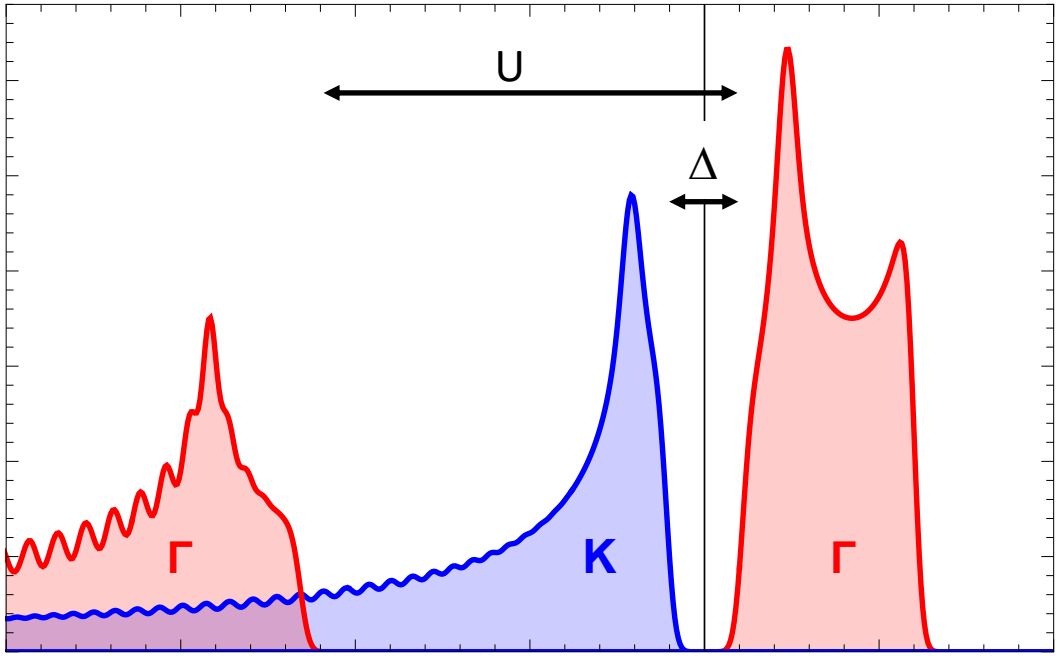
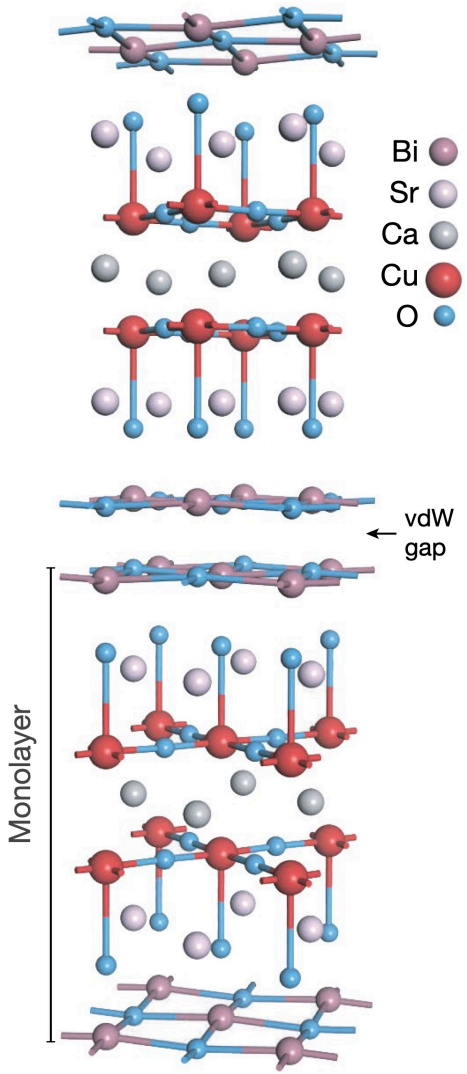


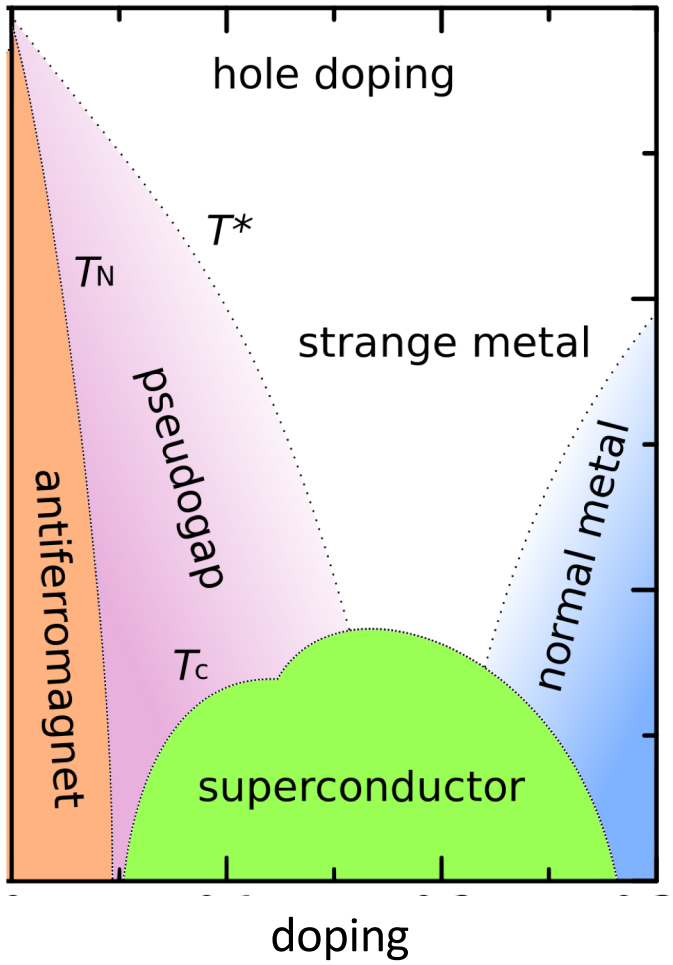
Charge-transfer insulators in moiré materials

Louk Rademaker

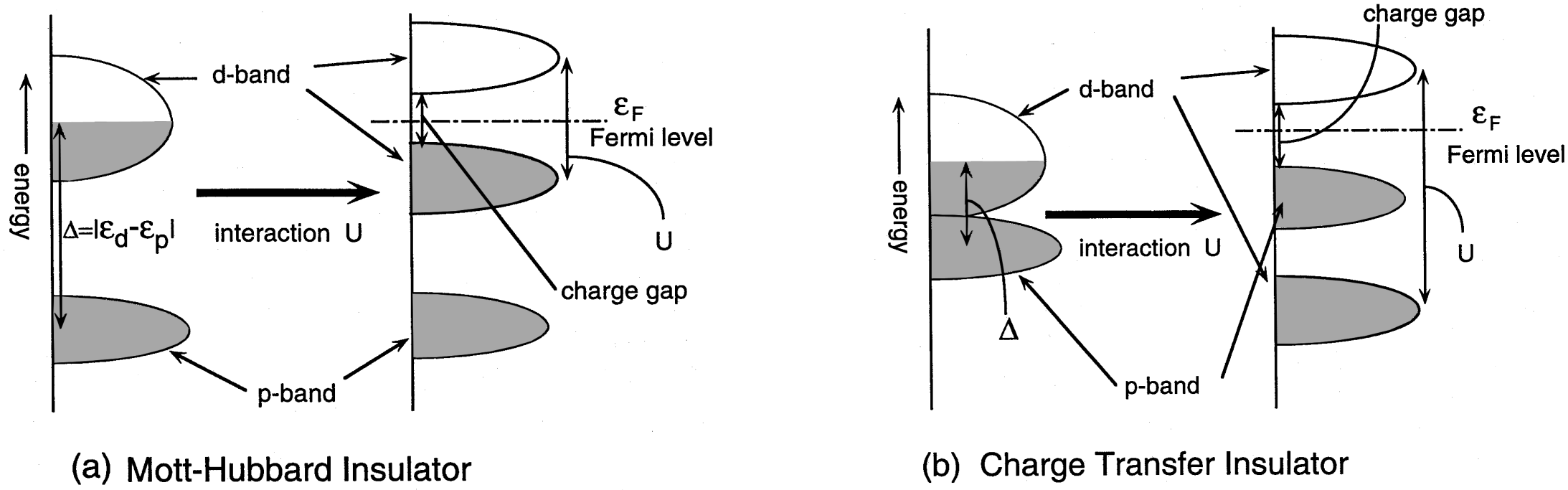
Monday 17 July 2023, Zaanen-Fest in Leiden

Strong correlations!





