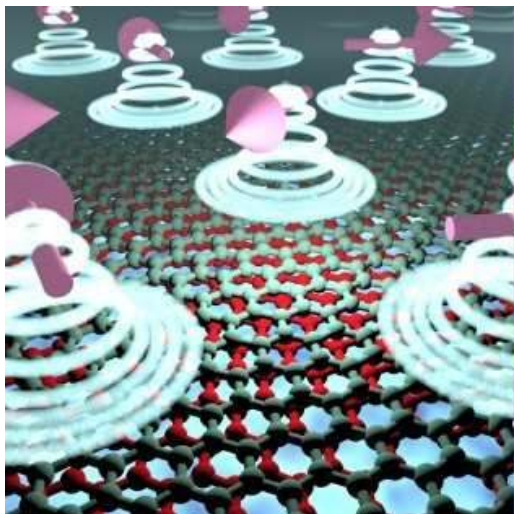


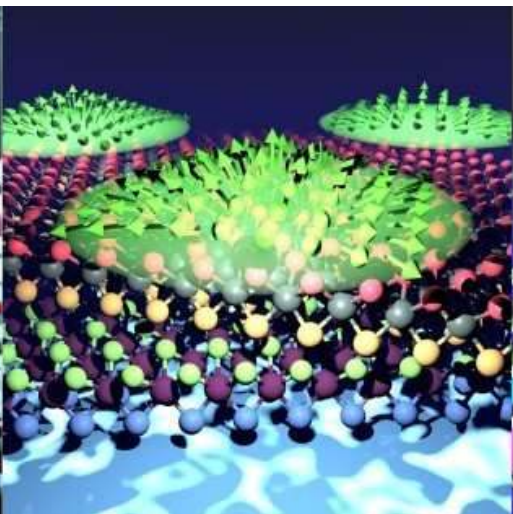
Correlated quantum materials design with magnetic twisted van der Waals heterostructures

Jose Lado

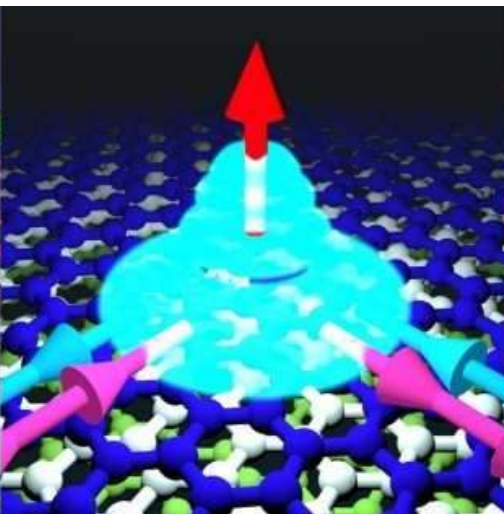
Department of Applied Physics, Aalto University, Finland



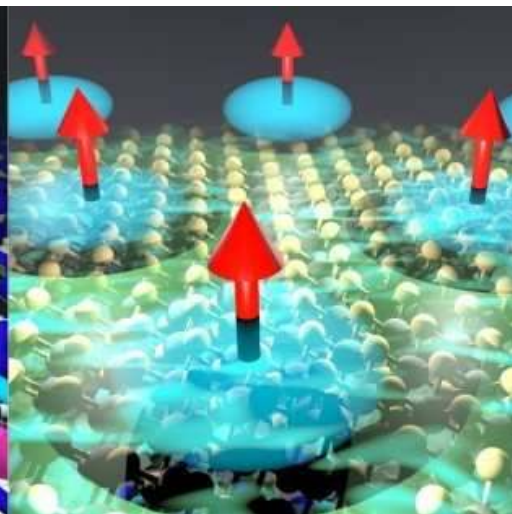
Phys. Rev. Lett. 126, 056803 (2021)



New J. Phys. 23 073038 (2021)



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



arXiv:2103.11989 (2021)

Graphene 2021, Grenoble, October 27th 2021

Complexity, universality and emergence

Psychology

Medicine

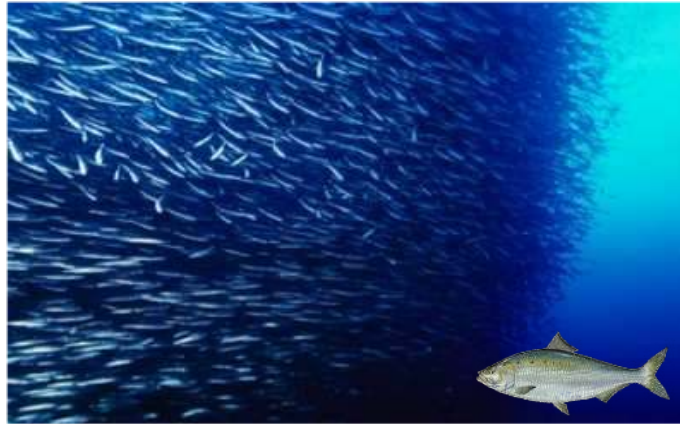
Biology

Chemistry

Physics

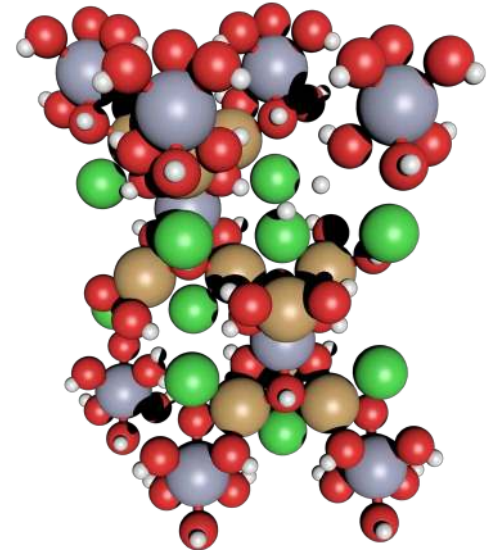
Complexity

Fish schools



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

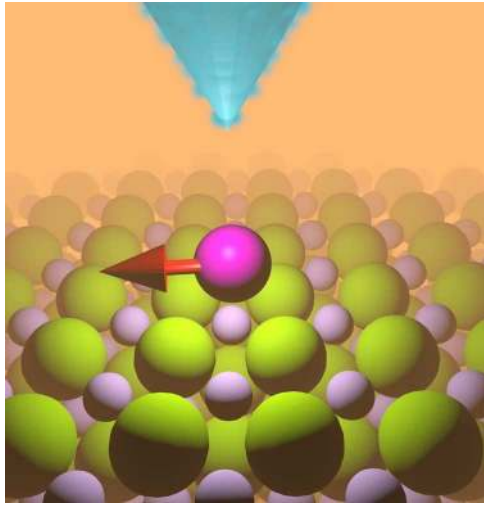
Complex compounds



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

Building quantum matter with artificial lattices

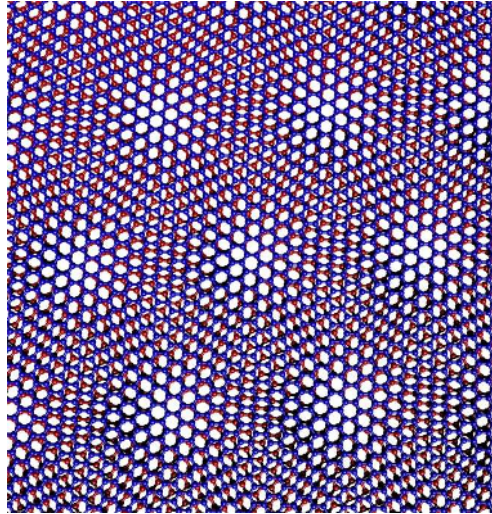
Atomic lattices



$a = 0.5 \text{ nm}$

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

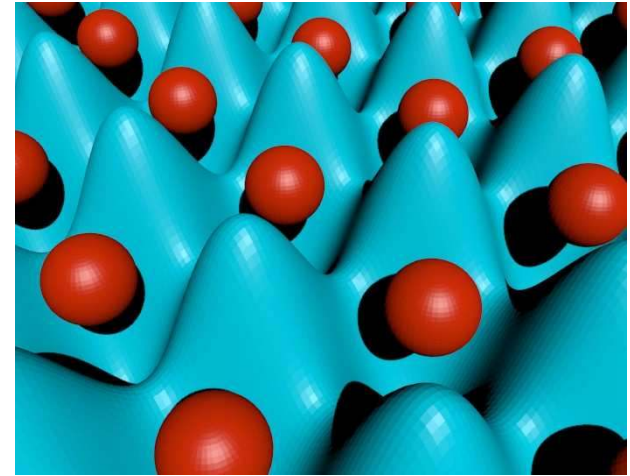
Twisted 2D moire materials



$a = 30 \text{ nm}$

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

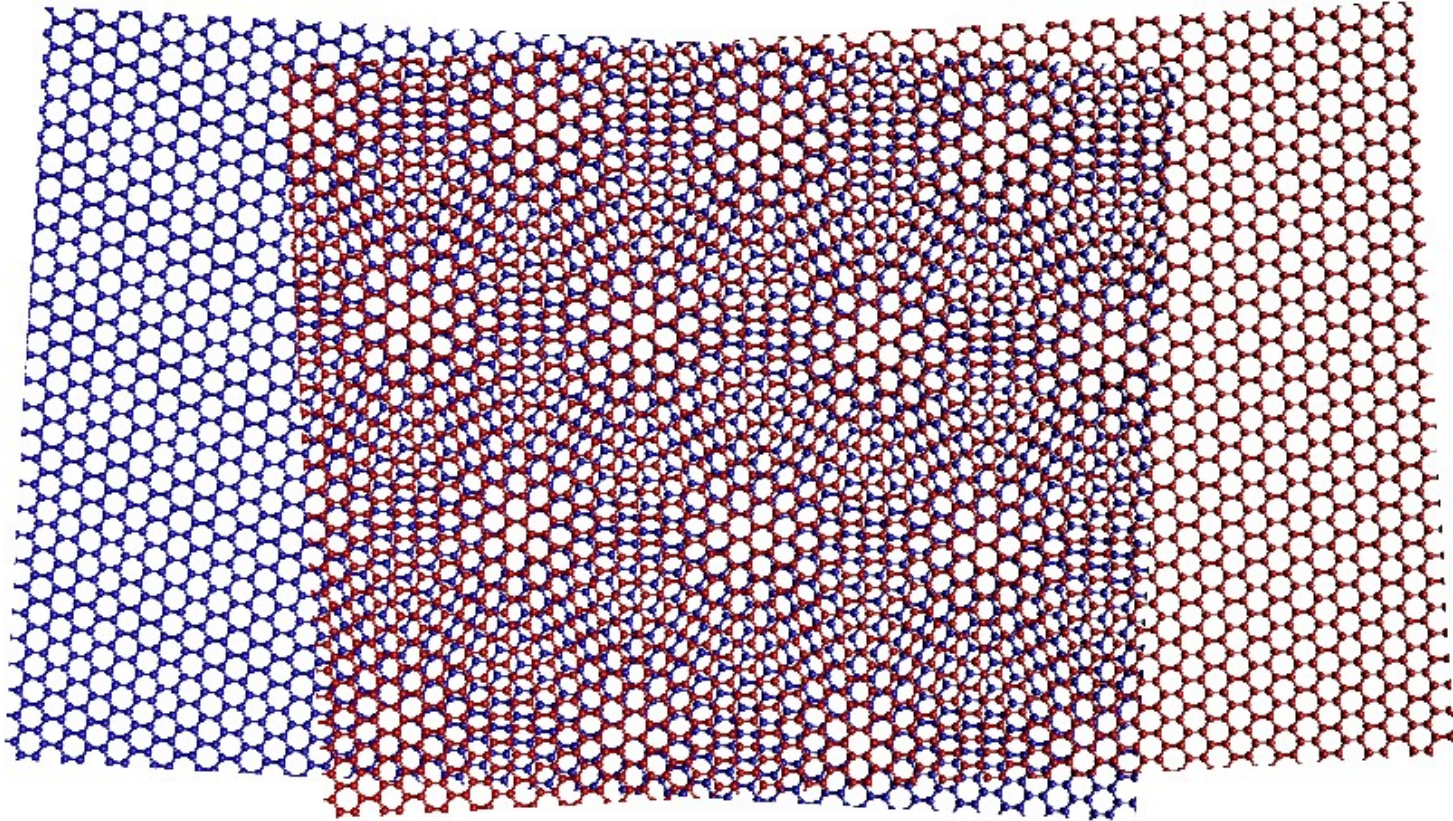
Cold atoms



$a = 1000 \text{ nm}$

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

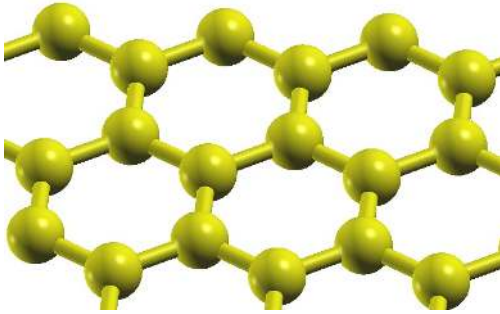
Twisted 2D materials as a platform for artificial quantum matter



The two-dimensional materials world

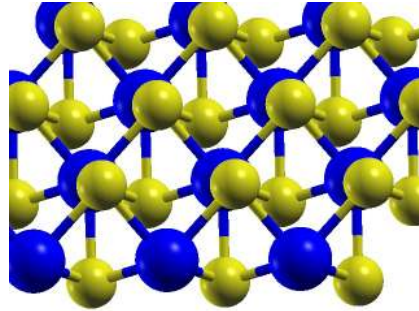
Semimetal

Graphene



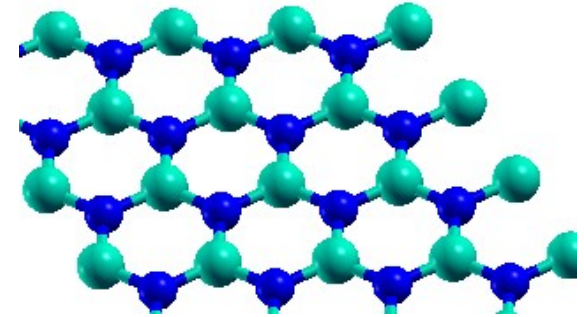
Superconductor

NbSe_2



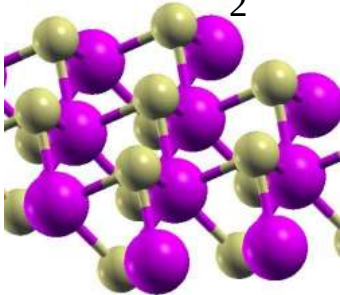
Insulator

BN



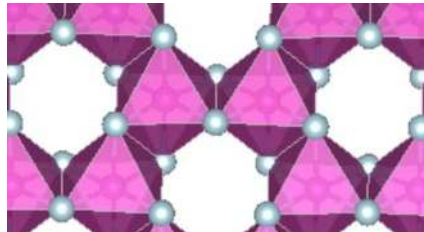
Semiconductor

WSe_2



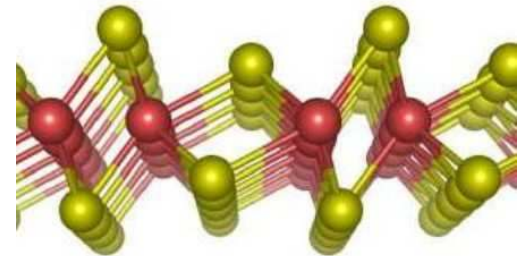
Ferromagnet

CrI_3



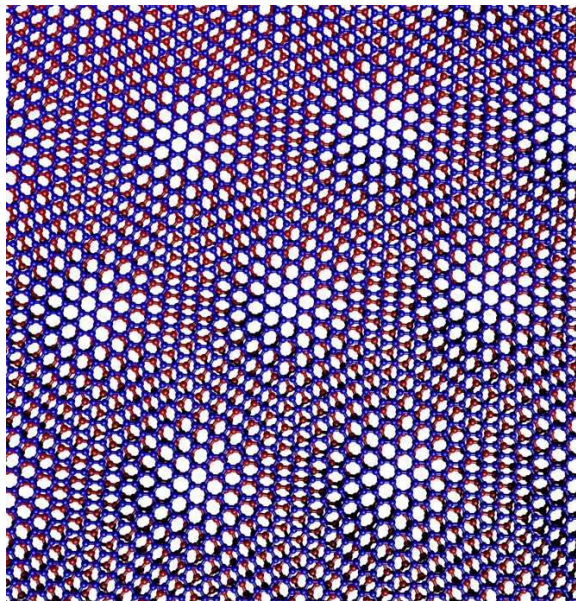
Quantum spin Hall insulator

WTe_2

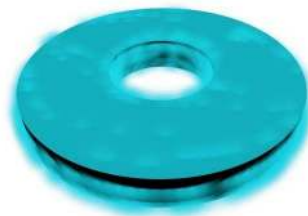


One material, a zoo of electronic phases

Twisted bilayer graphene

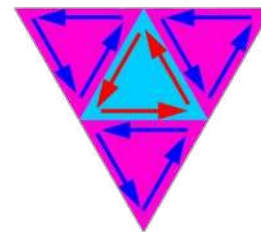


Superconductivity



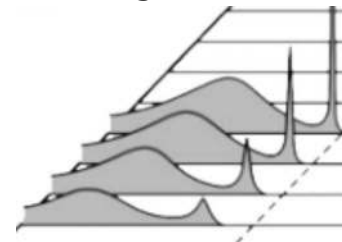
Nature 556, 43–50 (2018)

Topological networks



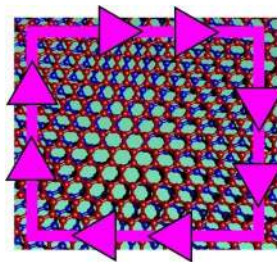
Nano Lett. 18, 11, 6725-6730 (2018)

Strange metals



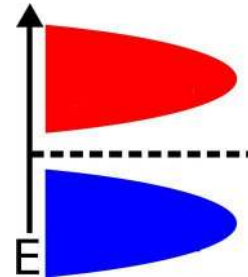
Phys. Rev. Lett. 124, 076801 (2020)

Chern insulators



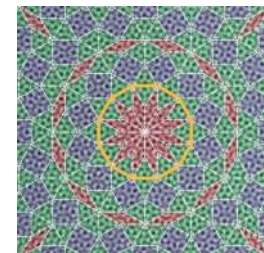
Science 365, 605-608 (2019)

Correlated insulators



Nature 556, 80–84 (2018)

