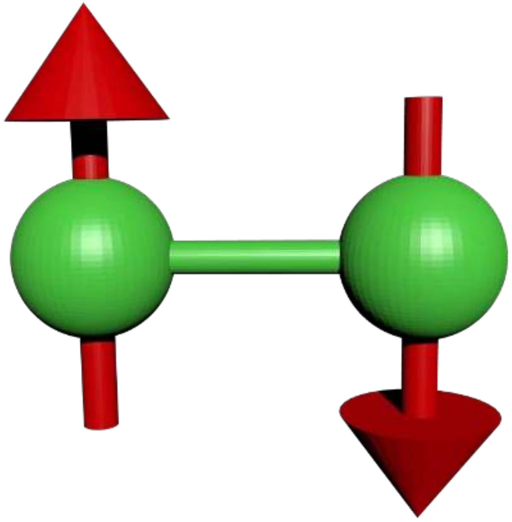
Frustration

A bird’s eye view on magnetism

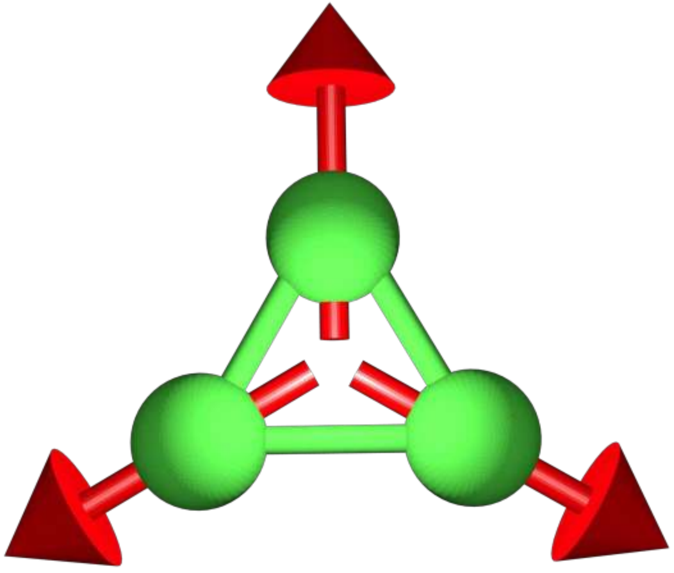
Ferromagnetism



Antiferromagnetism



Frustrated magnetism



Can we control the microscopic properties of a magnet?

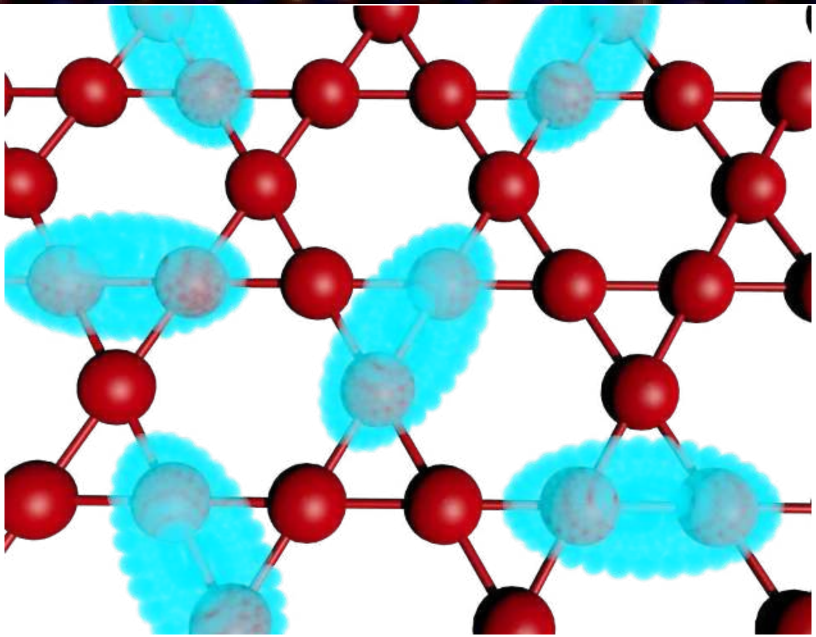
What is the best that can happen?

Quantum spin liquids

No magnetic ordering at T=0
Non-trivial topological properties
Fractional excitations
Macroscopic quantum state
“Ultra-quantum” matter

$$\mathcal{H} = \sum_{ij} \vec{S}_i \hat{J}_{ij} \vec{S}_j$$

Rep. Prog. Phys. 80, 016502 (2017)



 $\equiv |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$

Kitaev’s honeycomb

Annals of Physics 321.1 (2006)

Kagome Heisenberg

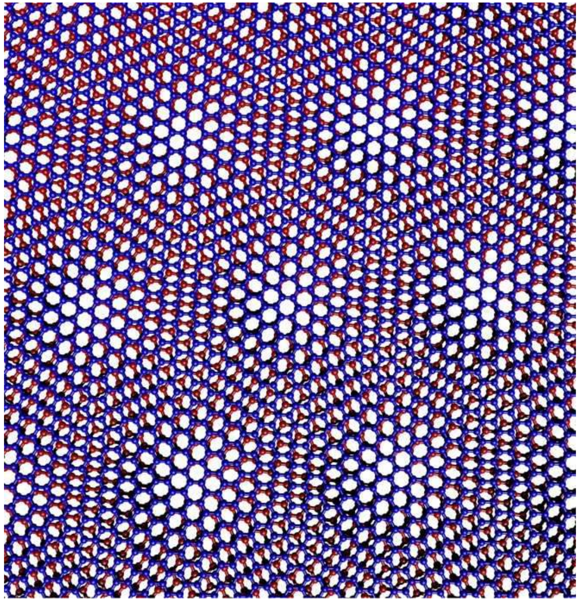
Science 332, 1173-1176 (2011)

Extended triangular Heisenberg

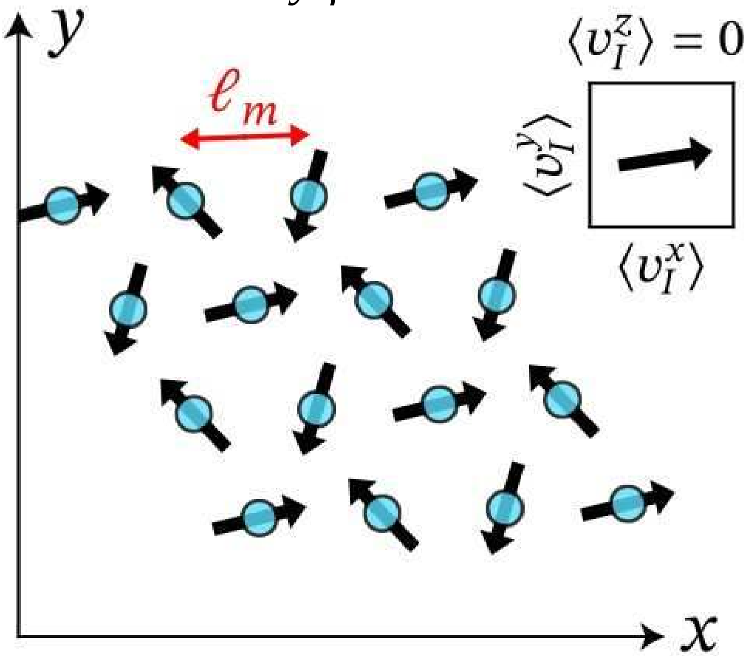
J. Phys. Soc. Jpn 83, 093707 (2014)

