Cascades: the unconventional normal state of magic angle twisted bilayer graphene

E. Bascones

Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC)

Work in collaboration with:

Anushree Datta
(ICMM-CSIC) and
Univ Paris-Cité &
Univ Paris-Saclay

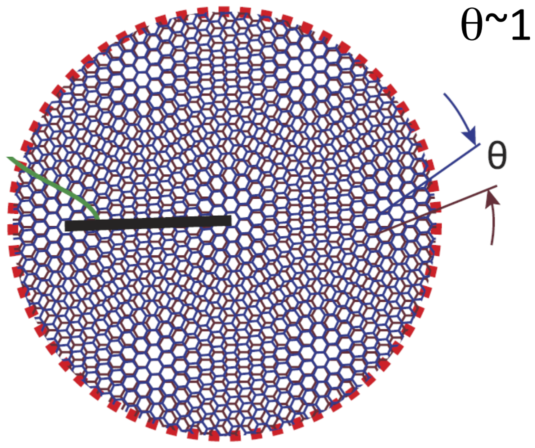
María José Calderón
(ICMM-CSIC)

Alberto Camjayi
(Uni. Buenos Aires)

A. Datta, MJ Calderón, A. Camjayi, EB,
Nature Comms (2023), arXiv:2301.13024

Flat bands in magic angle twisted bilayer graphene

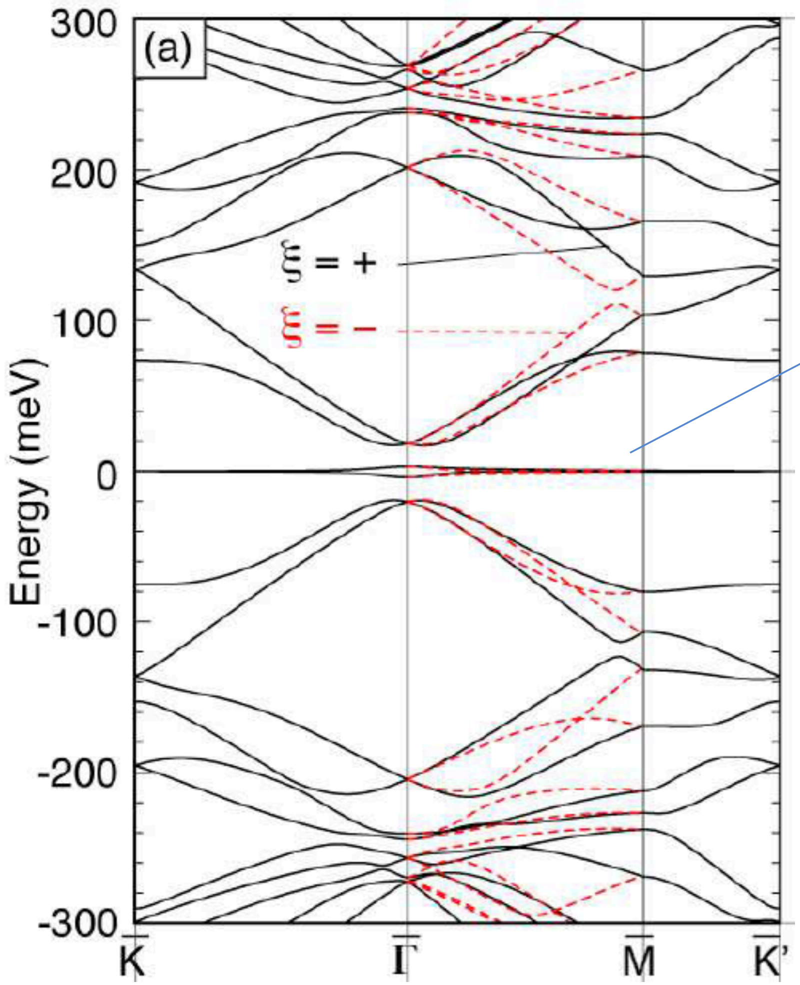
θ~1.1º



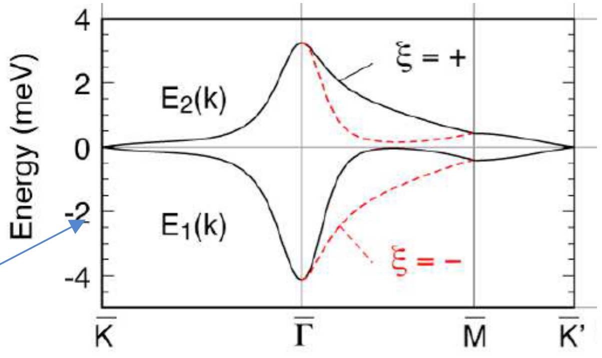
Moiré pattern

Large unit cell ~10.000 carbon atoms
(small Brillouin zone)

Many correlated states upong doping:
superconducting, insulating, ferromagnetic,
IVC, detected at low temperatures
(at most a few Kelvin)

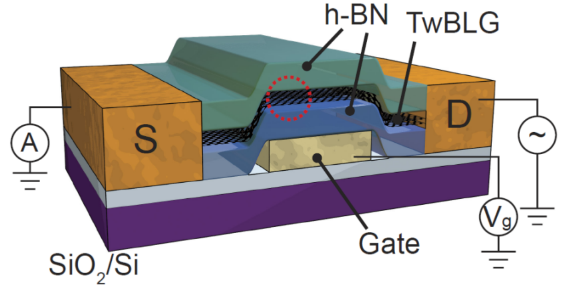


4 flat bands (2 per valley)



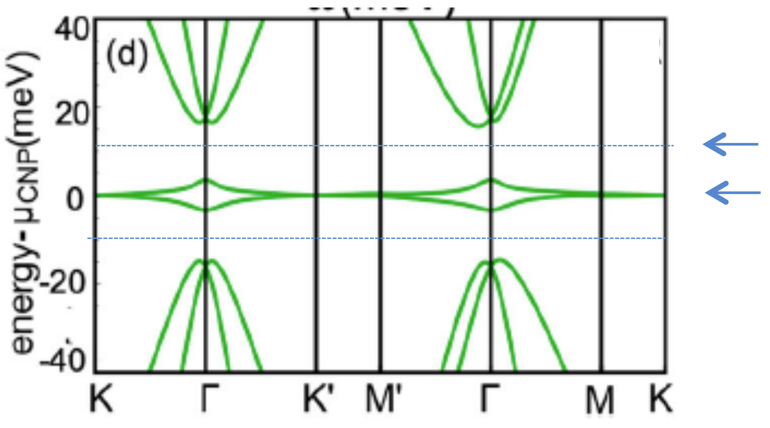
CNP (undoped)

Doping the flat bands with a gate

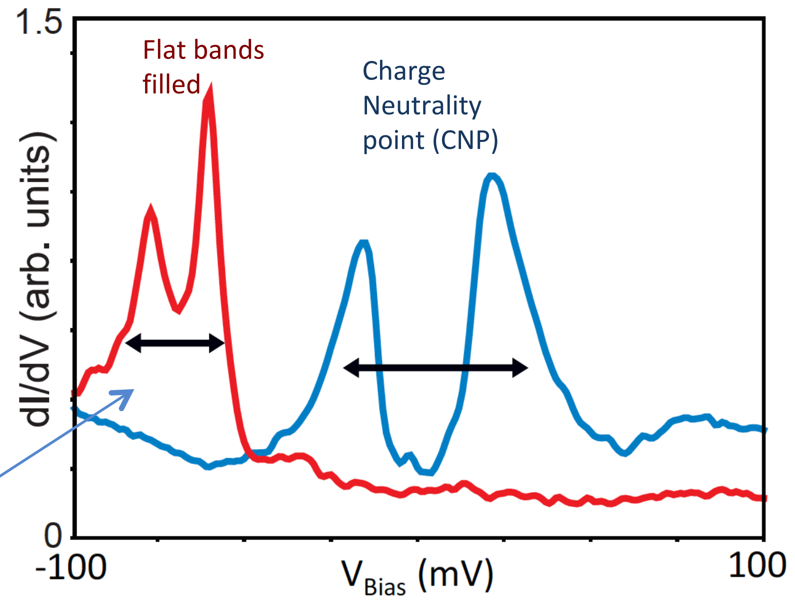


Suarez Morell et al, PRB 82, 121407 (2010), Bistritzer & Macdonald, PNAS 108, 12233 (2011), Cao et al, Nature 556, 80 (2018), Nature 556, 43 (2018)
Cao et al, PRX 8, 031087 (2016), Koshino et al, PRX 031037 (2018)

Spectral Weight Reorganization and Cascades from STM measurements in TBG



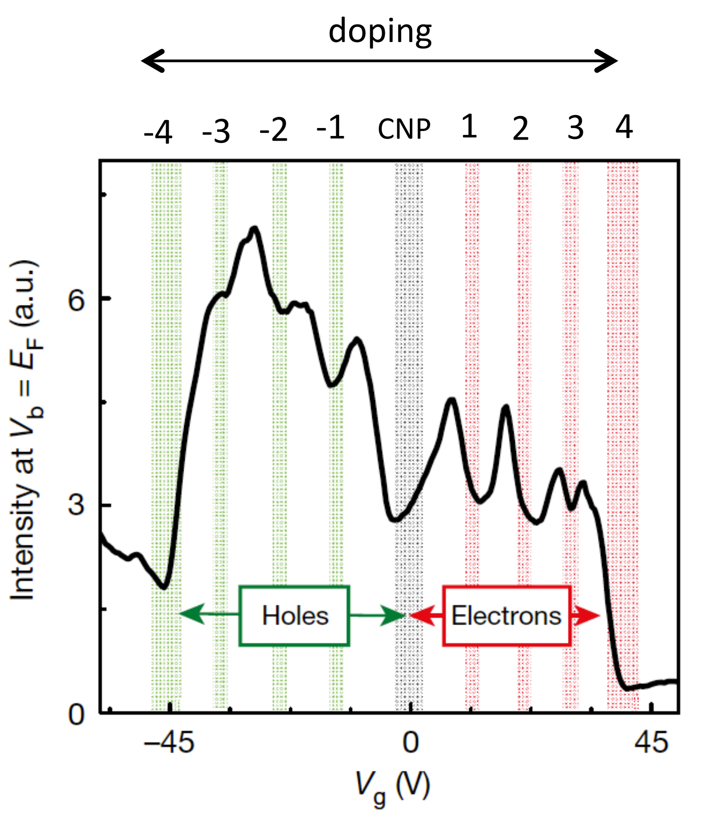
Doping dependent density of states



Two peaks due to the presence of two van Hove singularities

Choi et al, Nature Physics 15, 1174 (2019)

Minima in the density of states at the Fermi level at integer filling



Jiang et al (E. Andrei), Nature 573, 91 (2019)

leni.bascones@csic.es

Spectral Weight Reorganization in TBG: Cascades from STM measurements

Color plot of dI/dV (Density of states) as a function of energy and doping

Asymmetric resets at integer fillings

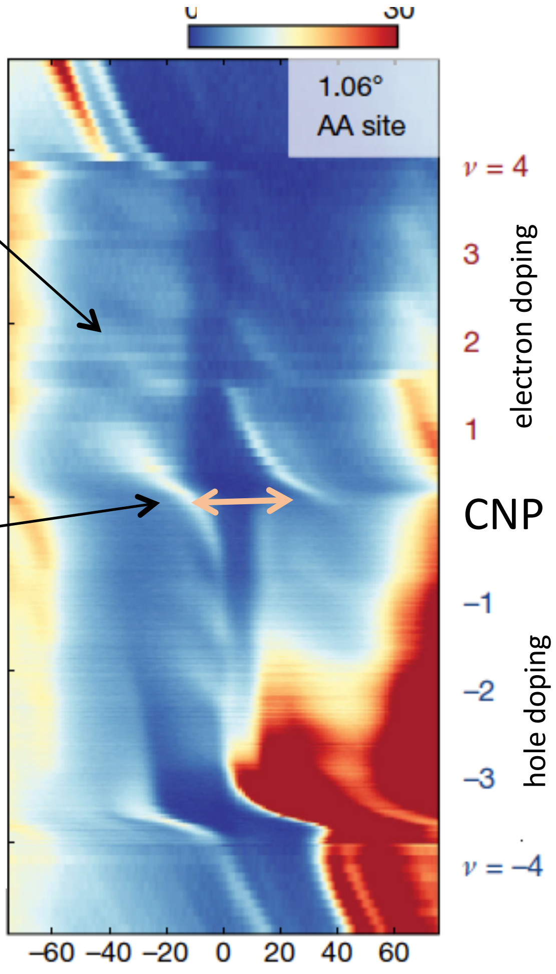
Spectral weight flow from ~30 meV
towards chemical potential
in the form of cascades
at positive and negative energies

Different shape at CNP

Wong et al, Nature
582, 198, (2020)

