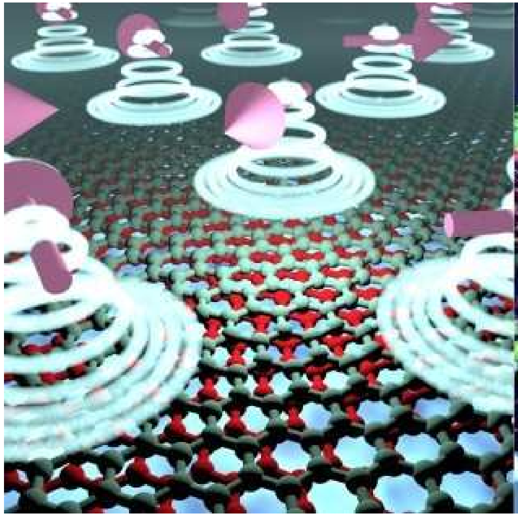
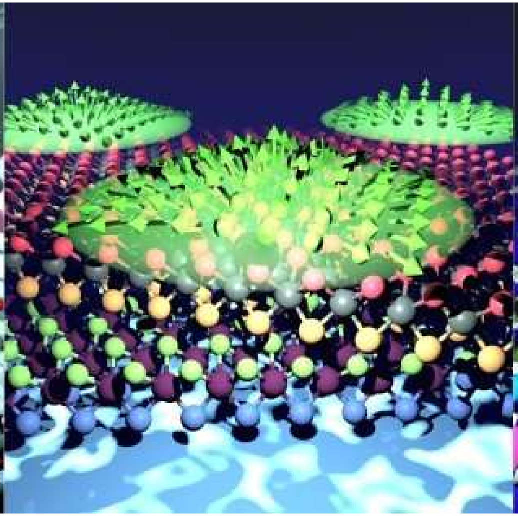
Correlated twisted spinorbitronics and heavy-fermions in van der Waals heterostructures

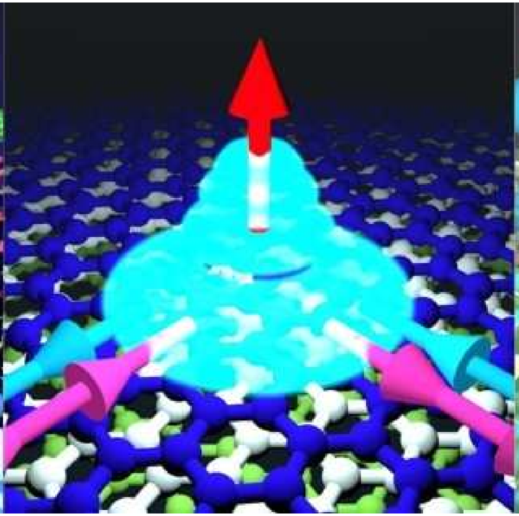
Jose Lado
Department of Applied Physics, Aalto University, Finland



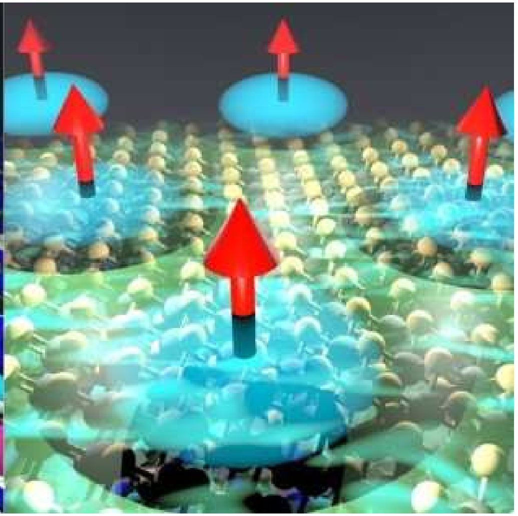
Phys. Rev. Lett. 126, 056803 (2021)



New J. Phys. 23 073038 (2021)



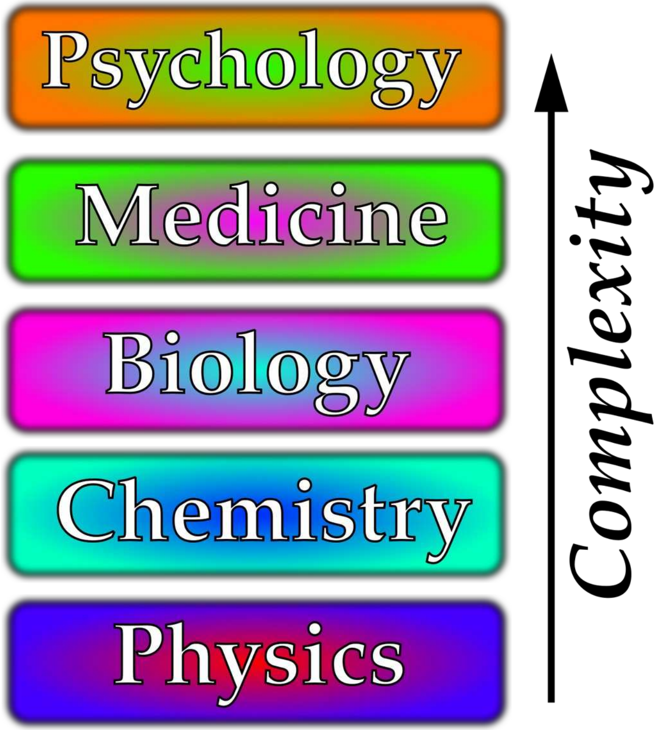
Phys. Rev. Lett. 127, 026401 (2021)



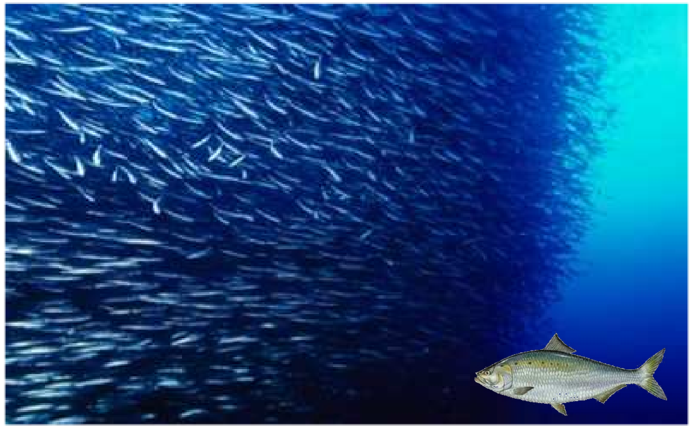
arXiv:2103.11989 (2021)

IFIMAC+ICMM Joint Seminars, Spain, October 14th 2021

Complexity, universality and emergence

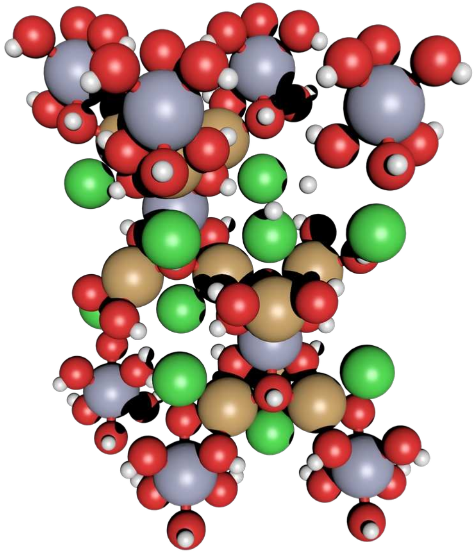


Fish schools



Phys. Rev. Lett. 120, 198101 (2018)

Complex compounds



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

Exotic physics in quantum materials

Quantum spin liquids

Unconventional superconductivity

Topological matter

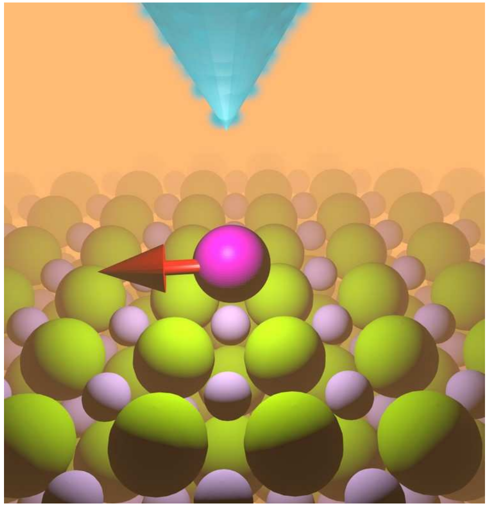
Topological quantum computing

Low consumption electronics

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

Building quantum matter with artificial lattices

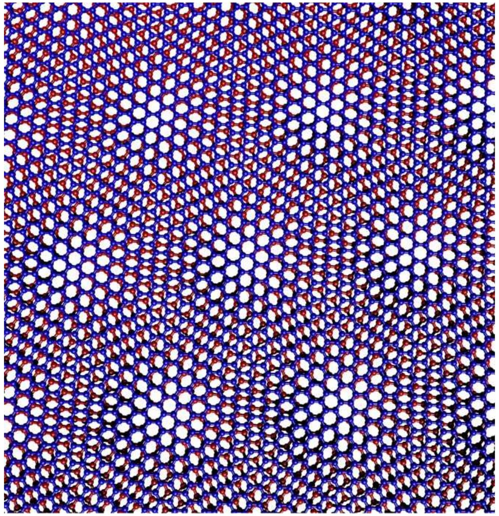
Atomic lattices



a = 0.5 nm

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

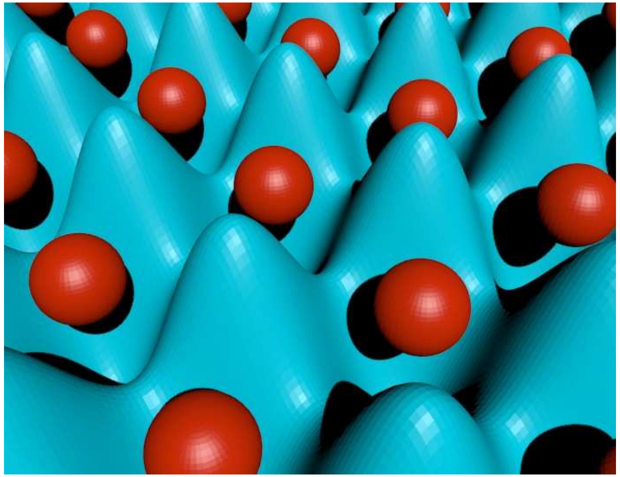
Twisted 2D moire materials



a = 30 nm

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

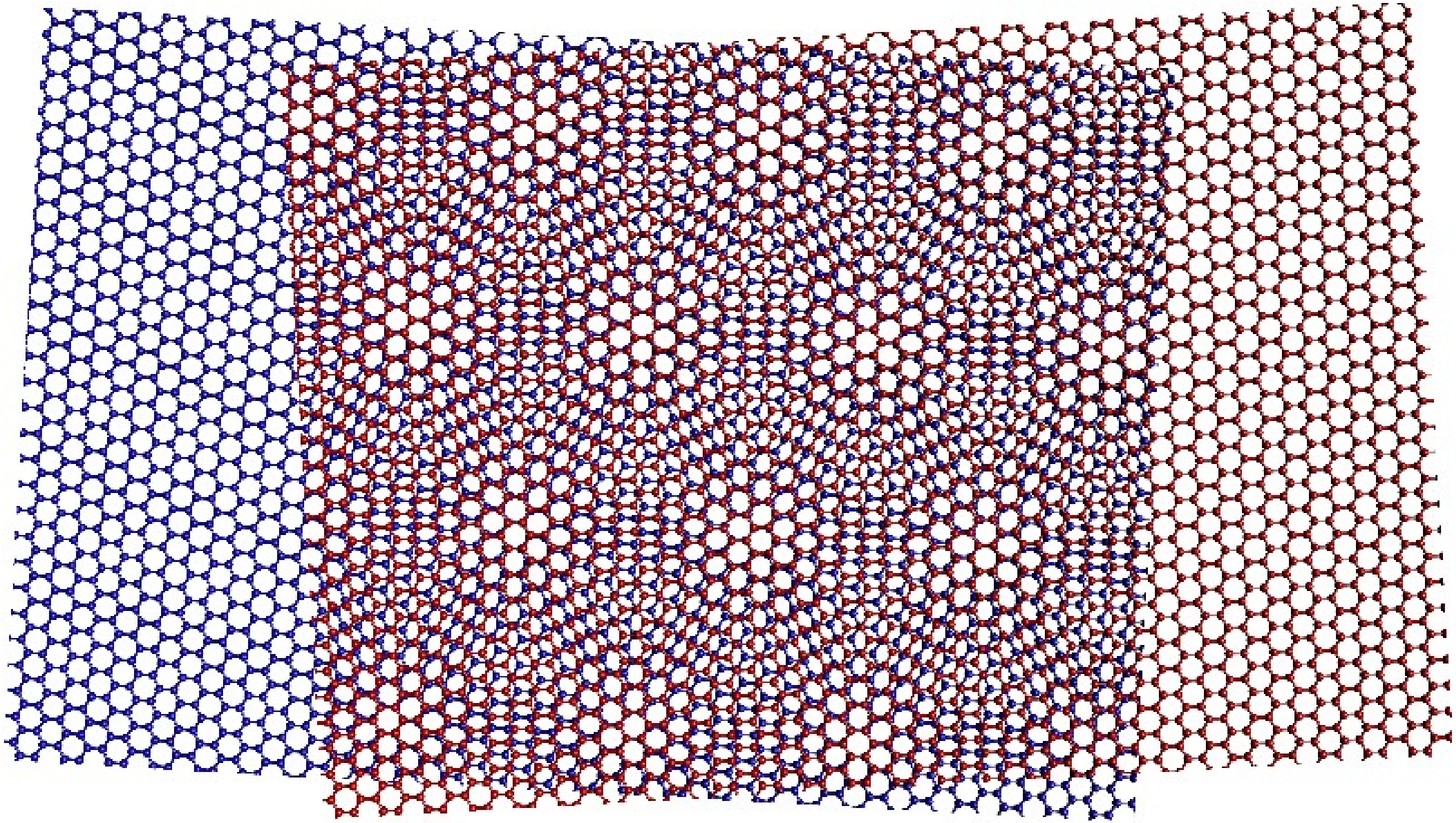
Cold atoms



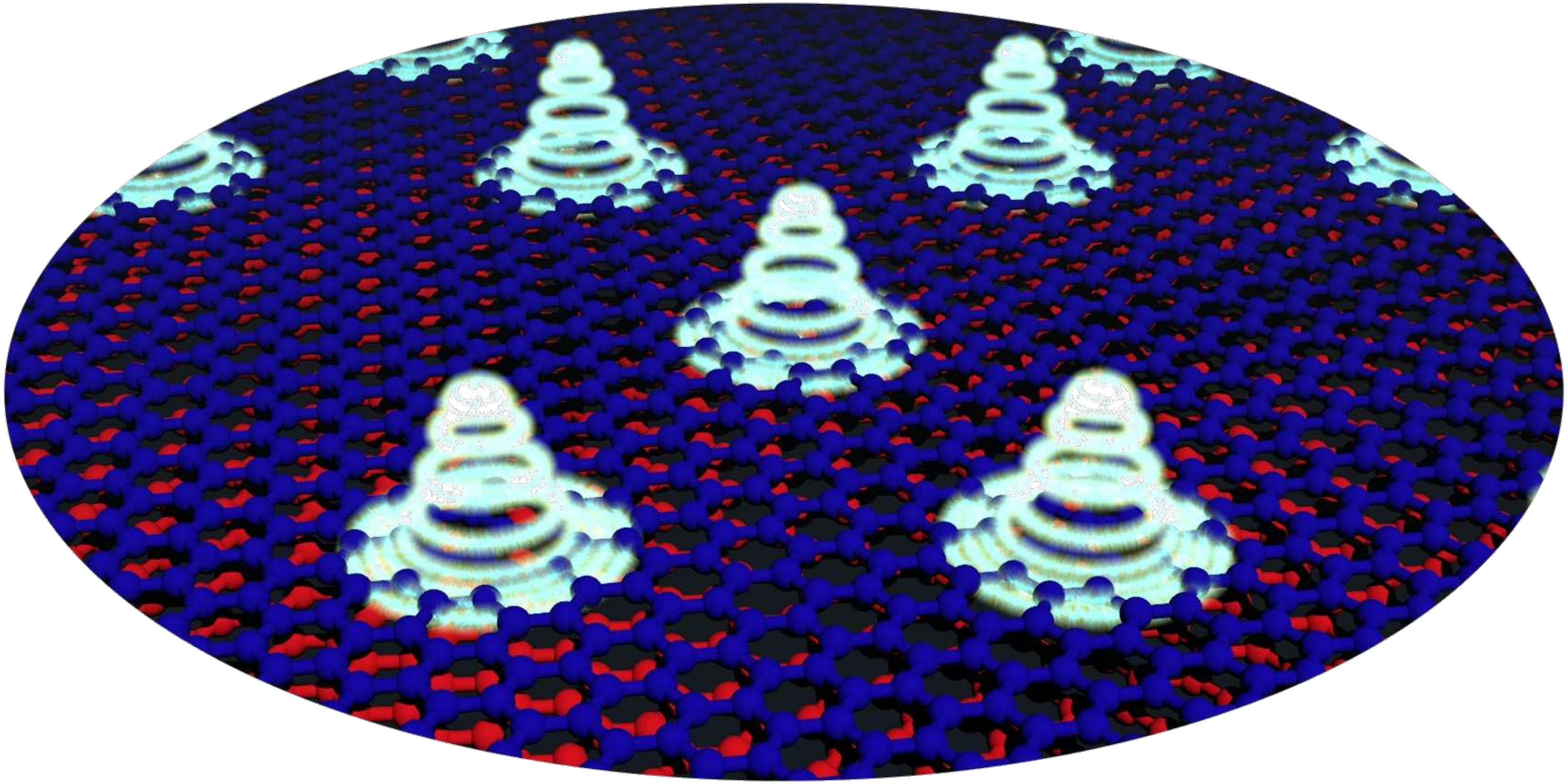
a = 1000 nm

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

Twisted 2D materials as a platform for artificial quantum matter



A new universe in each new twisted material

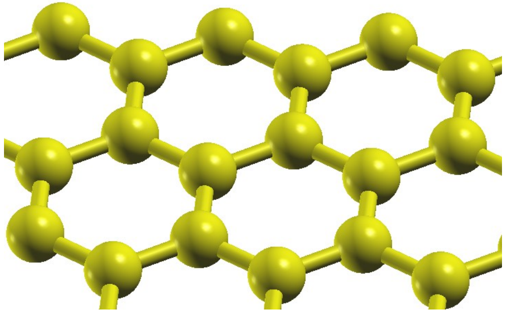


Each twisted material is a new universe for electrons, with laws that change from twist to twist

The two-dimensional materials world

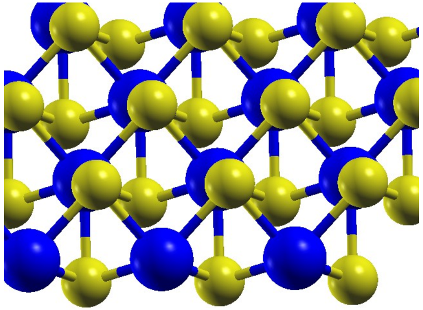
Semimetal

Graphene



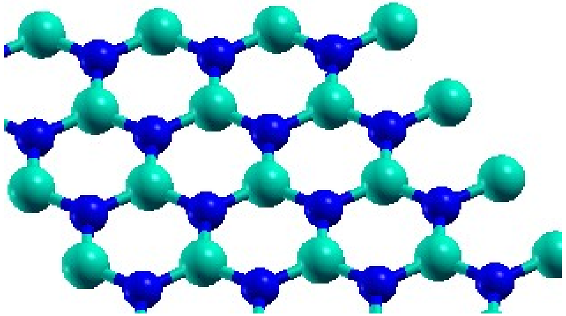
Superconductor

$NbSe_2$



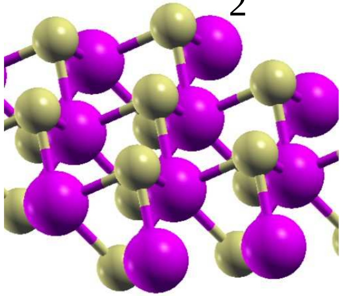
Insulator

BN



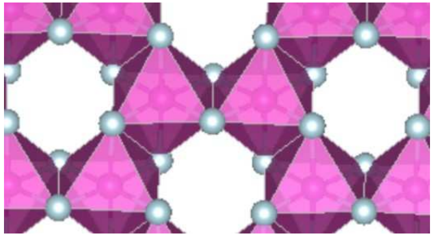
Semiconductor

WSe_2



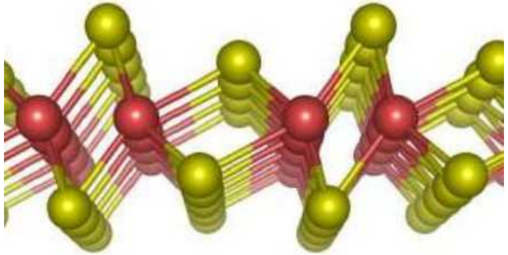
Ferromagnet

CrI_3



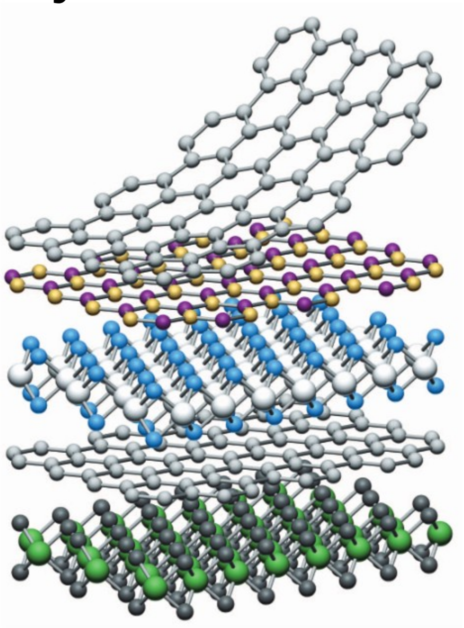
Quantum spin Hall insulator

WTe_2



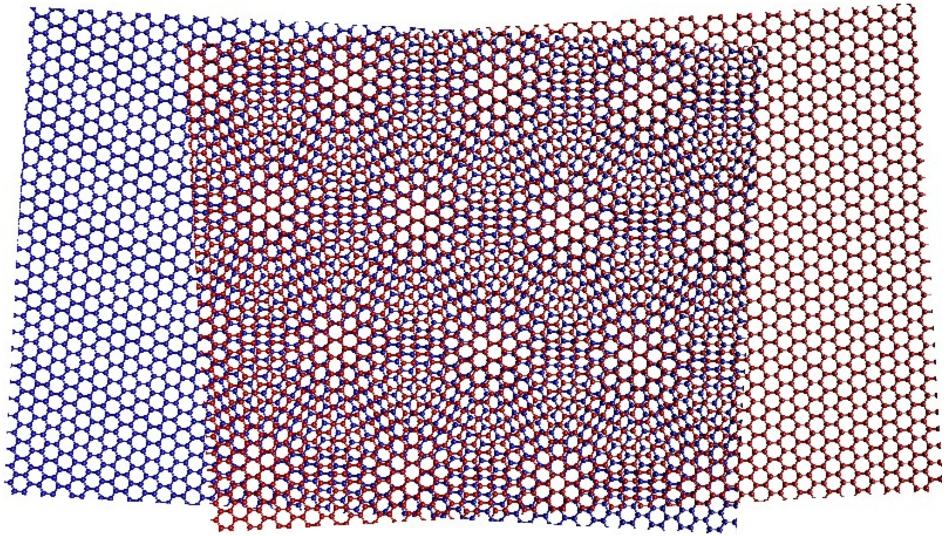
The flexibility of two-dimensional materials

They can be stacked



Nature 499.7459 419. (2013)

They can be rotated

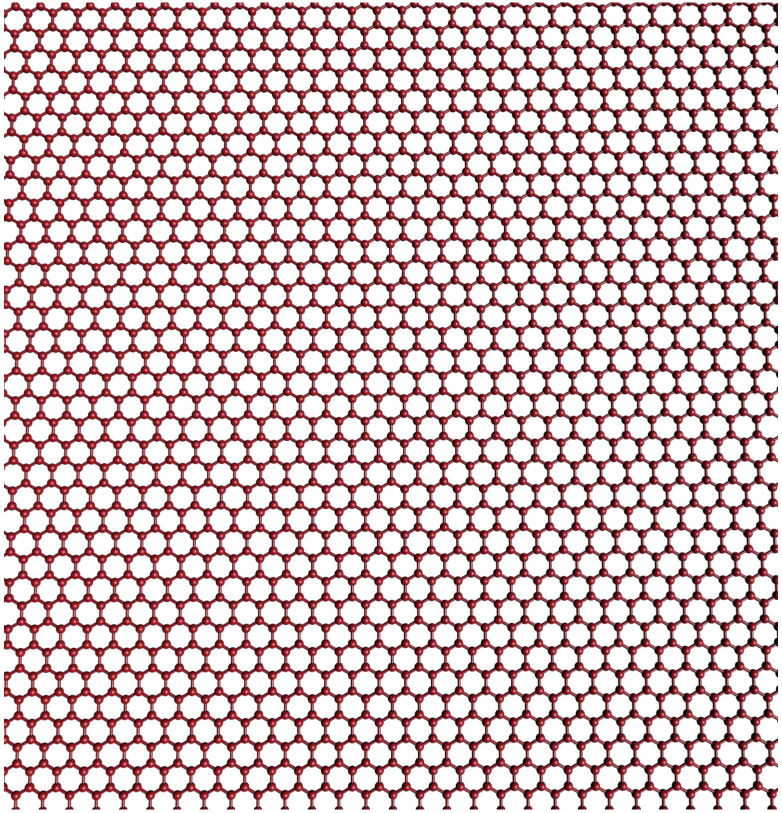


Science 361.6403 690-693. (2018)