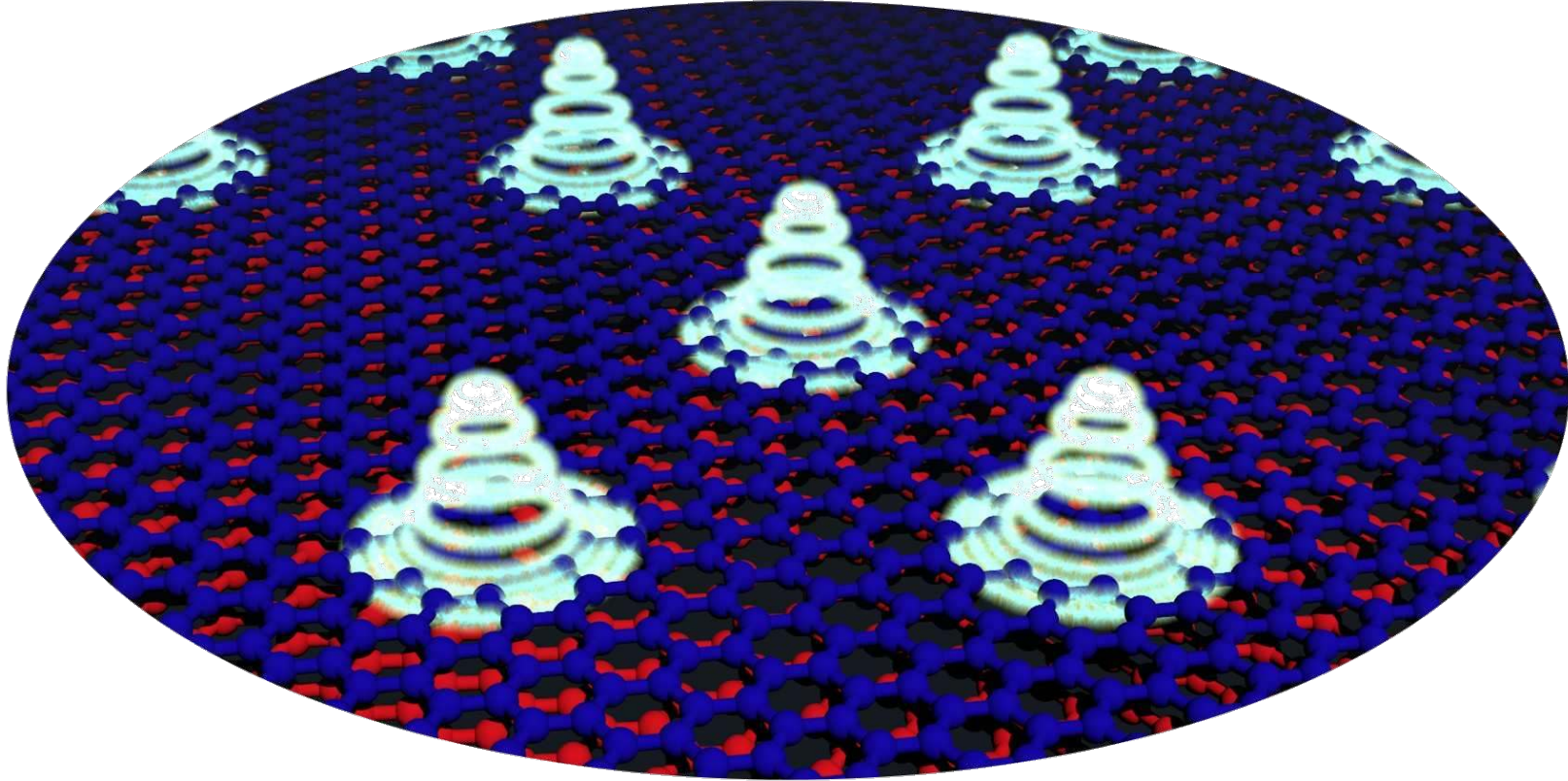
Quasicrystalline physics



Science 361 782-786 (2018)

Twisted graphene multilayers provide a powerful platform for emergent phenomena

A new universe in each new twisted material

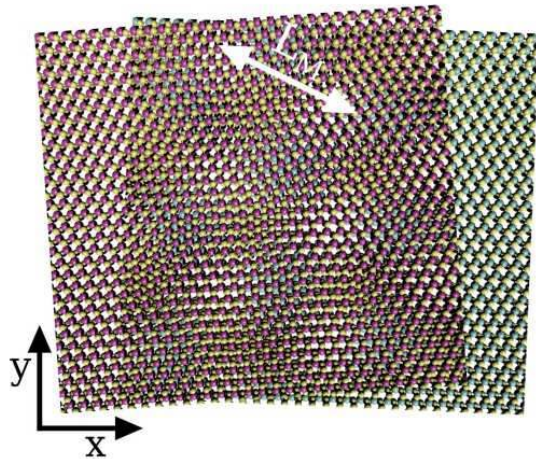


Each twisted material is a new universe for electrons, with laws that change from twist to twist

The generality of correlated physics in twisted 2D materials

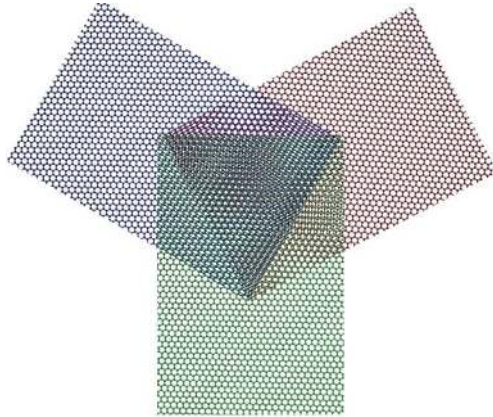
Superconductivity & correlated behavior found also in

Twisted dichalcogenides



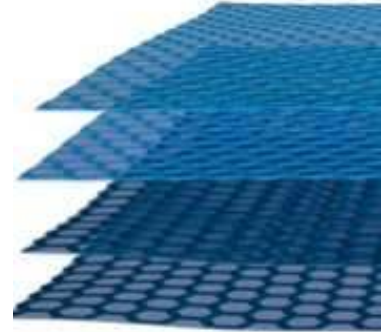
Nature 579, 359–363 (2020)

Twisted graphene trilayers



Nature 590, 249–255 (2021)

Twisted graphene tetralayers

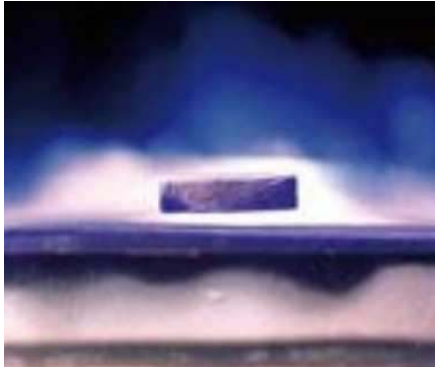


Nature 583, 221–225 (2020)

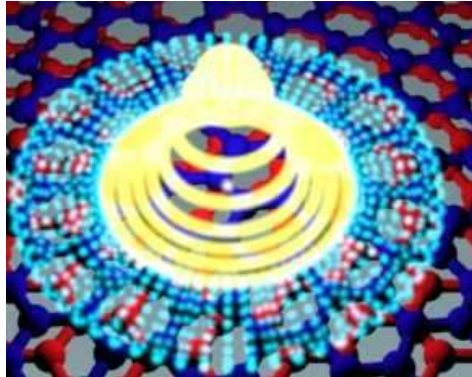
Some of new physics observed were only realized before in rare, heavy or even toxic compounds

The opportunities of twisted van der Waals materials

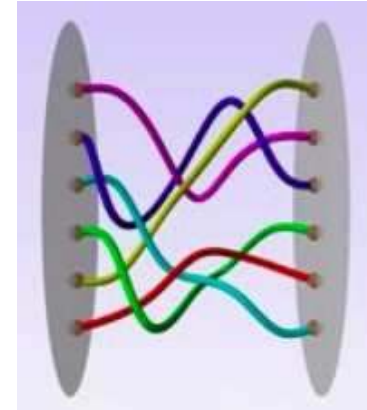
“Unveil” the nature of high T_c superconductivity (?)



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

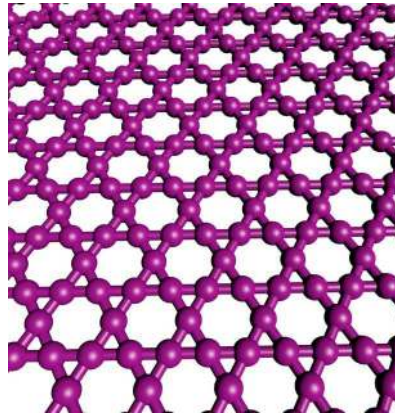
*The strength of
electronic correlations*

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



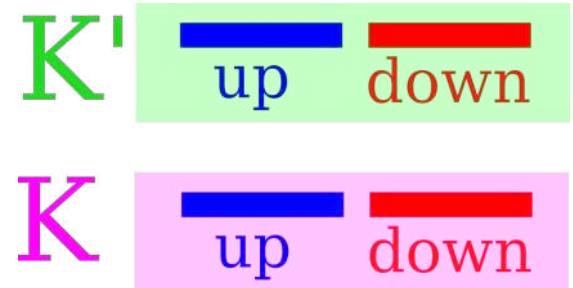
Twist angle control

*The details of the
electronic dispersion*



Interlayer bias

*The local quantum
degrees of freedom*



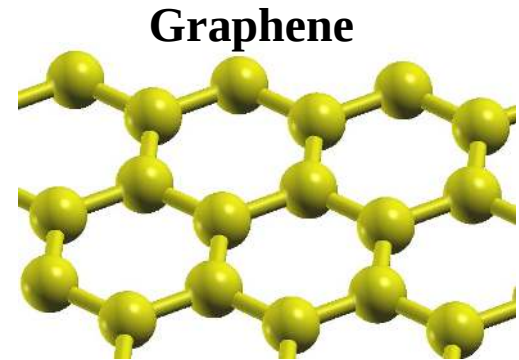
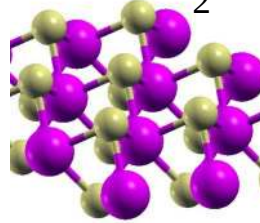
Magnetic encapsulation

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

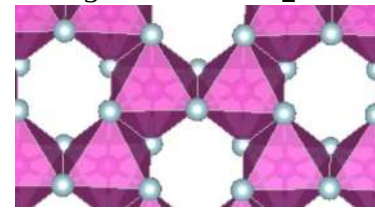
Designing quantum matter with twisted magnetic van der Waals materials



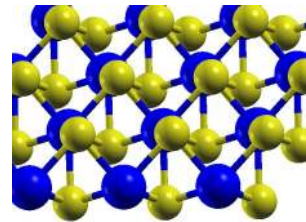
Semiconductor
 WSe_2



Magnet
 CrBr_3 , 1T-TaS₂, CrI_3



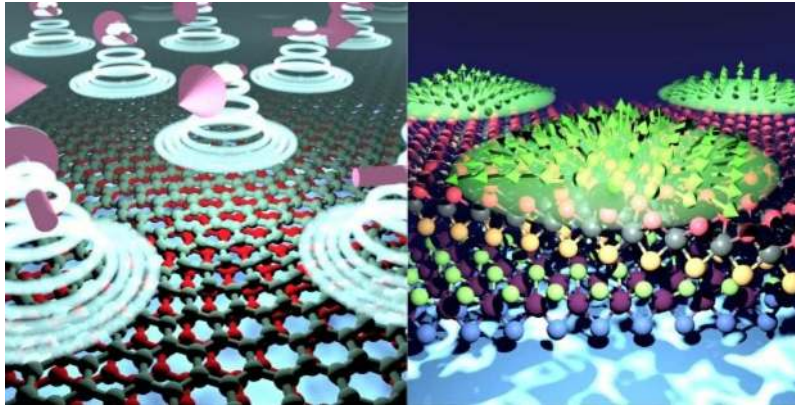
Metal
1H-TaS₂



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

Today's plan

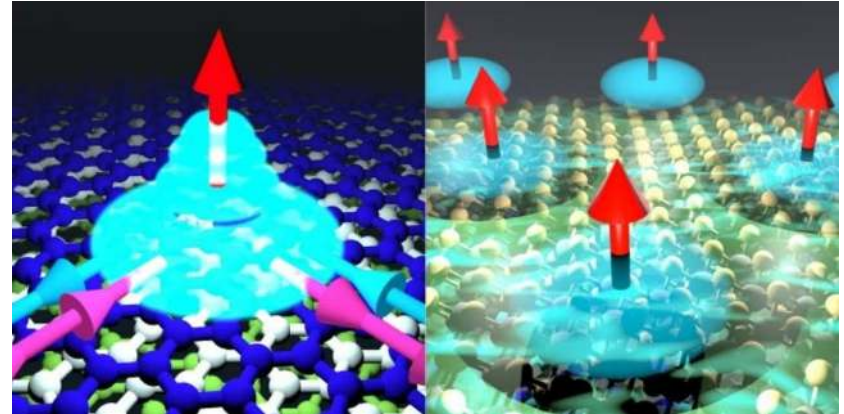
**Design of new correlated states
by magnetic encapsulation in
twisted materials**



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**

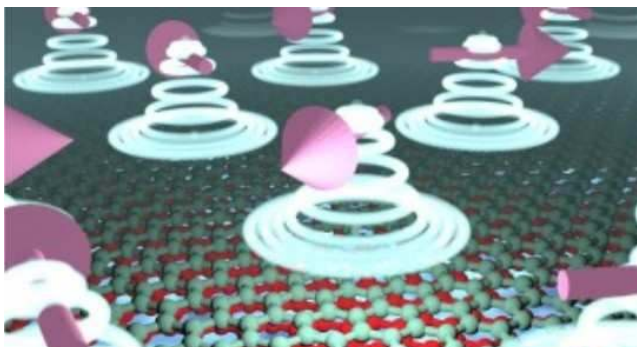


theory & experiment

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



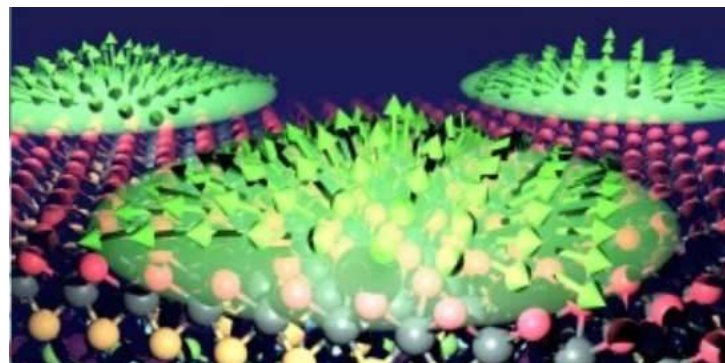
Gianni
Blatter



Oded
Zilberberg

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

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

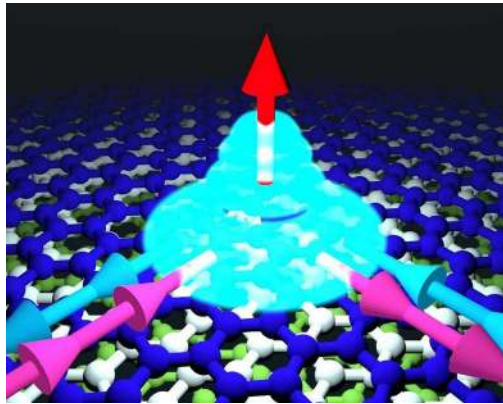


David
Soriano

New J. Phys. 23 073038 (2021)

Behind the scenes

Heavy fermions in twisted graphene trilayers

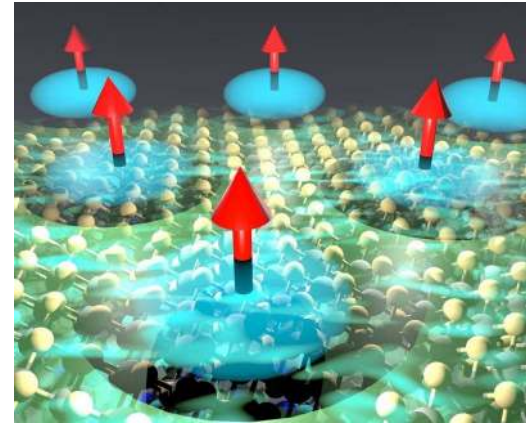


Aline Ramires



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

Heavy fermions in twisted dichalcogenide bilayers



V. Vaňo



S. Kezilebieke



P. Liljeroth



arXiv:2103.11989 (2021)

S. Ganguli



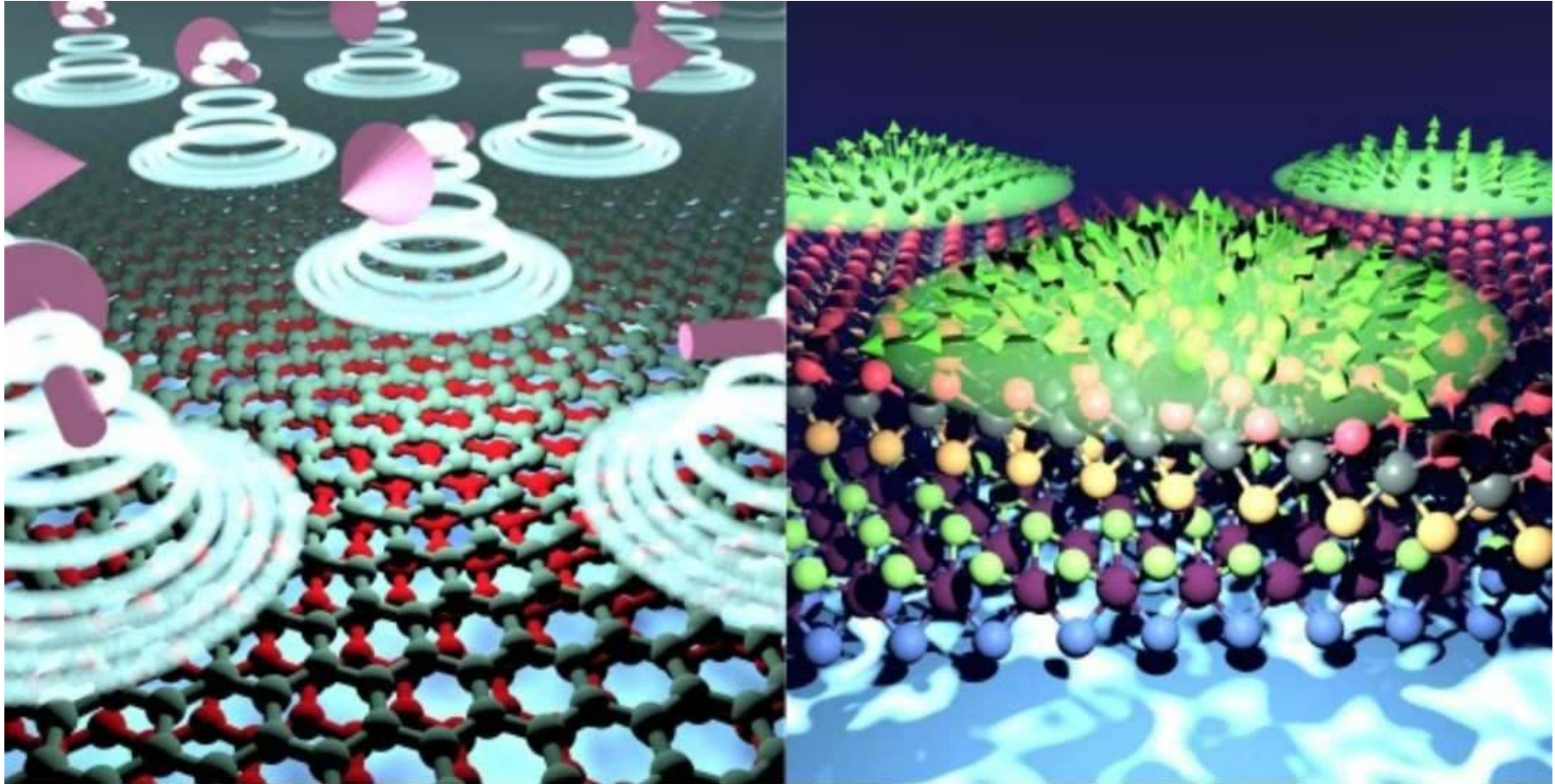
M. Amini



G. Chen



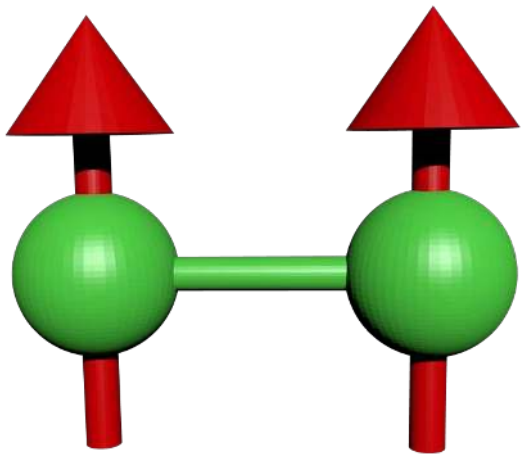
Design of new correlated states by magnetic encapsulation in twisted materials



