Engineering artificial heavy-fermion quantum matter in twisted van der Waals materials

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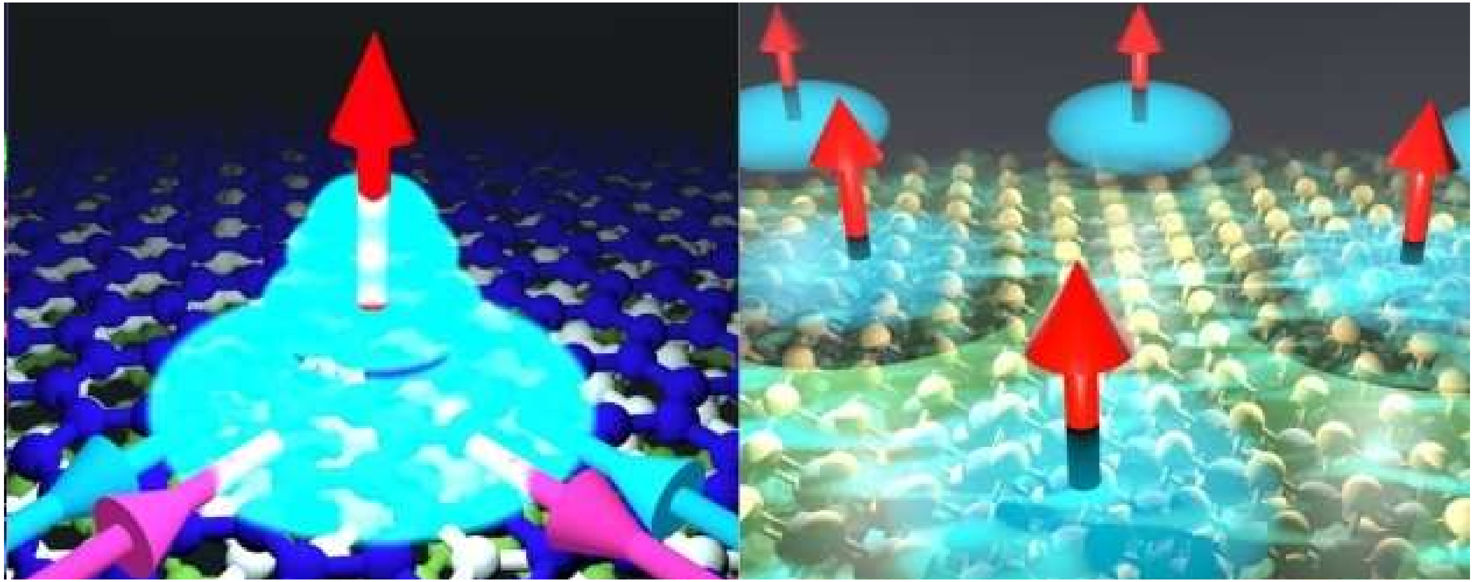
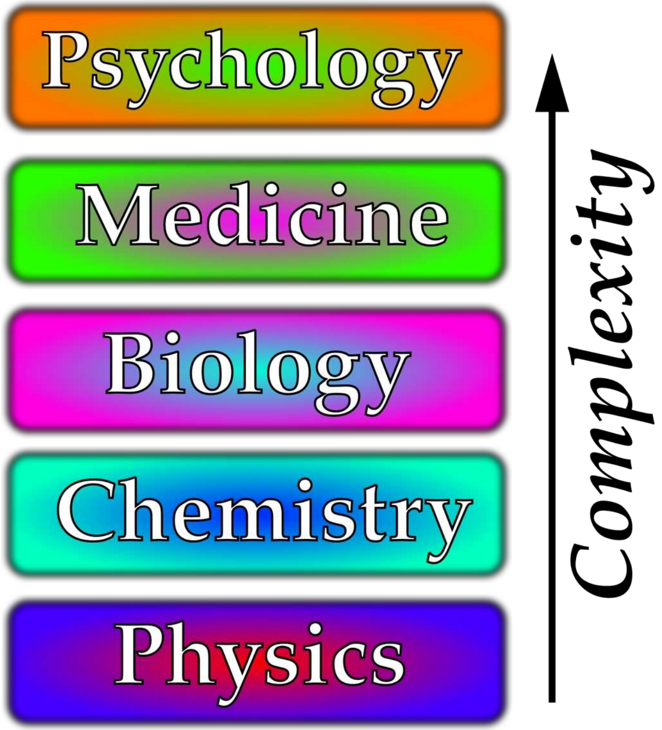


Phys. Rev. Lett. 127, 026401 (2021)

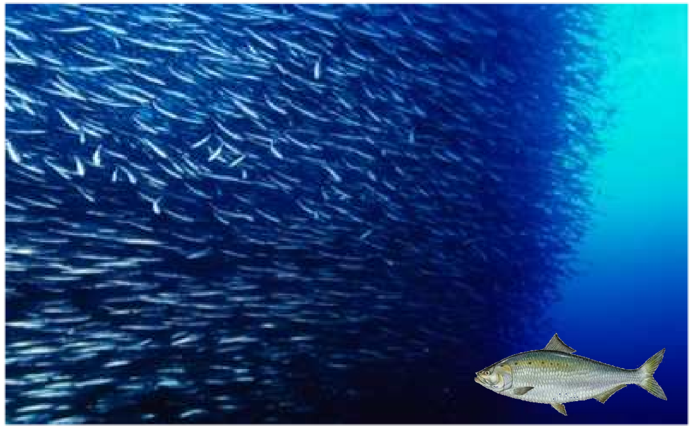
Nature 599, 582–586 (2021)

Correlations in Topological Quantum Matter, Lammi, Finland
September 7th 2022

Complexity, universality and emergence

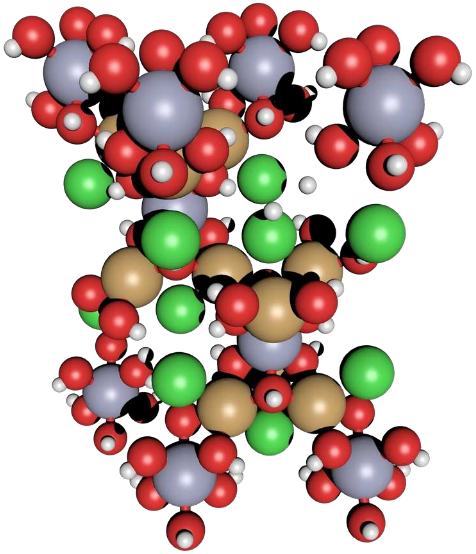


Fish schools



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

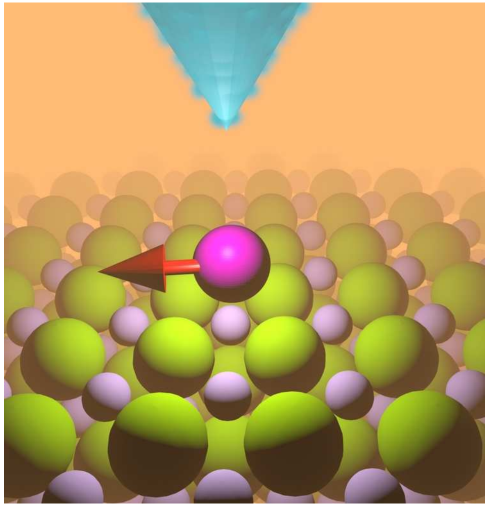
<u>Topological quantum computing</u>

<u>Low consumption electronics</u>

<u>New physics not yet realized in nature (fractional quantum particles)</u>

Building quantum matter with artificial lattices

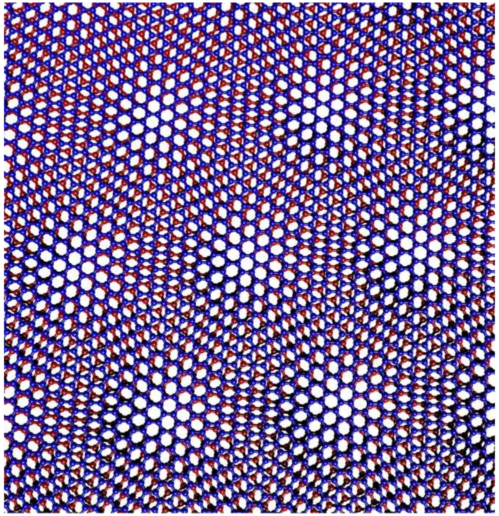
Atomic lattices



a = 0.5 nm

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

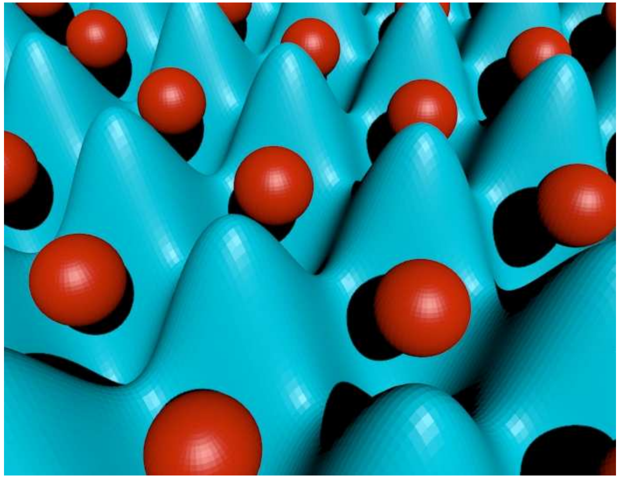
Twisted 2D moire materials



a = 30 nm

Phys. Rev. Lett. 99, 256802 (2007)
Nature Physics 6, 109–113 (2010)
PNAS 108 (30) 12233-12237 (2011)
Nature 556, 80–84 (2018)

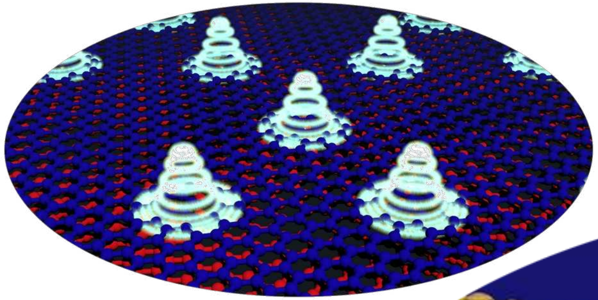
Cold atoms

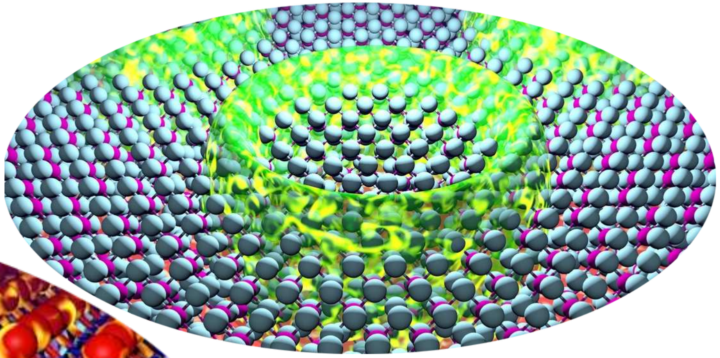


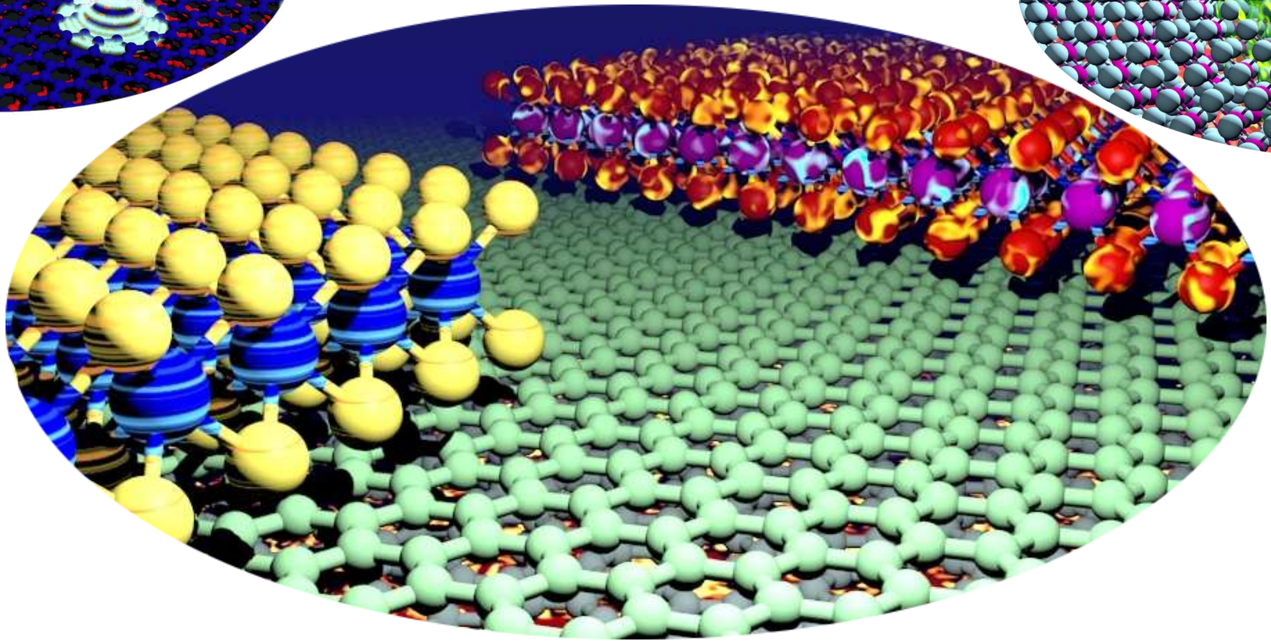
a = 1000 nm

Nature 545, 462–466 (2017)
Nature 455, 204–207 (2008)
Phys. Rev. Lett. 111, 185307 (2013)

A new universe in each van der Waals heterostructure





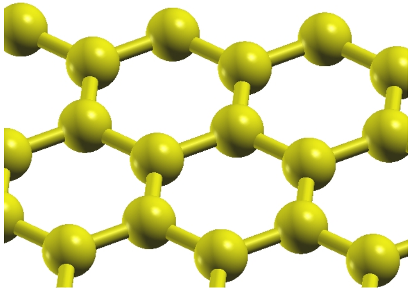


Each van der Waals heterostructure allows creating a whole new universe for electron

The two-dimensional materials world

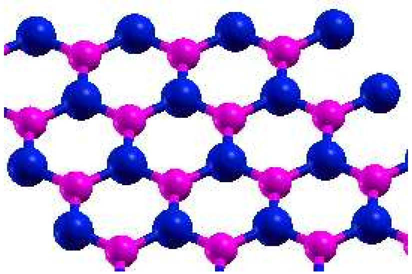
Semimetal

Graphene



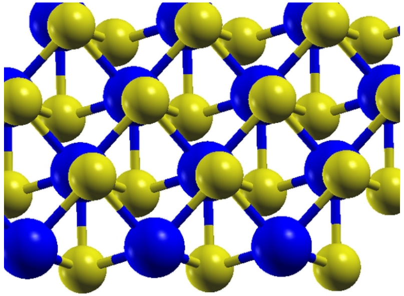
Insulator

BN



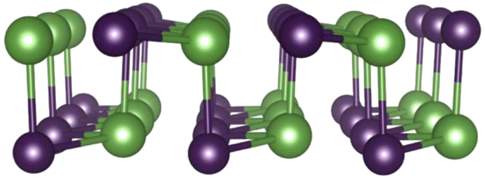
Superconductor

$NbSe_2$



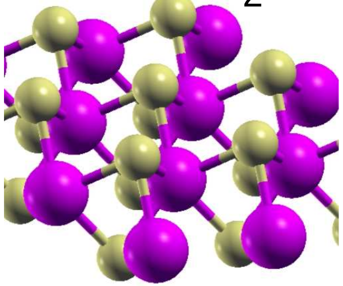
Ferroelectric

SnTe



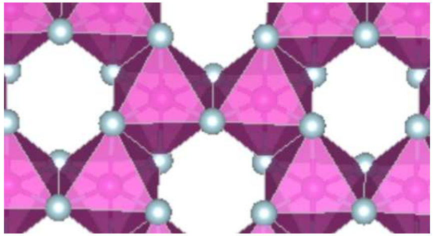
Semiconductor

WSe_2



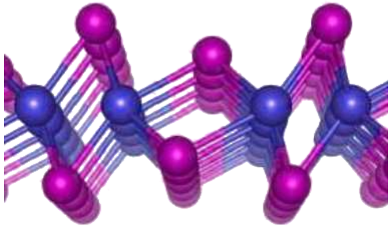
Ferromagnet

CrI_3



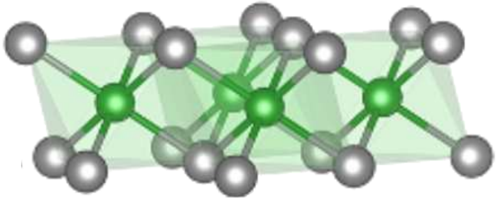
Quantum spin Hall insulator

WTe_2



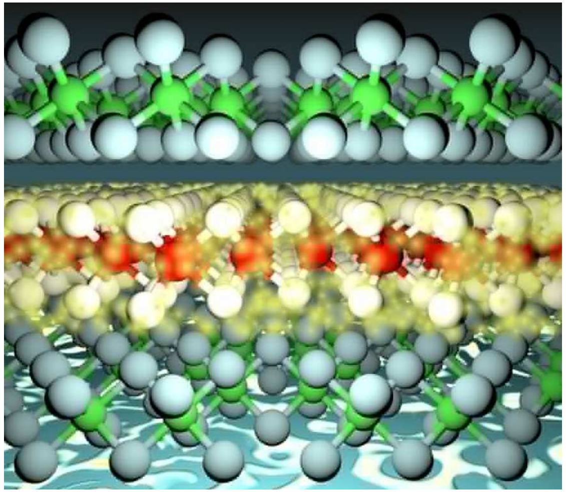
Multiferroic

NiI_2



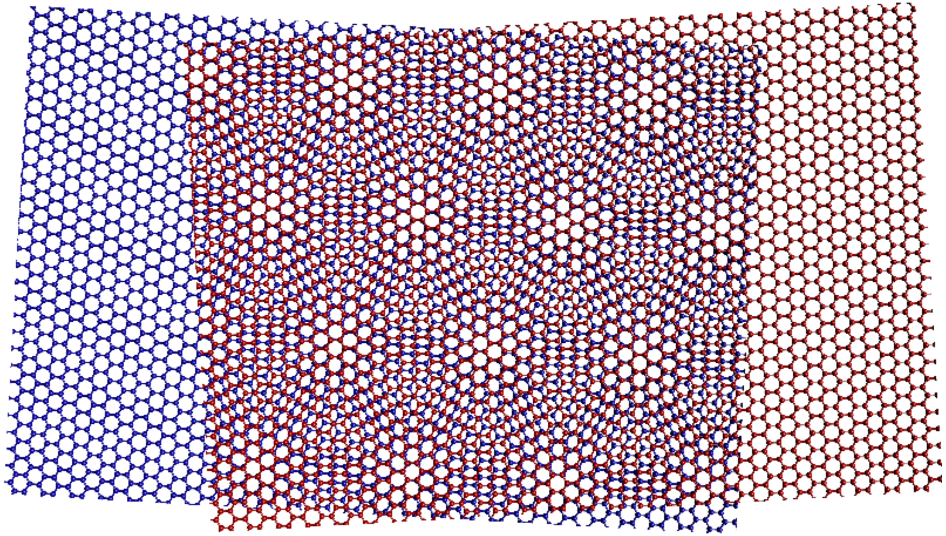
The flexibility of two-dimensional materials

They can be stacked



Nature 499.7459 419. (2013)

They can be rotated

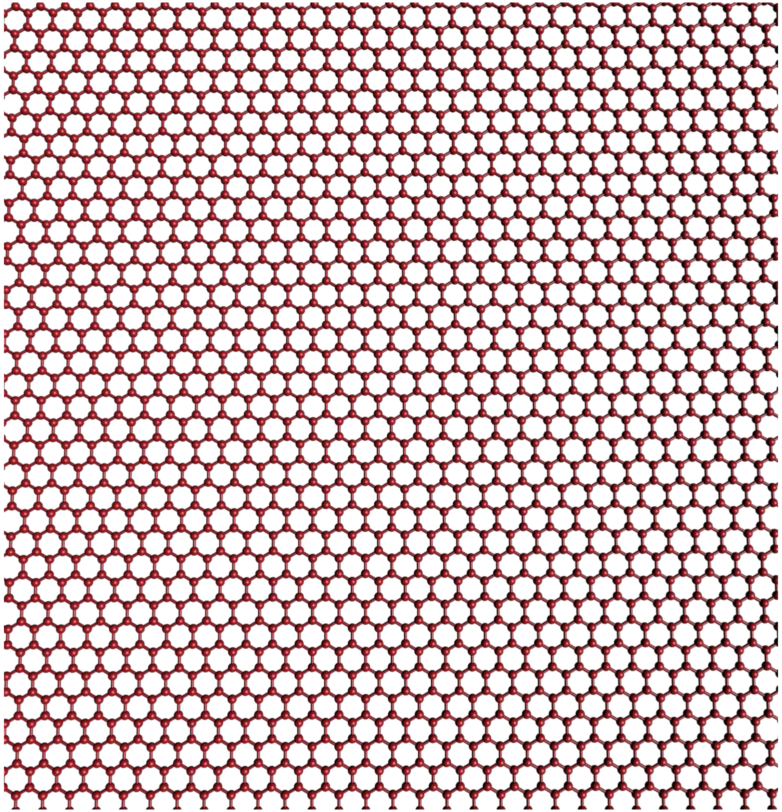


Science 361.6403 690-693. (2018)