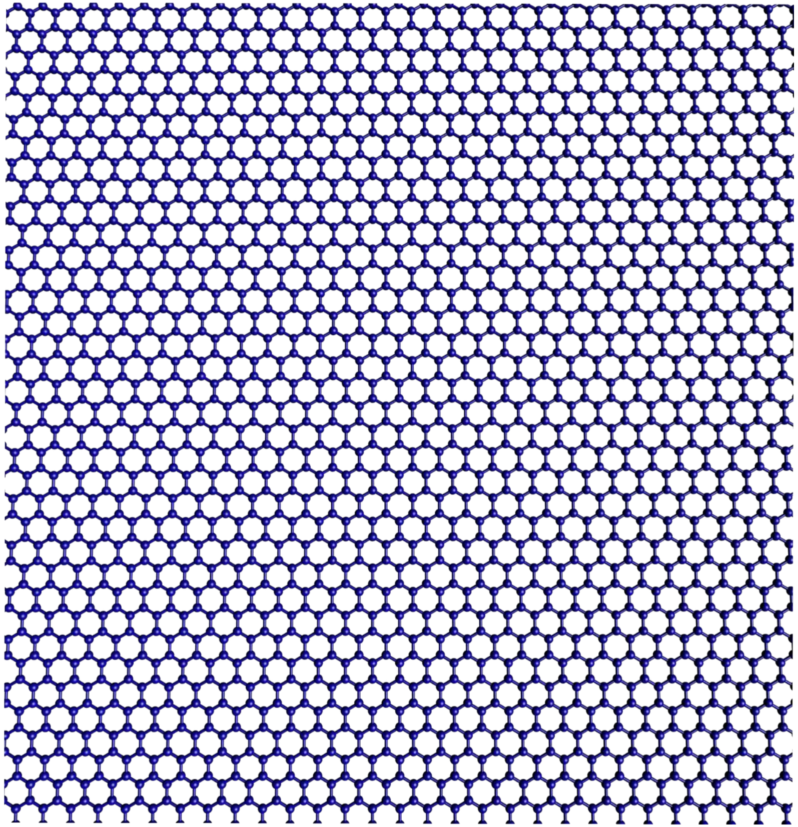
These are unique features of two-dimensional materials

Moire in twisted bilayer graphene

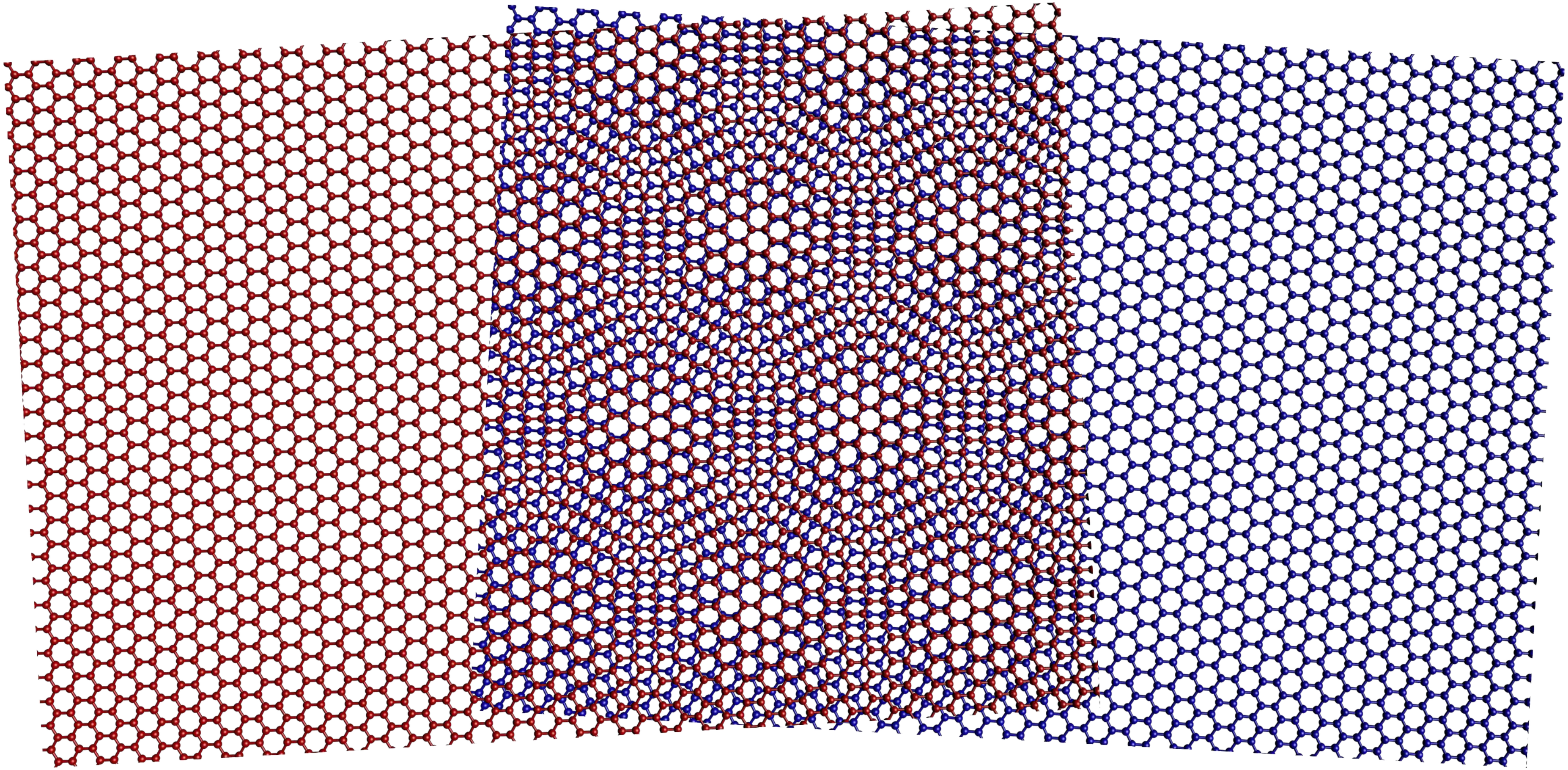
Upper graphene layer



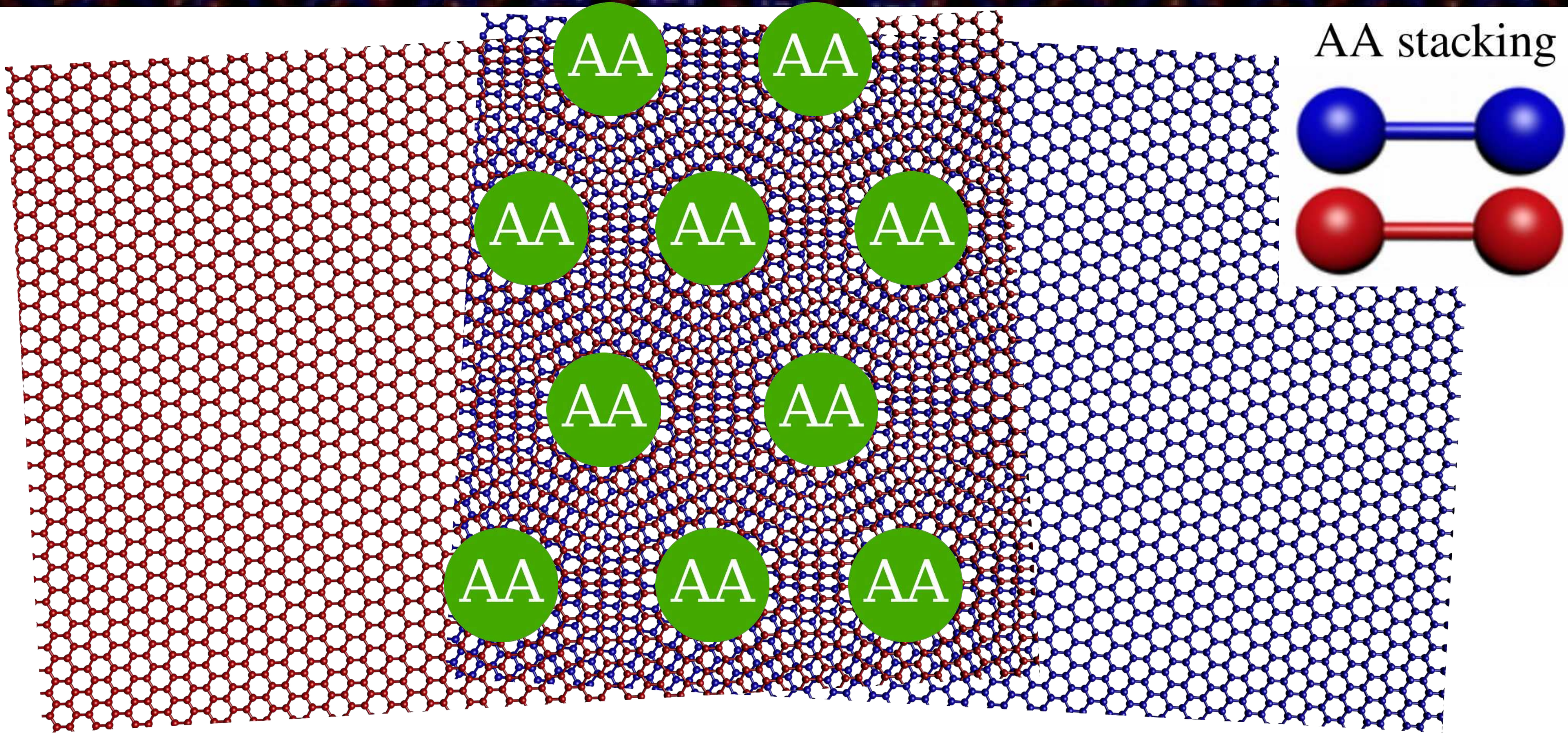
Lower graphene layer



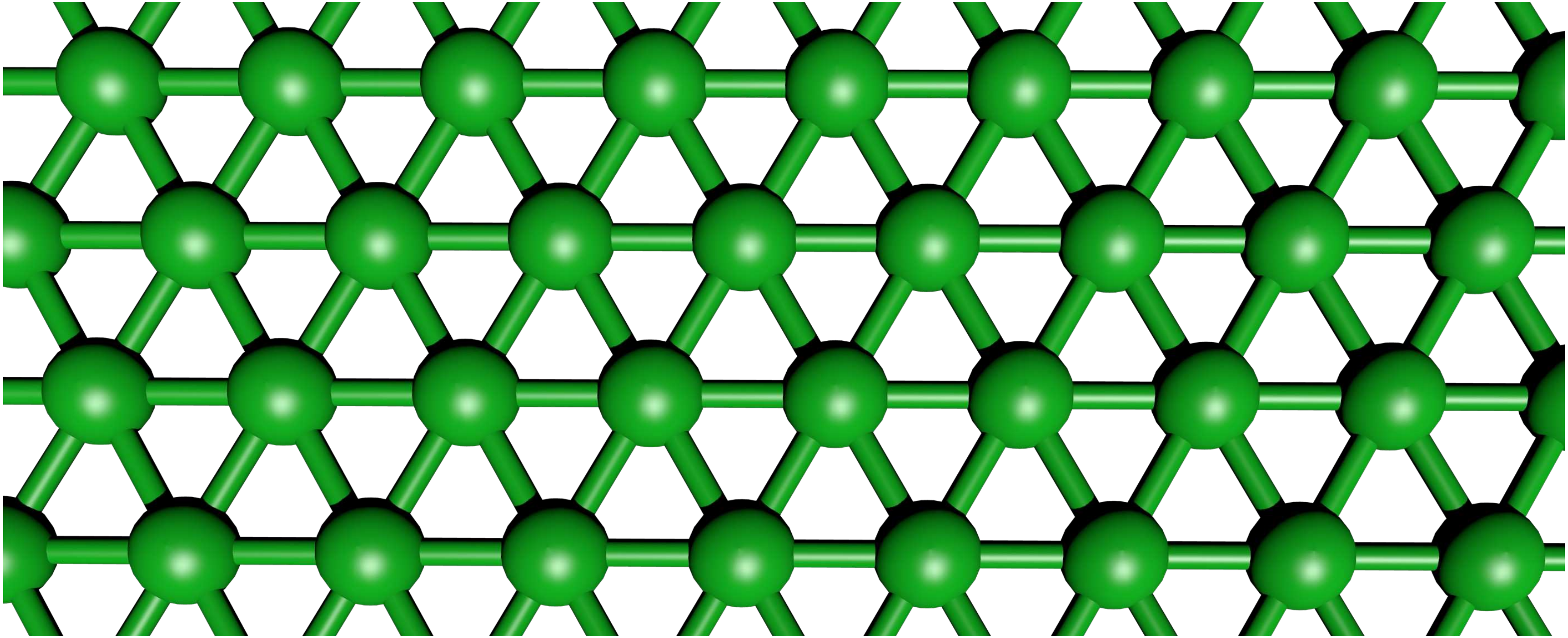
Moire in twisted bilayer graphene

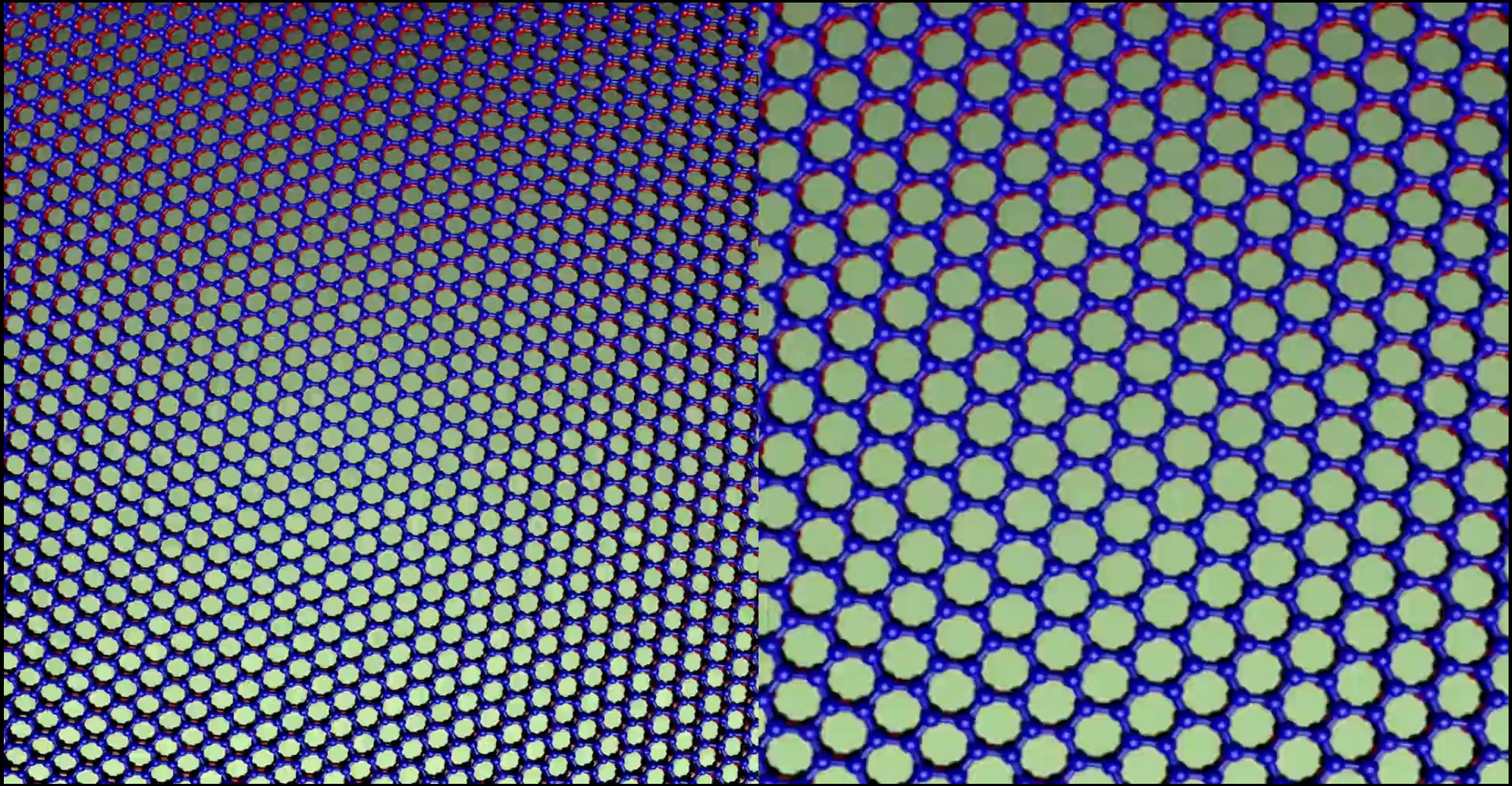


Moire in twisted bilayer graphene



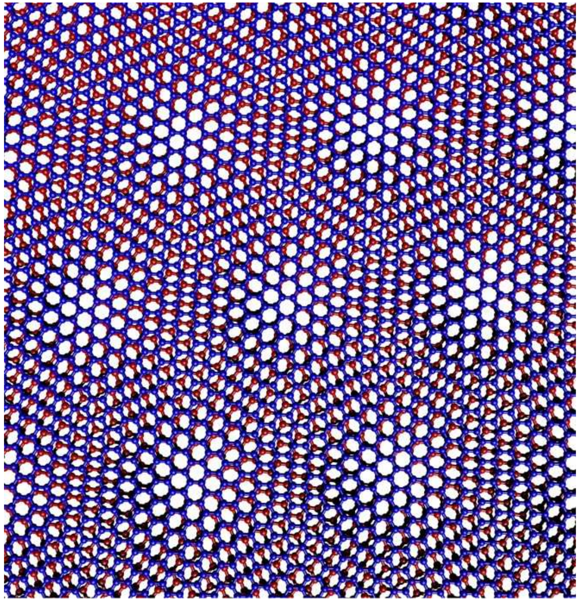
Moire in twisted bilayer graphene



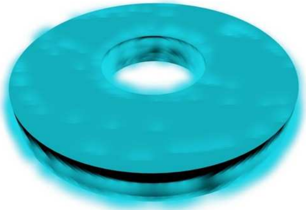


One material, a zoo of electronic phases

Twisted bilayer graphene

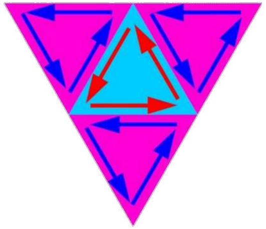


Superconductivity



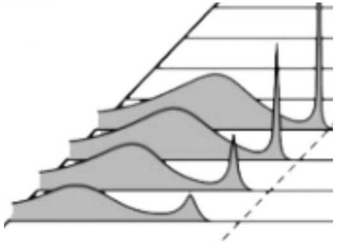
Nature 556, 43–50 (2018)

Topological networks



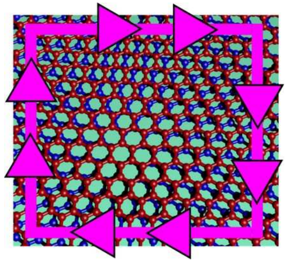
Nano Lett. 18, 11, 6725-6730 (2018)

Strange metals



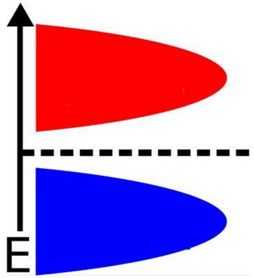
Phys. Rev. Lett. 124, 076801 (2020)

Chern insulators



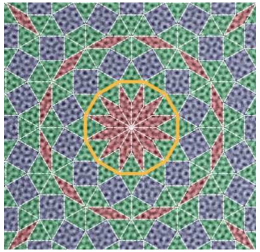
Science 365, 605-608 (2019)

Correlated insulators



Nature 556, 80–84 (2018)

Quasicrystalline physics



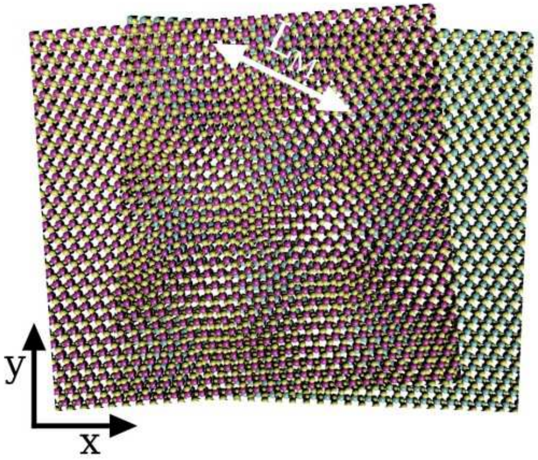
Science 361 782-786 (2018)

Twisted graphene multilayers provide a powerful platform for emergent phenomena

The generality of correlated physics in twisted 2D materials

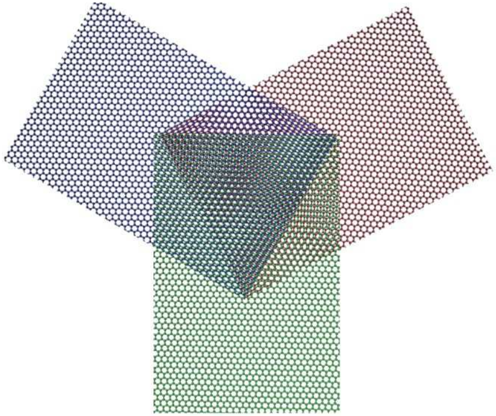
Superconductivity & correlated behavior found also in

Twisted dichalcogenides



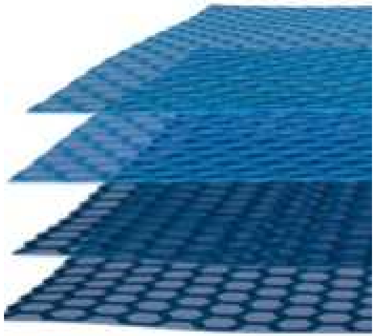
Nature 579, 359–363 (2020)

Twisted graphene trilayers



Nature 590, 249–255 (2021)

Twisted graphene tetralayers

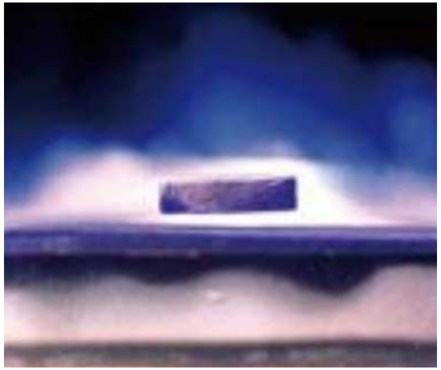


Nature 583, 221–225 (2020)

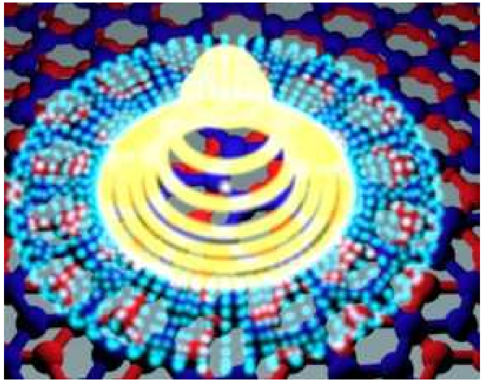
Some of new physics observed were only realized before in rare, heavy or even toxic compounds

The opportunities of twisted van der Waals materials

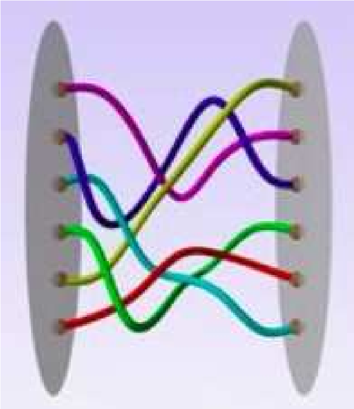
“Unveil” the nature of high T_C superconductivity (?)