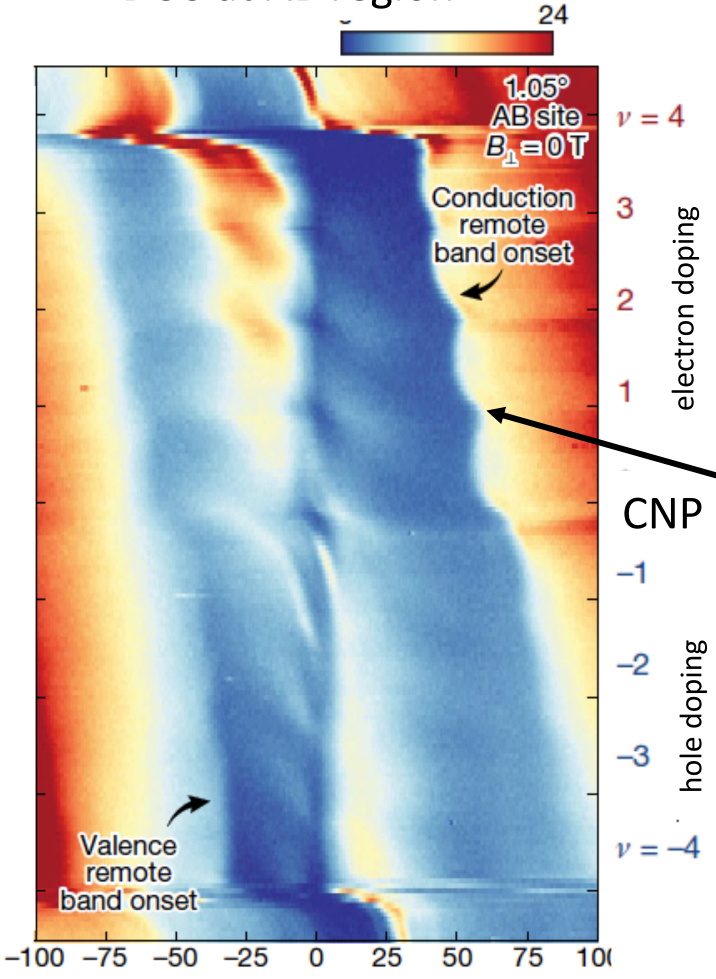
See also
Choi et al Nature 589, 536 (2021);
Nat Phys. 17,1375 (2021);
Polski et al, arXiv2205.05225

DOS at AA region

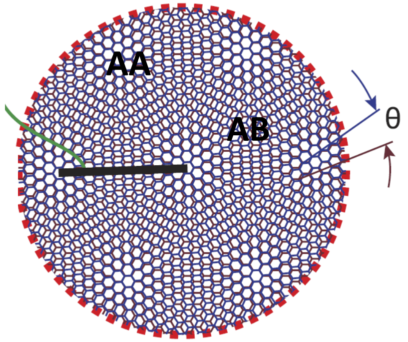


Energy from Fermi level

DOS at AB region



Energy from Fermi level

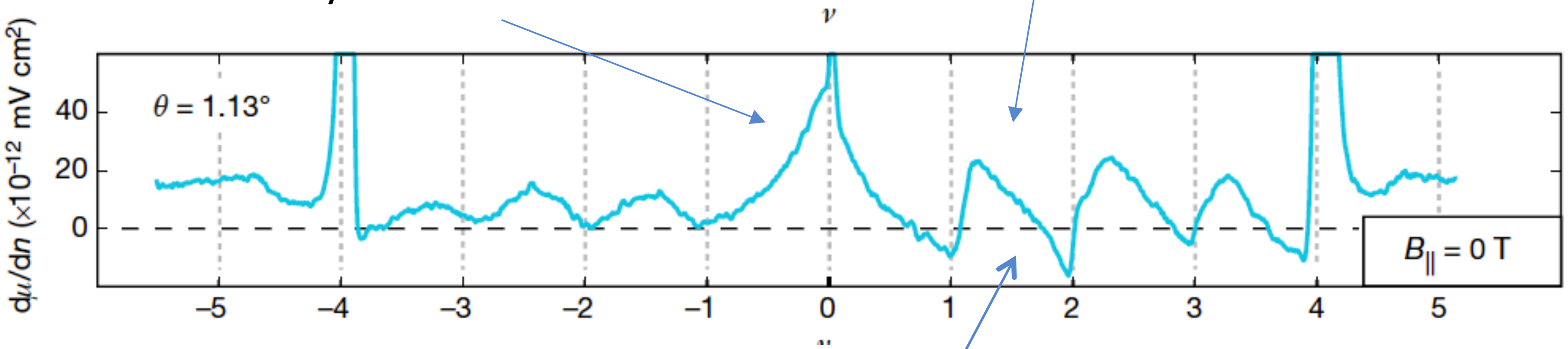


Oscillations of the remote bands energy (oscillations of the chemical potential)

Cascades in the inverse compressibility of TBG

Sawtooth asymmetric peaks in the inverse compressibility around integer fillings of the flat bands.

Symmetric at CNP



Zondiner et al, Nature 582, 203 (2020)

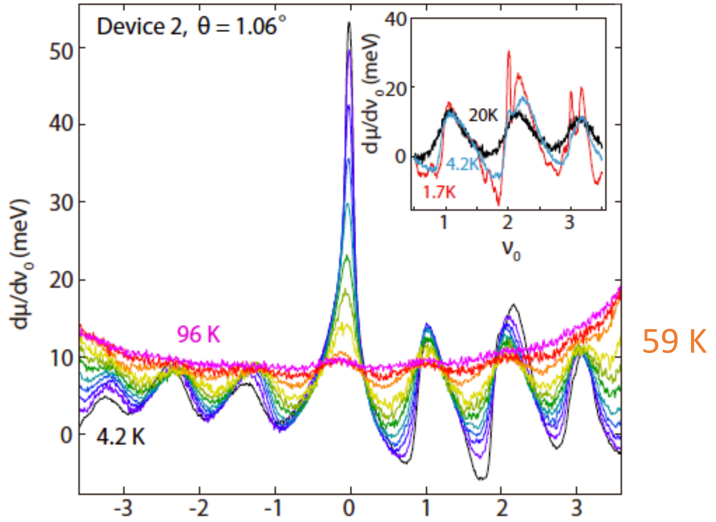
Negative inverse compressibility

Cascades (Dirac revivals) in TBG primarily interpreted with models which involve symmetry breaking in some way

Wong et al, Nature 582, 198, (2020), Zondiner et al, Nature 582, 203 (2020), Kang, Bernevig,Vafek, PRL 127, 266402 (2021);
Hong et al, PRL 129, 147001 (2022) Chichinadze (Chubukov) et al, npj Quant. Mat. 7, 114 (2022) ; Ingham et al (Scheurer), arXiv:2308.00748

Cascades in TBG resilient with temperature and resistive states

Inverse compressibility



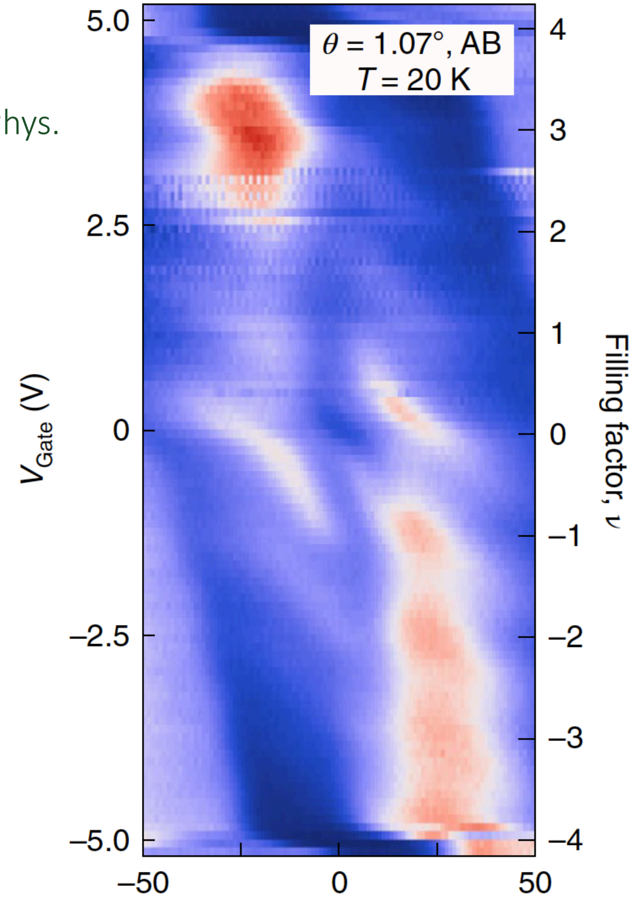
doping

Saito et al,
Nature 592, 220 (2021)

See also Rozen et al,
Nature 592, 214 (2021)

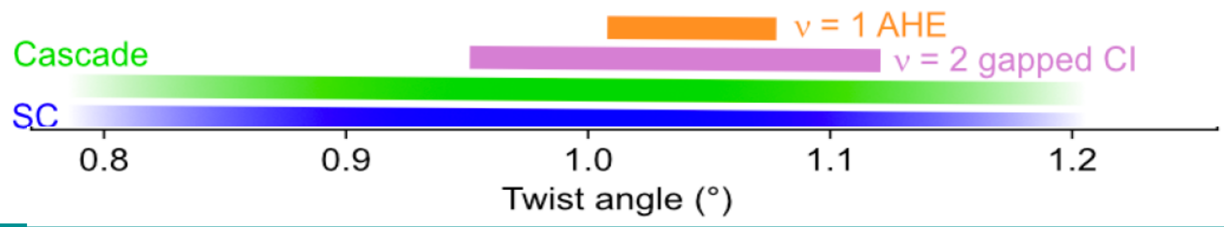
STM

Choi et al, Nat Phys.
17,1375 (2021)



Energy from Fermi level

Cascades are more resilient in temperature and twist angle than other correlated states (insulating, ferromagnetic, IVC) and involve larger energy scales (30 meV)

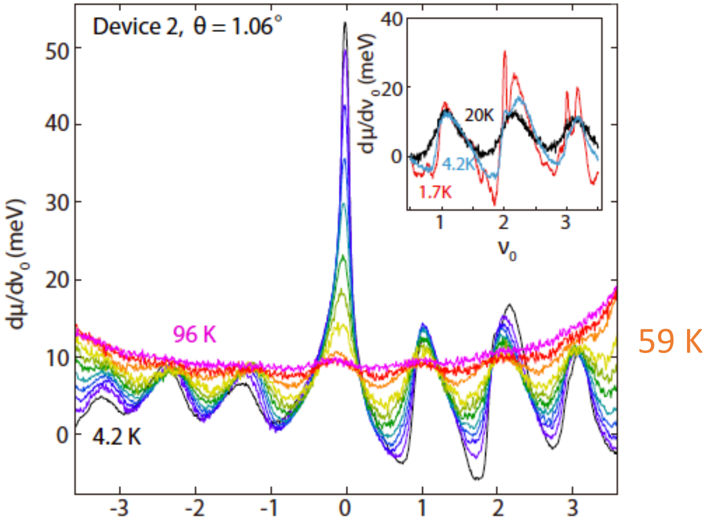


Polski et al, arXiv2205.05225

leni.bascones@csic.es

Cascades in TBG resilient with temperature and resistive states

Inverse compressibility



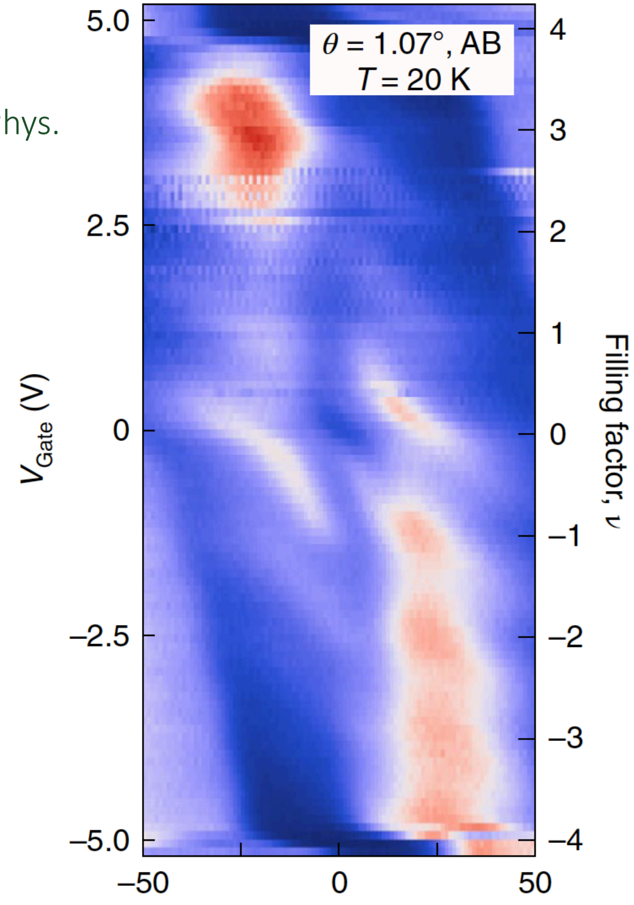
doping

Saito et al,
Nature 592, 220 (2021)

See also Rozen et al,
Nature 592, 214 (2021)

STM

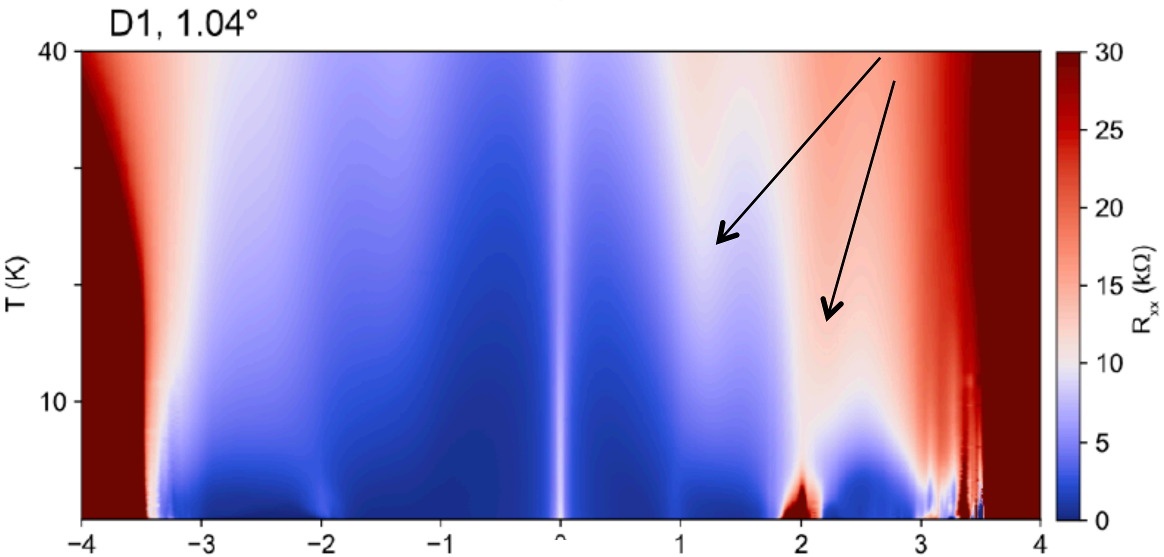
Choi et al, Nat Phys.
17,1375 (2021)