Frustrated valley magnetism

Moire structure



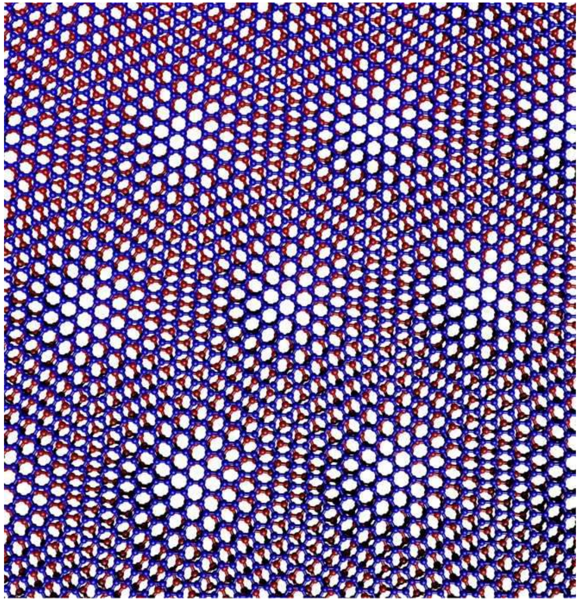
Valley-frustrated state



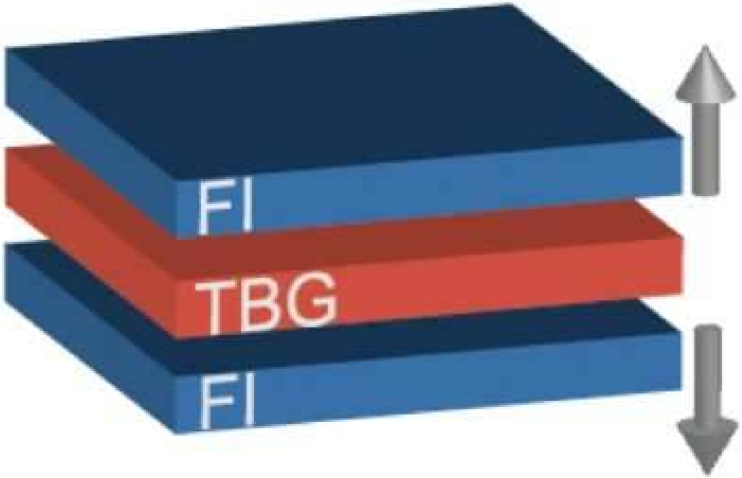
Can we create a controllable valley-only frustrated magnet?

Magnetically encapsulated twisted graphene bilayer

Moire structure



Magnetic encapsulation



CrI_3/twisted bilayer graphene/CrI_3

Let us focus on the antiferromagnetic configuration of the encapsulation

Magnetically encapsulated twisted graphene bilayer

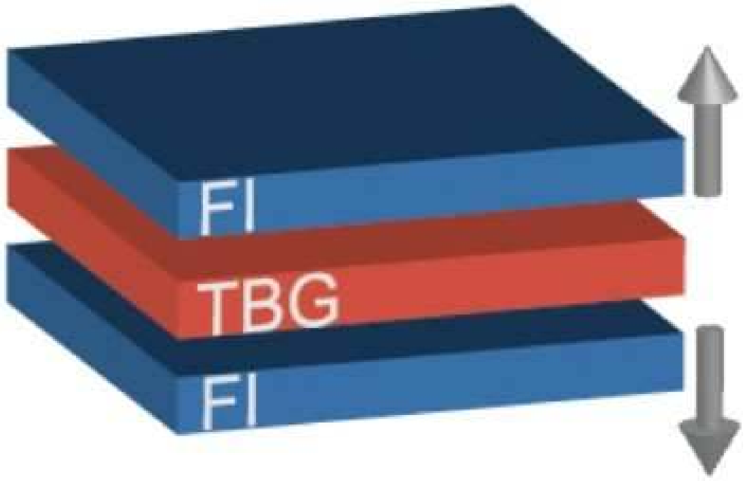
Magnetic encapsulation

$$H = H_0 + H_{\mathrm{J}} + H_{\mathrm{R}}$$

Kinetic energy

Exchange proximity effect

Rashba spin-orbit coupling

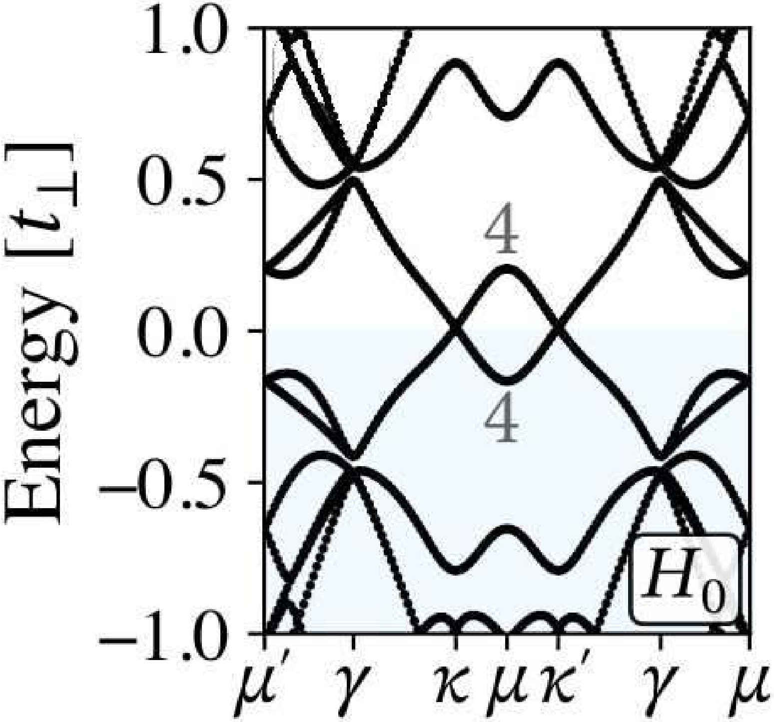


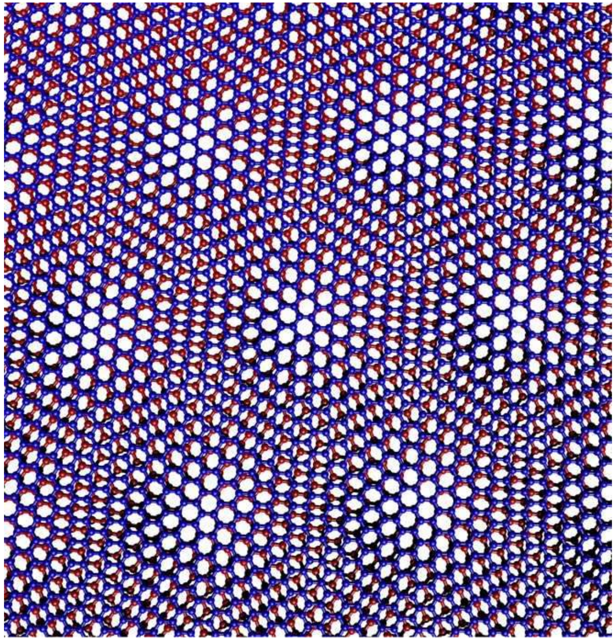
Valley frustration from combined twist engineering, exchange proximity and spin-orbit coupling.