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*

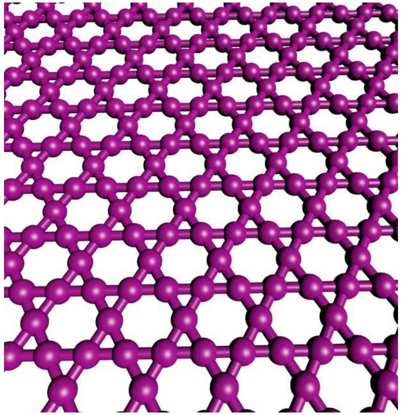
Designing quantum matter in twisted materials

The strength of electronic correlations

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

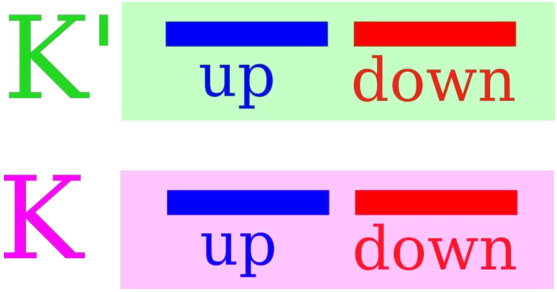
Twist angle control

The details of the electronic dispersion



Interlayer bias

The local quantum degrees of freedom

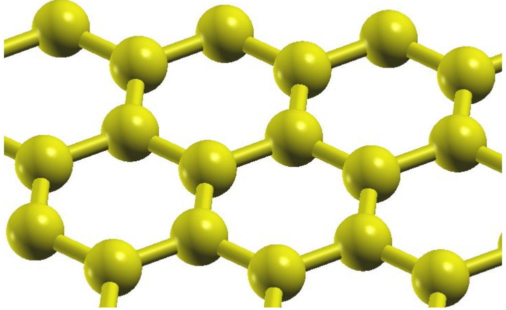


Magnetic encapsulation

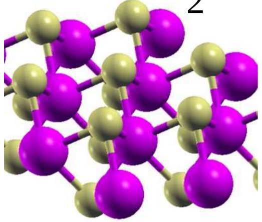
Goal: control local degrees of freedom via magnetic encapsulation a twisted material

Designing quantum matter with twisted magnetic van der Waals materials

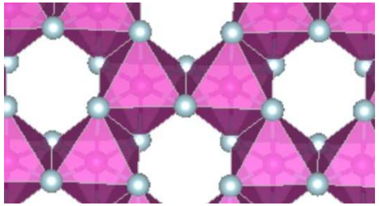
Graphene



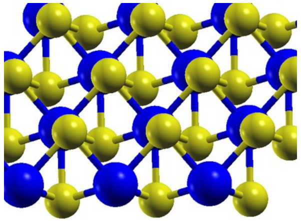
Semiconductor
WSe_2



Magnet
$CrBr_3$, 1T-TaS_2, CrI_3



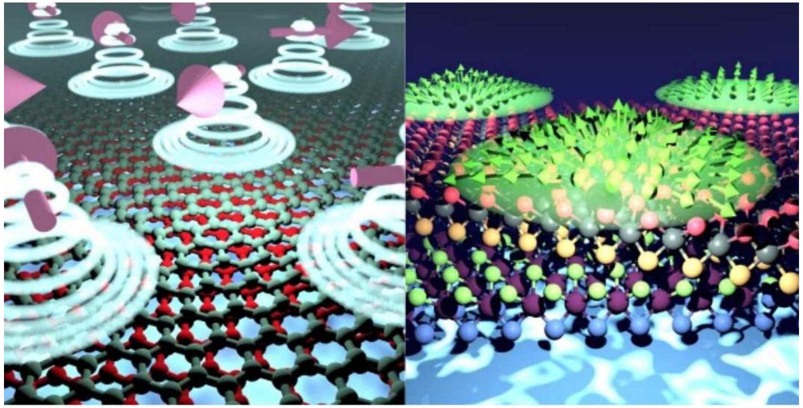
Metal
1H-TaS_2



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

Today's plan

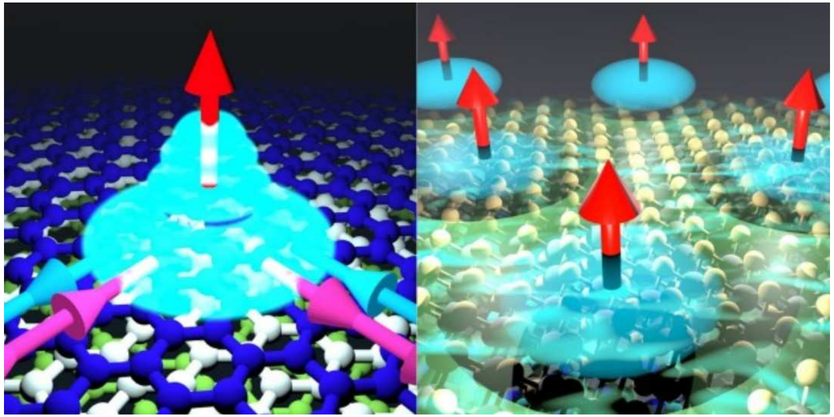
Design of new correlated states by magnetic encapsulation in twisted materials



theory

Phys. Rev. Lett. 126, 056803 (2021)
New J. Phys. 23 073038 (2021)

A new family of correlated states based on quantum magnetism: heavy fermions in twisted materials

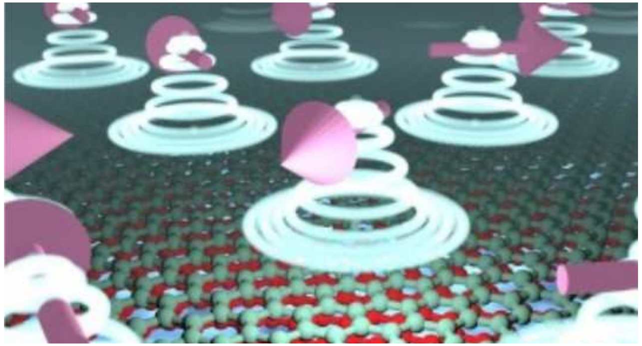


theory & experiment

Phys. Rev. Lett. 127, 026401 (2021)
arXiv:2103.11989 (2021)

Behind the scenes

Valley-mixing correlations in CrI_3/twisted BG/CrI_3



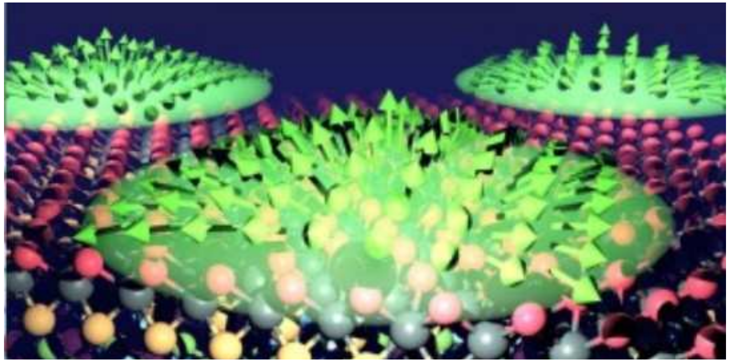
Tobias Wolf

Gianni Blatter

Oded Zilberberg

Phys. Rev. Lett. 126, 056803 (2021)

Correlated states dominated by spin-orbit coupling in twisted Janus dichalcogenide bilayers

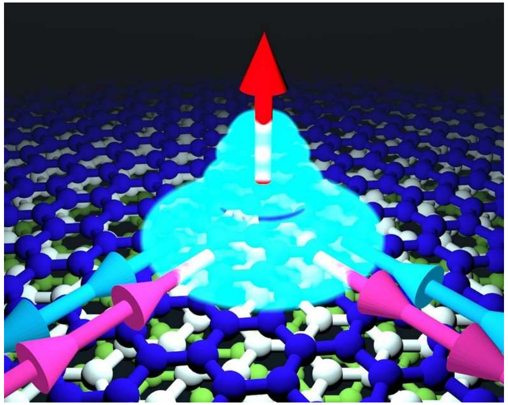


David Soriano

New J. Phys. 23 073038 (2021)

Behind the scenes

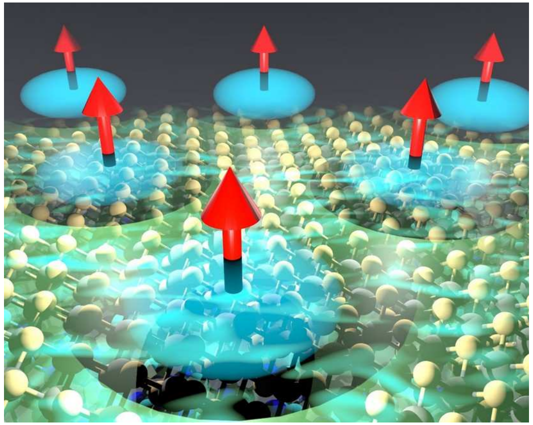
Heavy fermions in twisted graphene trilayers



Aline Ramires

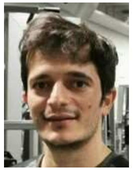
Phys. Rev. Lett. 127, 026401 (2021)

Heavy fermions in twisted dichalcogenide bilayers

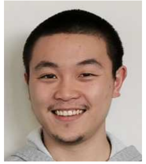


S. Ganguli

M. Amini



G. Chen



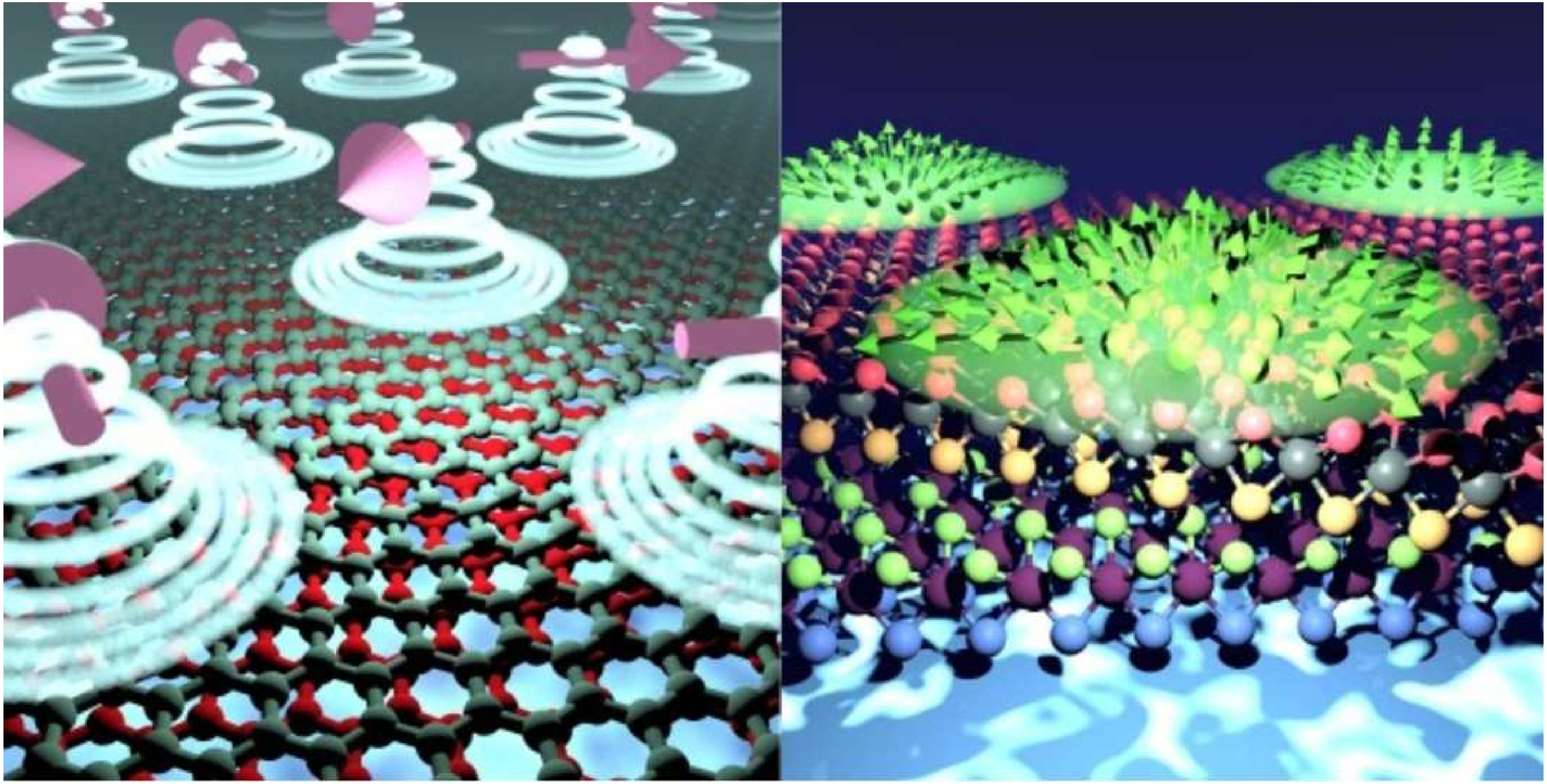
V. Vaňo

S. Kezilebieke

P. Liljeroth

arXiv:2103.11989 (2021)

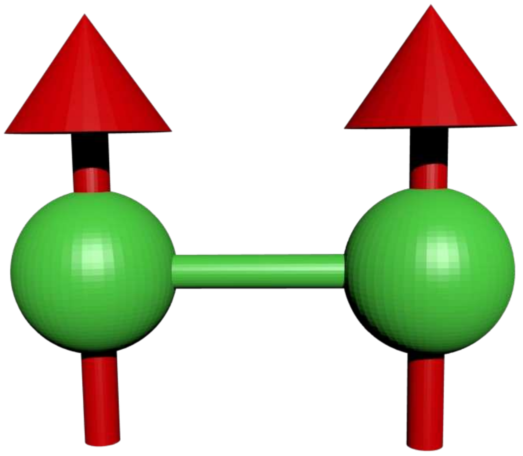
Design of new correlated states by magnetic encapsulation in twisted materials



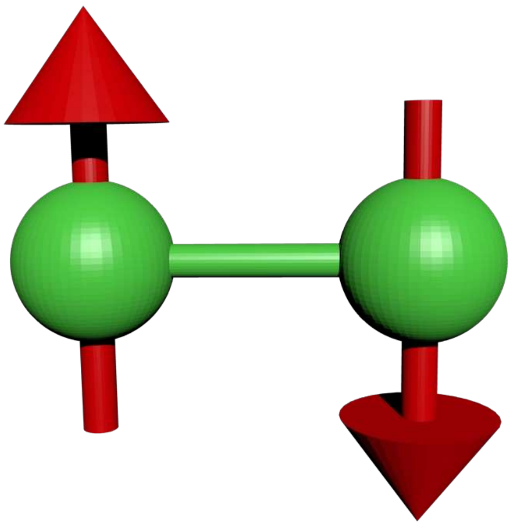
Frustration

A bird's eye view on magnetism

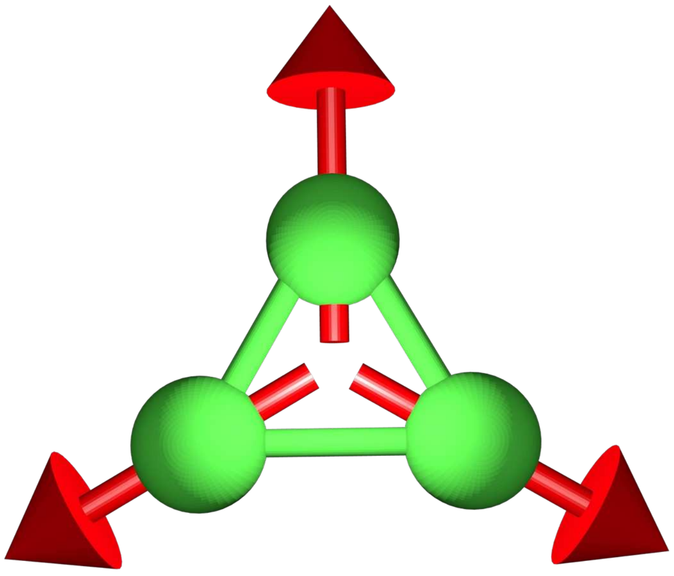
Ferromagnetism



Antiferromagnetism



Frustrated magnetism



Can we control the microscopic properties of a magnet?

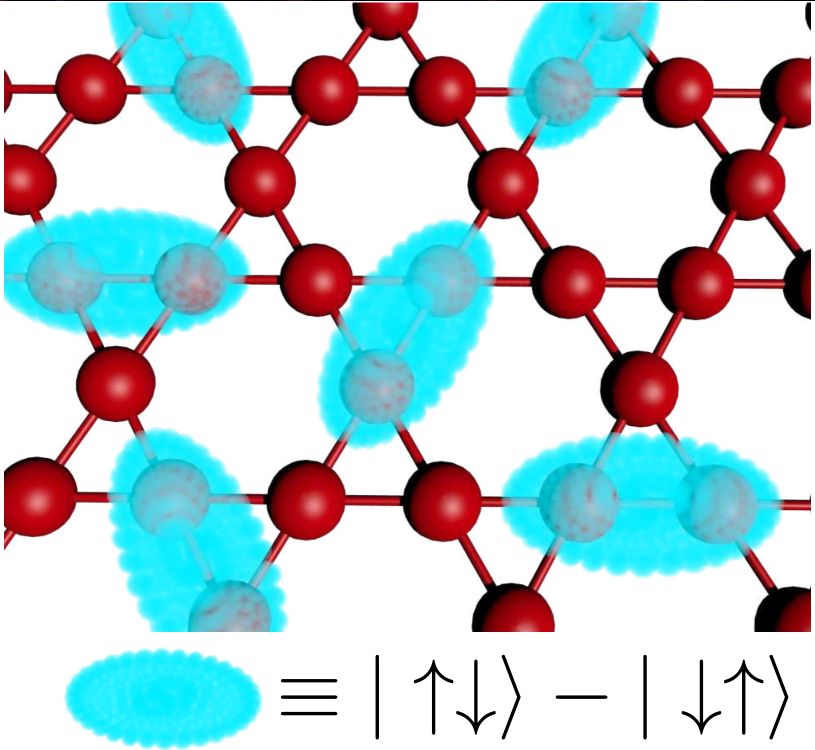
What is the best that can happen?

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)

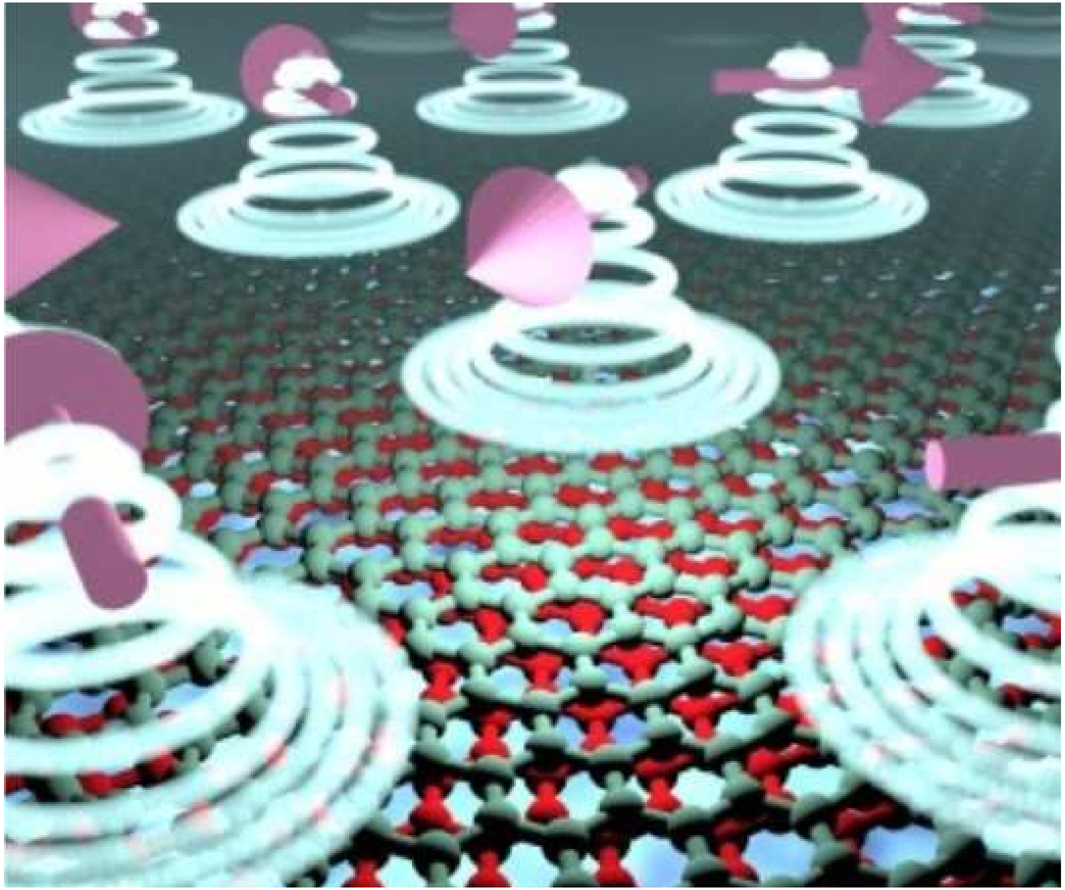
Kagome Heisenberg

Science 332, 1173-1176 (2011)

Extended triangular Heisenberg

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

Valley-mixing correlations in magnetically encapsulated tBG



Tobias Wolf

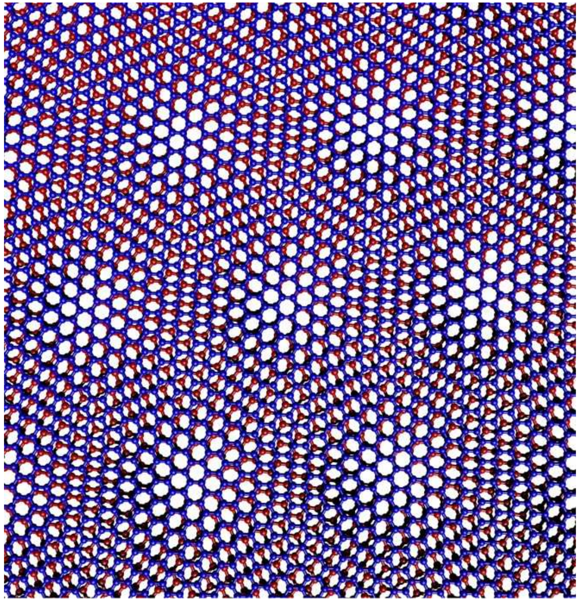
Gianni Blatter

Oded Zilberberg

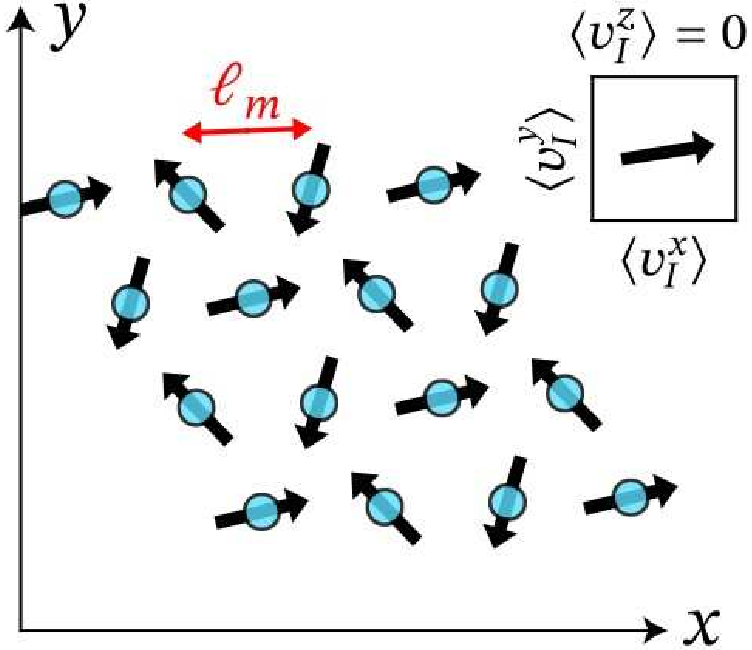
Phys. Rev. Lett. 126, 056803 (2021)

Frustrated valley magnetism

Moire structure



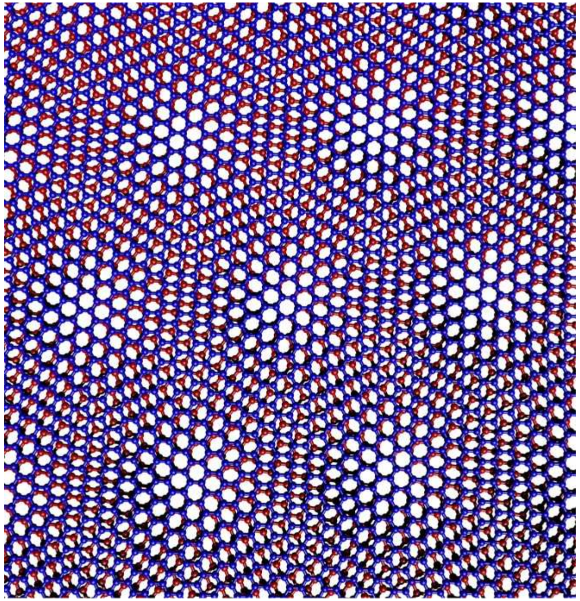
Valley-frustrated state



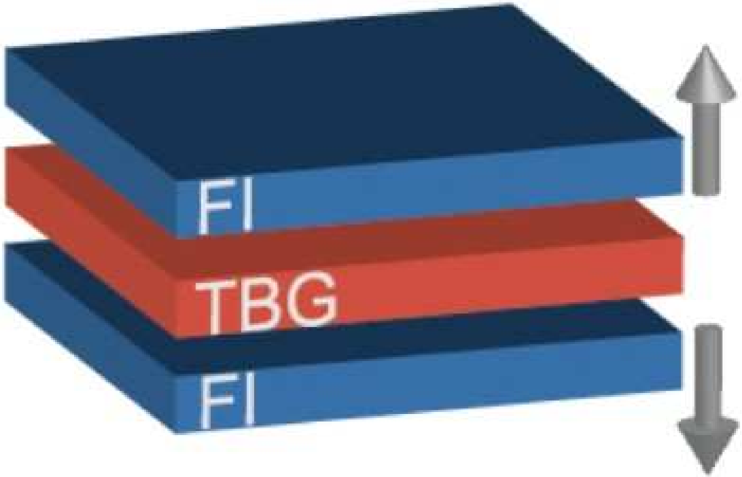
Can we create a controllable valley-only frustrated magnet?