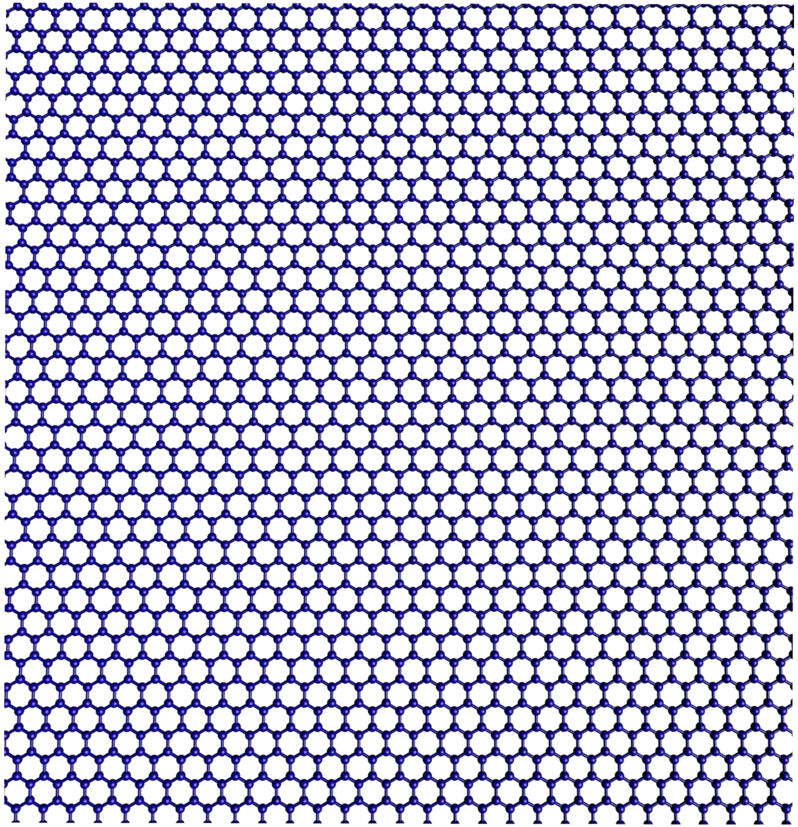
These are unique features of two-dimensional materials

Moire in twisted bilayer graphene

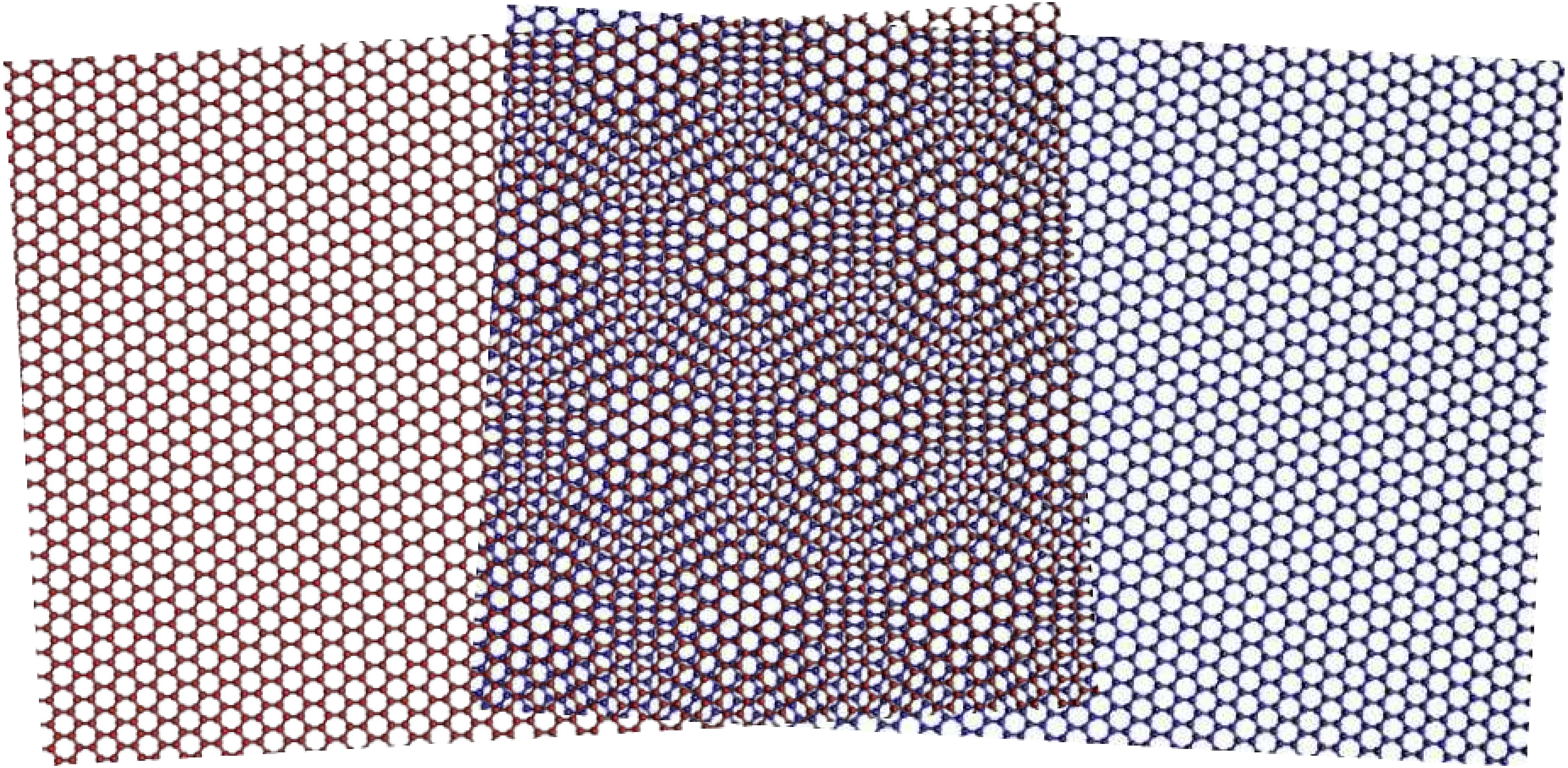
Upper graphene layer



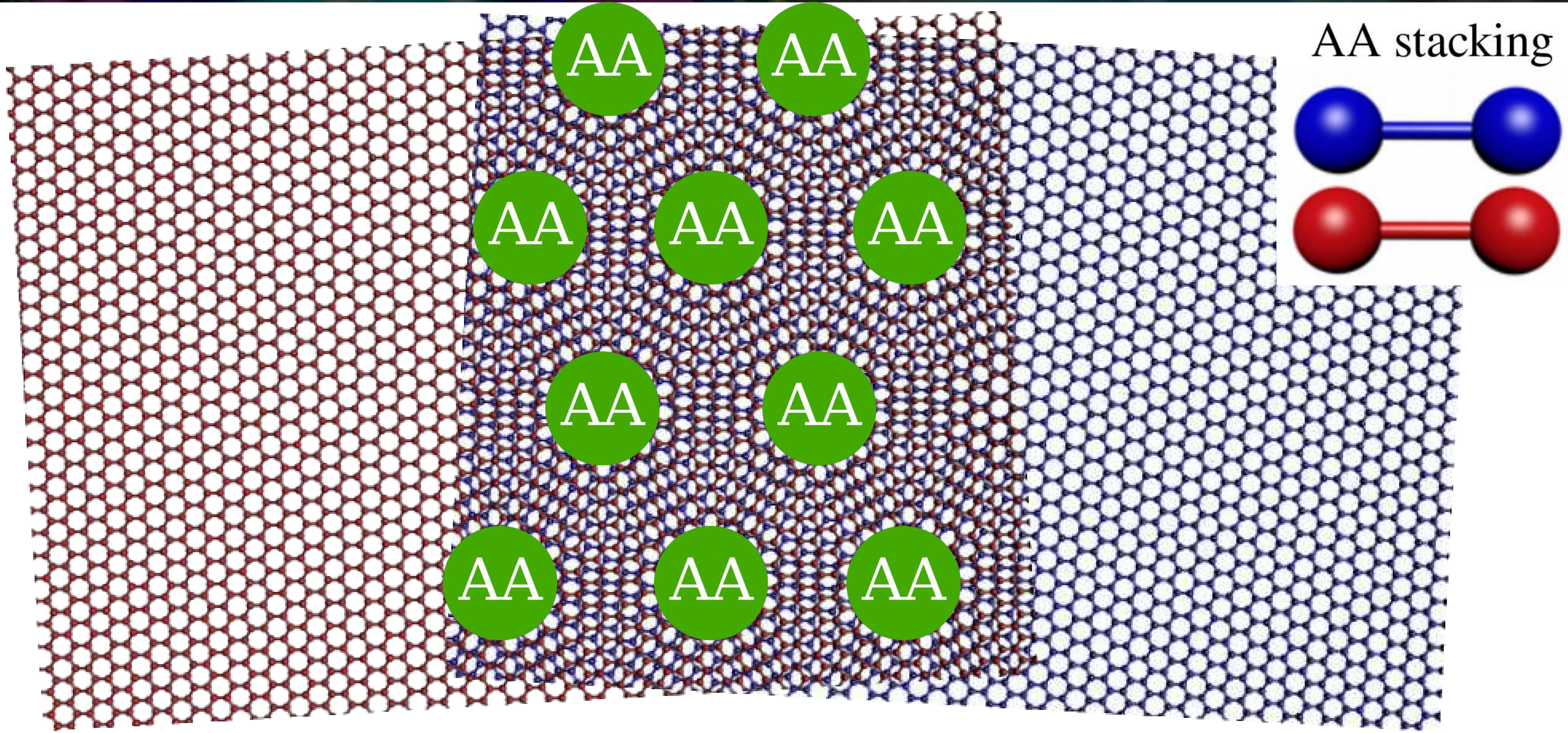
Lower graphene layer



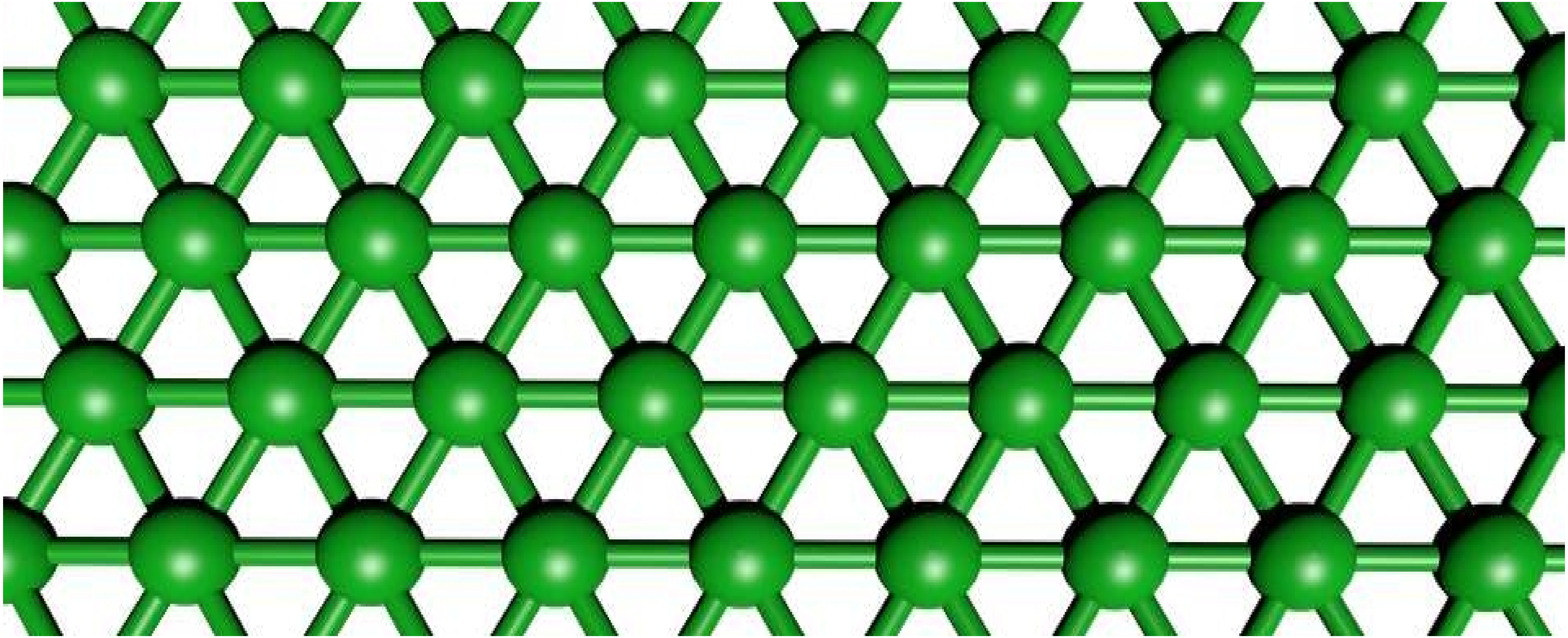
Moire in twisted bilayer graphene



Moire in twisted bilayer graphene

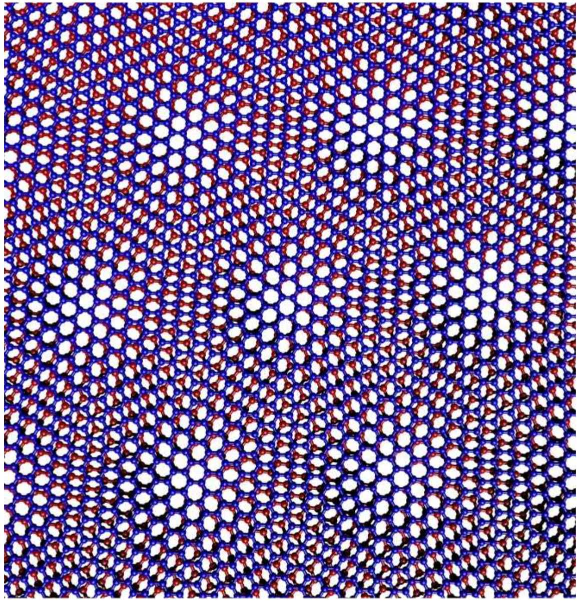


Moire in twisted bilayer graphene

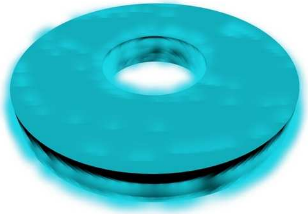


One material, a zoo of electronic phases

Twisted bilayer graphene

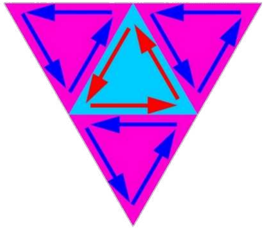


Superconductivity



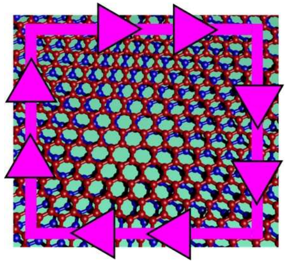
Nature 556, 43–50 (2018)

Topological networks



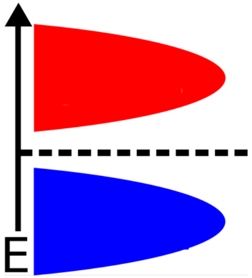
Nano Lett. 18, 11, 6725-6730 (2018)

Chern insulators



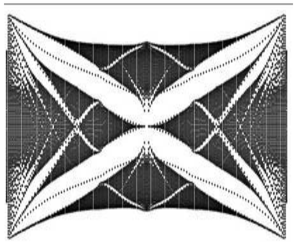
Science 365, 605-608 (2019)

Correlated insulators



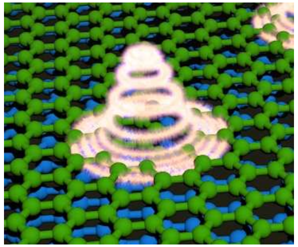
Nature 556, 80–84 (2018)

Quasicrystalline physics



Science 361, 782-786 (2018)

Fractional Chern insulators



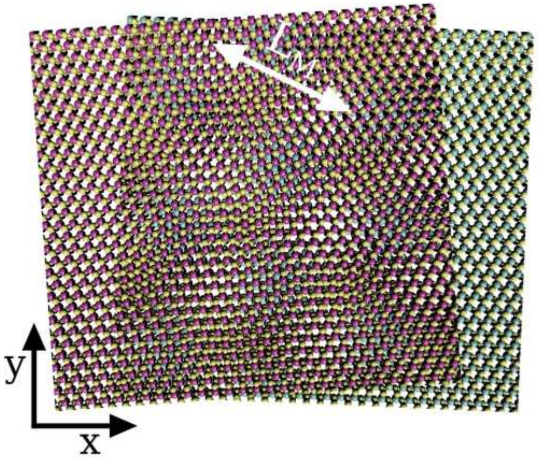
Nature 600, 439–443 (2021)

A bilayer of a van der Waals material realizes a variety of widely different electronic states

The generality of correlated physics in twisted 2D materials

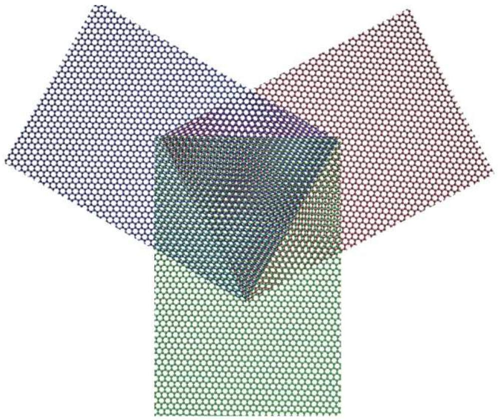
Superconductivity & correlated behavior found also in

Twisted dichalcogenides



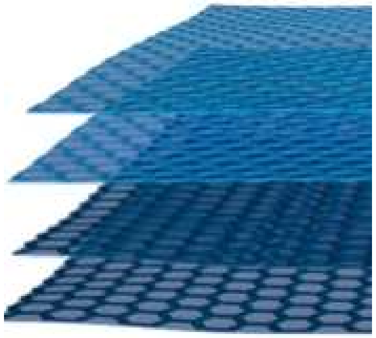
Nature 579, 359–363 (2020)

Twisted graphene trilayers



Nature 590, 249–255 (2021)

Twisted graphene tetralayers



Nature 583, 221–225 (2020)

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

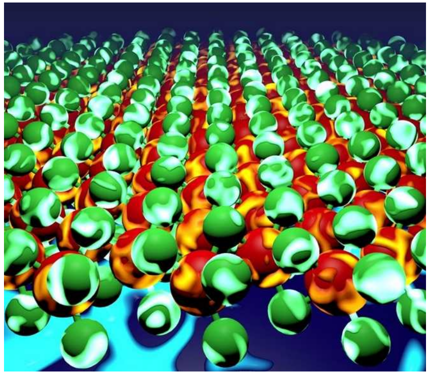
Controlling electronic states in van der Waals materials

Of course, we can use the typical knobs of bulk compounds

(pressure, chemical doping, etc)

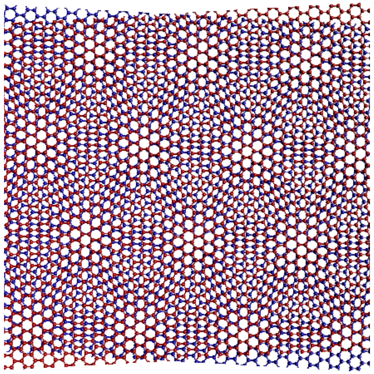
Most importantly, we can exploit the full tunability of van der Waals materials

Gating



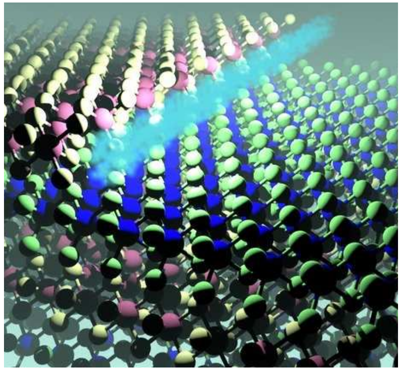
Science 306, 5696, 666-669 (2004)

Twist engineering



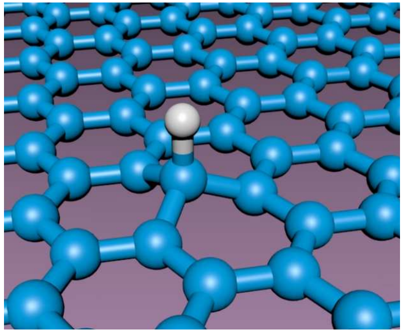
Nat, Rev, Mat, 6, 201–206 (2021)

Materials engineering



Nature 499, 419–425 (2013)

Atomic engineering

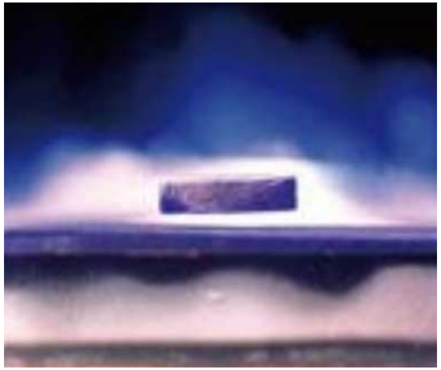


Science, 352(6284), 437-441 (2016)

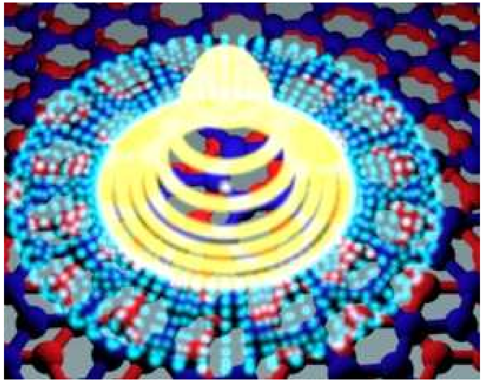
Allowing to independently control different features of the electronic structure

The opportunities of twisted van der Waals materials

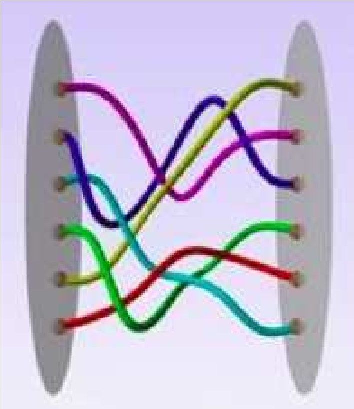
“Unveil” the nature of high T_C superconductivity (?)



Controllable exotic quantum matter (?)



A platform for topological quantum computing (?)