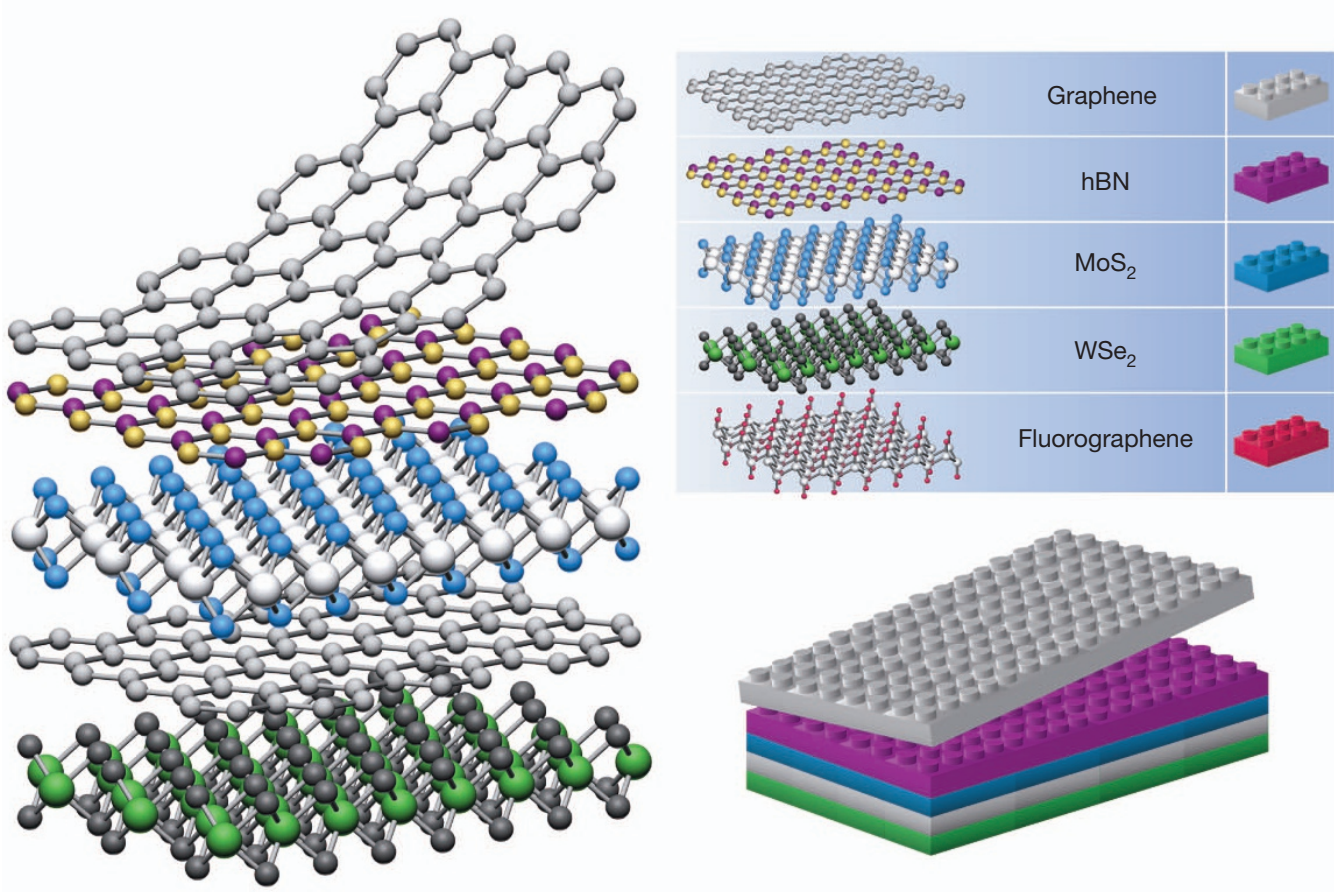
Charge-transfer insulation



Ref: Zaanen, Sawatzky, Allen PRL 1985; Imada RMP 1998

Van der Waals – moiré materials

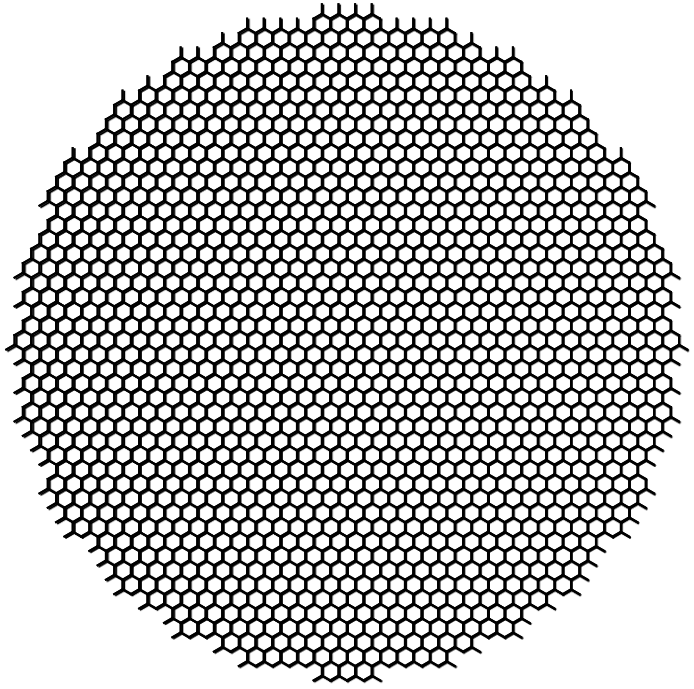
Van der Waals heterostructures: Atomic ‘LEGO’



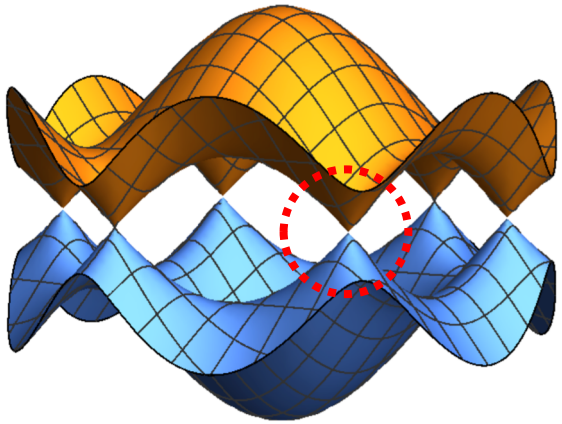
Ref: Geim Nature 2013

Moiré pattern

Twist or Lattice mismatch



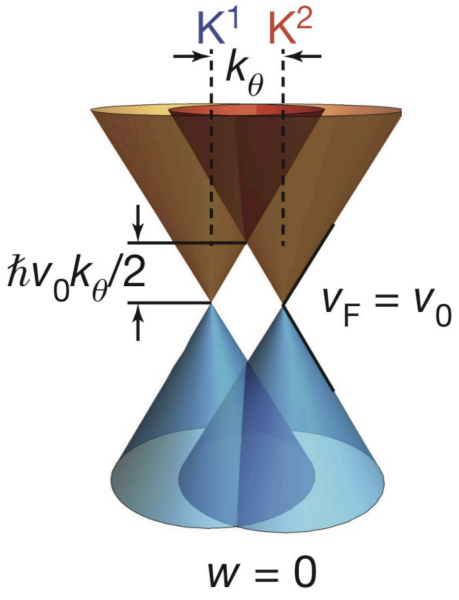
Monolayer graphene

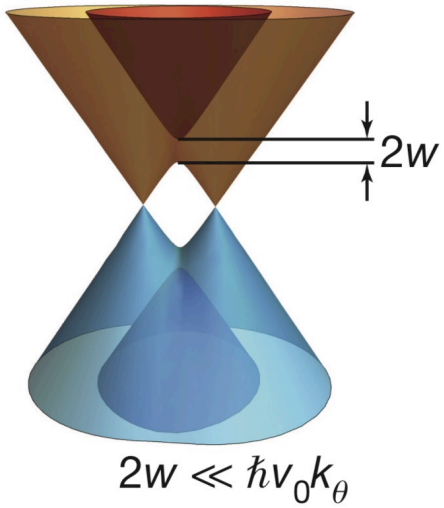


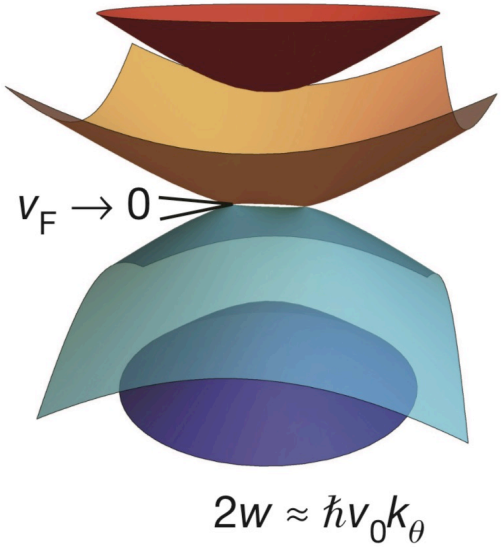
Dirac cone dispersion of **massless** electrons

$$H = v_F \vec{\sigma} \cdot \vec{k}$$

Twisted Bilayer Graphene (tBG)





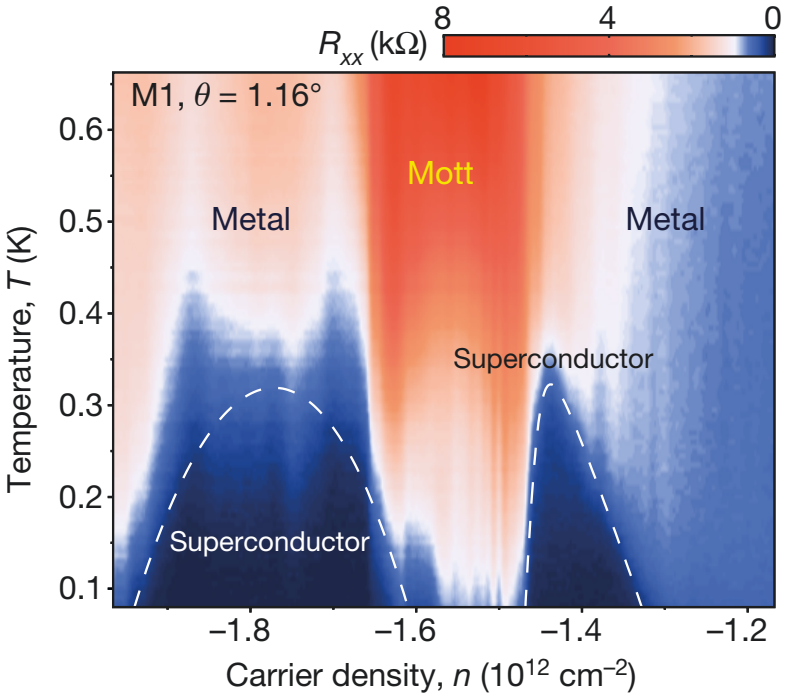


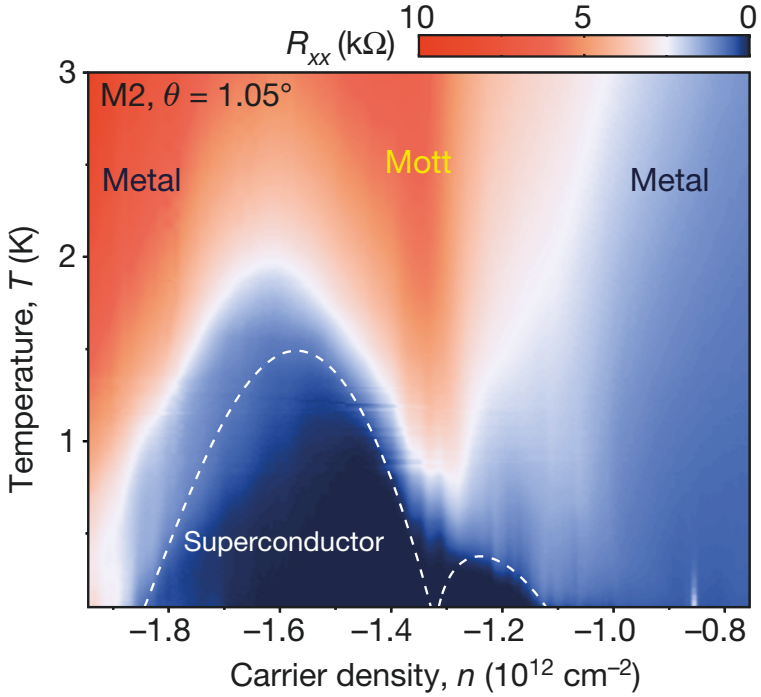
Dirac cones of each layer are **close** + Interlayer **hopping** = Topological **Flat bands**