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

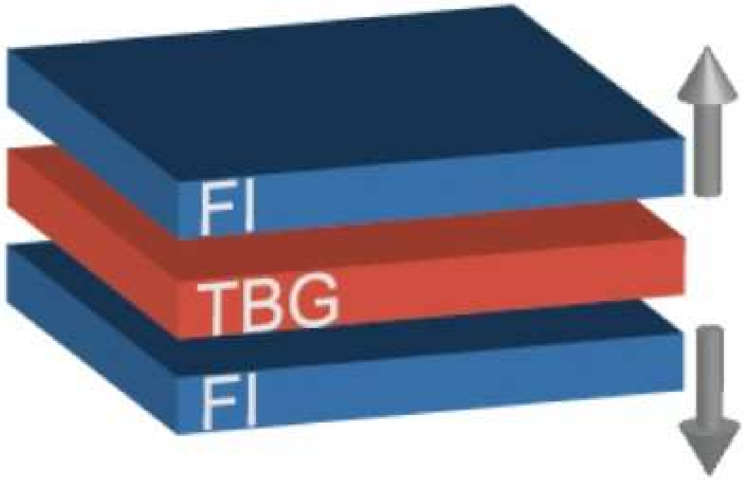
Magnetic encapsulation

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

Kinetic energy

Exchange proximity effect

Rashba spin-orbit coupling

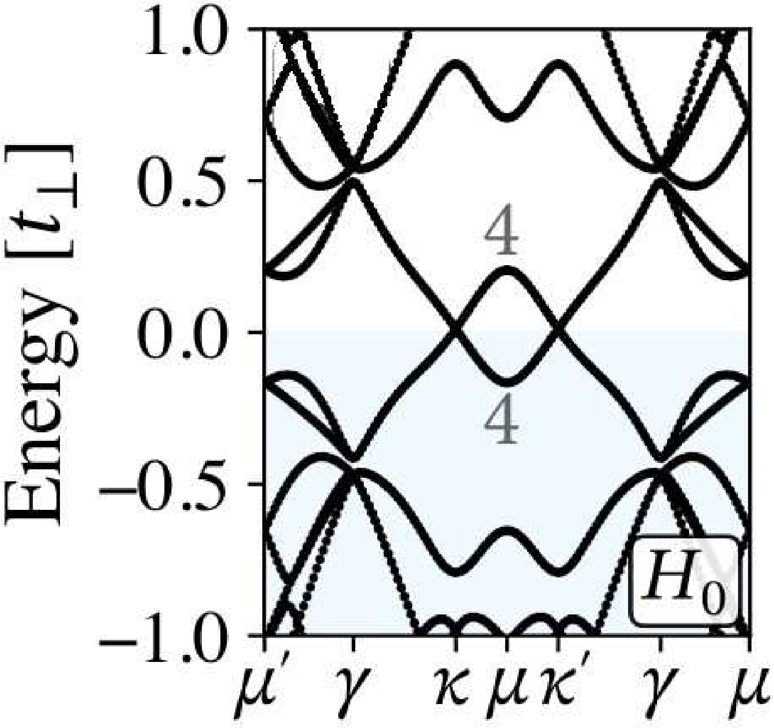


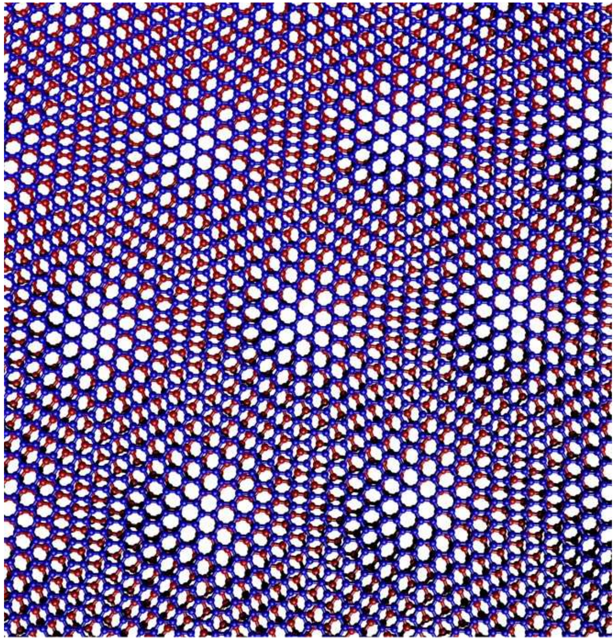
Valley frustration from combined twist engineering, exchange proximity and spin-orbit coupling.

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

Twisted graphene bilayer at 2 degrees

Without exchange field nor spin-obit coupling



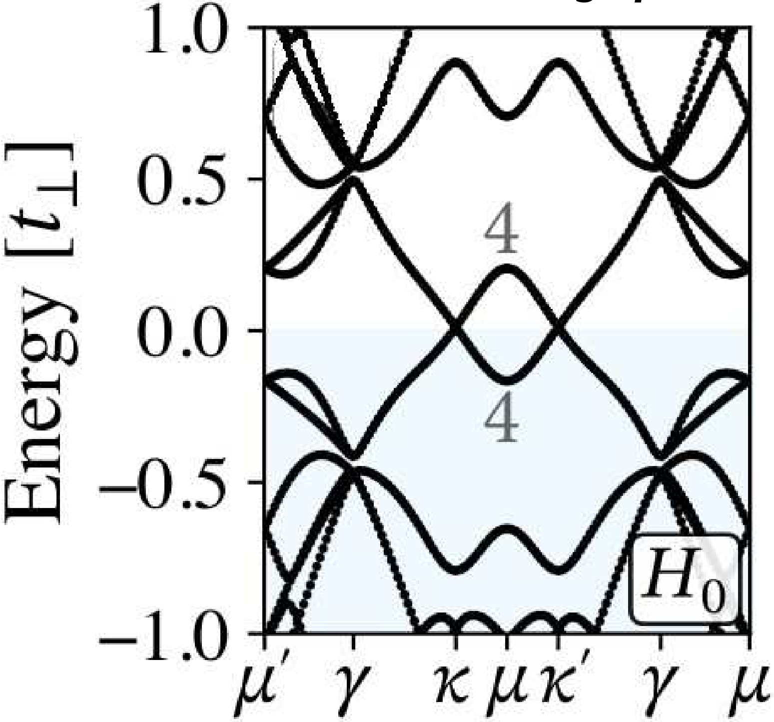


Phys. Rev Lett. 99 256802 (2007)
Phys. Rev. B 82, 121407(R) (2010)
PNAS 108 30 12233-12237 (2011)

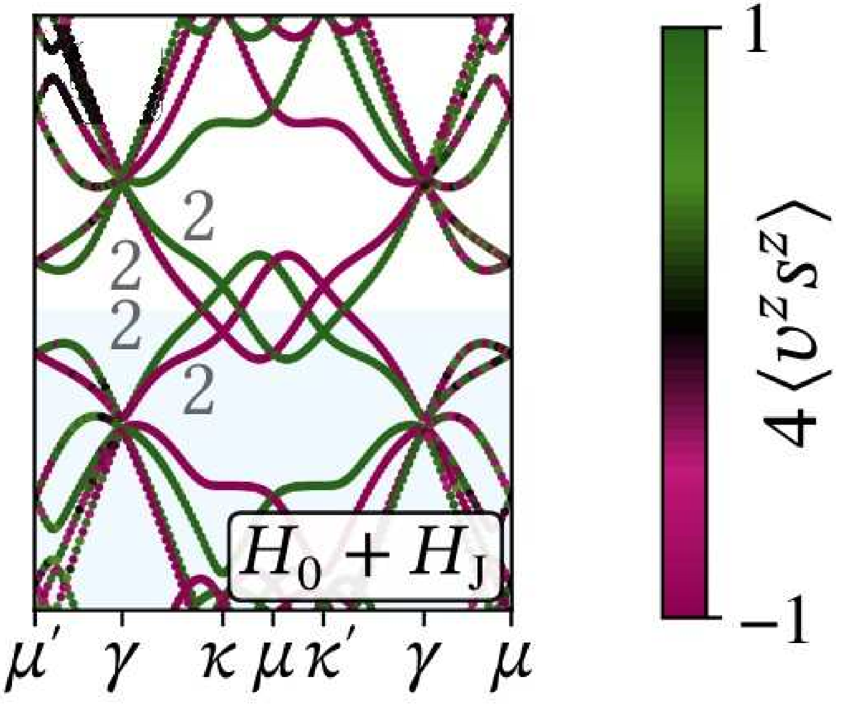
Renormalized Dirac cones

Twisted graphene bilayer at 2 degrees

Without exchange field



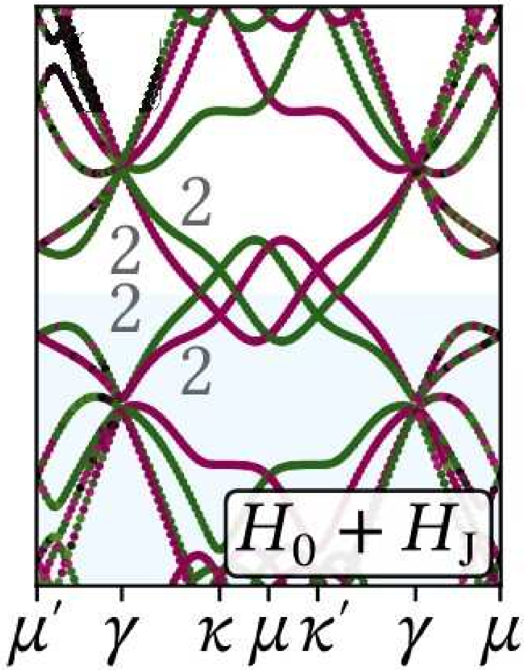
With exchange field



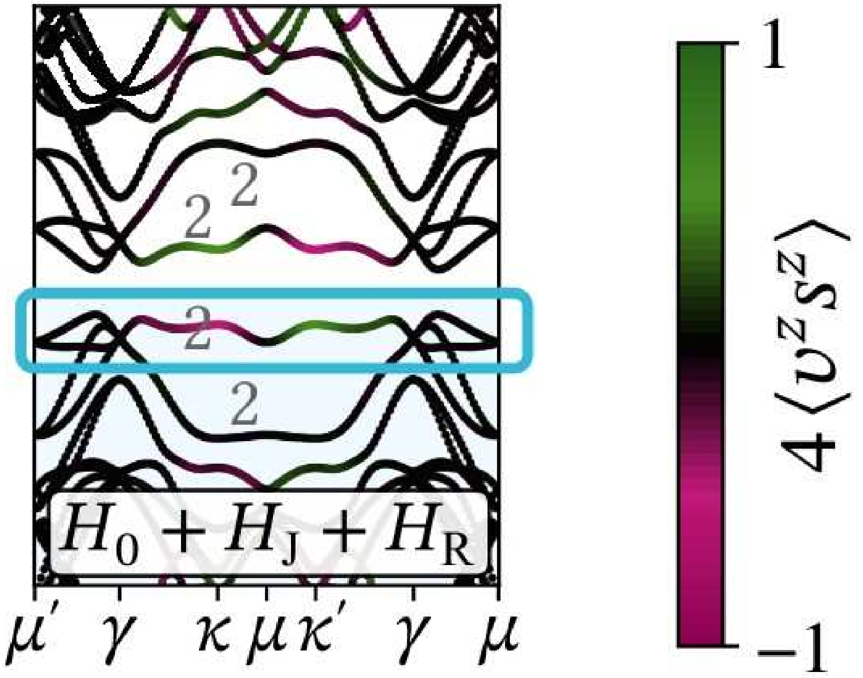
<u>Valley-spin splitting degeneracy lifting</u>

Valley-only correlated states in twisted graphene bilayers

Without Rashba SOC



With Rashba SOC

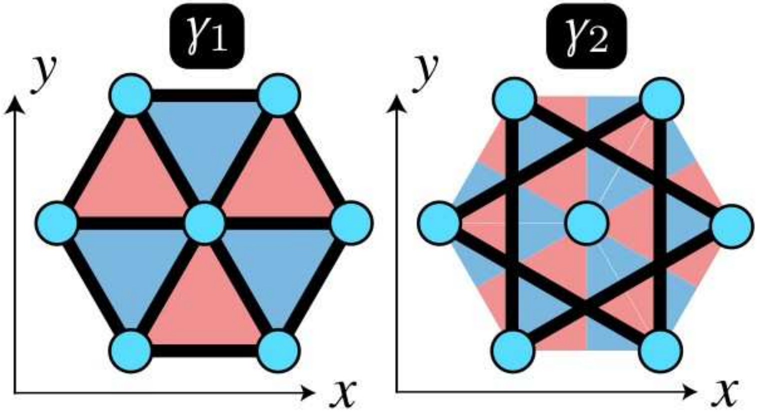


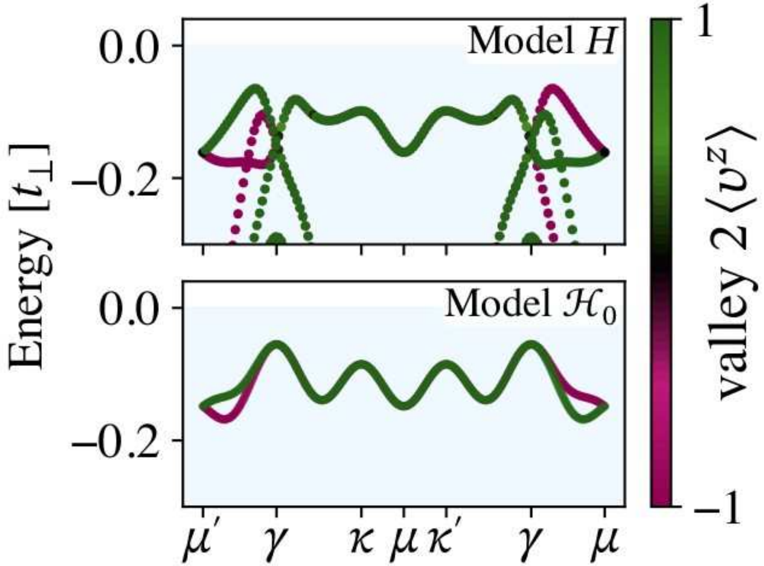
Nearly flat bands created from twist + exchange + spin-orbit coupling

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

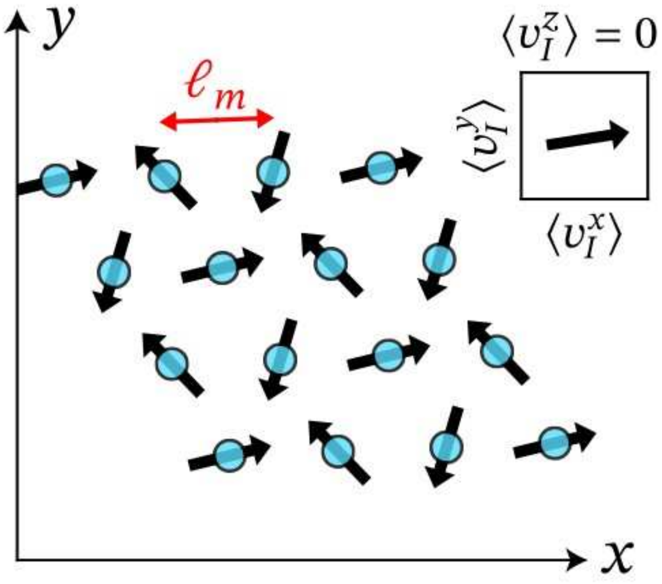
Impact of interactions

Lets add electronic interactions

Free Hamiltonian

Electronic interactions

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

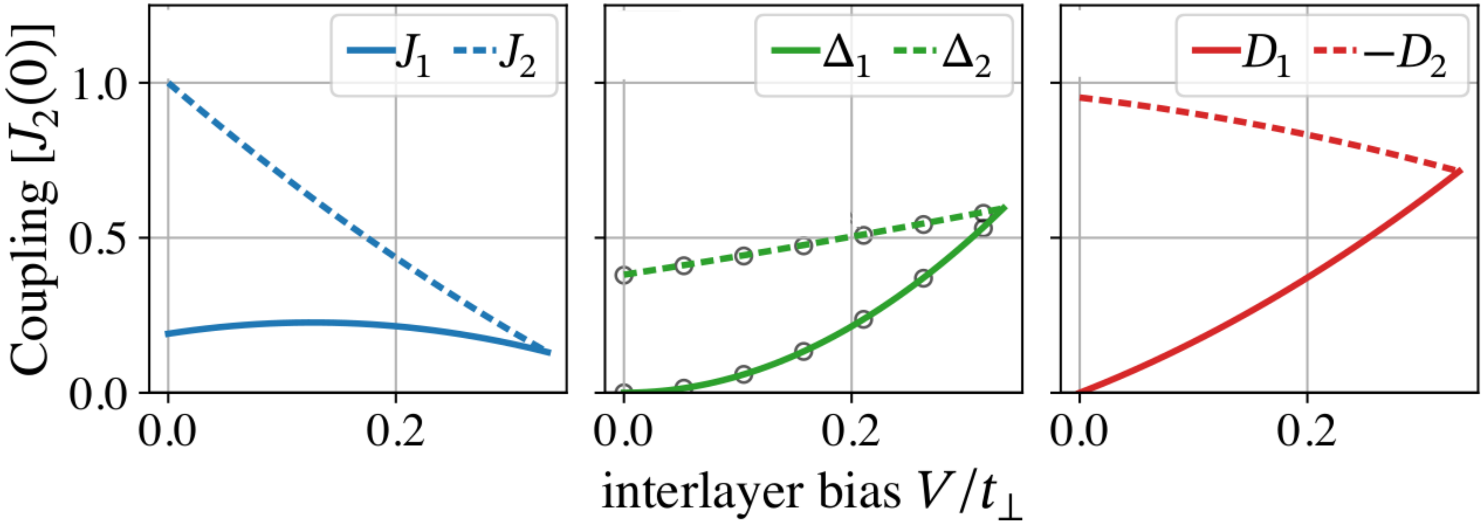


And compute the effective valley-Heisenberg Hamiltonian in the strong coupling limit

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

Controlling a valley-Heisenberg model electrically

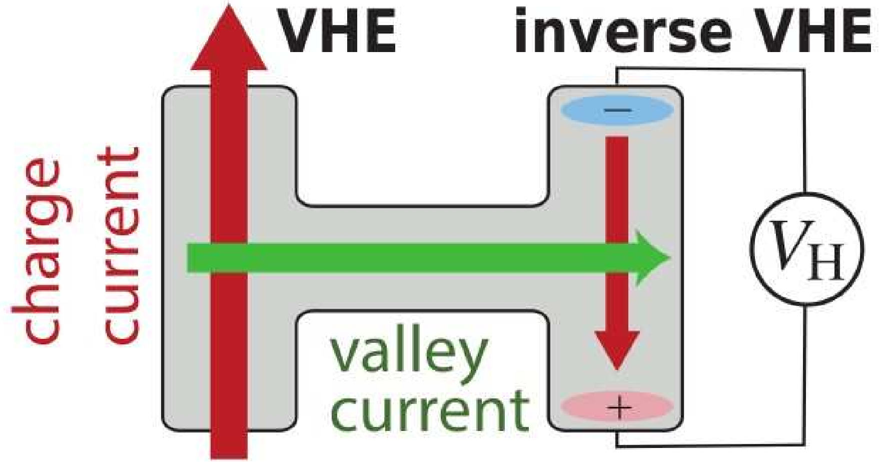
$$\mathcal{H}_v = \sum_{IJ} J_{IJ}\, \boldsymbol{v}_I \cdot \boldsymbol{v}_J + \Delta_{IJ}\, v_I^z v_J^z + \nu_{IJ}\, D_{IJ}\, (\boldsymbol{v}_I \times \boldsymbol{v}_J)_z$$



An interlayer bias provides a tunable anisotropic valley-Heisenberg model

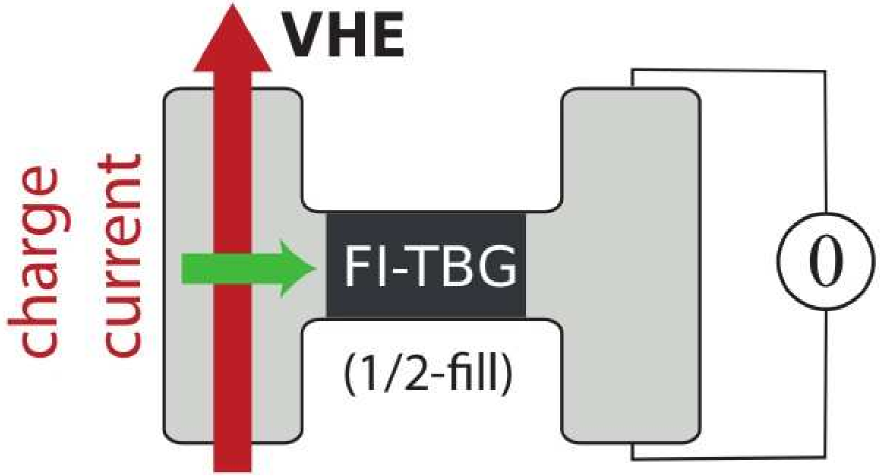
Detecting the valley spiral

No valley mixing



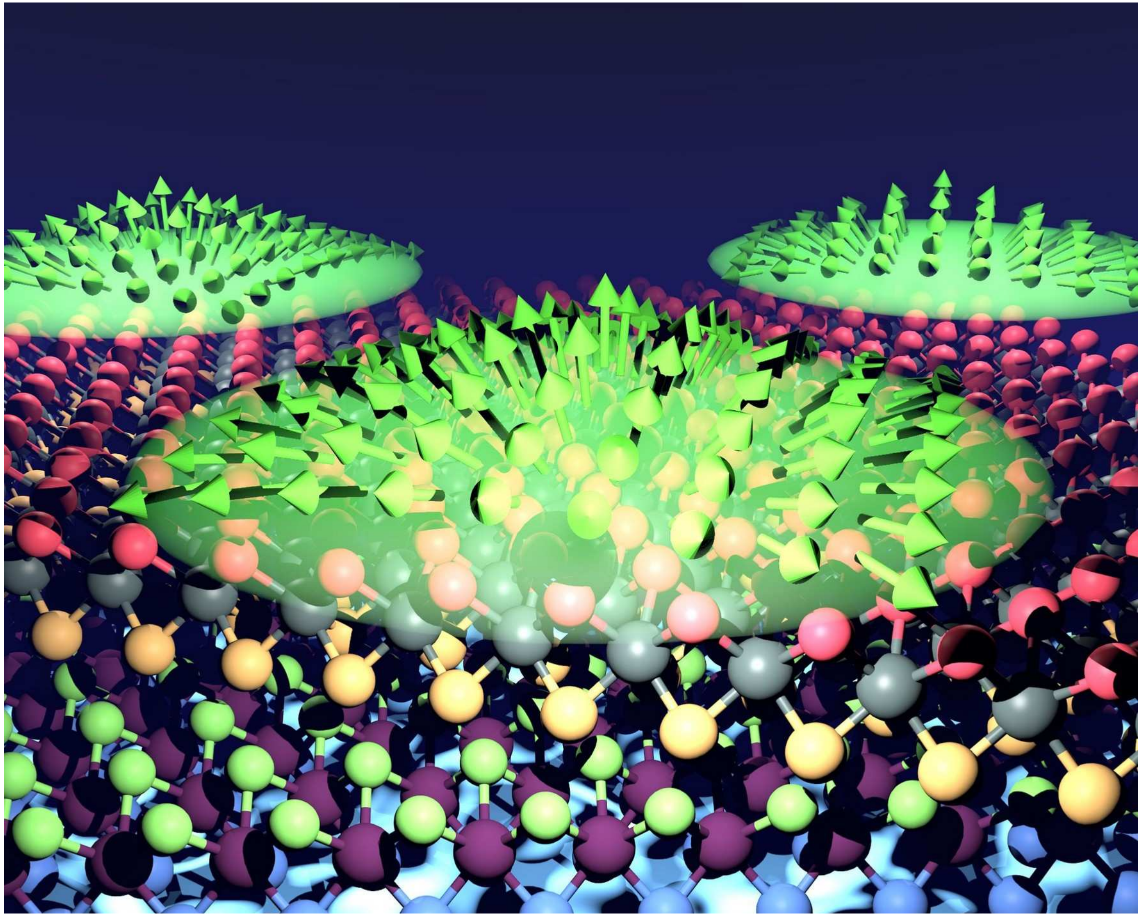
Finite non-local conductance

Finite valley mixing



Zero non-local conductance

Correlated states dominated by spin-orbit coupling in Janus dichalcogenides

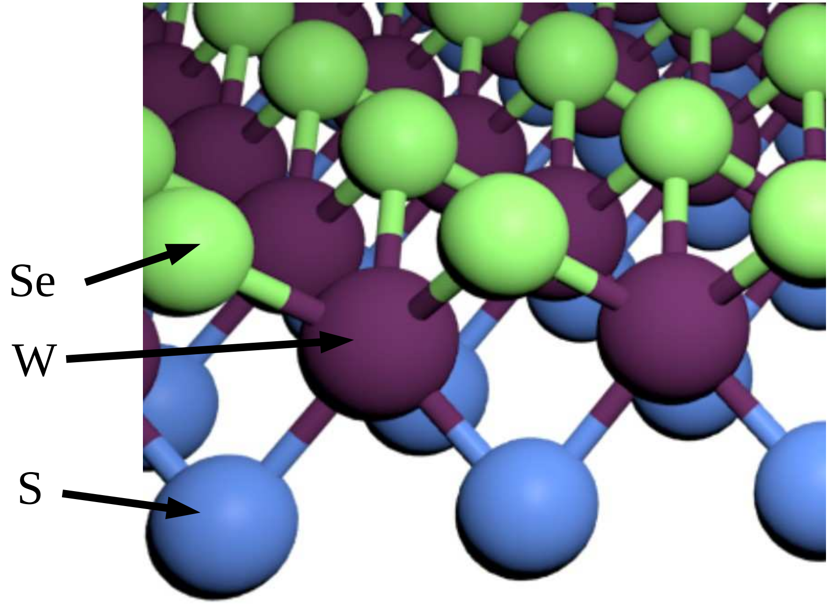


David Soriano

New J. Phys. 23 073038 (2021)