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

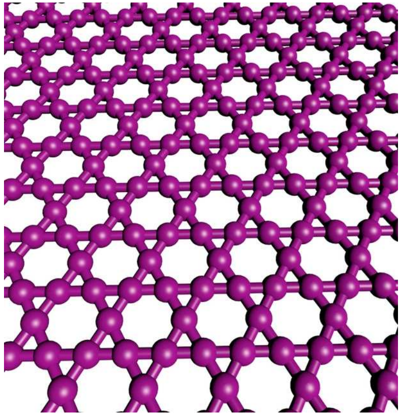
→ ***Control of single particle and many-body interactions***
→ ***Explore physics that only appear in rare or toxic compounds***

Designing quantum matter in twisted materials

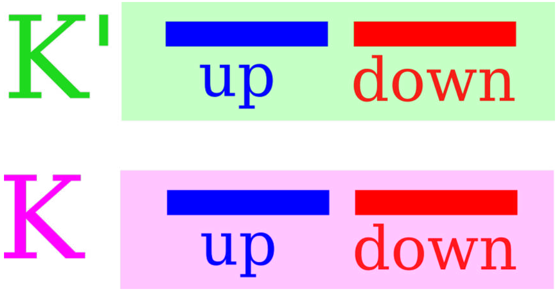
The strength of electronic correlations

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

The details of the electronic dispersion



The local quantum degrees of freedom



Twist angle control

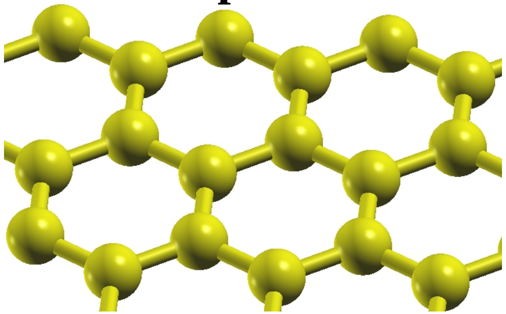
Interlayer bias

Magnetic 2D materials

Goal: engineer local quantum degrees of freedom via 2d magnetism

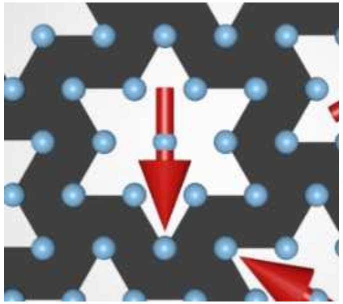
Designing heavy-fermion quantum matter with twisted magnetic van der Waals materials

Graphene



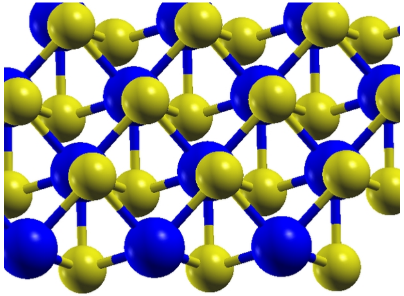
Magnet

$1T\text{-}TaS_2$



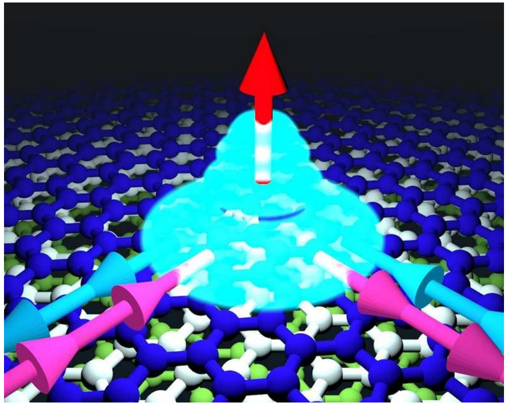
Metal

$1H\text{-}TaS_2$



Behind the scenes

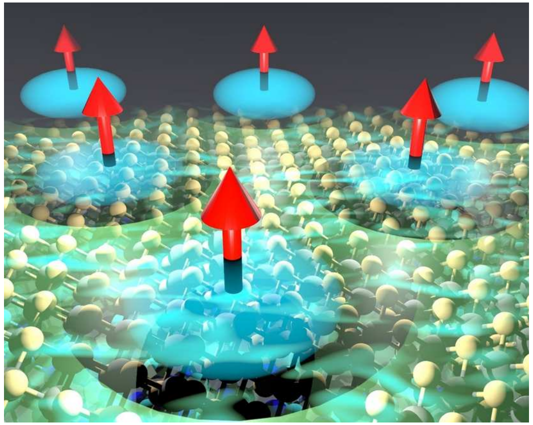
Heavy fermions in twisted graphene trilayers



Aline Ramires

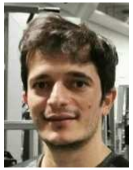
Phys. Rev. Lett. 127, 026401 (2021)

Heavy fermions in twisted dichalcogenide bilayers

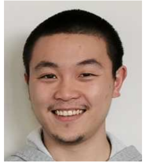


S. Ganguli

M. Amini



G. Chen



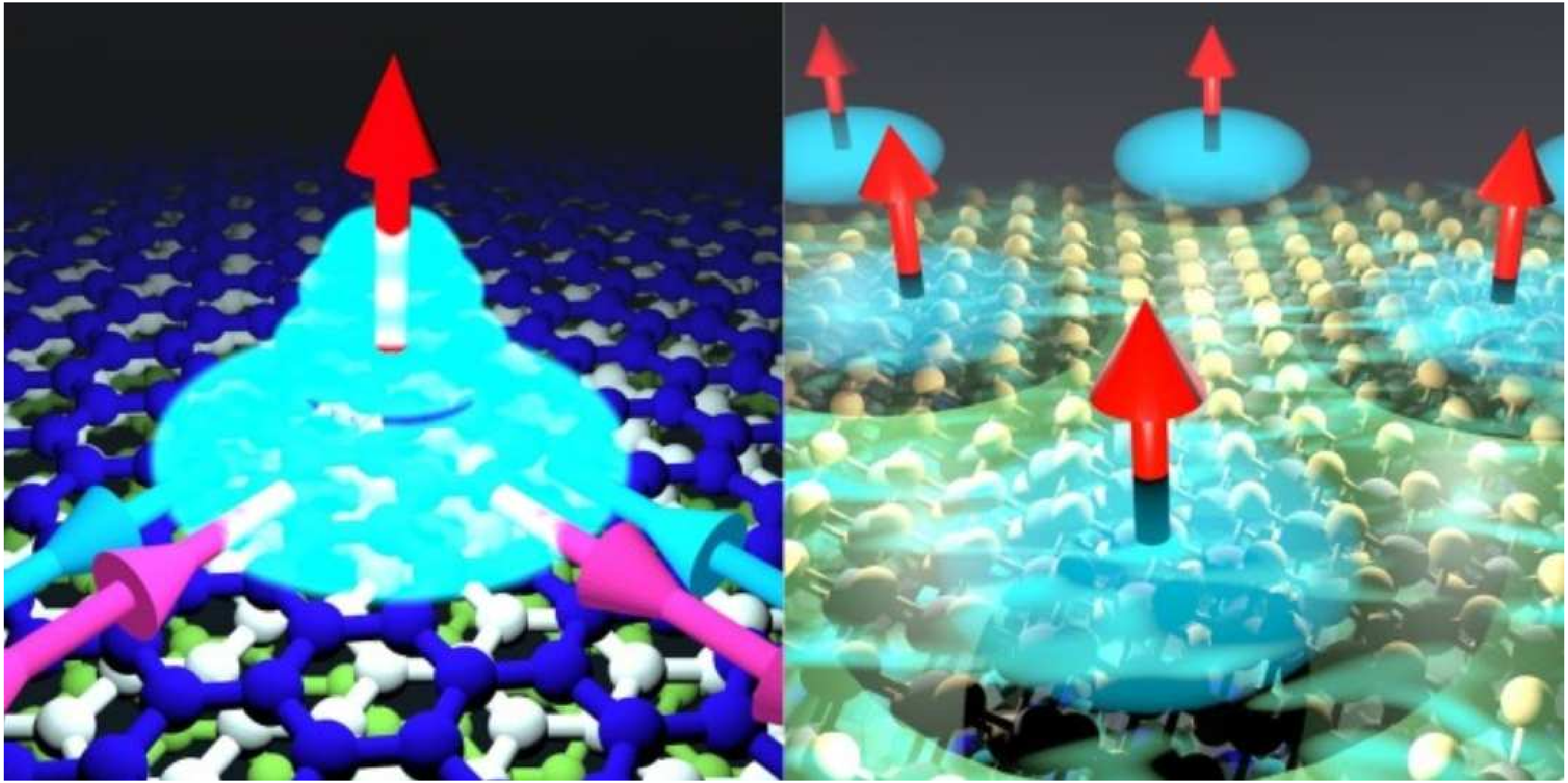
V. Vaňo

S. Kezilebieke

P. Liljeroth

Nature 599, 582–586 (2021)

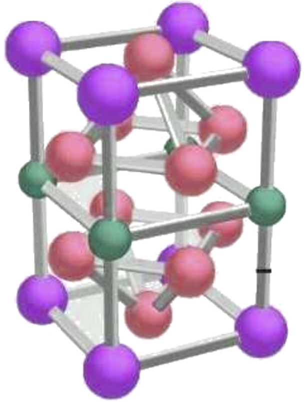
Heavy fermions in van der Waals materials



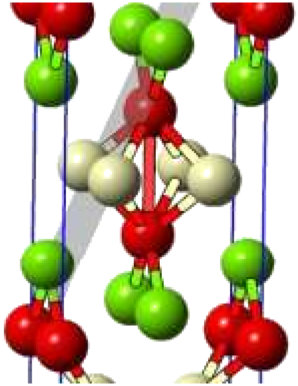
Searching for new heavy fermion compounds

We have a rich family of bulk heavy-fermion compounds

$CeCoIn_5$
Science 375, 6576, 76-81 (2021)



UTe_2
Nature 579, 523–527 (2020)

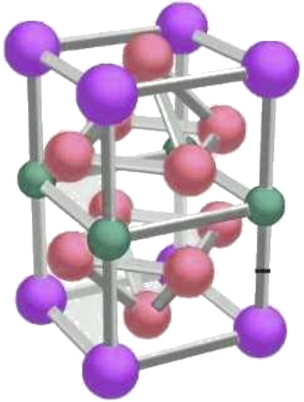


- Strongly correlated matter, dominated by Kondo lattice physics
- Unique system to realize quantum criticality and unconventional superconductivity
- Found in rare-earth compounds, such as UTe_2 or UPt_3

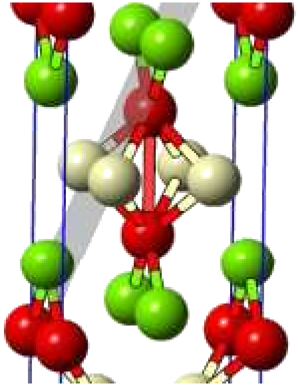
Searching for new heavy fermion compounds

We have a rich family of bulk heavy-fermion compounds

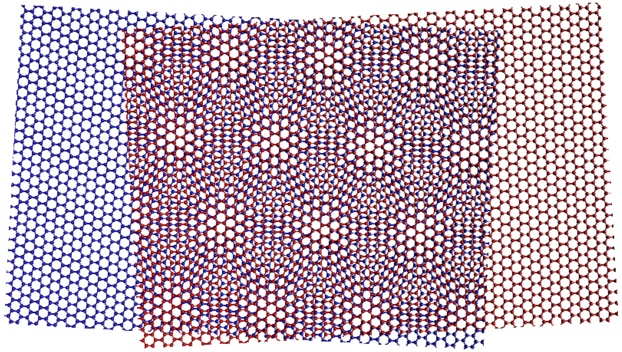
$CeCoIn_5$
Science 375, 6576, 76-81 (2021)

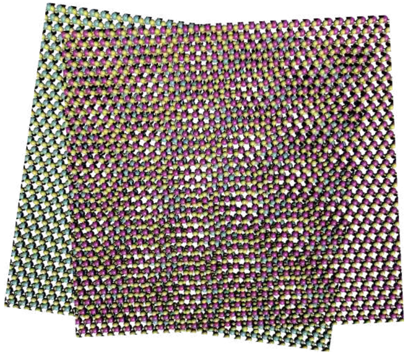


UTe_2
Nature 579, 523–527 (2020)



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

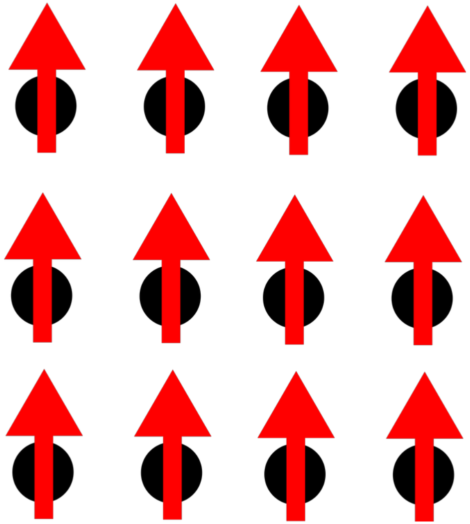




Phys. Rev. Lett. 127, 026401 (2021)
Nature 599, 582–586 (2021)
Phys. Rev. Research 3, 043173 (2021)
arXiv:2110.11962
arXiv:2207.00096

Building an artifcicial heavy fermion state

Lattice of Kondo impurities



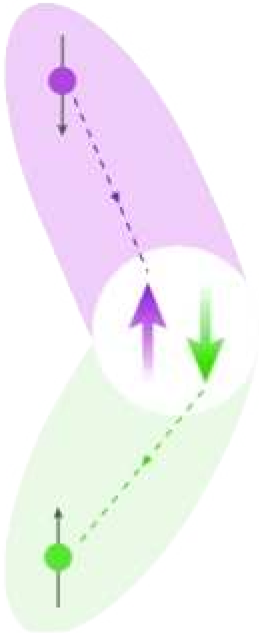
f-electrons in
rare-earth compounds

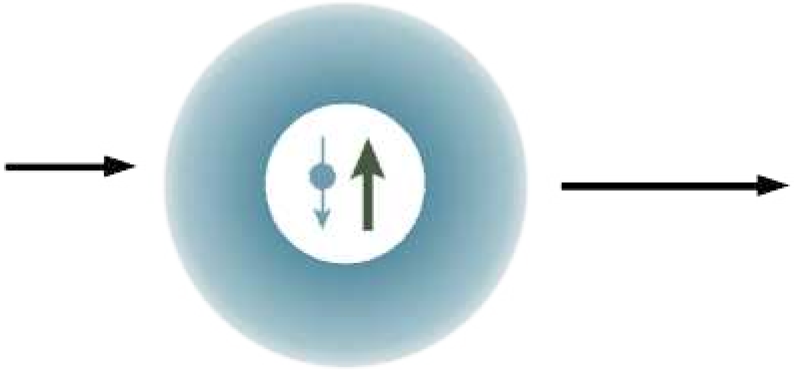
Dispersive electron gas

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

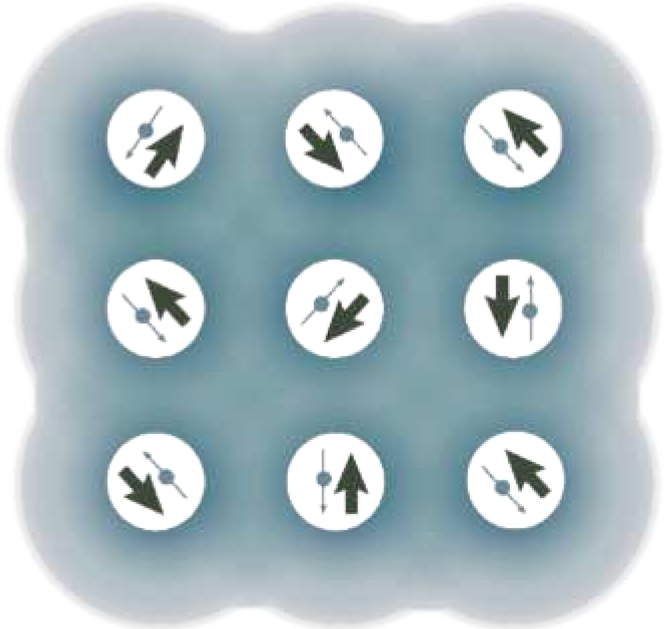
Building an artificial heavy fermion state

Conduction electrons form Kondo singlets with the impurities



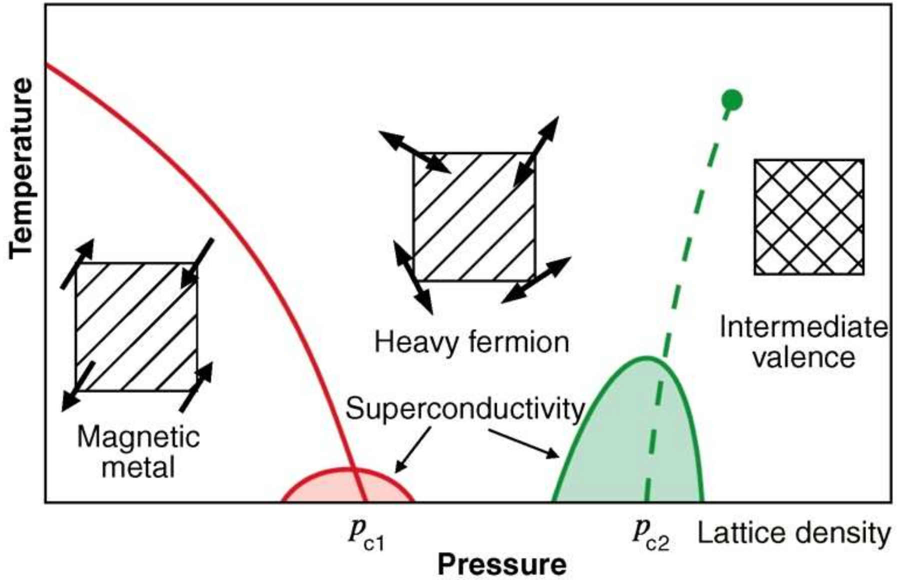


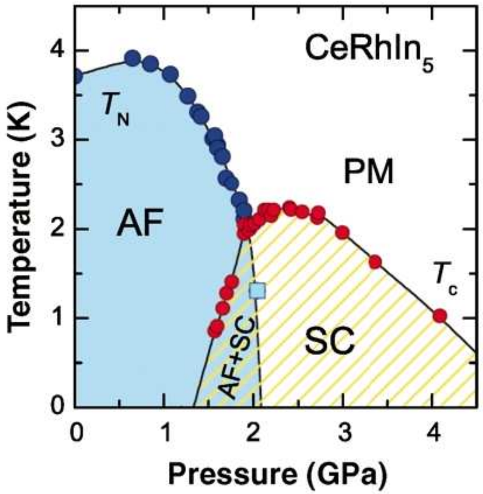
Kondo-lattice model



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

Basics of heavy fermion physics



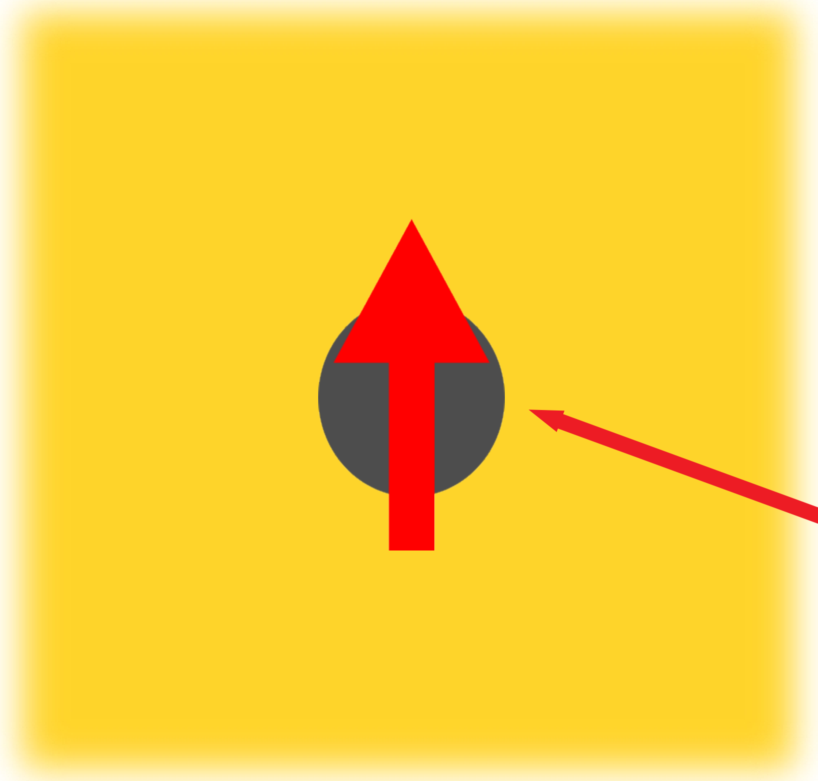


Science 332.6026, 196-200 (2011)

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

The Kondo lattice problem

The Kondo problem



Conduction electrons

$$H = -t \sum_{(i,j)\sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + \text{ H.c} \right)$$

Kondo coupling

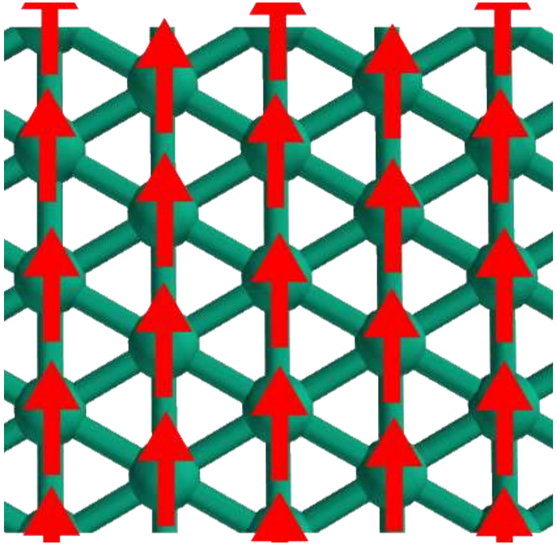
$$H_K = \sum_{\alpha\beta} \left(c^{\dagger}_{0\beta} \vec{\sigma}_{\beta\alpha} c_{0\alpha} \right) \cdot \vec{S}$$

We now take a quantum spin S=1/2

$$|GS\rangle \sim \frac{1}{\sqrt{2}} [| \Uparrow\downarrow\rangle - | \Downarrow\uparrow\rangle]$$

The Kondo lattice problem

Lattice of Kondo impurities



J_K

Dispersive electron gas

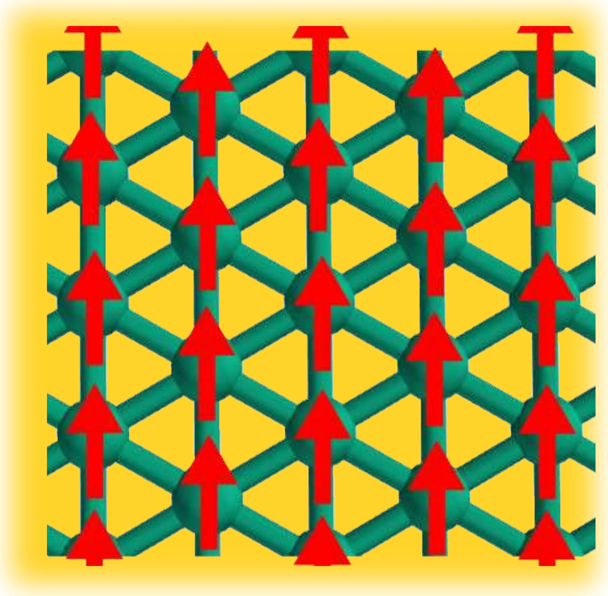
Both ingredients coupled through Kondo coupling

