Electronic topology and correlations in kagome metals

IBS-APCTP Conference on Advances in the Physics of Topological and Correlated Matter

19 September 2022

scattering.mit.edu

Outline

Intro. Quantum matter phenomena and the kagome lattice

Part 1 – Topological Dirac fermions and flat bands in kagome metals

Part 2 – van Hove singularity and electronic symmetry breaking in kagome superconductor AV_3Sb_5

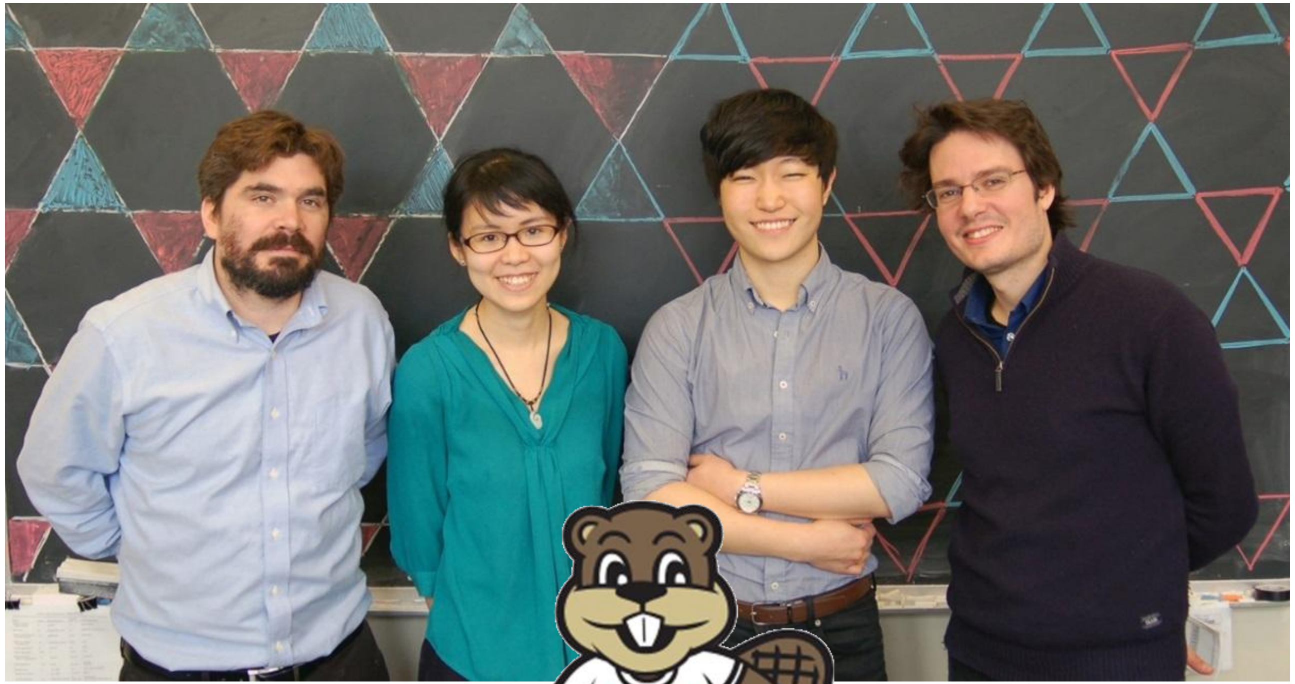
Acknowledgments – Part 1

IFW Dresden

M. Ghimire
M. Richter
J. van den Brink

Harvard

S. Fang
F. Von Cube
D. Bell



Materials discovery
Electronic transport

Linda Ye
Takehito Suzuki
Joe Checkelsky

Band structure spectroscopy

Mingu Kang

LBNL-ALS

C. Jozwiak
A. Bostwick
E. Rotenberg
J. Denlinger

Theory

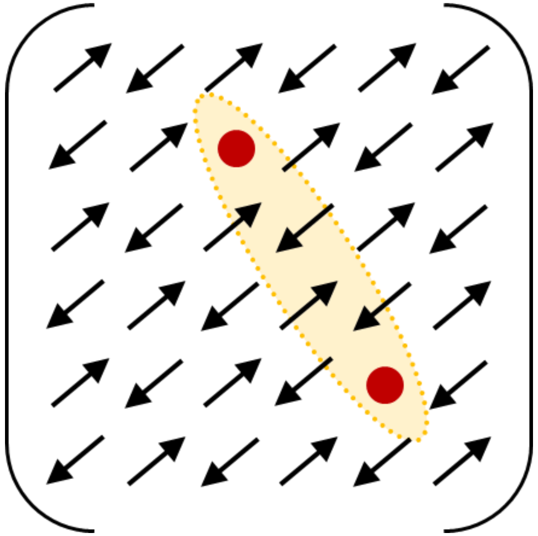
Junwei Liu
Shiang Fang
Tim Kaxiras
Liang Fu

Introduction

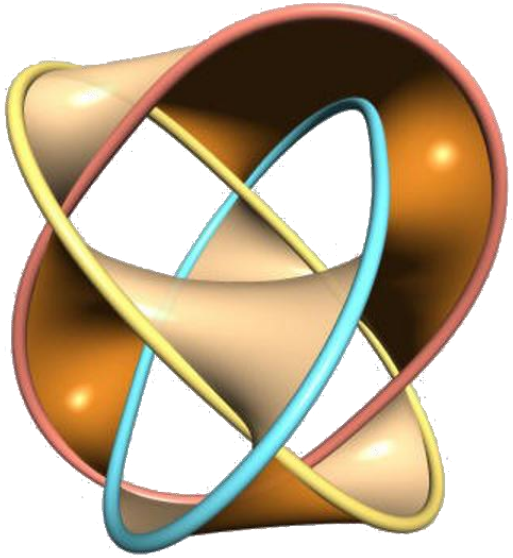
Quantum matter phenomena and the kagome lattice

Motivation. New physics from topology + correlations

Electronic correlations —— **Quantum matter** —— Electronic topology



Chern & axion insulator
Magnetic Weyl physics
Fractional quantum Hall effect
Topological order
Majorana fermions

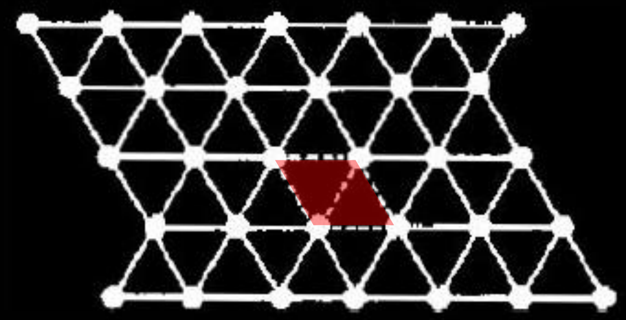


Mott insulator
Superconductivity
Charge-density-waves
Pair-density-waves
. . .

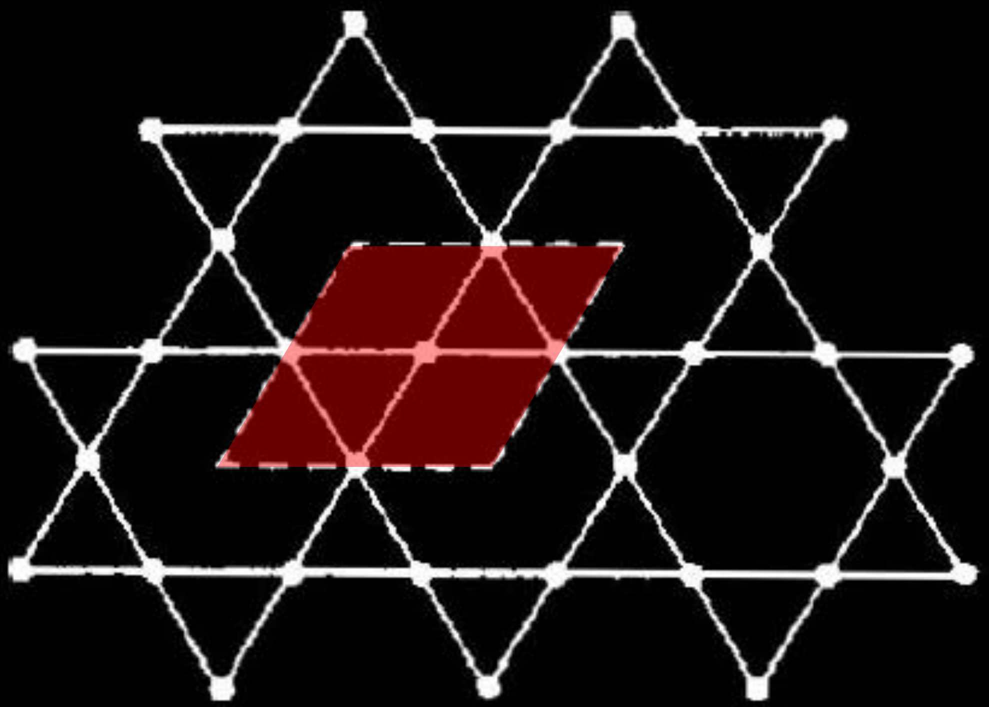
Quantum spin Hall
3D TI
Weyl SM
Nodal line SM
. . .