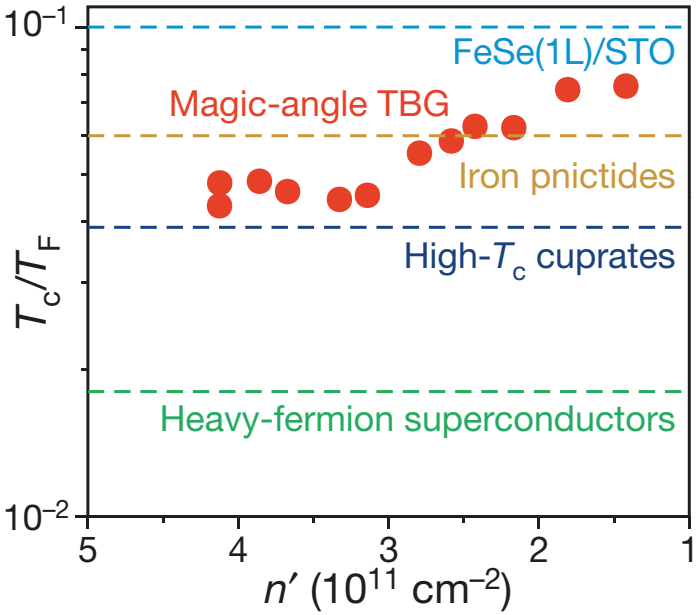
'Magic Angle' tBG

Ref: Bistritzer PNAS 2011; Cao Nature 2018

Mott (?) insulators and (High Tc) Superconductivity

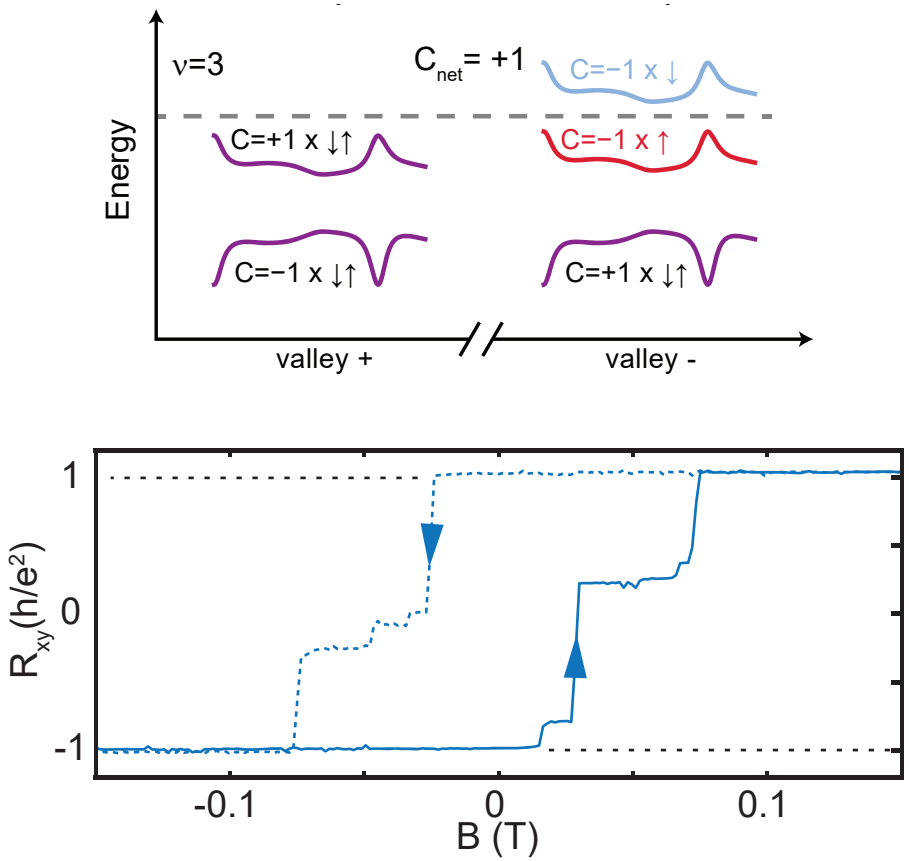




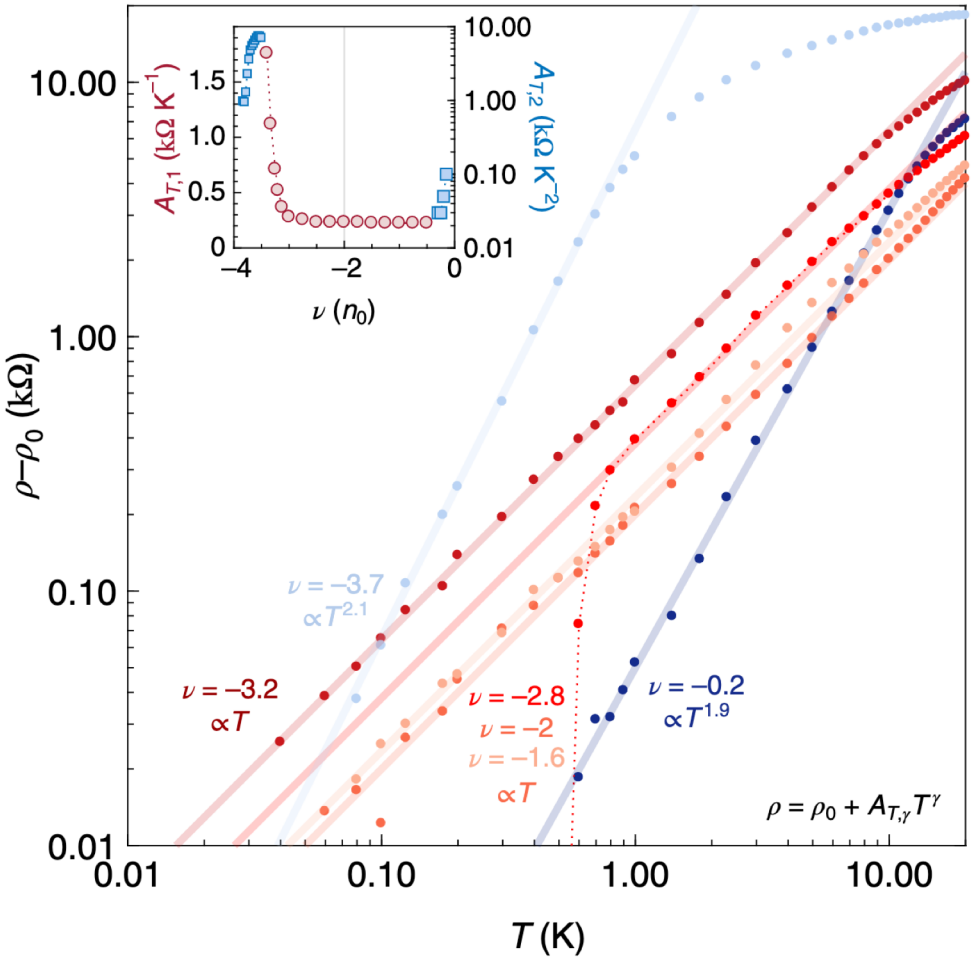


Ref: Cao Nature 2018

Quantum Anomalous Hall effect

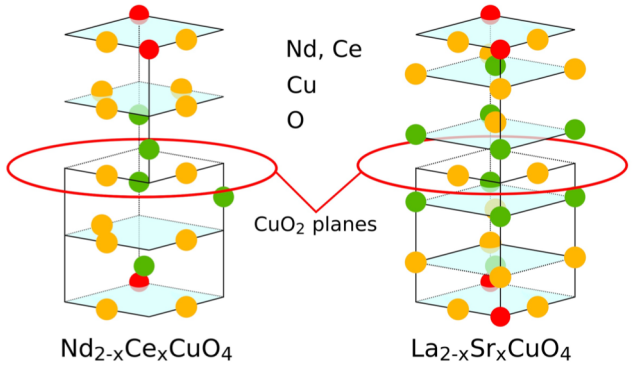


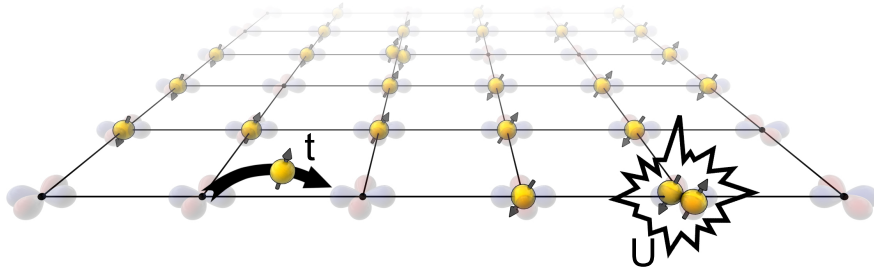
Strange metal

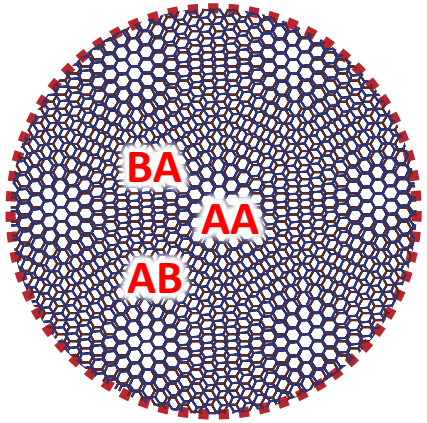


Ref: Serlin Science ’20; Jaoui Nat Phys ‘22

Tight-binding picture of tBG?