The Kondo lattice problem

The Kondo lattice problem

$$H = -t \sum_{(i,j)\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{ H.c } \right) + J \sum_{j,\alpha\beta} \left(c^\dagger_{j\beta} \vec{\sigma}_{\beta\alpha} c_{j\alpha} \right) \cdot \vec{S}_j$$

Conduction electrons



Kondo coupling

Kondo sites

Solving the Kondo lattice problem

$$H = -t \sum_{(i,j)\sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + \text{ H.c } \right) + J \sum_{j,\alpha\beta} \left(c^{\dagger}_{j\beta} \vec{\sigma}_{\beta\alpha} c_{j\alpha} \right) \cdot \vec{S}_j$$

Replace the spin sites by auxiliary fermions

$$S_{\alpha\beta}(j) \sim f^{\dagger}_{j\alpha} f_{j\beta} - \frac{n_f(j)}{N} \delta_{\alpha\beta}$$

This makes the effective Hamiltonian an "interacting" fermionic Hamiltonian

$$H \sim \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} - J \sum_{j,\alpha\beta} \left(c^{\dagger}_{j\beta} f_{j\beta} \right) \left(f^{\dagger}_{j\alpha} c_{j\alpha} \right)$$

Solving the Kondo lattice problem

Now we decouple the fermions with a mean-field approximation

$$H \sim \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} - J \sum_{j,\alpha\beta} \left(c^\dagger_{j\beta} f_{j\beta} \right) \left(f^\dagger_{j\alpha} c_{j\alpha} \right)$$

Obtaining a quadratic Hamiltonian

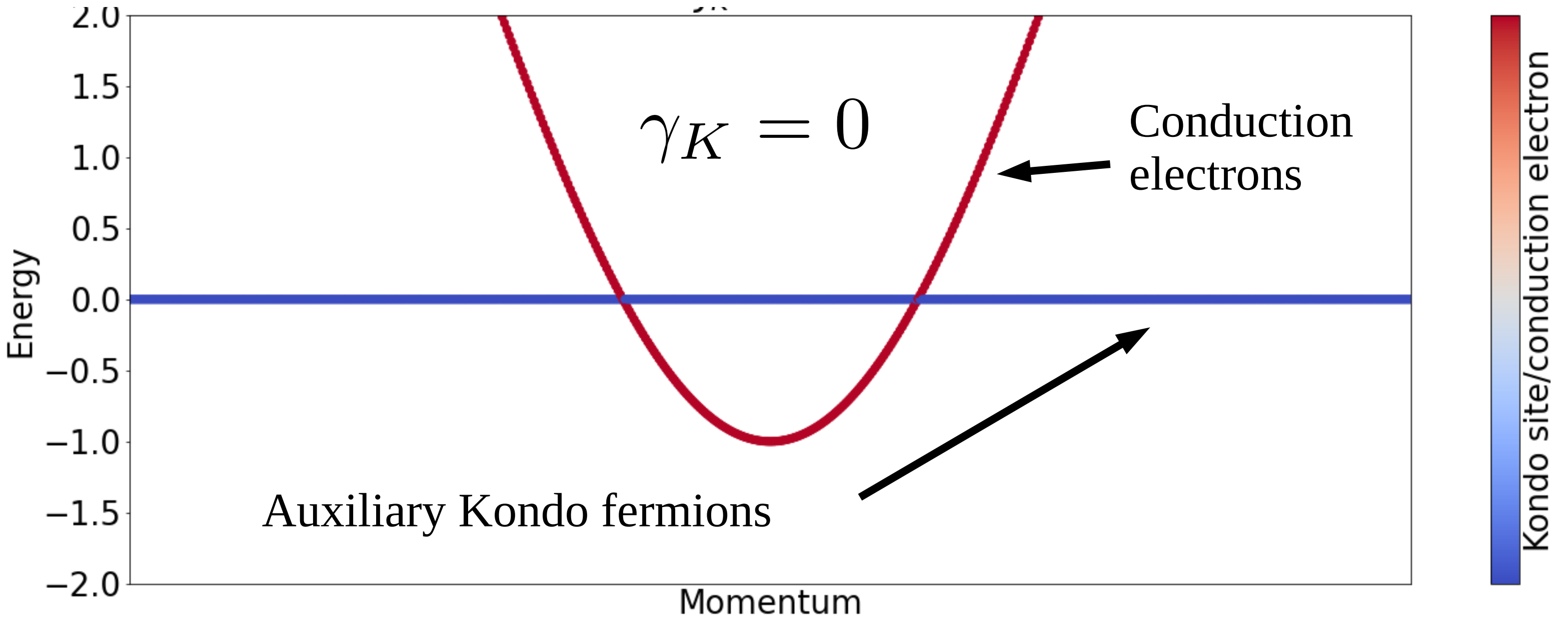
$$H \sim \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} - \gamma_K \sum_{\mathbf{k},\alpha} f^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + h.c.$$

Conduction band dispersion

Kondo hybridization

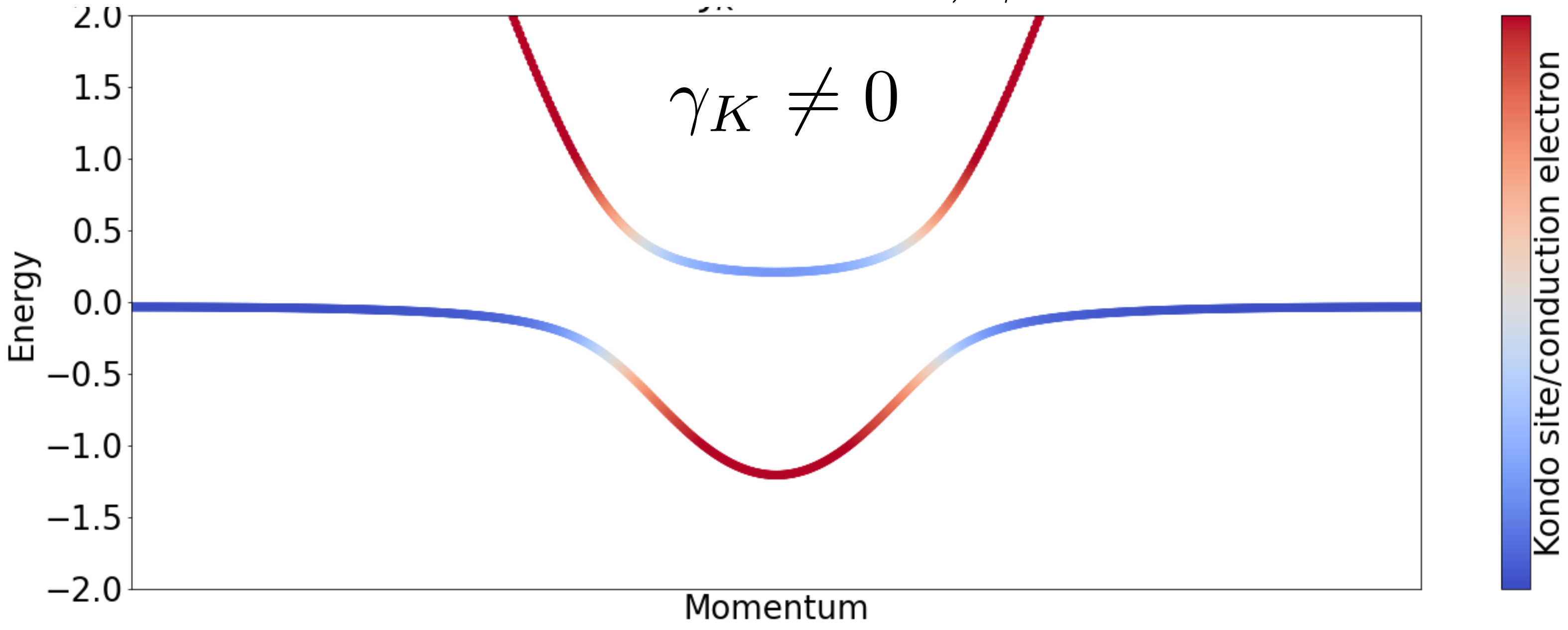
Electronic structure of the Kondo lattice problem

$$H \sim \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} - \gamma_K \sum_{\mathbf{k},\alpha\beta} f^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + h.c.$$



Electronic structure of the Kondo lattice problem

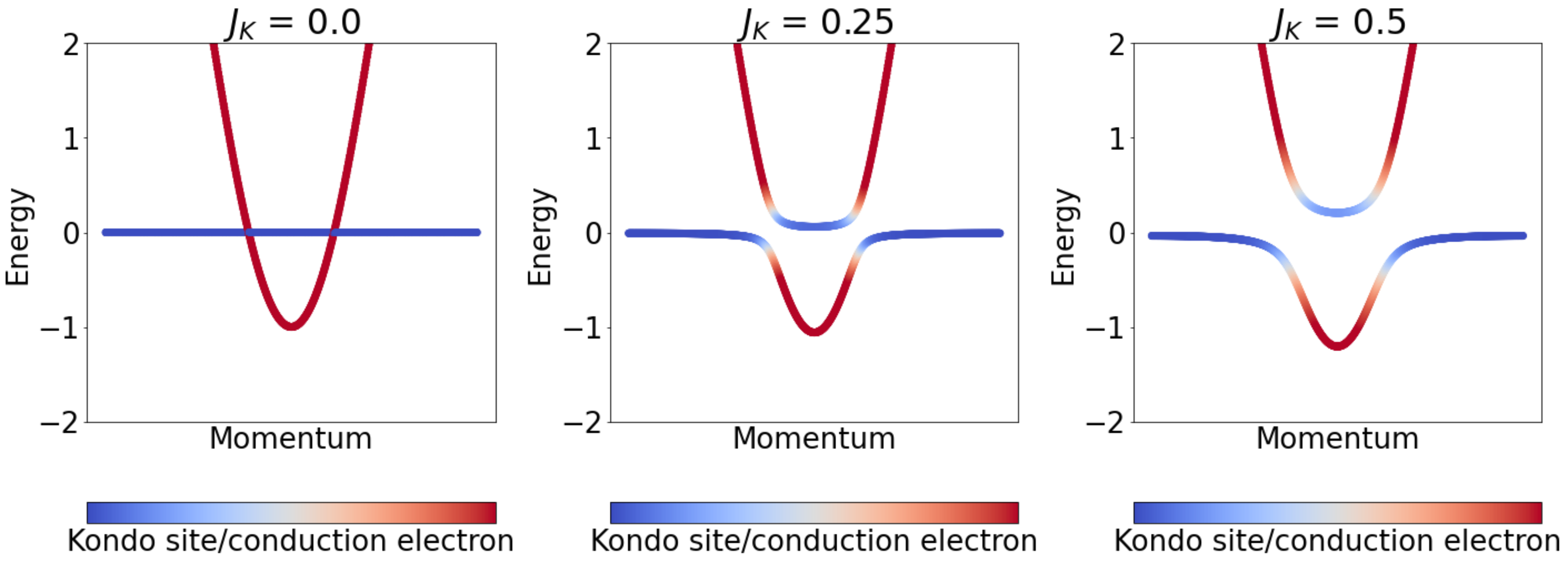
$$H \sim \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} - \gamma_K \sum_{\mathbf{k},\alpha\beta} f^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + h.c.$$



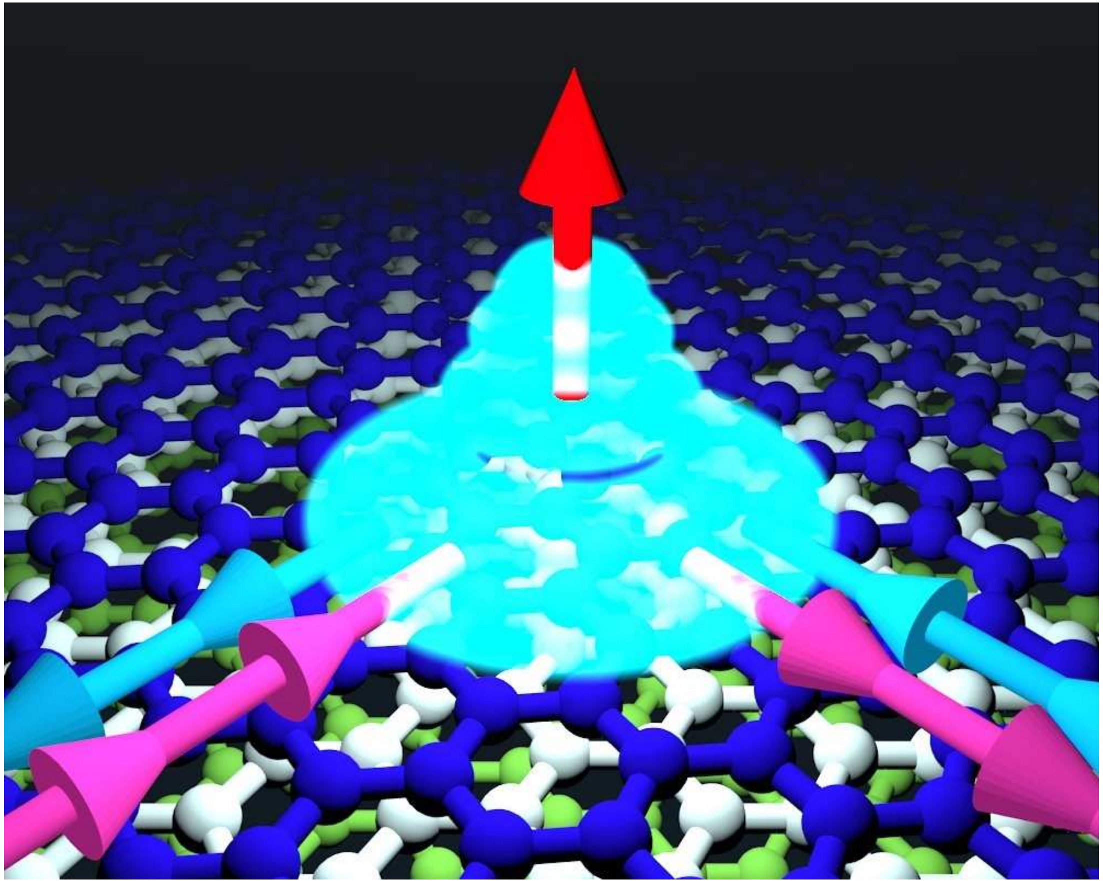
The Kondo coupling opens up a gap in the electronic structure

Dependence on the Kondo coupling

The heavy-fermion gap becomes bigger as the Kondo coupling increases



Heavy-fermions in twisted graphene trilayers

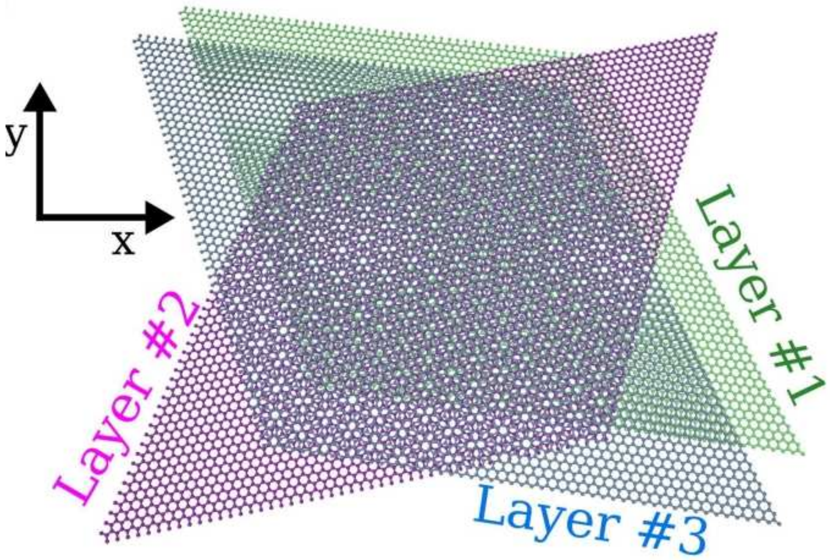


Aline Ramires

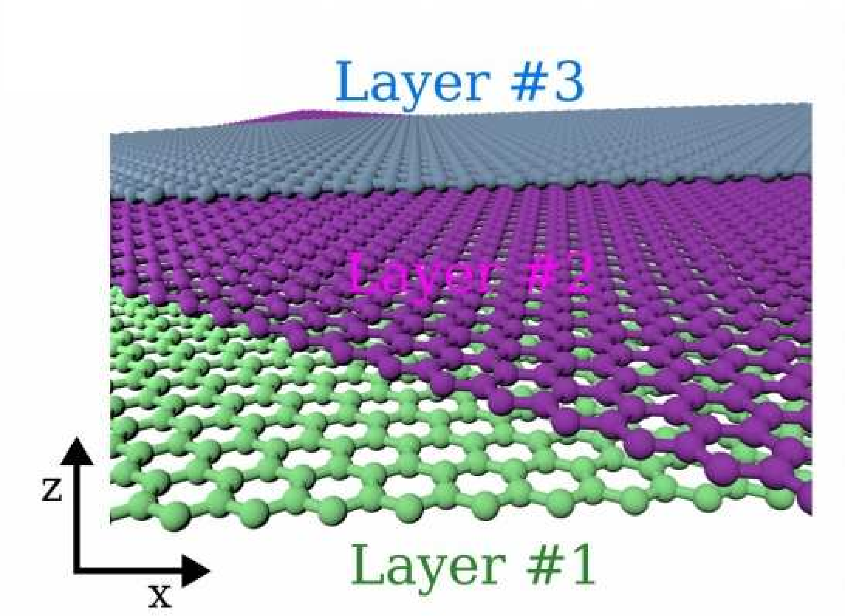
Phys. Rev. Lett. 127, 026401 (2021)