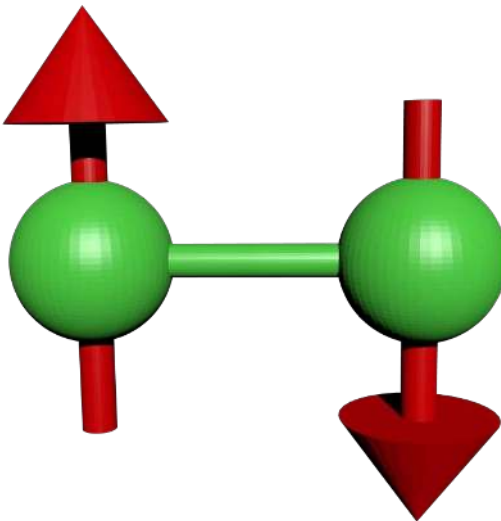
Frustration

A bird's eye view on magnetism

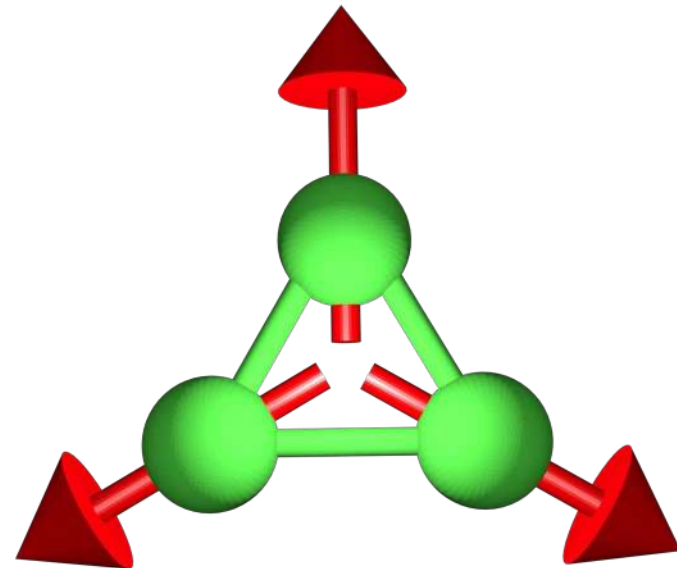
Ferromagnetism



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

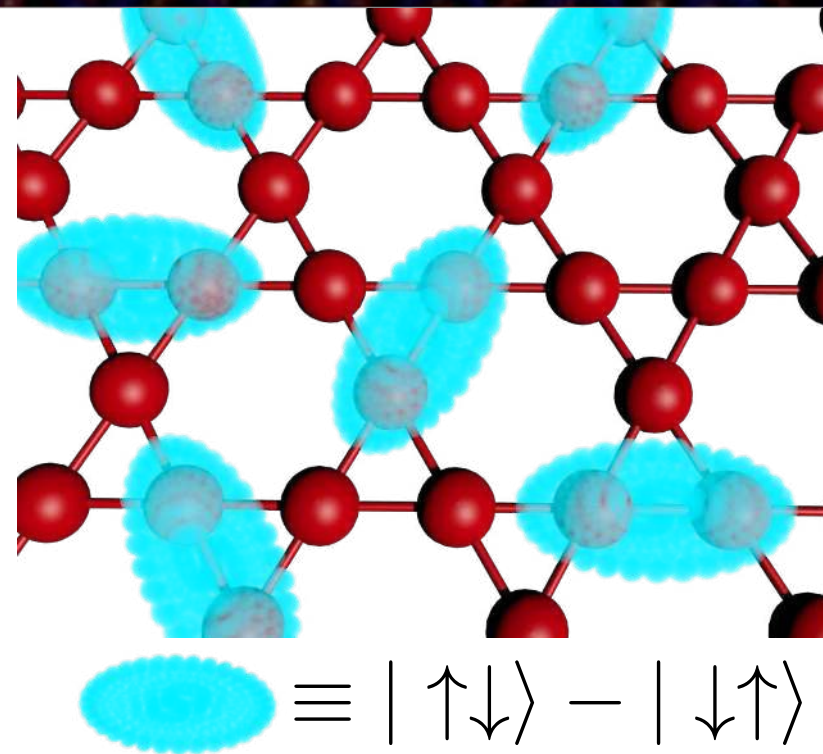
Fractional excitations

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)



Kitaev's honeycomb

Annals of Physics 321.1 (2006)

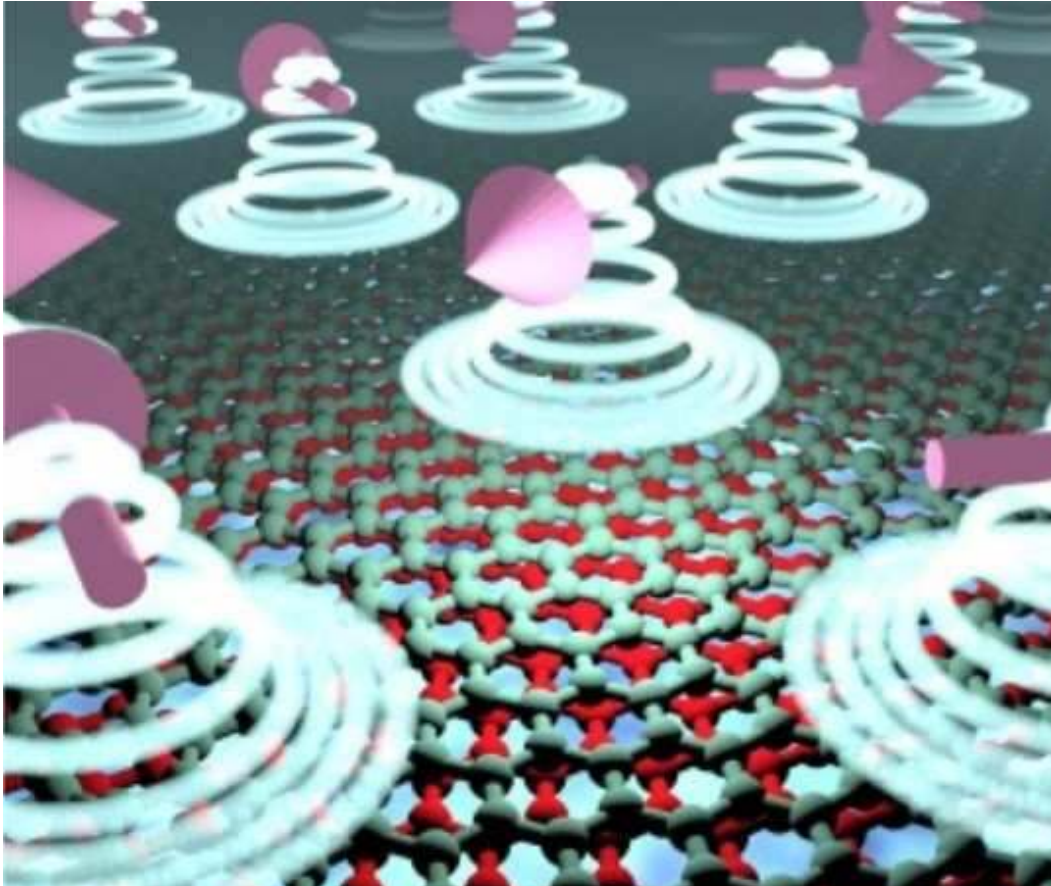
Kagome Heisenberg

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

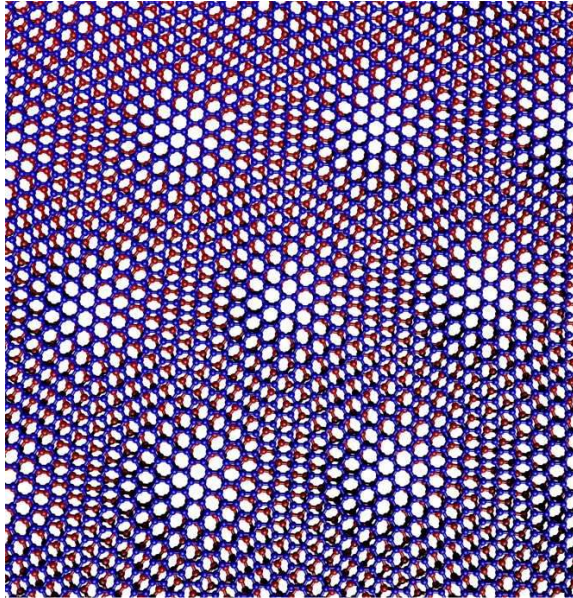


Oded
Zilberberg

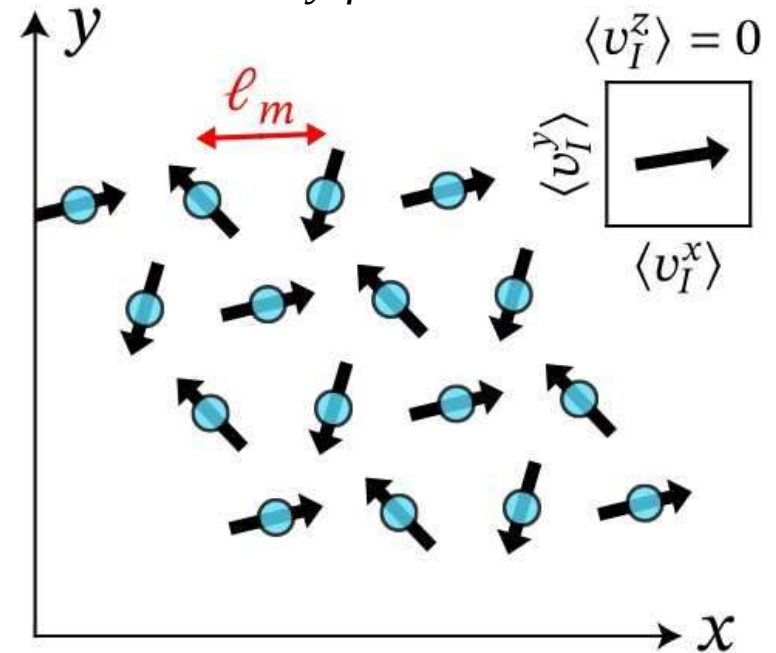
Phys. Rev. Lett. 126, 056803 (2021)

Frustrated valley magnetism

Moire structure



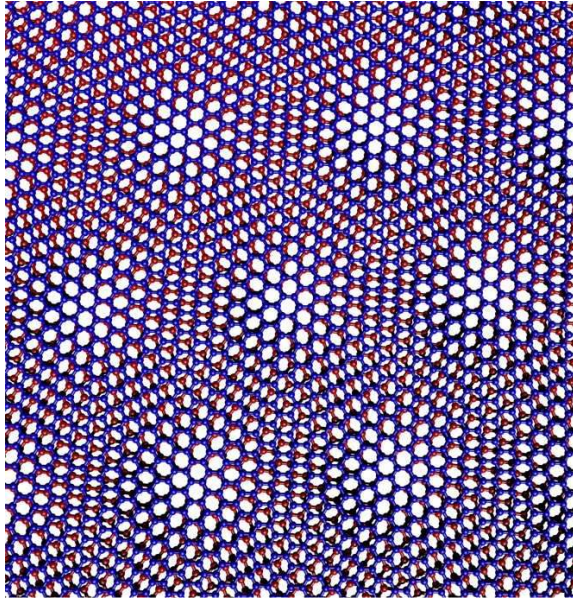
Valley-frustrated state



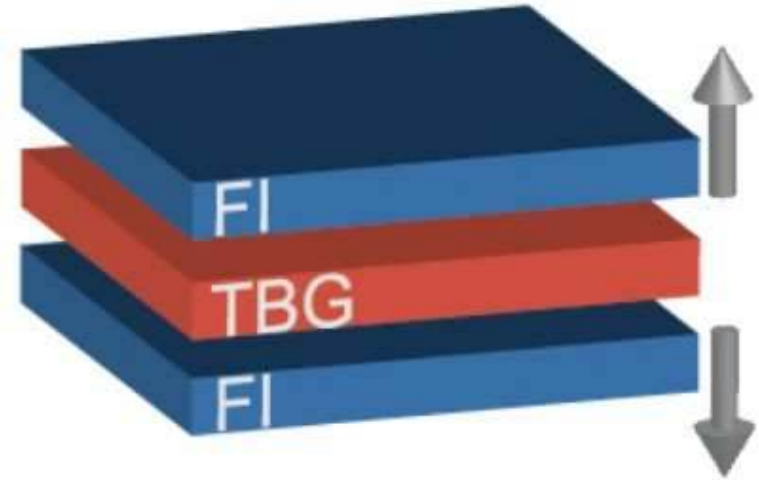
Can we create a controllable valley-only frustrated magnet?

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

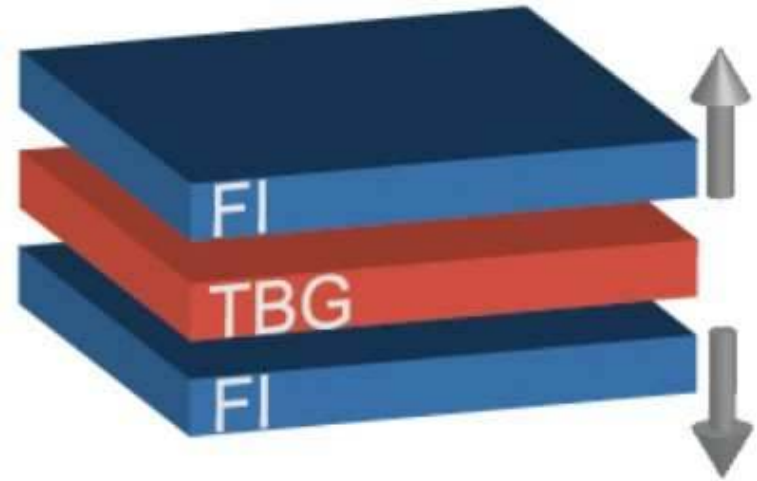
$$H = H_0 + H_J + H_R$$

Kinetic
energy

Exchange
proximity
effect

Rashba
spin-orbit
coupling

Magnetic encapsulation



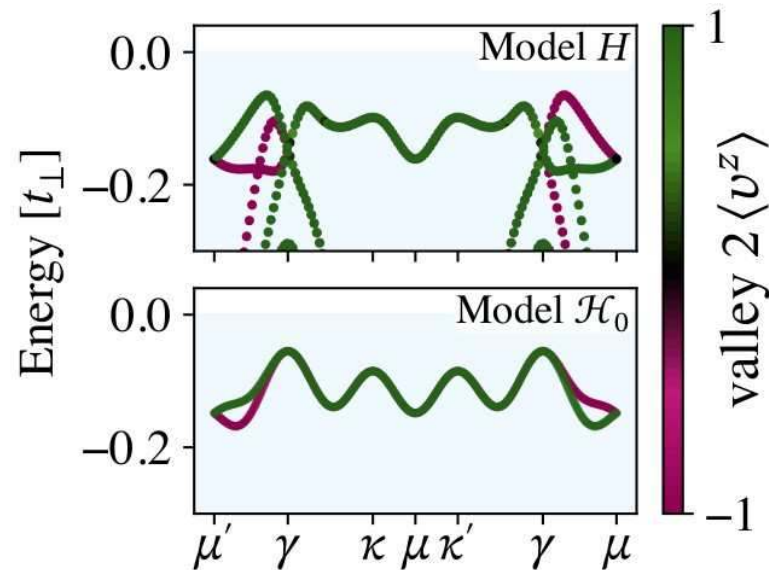
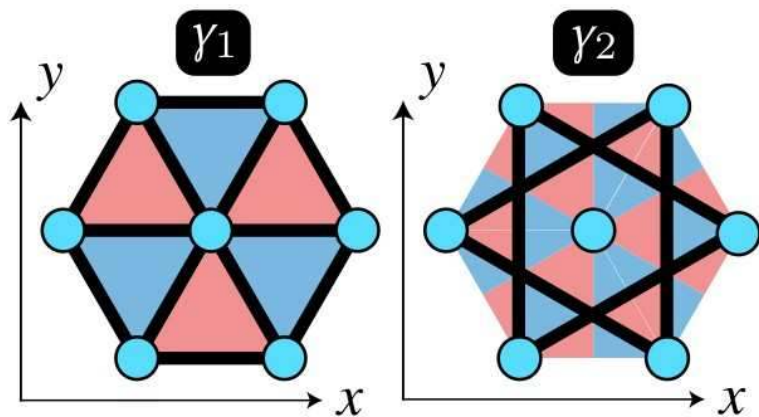
Valley frustration from combined twist engineering, exchange proximity and spin-orbit coupling.