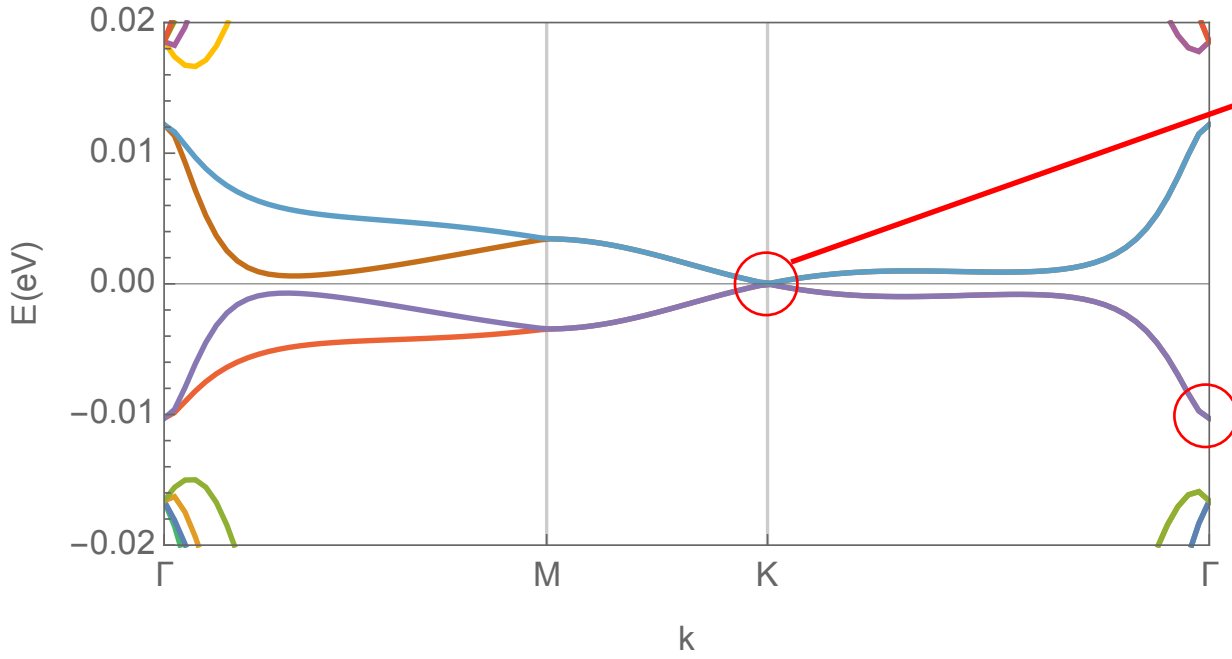


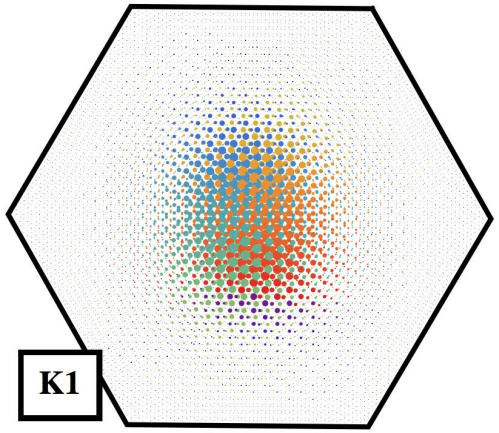


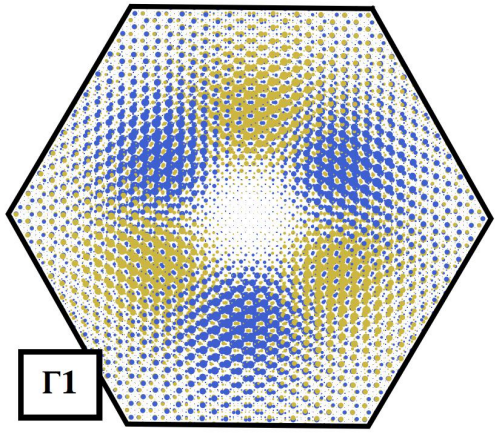
?

Multi-orbital picture

Density of states **at K** is peaked at **AA**







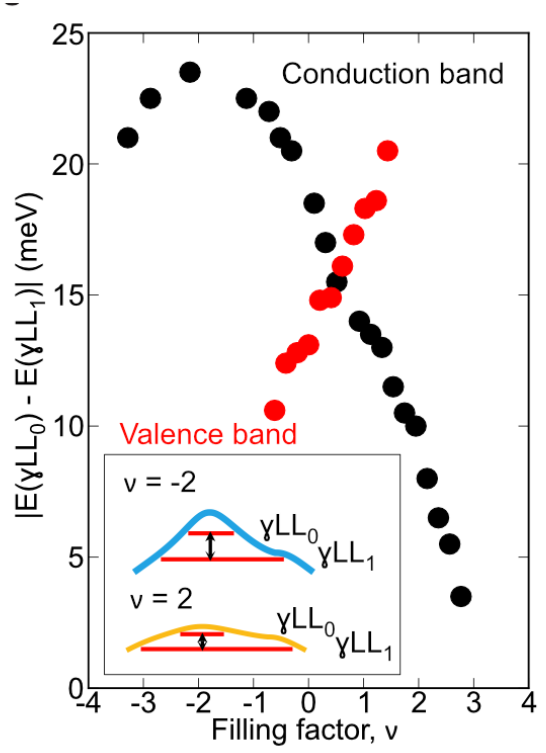
Density of states **at Γ** is peaked at **unit cell edge**

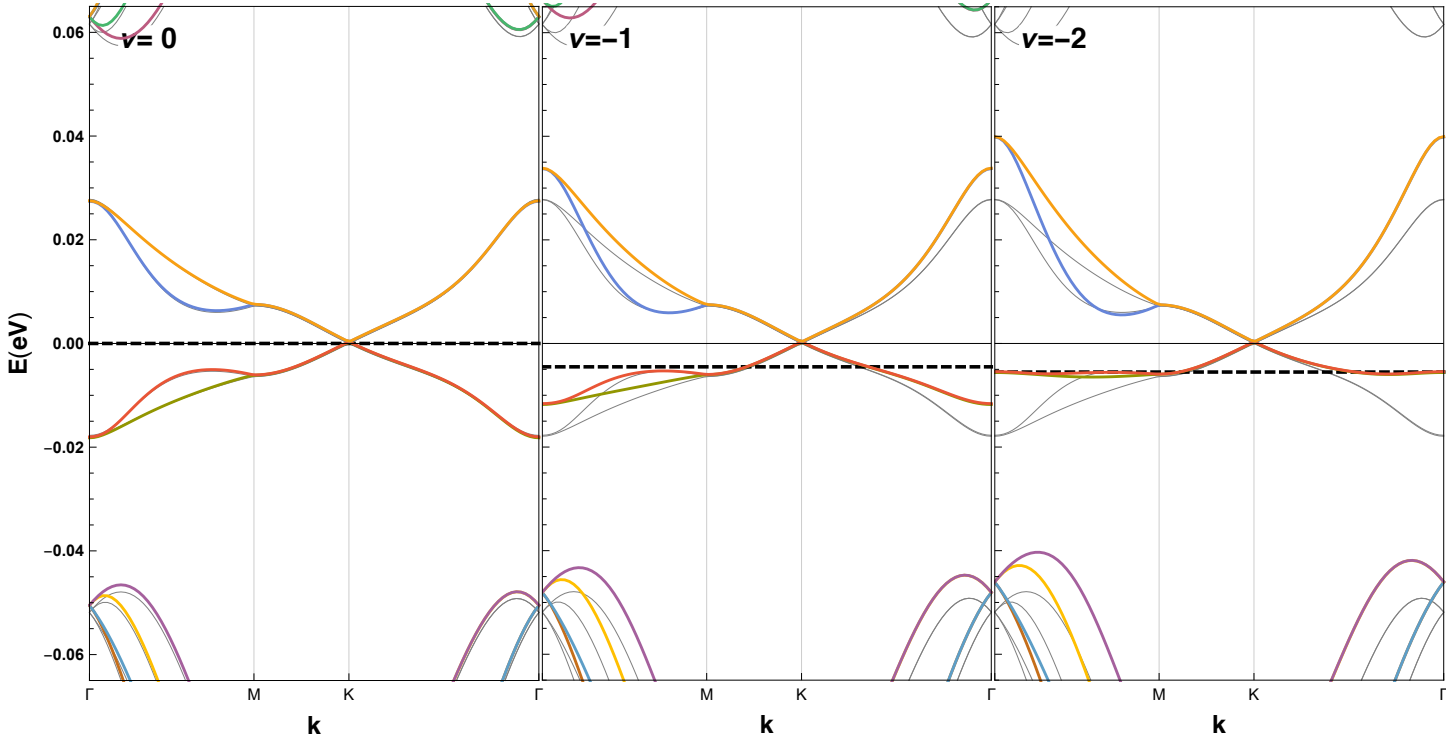
Ref: Rademaker, Mellado, PRB 2018; PRB 2019; Song Bernevig PRL 2022

Charge-transfer in tBG (weak coupling)

Need both **localized** (K, center) and **delocalized** (Γ, ring) orbitals to describe tBG