Lets focus on the regime $\alpha = 1.3^\circ - 2^\circ$

Twisted graphene bilayer at 2 degrees

Without exchange field nor spin-obit coupling



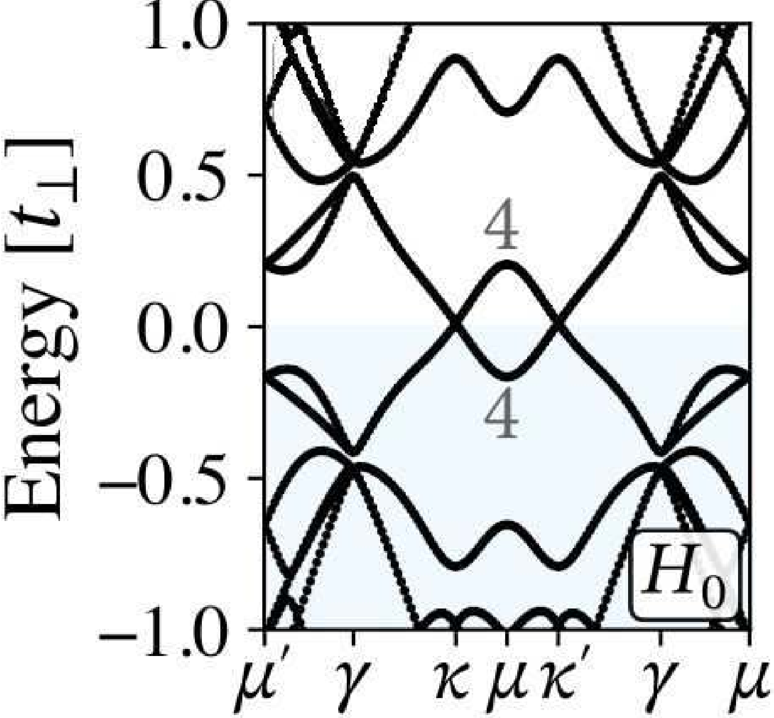


Phys. Rev Lett. 99 256802 (2007)
Phys. Rev. B 82, 121407(R) (2010)
PNAS 108 30 12233-12237 (2011)