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

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

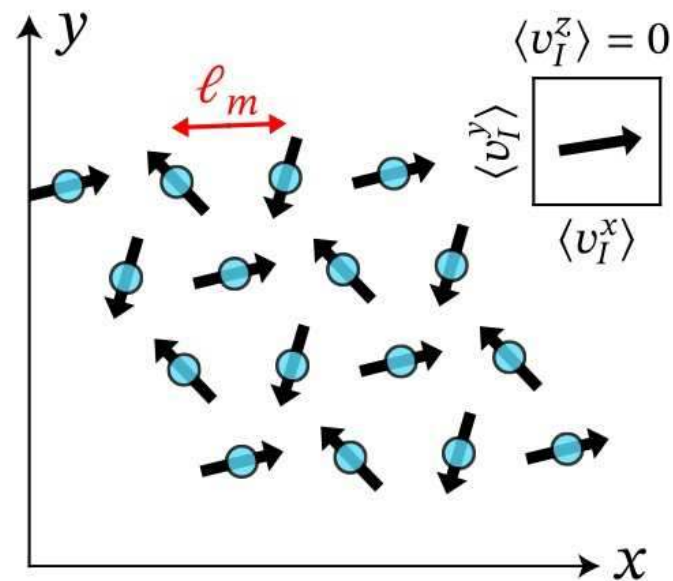
Impact of interactions

Lets add electronic interactions

Free
Hamiltonian

Electronic
interactions

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

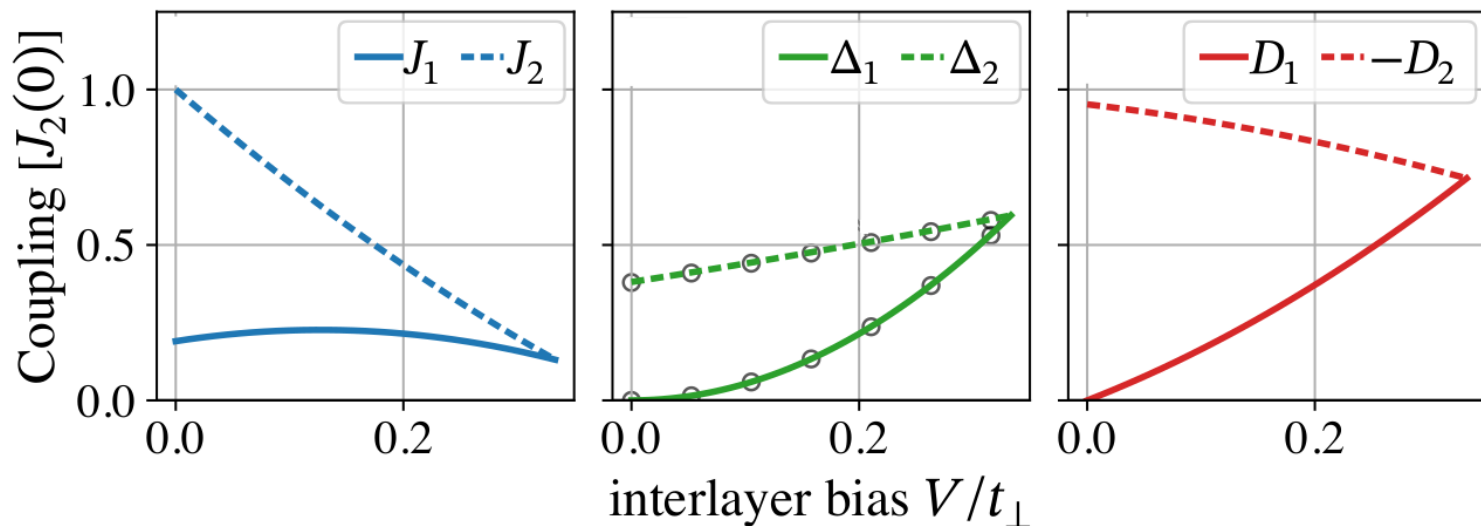


And compute the effective valley-Heisenberg Hamiltonian in the strong coupling limit

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

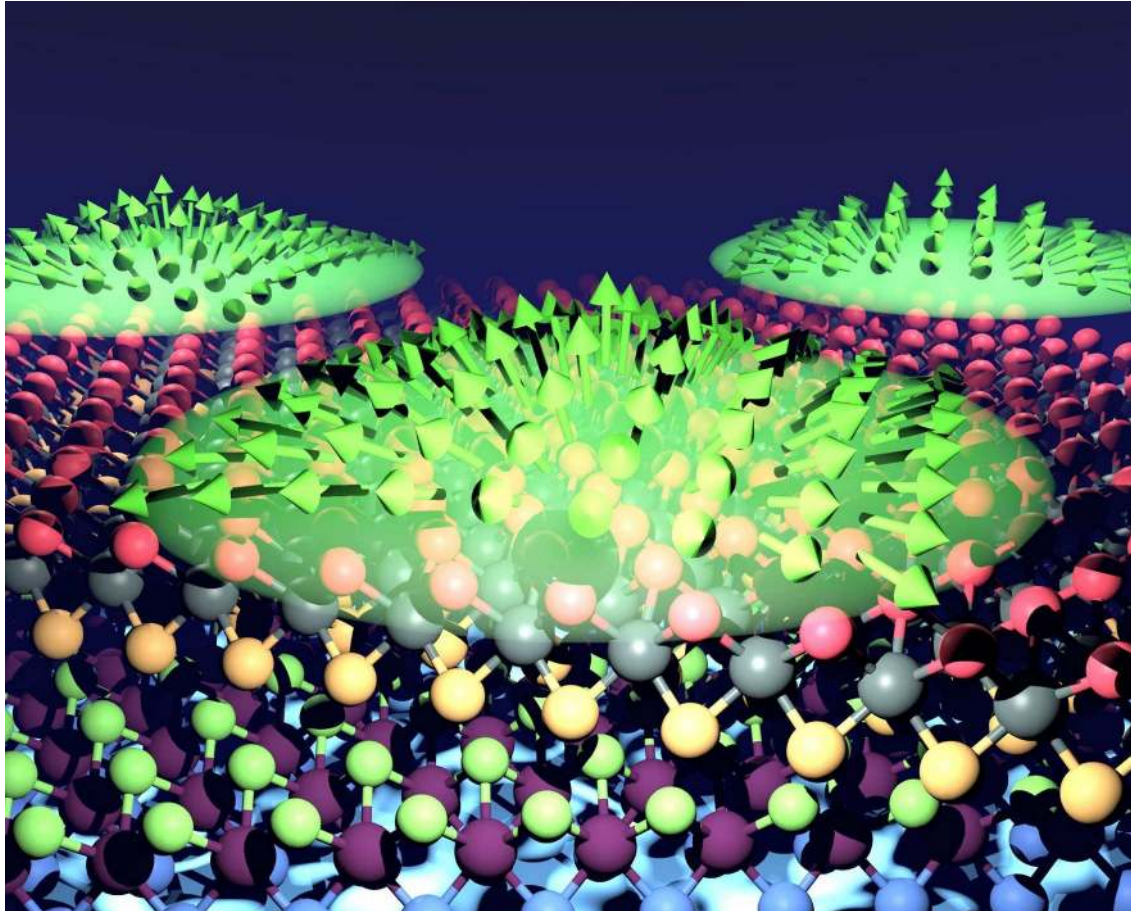
Controlling a valley-Heisenberg model electrically

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



An interlayer bias provides a tunable anisotropic valley-Heisenberg model

Correlated states dominated by spin-orbit coupling in Janus dichalcogenides

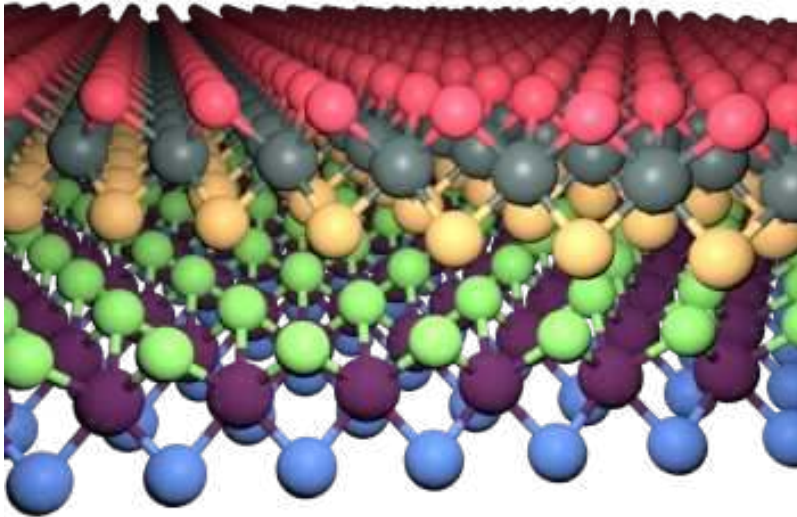


David Soriano

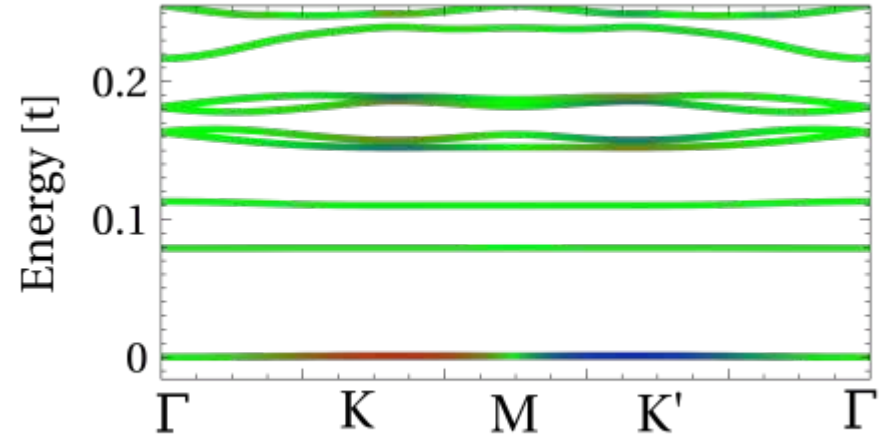
New J. Phys. 23 073038 (2021)

Twisted Janus bilayers

Twisted Janus bilayer

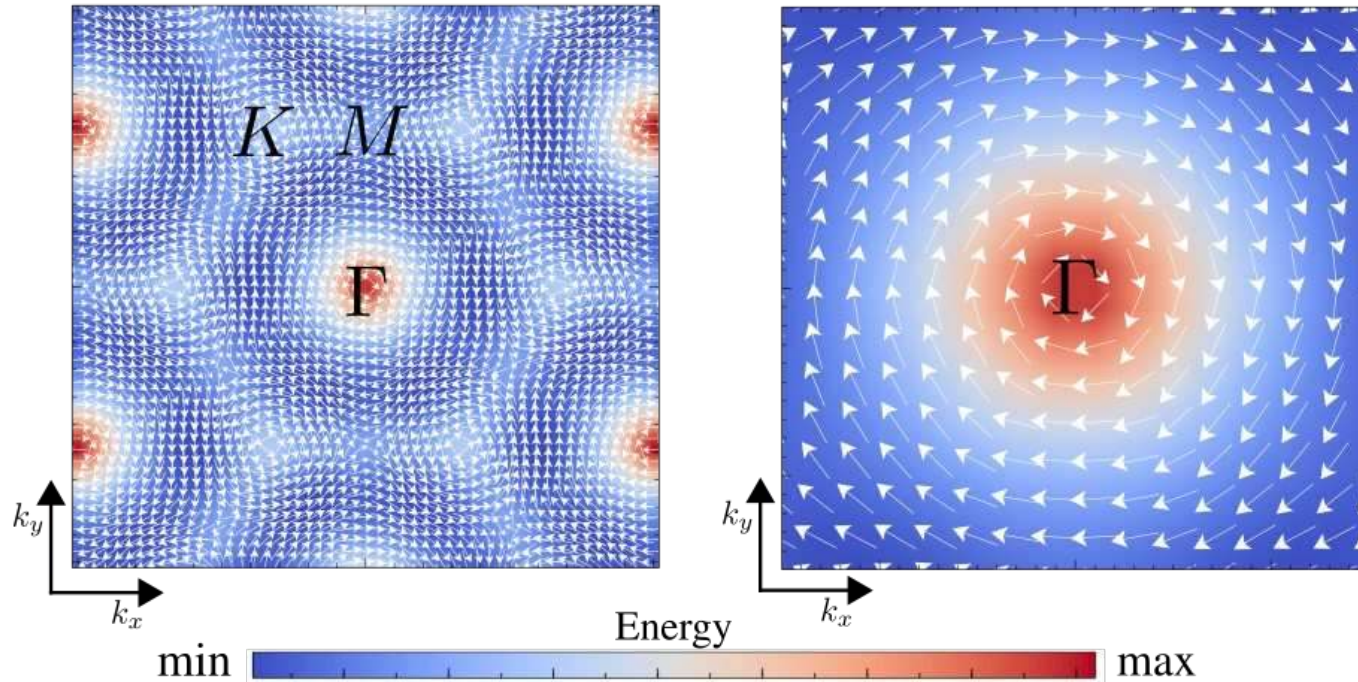


Band structure



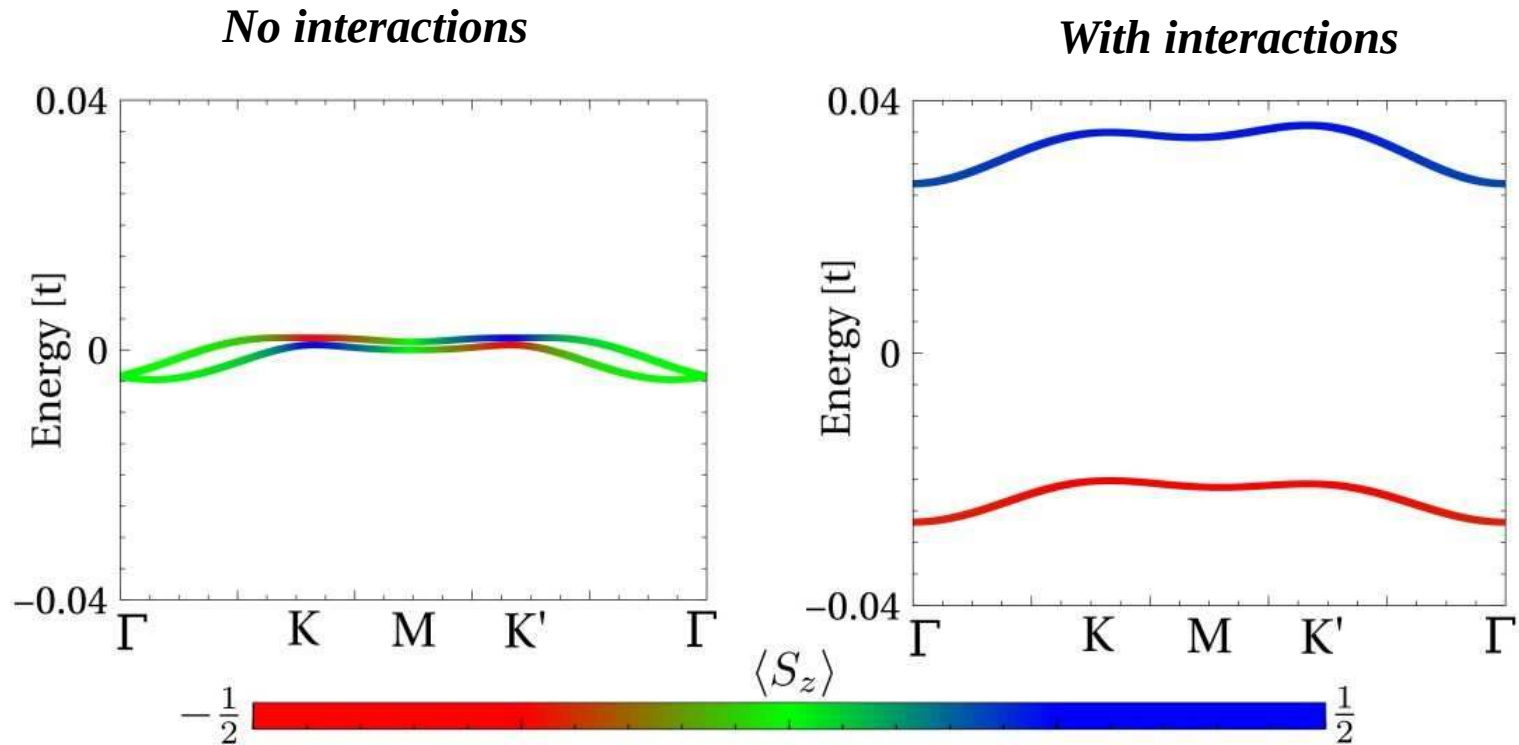
Flat bands emerge in a twisted Janus bilayer, inheriting the colossal Rashba SOC effects

Reciprocal space texture of the flat bands



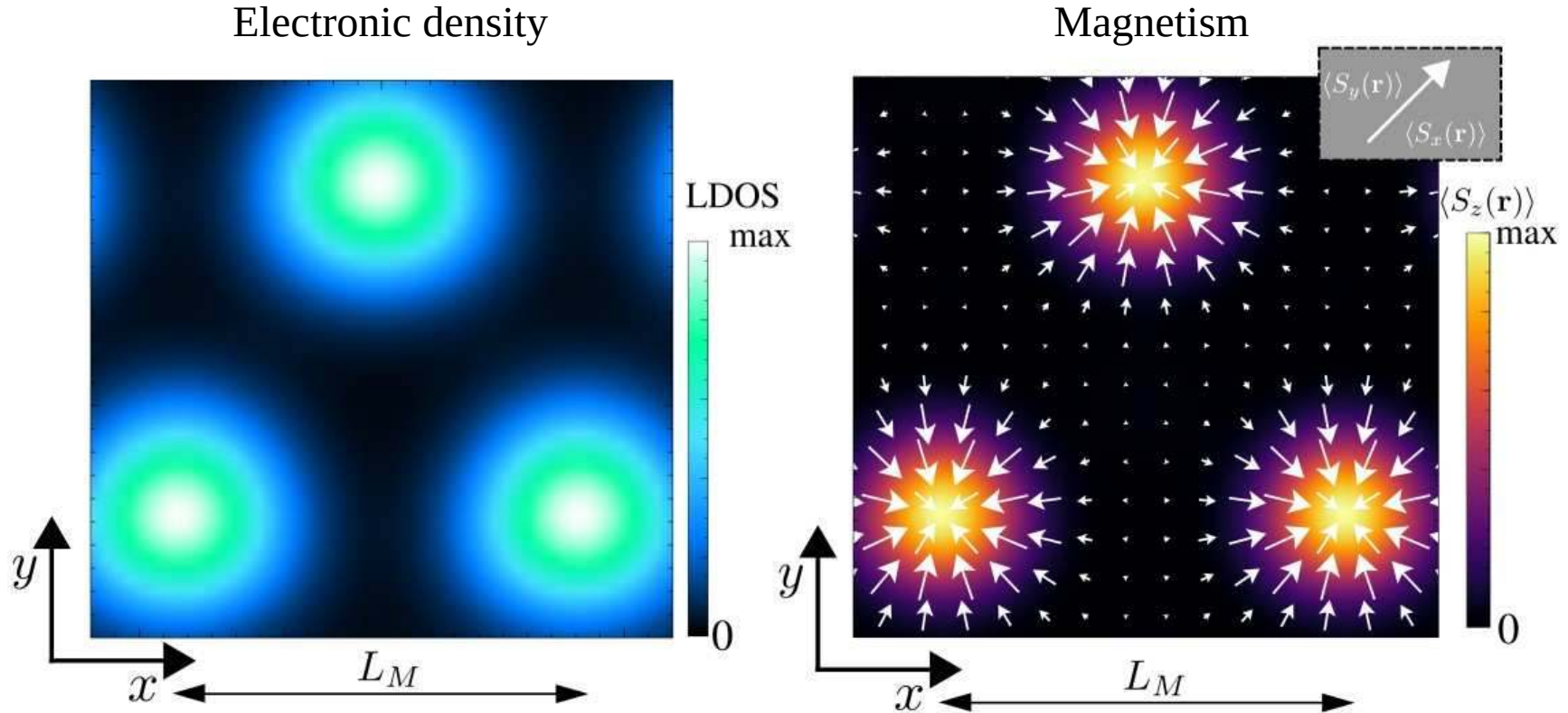
Flat bands are dominated by a strong spin-momentum texture, stemming from the Janus structure