Janus dichalcogenide monolayers

WSSe structure



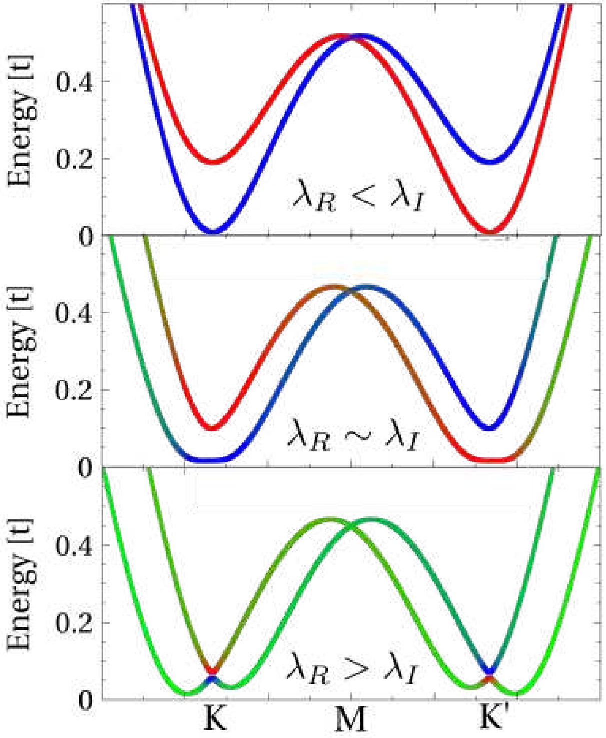
Intrinsic mirror symmetry breaking

Colossal Rashba SOC effects

Band structure

Rashba SOC
λ_R

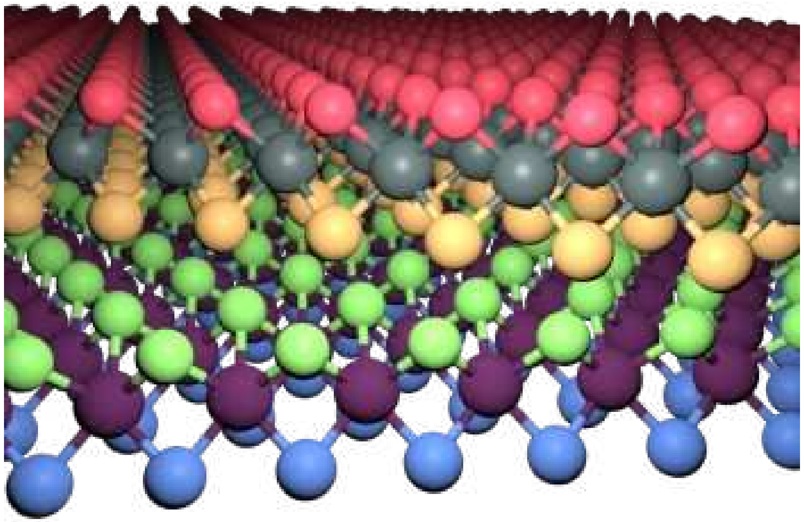
Ising SOC
λ_I



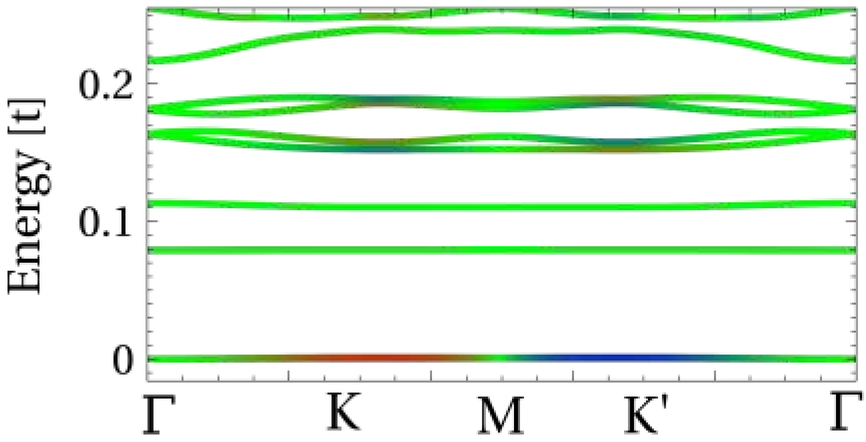
Rashba SOC strongly impact the low energy dispersion

Twisted Janus bilayers

Twisted Janus bilayer

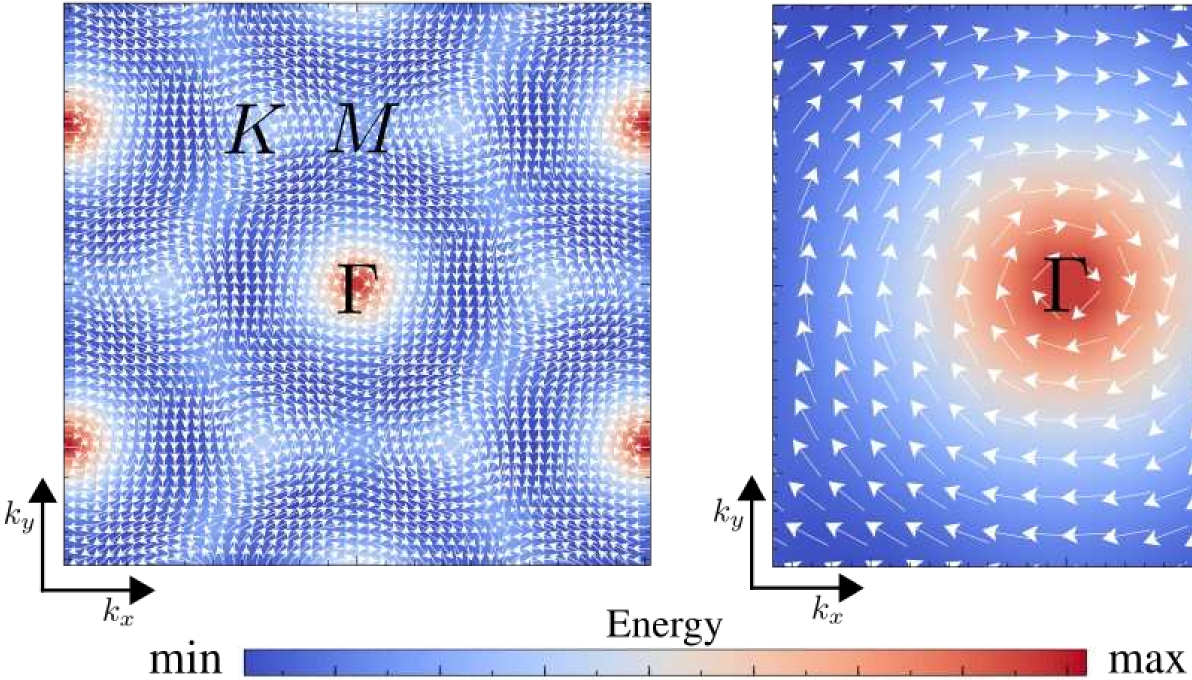


Band structure



Flat bands emerge in a twisted Janus bilayer, inheriting the colossal Rashba SOC effects

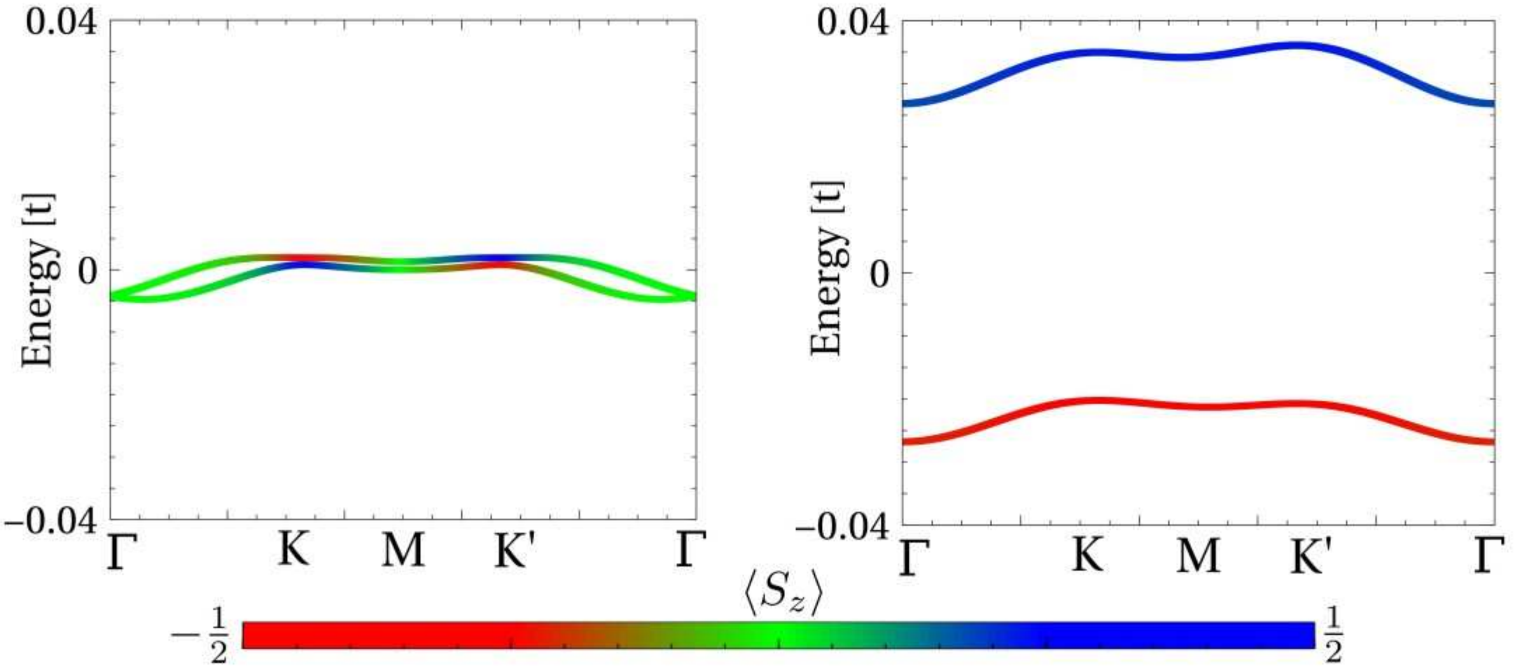
Reciprocal space texture of the flat bands



Flat bands are dominated by a strong spin-momentum texture, stemming form the Janus structure

Impact of interactions at low energies

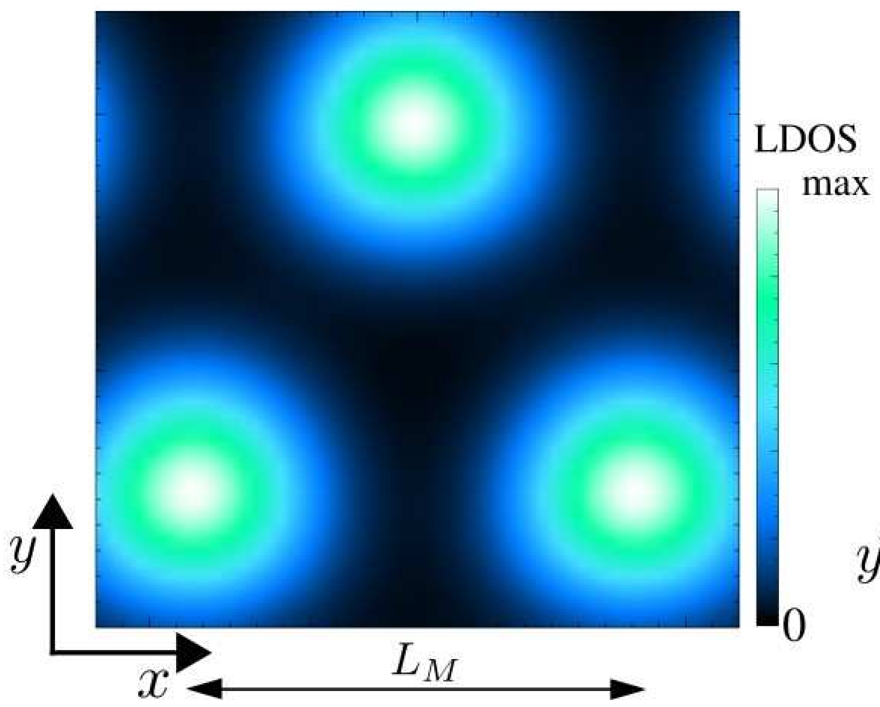
No interactions | *With interactions*



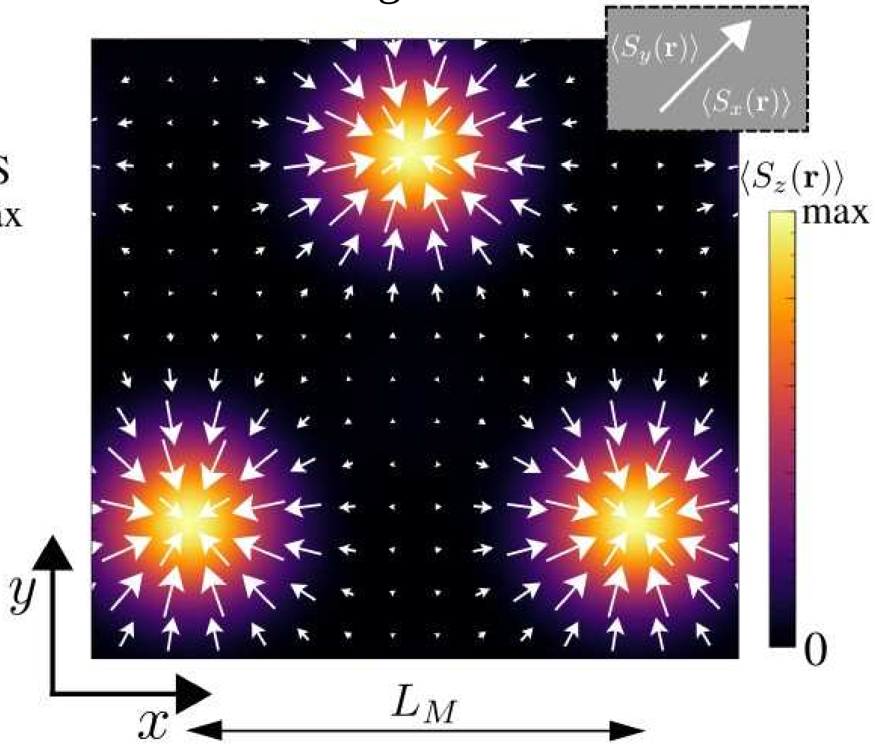
When including interactions in the full lattice model, a symmetry broken state arises

Real space profile when including interactions

Electronic density

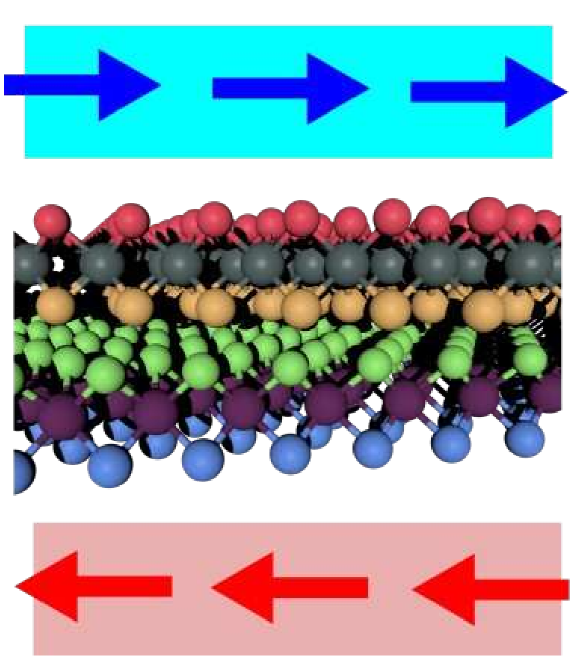


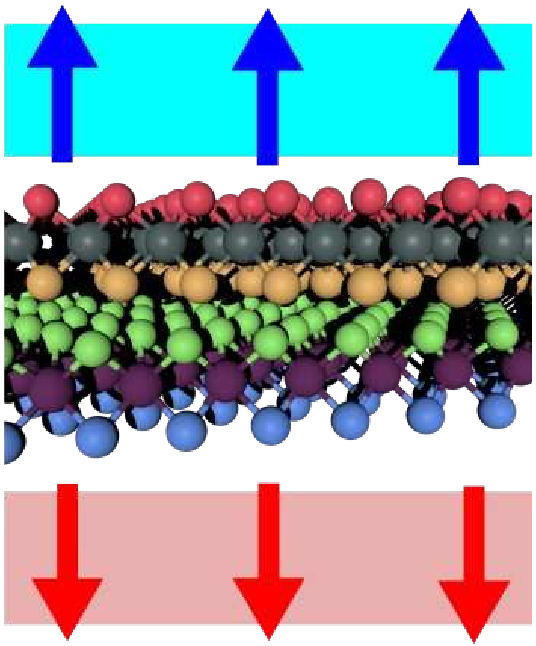
Magnetism



A moire meron magnetic structure appears due to the presence of interactions

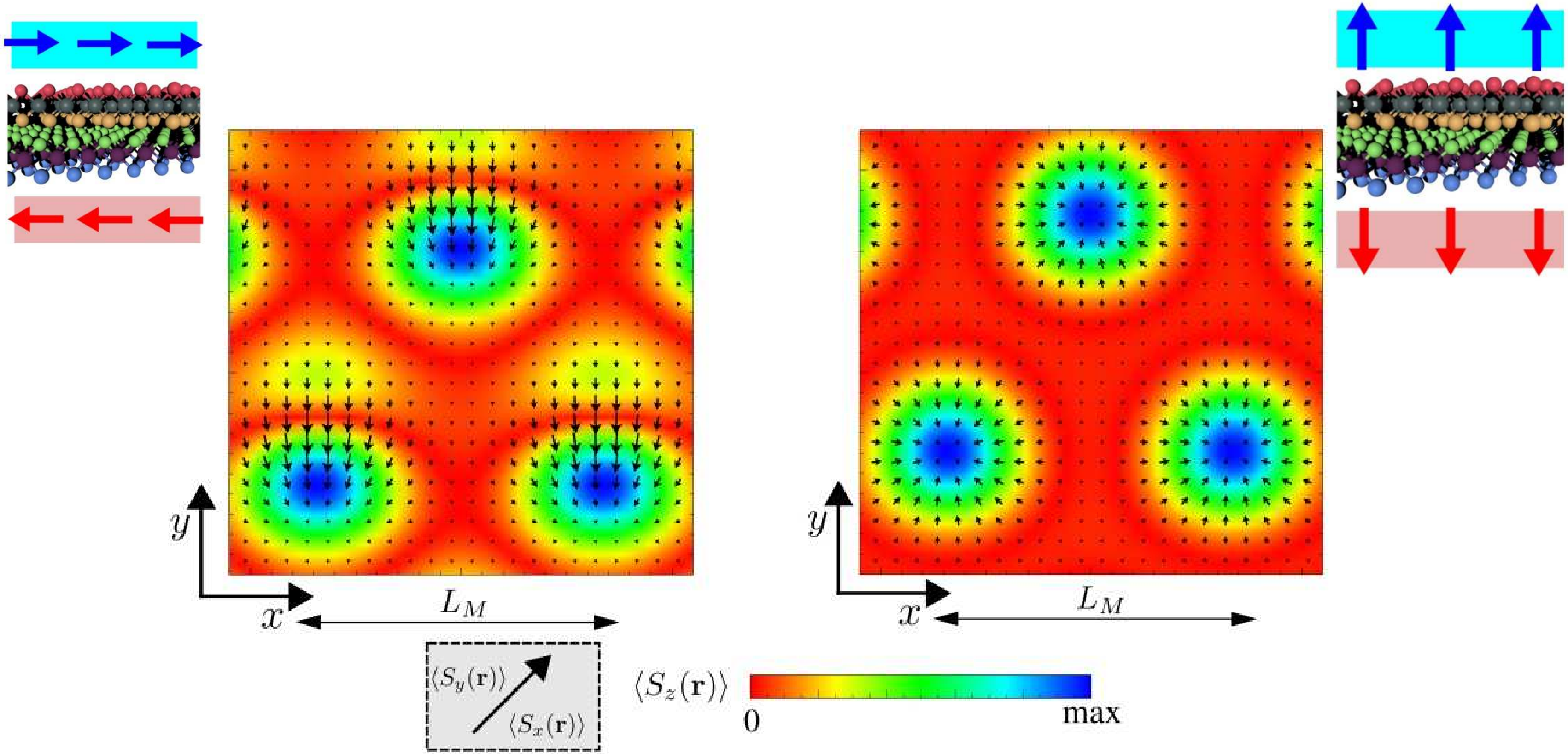
Control by magnetic encapsulation





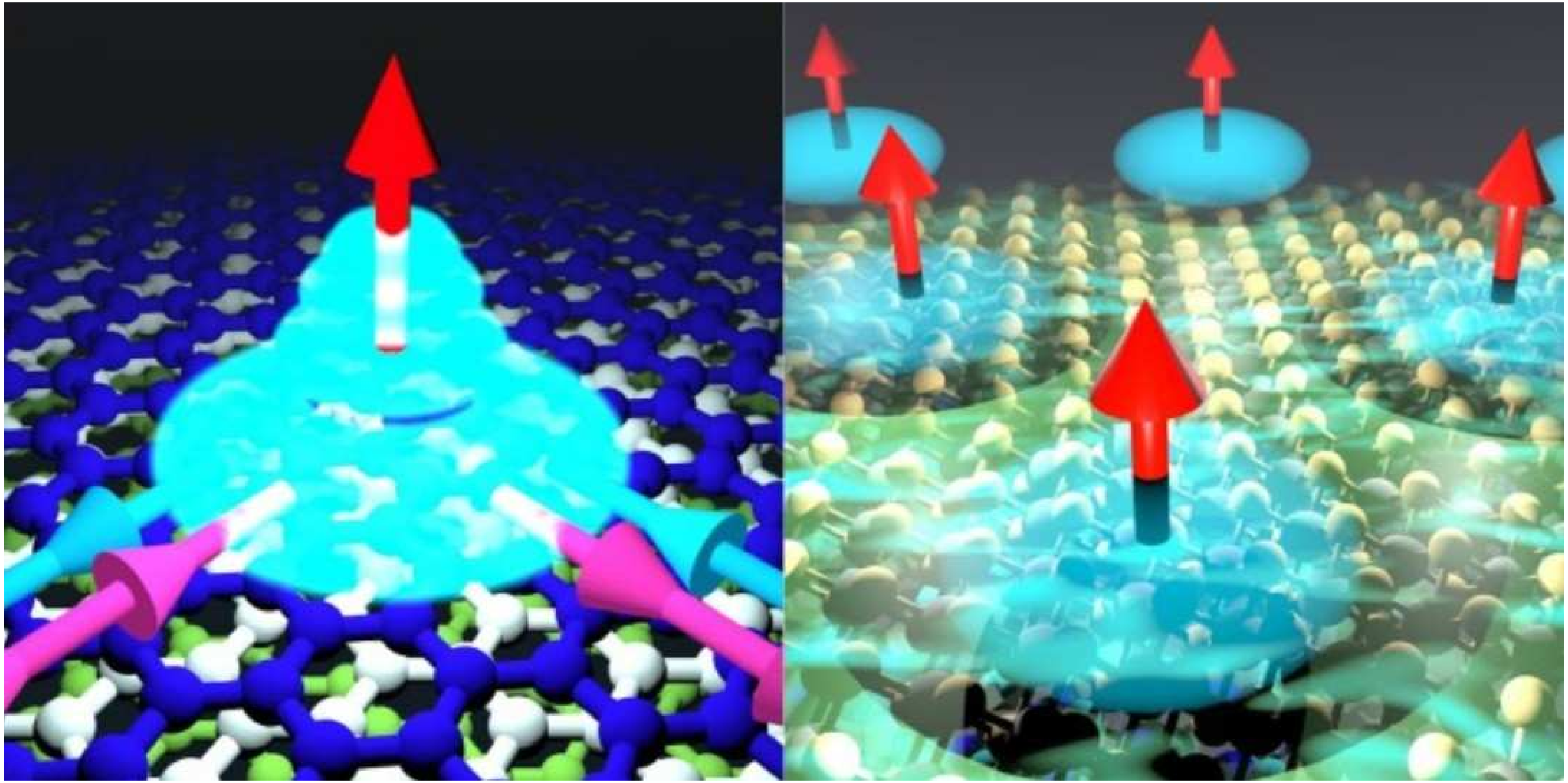
Let us explore the impact of a magnetic encapsulation in the correlated Janus bilayer

Control by magnetic encapsulation



Magnetic moire merons controlled by the magnetic encapsulation

A new family of correlated states based on quantum magnetism: heavy fermions in twisted materials



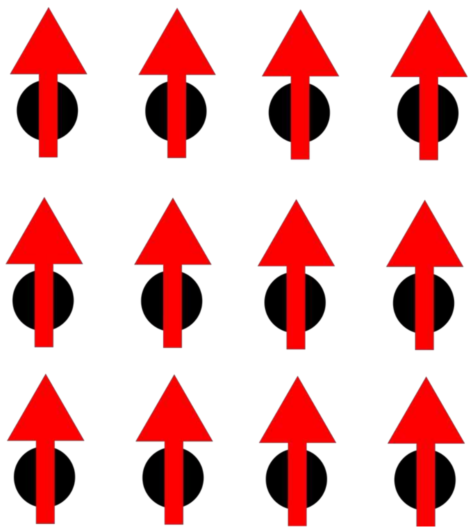
Basics of heavy fermion physics

- Strongly correlated matter, dominated by Kondo lattice physics
- Unique system to realize quantum criticality and unconventional superconductivity
- Found in rare-earth compounds, such as UTe_2 or UPt_3

Can we realize heavy-fermion physics with twisted two-dimensional materials?