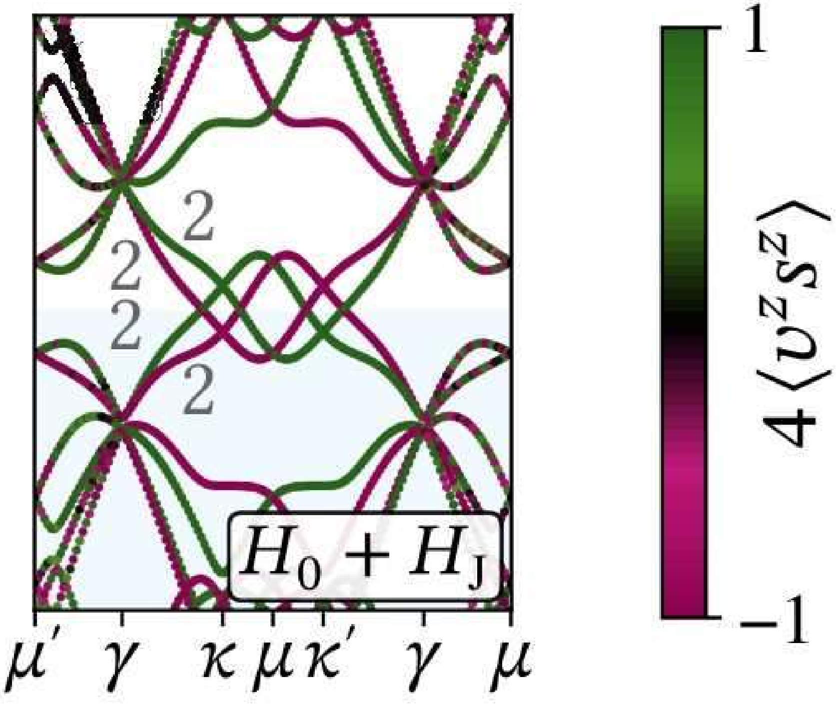
<u>Renormalized Dirac cones</u>

Twisted graphene bilayer at 2 degrees

Without exchange field

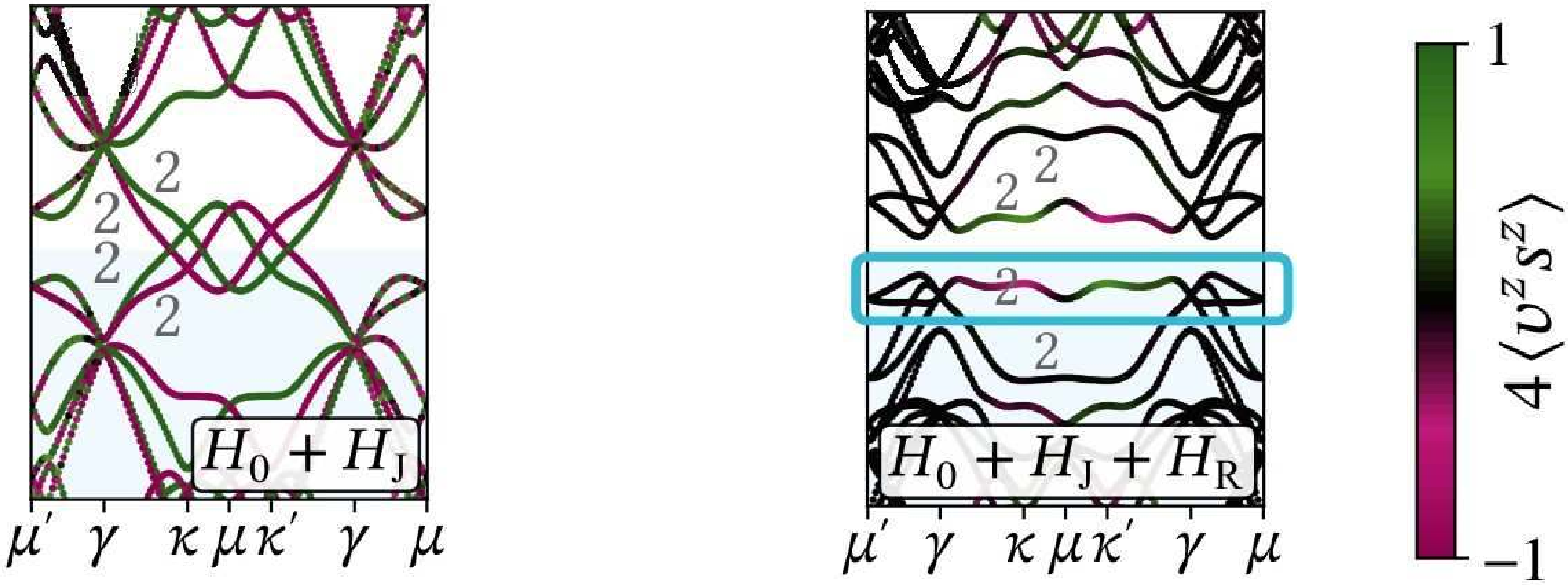


With exchange field



<u>Valley-spin splitting degeneracy lifting</u>

Valley-only correlated states in twisted graphene bilayers

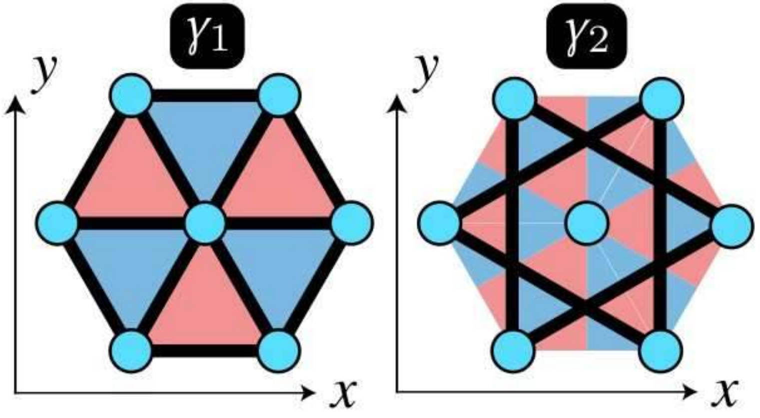


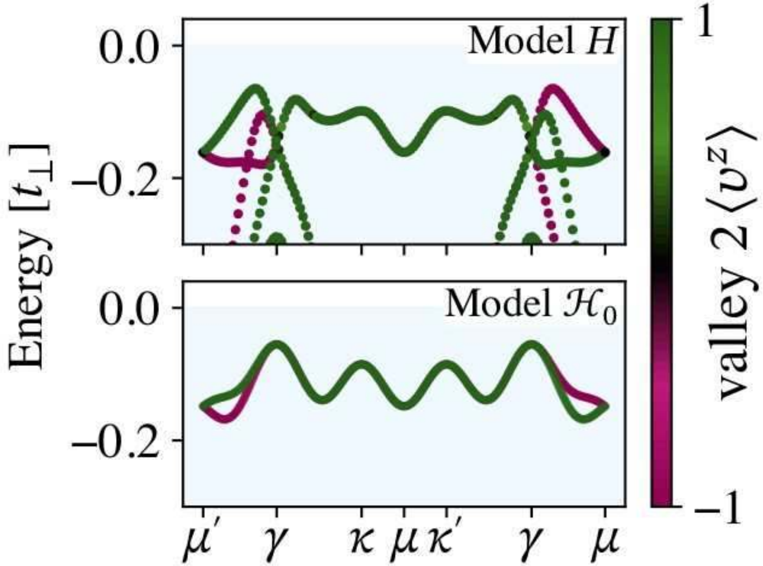
Nearly flat bands created from twist + exchange + spin-orbit coupling

Effective low energy valley model

Flux model in the triangular lattice

$$\mathcal{H}_0 = \sum_{\langle IJ \rangle} \gamma_1 \, \psi_I^\dagger e^{i\sigma^z \nu_{IJ} \phi_1} \psi_J + \sum_{\langle\langle IJ \rangle\rangle} \gamma_2 \, \psi_I^\dagger e^{i\sigma^z \nu_{IJ} \phi_2} \psi_J$$

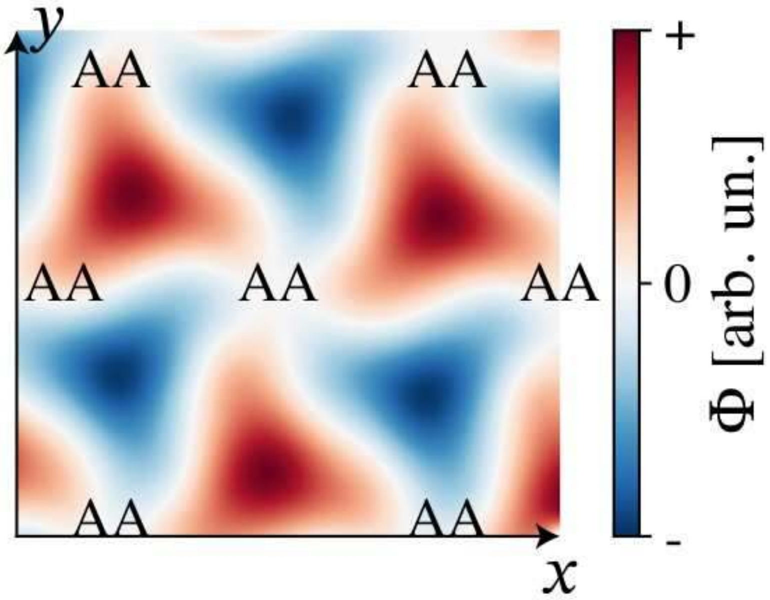




Two-band valley-only model in the triangular lattice

Real-space valley flux density

$$\mathcal{H}_0 = \sum_{\langle IJ \rangle} \gamma_1 \, \psi_I^\dagger e^{i\sigma^z \nu_{IJ} \phi_1} \psi_J + \sum_{\langle\langle IJ \rangle\rangle} \gamma_2 \, \psi_I^\dagger e^{i\sigma^z \nu_{IJ} \phi_2} \psi_J$$



Real space density of artificial valley gauge field

$$\mathcal{C} = \int_{-\infty}^{0} d\omega \int d^2\mathbf{r}\Phi(\mathbf{r},\omega)$$

$$\mathcal{C} = (\mathcal{C}_{\uparrow,K} + \mathcal{C}_{\downarrow,K}) - (\mathcal{C}_{\uparrow,K'} + \mathcal{C}_{\downarrow,K'})$$