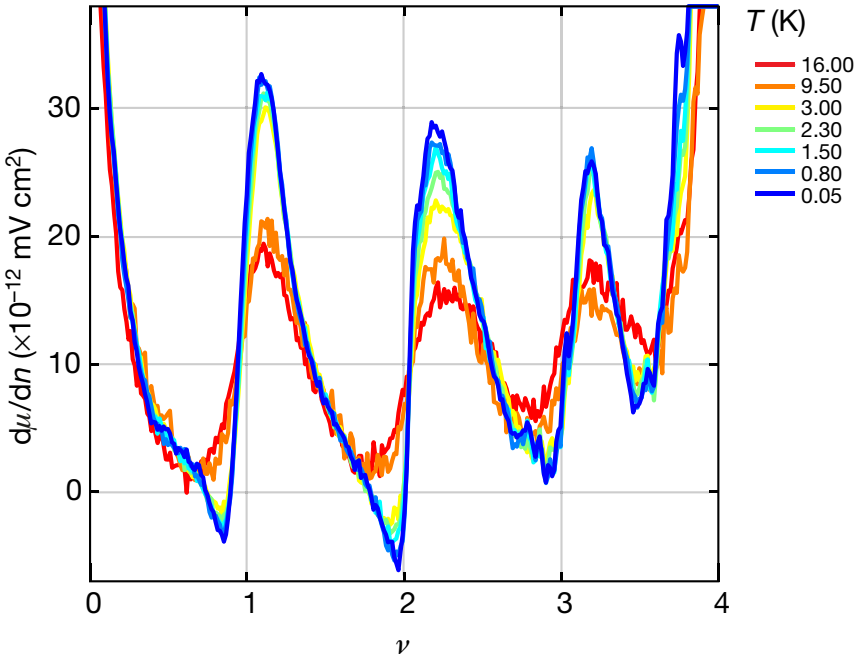
Hartree-Fock: **charge-transfer** causes reduction of effective bandwidth

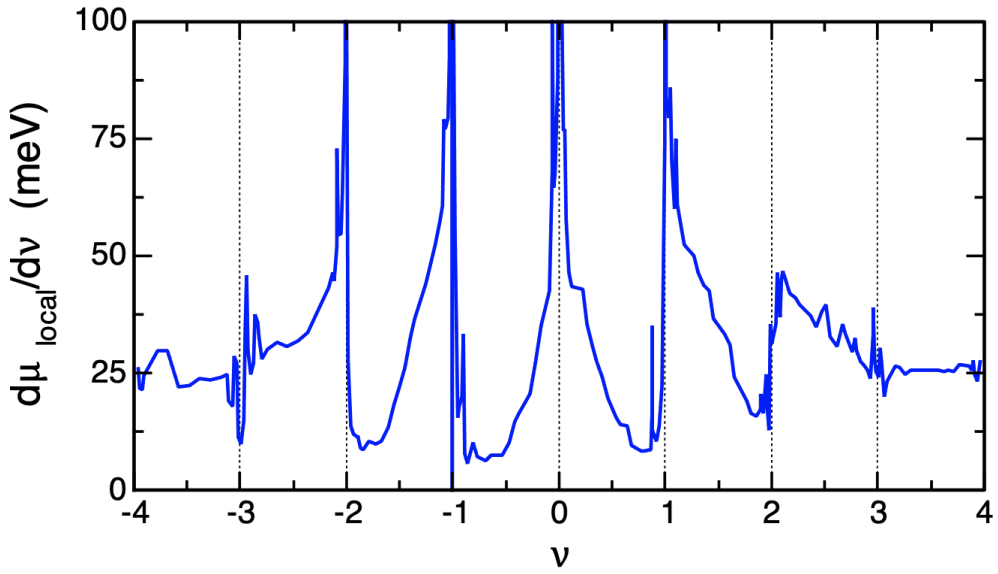




Ref: Rademaker, Mellado, PRB 2018; PRB 2019; Choi Nat Phys 2021

Charge-transfer in tBG (strong coupling)





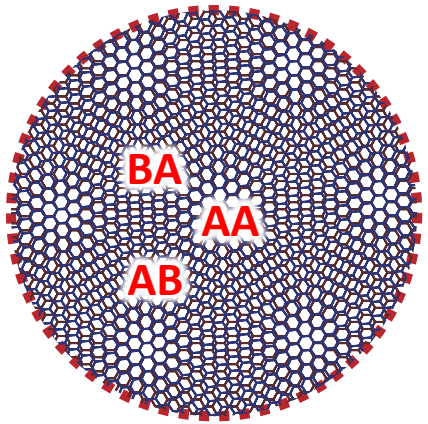
Experiments: **cascade** in inverse compressibility

Charge-transfer between localized and itinerant?

"topological heavy Fermion"?

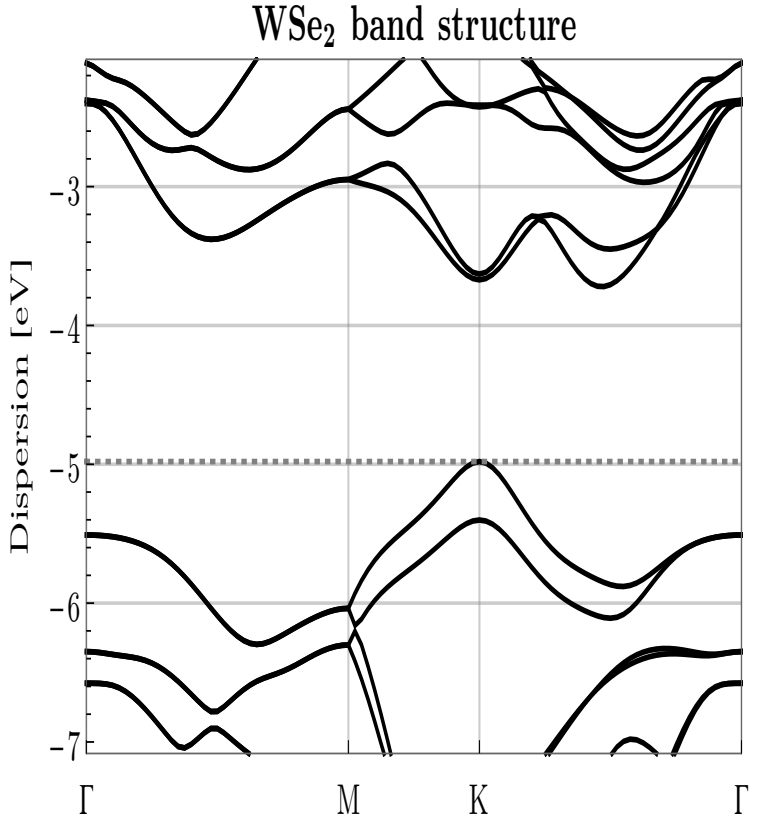
Ref: Song Bernevig PRL 2022; Datta Bascones 2301.13024; Zondiner Nature 2020

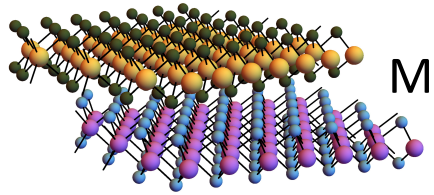
Outlook in tBG



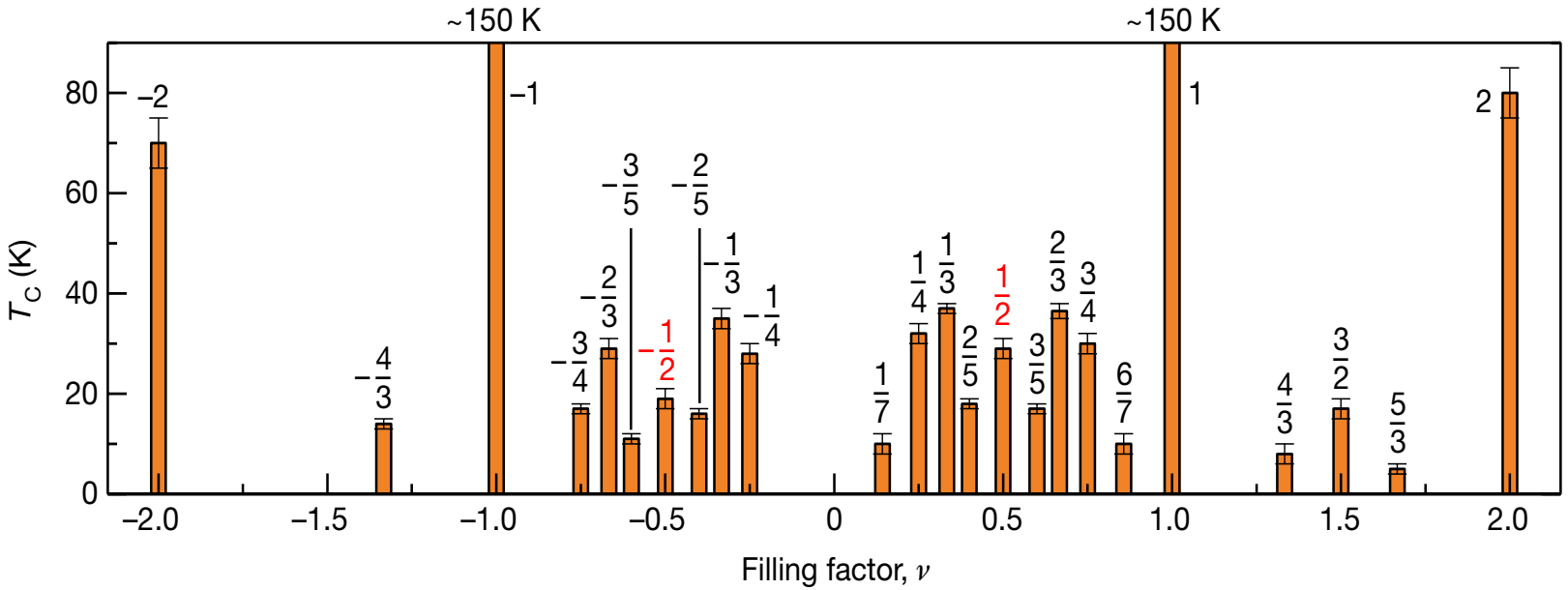
- Still debate on the **correct** effective tight-binding model
- Definitely **not "rigid band-shift"** model
- Need this to understand SC and strange metal
- Key role for **charge-transfer**!