Impact of interactions at low energies



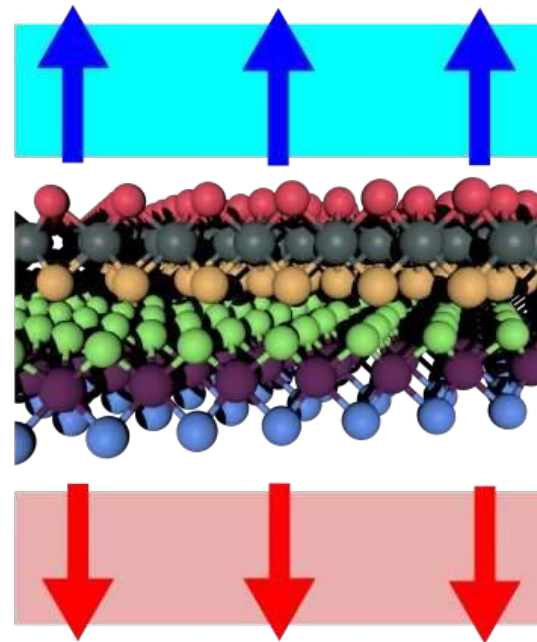
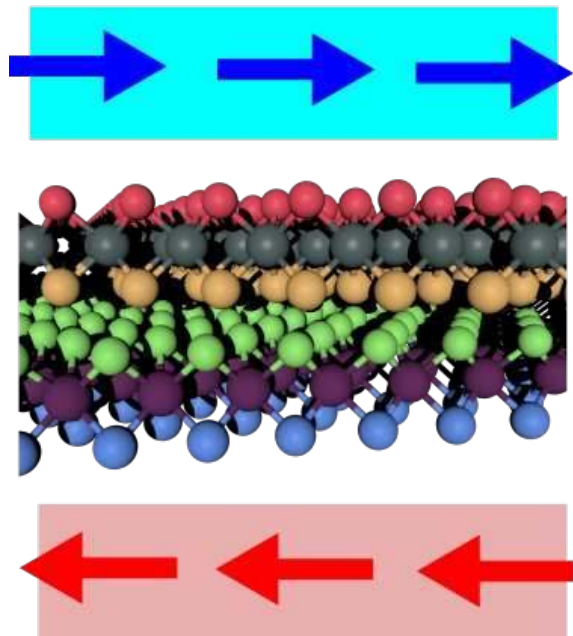
When including interactions in the full lattice model, a symmetry broken state arises

Real space profile when including interactions



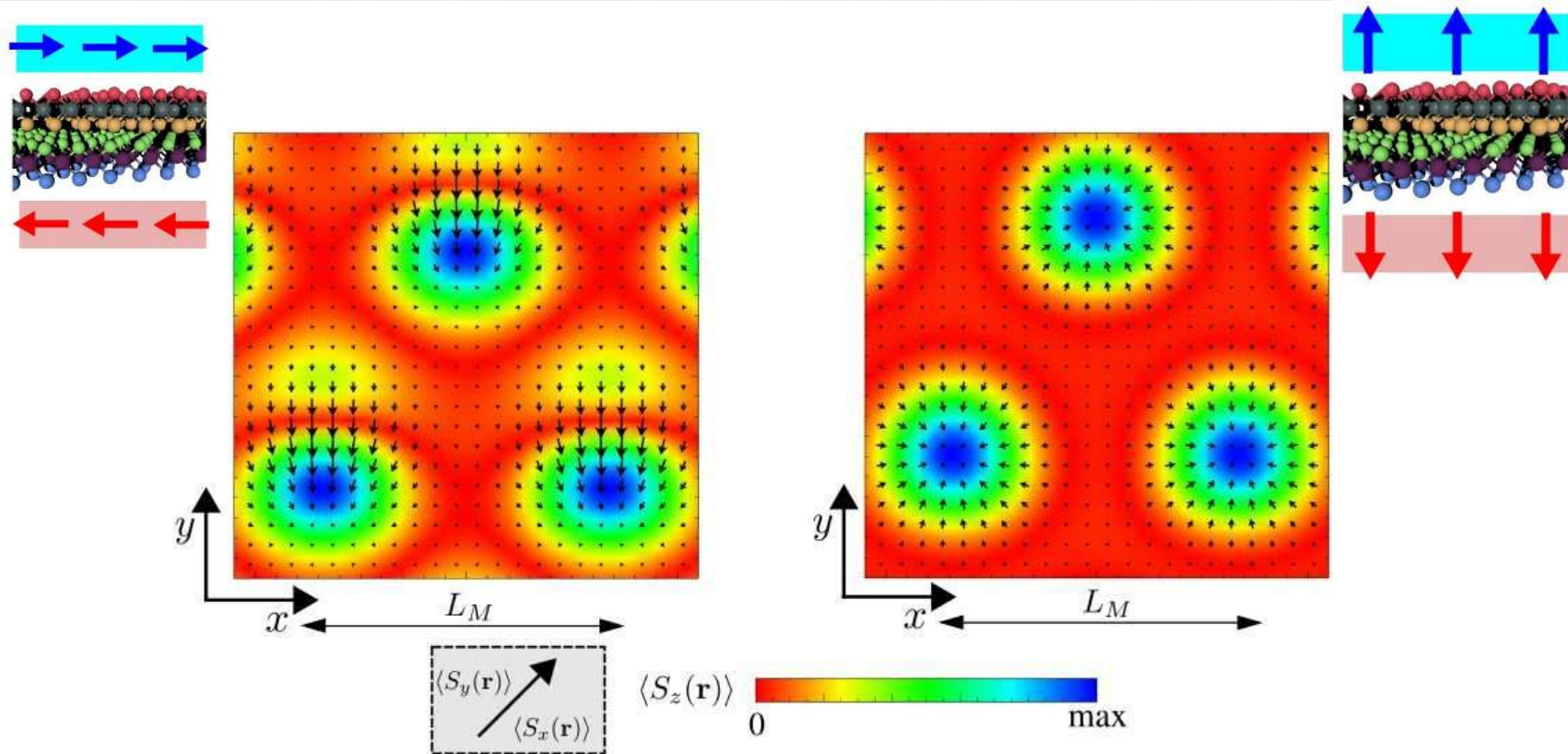
A moire meron magnetic structure appears due to the presence of interactions

Control by magnetic encapsulation



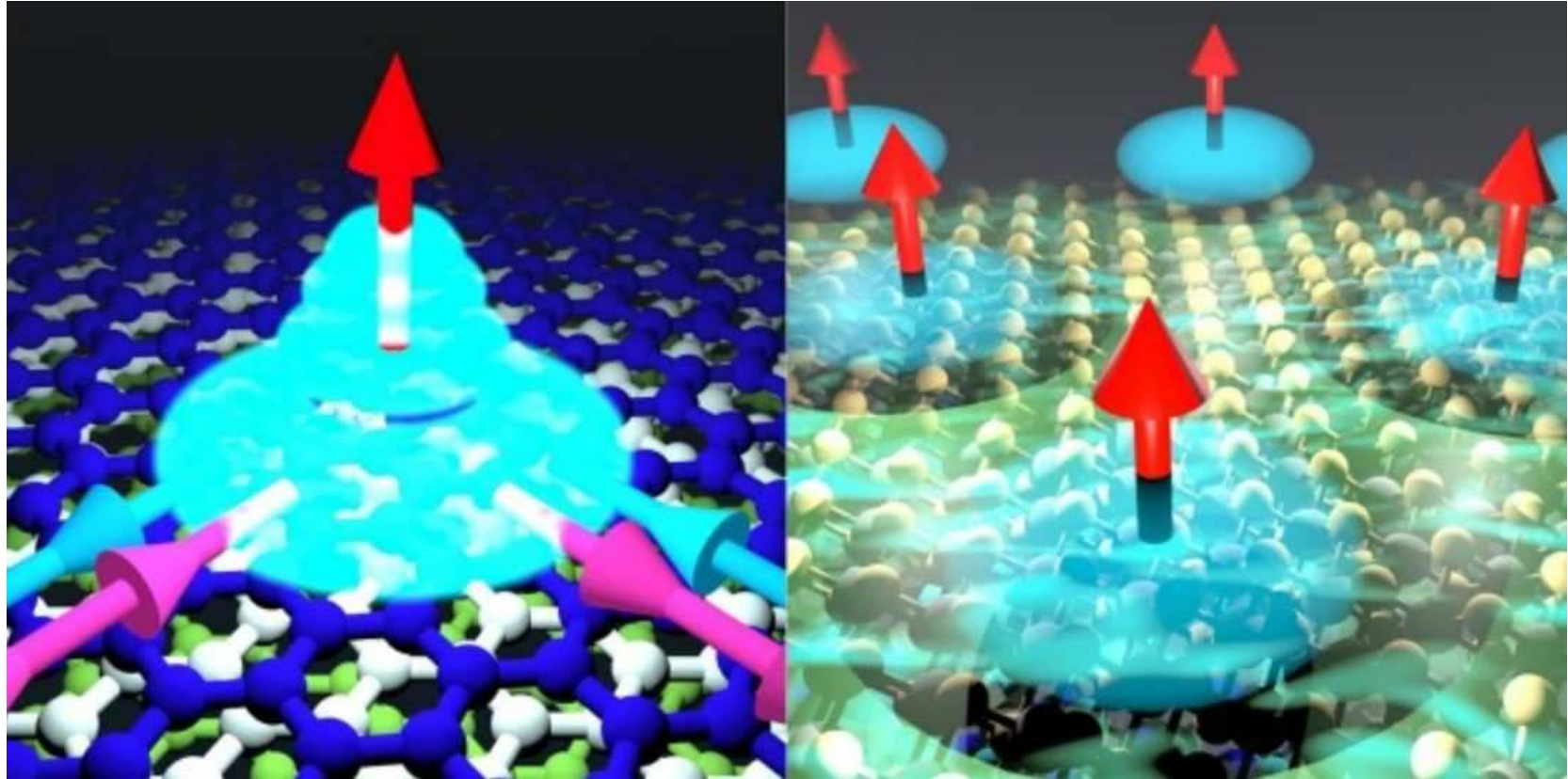
Let us explore the impact of a magnetic encapsulation in the correlated Janus bilayer

Control by magnetic encapsulation



Magnetic moiré merons controlled by the magnetic encapsulation

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



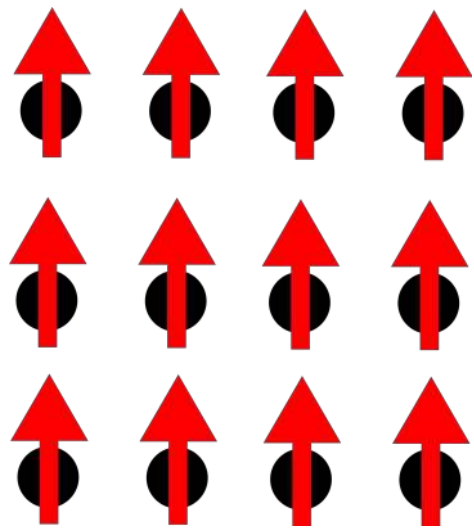
Basics of heavy fermion physics

- 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



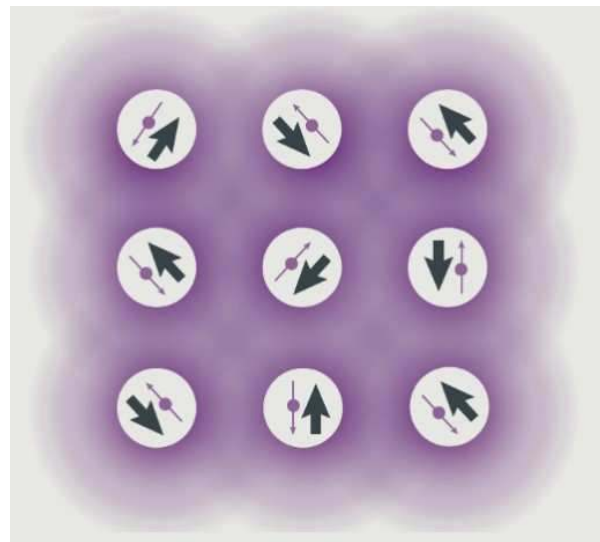
f-electrons in
rare-earth compounds

Dispersive electron gas



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

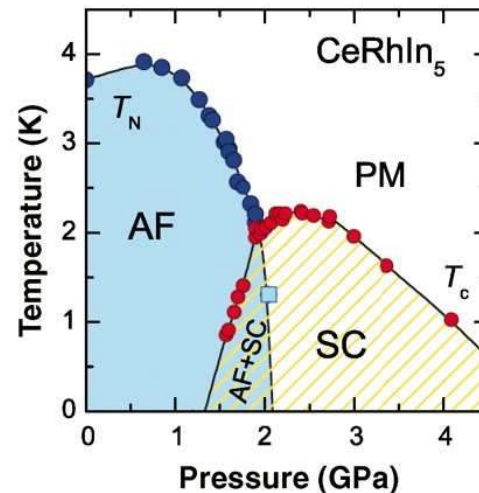
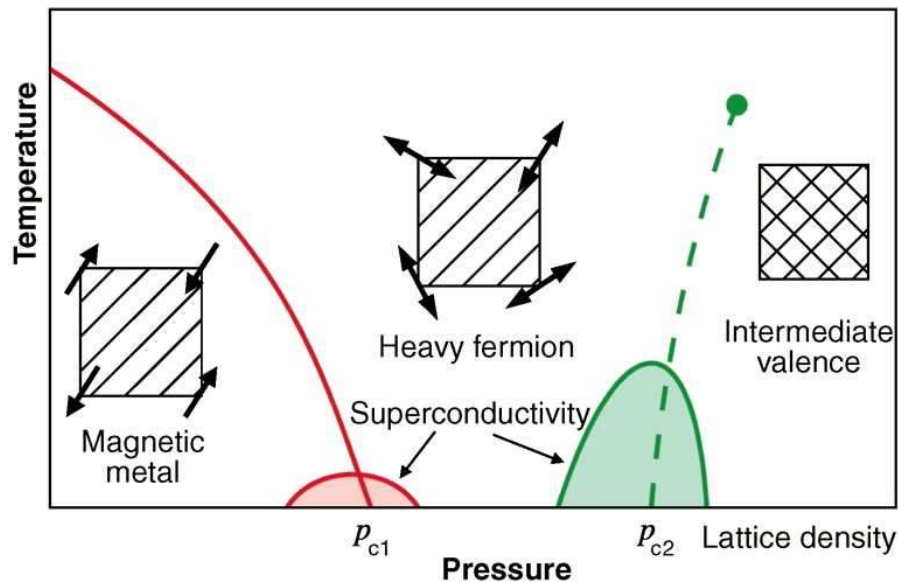
Kondo-lattice model



Associated with Kondo lattice physics:

- Colossal mass enhancement
- Quantum criticality
- Unconventional superconductivity

Basics of heavy fermion physics

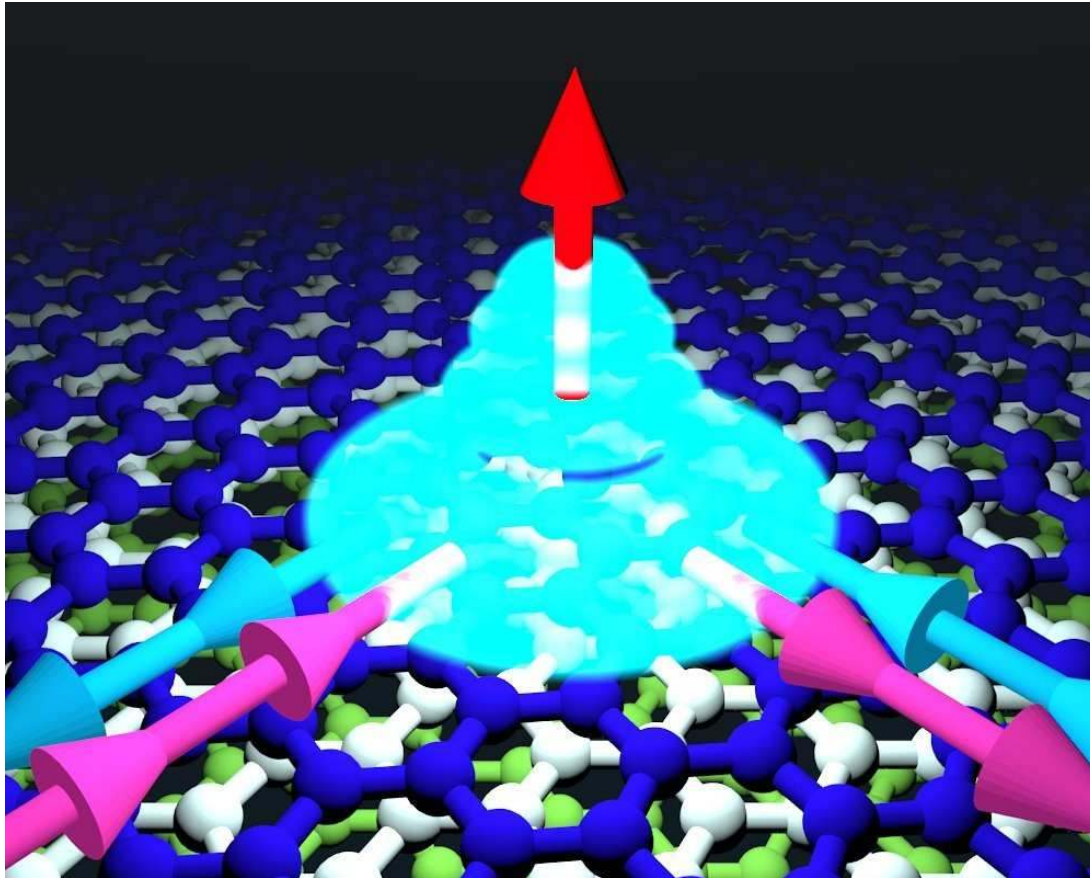


Science 332.6026, 196-200 (2011)