Applying an interlayer bias controls the valley-flux of the effective model

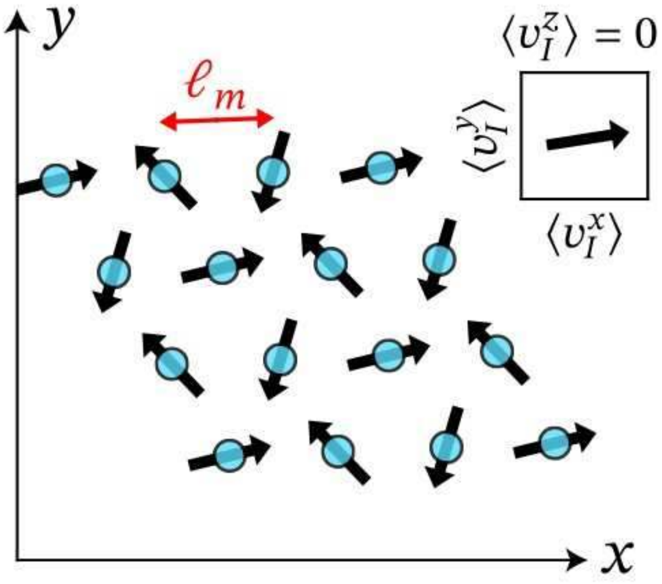
Impact of interactions

Lets add electronic interactions

Free Hamiltonian

Electronic interactions

$$\bar{H} = H + H_{int}$$

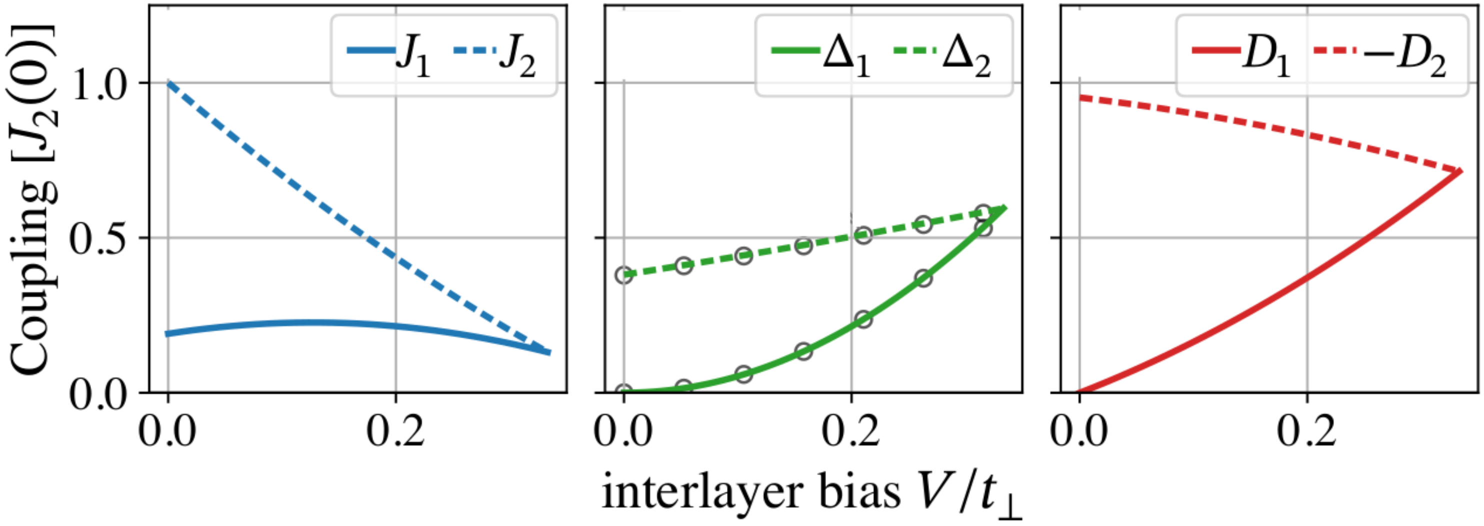


And compute the effective valley-Heisenberg Hamiltonian in the strong coupling limit

$$\mathcal{H}_v = \sum_{IJ} J_{IJ}\, \boldsymbol{v}_I \cdot \boldsymbol{v}_J + \Delta_{IJ}\, v_I^z v_J^z + \nu_{IJ}\, D_{IJ}\, (\boldsymbol{v}_I \times \boldsymbol{v}_J)_z$$

Controlling a valley-Heisenberg model electrically

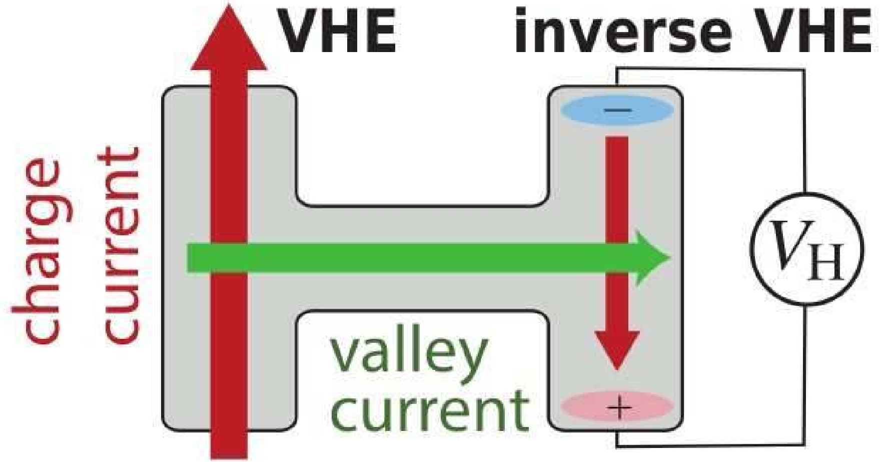
$$\mathcal{H}_v = \sum_{IJ} J_{IJ}\, \boldsymbol{v}_I \cdot \boldsymbol{v}_J + \Delta_{IJ}\, v_I^z v_J^z + \nu_{IJ}\, D_{IJ}\, (\boldsymbol{v}_I \times \boldsymbol{v}_J)_z$$