Intro. The 2D kagome network: lattice structure

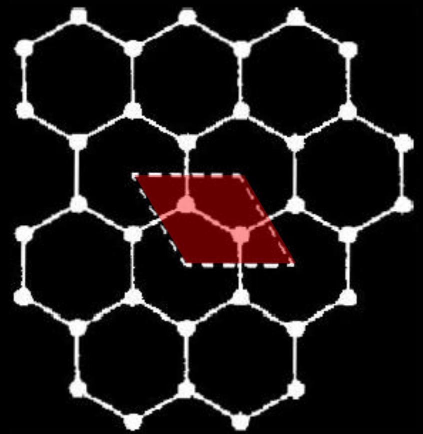
Triangular



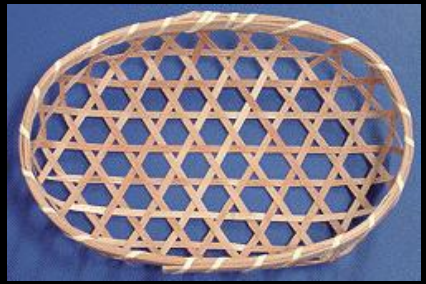
Kagome



Honeycomb

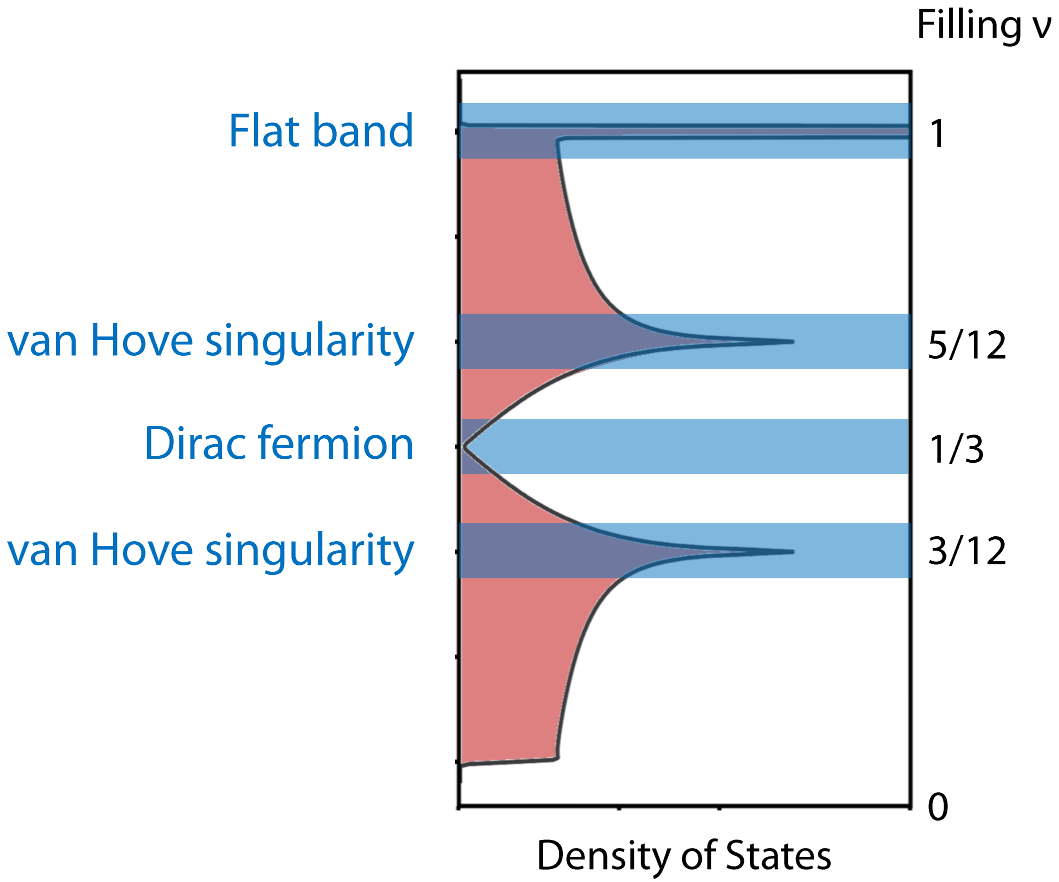


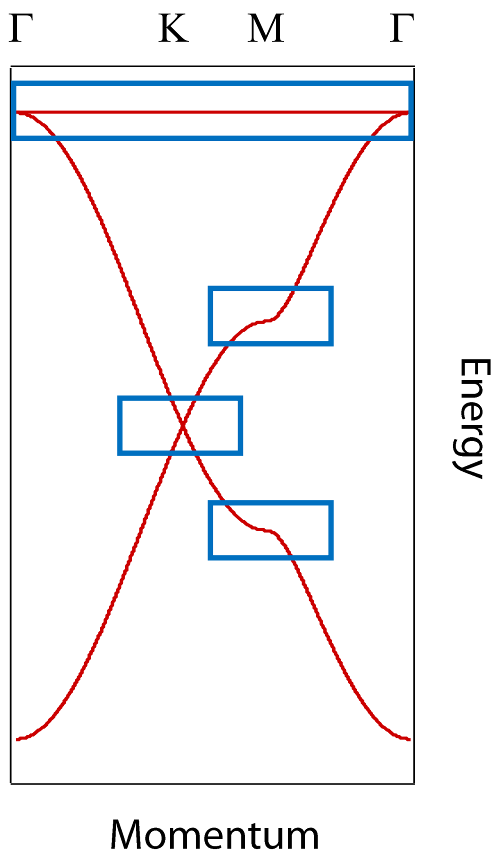
Japanese basket
weaving pattern

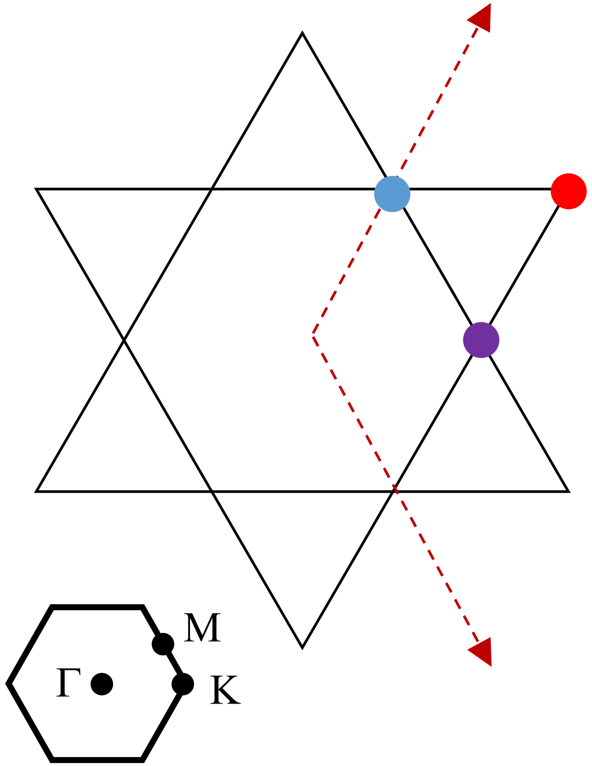


Intro. The 2D kagome network: electronic structure

Kagome lattice



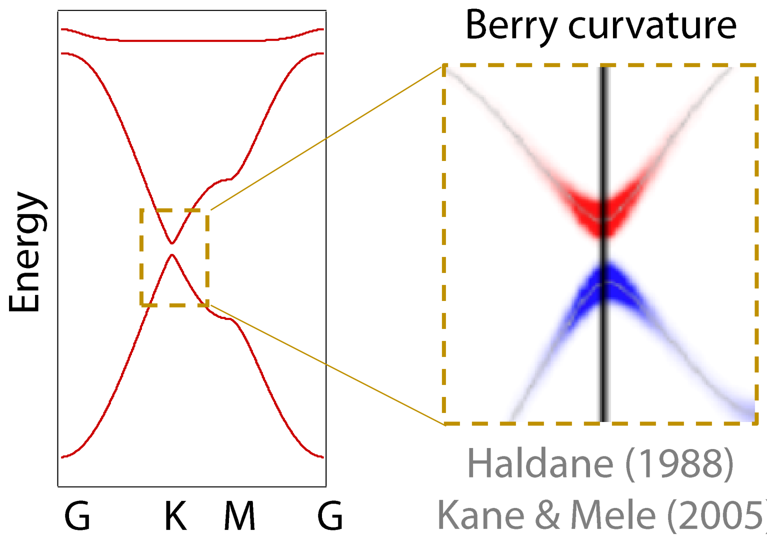




Dirac fermions + vHS + **flat band**

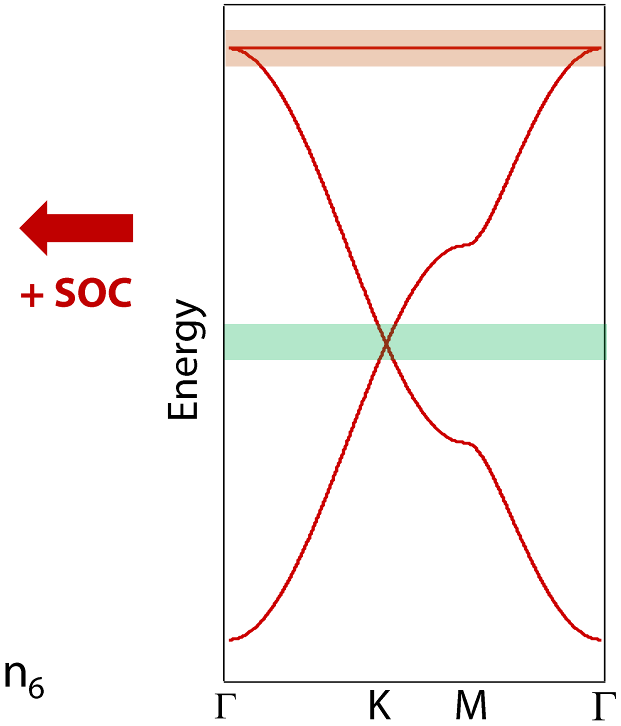
Intro. The 2D kagome net as a new platform for quantum matter

Nontrivial topology



Haldane (1988)
Kane & Mele (2005)

Kagome lattice



Chern physics	Fe_3Sn_2, $TbMn_6Sn_6$
Magnetic Weyl fermions	Mn_3Sn, $Co_3Sn_2S_2$
Topological flat bands	(Co,Fe)Sn

Nat. Mat. **16,** 1090 (2017)
Nature **555,** 638 (2018)
Nat. Mat. **19,** 163 (2019)

Science **365,** 1282 (2019)
Nature **583,** 533 (2020)
Nat. Comm. **11,** 4004 (2020)

Intro. The 2D kagome net as a new platform for quantum matter

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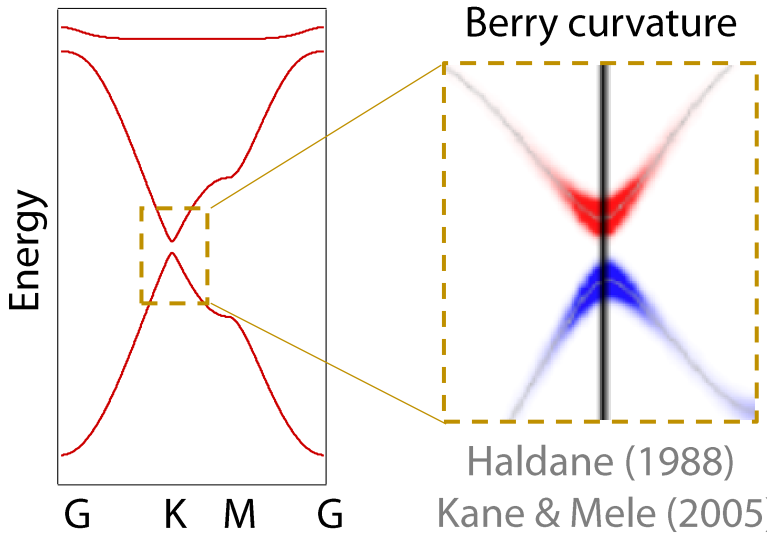
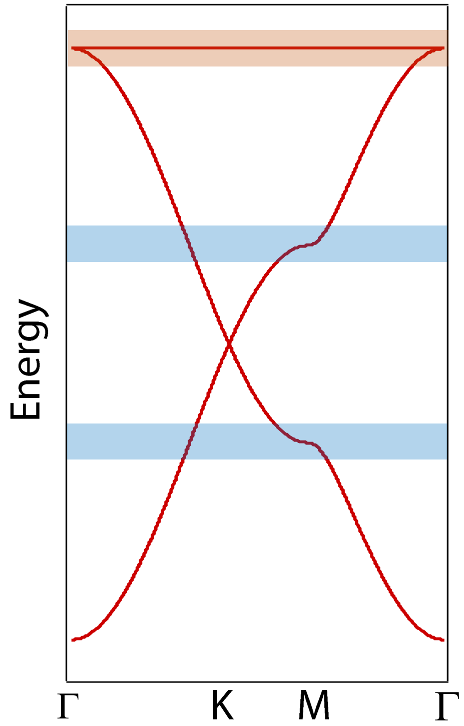


Haldane (1988)
Kane & Mele (2005)

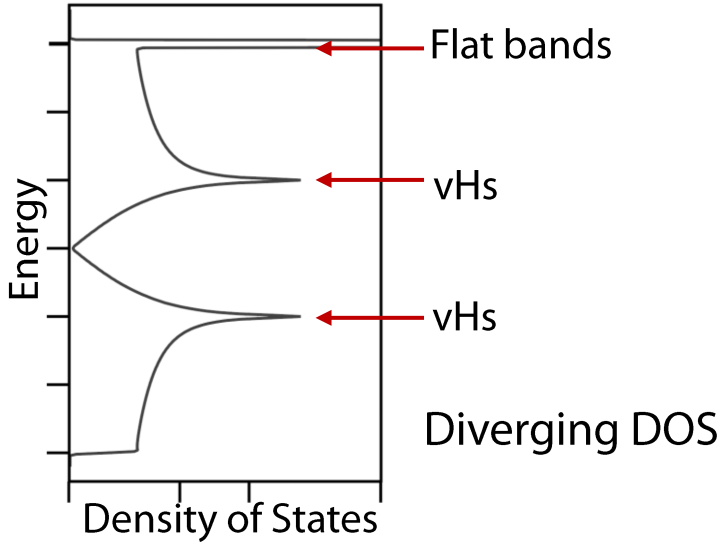
+ SOC

Kagome lattice



Filling control

Electronic symmetry breaking



Chern physics — Fe_3Sn_2, $TbMn_6Sn_6$

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Science **365,** 1282 (2019)
Nature **583,** 533 (2020)
Nat. Comm. **11,** 4004 (2020)

AV_3Sb_5 (A = K,Rb,Cs)

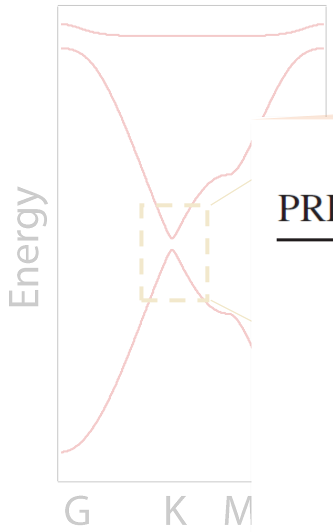
B. R. Ortiz *et al.*, Phys. Rev. Lett. **125,** 247002 (2020)

Charge order
Superconductivity
Stripe ordering
Nematicity

Orbital order
Pair density wave
Anomalous Hall effect

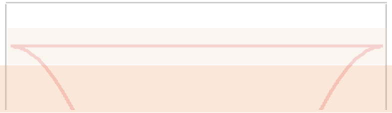
Intro. The 2D kagome net as a new platform for quantum matter

Nontrivial topology

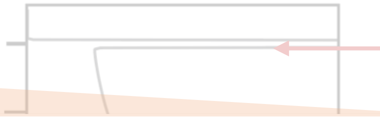


Berry curvature

Kagome lattice



Electronic symmetry breaking



Selected for a Viewpoint in *Physics*

PRL **106,** 236802 (2011) PHYSICAL REVIEW LETTERS week ending 10 JUNE 2011

High-Temperature Fractional Quantum Hall States

Evelyn Tang,[1] Jia-Wei Mei,[1,2] and Xiao-Gang Wen[1]

[1]*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
[2]*Institute for Advanced Study, Tsinghua University, Beijing, 100084, People's Republic of China*

(Received 14 December 2010; published 6 June 2011)

We show that a suitable combination of geometric frustration, ferromagnetism, and spin-orbit interactions can give rise to nearly flatbands with a large band gap and nonzero Chern number. Partial filling of the flatband can give rise to fractional quantum Hall states at high temperatures (maybe even room temperature). While the identification of material candidates with suitable parameters remains open, our work indicates intriguing directions for exploration and synthesis.