Associated with Kondo lattice physics:

- Colossal mass enhancement of electrons
- Quantum criticality
- Unconventional (topological) superconductivity

Heavy-fermions in twisted graphene trilayers



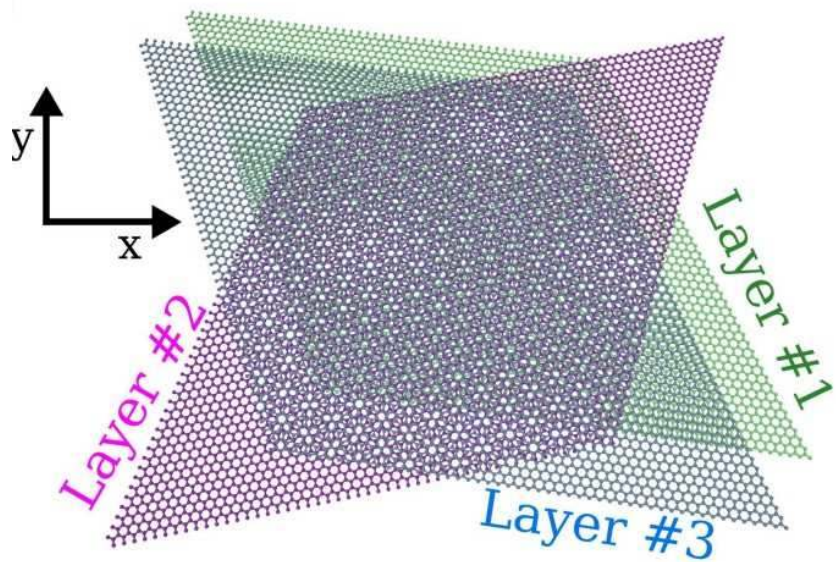
Aline Ramires



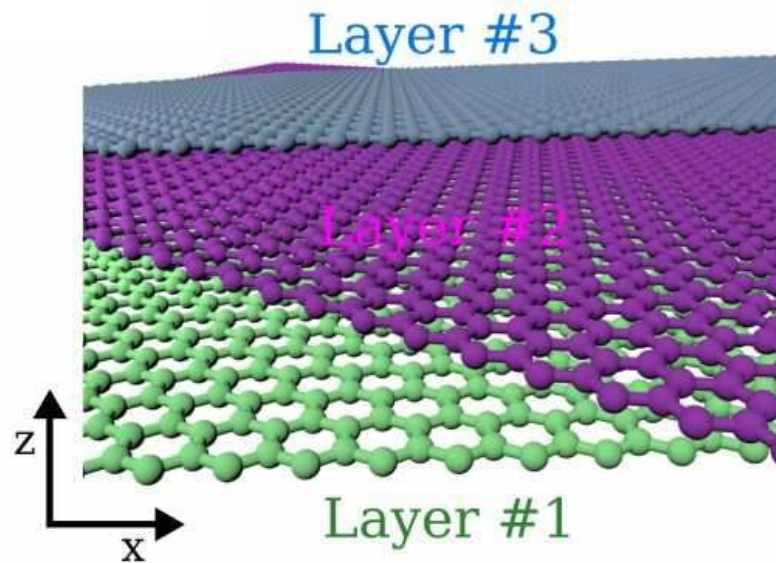
Phys. Rev. Lett. 127, 026401 (2021)

Heavy-fermions in twisted graphene trilayers

Top view

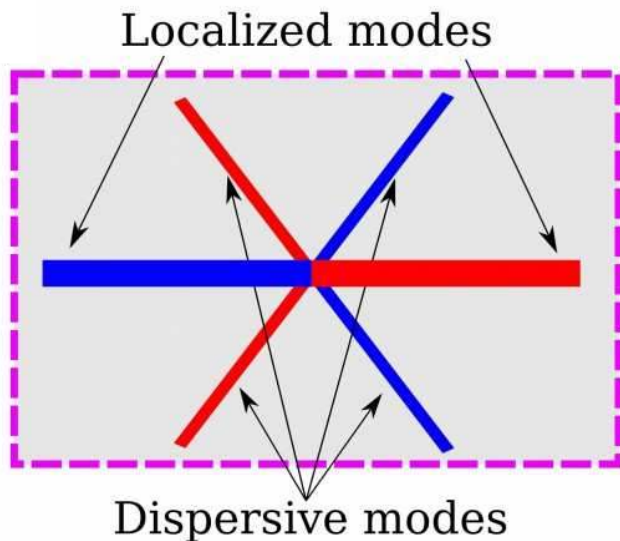


Lateral view

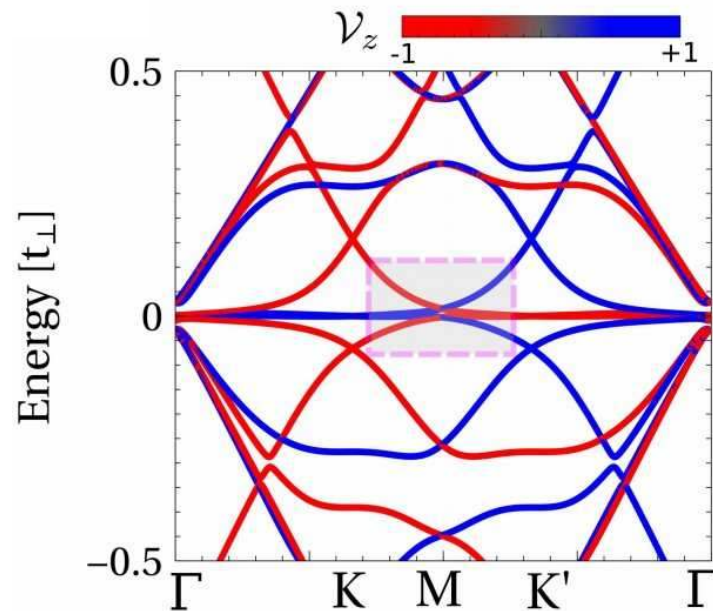


Heavy-fermions in twisted graphene trilayers

Low energy model

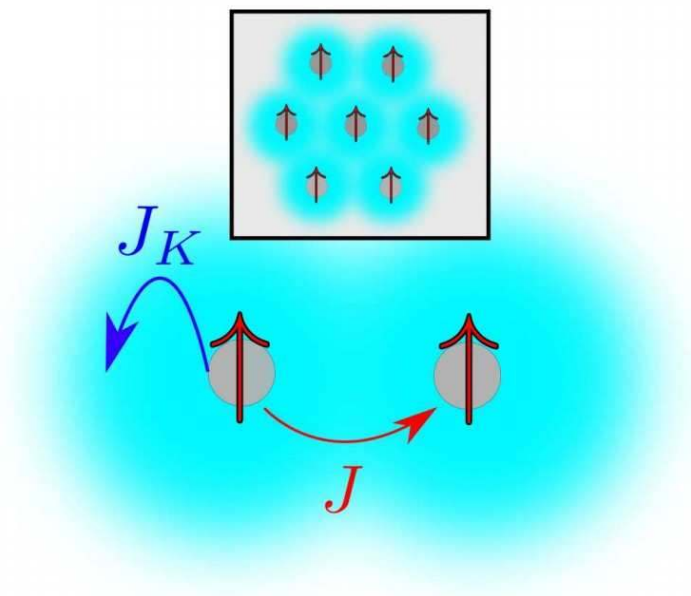


Electronic structure in the presence of an electric bias

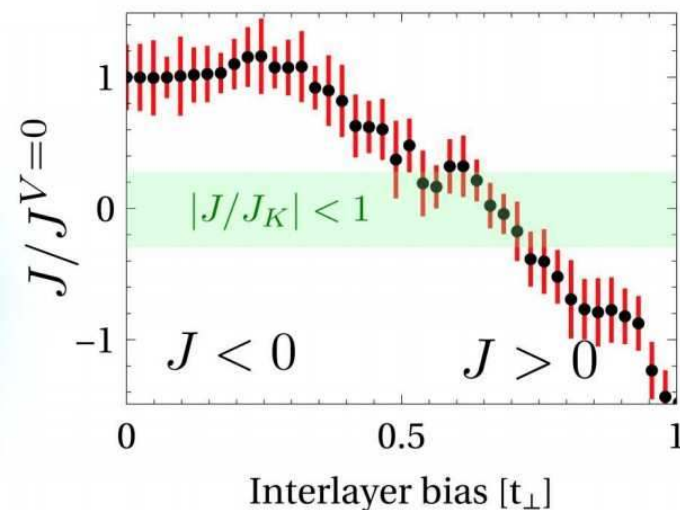


Kondo lattice model in the presence of interactions

Interactions of the Kondo lattice model



Electric control of the Kondo regime

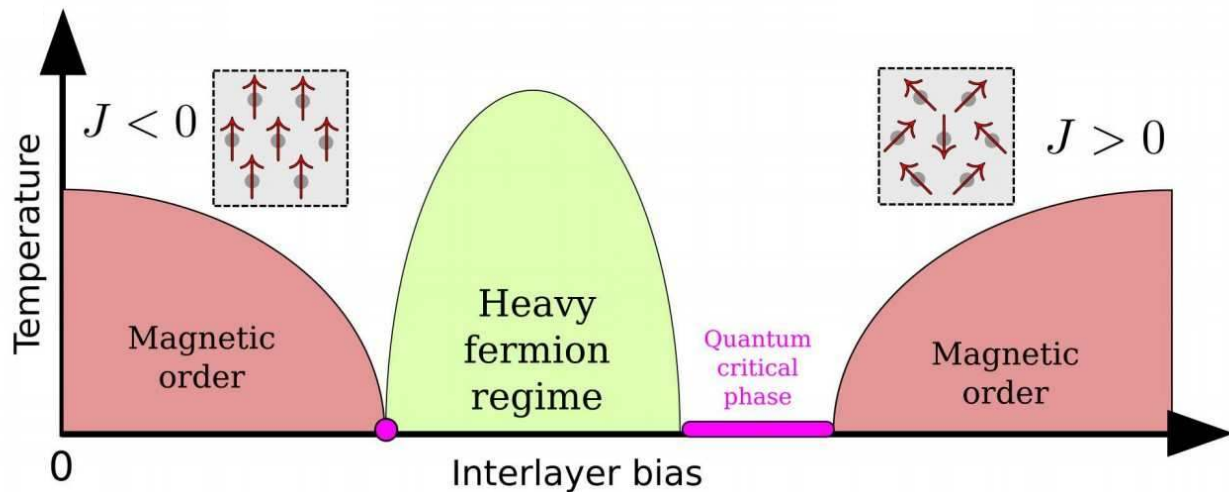


A heavy fermion regime appears when the Kondo coupling dominates over the exchange coupling