Basics of heavy fermion physics

Lattice of Kondo impurities



f-electrons in
rare-earth compounds

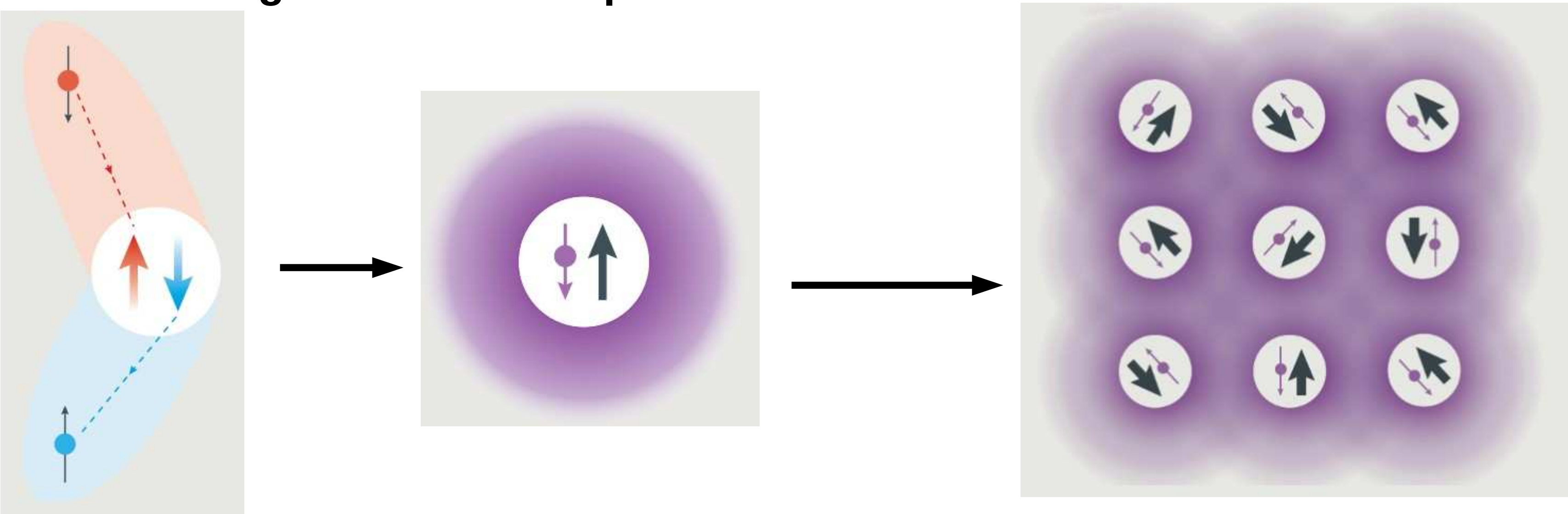
Dispersive electron gas

s/p/d-electrons in
rare-earth compounds

Basics of heavy fermion physics

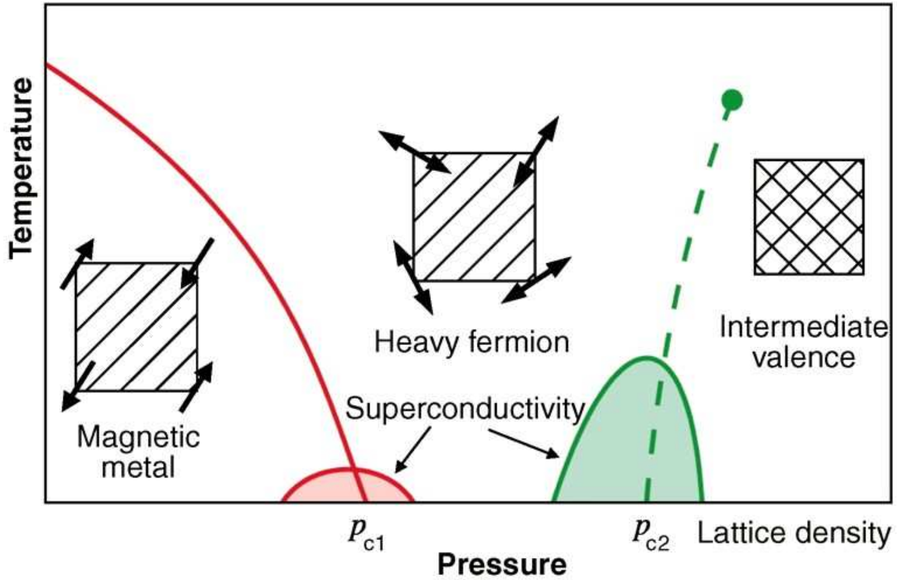
Conduction electrons form Kondo singlets with the impurities

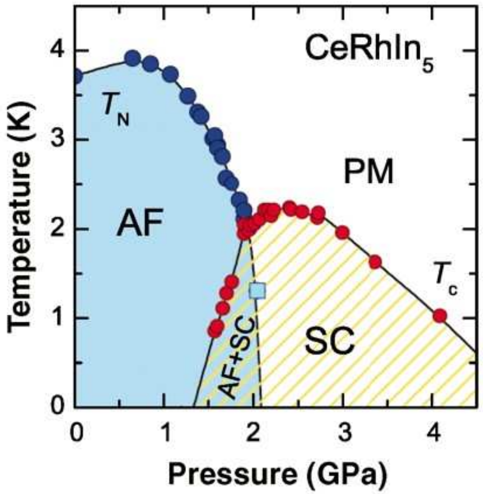
Kondo-lattice model



Associated with Kondo lattice physics:
- Colossal mass enhancement of electrons
- Quantum criticality
- Unconventional (topological) superconductivity

Basics of heavy fermion physics

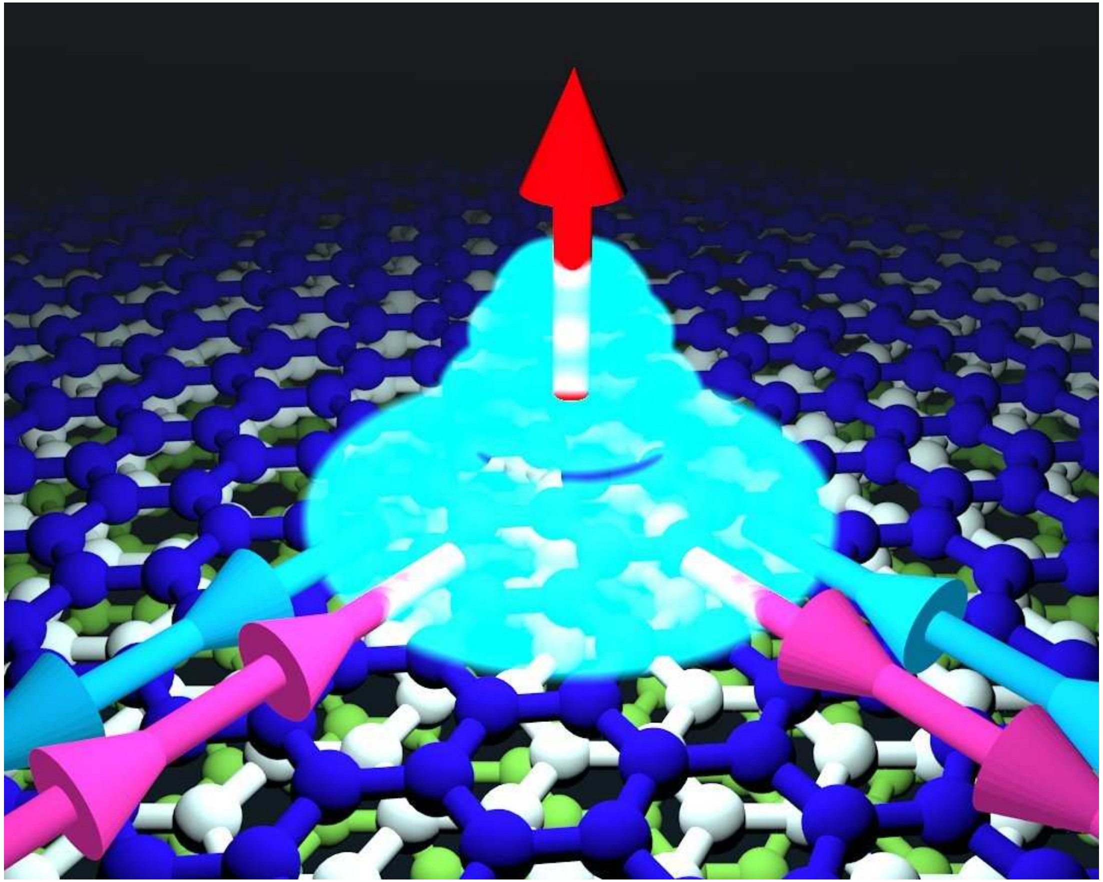




Science 332.6026, 196-200 (2011)

Associated with Kondo lattice physics:
- Colossal mass enhancement of electrons
- Quantum criticality
- Unconventional (topological) superconductivity

Heavy-fermions in twisted graphene trilayers

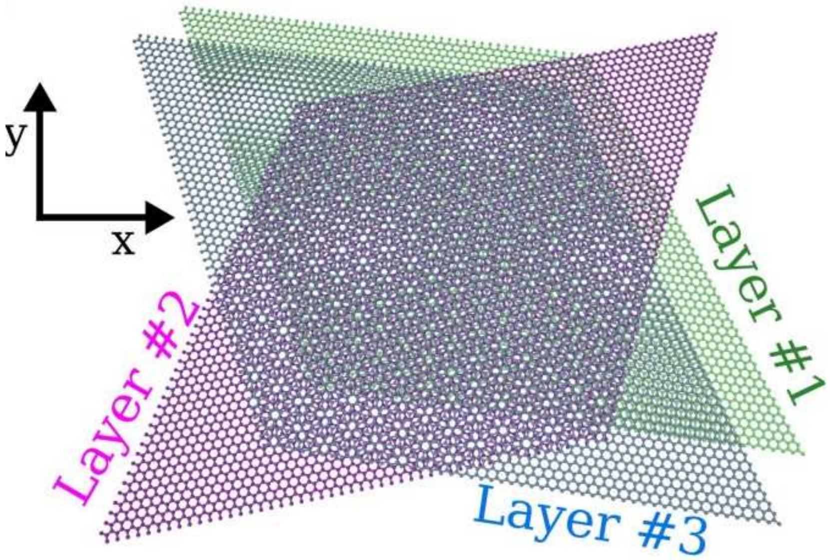


Aline Ramires

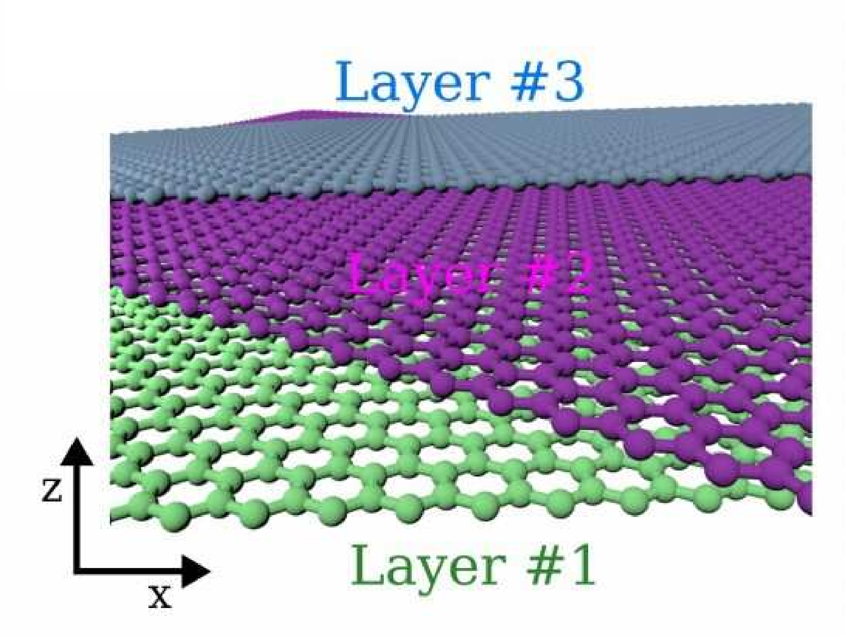
Phys. Rev. Lett. 127, 026401 (2021)

Heavy-fermions in twisted graphene trilayers

Top view

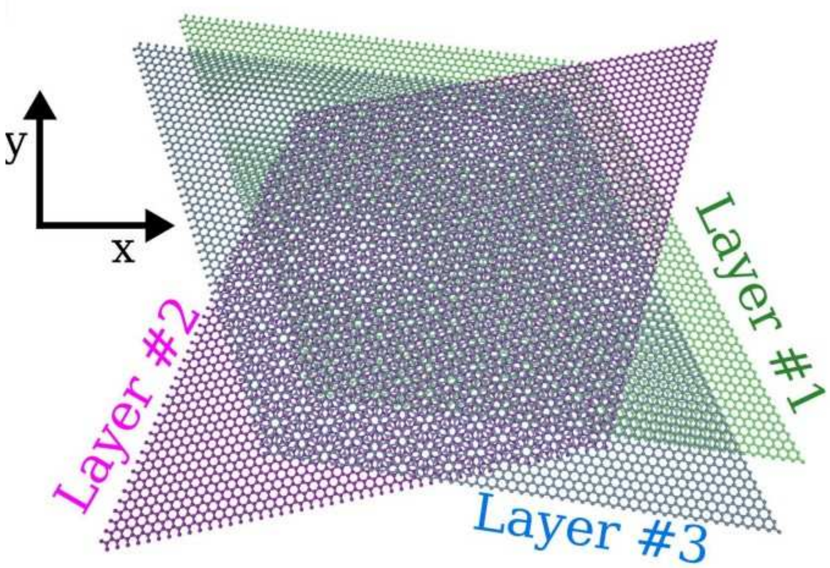


Lateral view

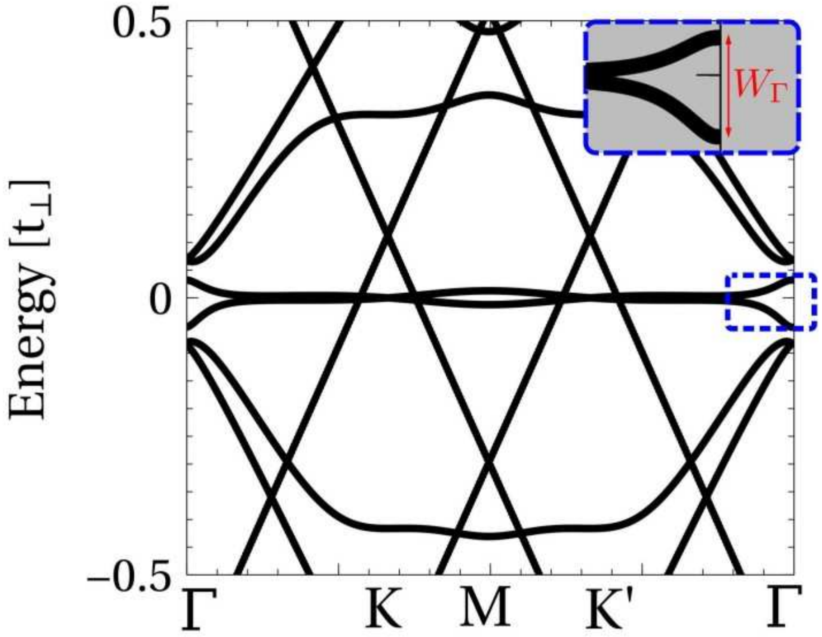


Heavy-fermions in twisted graphene trilayers

Top view

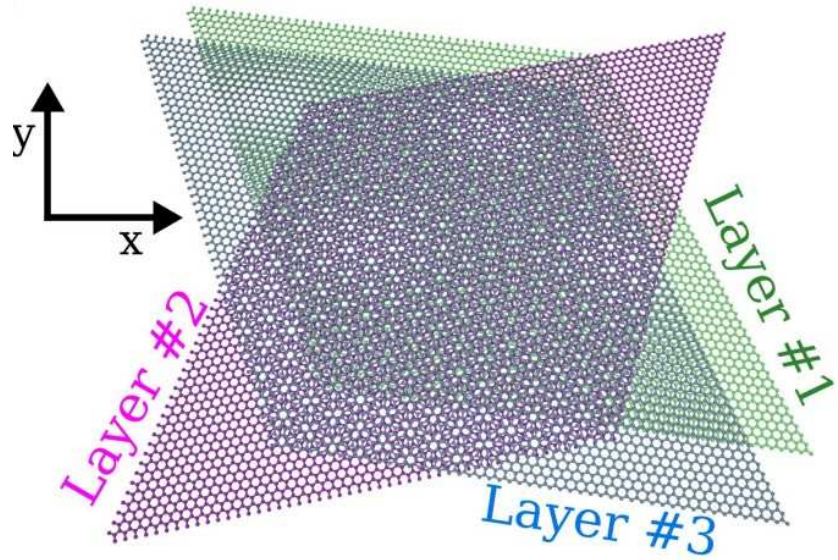


Band structure

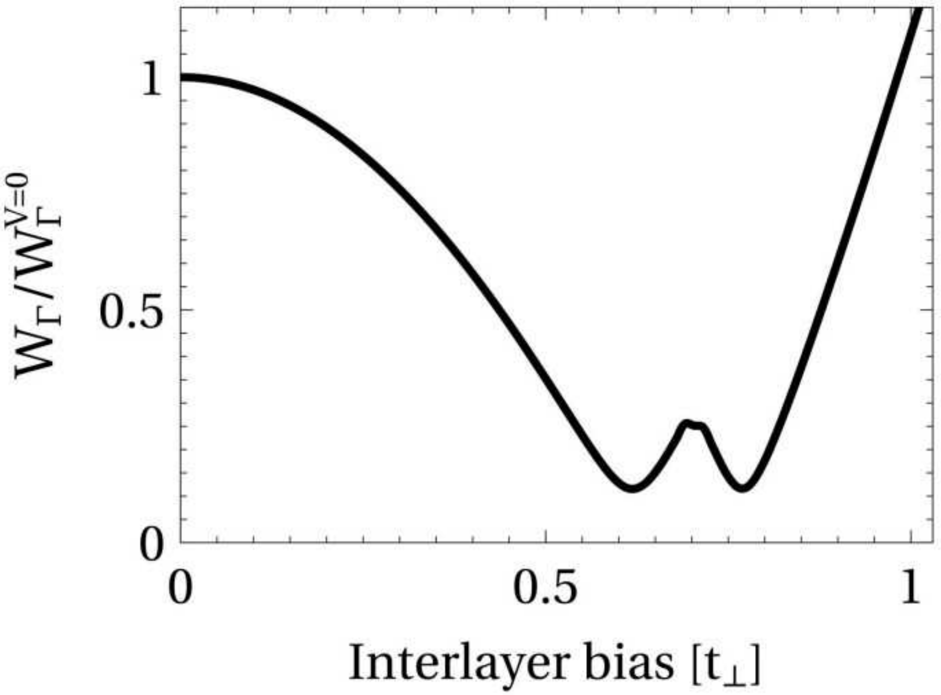


Heavy-fermions in twisted graphene trilayers

Top view



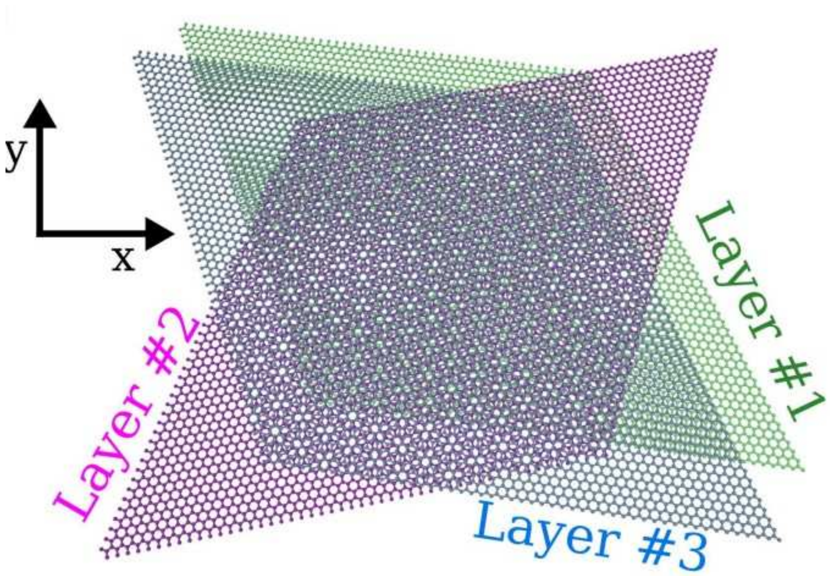
Bandwidth of nearly flat bands



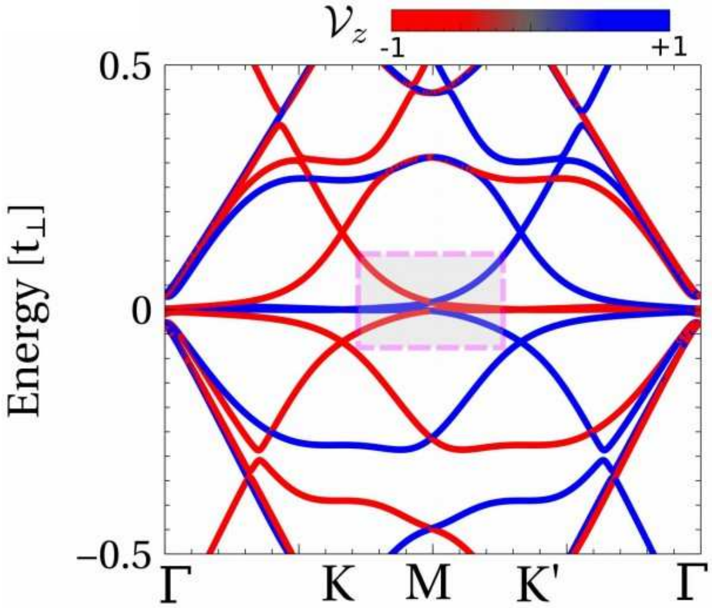
Band flattening as an interlayer bias is applied