...ging DOS

Chern physics

Magnetic Wey...

...2 (2020)

Topological flat bands

Nat. Mat. **16,** 1090 (2017)
Nature **555,** 638 (2018)
Nat. Mat. **19,** 163 (2019)

(Co,Fe)Sn

Science **365,** 1282 (2019)
Nature **583,** 533 (2020)
Nat. Comm. **11,** 4004 (2020)

Charge order
Superconductivity
Stripe ordering
Nematicity

Orbital order
Pair density wave
Anomalous Hall effect

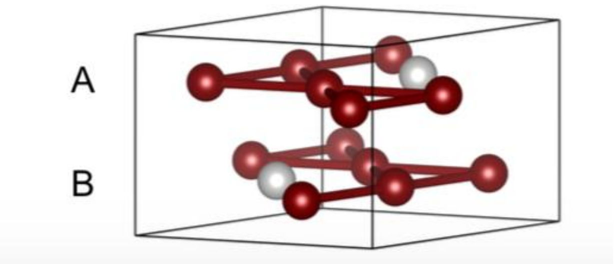
Intro. Materials hosts for the 2D kagome network

Transition metal stannides

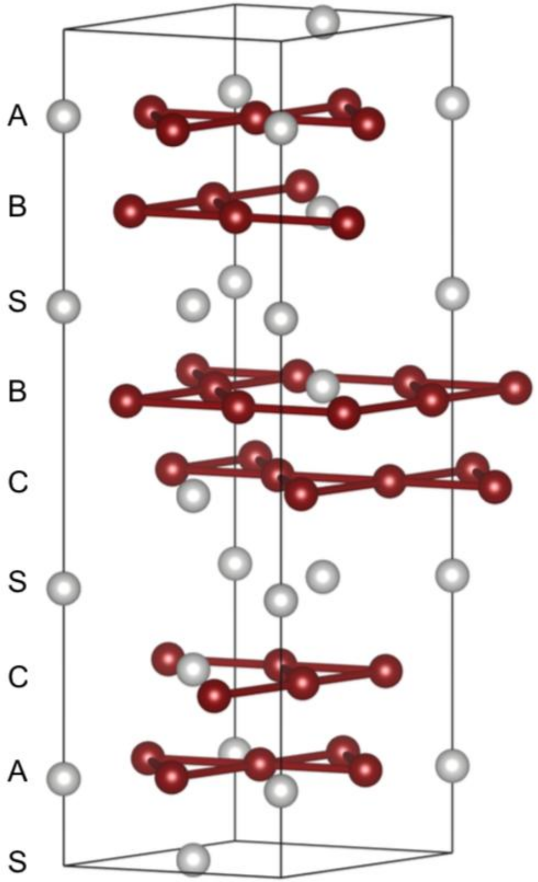
Tm_mX_n

- Tm : Fe, Mn, Co
- X : Ge, Sn

$m:n=3:1$

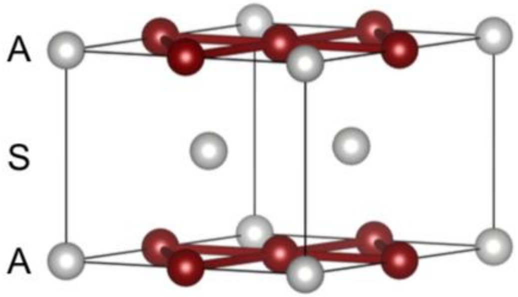


$m:n=3:2$



Bulk stacking of kagome layers

$m:n=1:1\ (3:3)$



Strong interlayer coupling

Weak interlayer coupling

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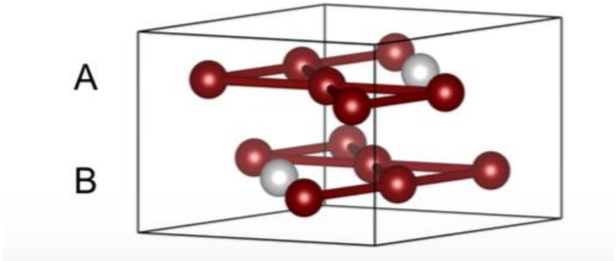
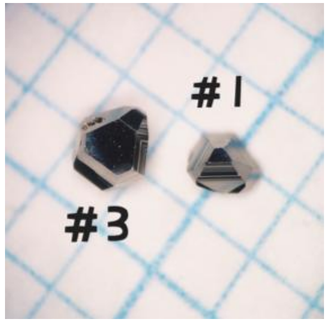
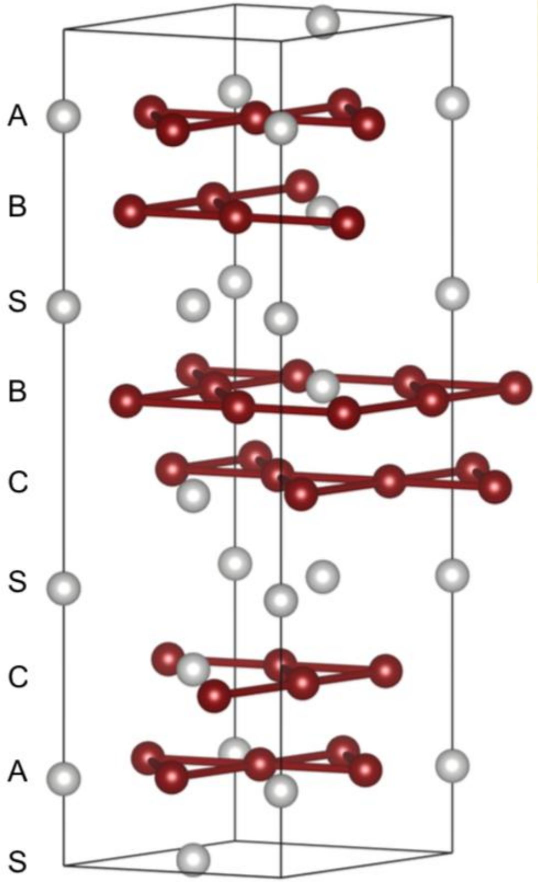
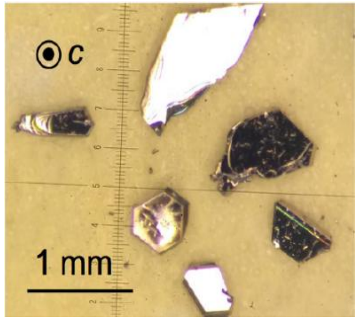


Mn_3Sn
noncollinear AFM



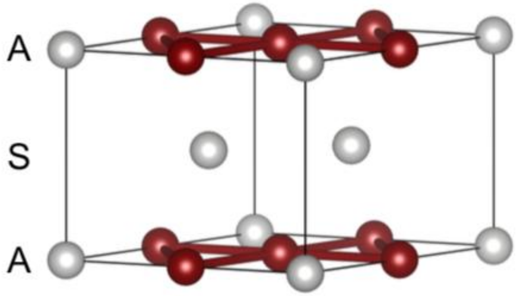
$m : n = 3 : 2$



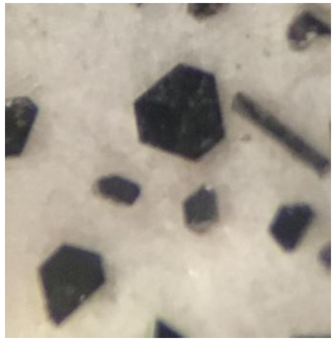


Fe_3Sn_2
collinear FM

$m : n = 1 : 1\ (3 : 3)$



FeSn
collinear AFM



Intro. Materials hosts for the 2D kagome network

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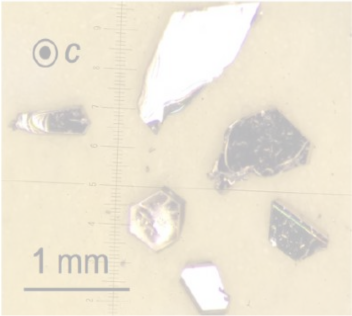
Tm_mX_n

Tm : Fe, Mn, Co

X : Ge, Sn

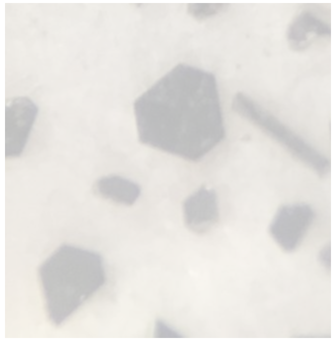


Fe_3Sn_2
collinear FM

- Various form of intrinsic **magnetism** ✓
- **Spin-orbit coupling** from 3*d*-orbitals ✓
- **Intermediate** Coulomb interactions ✓

Mn_3Sn
noncollinear AFM

FeSn
collinear AFM



Part 1

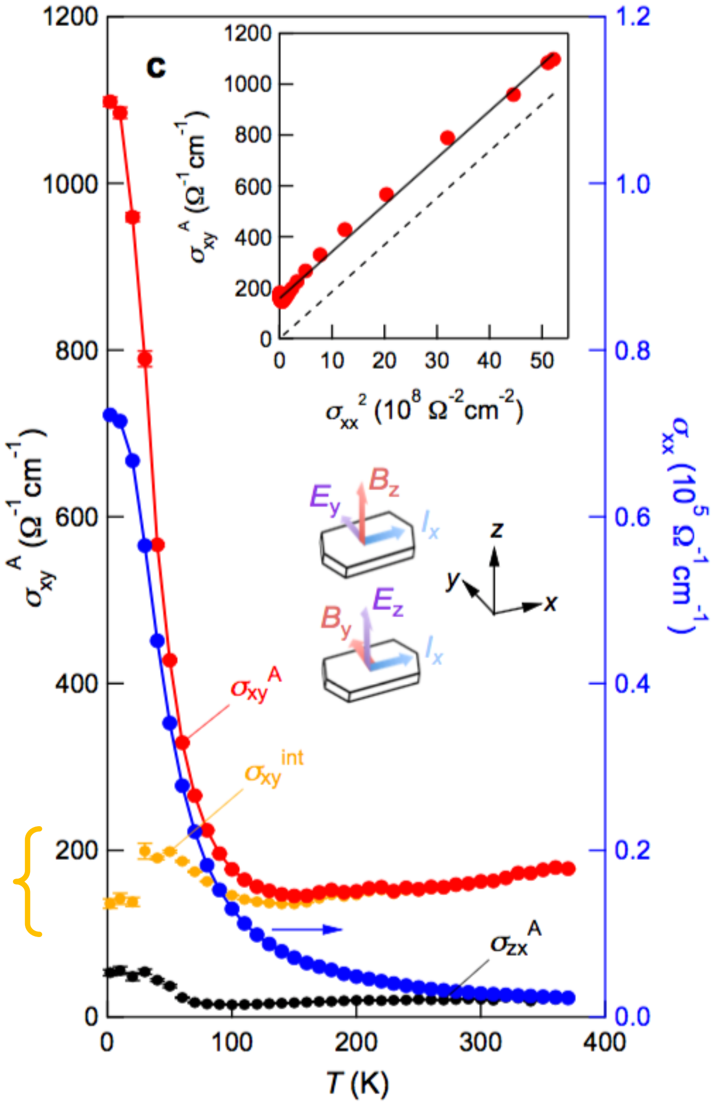
Topological Dirac fermions and flat bands in kagome metals

Transport signatures of topology in kagome metal Fe_3Sn_2

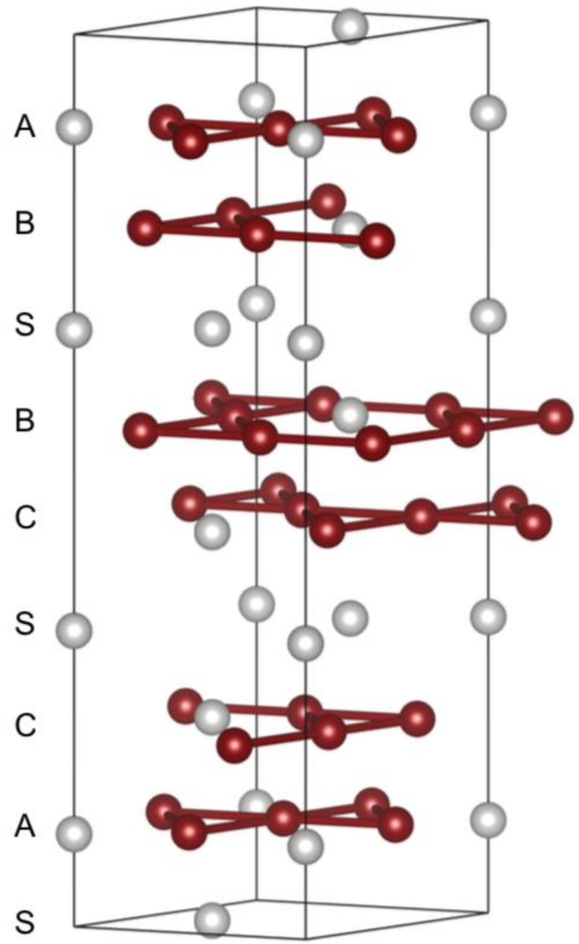
It all started with some interesting magnetotransport data…
(**Checkelsky** lab)

A possible manifestation of band topology?