Energy from Fermi level

Resistivity

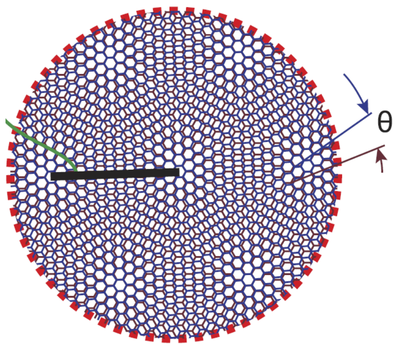
Resistive states



doping

Polski et al,
arXiv2205.05225

Take home message: The cascades constitute the normal state of TBG (no symm. breaking)



Cascades already present
in the normal state
& consequence of local physics:
Formation of local moments &
Heavy quasiparticles

T

Normal state

Ordered state (Symmetry breaking)

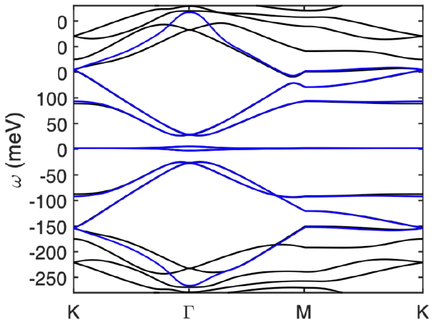
Doping or tuning parameter

Superconducting
Ferromagnetic
Intervalley order, …

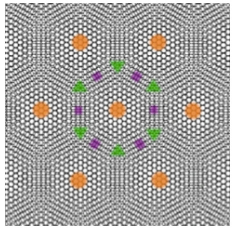
leni.bascones@csic.es

Multi-orbital models for Twisted Bilayer Graphene

Moiré orbital models for TBG with 5, 6, 8 and 10 orbitals per valley

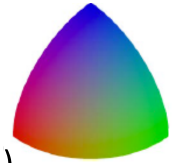


C_3, C_{2T} and M_{2y} symmetry in each valley



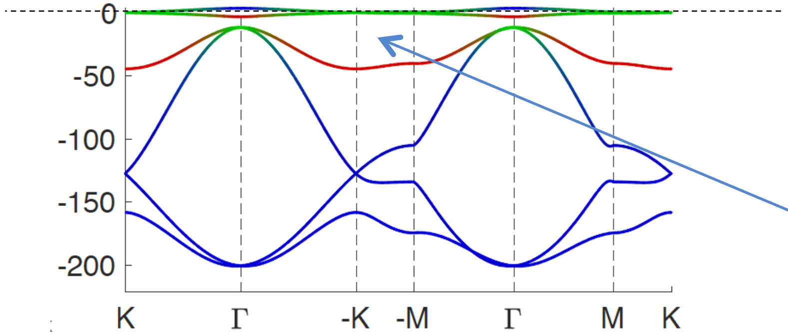
6 orbital model

3 s orbitals (Kagome)



1 p_z orbital (Triangular-AA)

p+ & p- orbitals (Triangular-AA)



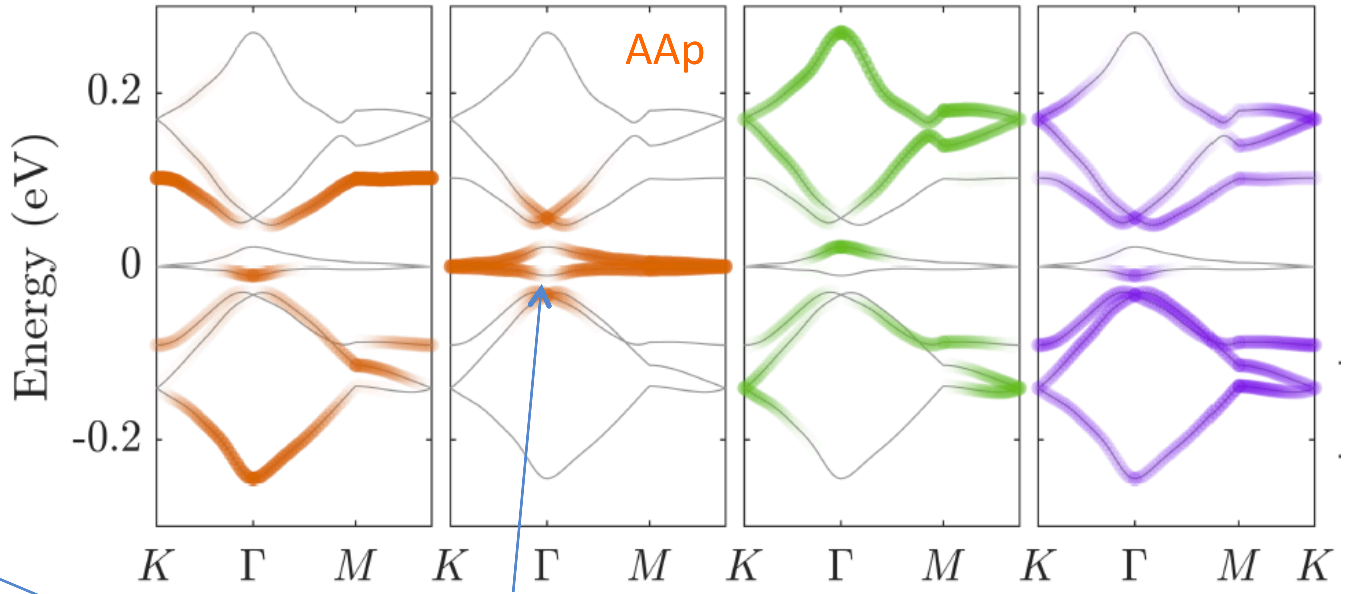
8 orbital model

1 s orbital Triangular (AA)

p+ and p- orbitals Triangular (AA)

2 Pz orbitals Honeycomb (AB/BA)

3 s orbitals Kagome (DW)

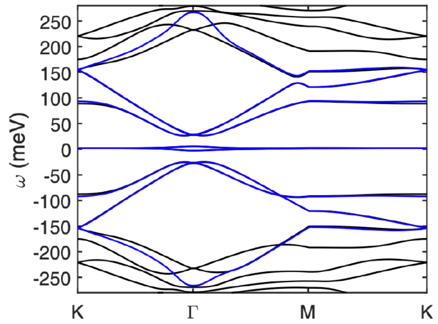


Flat bands: p+ and p- orbitals @ Triangular lattice AA (AAp orbitals) everywhere except at Γ (Fragile topology in TBG)

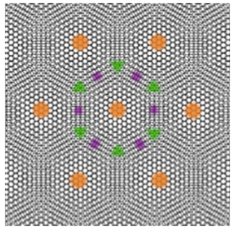
L. Zou, H.C. Po, A. Vishwanath, T. Senthil, PRB 98, 085435 (2018), Z. Song, AZ. Wang, W. Shi, G. Li, C. Fang, B.A. Bernevig 123, 036401 (2019), H.C. Po, L. Zou, T. Senthil, A. Vishwanath, PRB 99, 195455 (2019); S. Carr, S. Fang, Z. Zhu, E. Kaxiras, PRR 1, 013001 (2019), S. Carr, S. Fang, H.C. Po, A. Vishwanath, E. Kaxiras, PRR 1, 033072 (2019)

Multi-orbital models for Twisted Bilayer Graphene

Orbital models for TBG with
5, 6, 8 and 10 orbitals per valley



C_3, C_{2T} and M_{2y}
symmetry in each valley

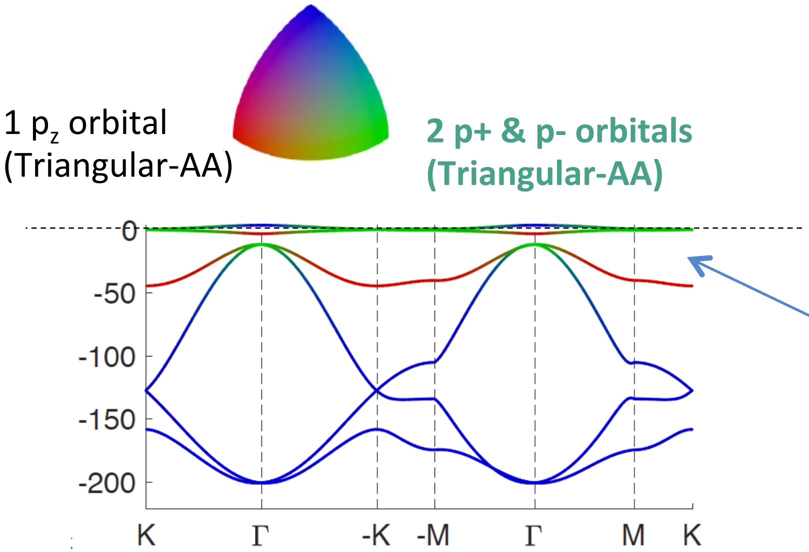


6 orbital model

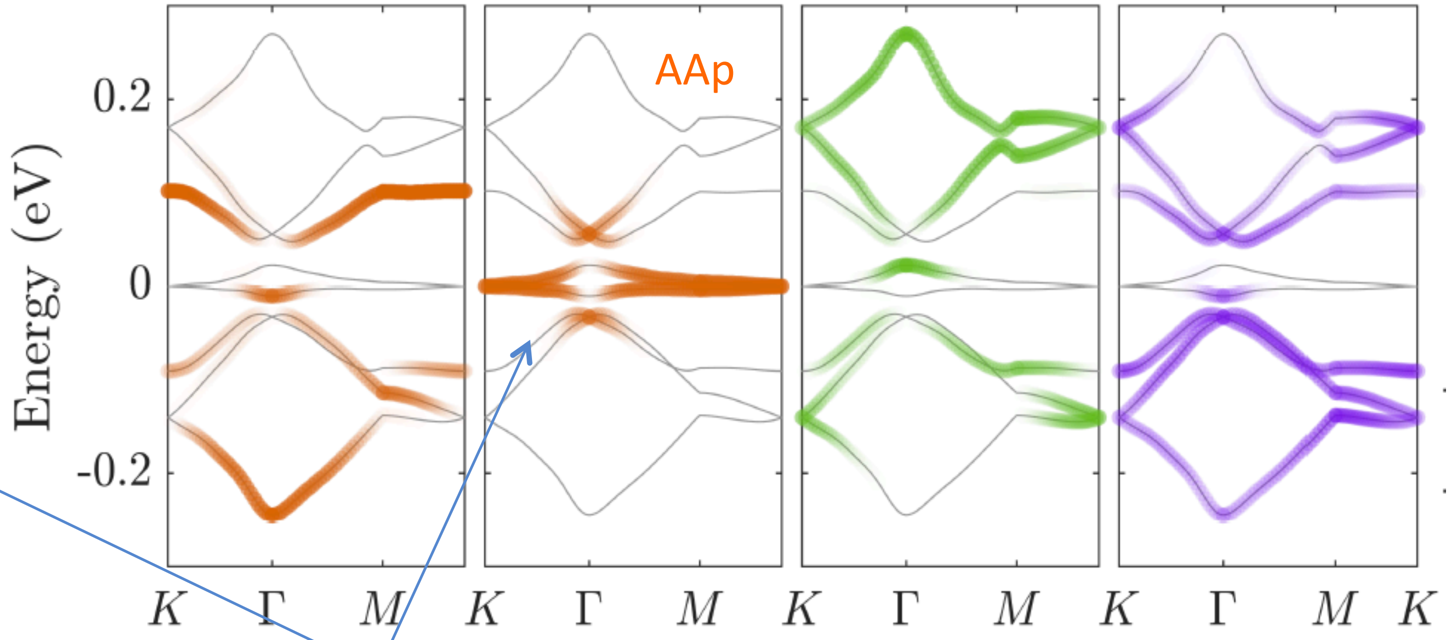
3 s orbitals (Kagome)

1 p_z orbital
(Triangular-AA)

2 p+ & p- orbitals (Triangular-AA)



8 orbital model



At each valley: 2 flat orbitals coupled to more dispersive electrons

M. Haule, E. Andrei, K. Haule, arXiv:1901.09852 (2019): Heavy fermion like description

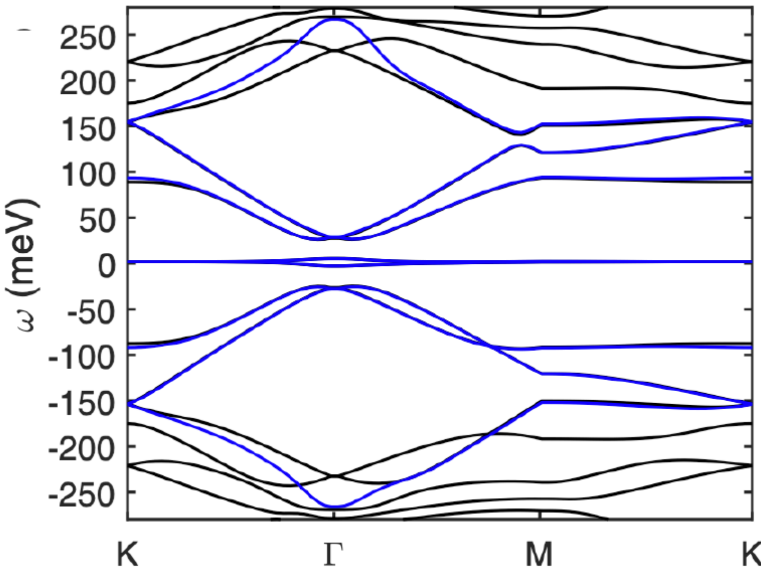
8 orbital model (per valley) for Magic AngleTBG

θ ~1.08º

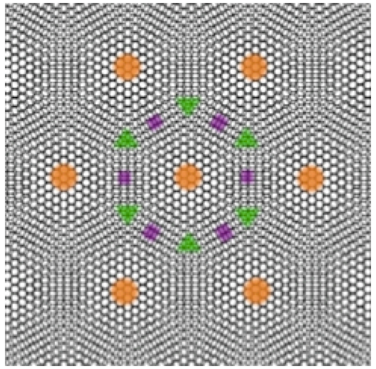
AA/AB tunneling

w_0/w_1=0.78

Includes C_3, C_{2T} and M_{2y} symmetry in each valley



8 orbitals per valley (16 in total) in triangular, honeycomb and kagome lattices.