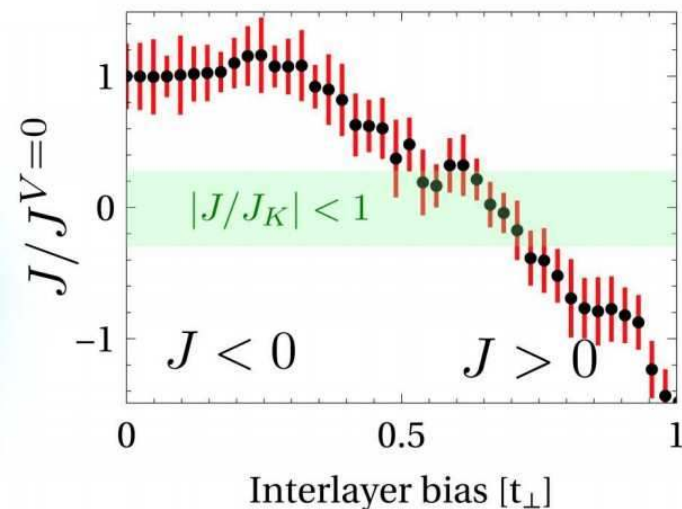
$$|J/J_K| < 1$$

Heavy-fermions in twisted graphene trilayers

Heavy-fermion (Doniach) phase diagram

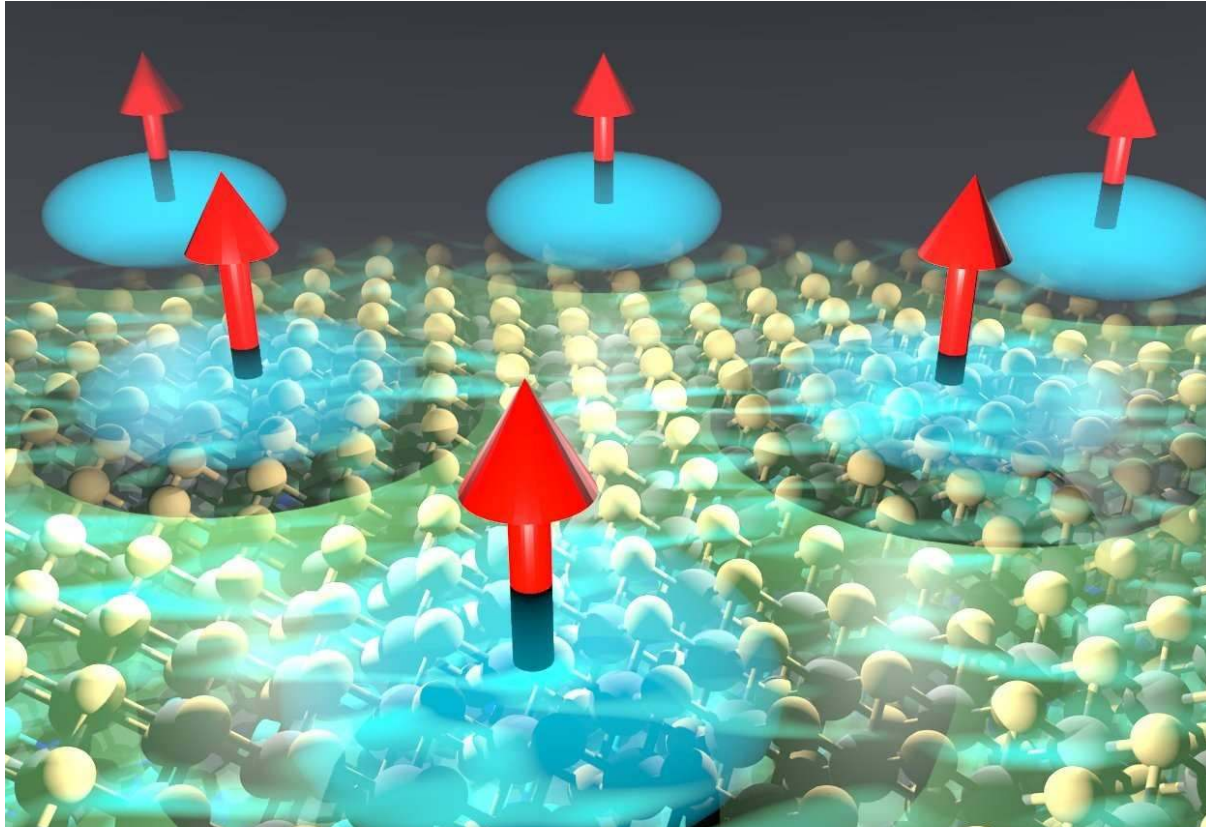


Electric control of the Kondo regime



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-TaS₂

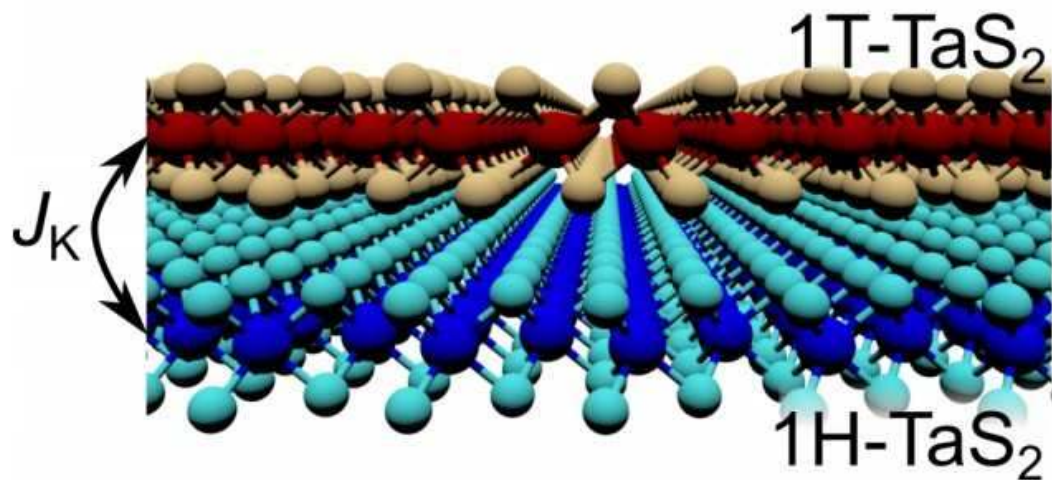
Two-dimensional electron gas



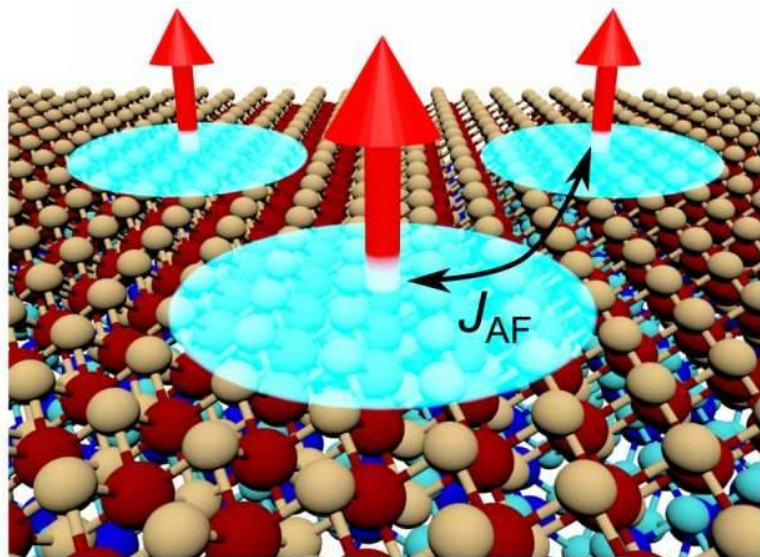
1H-TaS₂

Heavy-fermions in dichalcogenide bilayers

Interlayer coupling create
the Kondo coupling



Intralayer exchange between
local moments

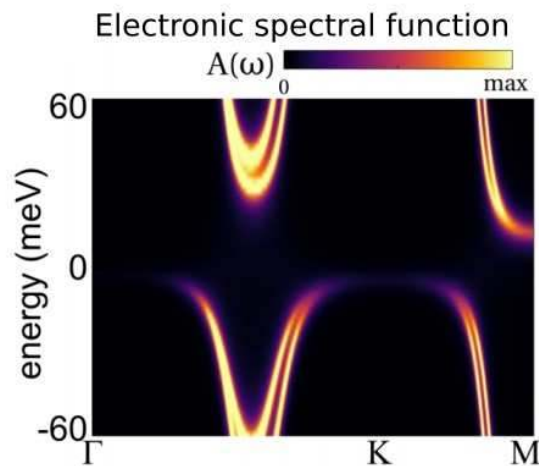
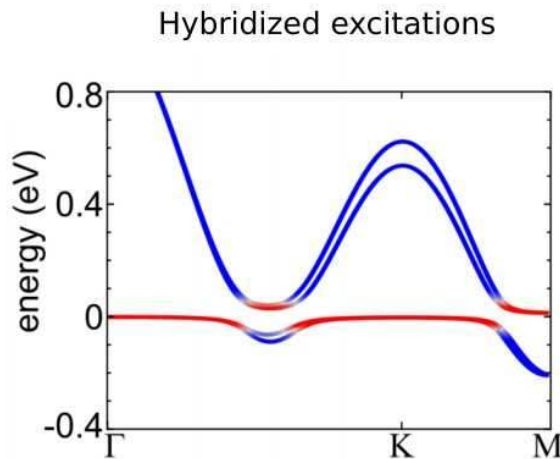
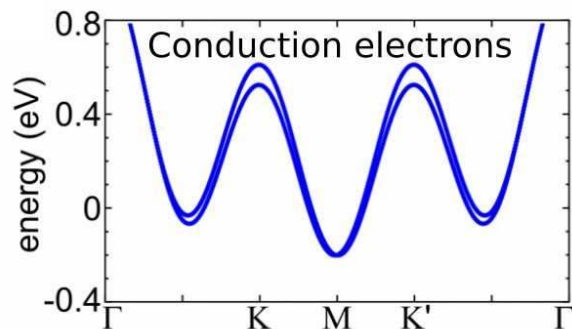
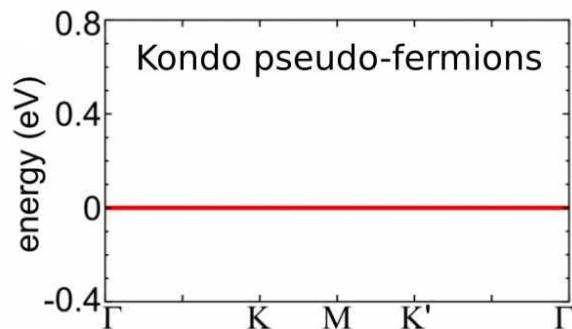


The bilayer realizes all the ingredients for heavy-fermion physics

Brief theory of heavy-fermions

Kondo physics introduces resonant pseudo-fermions at the chemical potential

Leading to the opening of a heavy-fermion gap

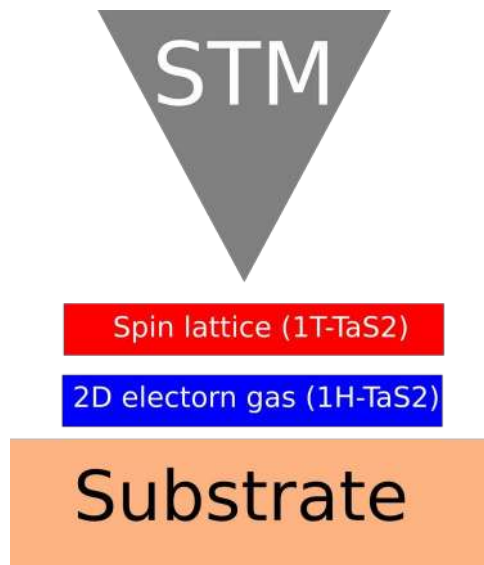


Experimental signatures of heavy-fermion physics

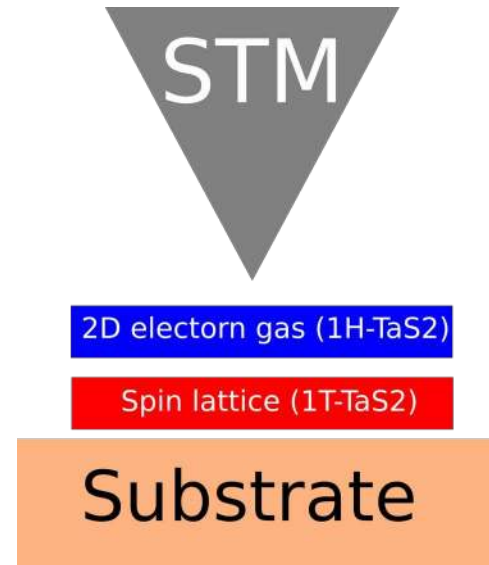
- Kondo physics in the magnetic lattice
- Gap opening in the metallic layer

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

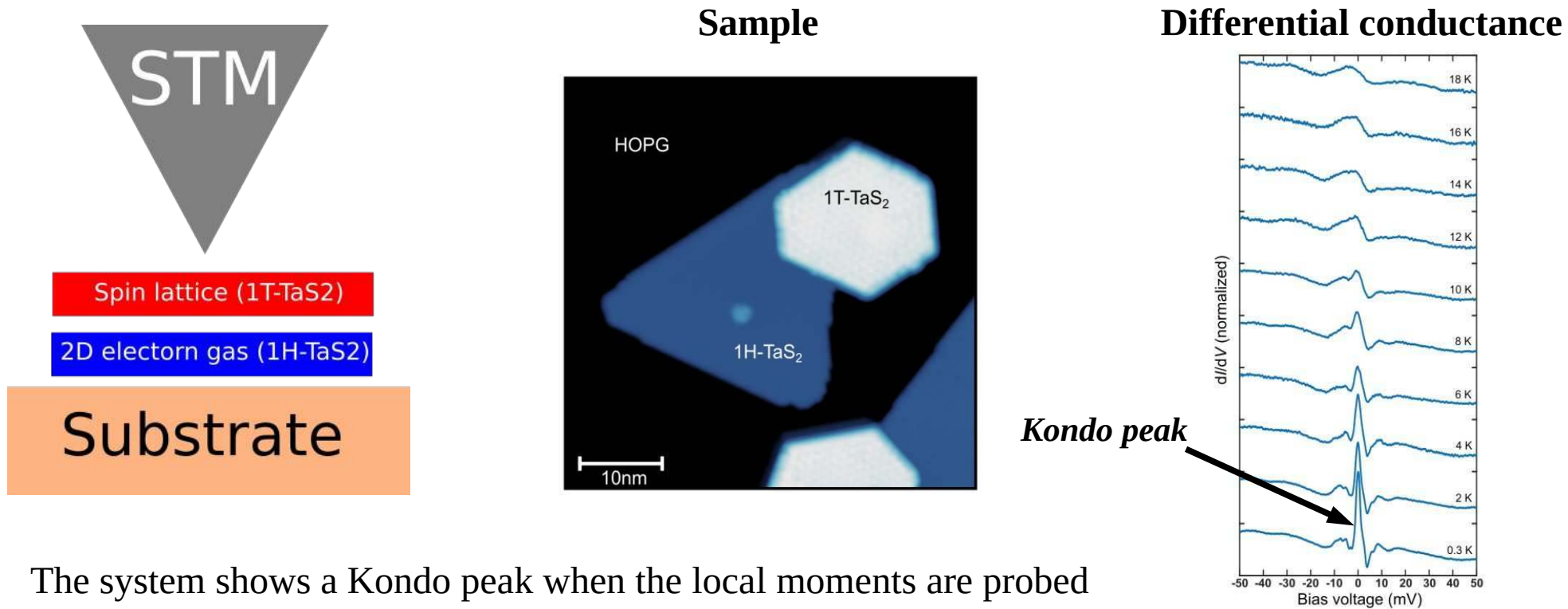
Probing the Kondo peak



Probing the heavy-fermion gap

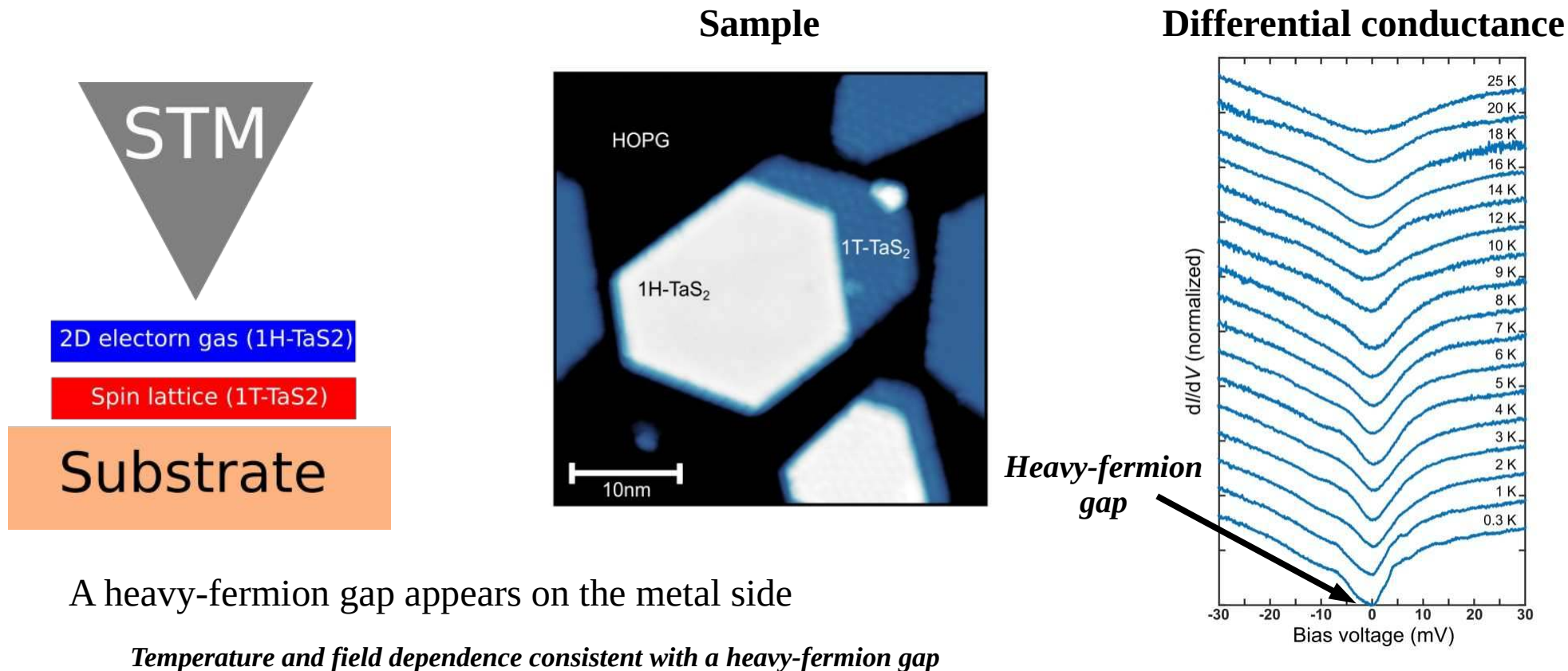


Kondo physics in the magnetic lattice

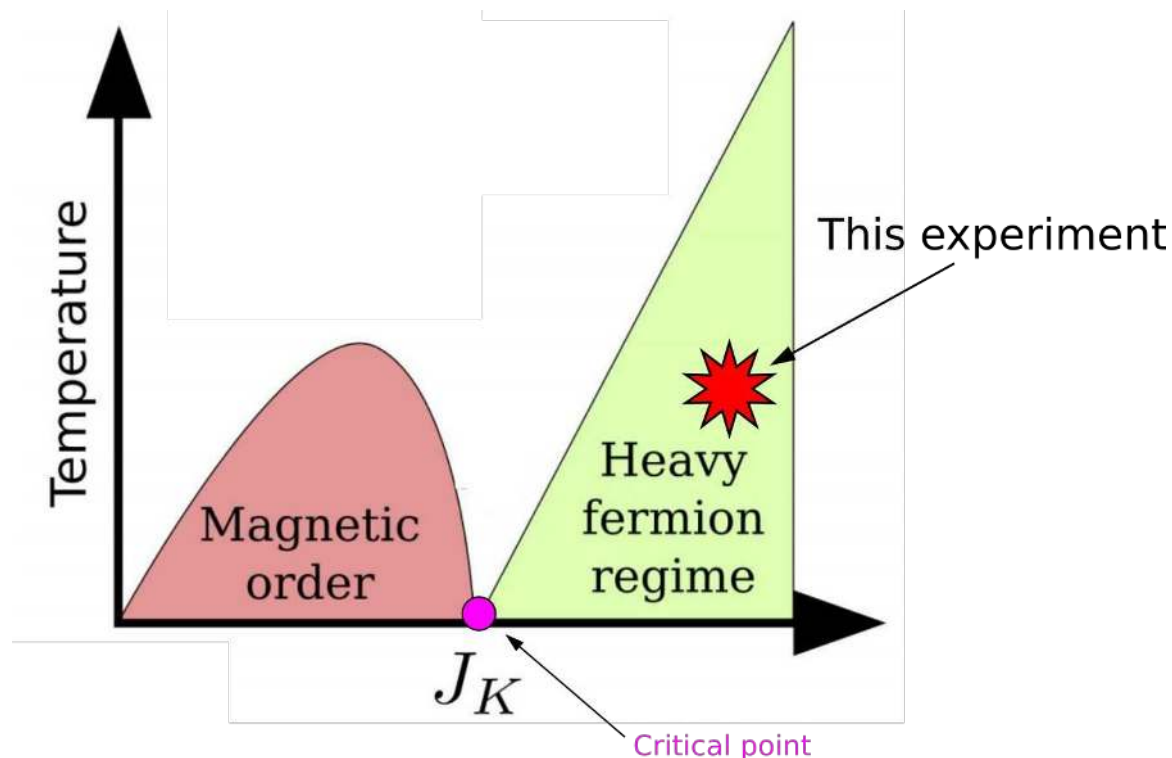


Temperature and field dependence consistent with Kondo

Heavy-fermion gap in the 2D electron gas



Next steps in van der Waals heavy-fermions

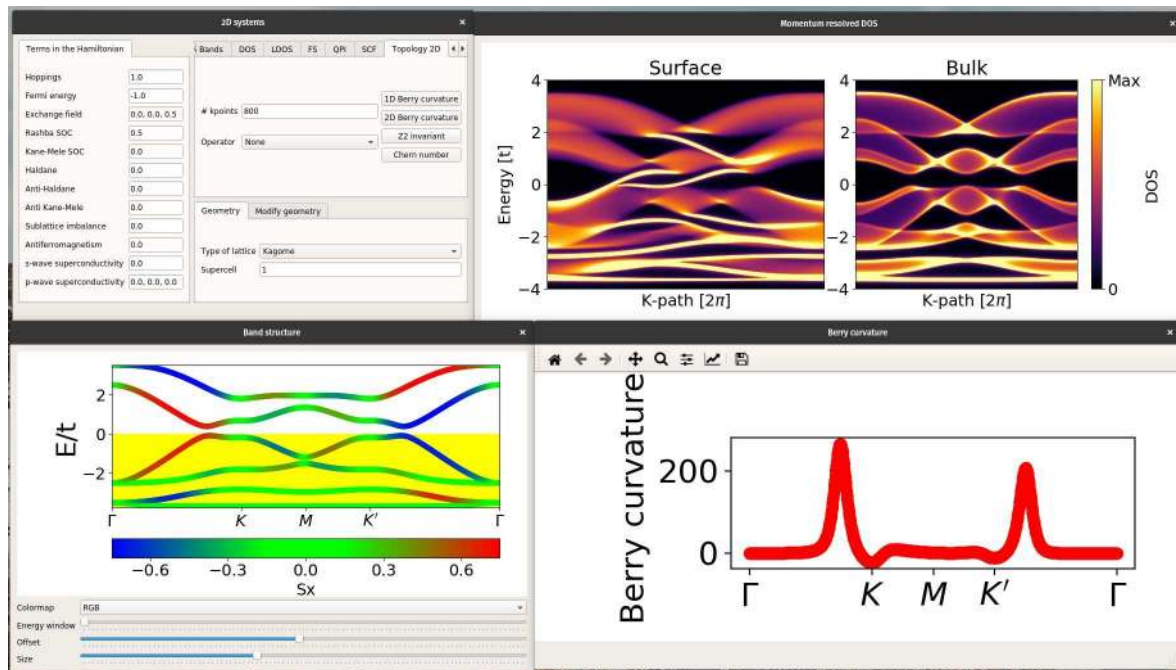
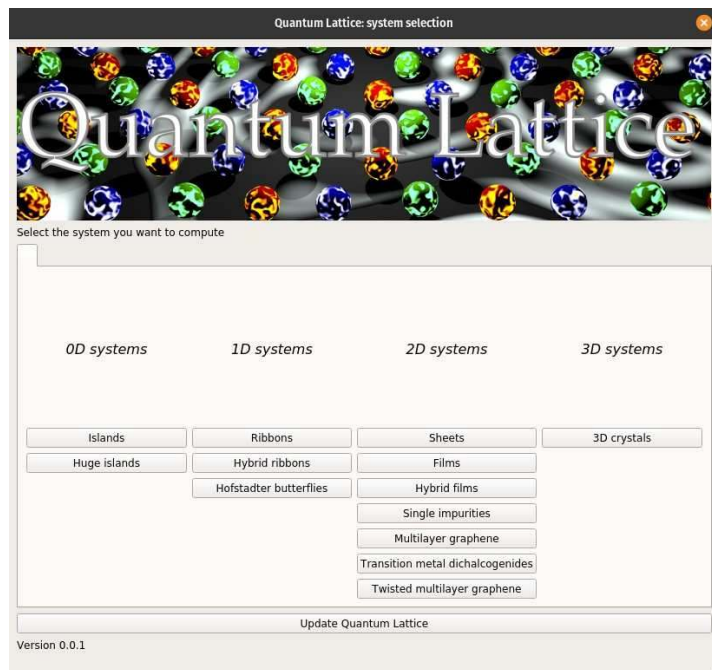


Can we push this system to the critical and ultimately topological superconducting regimes?