Temperature-independent intrinsic anomalous Hall conductance

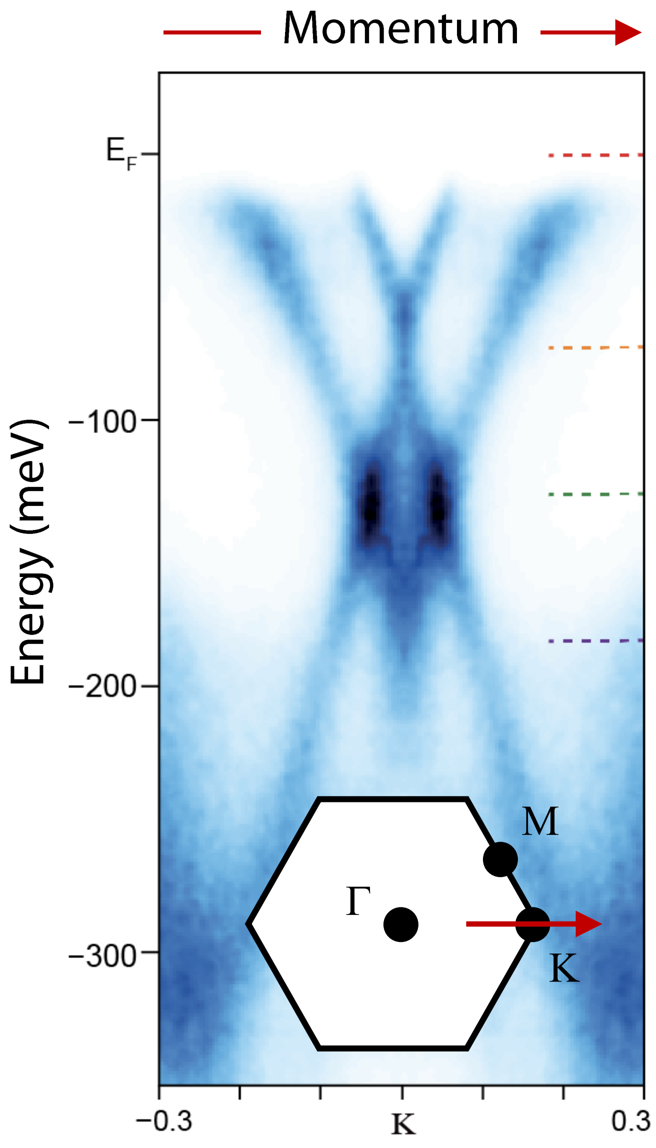


Fe_3Sn_2

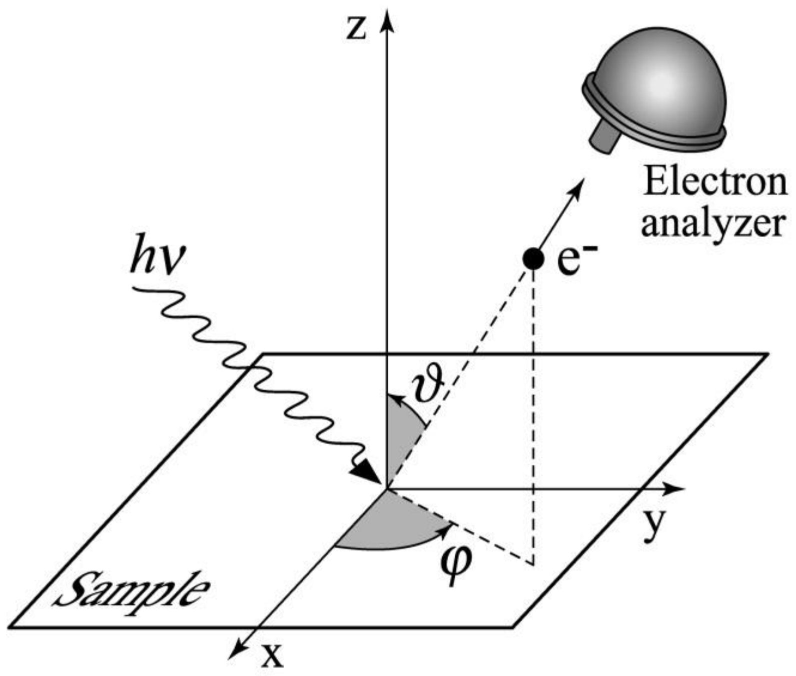


L. Ye[*], M. Kang[*], *et al.*, *Nature* **555**, 638 (2018)

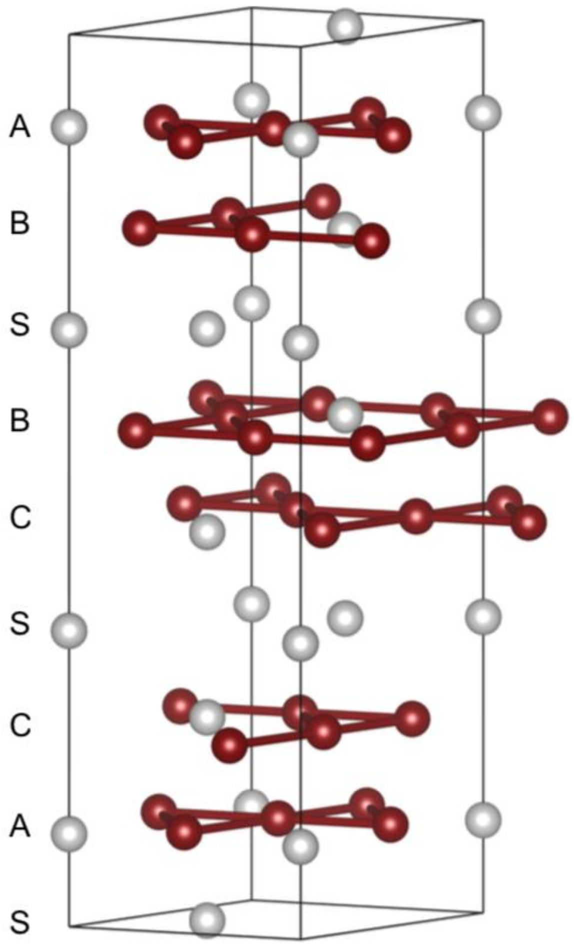
Observation of Massive Dirac fermions in Fe_3Sn_2



Angle-resolved Photoemission Spectroscopy (ARPES)



Fe_3Sn_2



L. Ye*, M. Kang*, *et al.*, *Nature* **555**, 638 (2018)

Observation of Massive Dirac fermions in Fe_3Sn_2

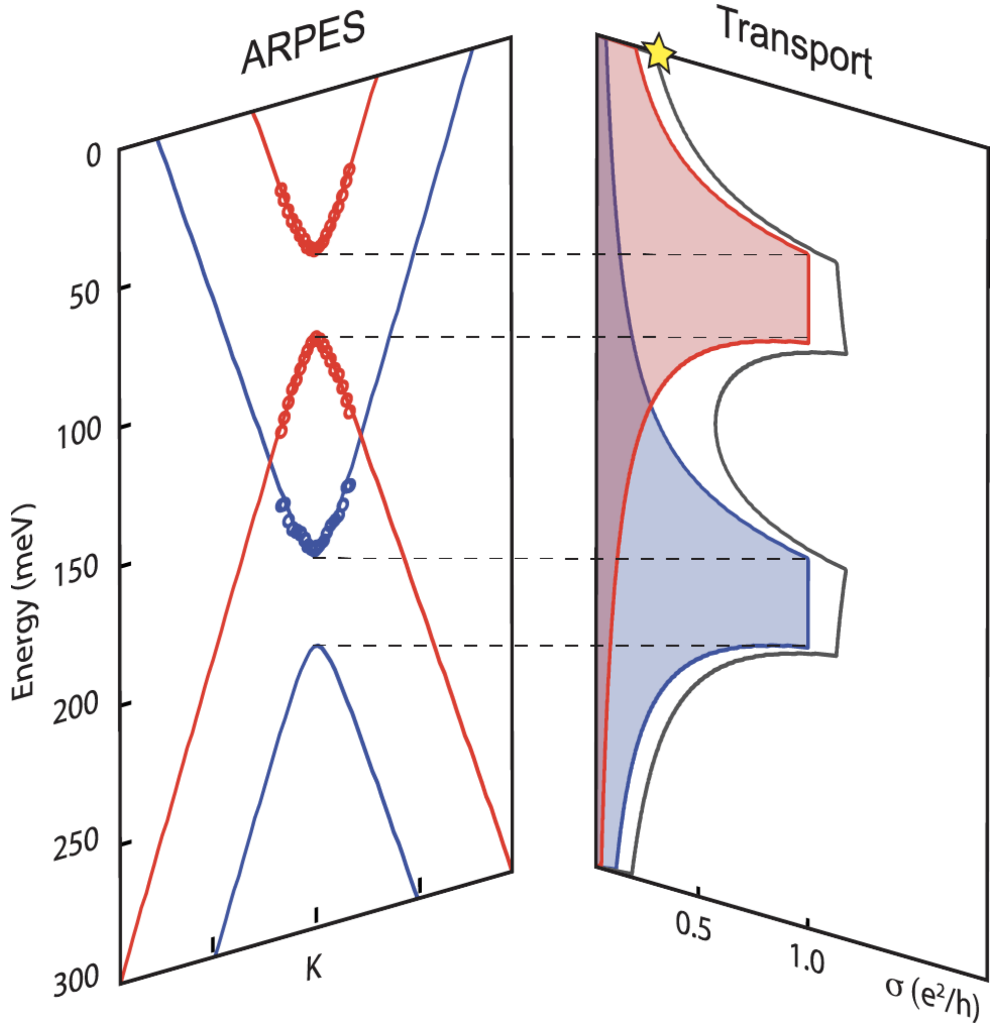
Calculating AHC from experimental band structures

$k \cdot p$ Hamiltonian : $H_D = [\hbar v_F(k_x\sigma_y - k_y\sigma_x)] \otimes I + E_0\tau_x + m\sigma_z$

Calculated AHC : $\sigma_{xy} = \frac{e^2}{2h}\frac{\Delta/2}{\sqrt{((\Delta/2))^2 + (\hbar v_F k_F)^2}}$

With input from exp. band structure: $\sigma_{xy}^{cal} = 0.31\ e^2/h$

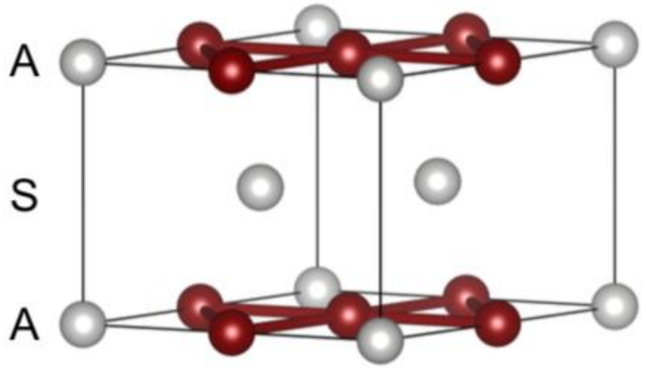
Close agreement to transport value: $\sigma_{xy}^{int} = 0.27\ e^2/h$