Heavy-fermions in twisted graphene trilayers

Top view

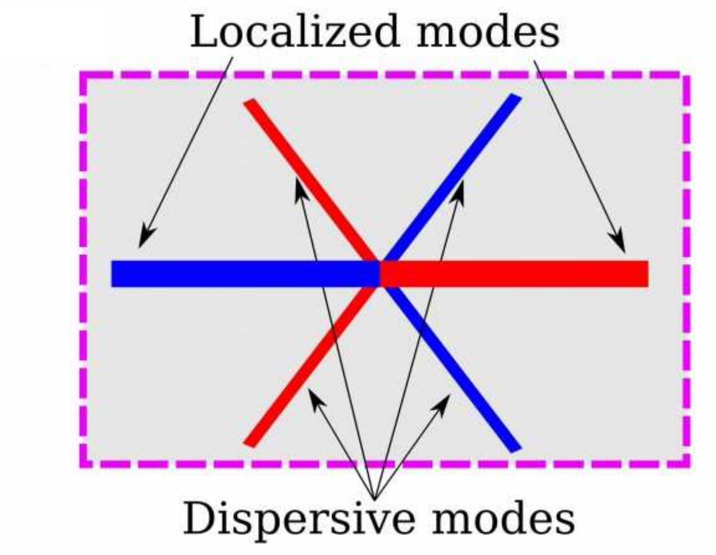


Electronic structure in the presence of an electric bias

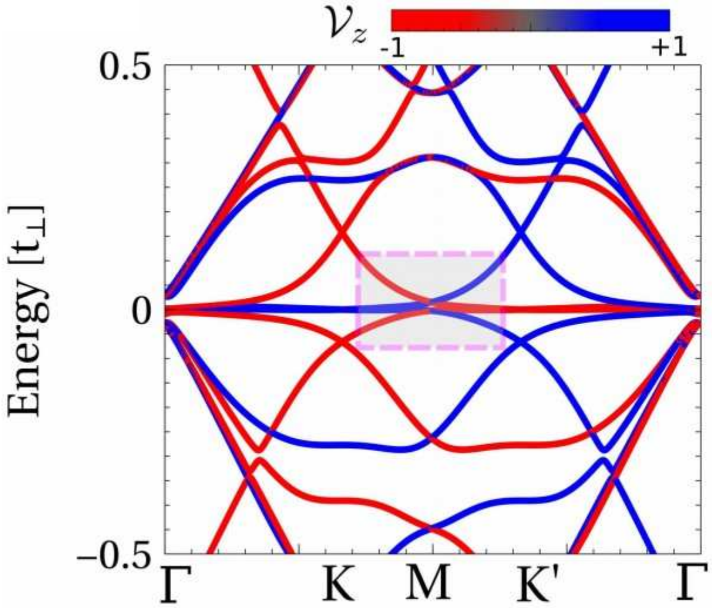


Heavy-fermions in twisted graphene trilayers

Low energy model

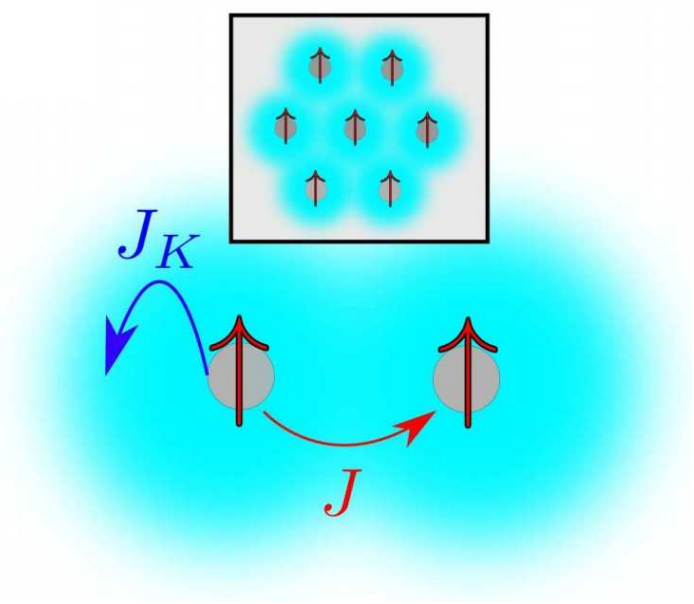


Electronic structure in the presence of an electric bias

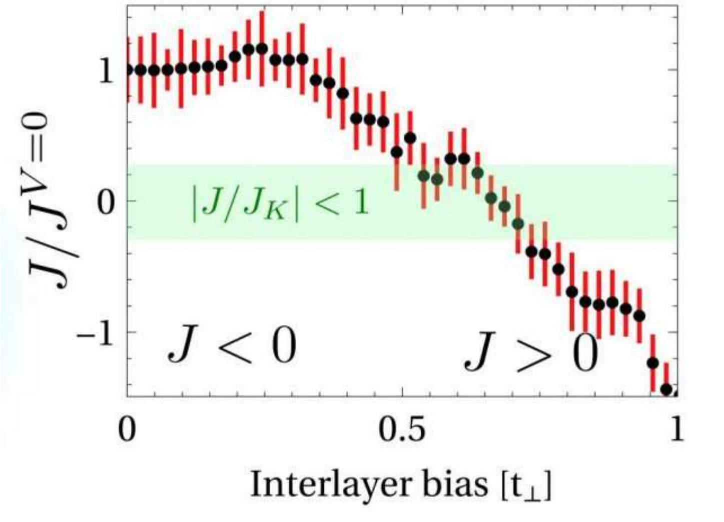


Kondo lattice model in the presence of interactions

Interactions of the Kondo lattice model



Electric control of the Kondo regime

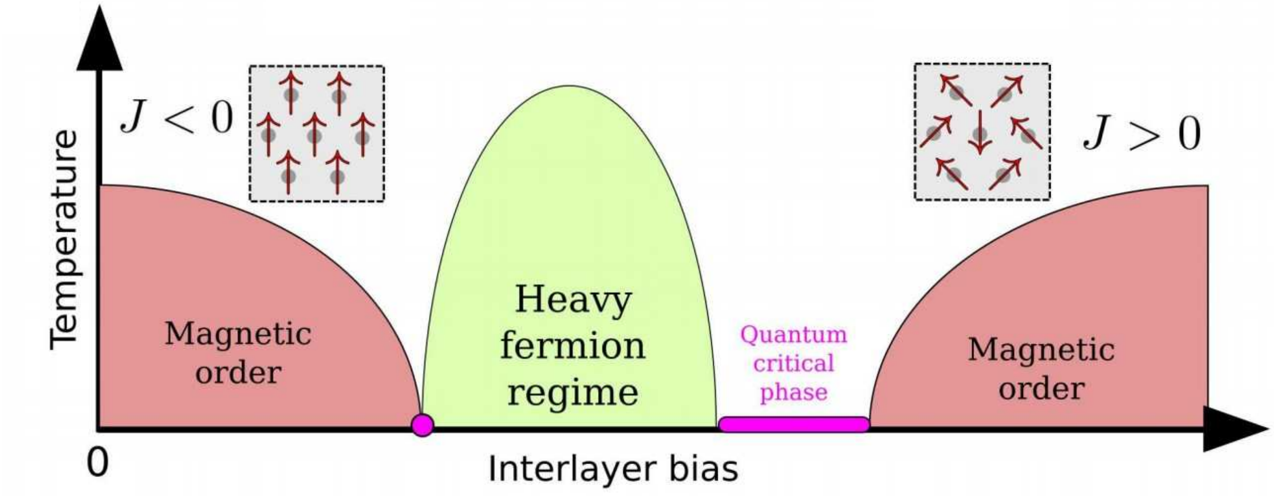


A heavy fermion regime appears when the Kondo coupling dominates over the exchange coupling

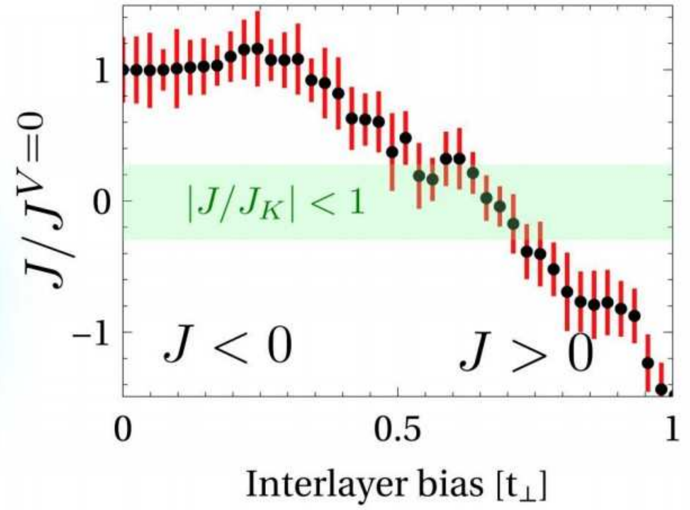
$$|J/J_K| < 1$$

Heavy-fermions in twisted graphene trilayers

Heavy-fermion (Doniach) phase diagram

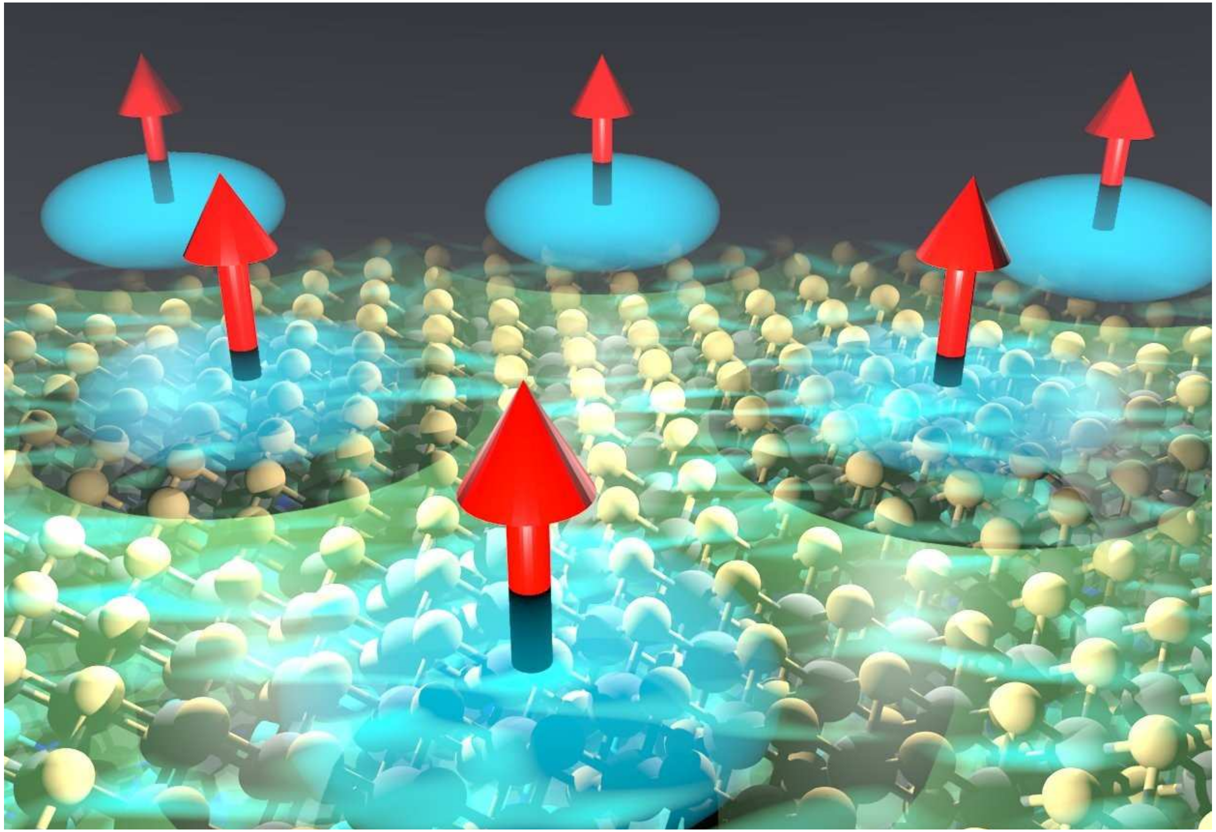


Electric control of the Kondo regime



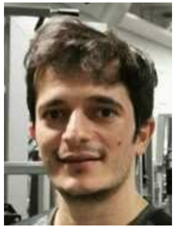
The full phase diagram of the heavy fermion system can be explored in a single twisted graphene, by tuning the system with an electric bias

Heavy-fermions in a van der Waals dichalcogenide heterostructure

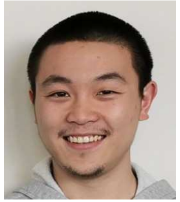


S. Ganguli

M. Amini



G. Chen



V. Vaňo

S. Kezilebieke

P. Liljeroth

arXiv:2103.11989 (2021)

Heavy-fermions in dichalcogenide bilayers

Triangular lattice of local magnetic moments

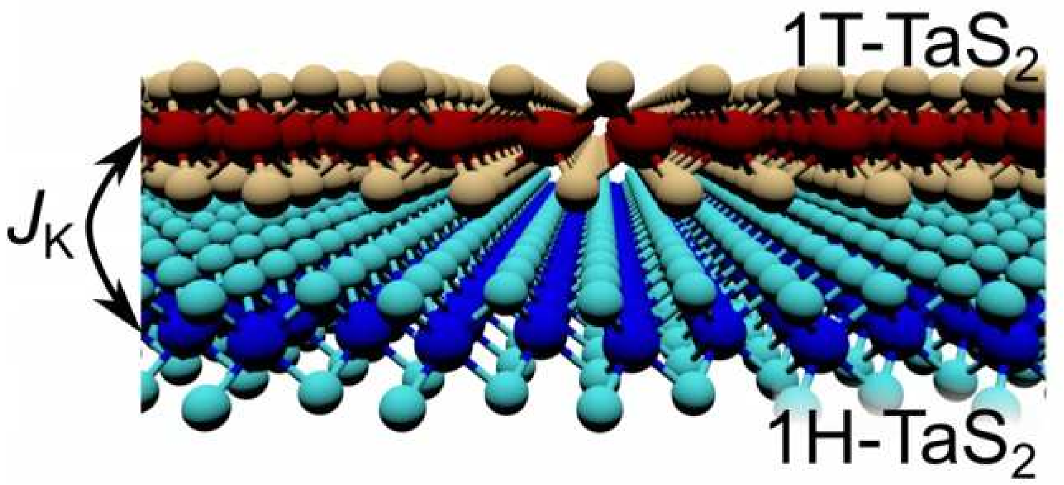
1T-TaS_2

Two-dimensional electron gas

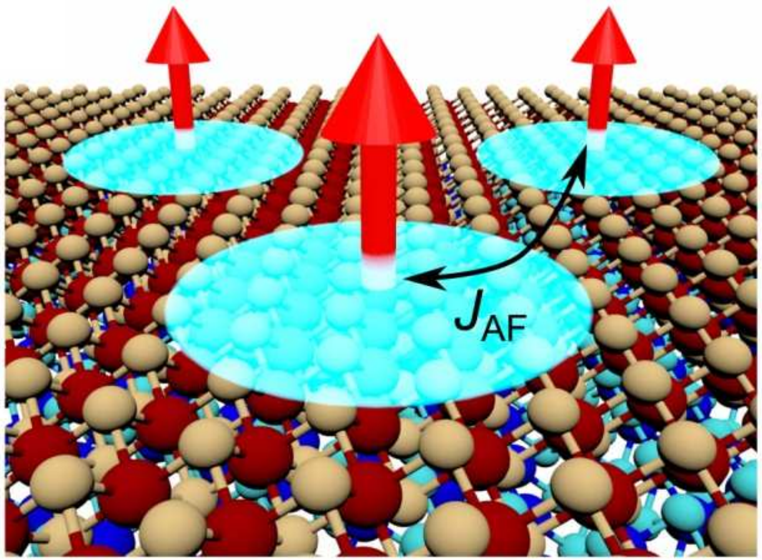
1H-TaS_2

Heavy-fermions in dichalcogenide bilayers

Interlayer coupling create the Kondo coupling



Intralayer exchange between local moments

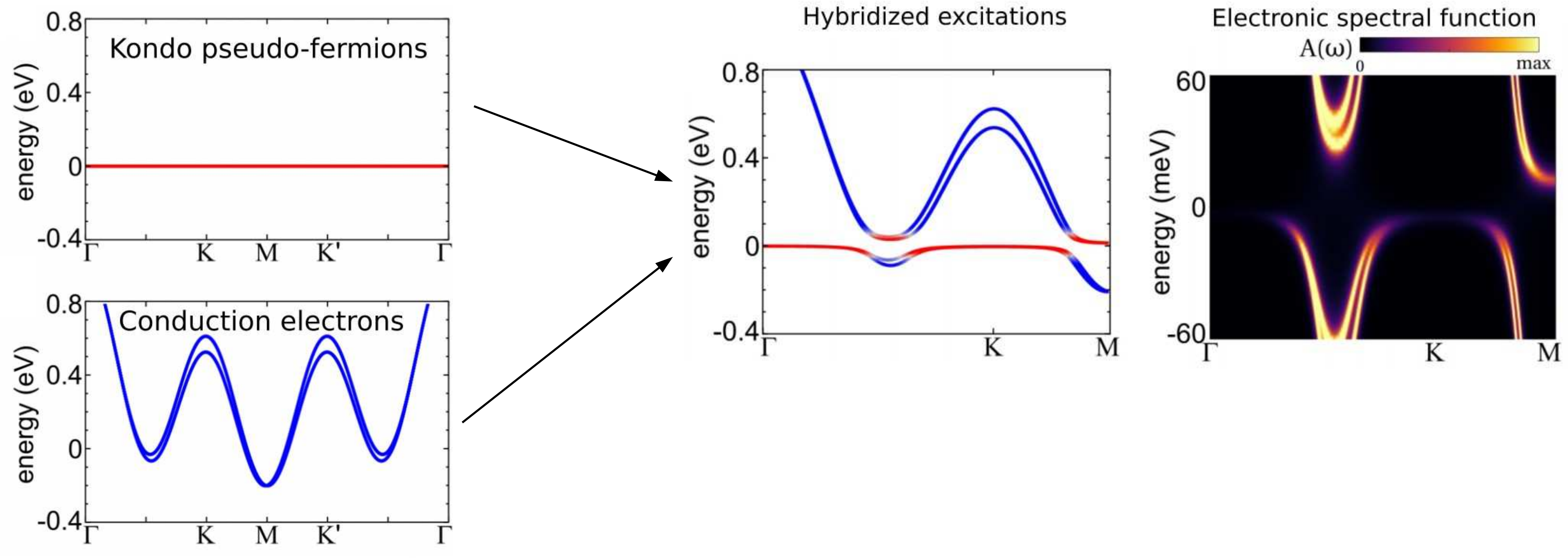


The bilayer realizes all the ingredients for heavy-fermion physics

Brief theory of heavy-fermions

Kondo physics introduces resonant pseudo-fermions at the chemical potential

Leading to the opening of a heavy-fermion gap

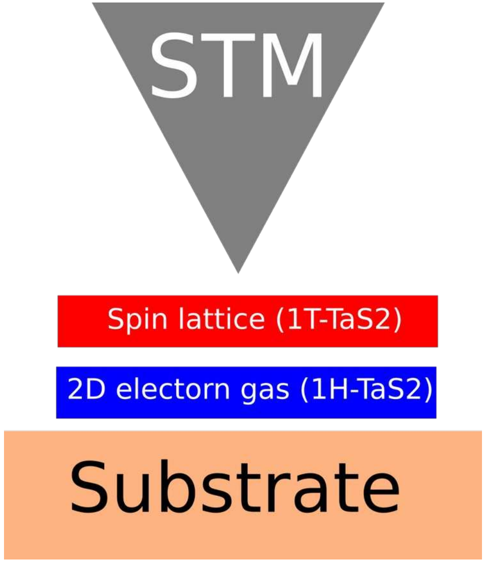


Experimental signatures of heavy-fermion physics

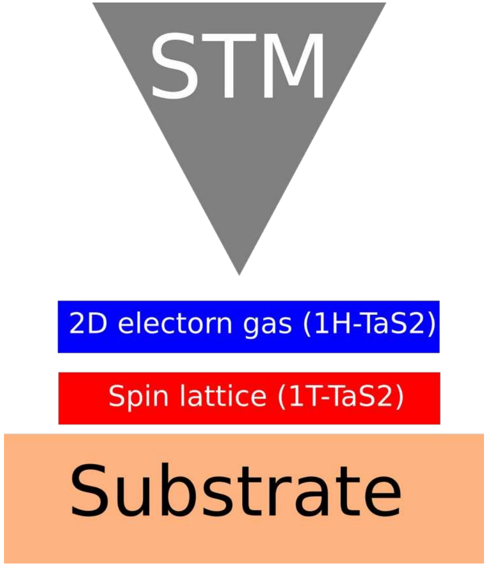
- Kondo physics in the magnetic lattice
- Gap opening in the metallic layer

Both signatures can be probed with scanning tunnel microscopy by growing two heterostructures

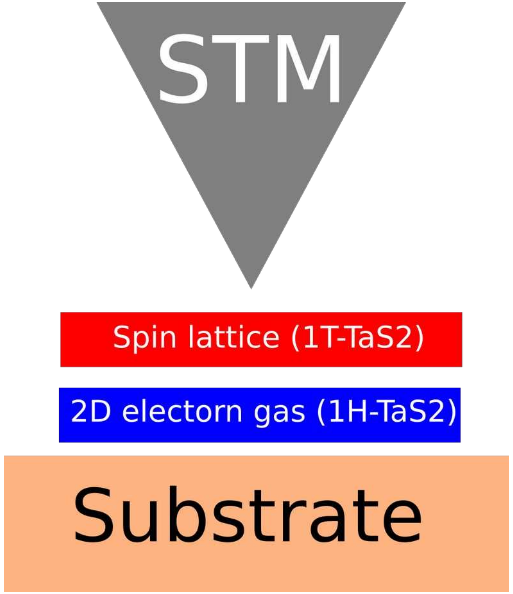
Probing the Kondo peak



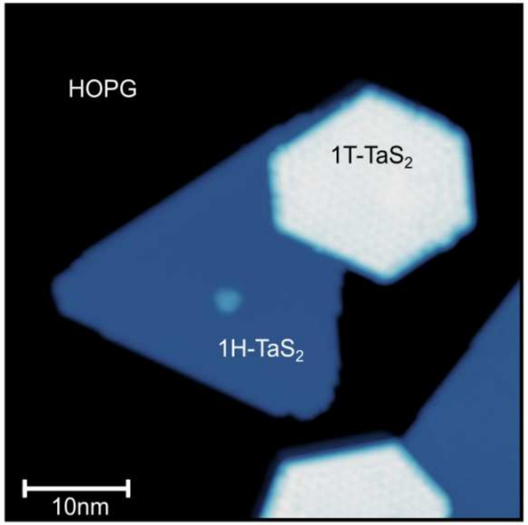
Probing the heavy-fermion gap



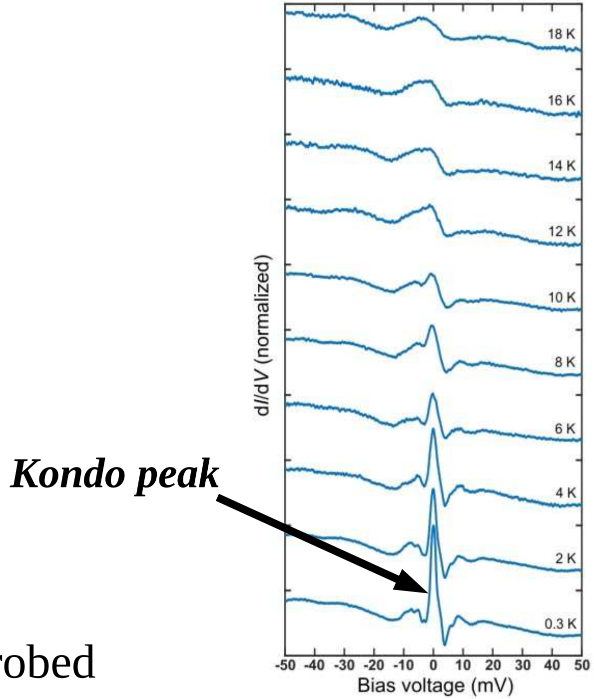
Kondo physics in the magnetic lattice



Sample



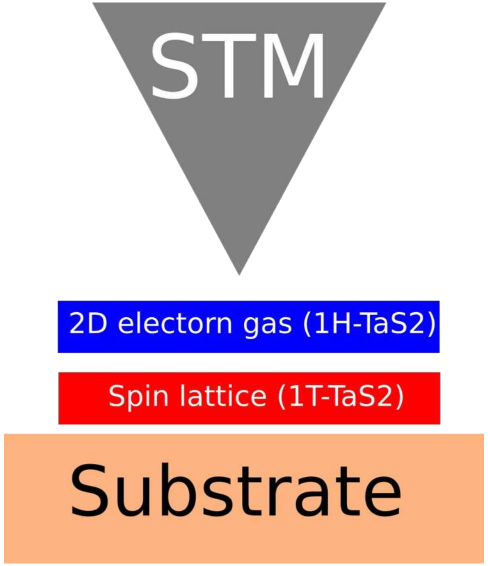
Differential conductance



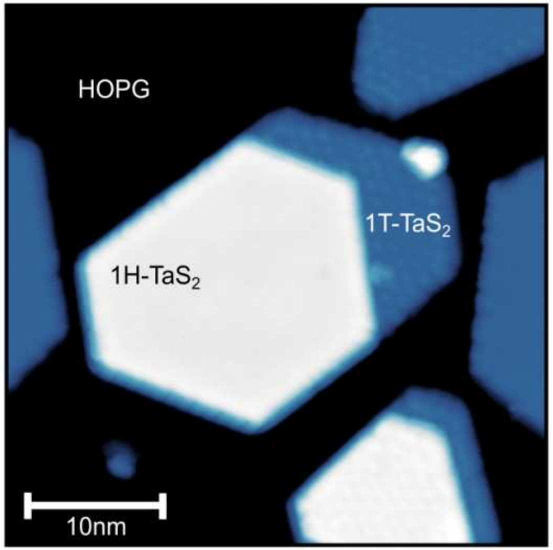
The system shows a Kondo peak when the local moments are probed

Temperature and field dependence consistent with Kondo

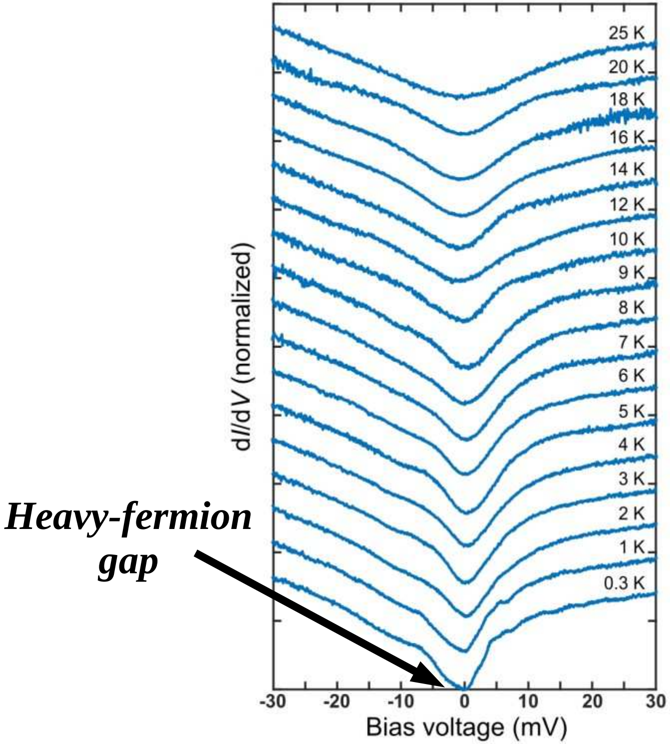
Heavy-fermion gap in the 2D electron gas