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

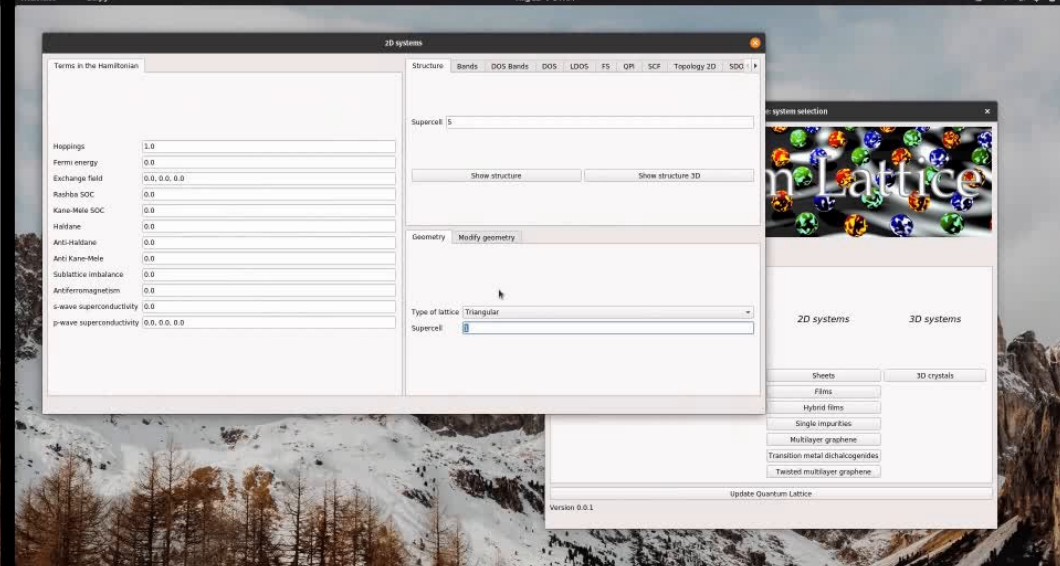
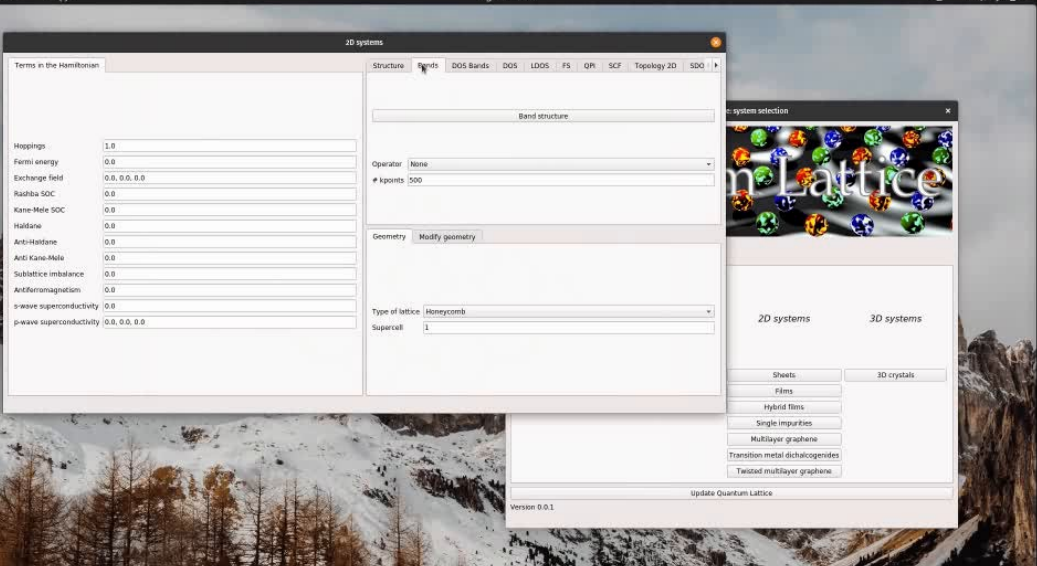
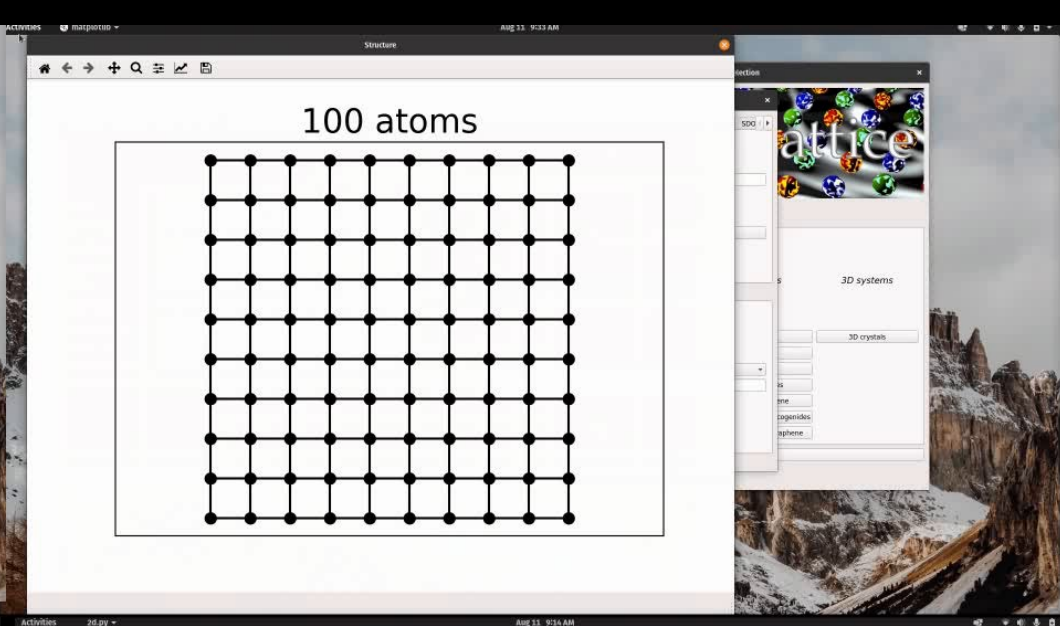
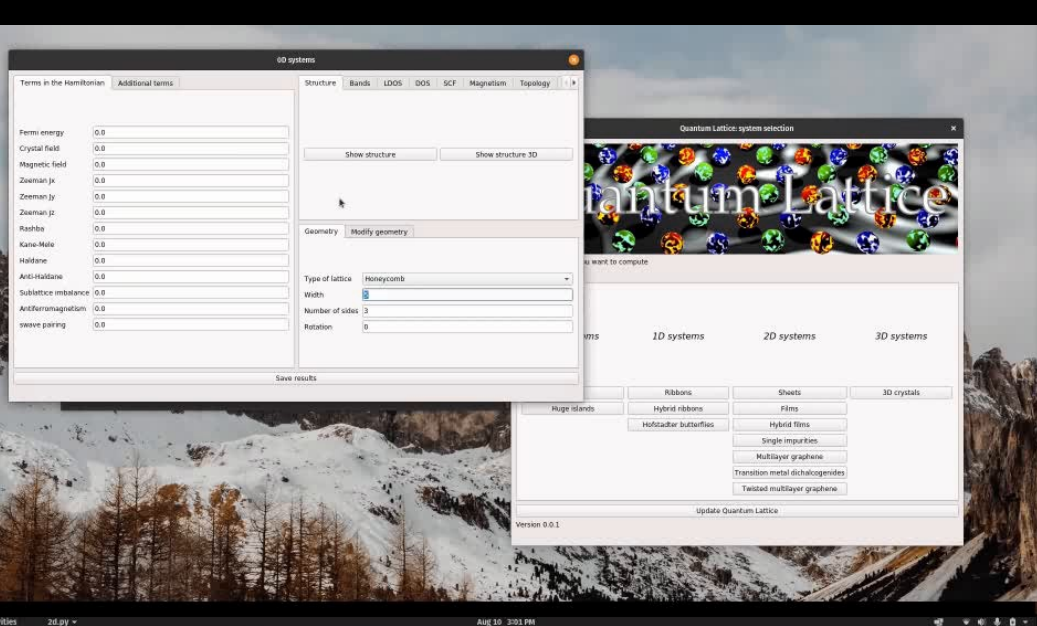
Computing electronic
properties

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>



Hamiltonian

Interlayer

Electric bias

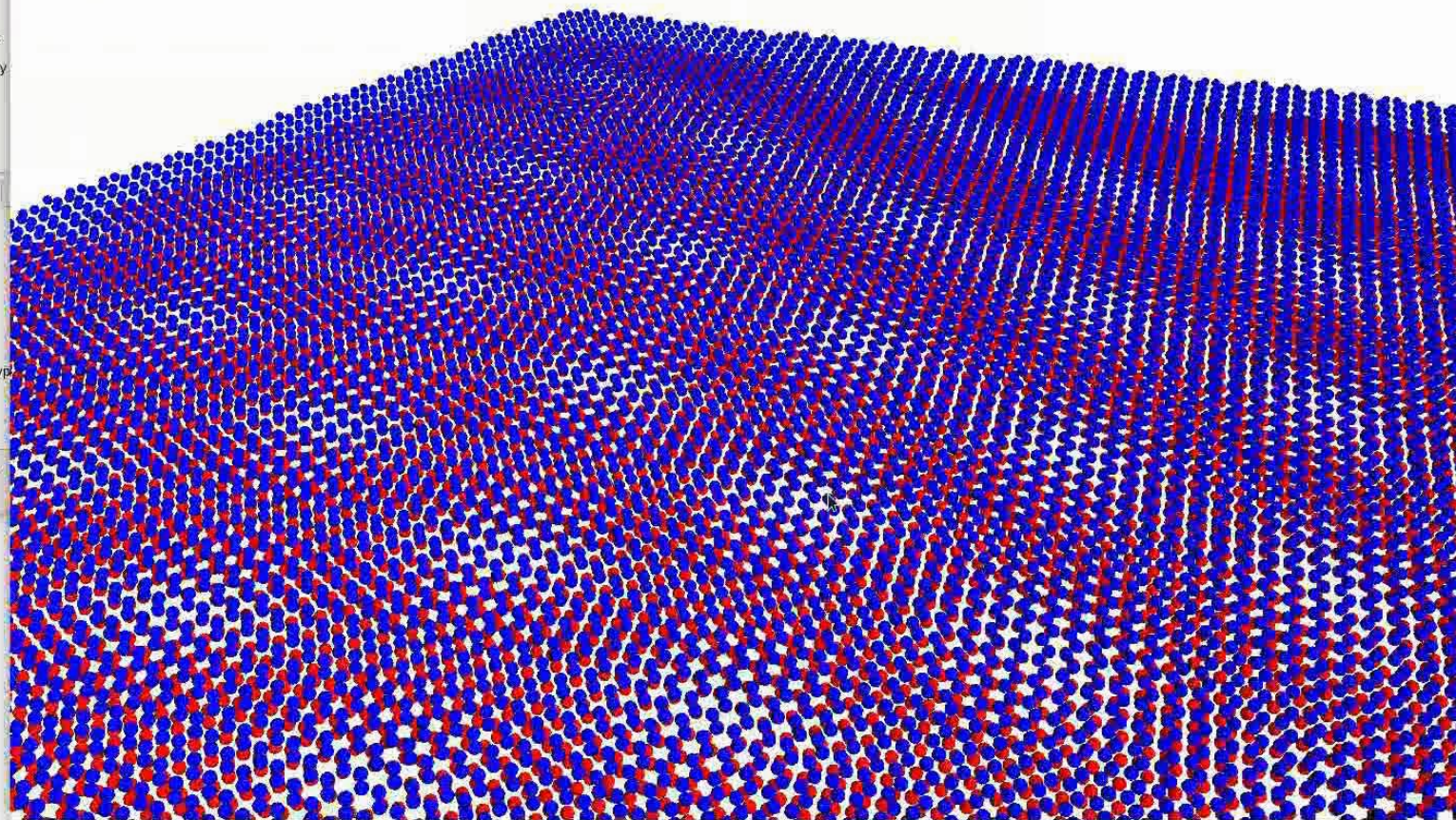
Fermi energy

Geometry

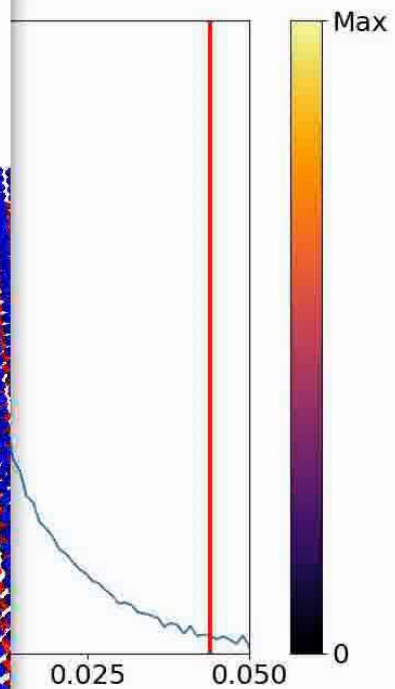
Cell size

Multilayer type

Parallelization

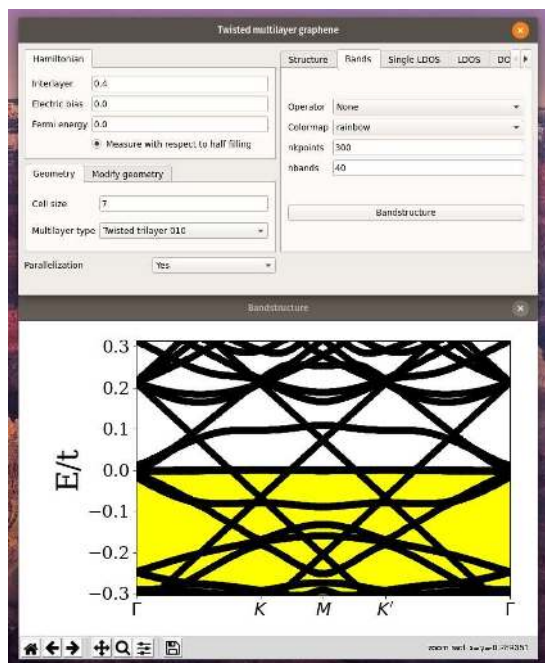


IPR

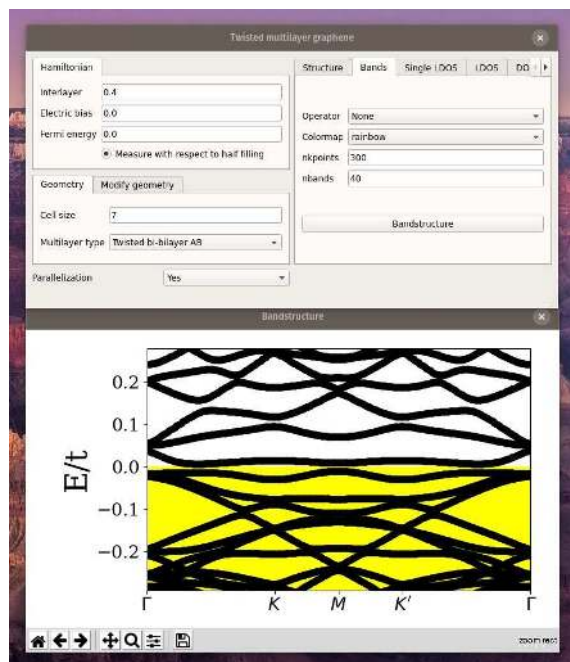


Twisted multilayers

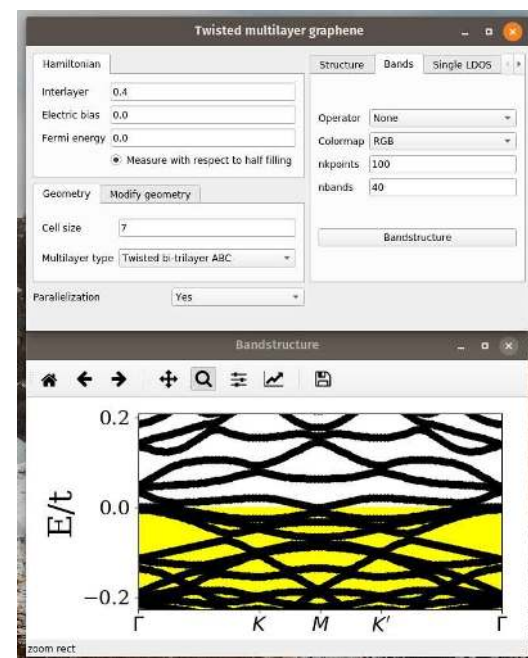
Twisted trilayer graphene



Twisted bi-bilayer graphene

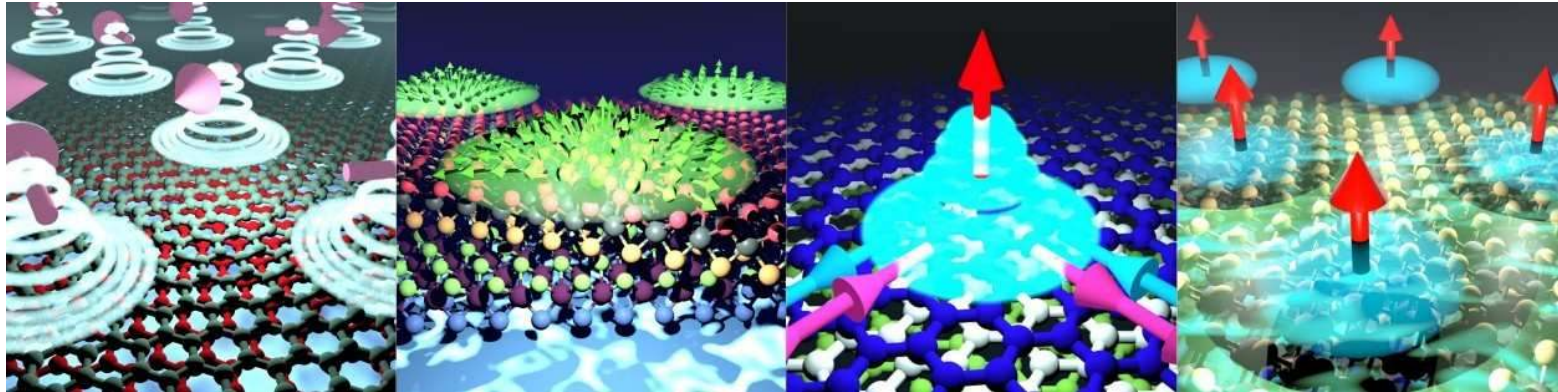


Twisted bi-trilayer graphene



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!

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

Funding from