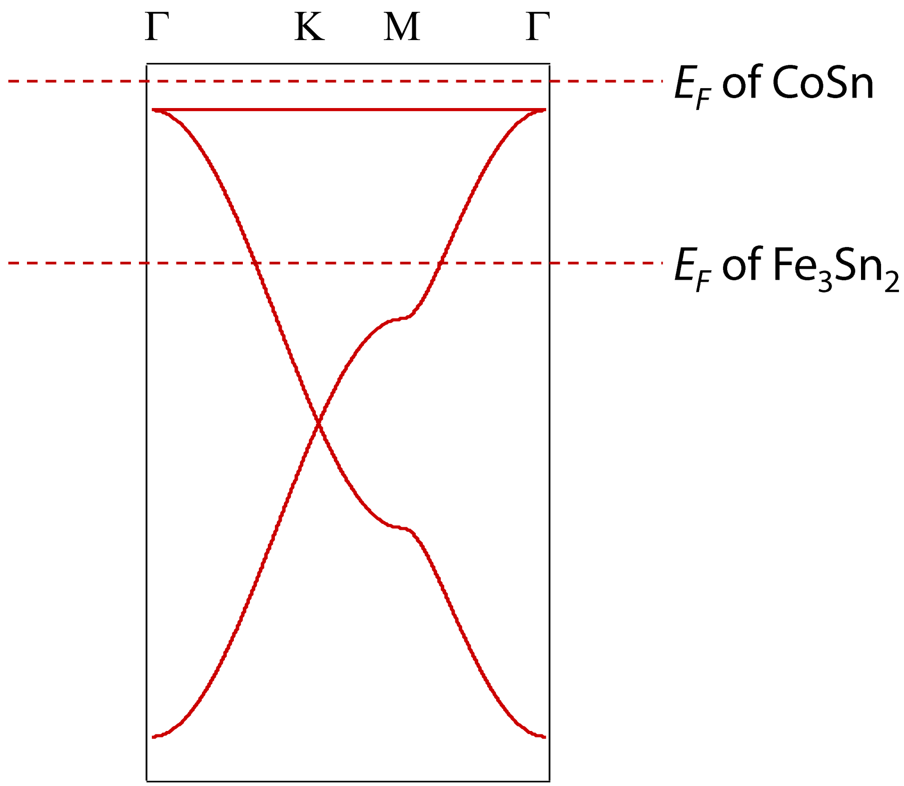
In search of the flat bands…

Chemical potential tuning via electron filling

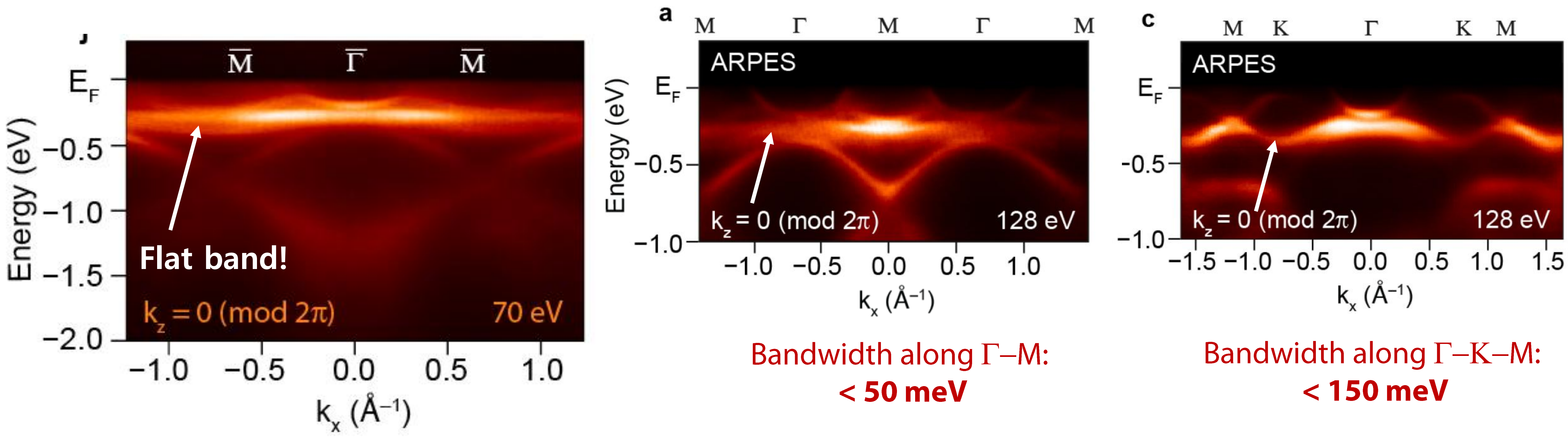
1. Simplest structure with isolated 2D kagome layers + 2. Fermi level tuning (electron filling)



CoSn



Topological flat bands in **CoSn**



Bandwidth along Γ–M:
< 50 meV

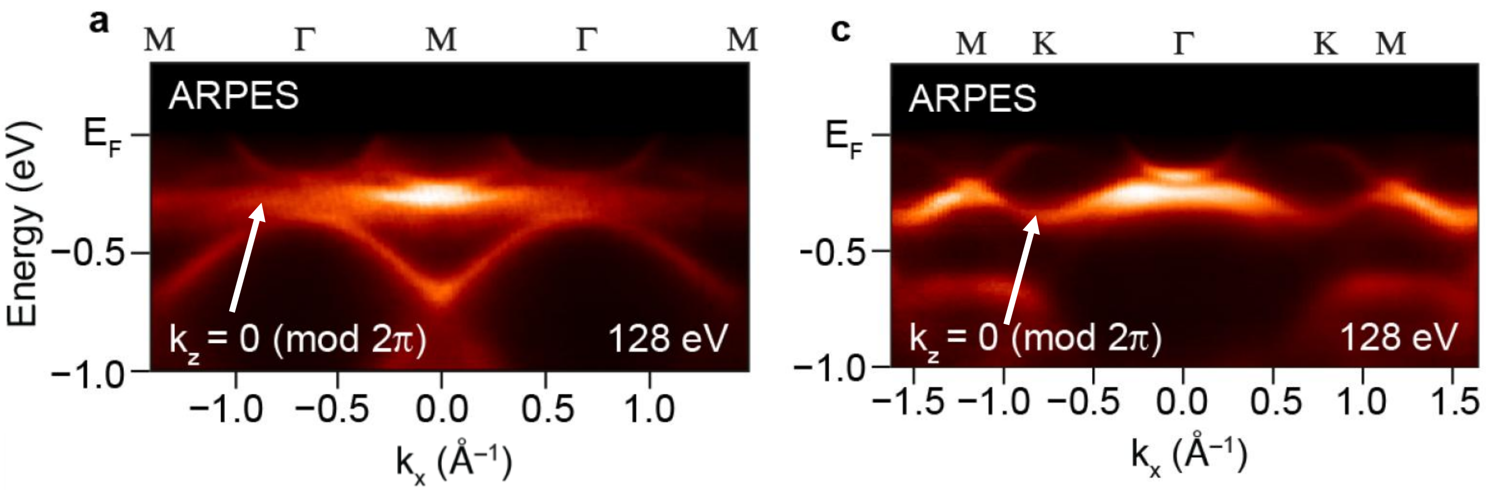
Bandwidth along Γ–K–M:
< 150 meV

- We could **directly observe the flat band** near the Fermi level at the -0.27 eV binding energy

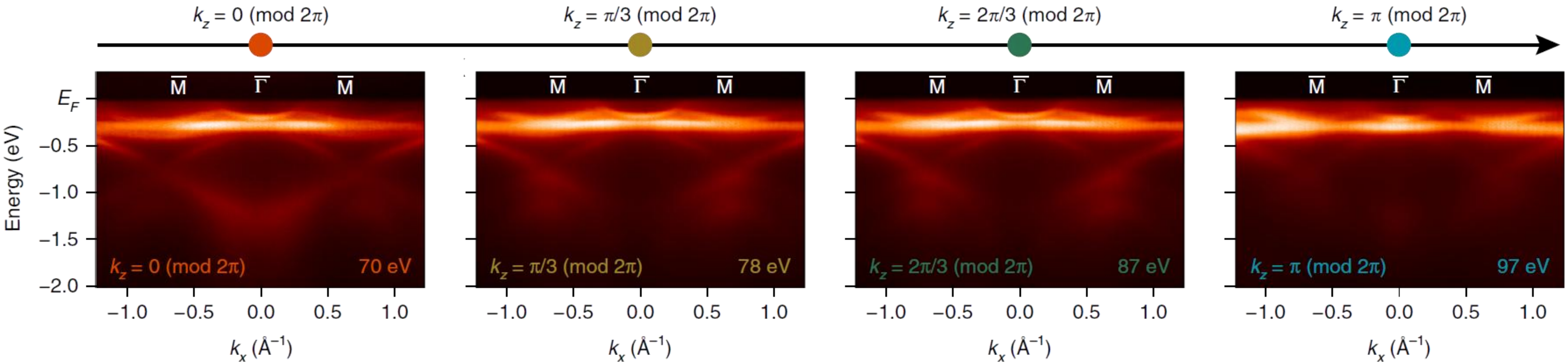
- Flat band **acquires small dispersion only near the K point** (likely due to NNN hopping).

M. Kang, S. Fang, L. Ye, *et al.*, *Nature Comm.* **11**, 4004 (2020)

Topological flat bands in **CoSn**

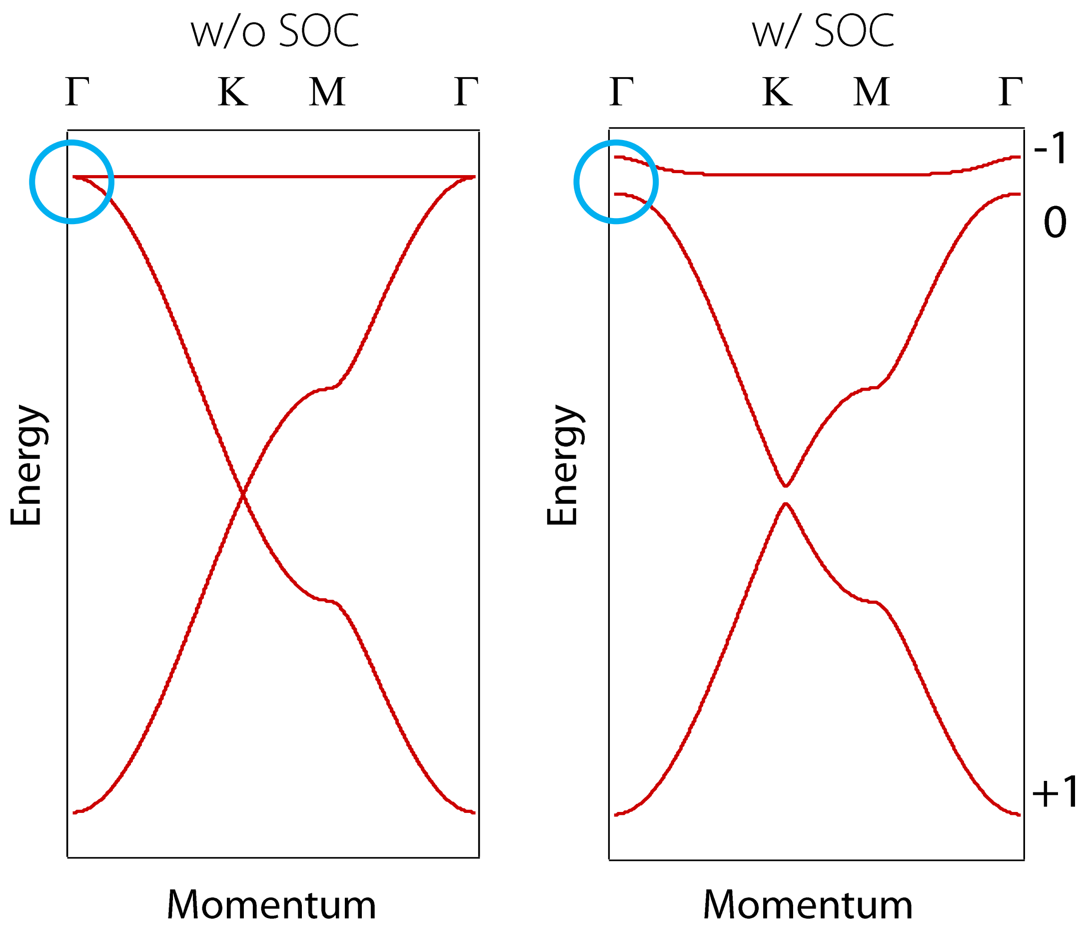


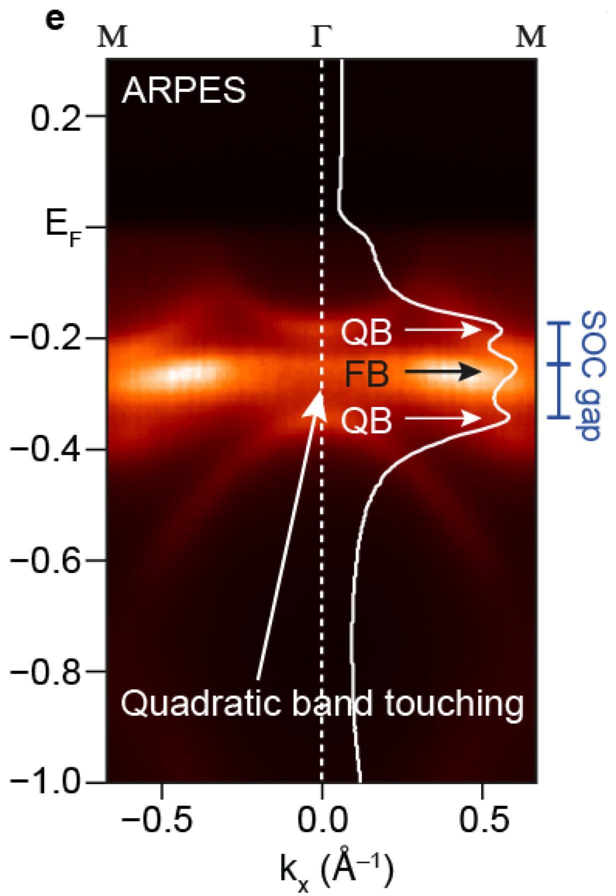
No dependence on out-of-plane momentum (k_z)