Heavy-fermions in twisted graphene trilayers

Top view

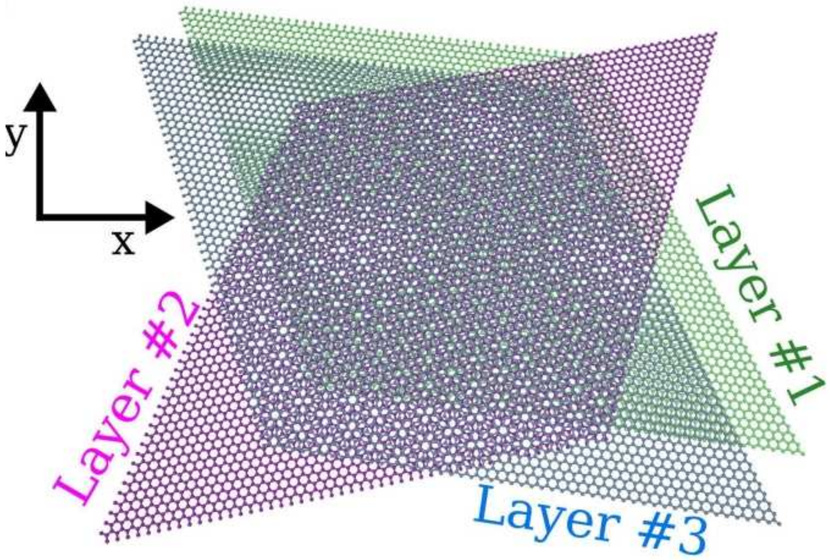


Lateral view

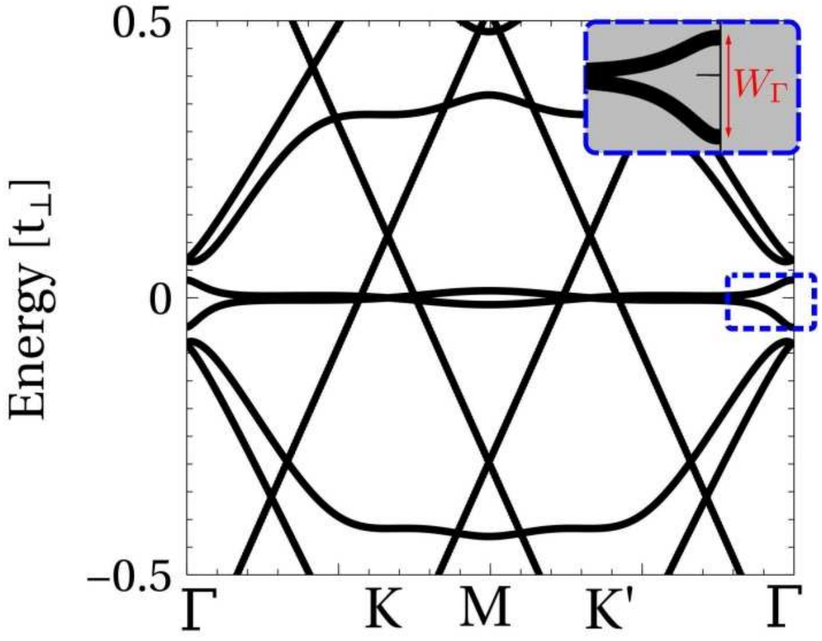


Heavy-fermions in twisted graphene trilayers

Top view

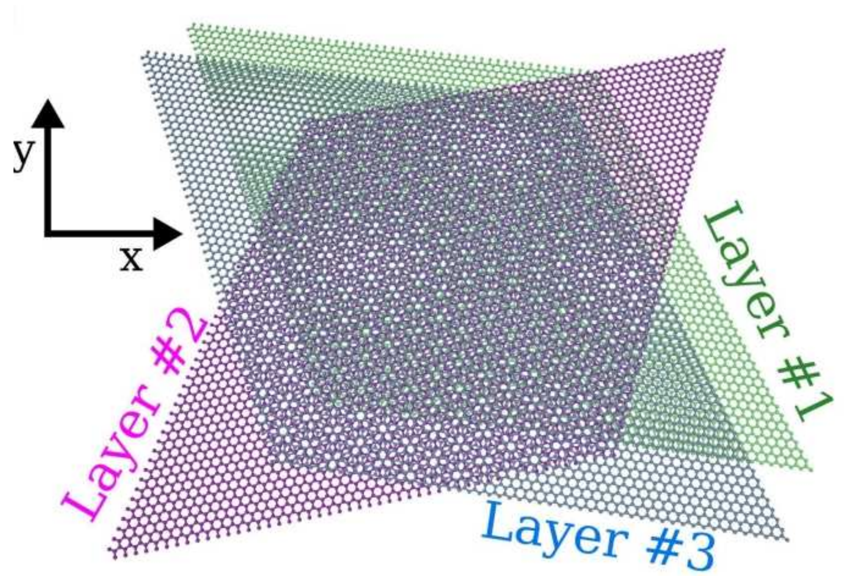


Band structure

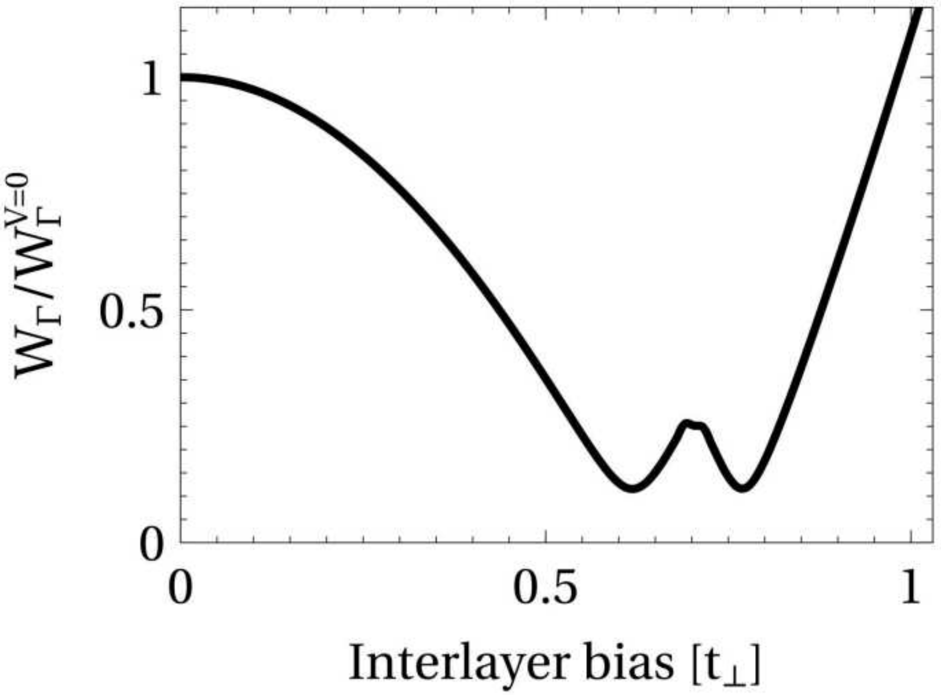


Heavy-fermions in twisted graphene trilayers

Top view



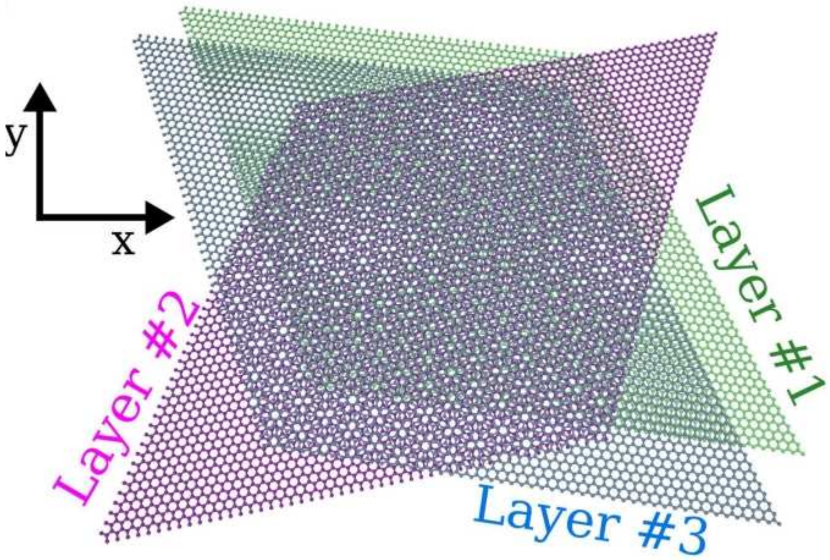
Bandwidth of nearly flat bands



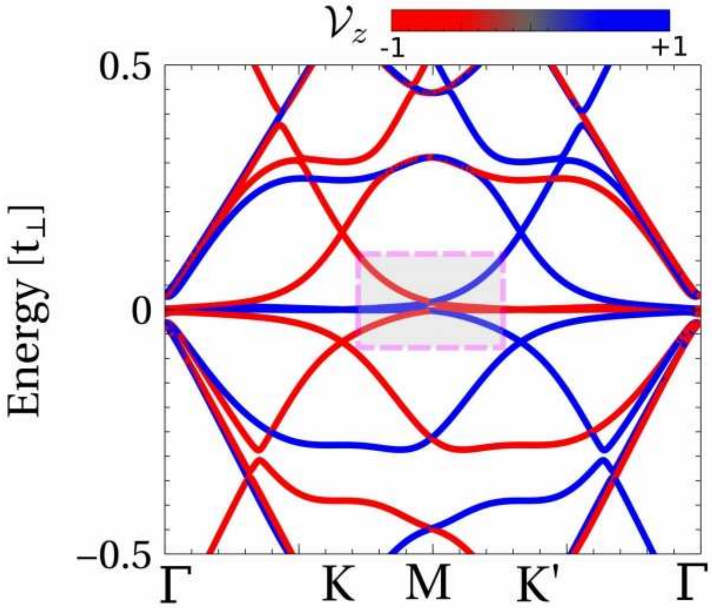
Band flattening as an interlayer bias is applied

Heavy-fermions in twisted graphene trilayers

Top view

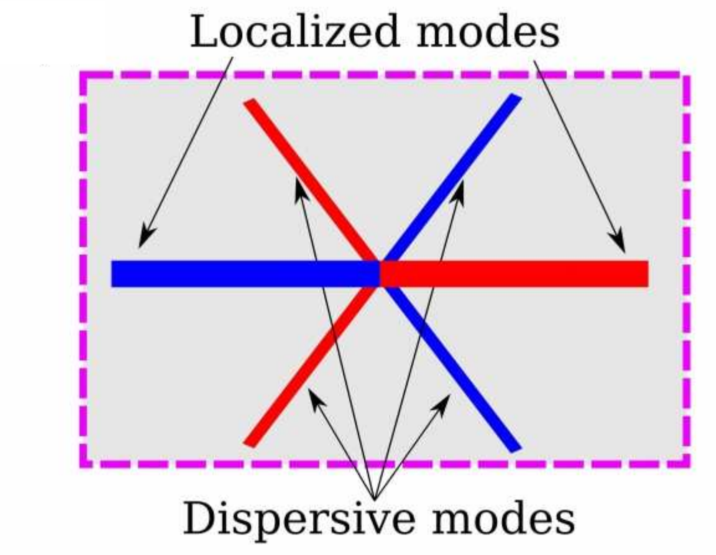


Electronic structure in the presence of an electric bias

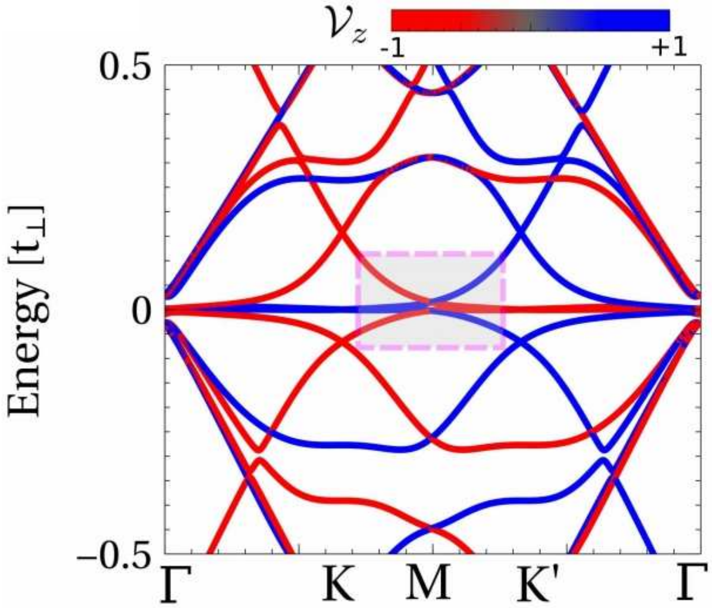


Heavy-fermions in twisted graphene trilayers

Low energy model

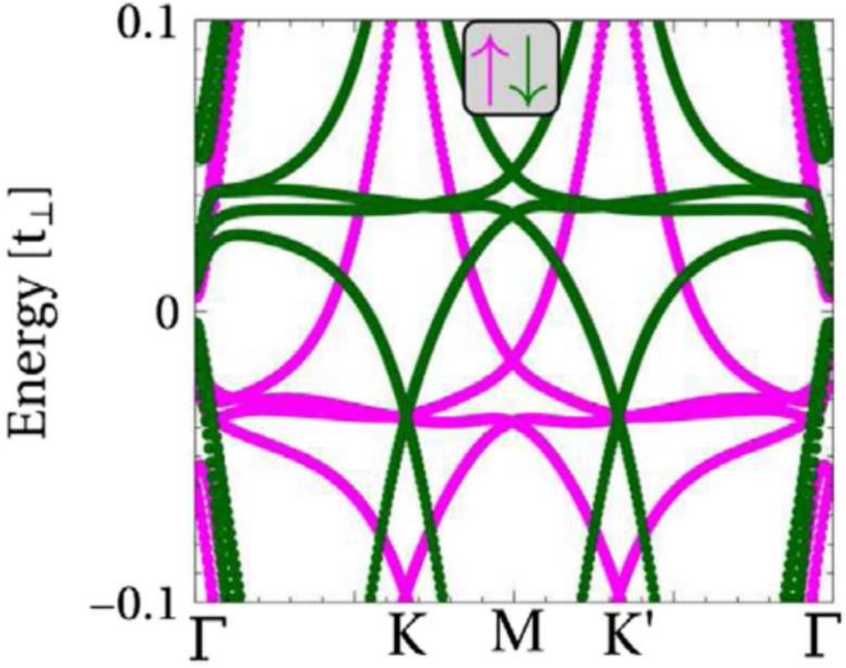


Electronic structure in the presence of an electric bias

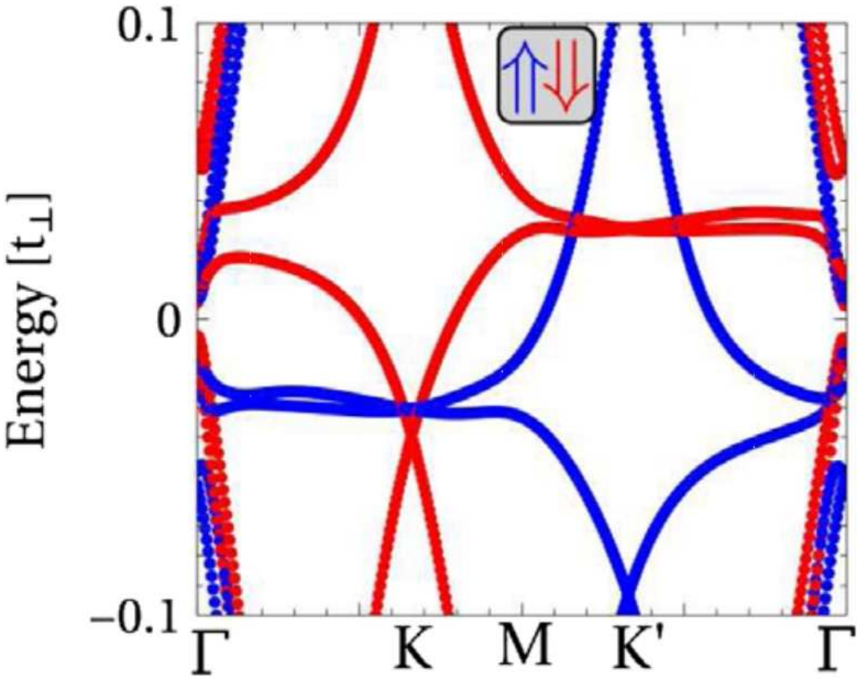


Mean-field electronic structure at half filling

Promoting spin moment formation



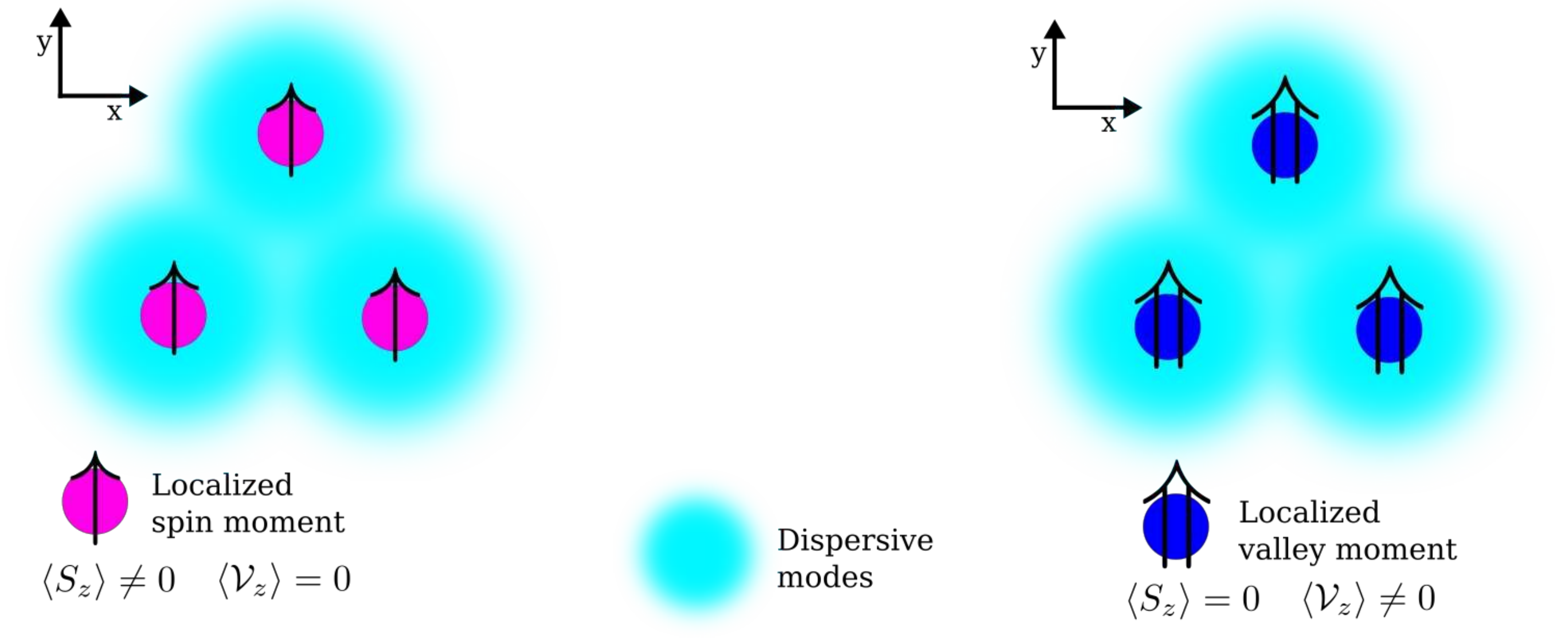
Promoting valley moment formation



Local spin and valley moments appear when including electronic interactions at the mean-field level

Mean-field electronic structure at half filling

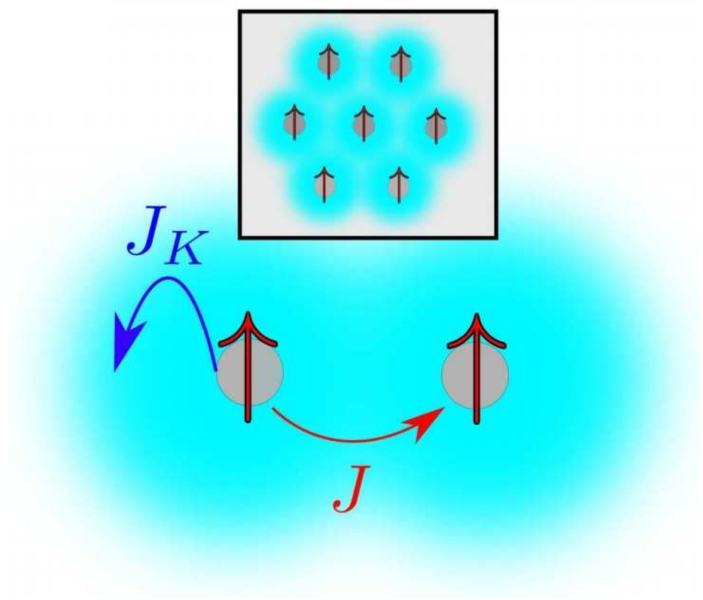
Promoting spin moment formation | **Promoting valley moment formation**



Local spin and valley moments appear when including electronic interactions at the mean-field level

Kondo lattice model in the presence of interactions

Interactions of the Kondo lattice model



Kondo coupling

Exchange coupling

$$H = H_{\text{dispersive}} + J_K \sum_{\langle i\alpha \rangle} \mathbf{S}_i \cdot \mathbf{s}_\alpha + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Promotes
Kondo screening

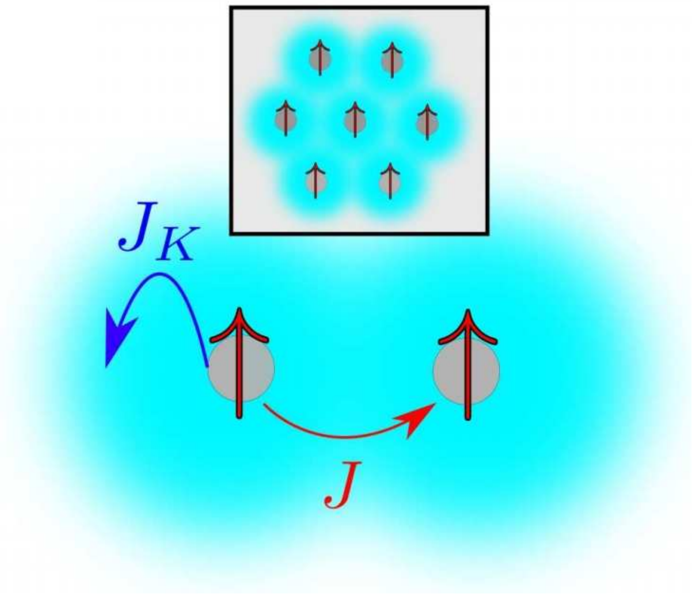
Promotes
magnetic order

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

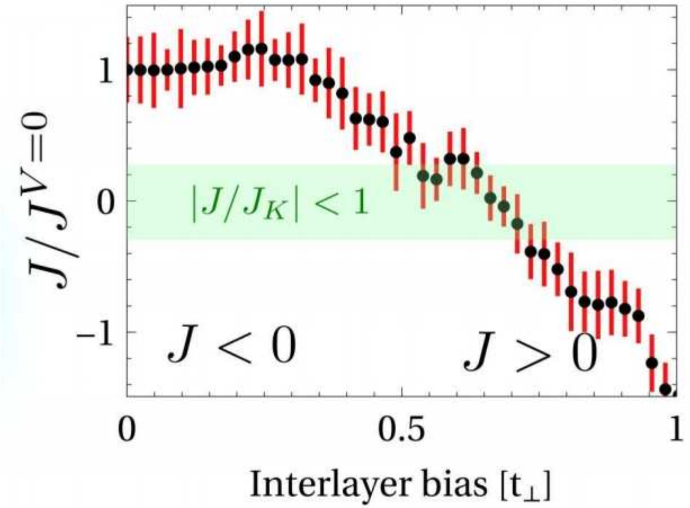
$$|J/J_K| < 1$$

Kondo lattice model in the presence of interactions

Interactions of the Kondo lattice model



Electric control of the Kondo regime

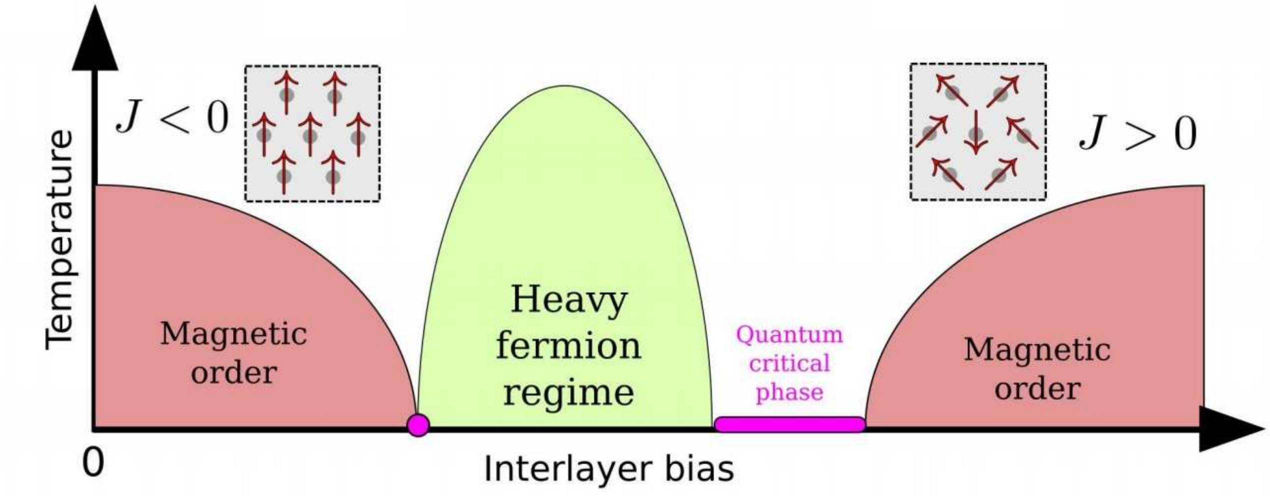


A heavy fermion regime appears when the Kondo coupling dominates over the exchange coupling