More moiré in TMDs





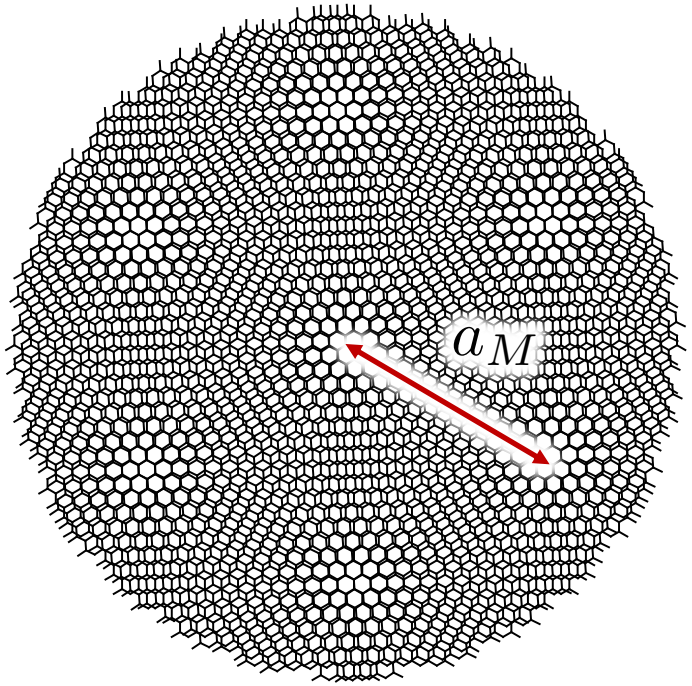
Moiré material from aligned **WS_2/WSe_2** “heterobilayers”



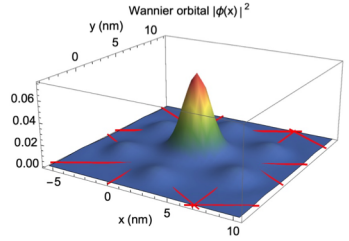
Ref: Rademaker PRB 2022; Xu Nature 2020

Natural Strong Correlations

Moiré unit cell

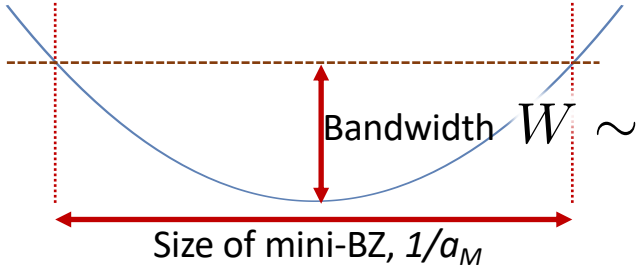


Coulomb Interaction



$$U \sim 1/a_M$$

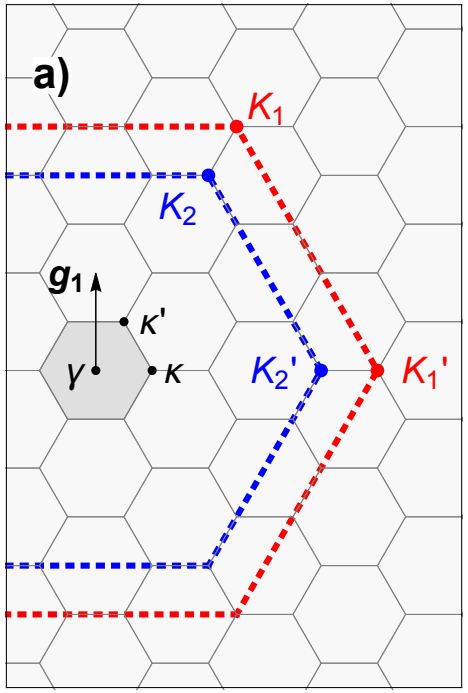
Effective bandwidth



$$W \sim 1/a_M^2$$

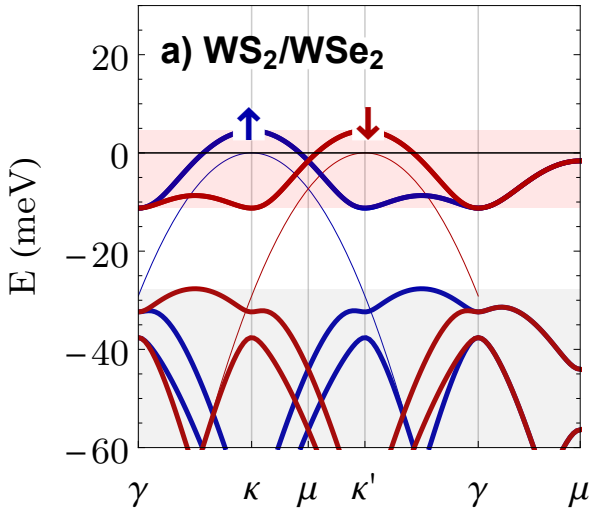
Small twist angle = Large Moiré unit cell = Strong correlations $U/W \sim a_M$

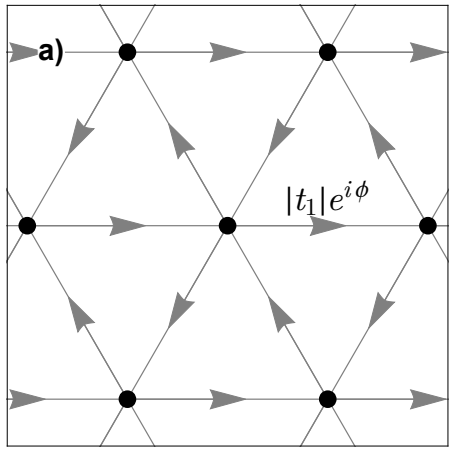
Simple effective model at K



Hopping model on **triangular lattice** with **spin-orbit coupling**

$$H = t_1 \sum_{\langle ij \rangle \sigma} e^{i\phi\sigma^z \nu_{\langle ij \rangle}} c^\dagger_{i\sigma} c_{j\sigma}$$

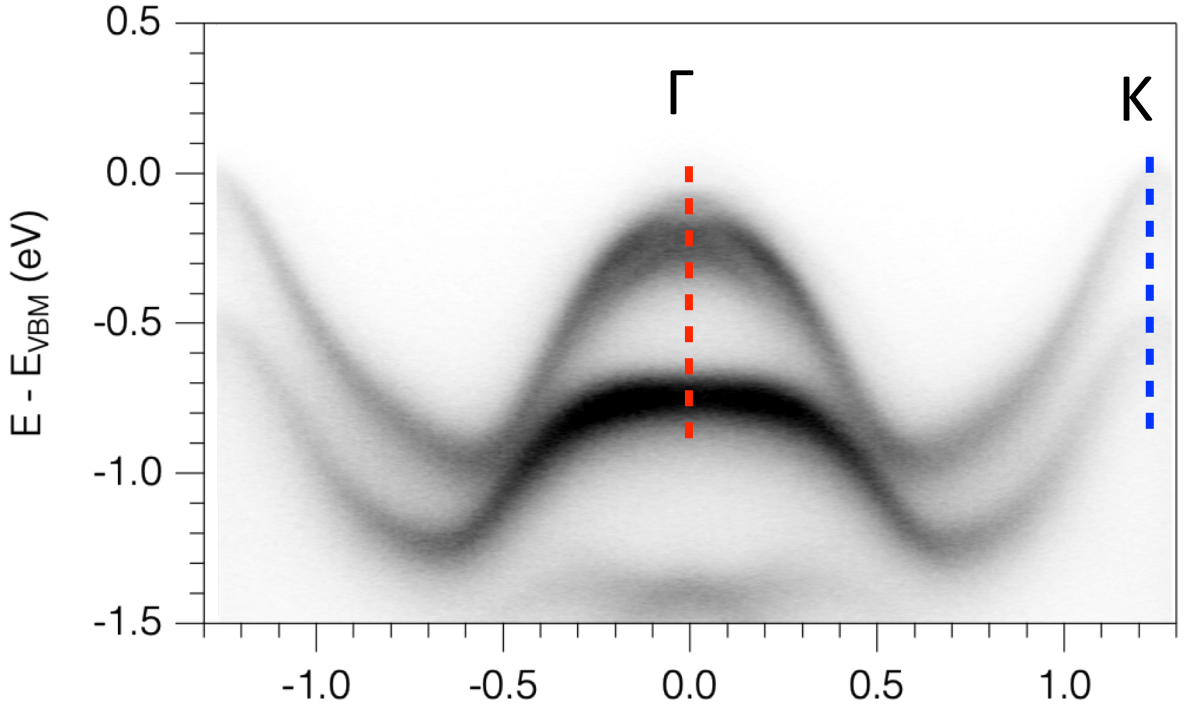


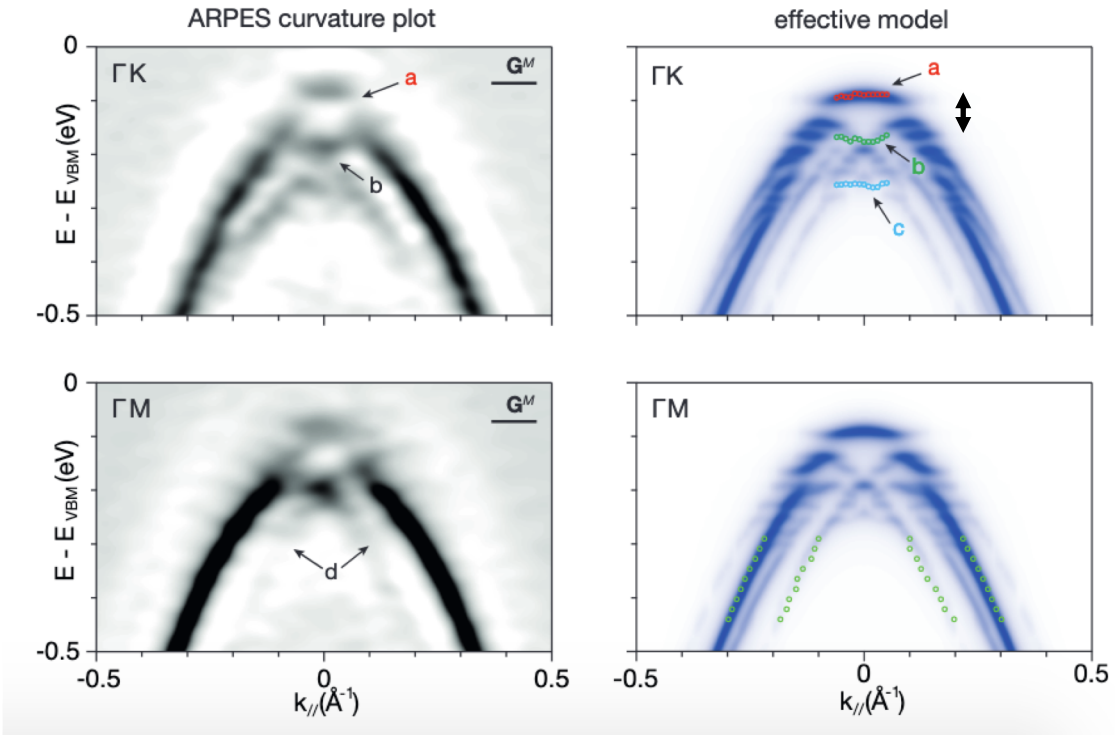


Ref: Rademaker PRB '22

ARPES results on twisted bilayer WSe2

Moiré bands at Γ **are more correlated** but moiré bands at **K are higher in energy**