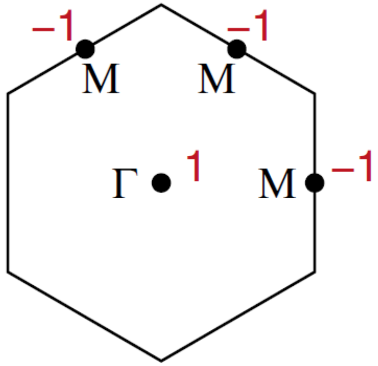


M. Kang, S. Fang, L. Ye, *et al.*, *Nature Comm.* **11**, 4004 (2020)

Topological flat bands in **CoSn**







Topo index $Z_2 = 1$

SOC opens an **80 meV gap** at the quadratic band touching point

Flat band is **topologically nontrivial**

Part 2

van Hove singularity and electronic symmetry breaking

Acknowledgments – Part 3

Theory

U. Wurzburg / Flatiron

Giorgio Sangiovanni
Domenico Di Sante

Harvard

Tim Kaxiras

Synthesis

UCSB

Brenden Ortiz
Stephen Wilson

Band structure theory

Shiang Fang

Band structure spectroscopy

Mingu Kang

Synchrotron-ARPES

LBNL-ALS

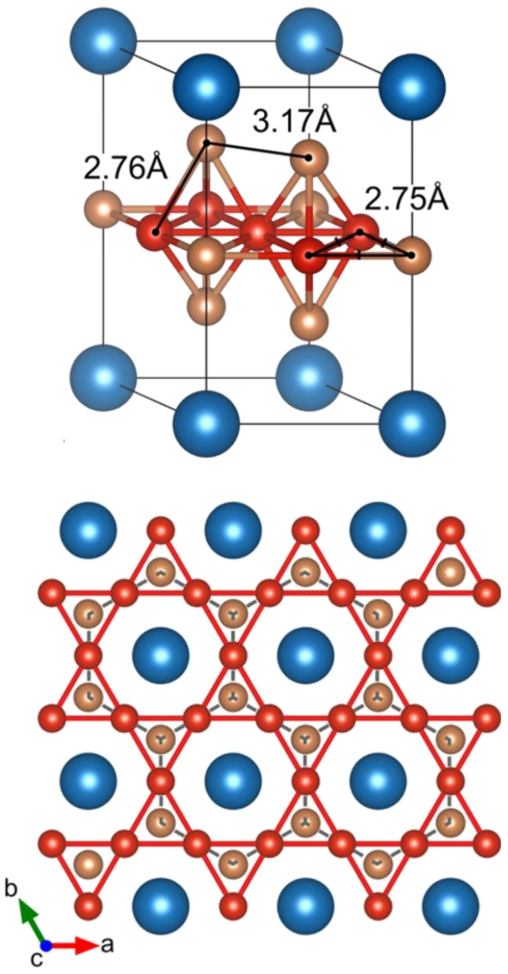
Sae Hee Ryu
Chris Jozwiak
Aaron Bostwick
Eli Rotenberg

POSTECH

Jeong-Kyu Kim
Jimin Kim
Jonggyu Yoo
Jae-Hoon Park
Byeong-Gyu Park

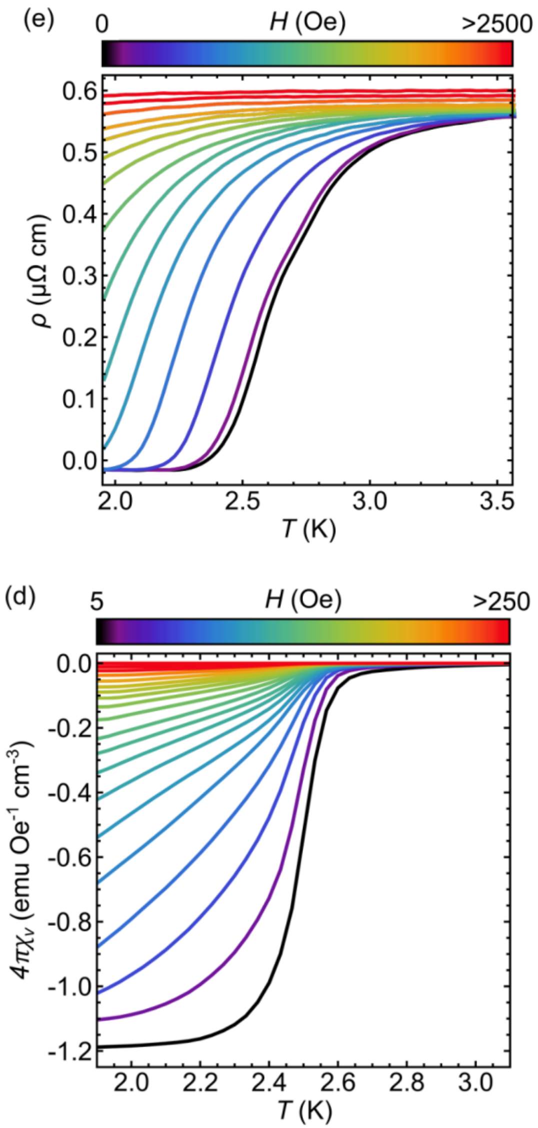
Quantum matter in AV_3Sb_5 – CDW & superconductivity

CsV_3Sb_5

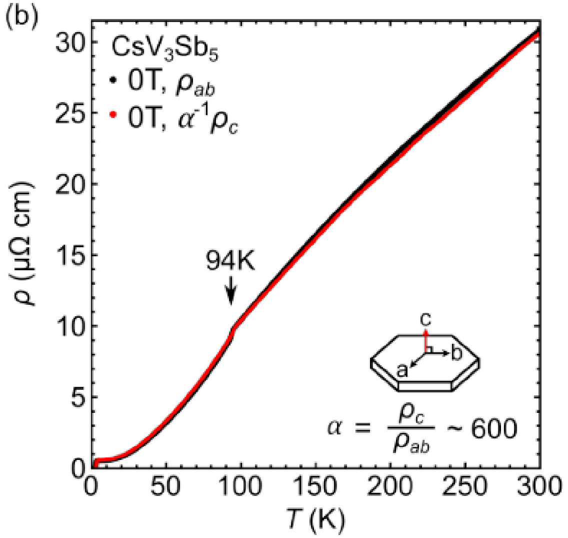


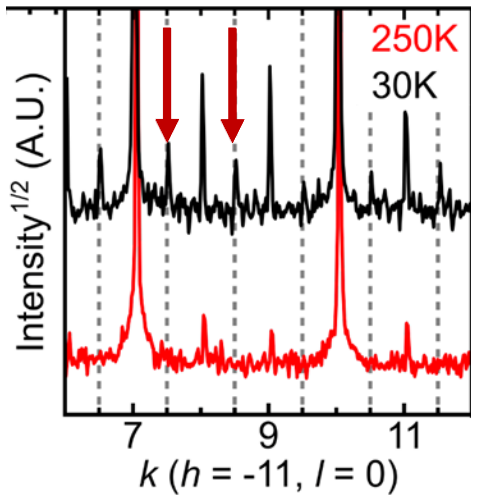
Ortiz et al., PRL **125,** 247002 (2020)

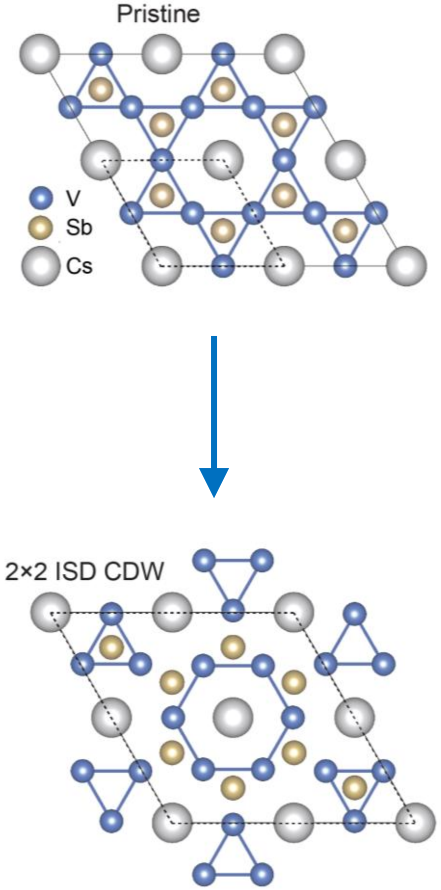
Superconductivity at 3 K



Charge order at 94 K - Q=(0.5,0,L)







Quantum matter in AV_3Sb_5

≈ 94 K
Charge order

≈ 94~70 K
Loop current order

≈ 60 K
Uniaxial stripe order

≈ 35 K
Electronic nematicity

≈ 2.5 K
Superconductivity, PDW

STM: *Nat. Mat.* **20**, 1353-1357 (2021).
XRD: *Phys. Rev. X* **11,** 031050 (2021).

STM: *Nature* **599**, 216-221 (2021).
STM: *Phys. Rev. B* **104,** 035131 (2022).

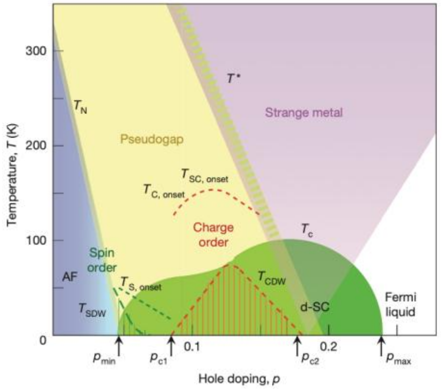
STM: *Nature* **599,** 222-228 (2021).

mSR: *Nature* **602,** 245-250 (2022).
mSR: *ArXiv:2107.10714* (2021).

Strain: *Nature* **604**, 59-64 (2022).
STM: *Nat. Phys.* **18,** 1-6 (2022).

- **Cuprates High T_c SC**

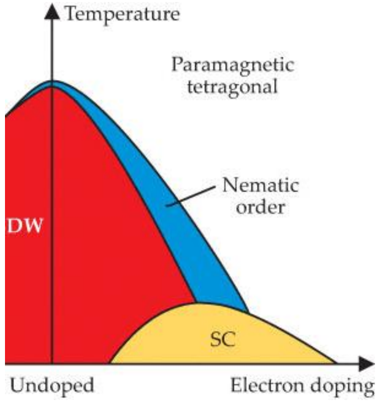
(1986 ~)



Keimer *et al.* (2015)

- **Fe-based High T_c SC**

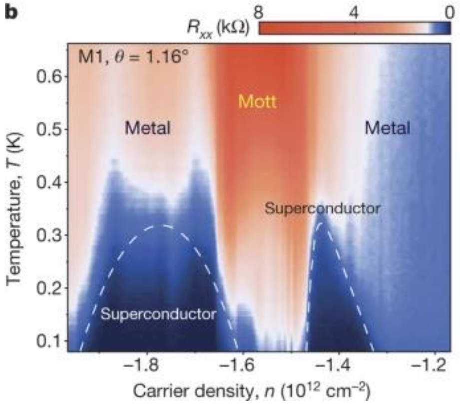
(2008 ~)



Kamihara *et al.* (2008)

- **Twisted Moire superlattices**

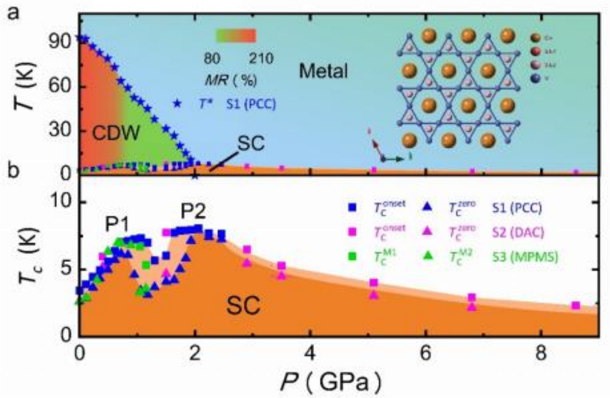
(2018 ~)



Y. Cao *et al.* (2018)

- **Kagome metal AV_3Sb_5**

(2020 ~)