An interlayer bias provides a tunable anisotropic valley-Heisenberg model

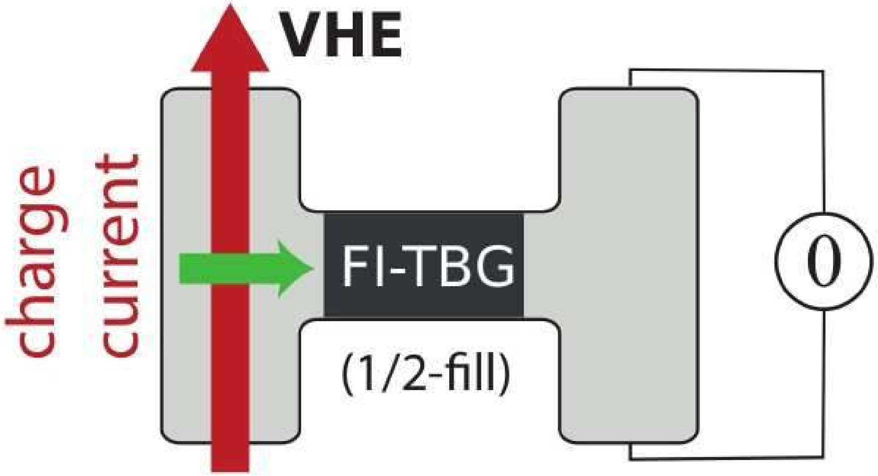
Detecting the valley spiral

No valley mixing



Finite non-local conductance

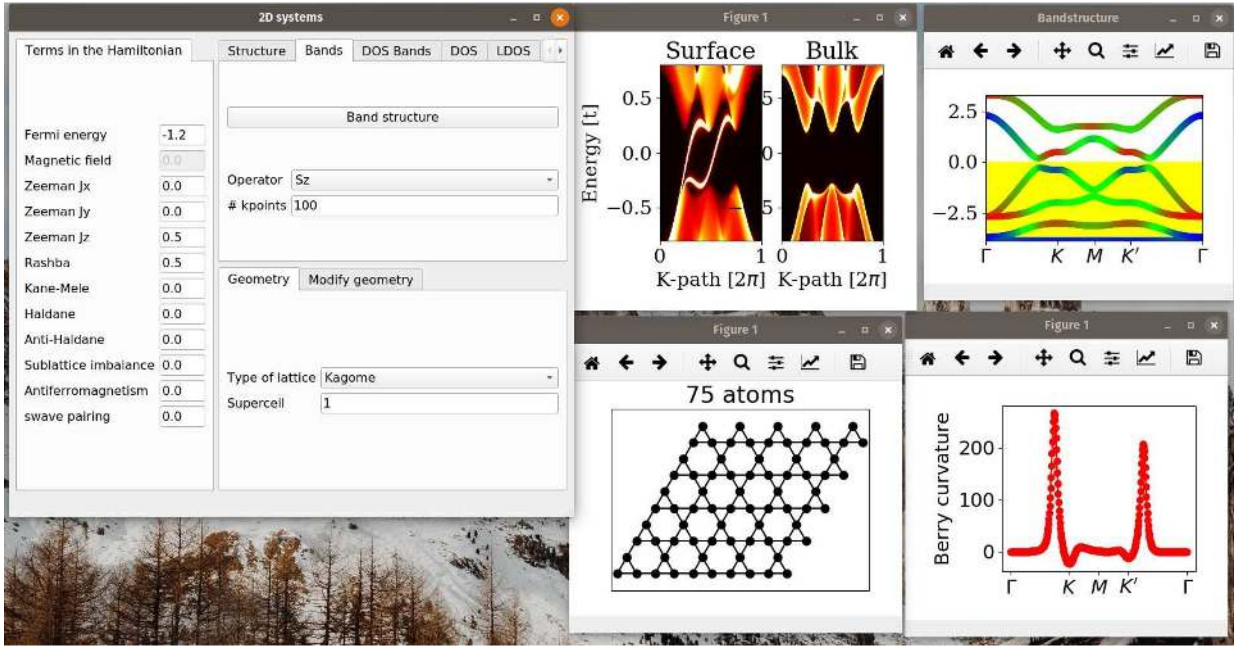
Finite valley mixing



Zero non-local conductance

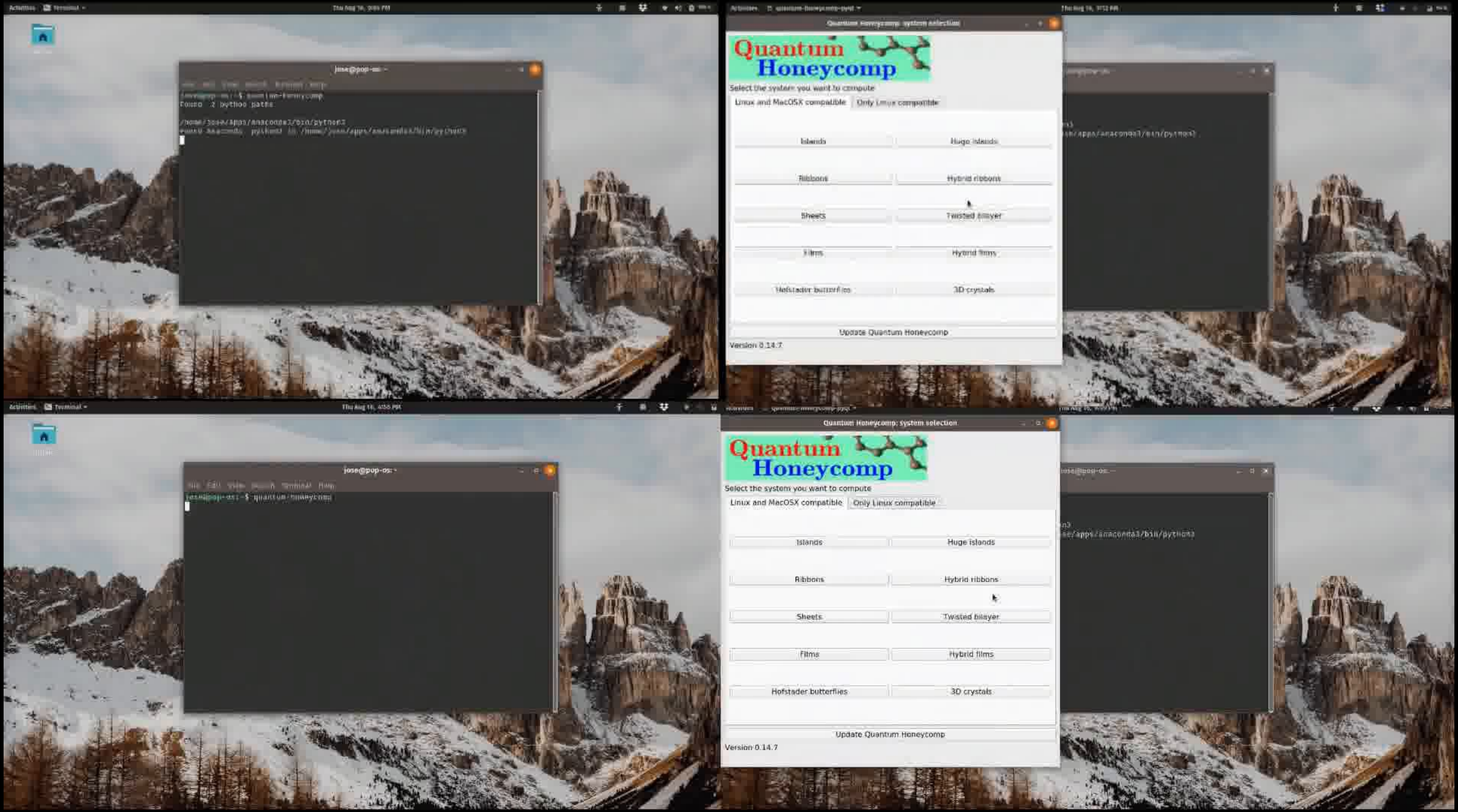