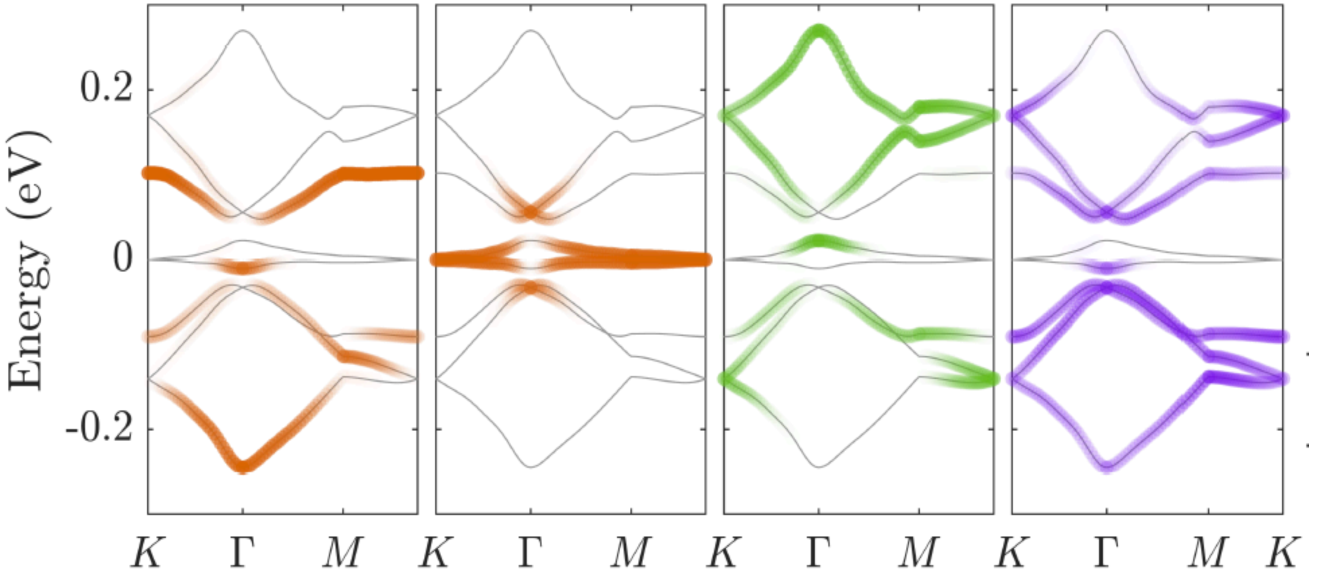
8 orbital model

1 s orbital Triangular (AA)

2 p+ 2p- orbitals Triangular (AA)

2 Pz orbitals Honeycomb (AB/BA)

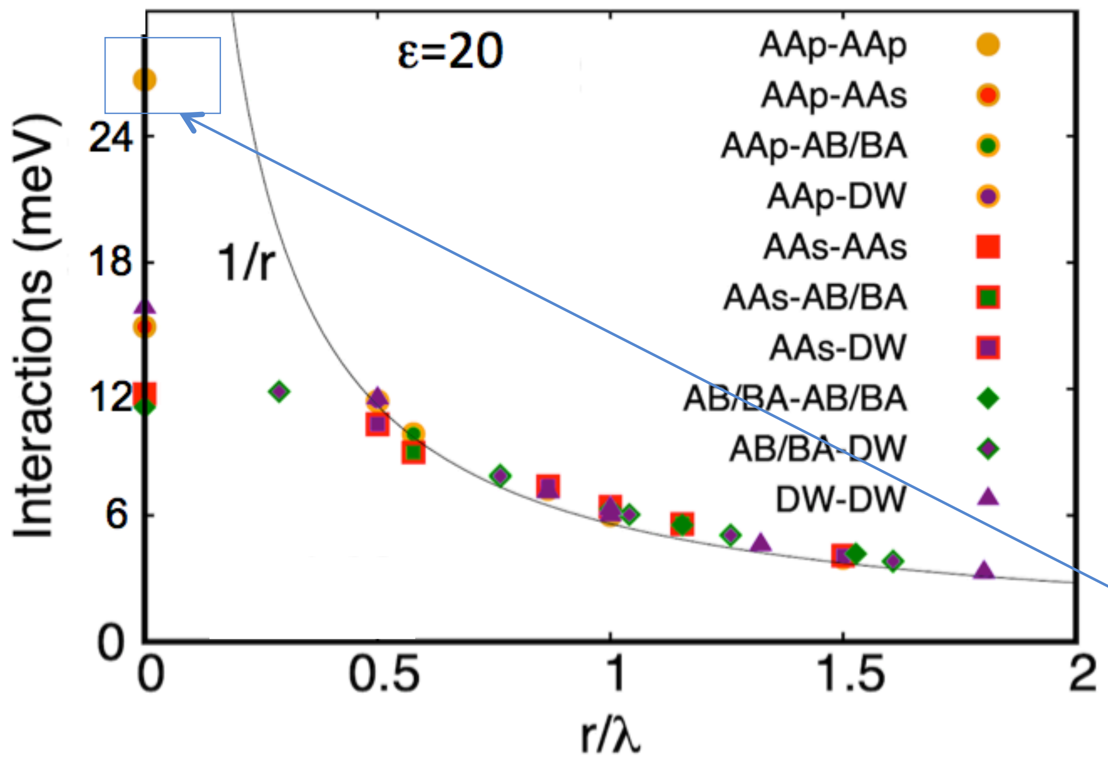
3 s orbitals Kagome (DW)



Wannierization adapted from S. Carr, S. Fang, H.C. Po, A. Vishwanath, E. Kaxiras, PRR 1, 033072 (2019)

Interactions in the 8 orbital model (per valley) in Twisted Bilayer Graphene

All density-density interactions
intra and inter moiré unit cell, Intra and inter orbital
(1/r interaction between rhe electrons in the carbon atoms)



Smaller Hund´s & Exchange

λ: moire lattice constant

AA-s triangular | AA-p+ and p- (triangular lattice) | AB/BA-pz honeycomb | DW-s

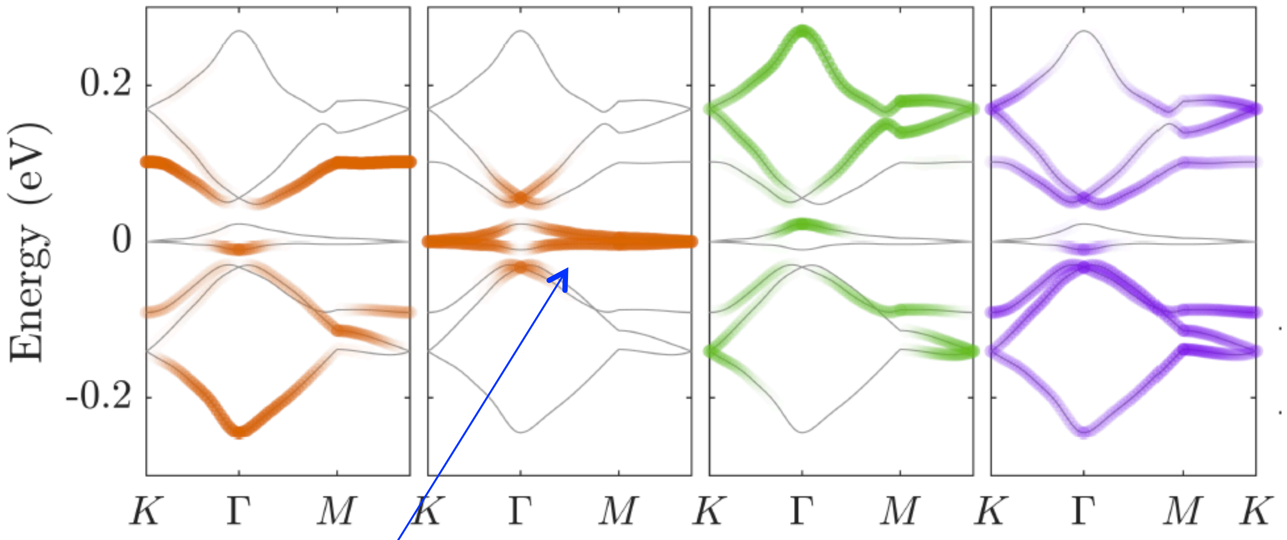


Fig from: S. Carr, et al PRR 1, 033072 (2019)

AA-p Intra-moiré
Interaction and small bandwidth

Only these AAp orbitals can give rise to Mott like physis (local moments)

M.J. Calderón, & EB, PRB 102,155149 (2020)

leni.bascones@csic.es

Interactions in the 8 orbital model (per valley) for TBG

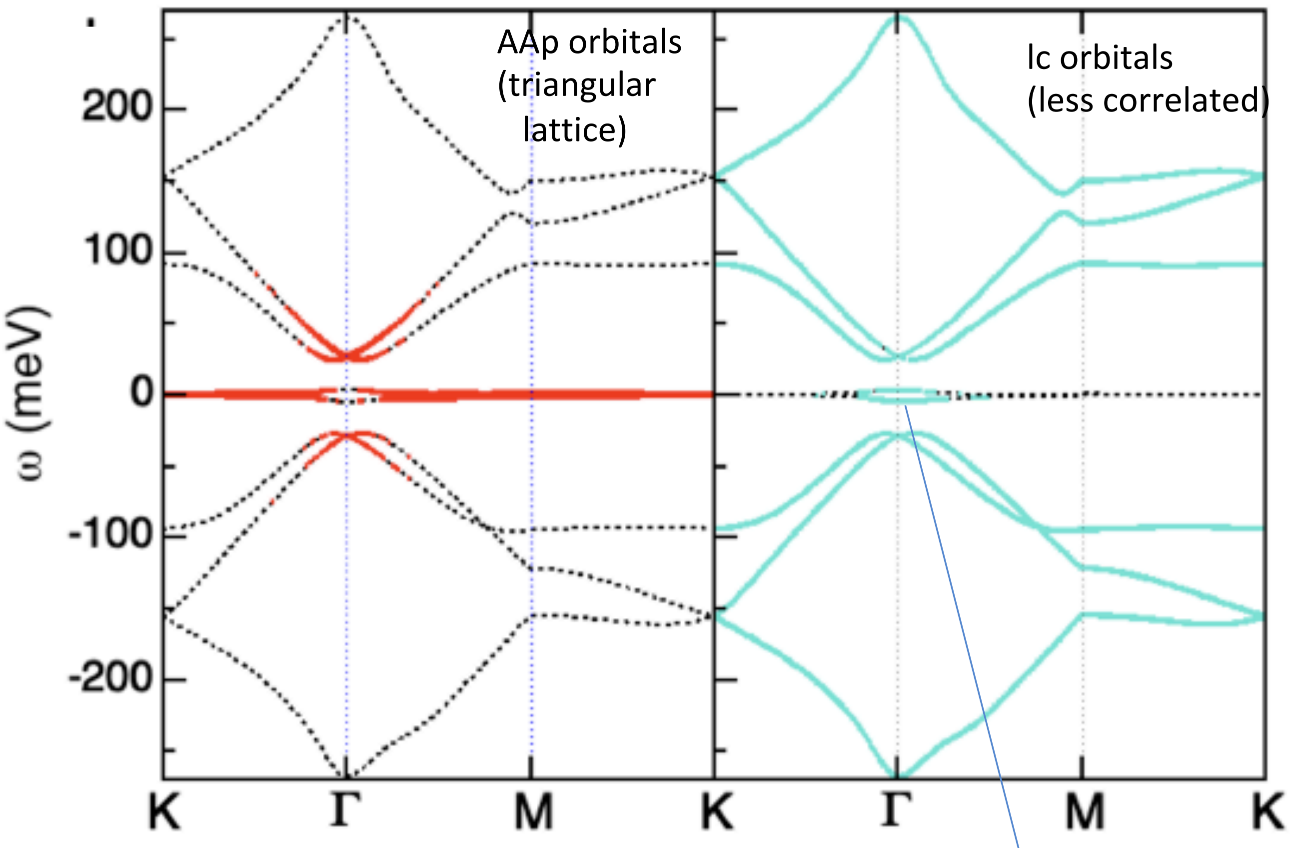
4 AAp (p+ and p-) strongly correlated orbitals (2 per valley)

coupled to and interacting with

12 less correlated (lc) orbitals, 6 per valley

↓

Extended heavy-fermion like model



lc orbitals at Γ of the flat bands: Fragile topology

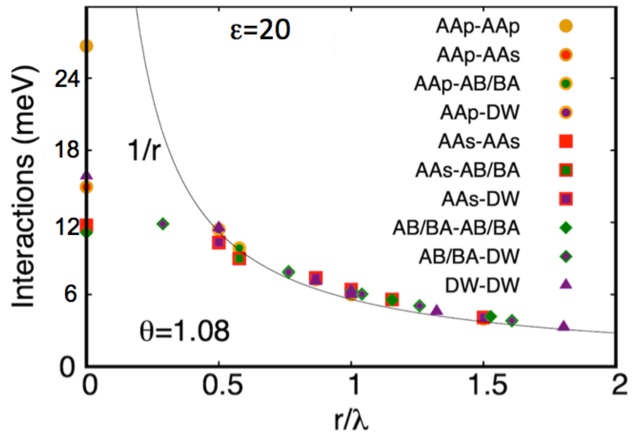
See also: M. Haule, E. Andrei, K. Haule, arXiv:1901.09852 (2019), Song and Bernevig, PRL 129, 047601 (2022)