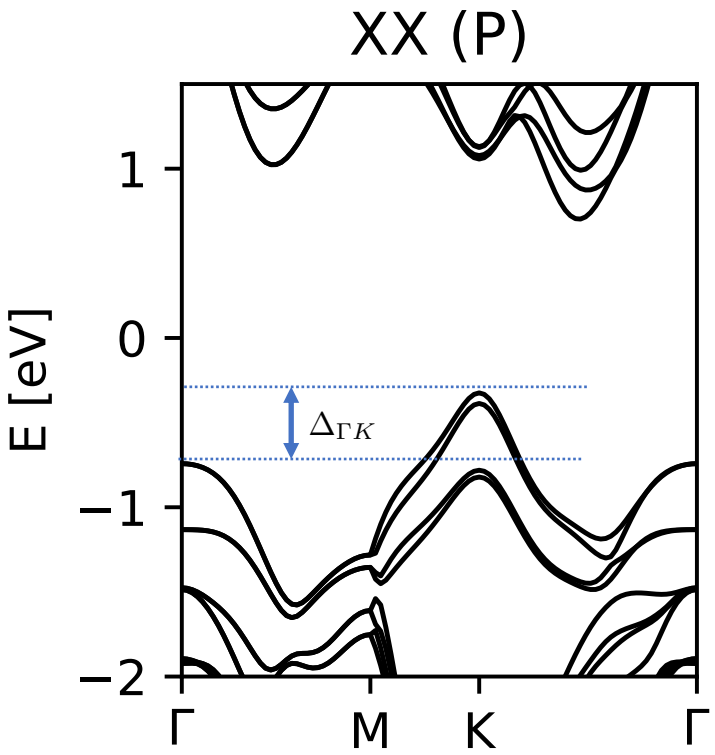




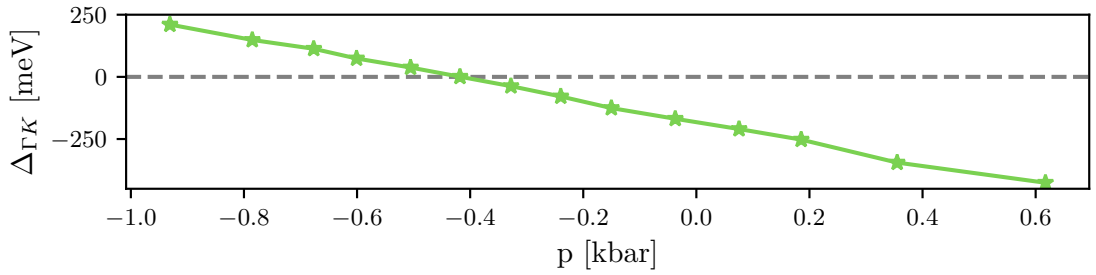
V_0 = 40 – 60 meV

Ref: Gatti, Rademaker et al PRL 2023

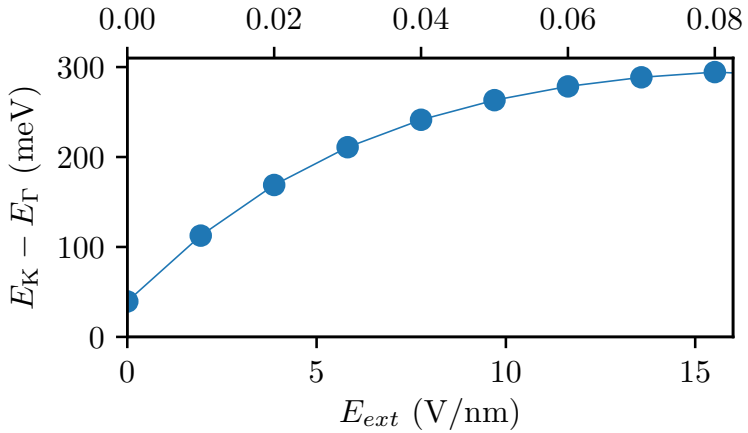
Idea: tune the valley charge-transfer



Energy offset between valleys



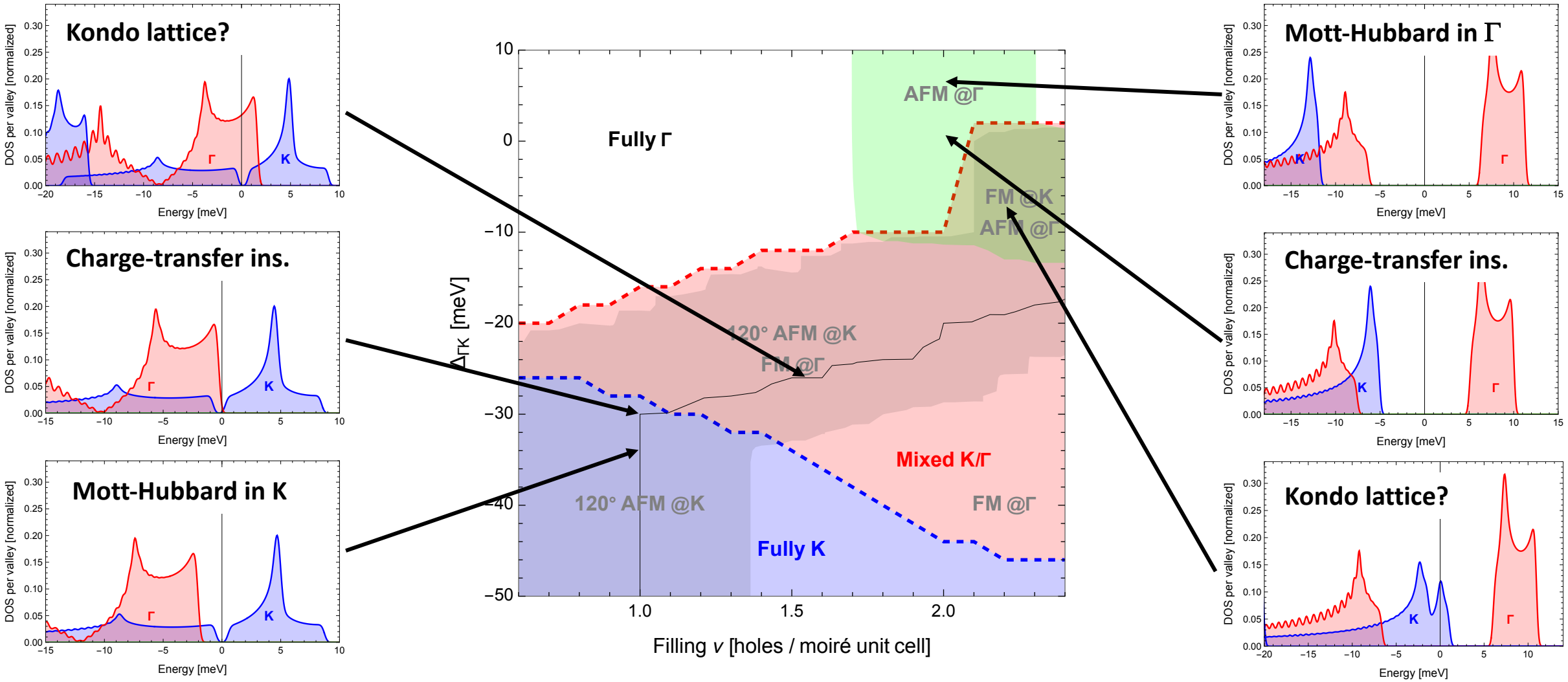
Pressure



Electric field

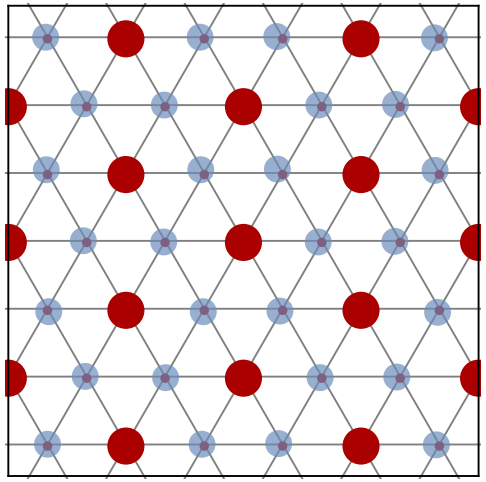
Ref: Brzezinska, Gibertini, Rademaker, arXiv:2023