Computing electronic properties

A user interface to compute electronic properties

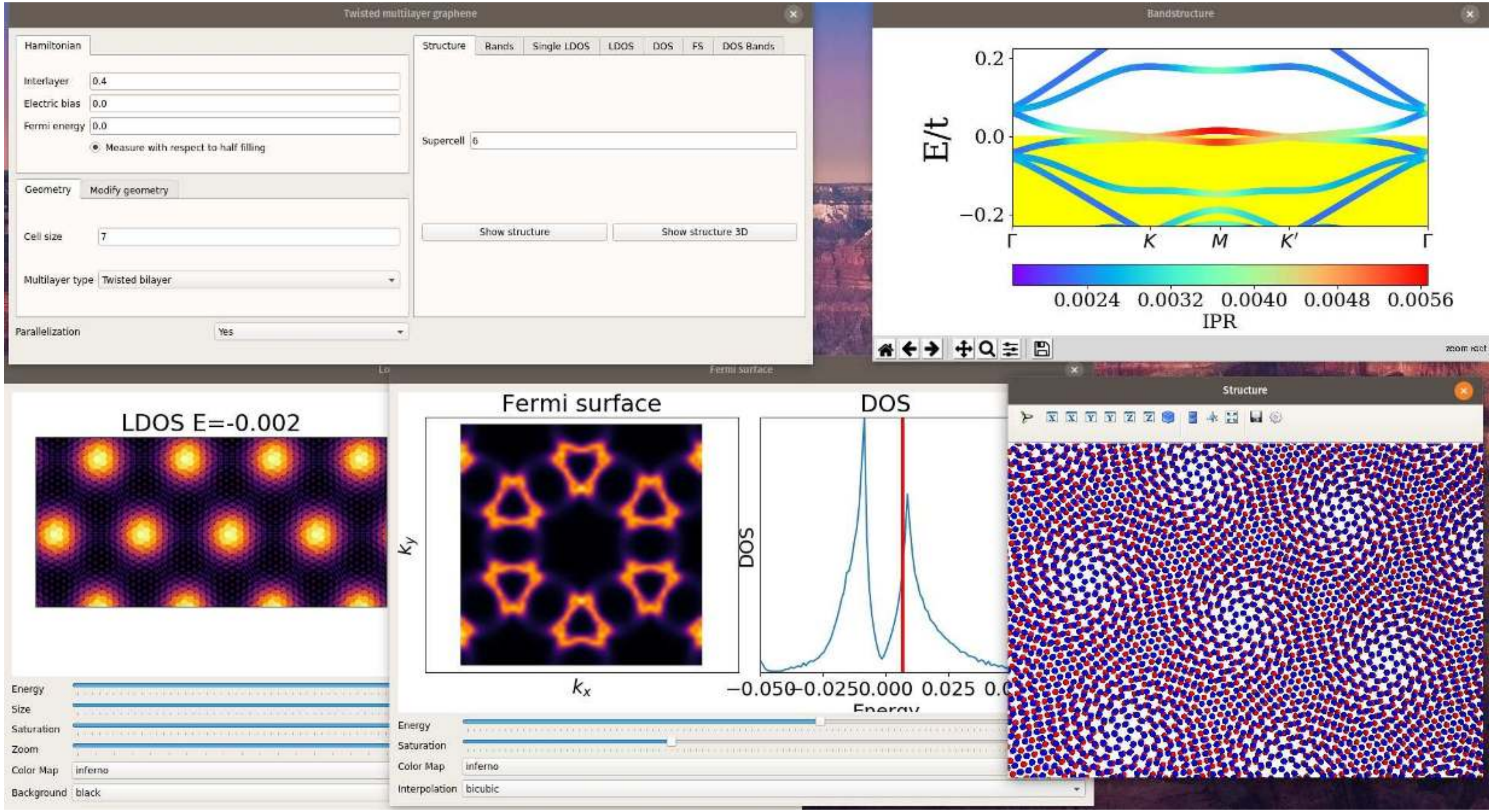


Quantum Honeycomp: open source interactive interface for tight binding modeling

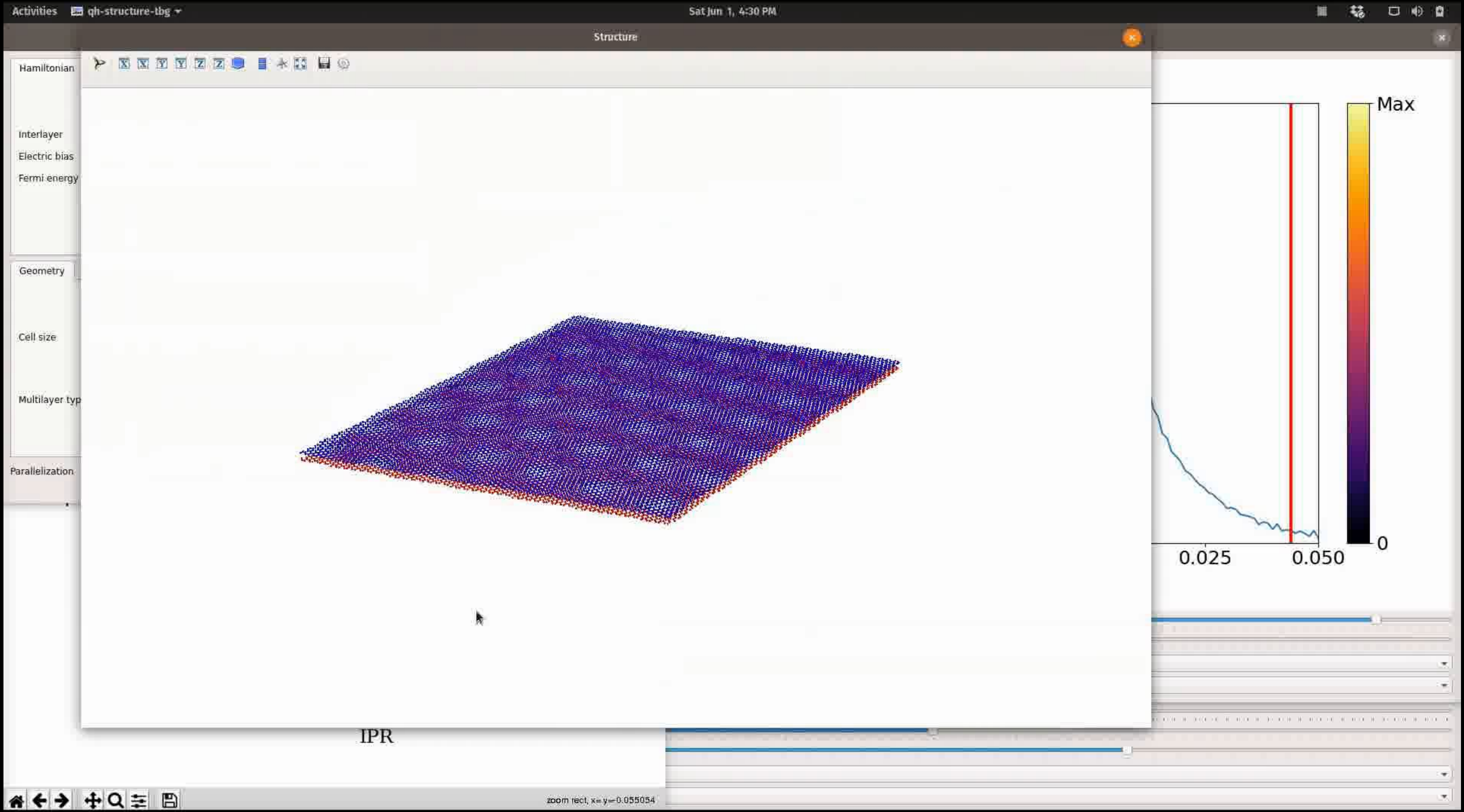
https://github.com/joselado/quantum-honeycomp