M.J. Calderón, & EB, PRB 102,155149 (2020)

A. Datta, MJ Calderón, A. Camjayi, EB, Nature Comms 14, 5036 (2023)

DMFT + Hartree Description for 8 orbital model per valley for TBG

Only density-density interactions included



DMFT + Hartree Description

DMFT (self-consistent)
Intra and inter-orbital
onsite interaction U
among AA-p orbitals
(Four correlated orbitals)

CTQMC-DMFT

Haule PRB 75,155113 (2007)

Hartree

Any other interaction
(including intersite), some
involve the correlated orbitals

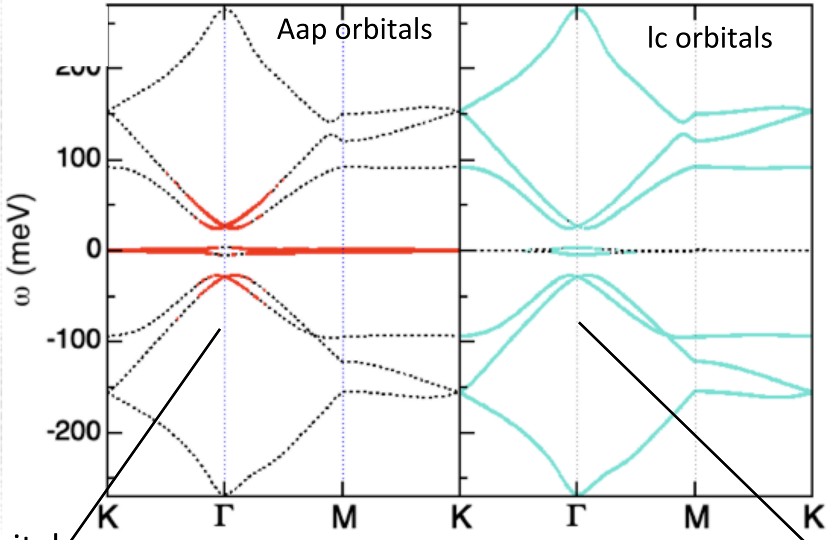
Self-consistency

@ T=6 K   ε=20   U=27 meV

Focus on the "normal" state without symmetry breaking
Lack of symmetry breaking imposed

A. Datta, MJ Calderón, A. Camjayi, EB, Nature Comms 14, 5036 (2023)

Cascades and oscillations in the Density of States

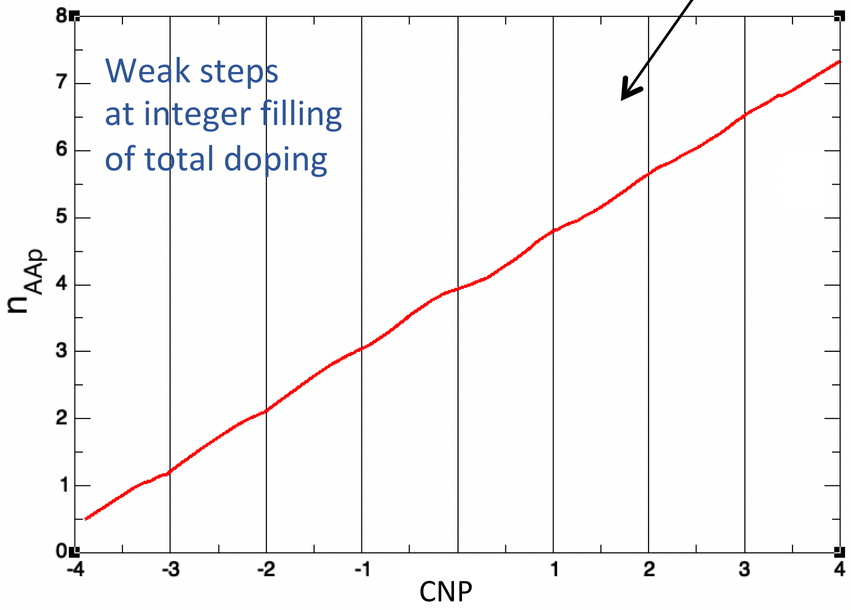


No symmetry breaking allowed

ε=20

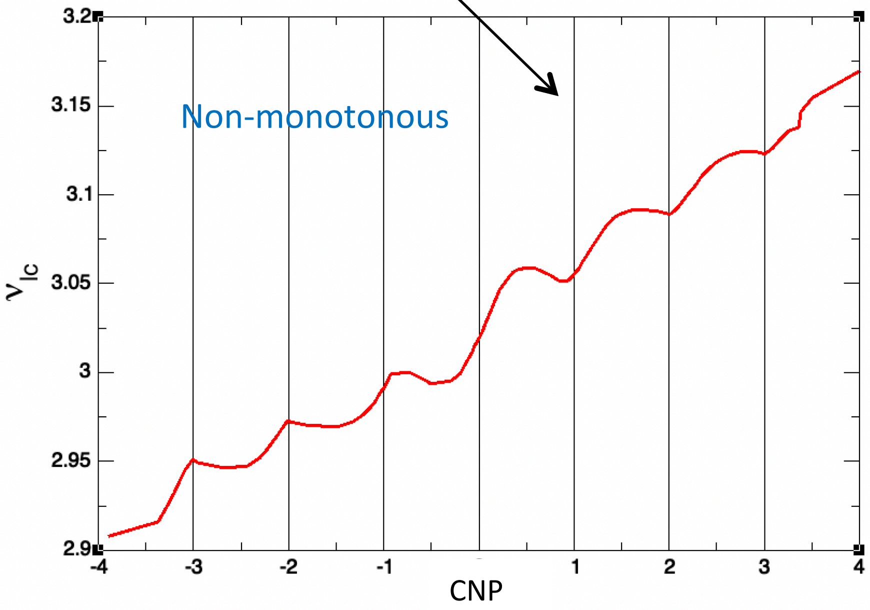
U=26.7 meV

Filling of strongly correlated Aap orbitals



Total doping

Filling of less correlated lc orbitals



Total doping

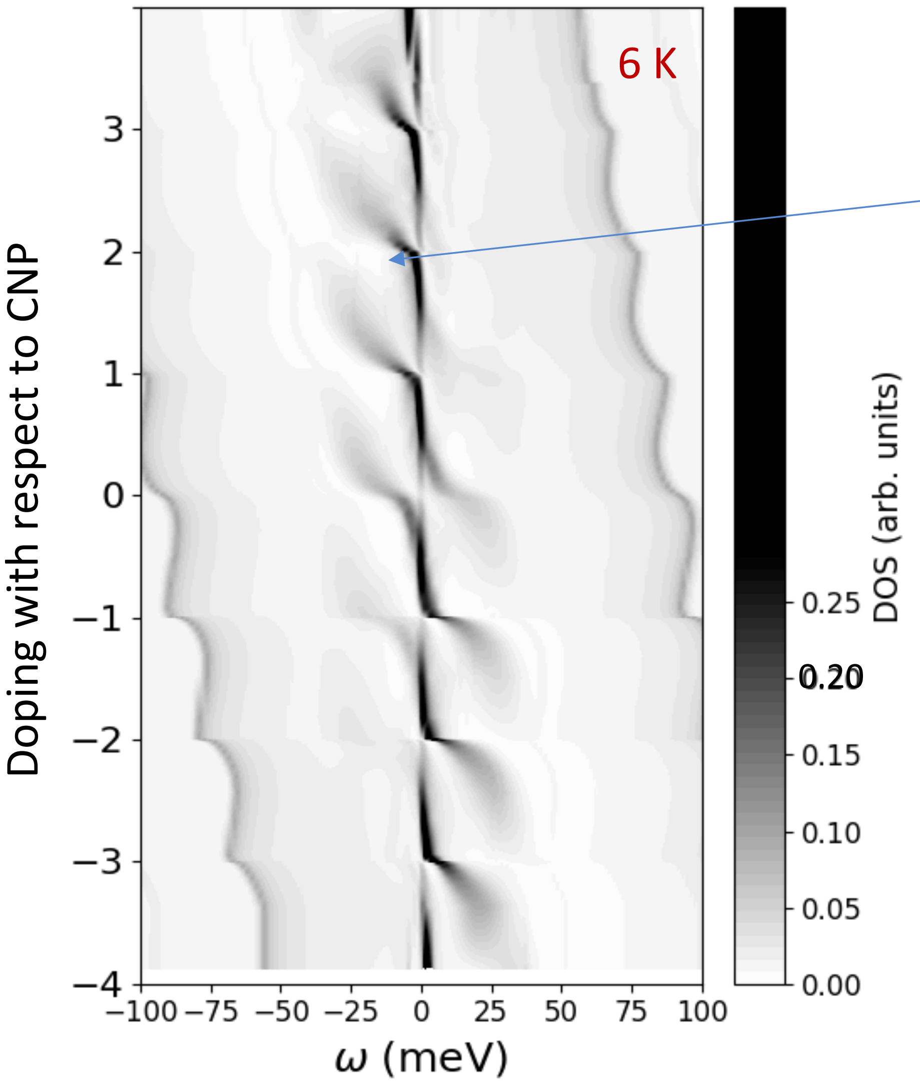
A Datta, MJ Calderón, A. Camjayi, EB, Nature Comms 14, 5036 (2023)

See also: Hu et al, arXiv: 2301.04669, 2301.04673

Total Density of States (DMFT + Hartree)

ε=20 U=27 meV

No symmetry breaking allowed



Energy with respect to the chemical potential

Strong reorganization of the spectral weight up to energies~ U Hubbard bands

A Datta, MJ Calderón, A. Camjayi, EB, Nature Comms 14, 5036 (2023)

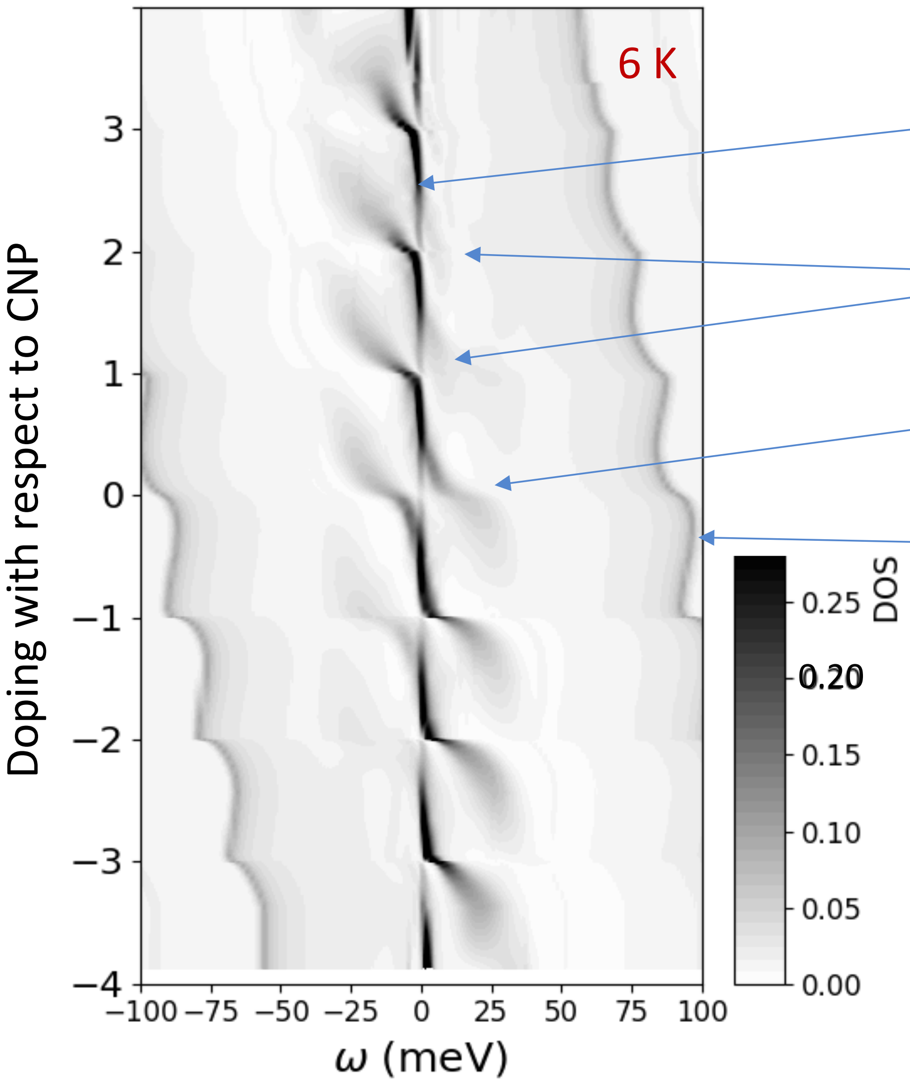
leni.bascones@csic.es

Cascades and oscillations in the Density of States

Total Density of States (DMFT + Hartree)