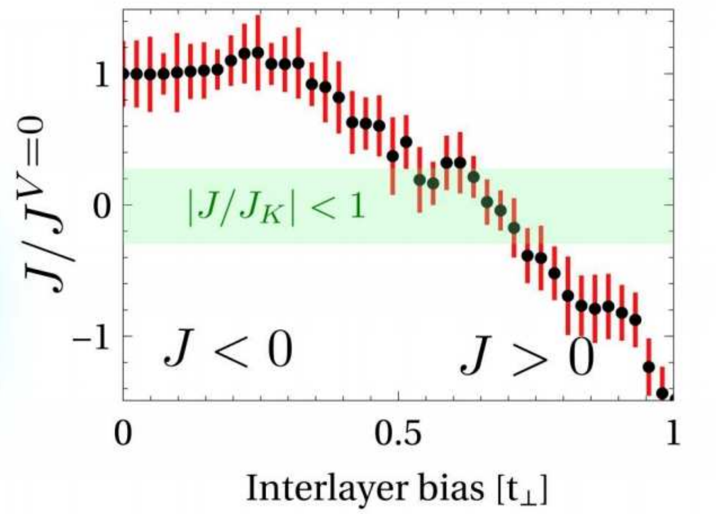
$$|J/J_K| < 1$$

Heavy-fermions in twisted graphene trilayers

Heavy-fermion (Doniach) phase diagram



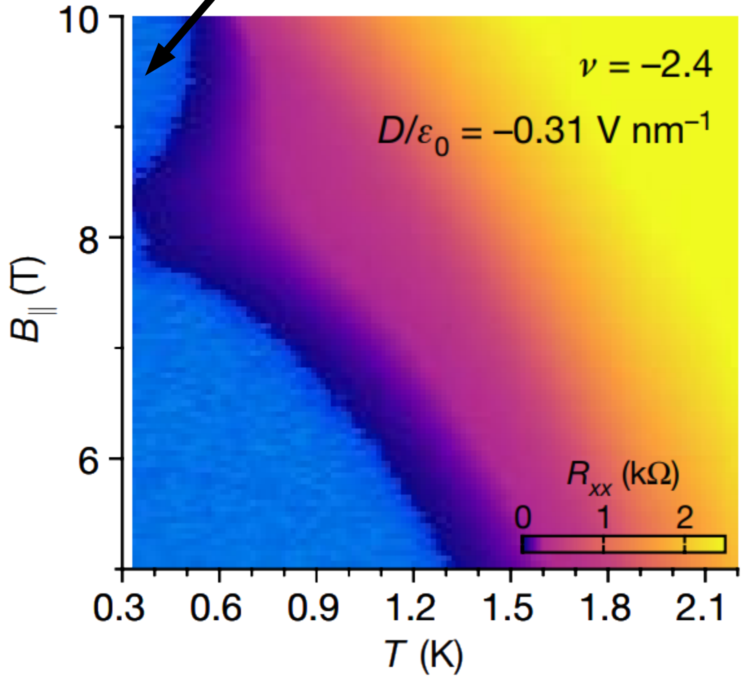
Electric control of the Kondo regime



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

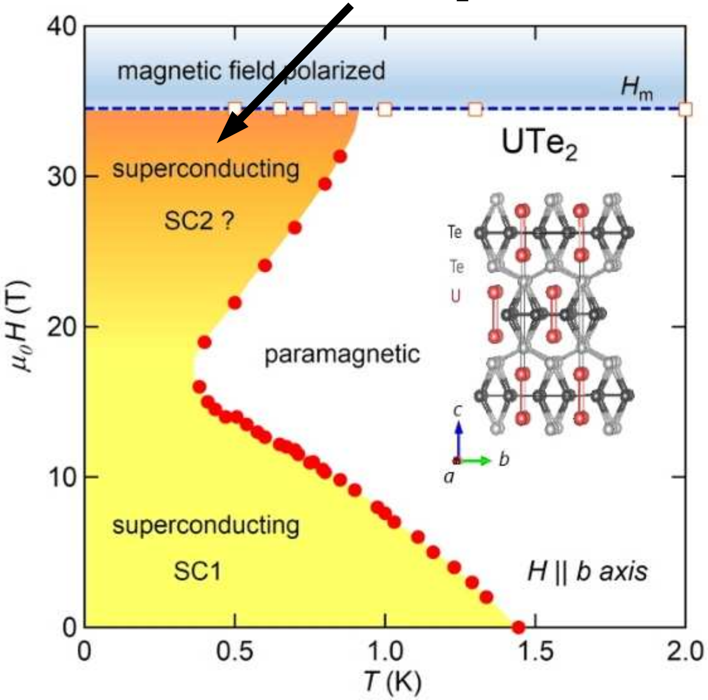
An experimental signature of heavy-fermion physics: spin-triplet superconductivity

Reentrant superconductivity in twisted trilayer graphene



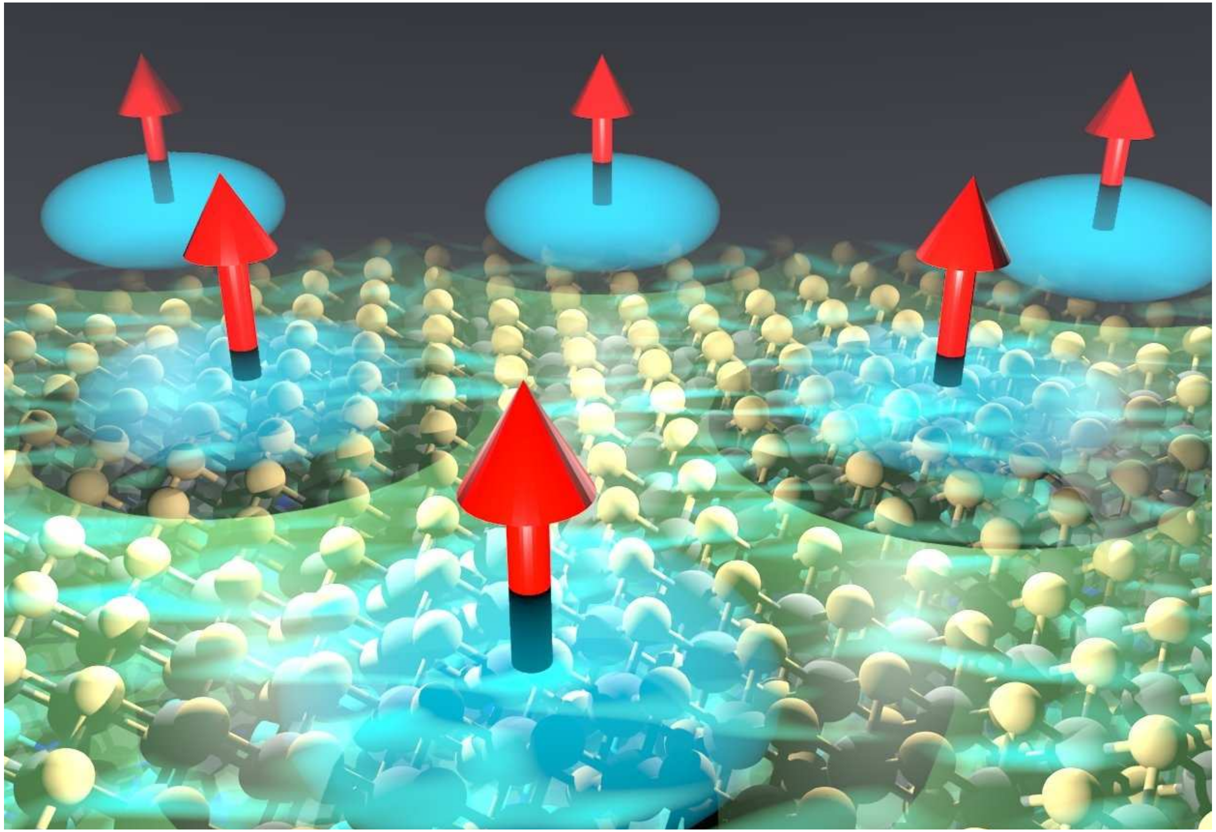
Nature 595, 526–531 (2021)

Reentrant superconductivity in UTe_2



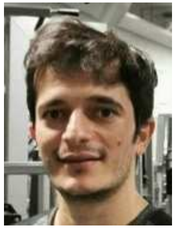
Nat. Phys. 15, 1250 (2019)
Science 365, 684 (2019)

Heavy-fermions in a van der Waals dichalcogenide heterostructure

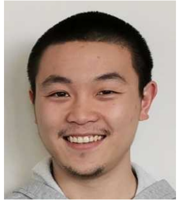


S. Ganguli

M. Amini



G. Chen



V. Vaňo

S. Kezilebieke

P. Liljeroth

Nature 599, 582–586 (2021)

Heavy-fermions in dichalcogenide bilayers

Triangular lattice of local magnetic moments

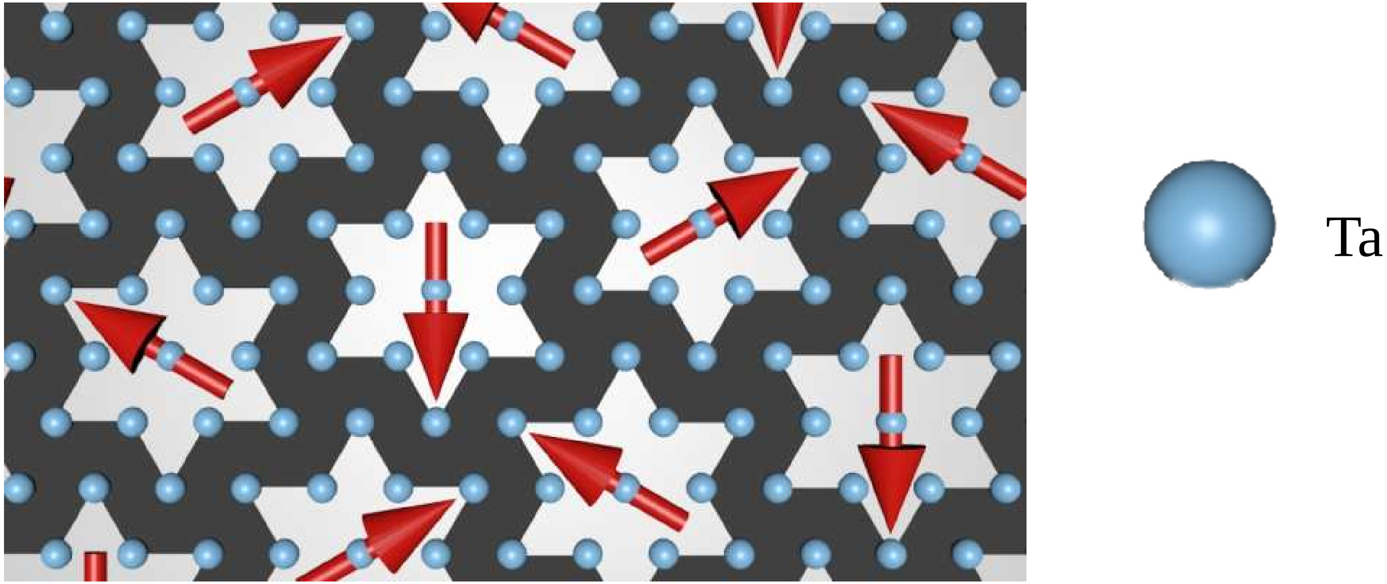
1T-TaS_2

Two-dimensional electron gas

1H-TaS_2

Moment formation in 1T-TaS_2

Charge-density wave reconstruction, leading to a localized orbital in a $\sqrt{13} \times \sqrt{13}$ unit cell



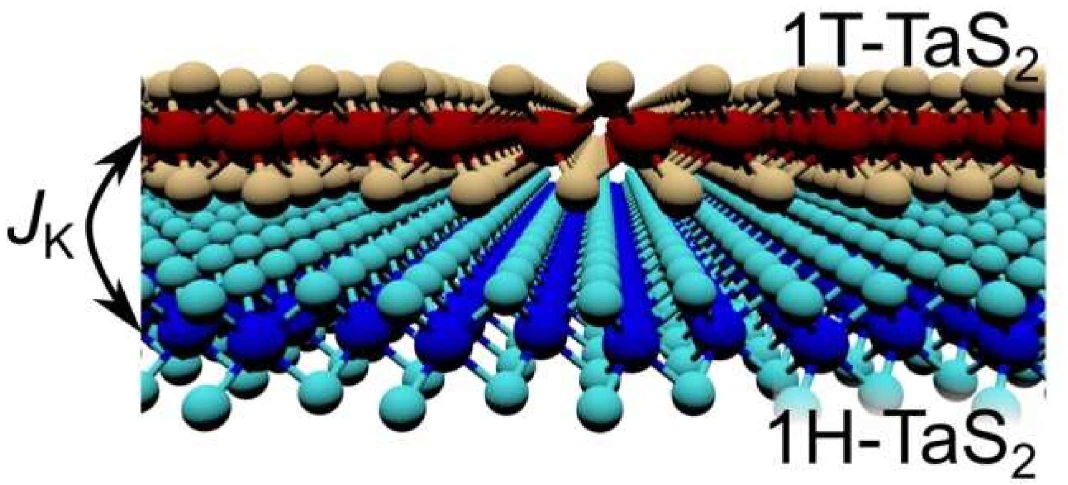
Strong interactions give rise to local moment formation

Effectively described by an S=1/2 Heisenberg model in a triangular lattice

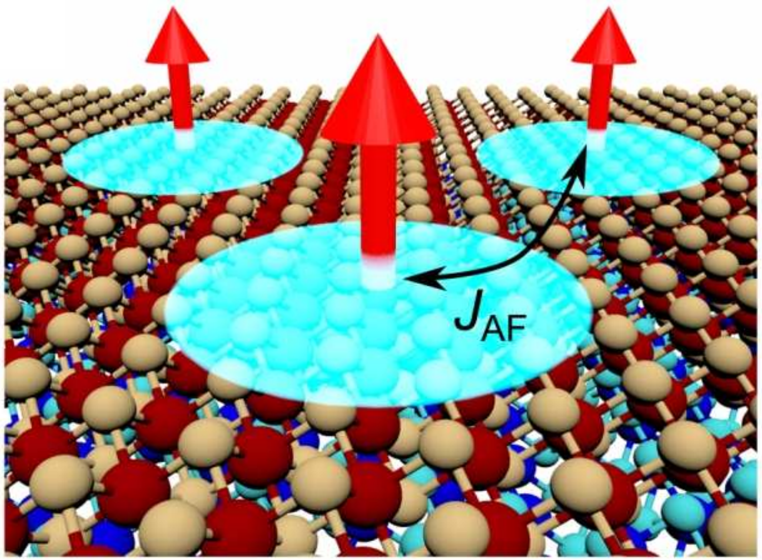
PNAS 114.27 (2017)
Phys. Rev. X 7, 041054 (2017)
Phys. Rev. B 96, 195131 (2017)

Heavy-fermions in dichalcogenide bilayers

Interlayer coupling creates the Kondo coupling



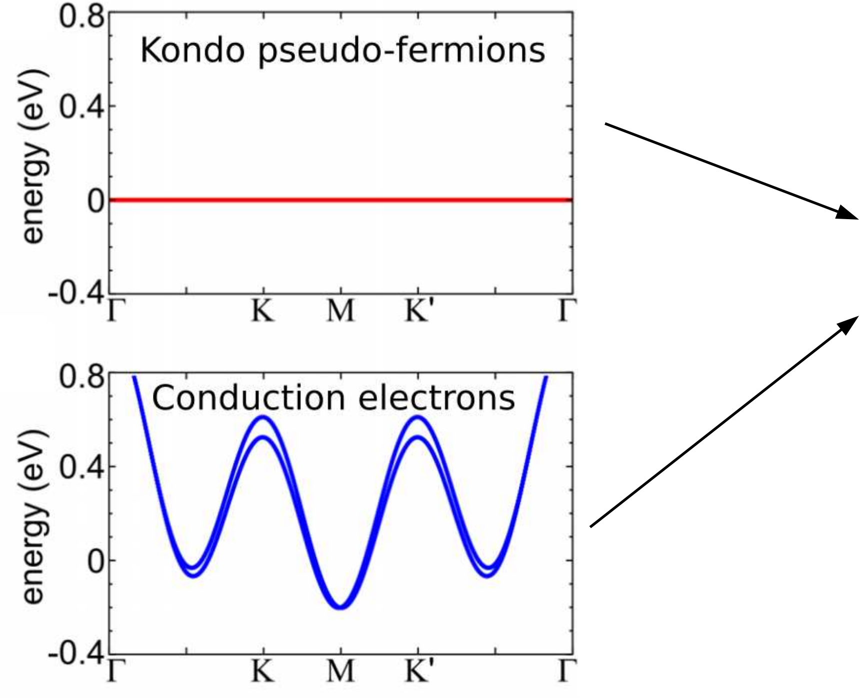
Intralayer exchange between local moments



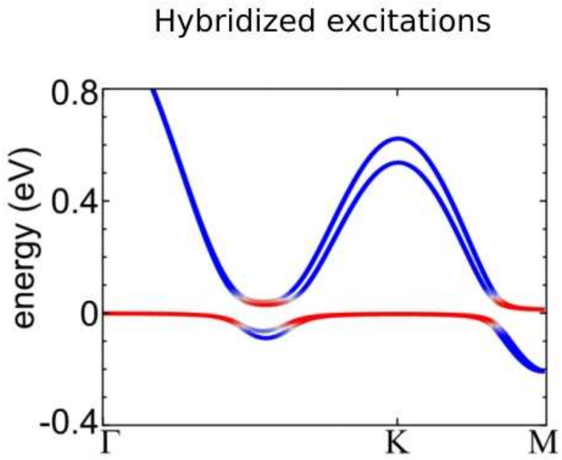
The bilayer realizes all the ingredients for heavy-fermion physics

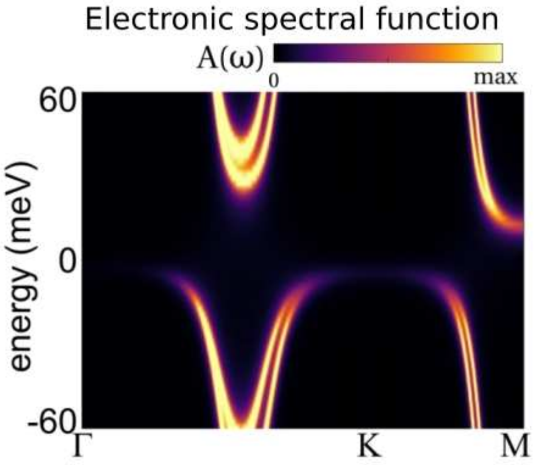
Brief theory of heavy-fermions

Kondo physics introduces resonant pseudo-fermions at the chemical potential

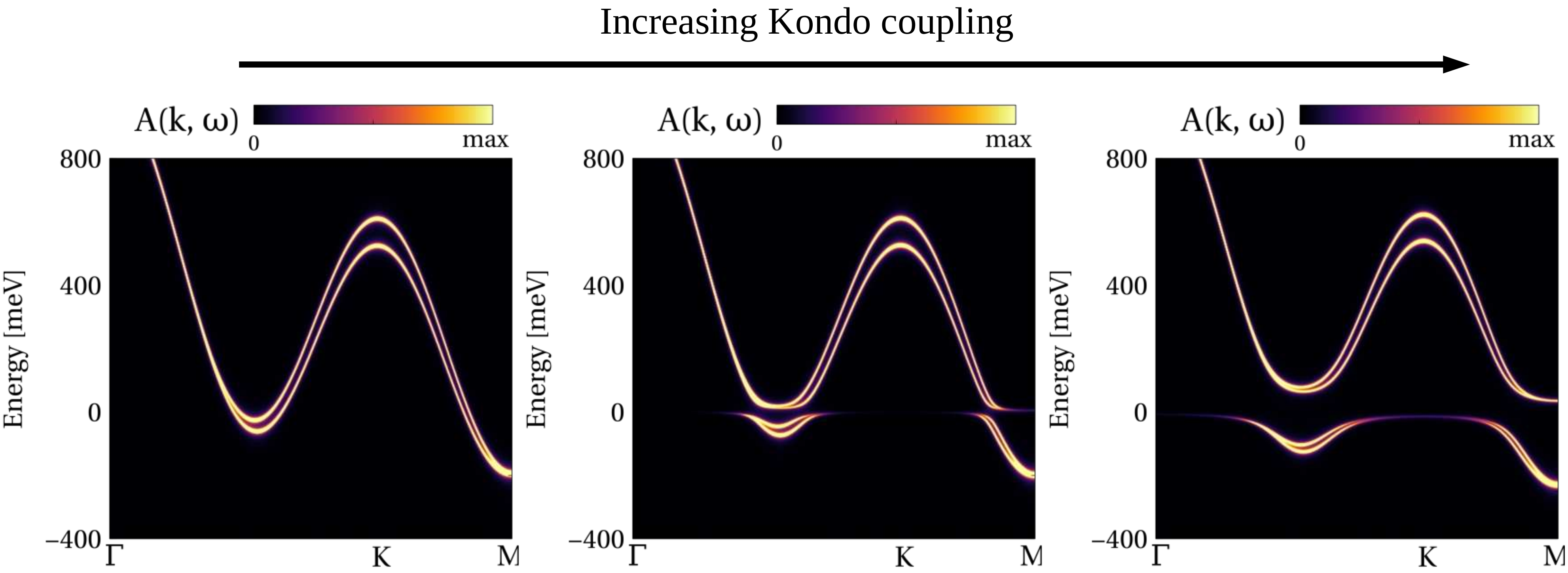


Leading to the opening of a heavy-fermion gap





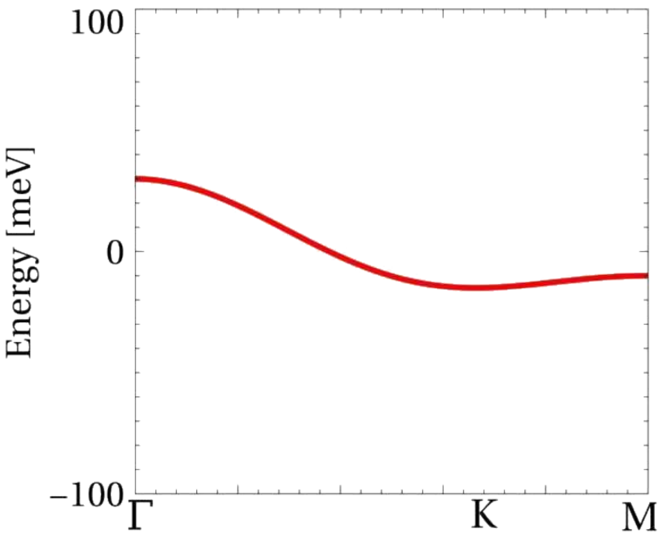
Heavy-fermion hybridization gap



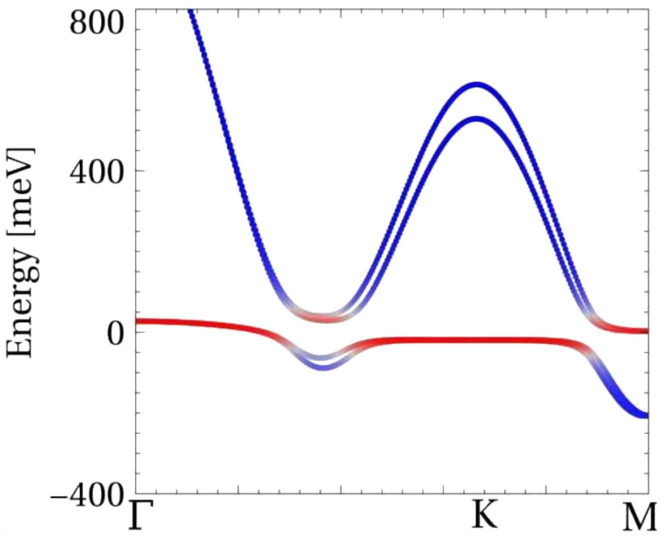
The Kondo coupling leads to a heavy-fermion gap opening in the metal