Quantum Honeycomp: system selection
Quantum
Honeycomp
Select the system you want to compute
Linux and MacOSX compatible
Only Linux compatible
Islands
Huge islands
Ribbons
Hybrid ribbons
Sheets
Twisted bilayer
Films
Hybrid films
Hofstader butterflies
3D crystals
Update Quantum Honeycomp
Version 0.14.7
jose@pop-os: ~

Twisted bilayer with the user interface

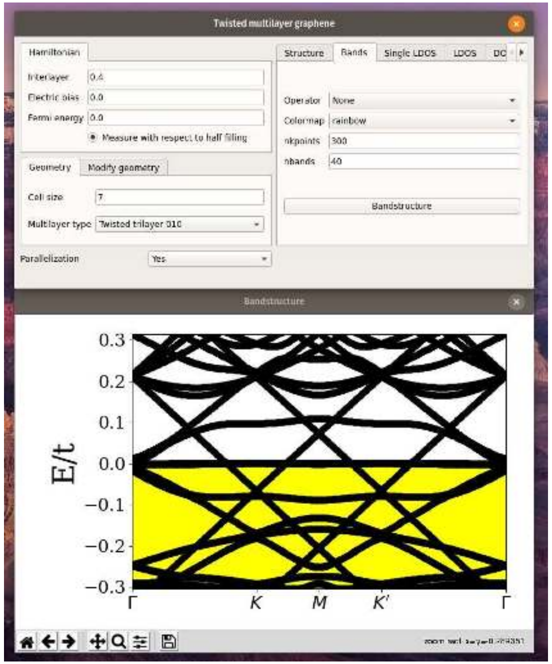


https://github.com/joselado/quantum-honeycomp

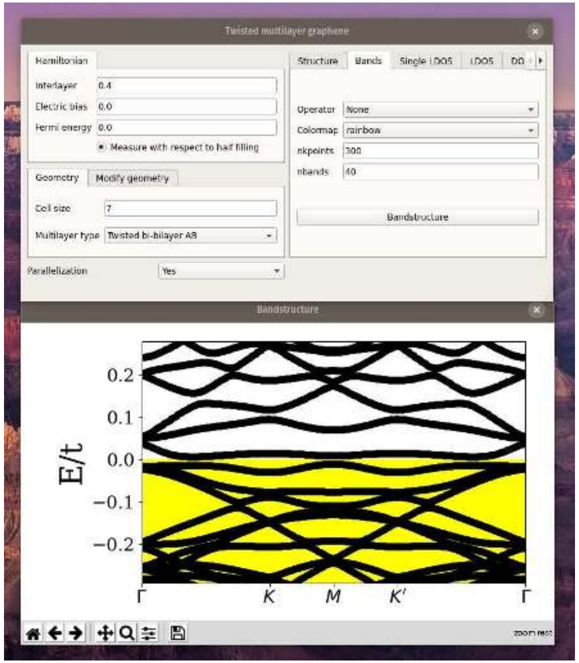

Activities
qh-structure-tbg
Sat Jun 1, 4:30 PM
Structure
Hamiltonian
Interlayer
Electric bias
Fermi energy
Geometry
Cell size
Multilayer typ
Parallelization
Max
0
0.025
0.050
IPR
zoom rect, x= y=0.055054

Twisted multilayers

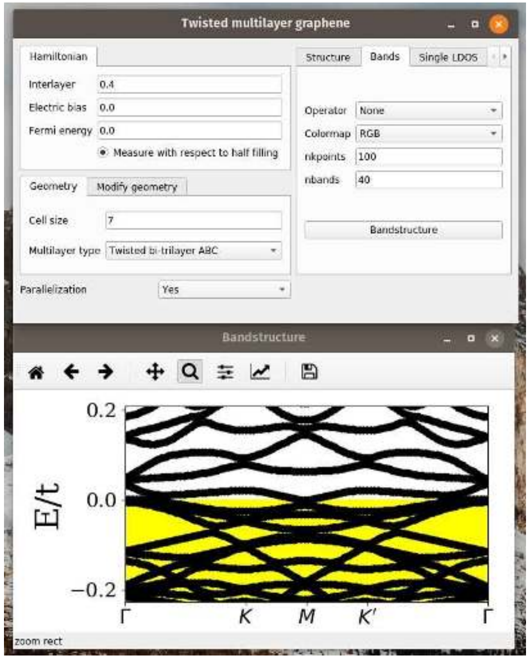
Twisted trilayer graphene



Twisted bi-bilayer graphene



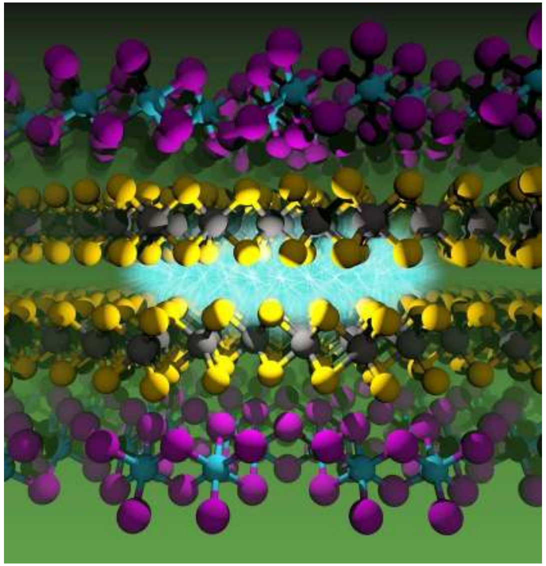
Twisted bi-trilayer graphene



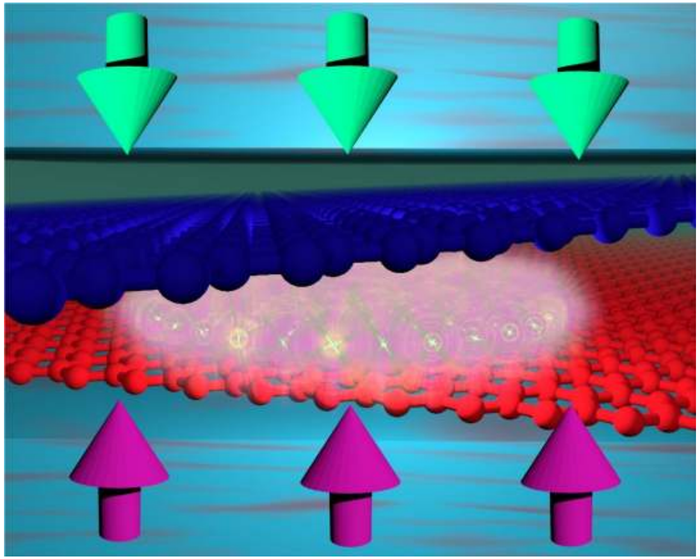
https://github.com/joselado/quantum-honeycomp

Take home

Magnetically encapsulated twisted van der Waals materials provide a platform to control the microscopic degrees of freedom of correlated states.



arXiv:2006.09953



arXiv:2008.06441

Thank you!

Funding from SUOMEN AKATEMIA