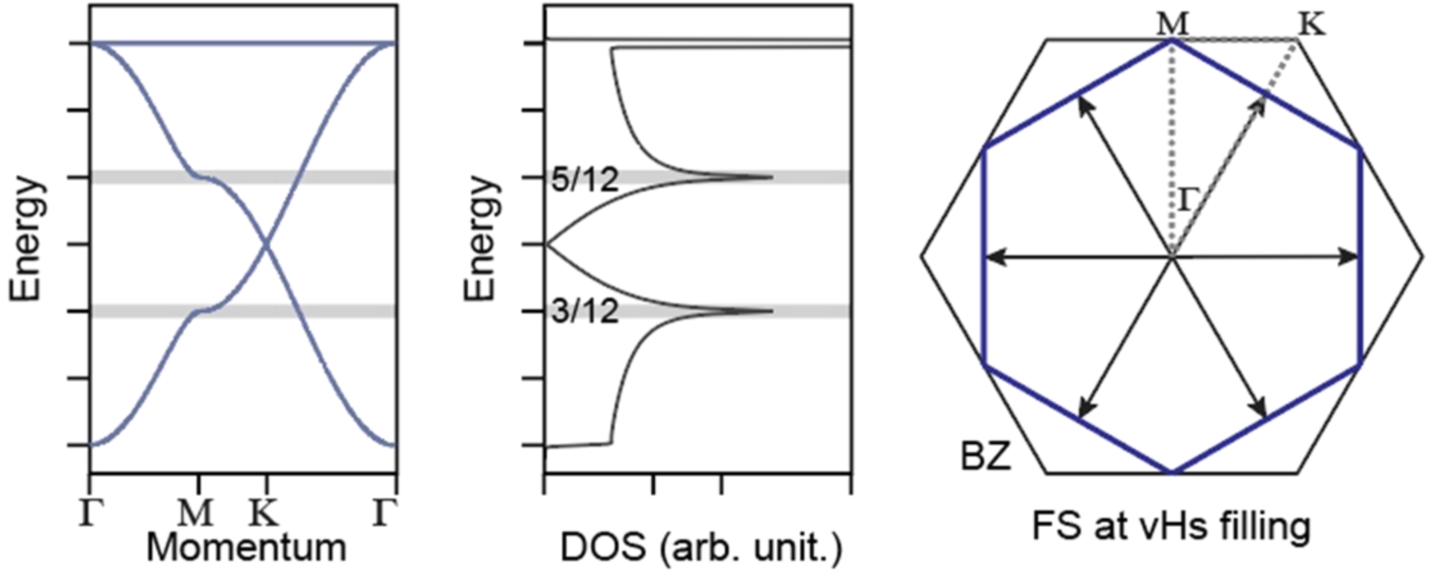
B. Ortiz *et al.* (2020)

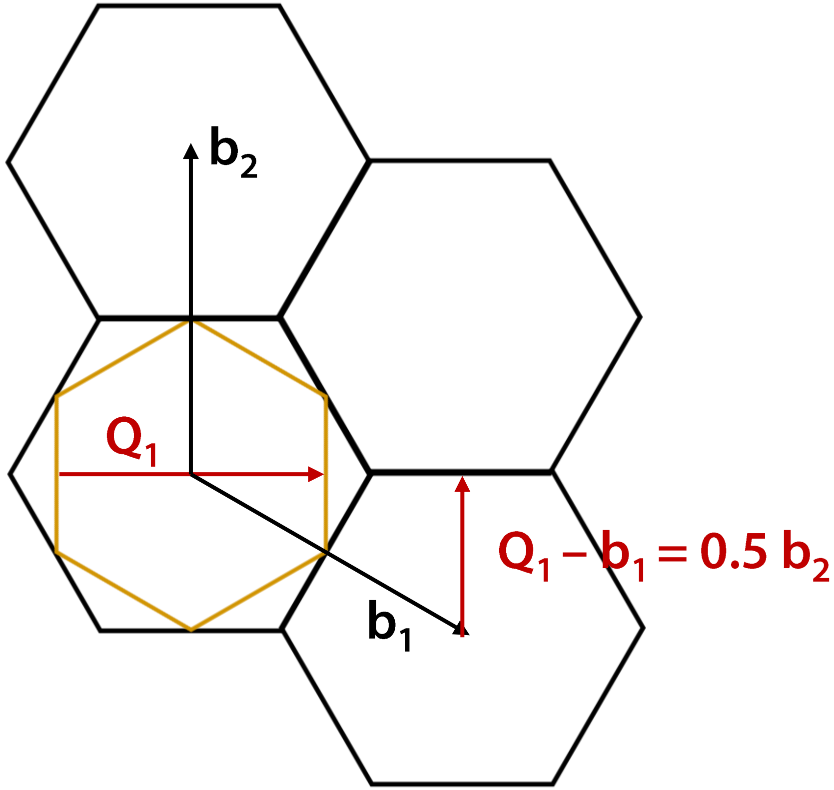
Iridate (2008)

Nickelate SC (2019)

AV_3Sb_5 – Fermiology & symmetry breaking

What's the role of the electronic band structure in the formation of the CDW state?





At the **van Hove singularity fillings** (5/12, 3/12) one finds:

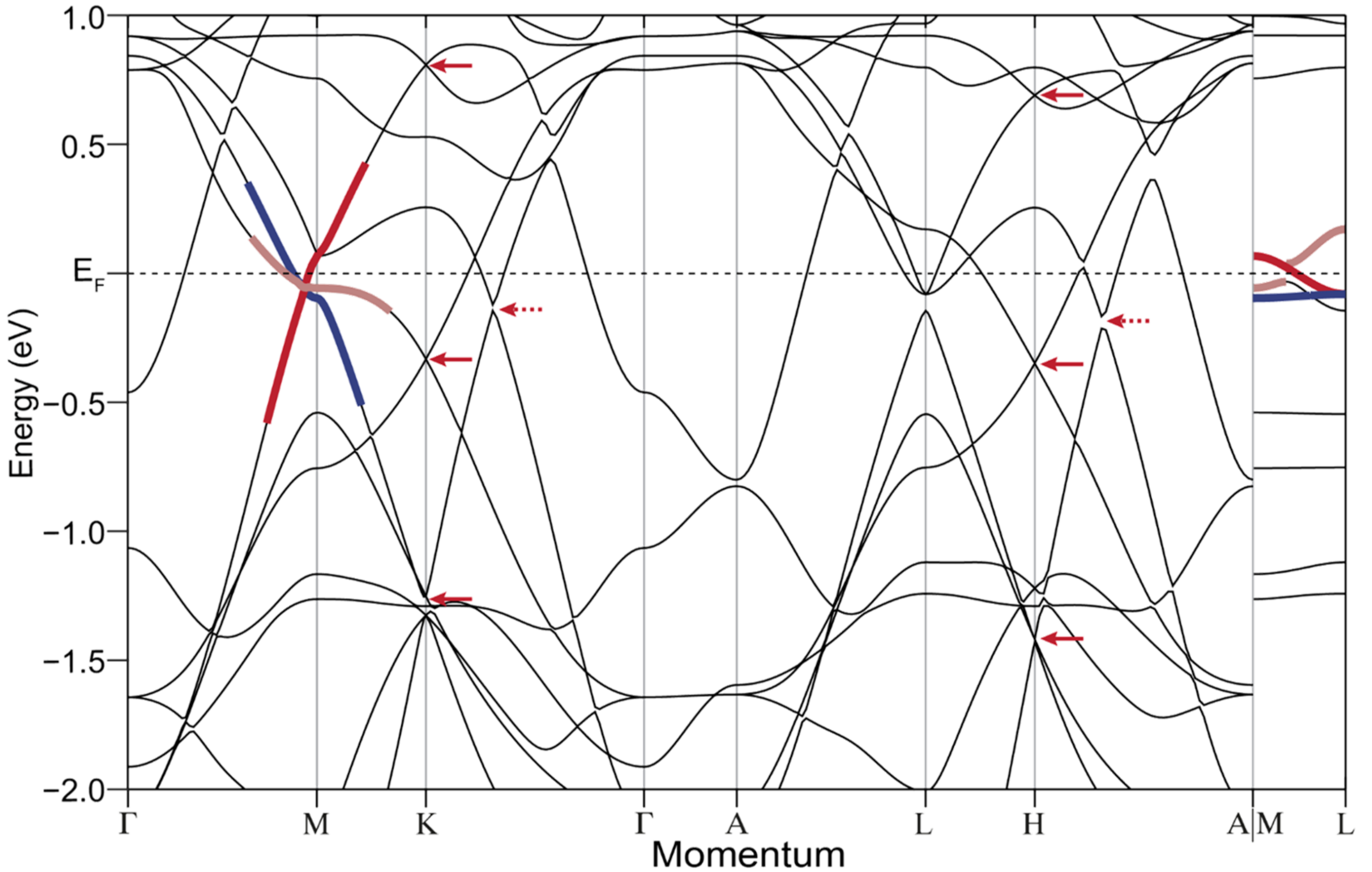
1) Diverging density of states
2) Perfectly nested Fermi surface

Ideal conditions for **electronic instabilities**

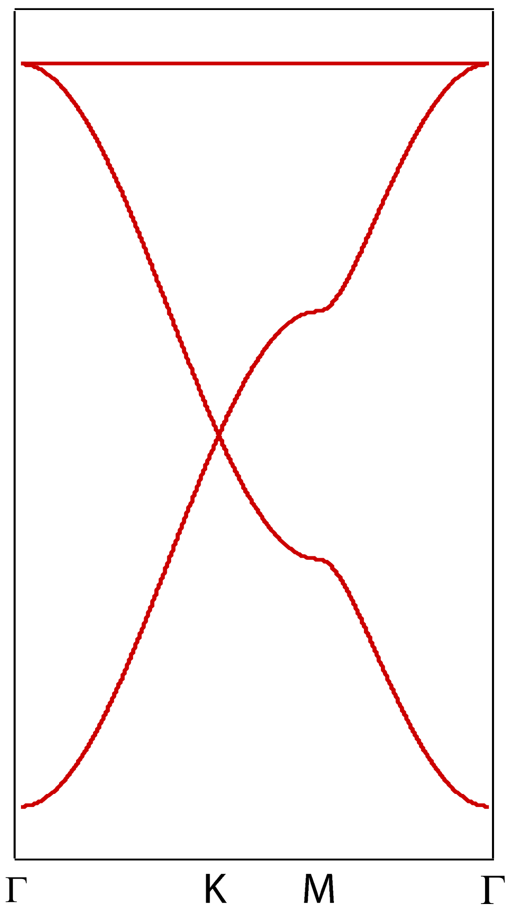
Nesting wave vector **Q = (1/2, 0)**, consistent with 2x2 charge order