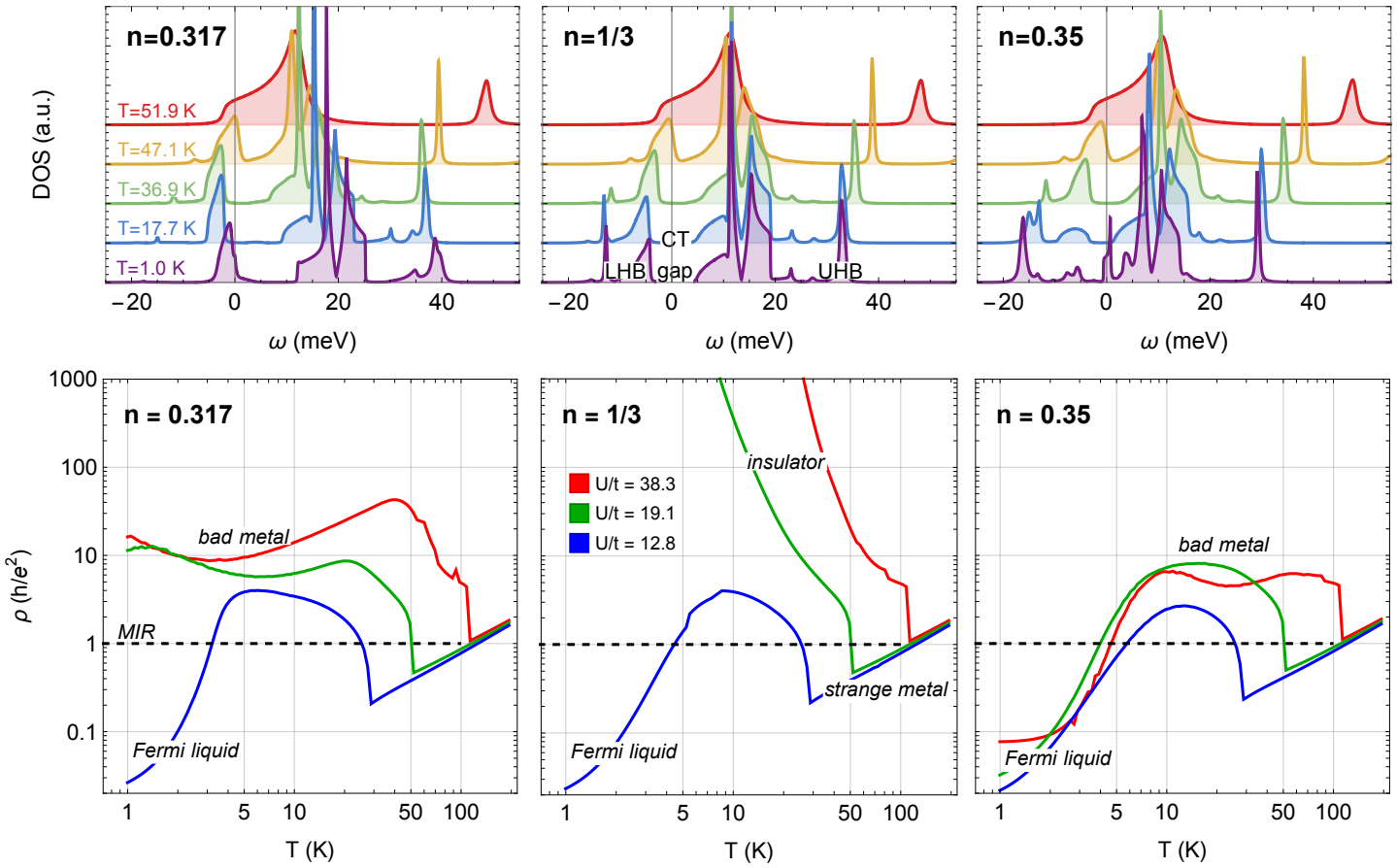
Mean field theory result: tuning valley charge-transfer



Ref: Brzezinska, Gibertini, Rademaker, arXiv:2023

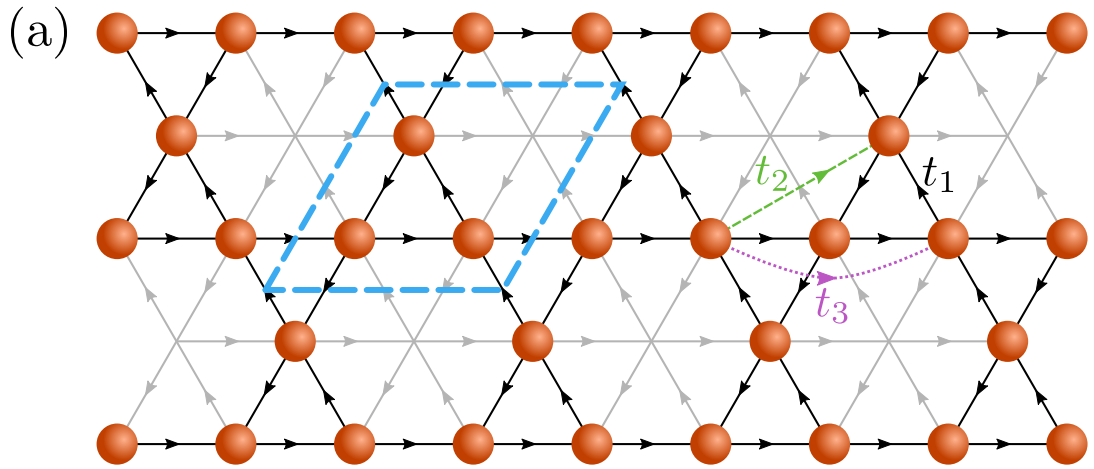
Charge-transfer Wigner crystals

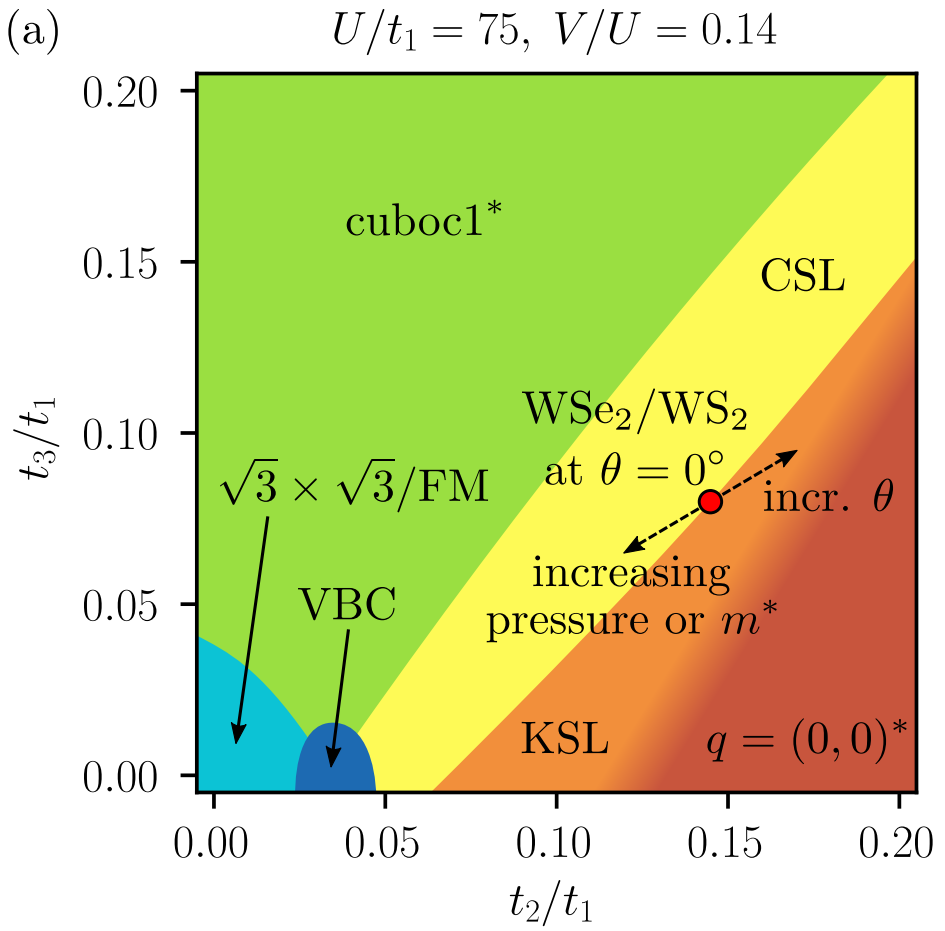




Ref: Tsang, Tan, Dobrosavljevic, Rademaker; arXiv:2210.07926

Chiral spin liquid





Ref: Motruk, Rossi, Abanin, Rademaker, PRR 2023

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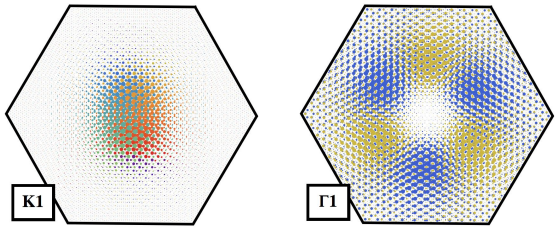
Julia Issing
Simone Lisi
Felix Baumberger
Alberto Morpurgo

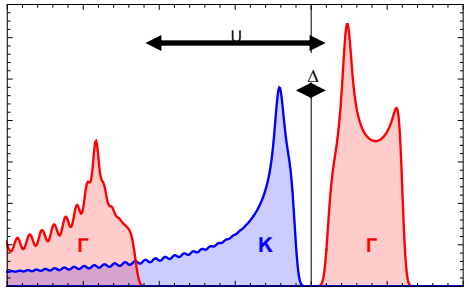
Modena, Italy
Marco Gibertini

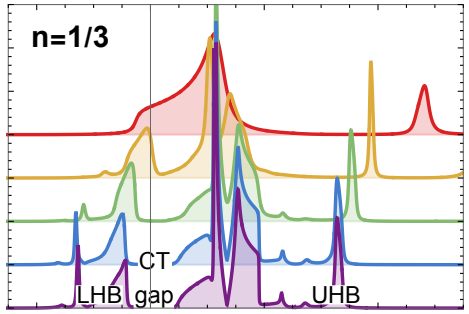
Grenoble, France
Simone Fratini

L'Aquila, Italy
Sergio Ciuchi

Conclusion: Tuning Charge-Transfer in Moiré Materials







Moire materials allow us to **surpass chemistry!**

Twisted bilayer graphene:

Charge-transfer between **localized** and **itinerant** electrons

Rademaker, Mellado PRB 2018

TMD bilayers:

Tunable charge-transfer between G and K valleys

Gatti, Rademaker et al PRL 2023

Brzezinska, Gibertini, Rademaker, arXiv:2023

Wigner-Mott charge transfer insulators

Tsang, Tan, Dobrosavljevic, Rademaker; arXiv:2210.07926