ε=20 U=27 meV

No symmetry breaking allowed



Energy with respect to the chemical potential

Spectral weight flows towards the chemical potential in the form of cascades at positive and negative energies

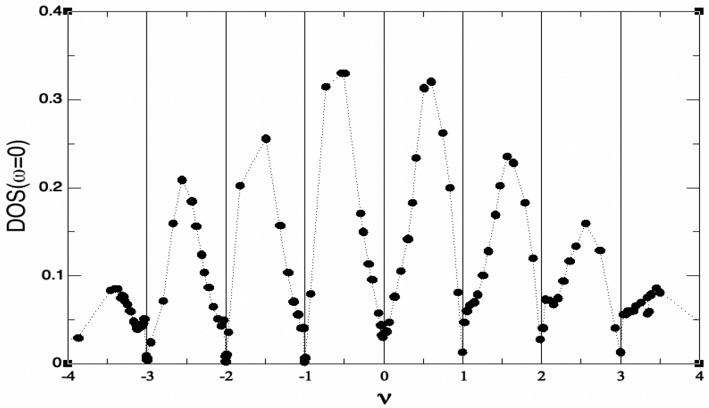
Asymmetric resets in the Density of States at integer dopings

Different shape at CNP

Oscillations of the remote bands

A Datta, MJ Calderón, A. Camjayi, EB, Nature Comms 14, 5036 (2023)

Suppression of DOS at Fermi level



See also:
Jiang et al, Nature 573, 91 (2019),
Hu et al, arXiv:2301.04673

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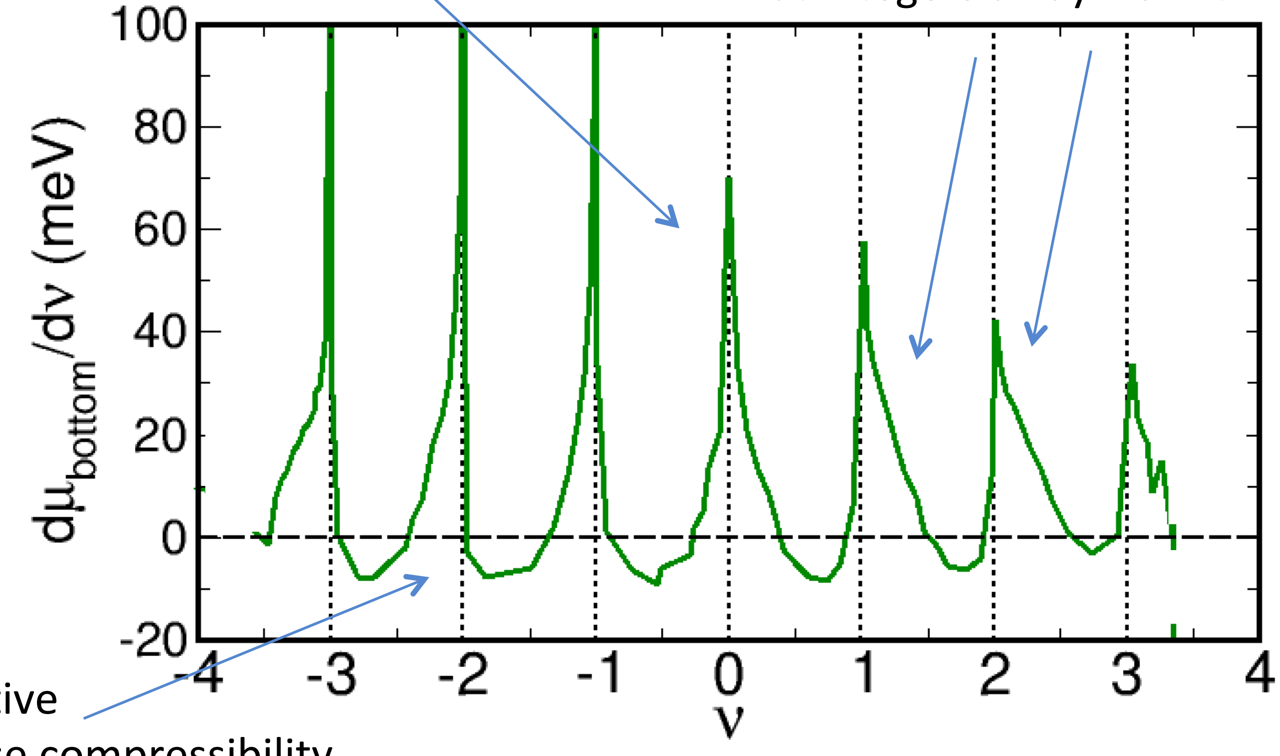
Sawtooth peaks in the inverse compressibility

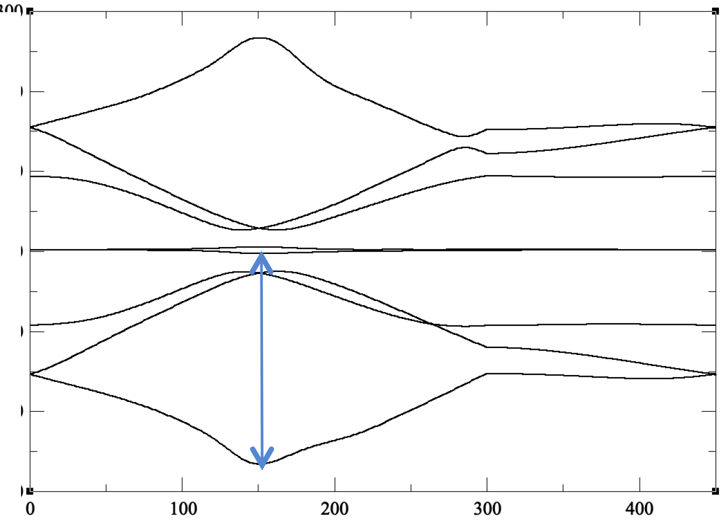
Symmetric peak at CNP

Sawtooth asymmetric peaks at integers away from CNP



doping

Negative Inverse compressibility



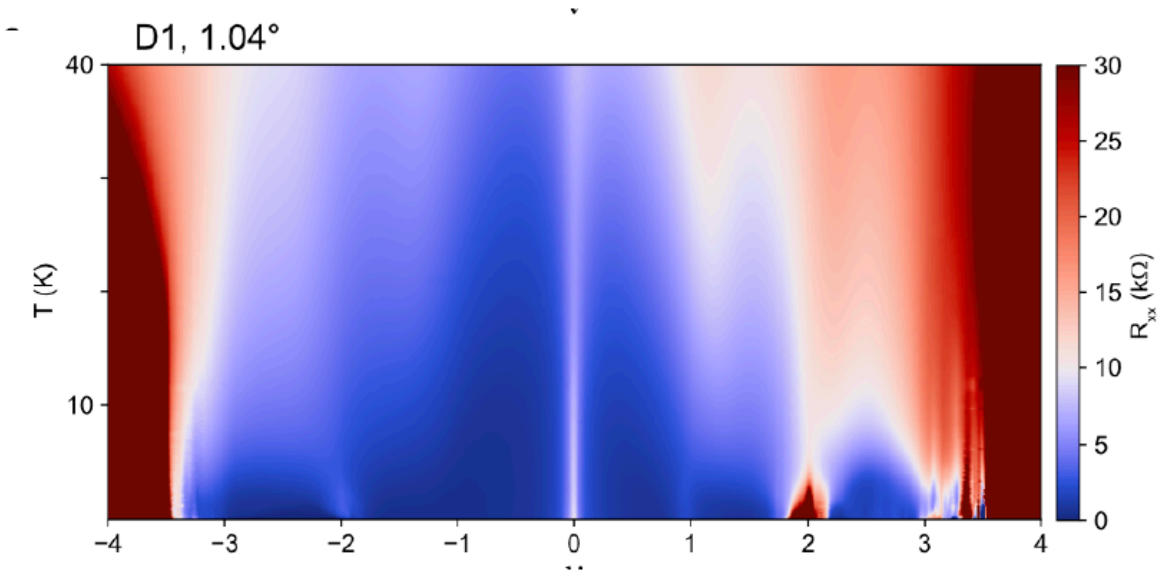
ε=20 U=26.7 meV

No symmetry breaking allowed

A. Datta, MJ Calderón, A. Camjayi, EB,
B. Nature Comms 14, 5036 (2023)

Negative inverse compressibility also Rai et al, 2309.08509

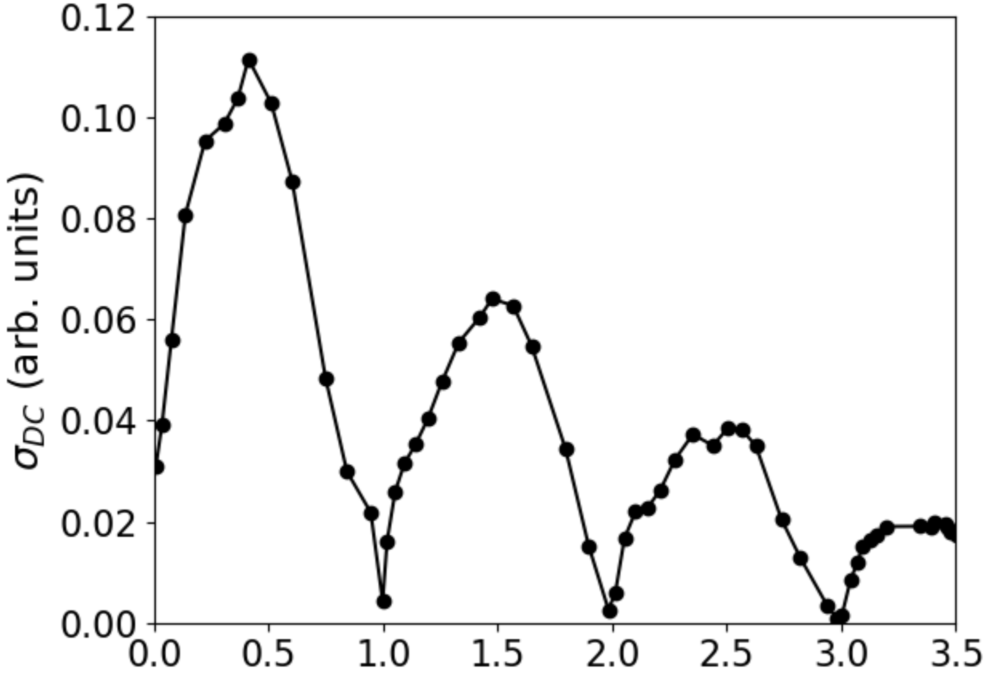
Resistive states without symmetry breaking



Polski et al, arXiv2205.05225

Recent unpublished data

d.c conductivity



CNP

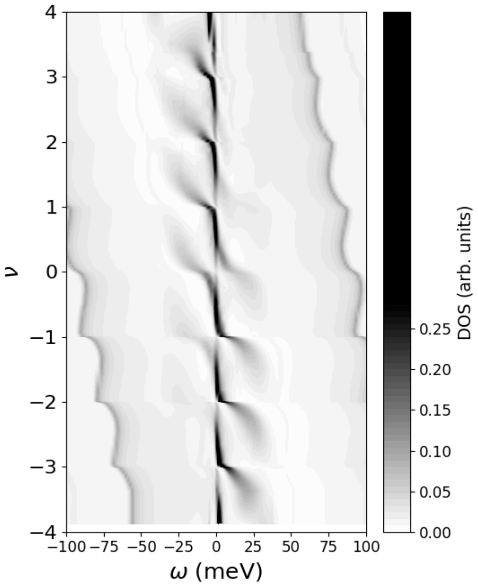
doping

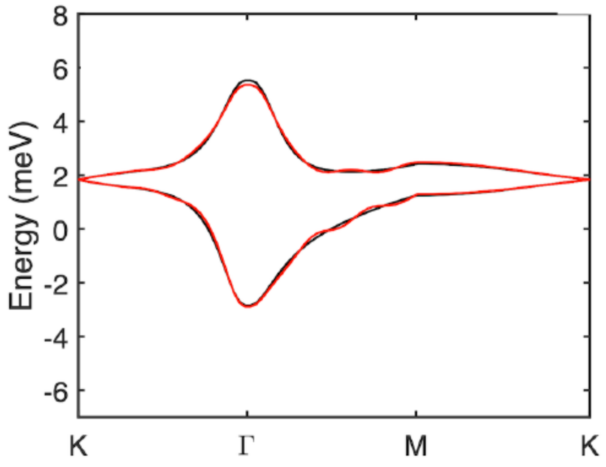
Resistive states
in transport at integer fillings