Heavy-fermion hybridization gap

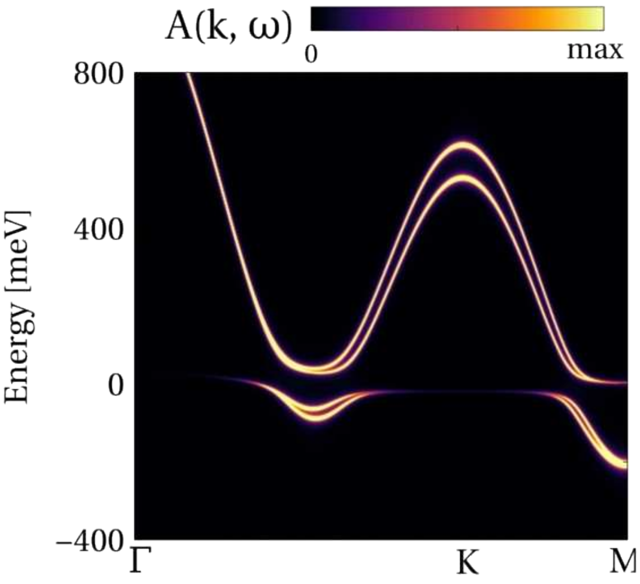
Kondo pseudofermions



Hybridized excitations



Conduction spectral function



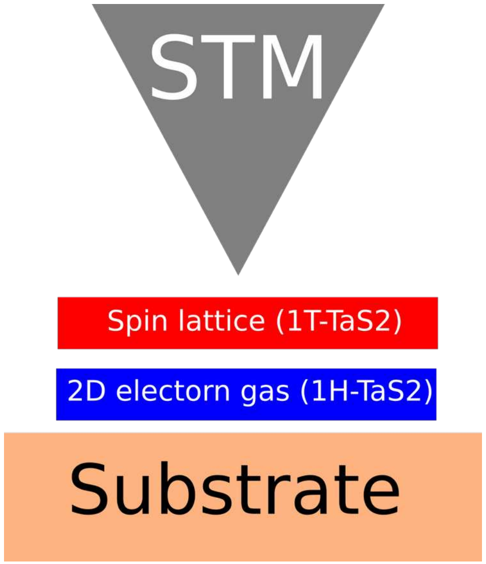
The gap remains open when including a small psedofermion dispersion

Experimental signatures of heavy-fermion physics

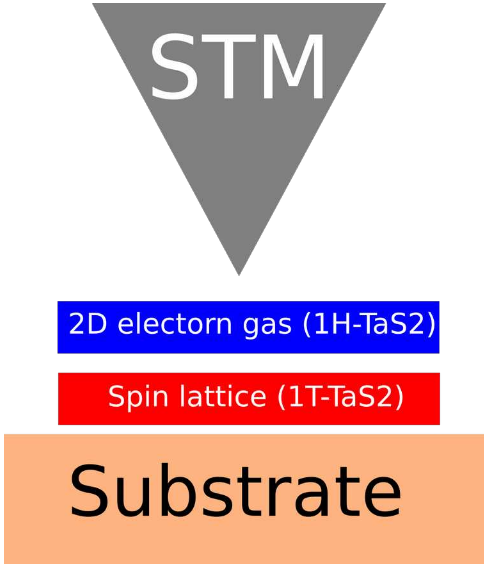
- Kondo physics in the magnetic lattice
- Gap opening in the metallic layer

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

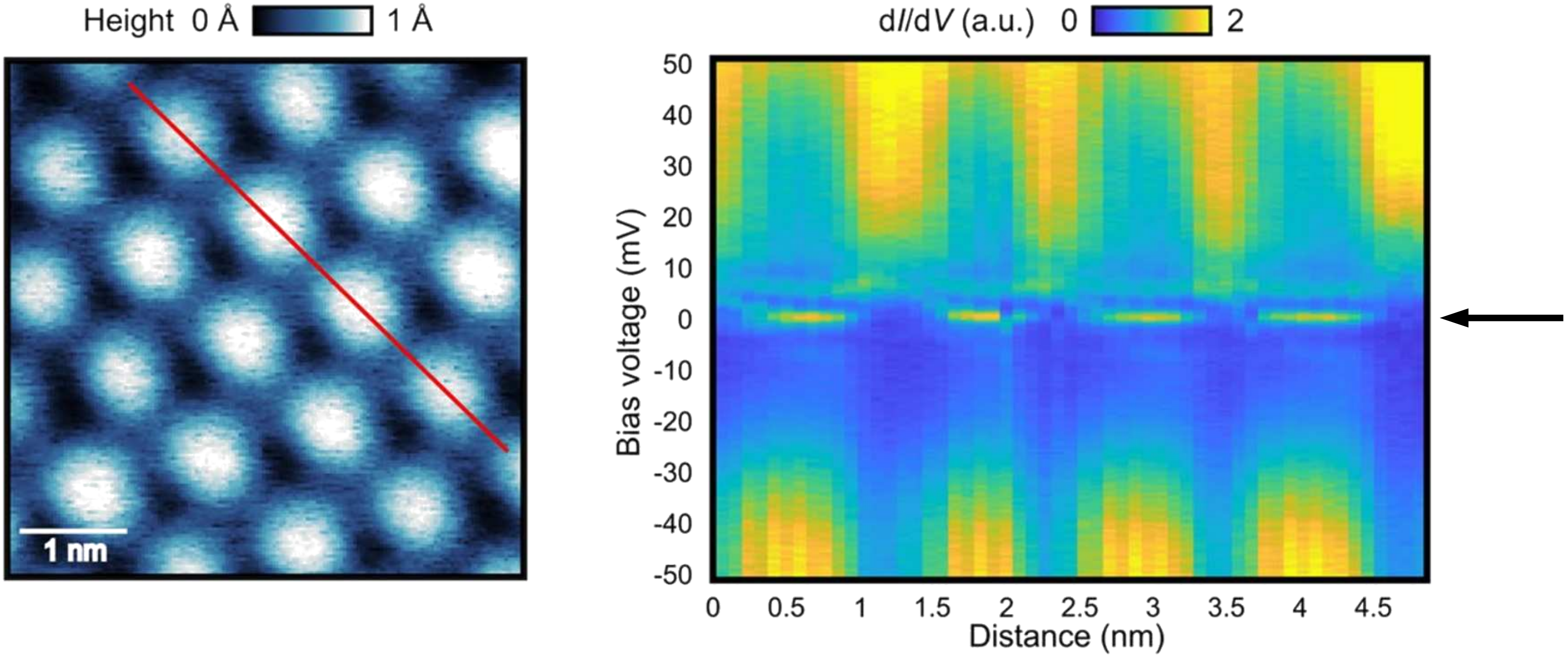
Probing the Kondo peak



Probing the heavy-fermion gap

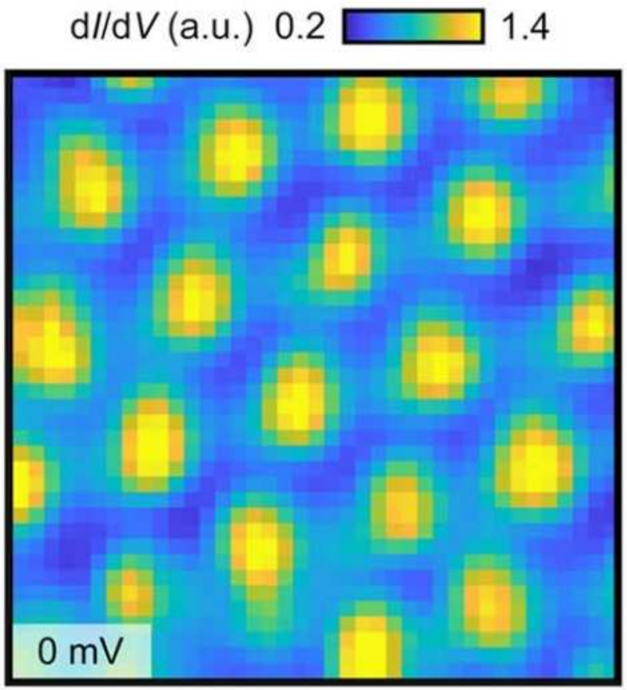


Grid spectroscopy of 1T-1H

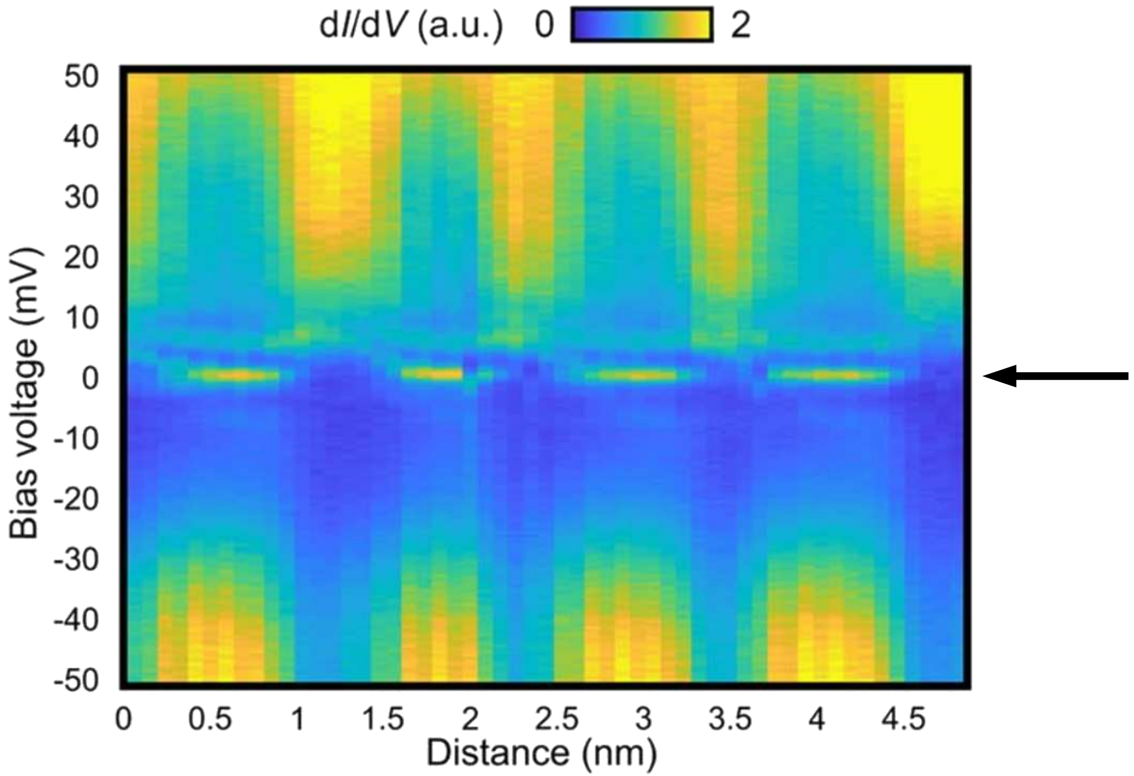


Zero bias (Kondo) peak appearing with the CDW periodicity

Grid spectroscopy of 1T-1H

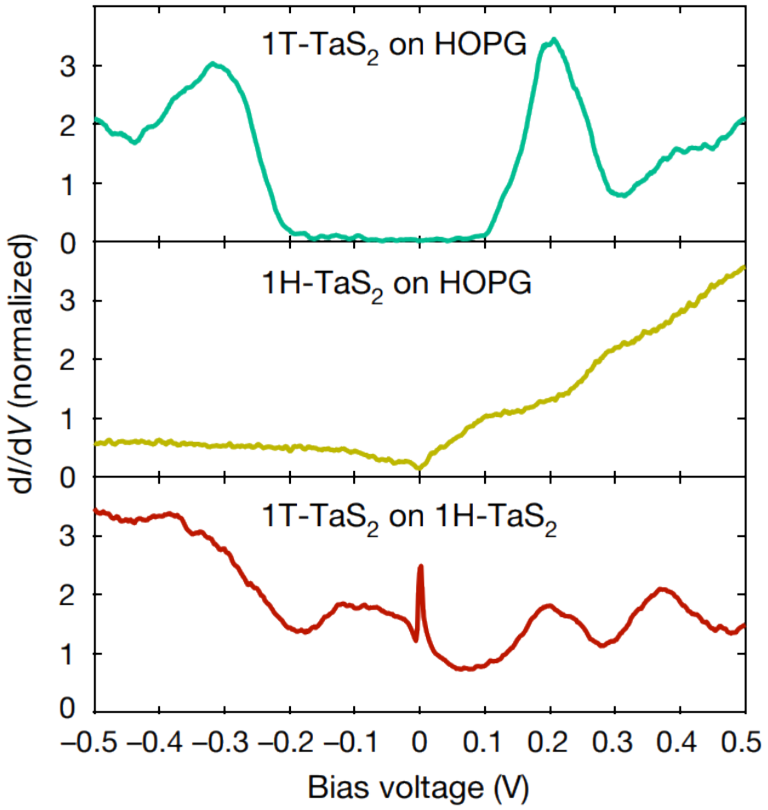


dI/dV (V=0)



Zero bias (Kondo) peak appearing with the CDW periodicity

Zero bias Kondo peak

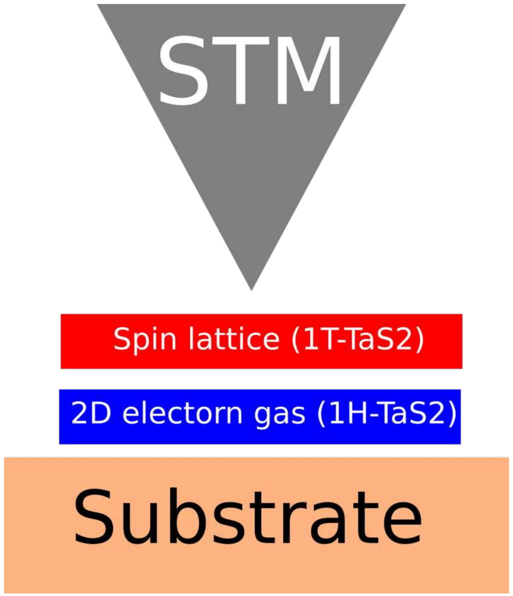


1T @ HOPG: Mott insulator

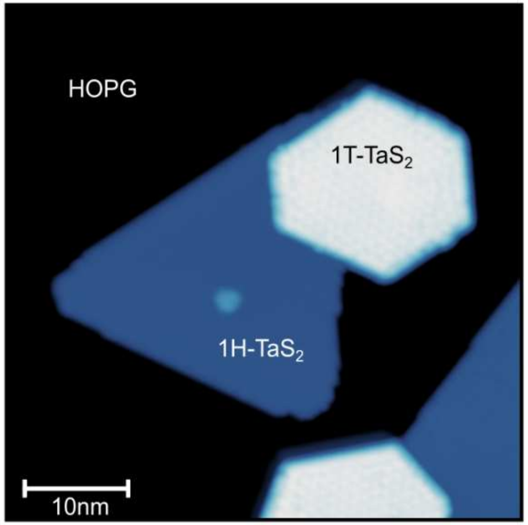
1H @ HOPG: Metal
(with a SC state at very low T)

1T @ 1H: Kondo peak

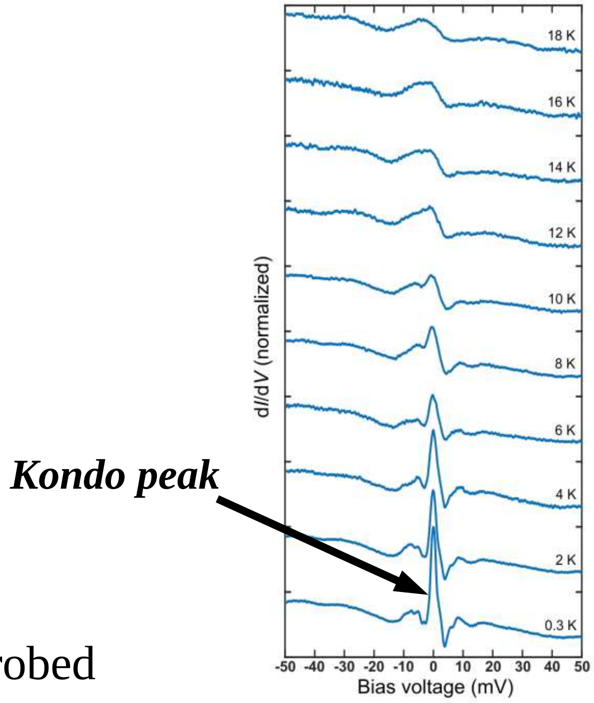
Kondo physics in the magnetic lattice



Sample



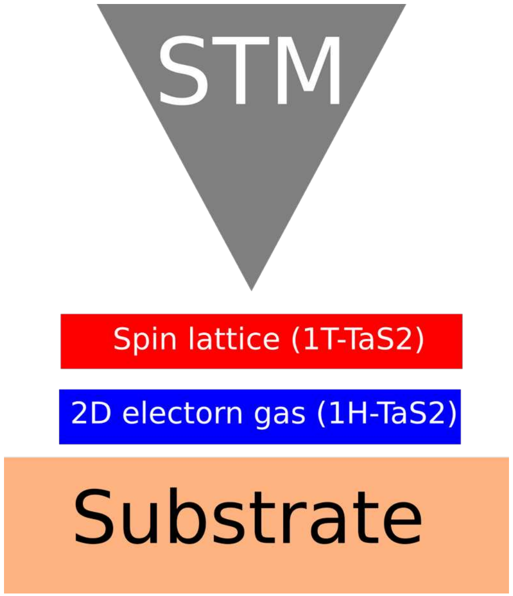
Differential conductance

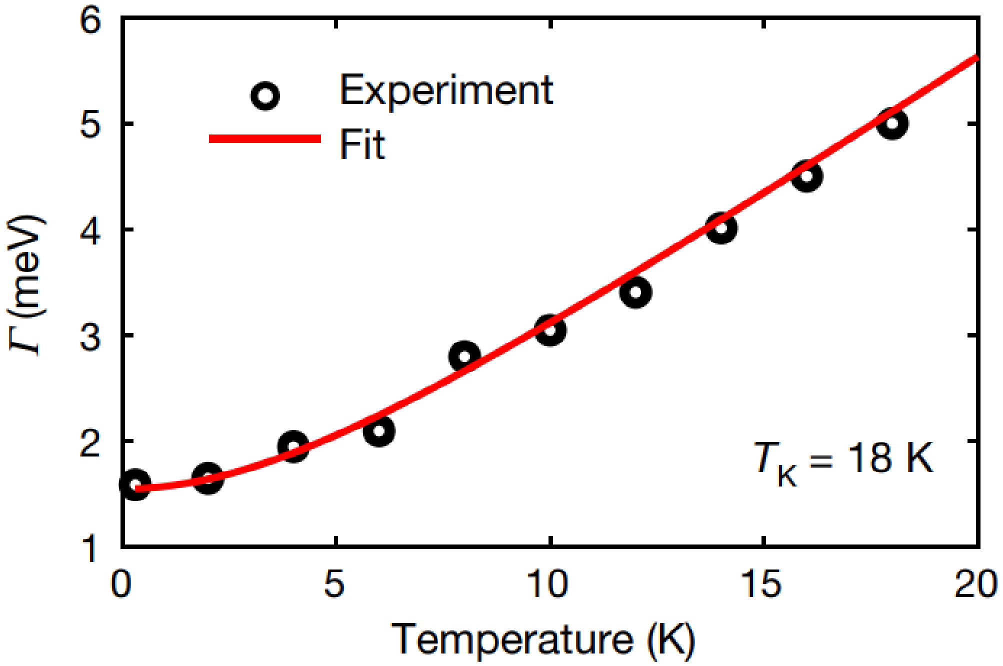


The system shows a Kondo peak when the local moments are probed

Temperature and field dependence consistent with Kondo

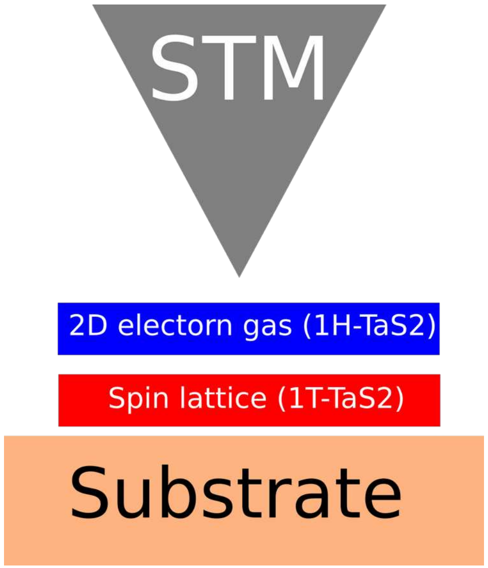
Kondo physics in the magnetic lattice



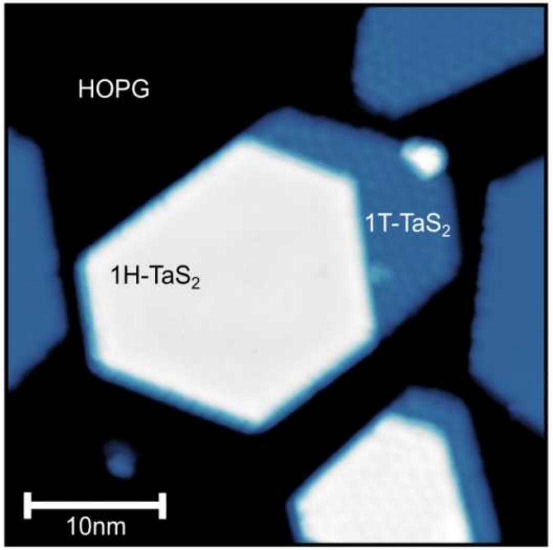


The Kondo peak follows the expected temperature dependence

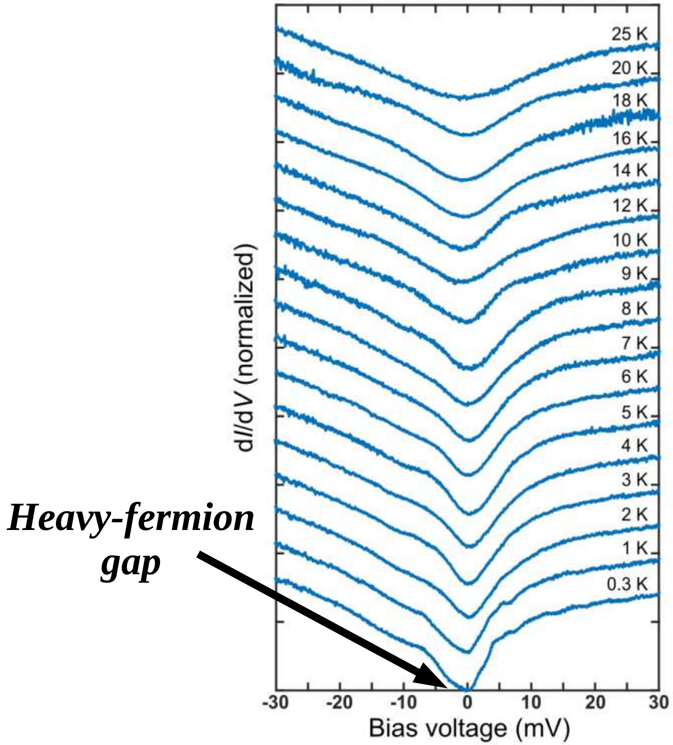
Heavy-fermion gap in the 2D electron gas