Sample



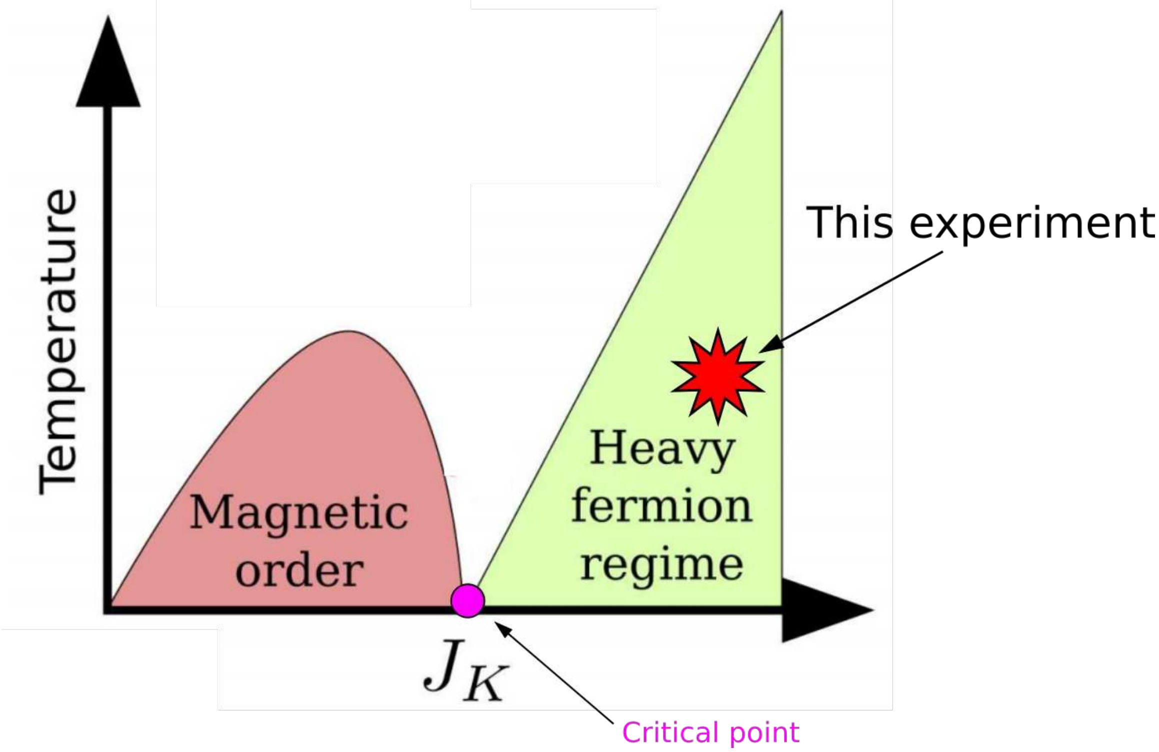
Differential conductance



A heavy-fermion gap appears on the metal side

Temperature and field dependence consistent with a heavy-fermion gap

Next steps in van der Waals heavy-fermions

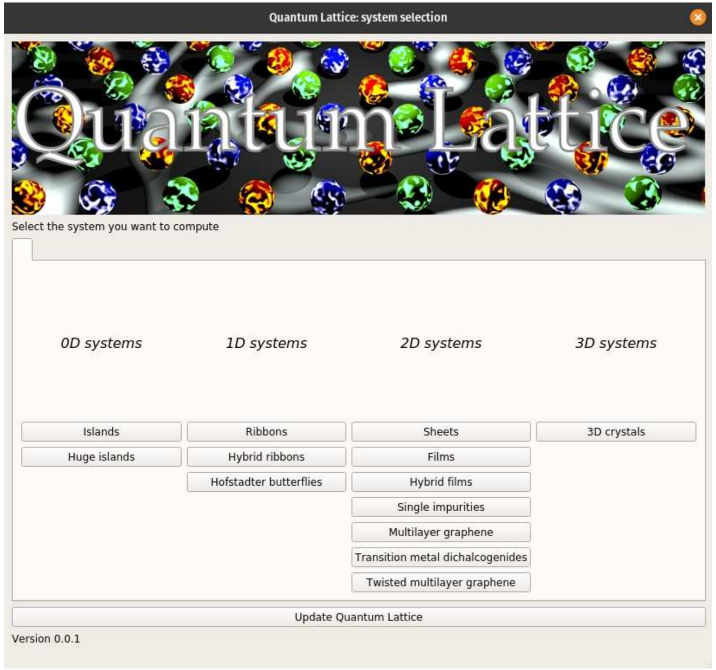


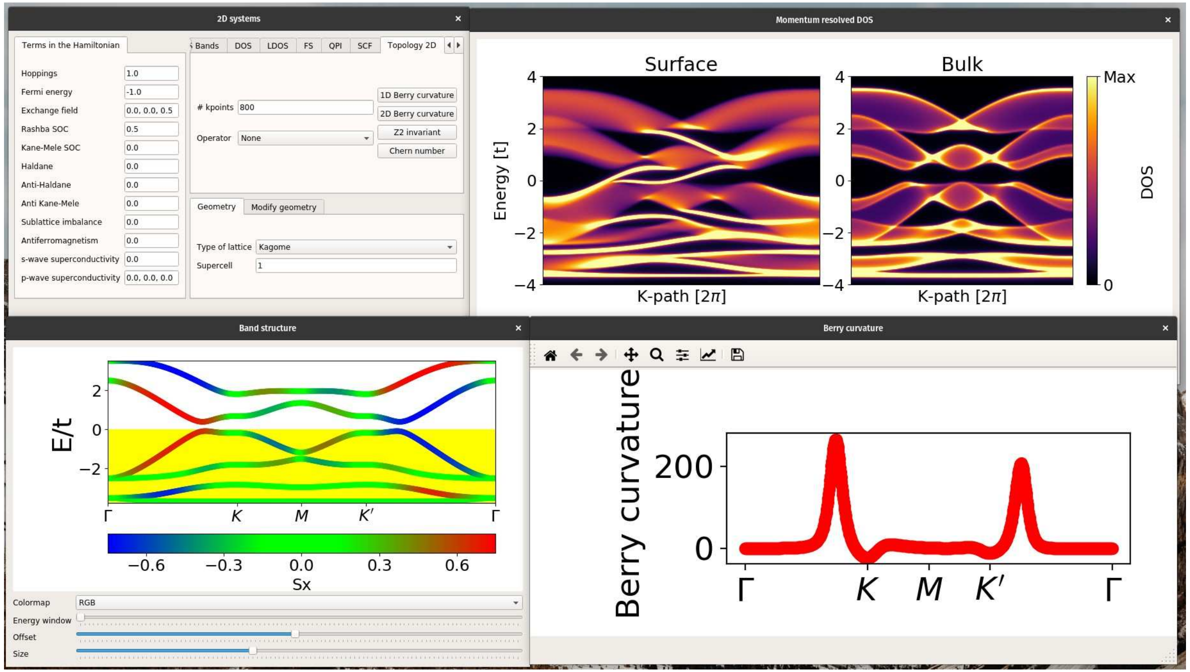
Can we push this system to the critical and ultimately topological superconducting regimes?

(twist, material engineering, gating, etc...)

Computing electronic properties

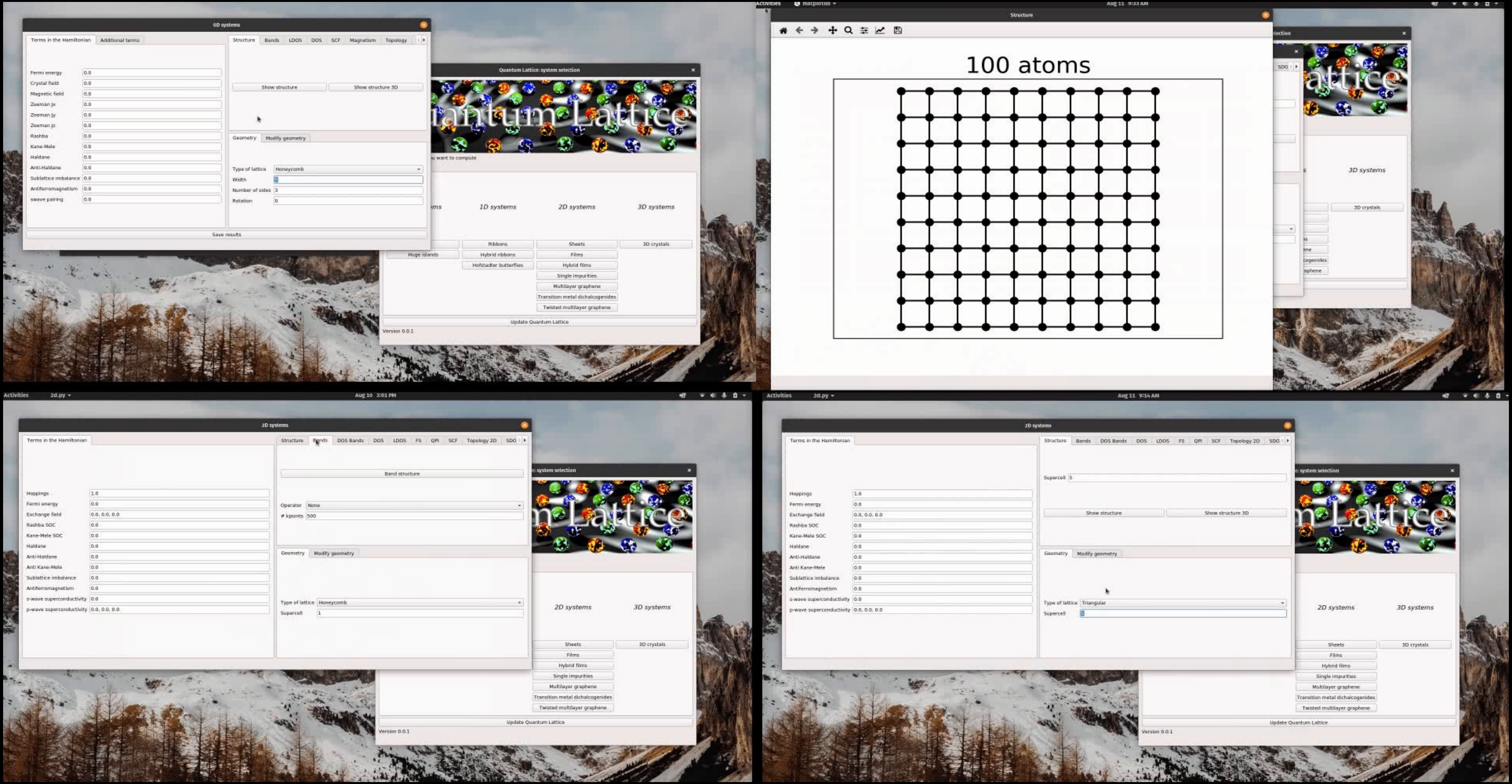
Quantum Lattice: A user interface to compute electronic properties



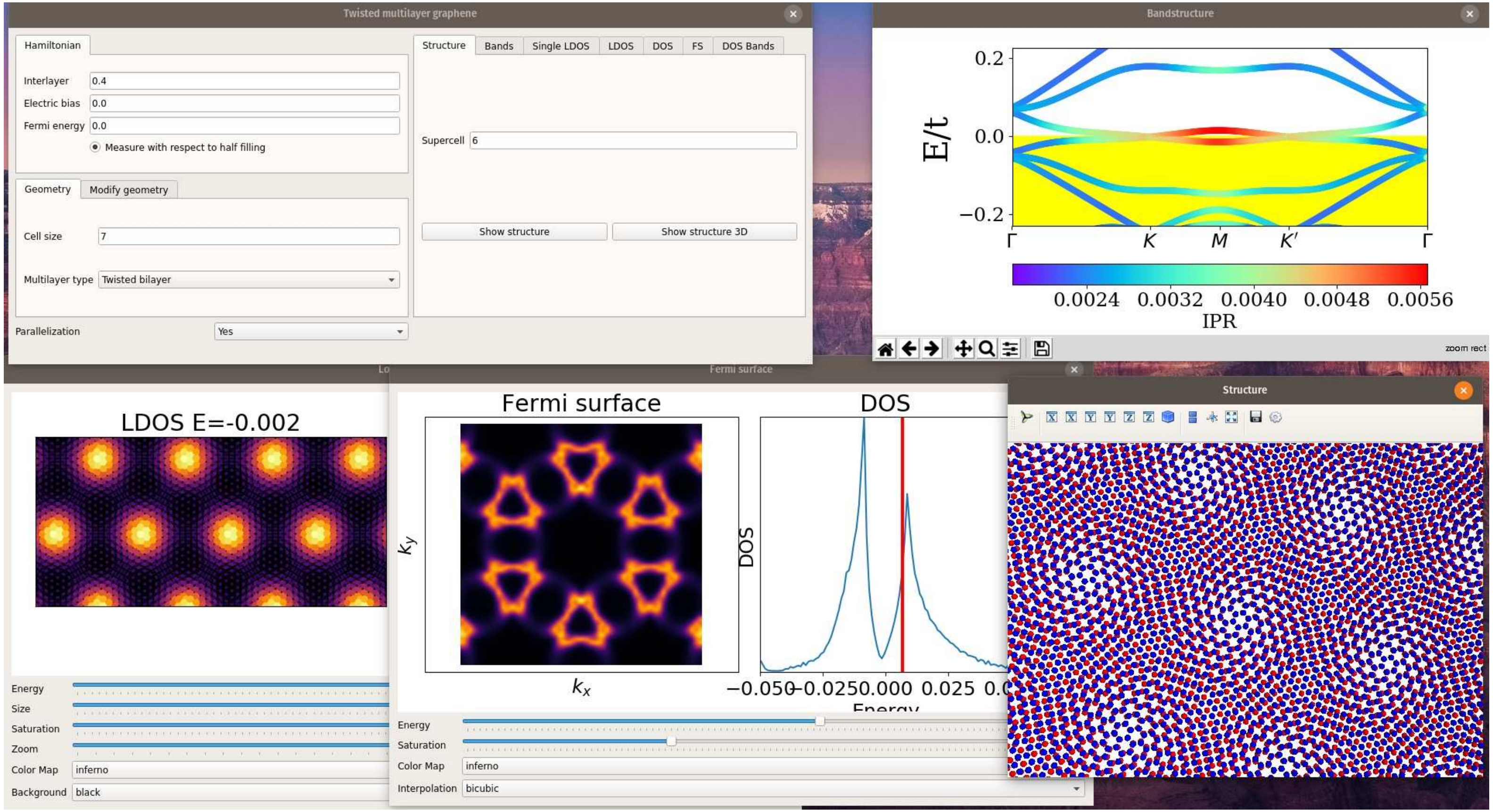


Quantum Lattice: open source interactive interface for tight binding modeling

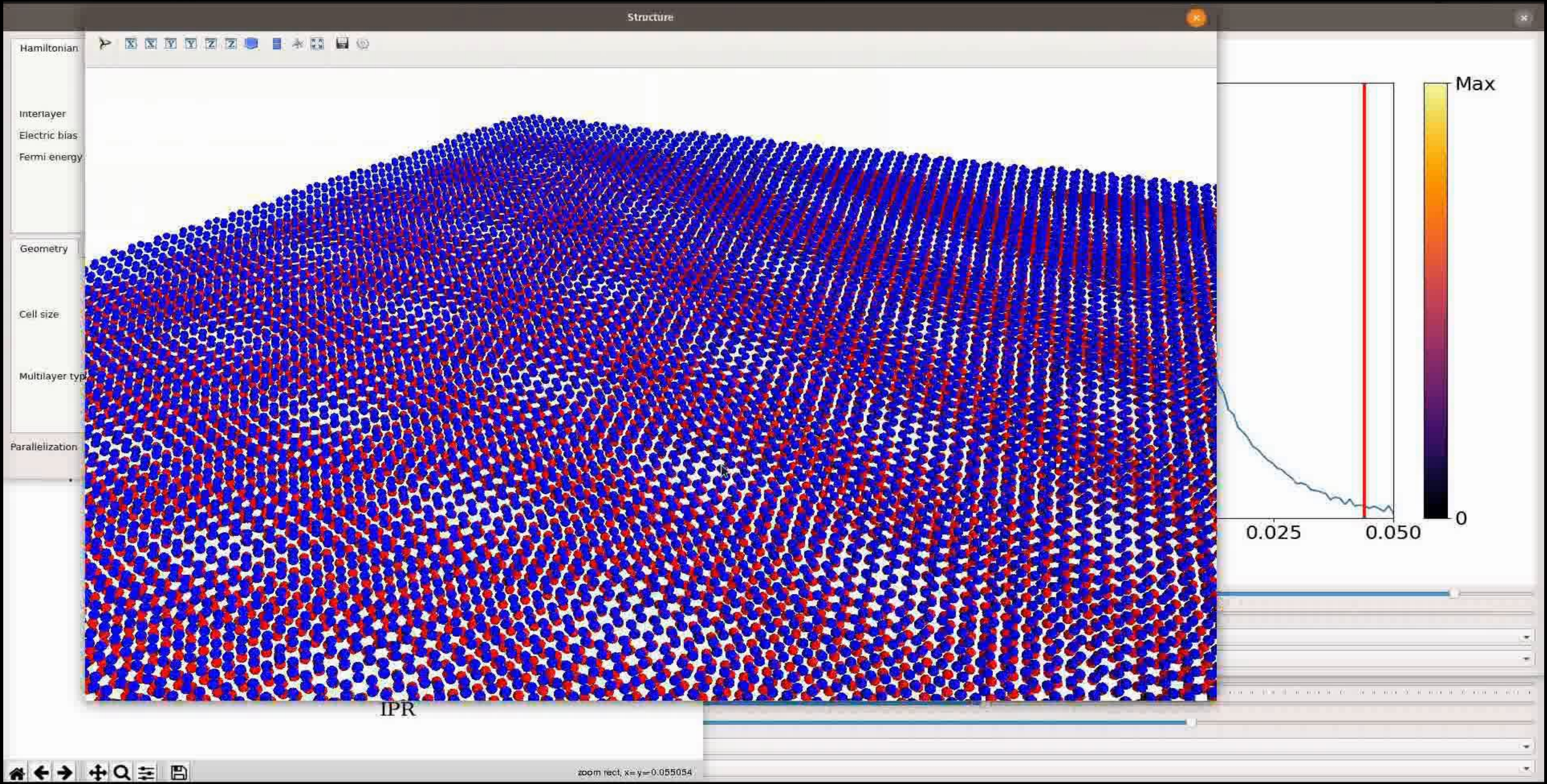
https://github.com/joselado/quantum-lattice


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

Twisted bilayer with the user interface

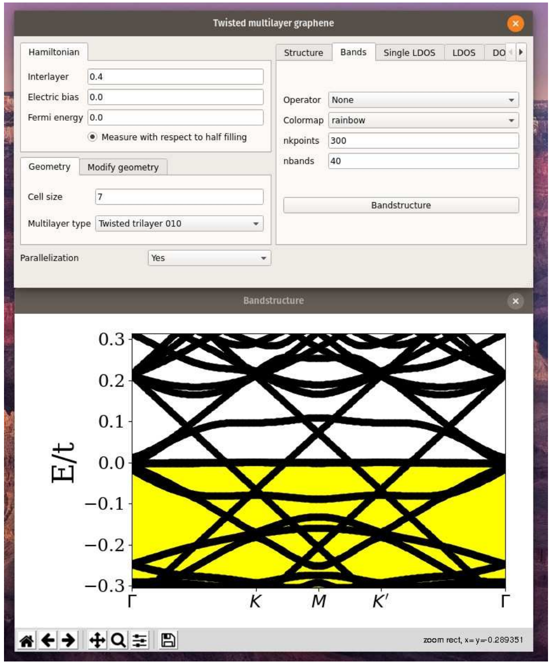


https://github.com/joselado/quantum-lattice

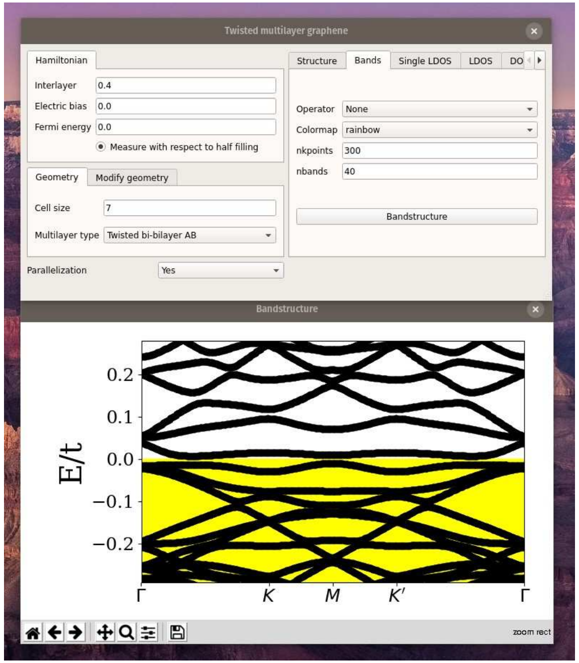

Structure
Hamiltonian
Interlayer
Electric bias
Fermi energy
Geometry
Cell size
Multilayer typ
Parallelization
Max
0
0.025
0.050
IPR
zoom rect, x=y=0.055054

Twisted multilayers

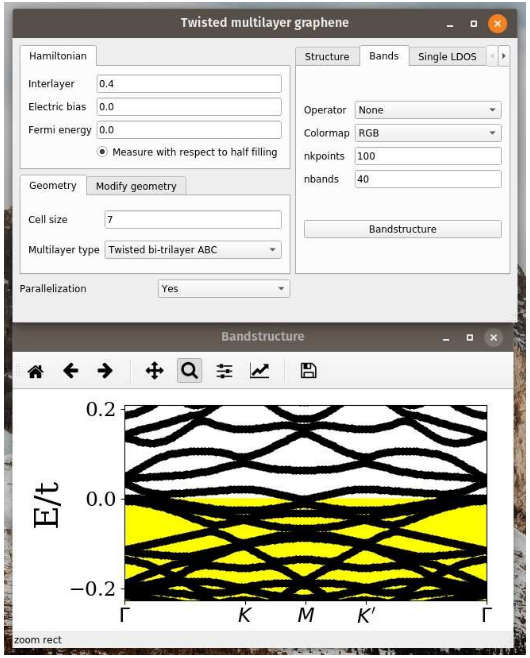
Twisted trilayer graphene



Twisted bi-bilayer graphene



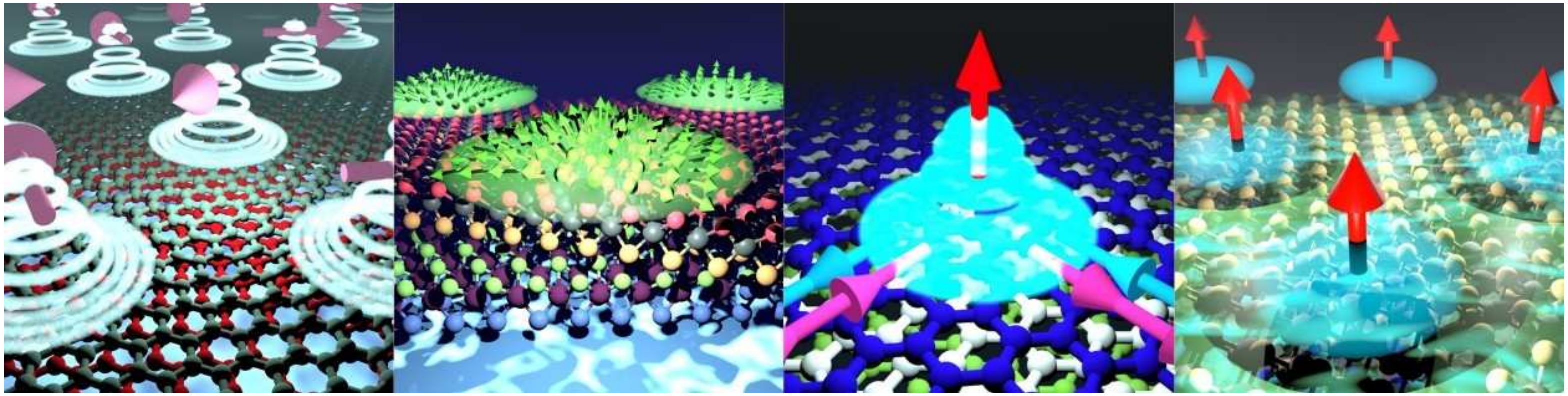
Twisted bi-trilayer graphene



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

Take home

Magnetic twisted van der Waals materials provide a platform to engineer a new family of correlated states, including exotic heavy-fermion physics



Thank you!

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SUOMEN AKATEMIA

Phys. Rev. Lett. 126, 056803 (2021)
New J. Phys. 23 073038 (2021)
Phys. Rev. Lett. 127, 026401 (2021)
arXiv:2103.11989 (2021)