Momentum selective incoherence in the band spectrum

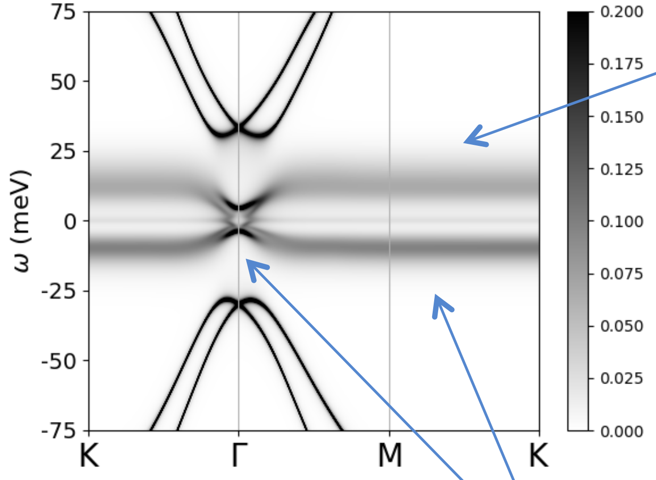
ε=20 U=26.7 meV

No symmetry breaking allowed



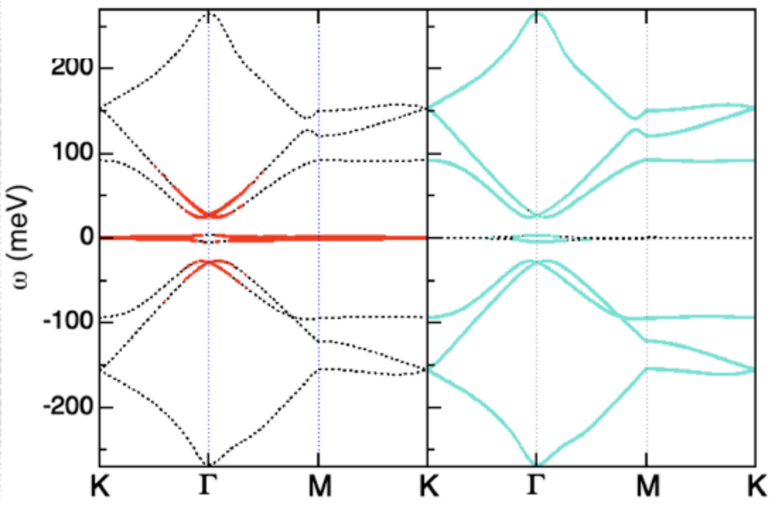


Charge Neutrality Point (no doping)



Incoherent
Local moment

Momentum
selective incoherence



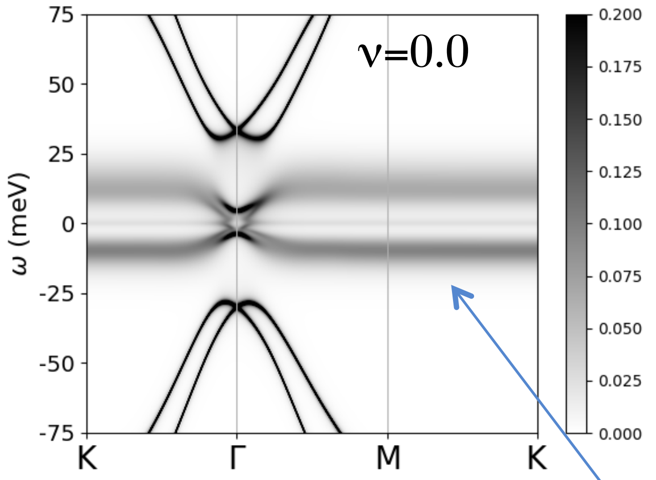
See also Hofmann et al, PRX 12, 011061 (2022)

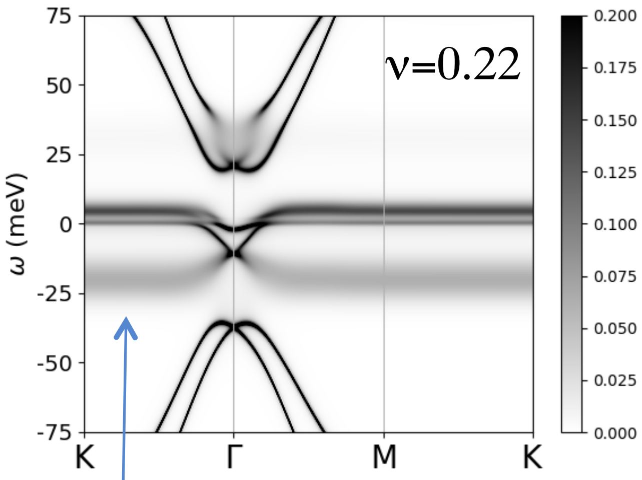
A. Datta, MJ Calderón, A. Camjayi, EB,
B. Nature Comms 14, 5036 (2023)

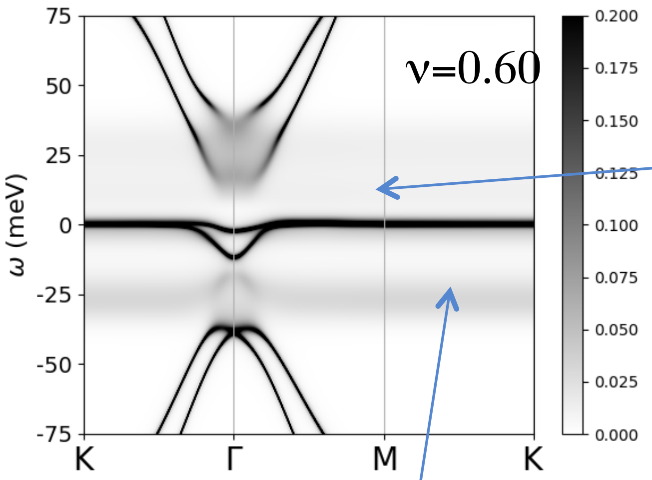
Momentum selective incoherence in the band spectrum and resets in the bands

ε=20 U=26.7 meV

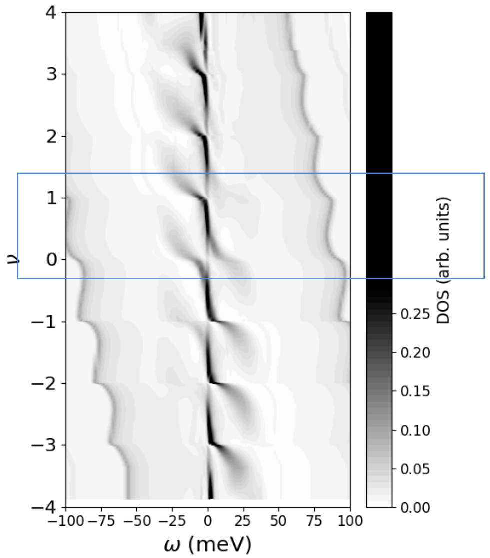
No symmetry breaking allowed





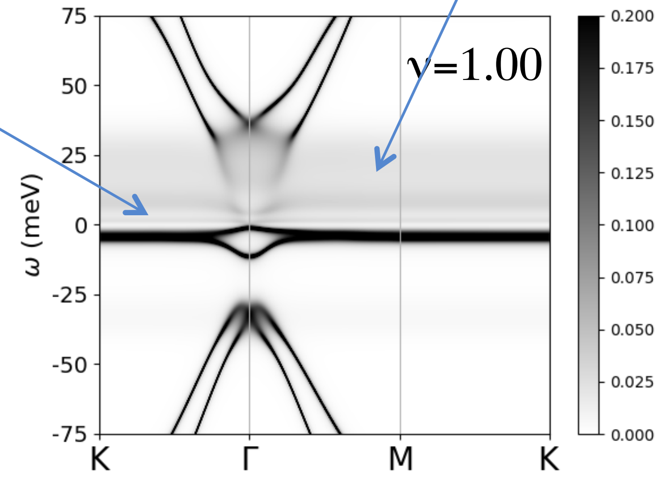


Band flattening when approaching Integer fillings from smaller doping



Incoherent Local moment

Tendency to form a heavy quasiparticle



A. Datta, MJ Calderón, A. Camjayi, EB, Nature Comms 14, 5036 (2023)

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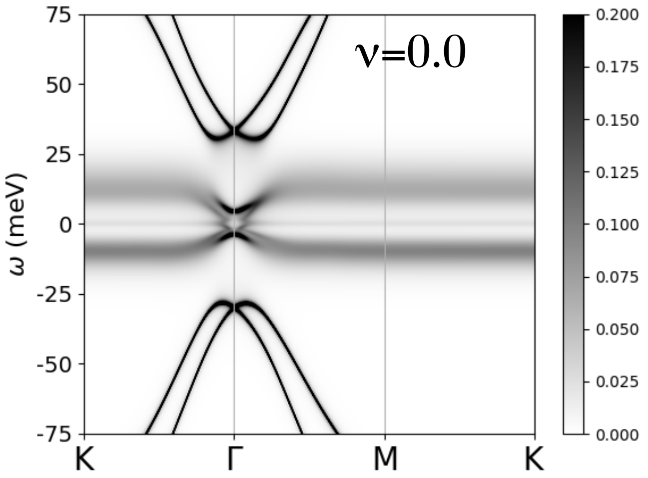
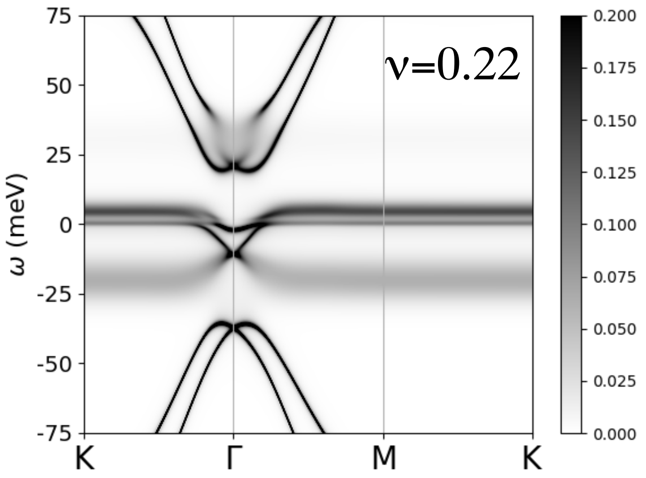
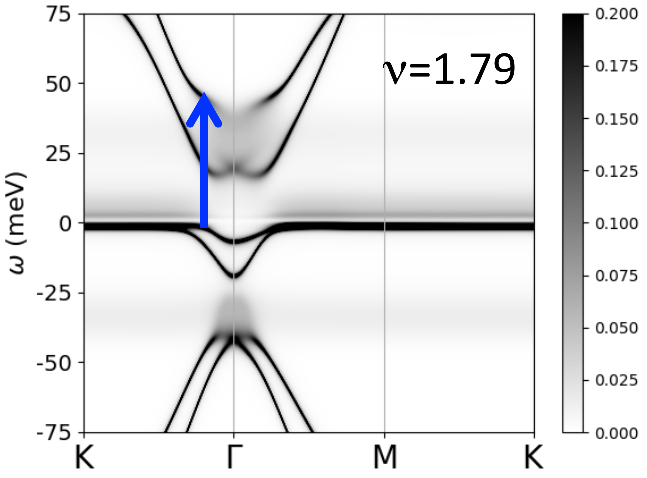
Cascades in the optical spectrum of Twisted Bilayer Graphene

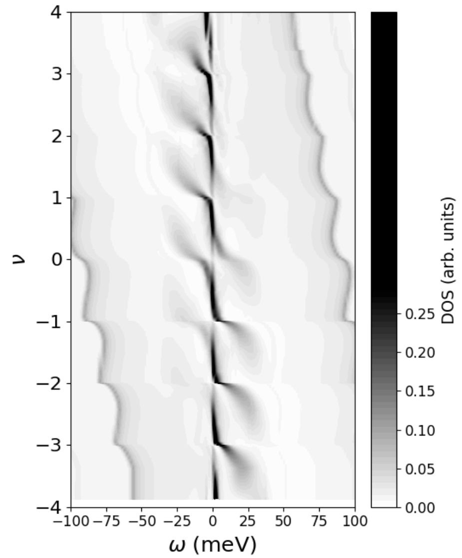
ε=20 U=26.7 meV

No symmetry breaking allowed









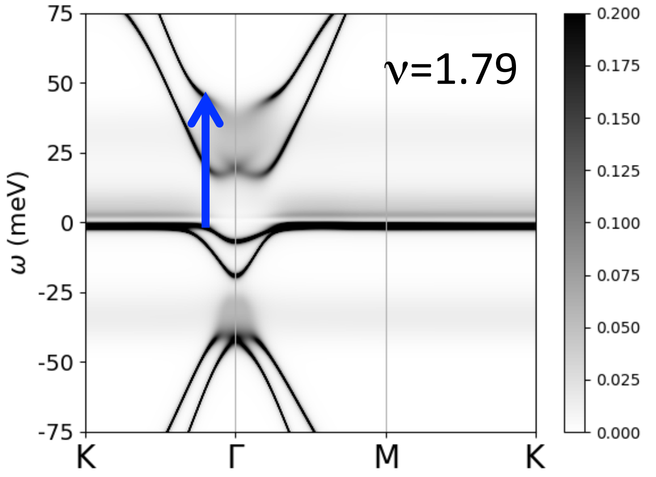
- Resets in the spectral weight with oscillations in energies
- Doping dependent momentum selective incoherence