Sample



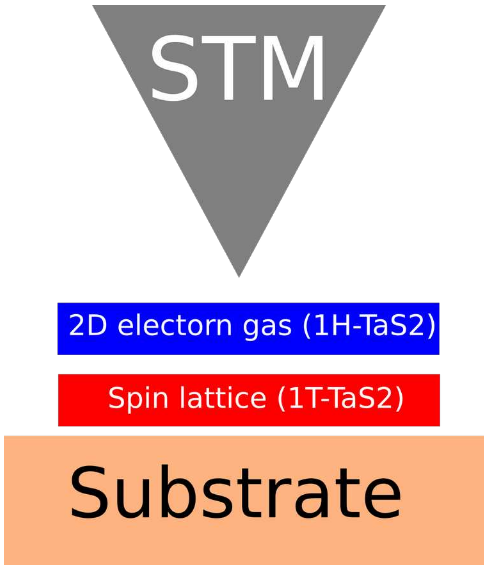
Differential conductance

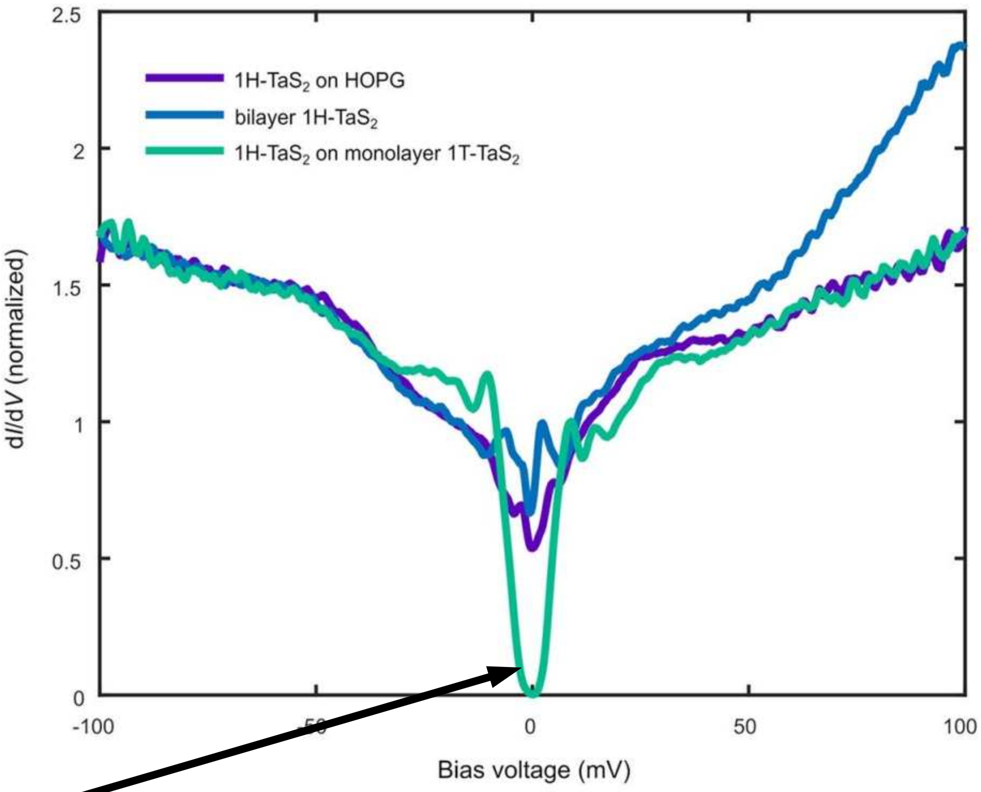


A heavy-fermion gap appears on the metal side

Temperature and field dependence consistent with a heavy-fermion gap

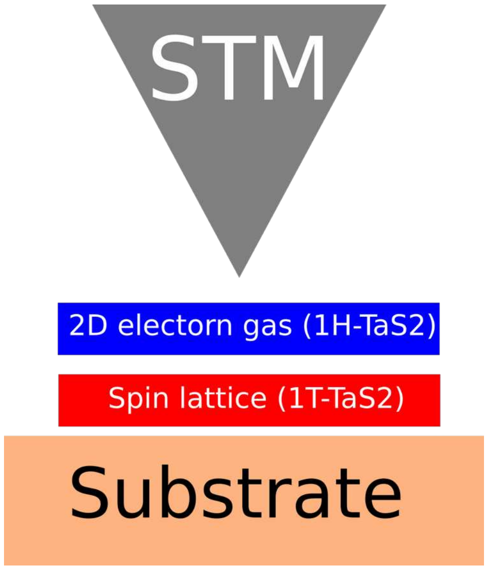
Heavy-fermion gap in the 2D electron gas

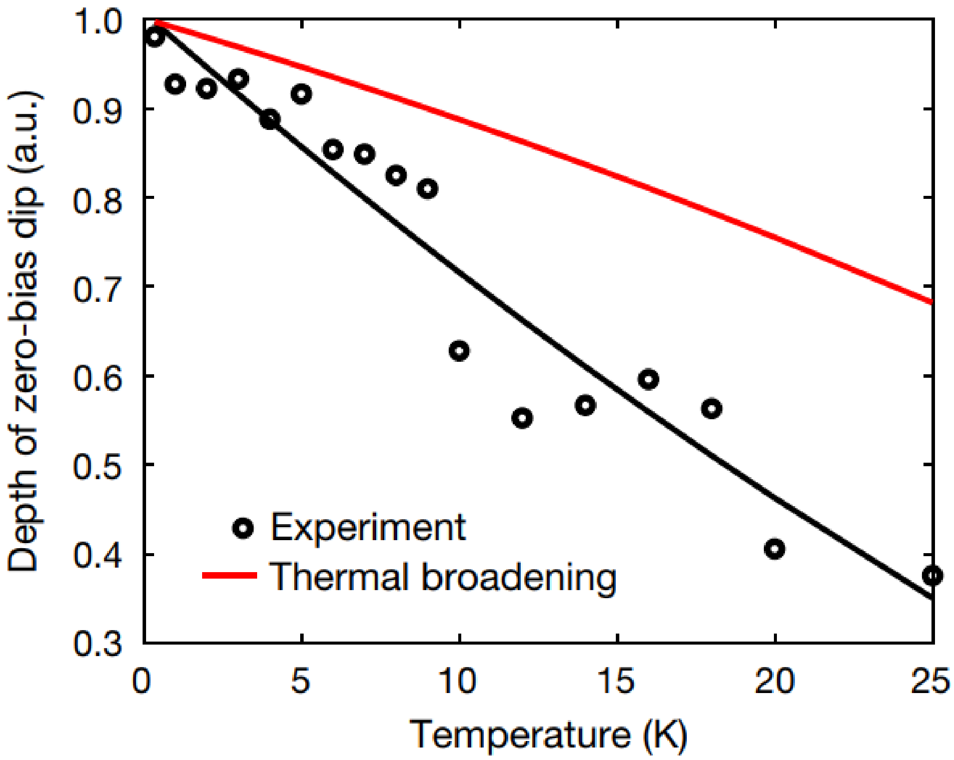




Heavy-fermion gap

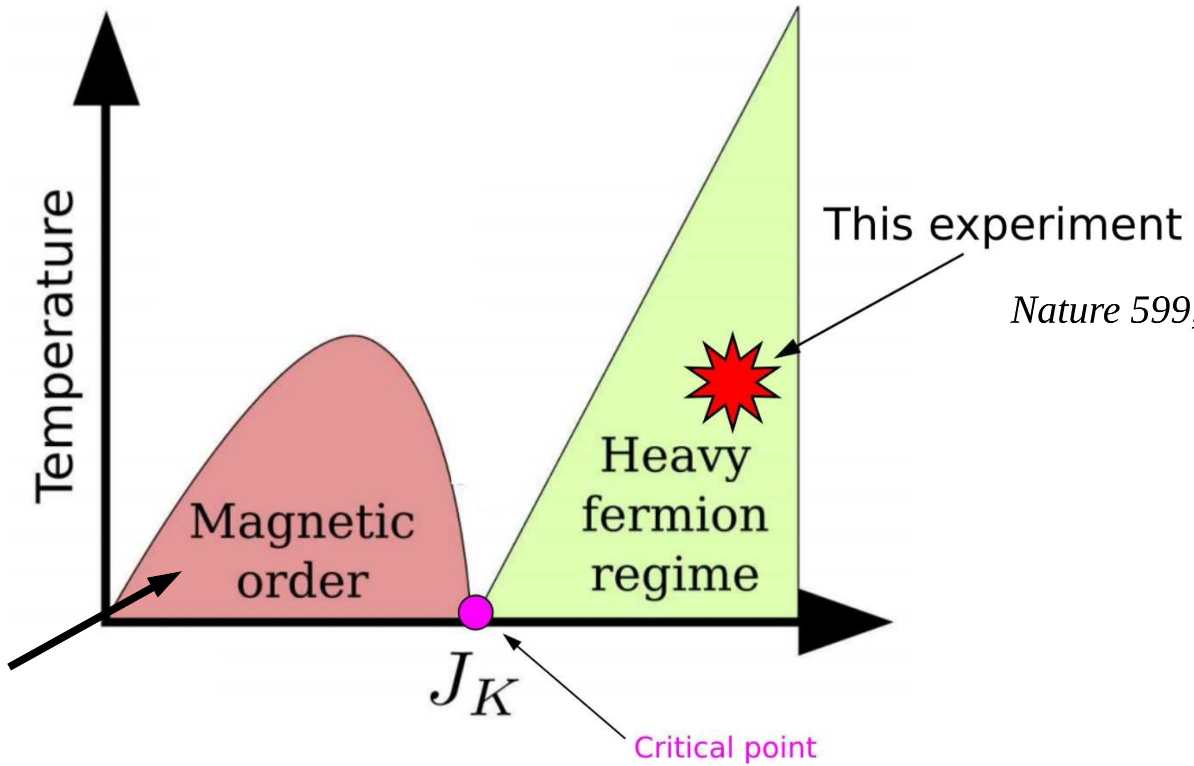
Heavy-fermion gap in the 2D electron gas





The gap shows a temperature dependence beyond thermal broadening, expected from a heavy-fermion gap

Next steps in van der Waals heavy-fermions



Nature 599, 582–586 (2021)

arXiv:2207.00096

Can we push this system to critical and different unconventional superconducting regimes?

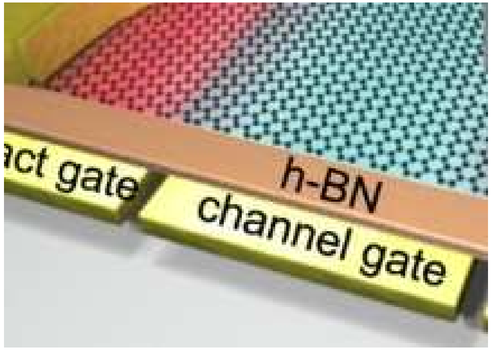
Controlling the heavy-fermion state

Of course, we can use the typical knobs of bulk heavy fermion compounds

(pressure, chemical doping, etc)

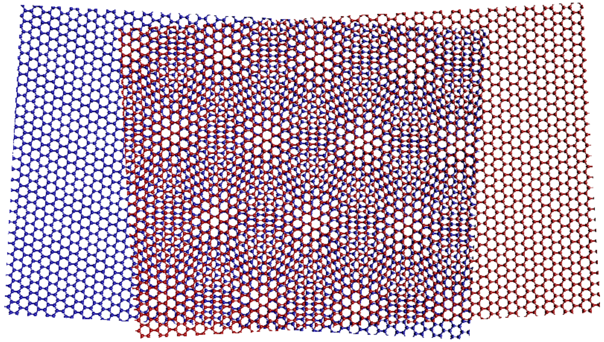
Most importantly, we can exploit the full tunability of van der Waals materials

Gating



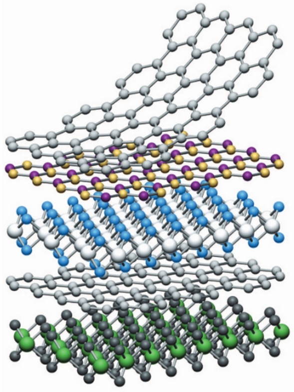
Science 306, 5696, 666-669 (2004)

Twist engineering



Nature Reviews Materials 6, 201–206 (2021)

Materials engineering

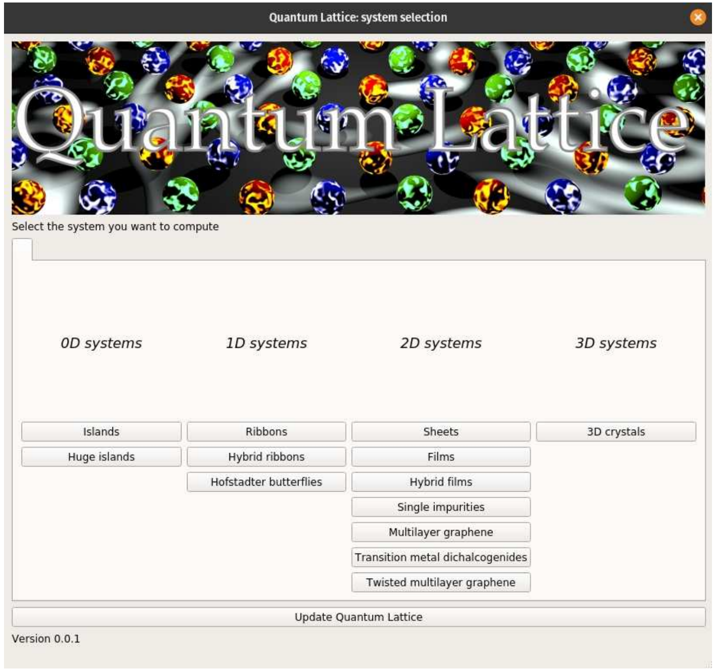


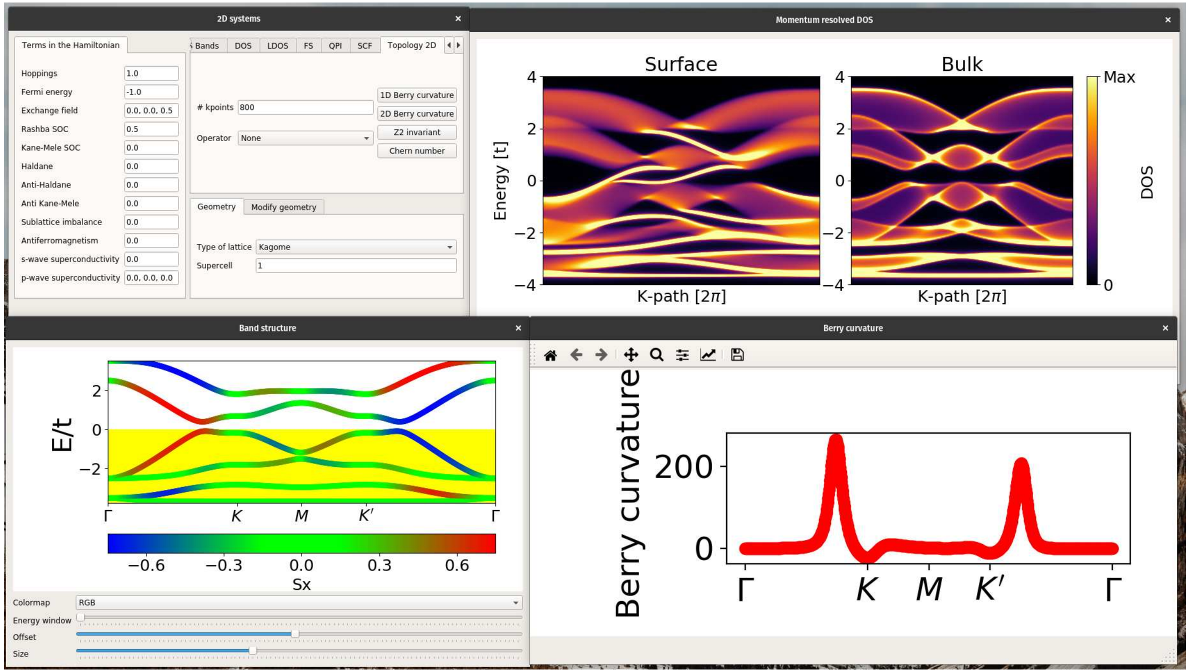
Nature 499, 419–425 (2013)

Allowing to independently control Kondo coupling, exchange coupling, doping and electronic dispersion

Computing electronic properties

Quantum Lattice: A user interface to compute electronic properties

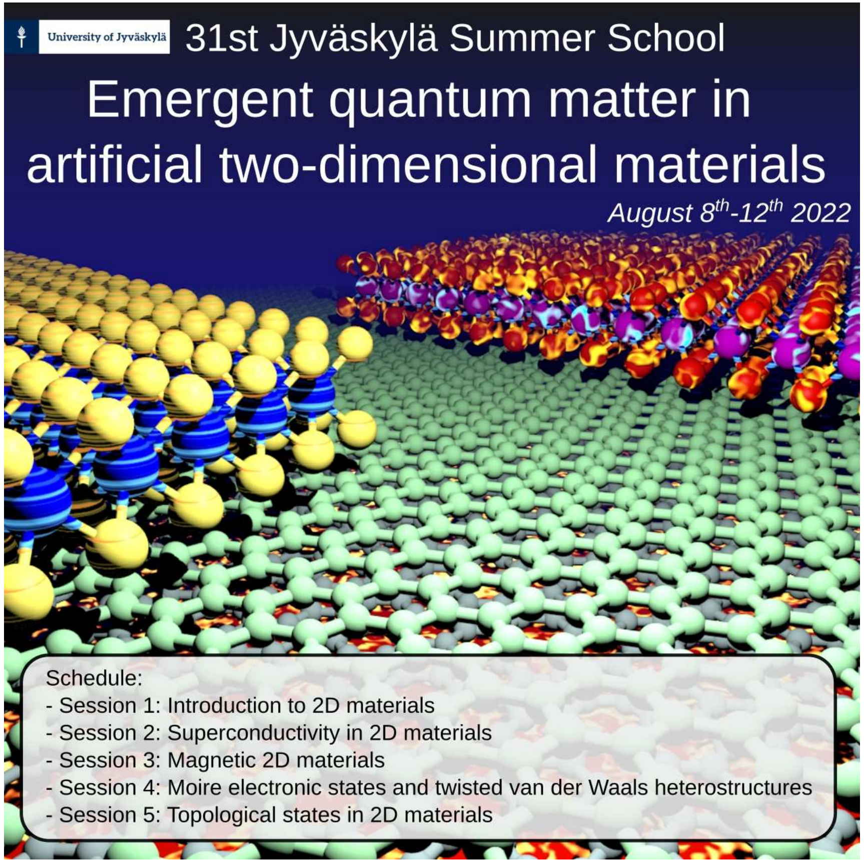




Quantum Lattice: open source interactive interface for tight binding modeling

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

Quantum matter in van der Waals materials school



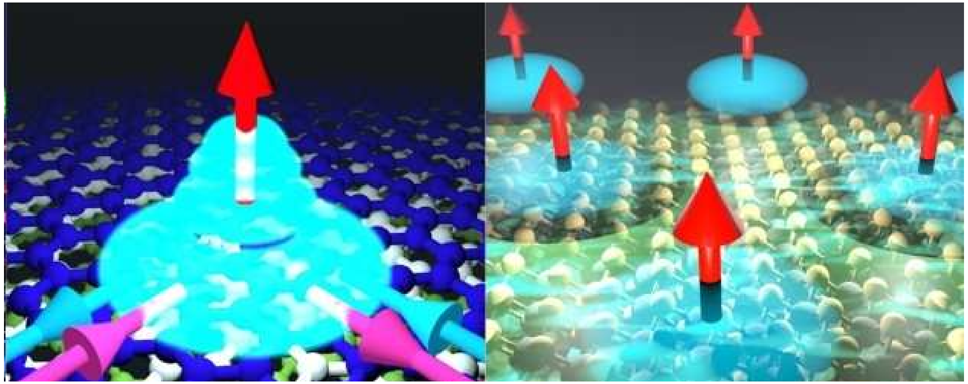
Recordings available at

https://www.youtube.com/channel/UCgnB-4CcqRQnvTi7P0cUakQ

- Session 1: Introduction to 2D materials
- Session 2: Superconductivity in 2D materials
- Session 3: Magnetic 2D materials
- Session 4: Moire electronic states and twisted van der Waals heterostructures
- Session 5: Topological states in 2D materials

Take home

Van der Waals heterostructures provide a platform to engineer heavy-fermion physics, opening a pathway to a whole new family of emergent quantum states



Thank you!

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SUOMEN AKATEMIA

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Nature 599, 582–586 (2021)