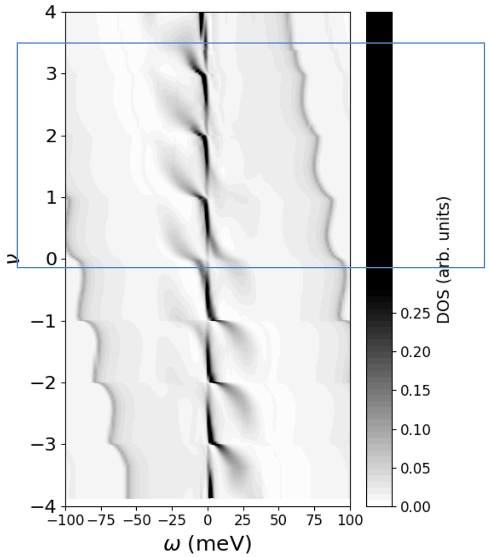
A. Datta, MJ Calderón, A. Camjayi, EB, Nature Comms 14, 5036 (2023)

leni.bascones@csic.es

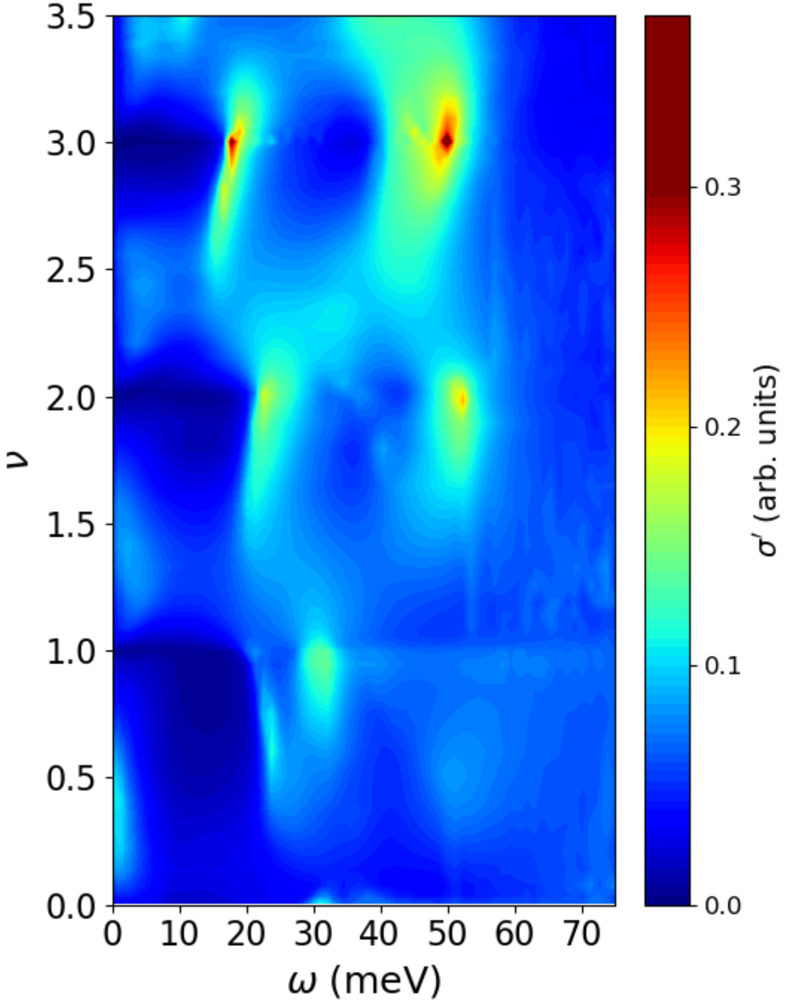
Cascades in the optical spectrum of Twisted Bilayer Graphene

New unpublished data

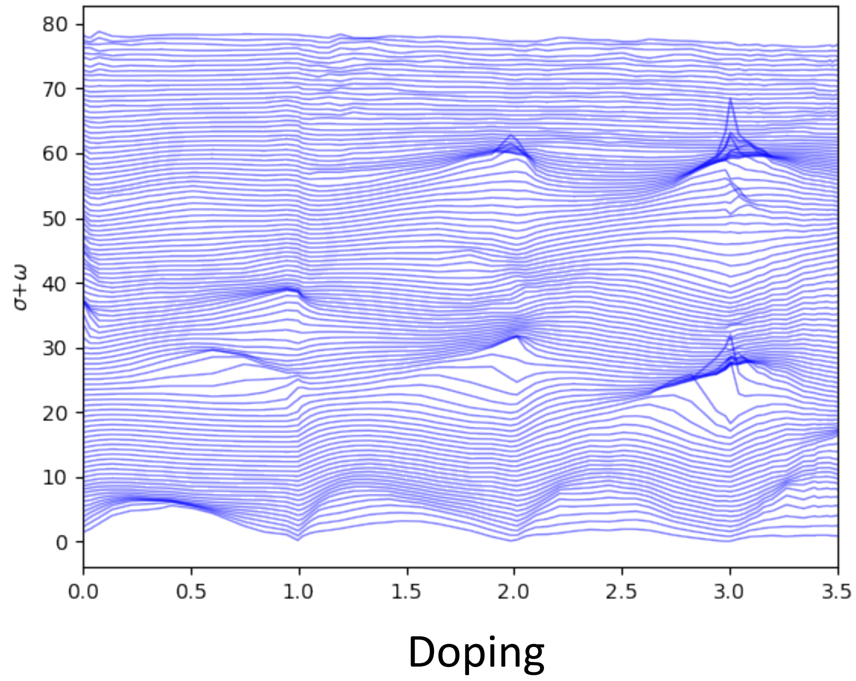




Optical Conductivity



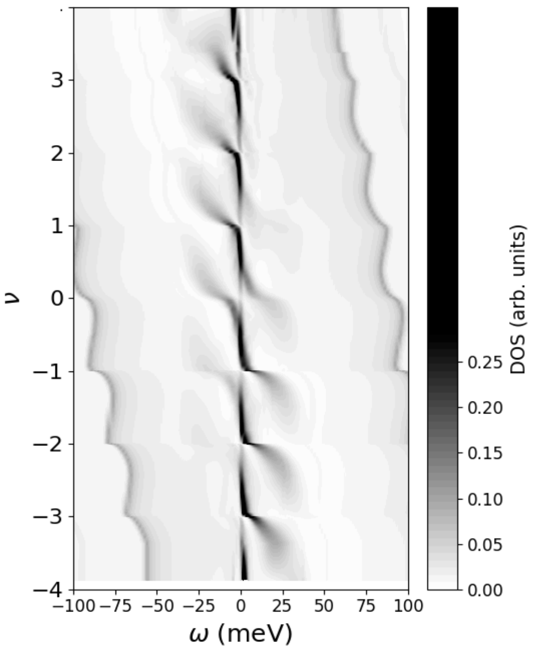
Optical Conductivity



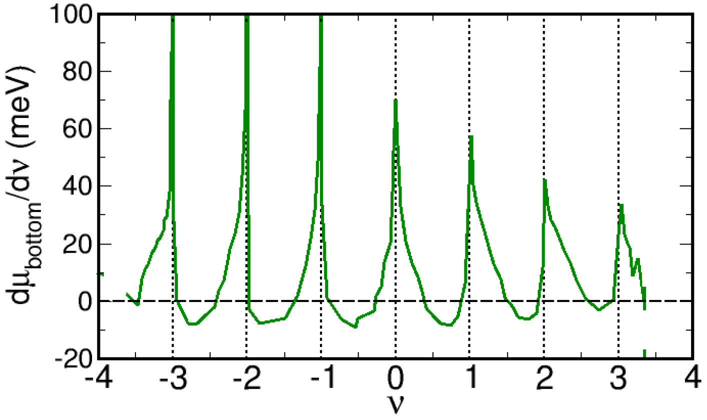
Summary

DMFT + Hartree calculations for multiorbital model for TBG.
(Extended heavy fermion like model): AAp correlated orbitals + less correlated (lc) orbitals

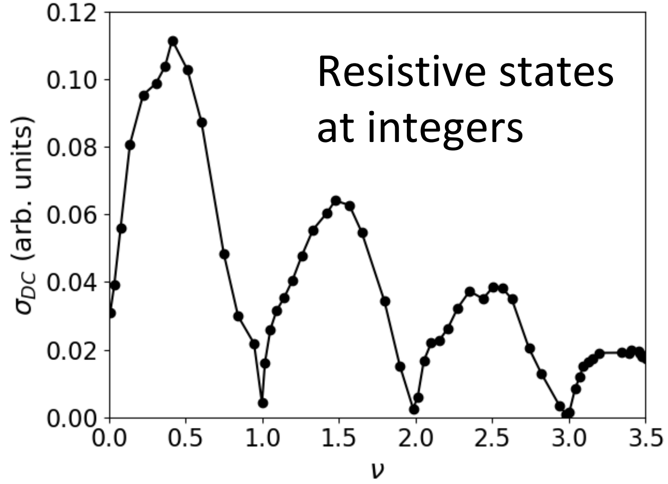
Reorganization of DOS



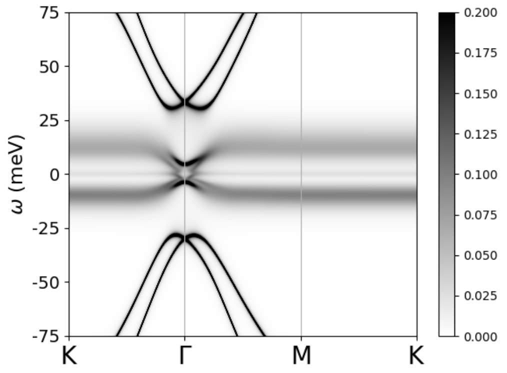
Sawtooth in inverse compressibility



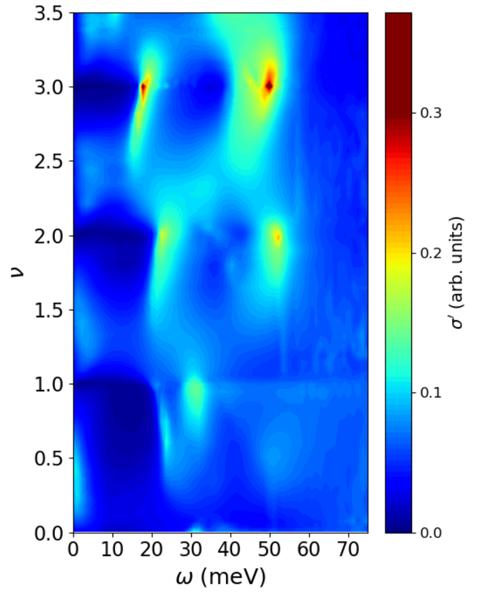
Resistive states at integers



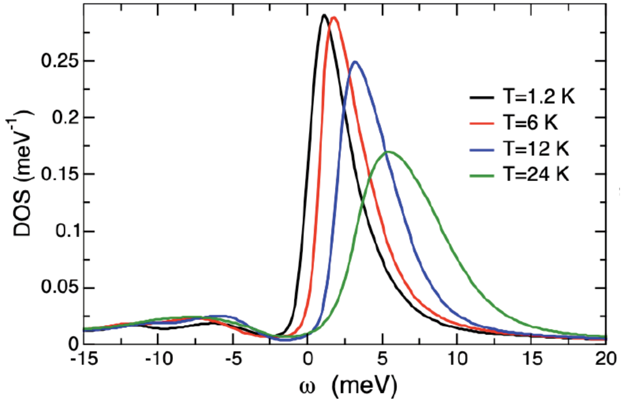
Momentum selective incoherence



Cascades in the optical spectrum



Local moments resilient with temperature



A Datta, MJ Calderón, A. Camjayi, EB, Nature Comms 145036 (2023)

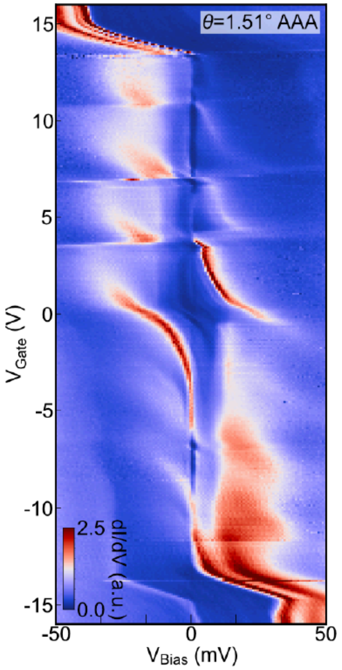
leni.bascones@csic.es

… and more

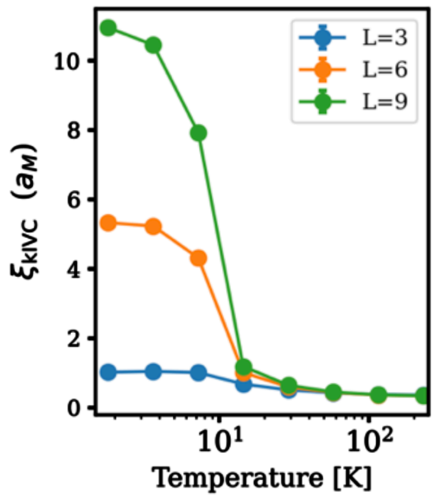
- Similar physics expected in twisted trilayer graphene

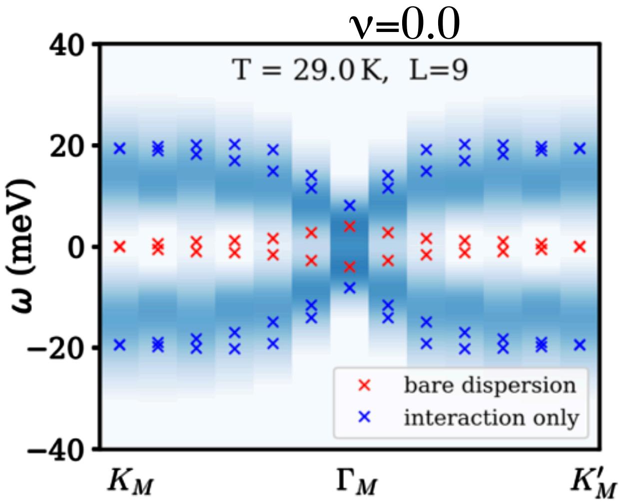
Kim et al, Nature 606, 494–500 (2022).

Yu et al, PRB 108 , 035129 (2023)



- Different numerics, similar results at CNP





Determinant Quantum Montecarlo

Hofmann et al, PRX 12, 011061 (2022)

Our work: DMFT+Hartree