Electronic band structure of CsV_3Sb_5 – **DFT (undistorted)**

Reality

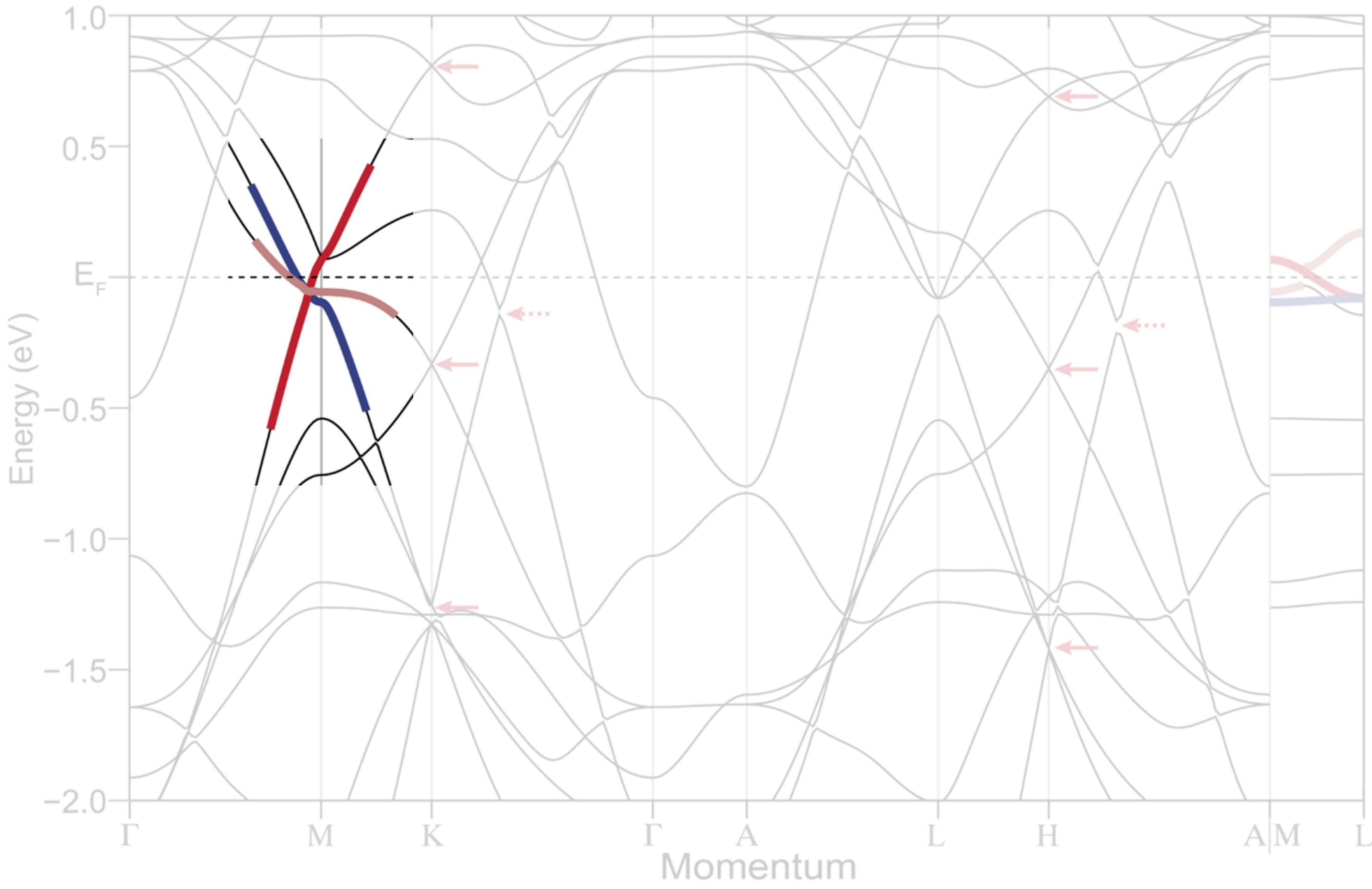


Expectation



M. Kang, S. Fang, …, RC. *Nature Physics* **18**, 301 (2021)

Electronic band structure of CsV_3Sb_5 – **DFT (undistorted)**

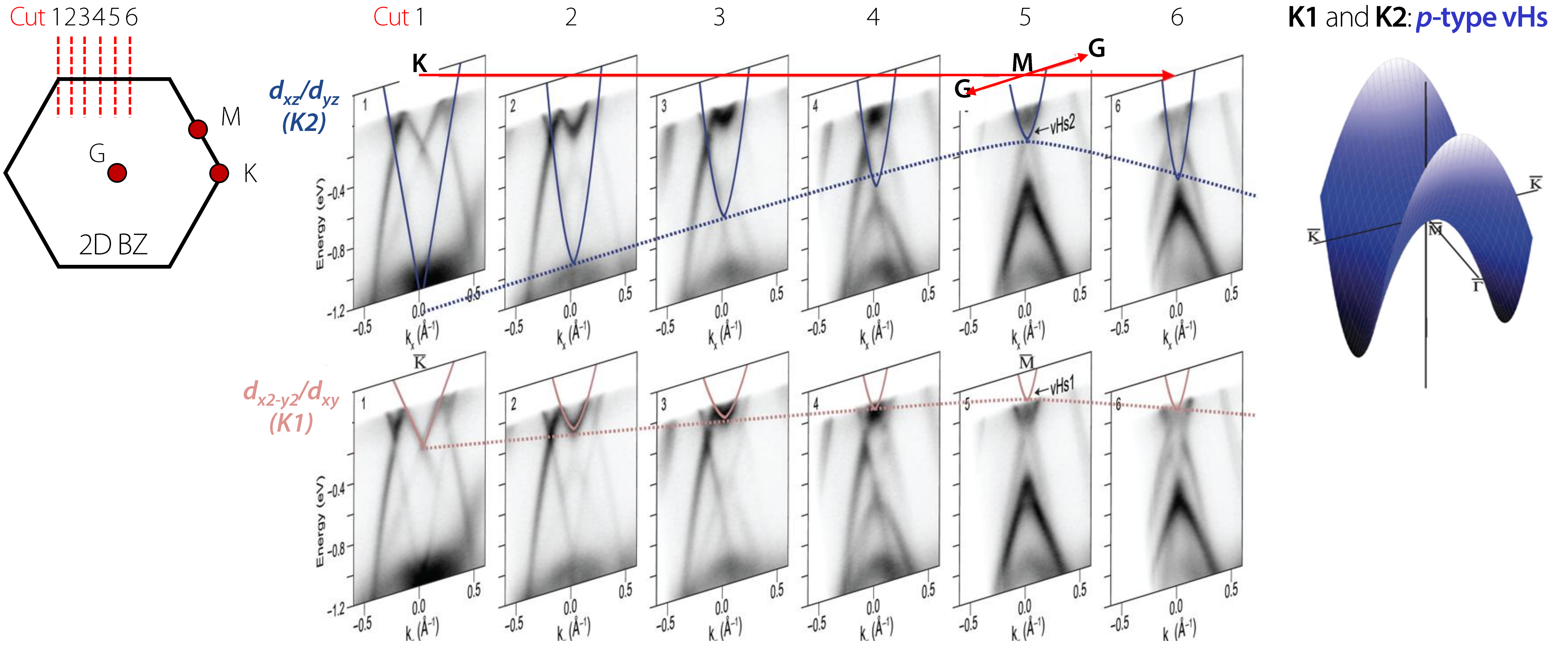


Three main kagome-derived bands from V-3d orbitals:

- **K1** band – has $d_{xy}/d_{x2\text{-}y2}$ (in-plane) character and a ***p*-type vHs near E_F** at the *M* point
- **K2** band – has d_{xz}/d_{yz} (out-of-plane) character and a ***p*-type vHs near E_F** at the *M* point
- **K2'** band has d_{xz}/d_{yz} (out-of-plane) character and a ***m*-type vHs near E_F** at the *M* point

M. Kang, S. Fang, …, RC. *Nature Physics* **18**, 301 (2021)

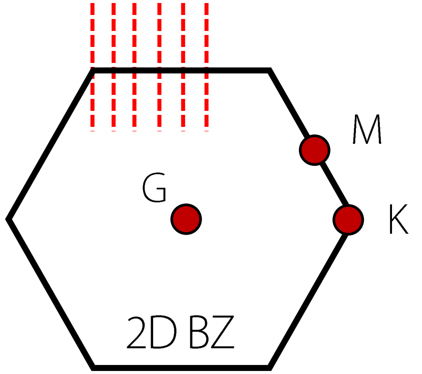
Electronic band structure of CsV_3Sb_5 – **van Hove singularities**

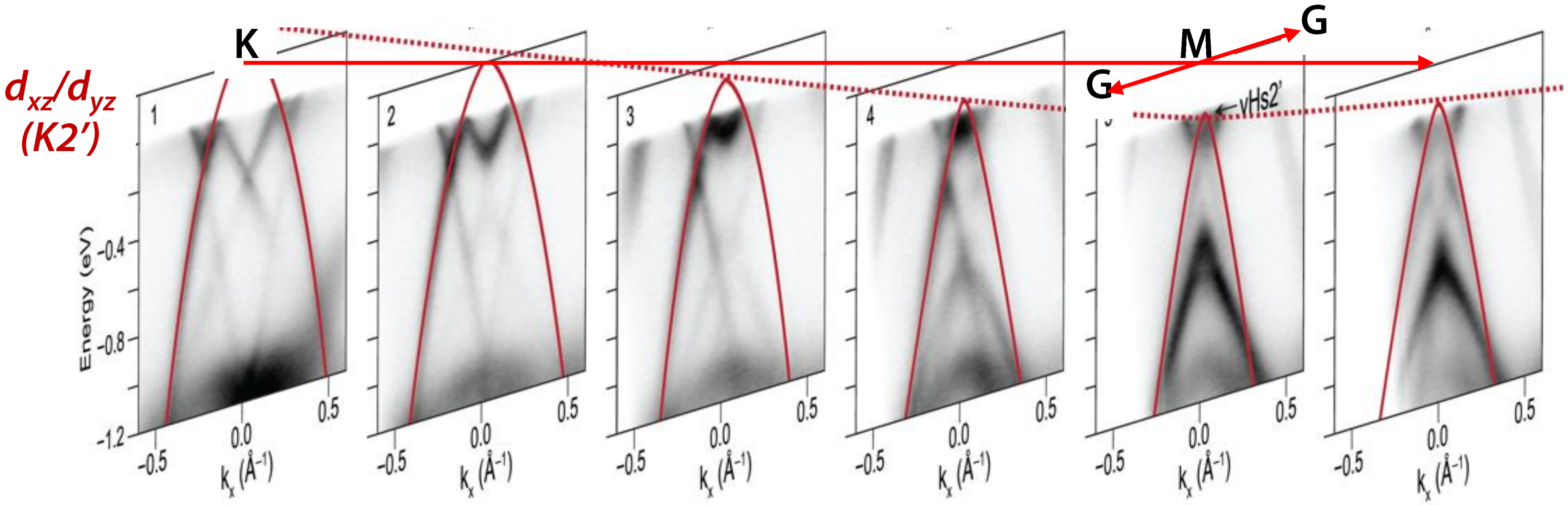


Hole-like dispersion along **K-M-K**.

Electron-like dispersion along **G-M-G**.

Electronic band structure of CsV_3Sb_5 – **van Hove singularities**

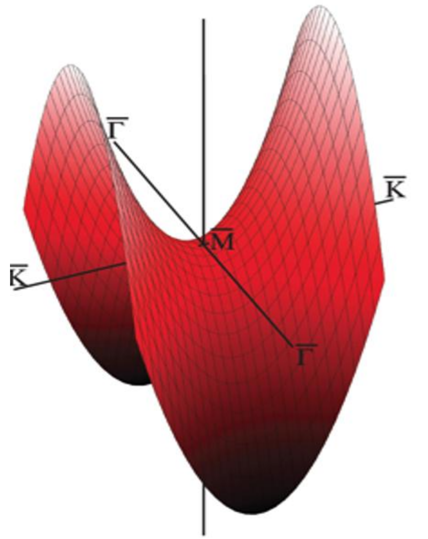




Electron-like dispersion along **K-M-K**.

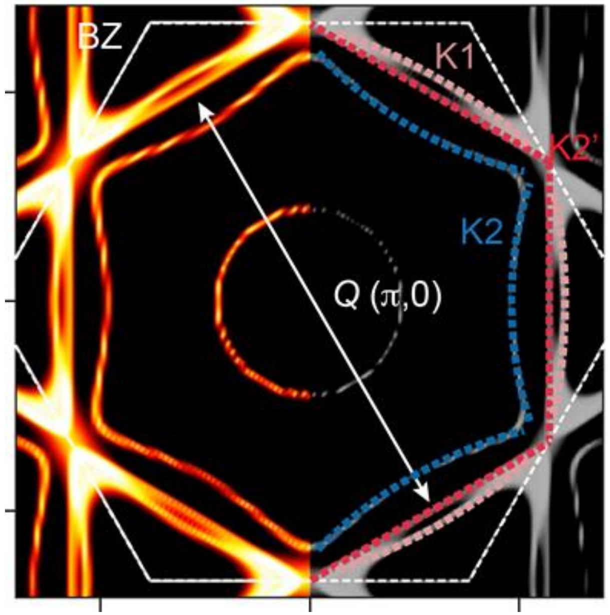
Hole-like dispersion along **G-M-G**.

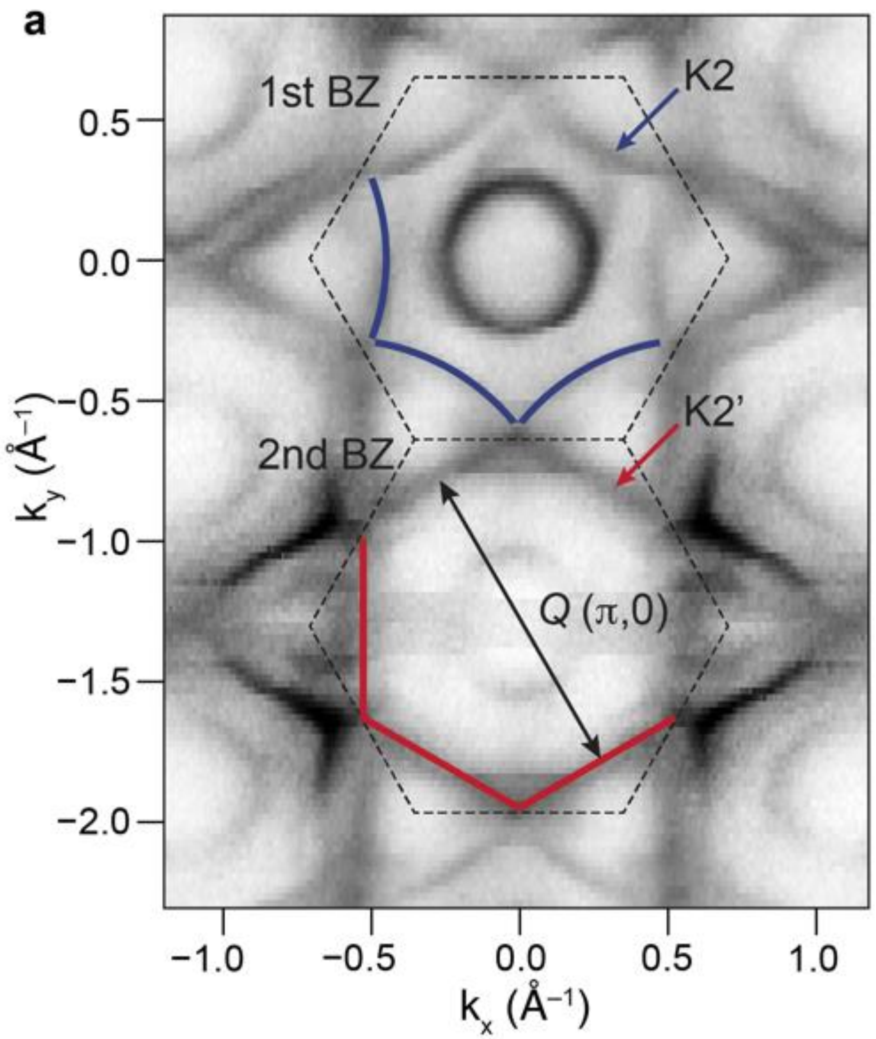
K2': ***m*-type vHs**

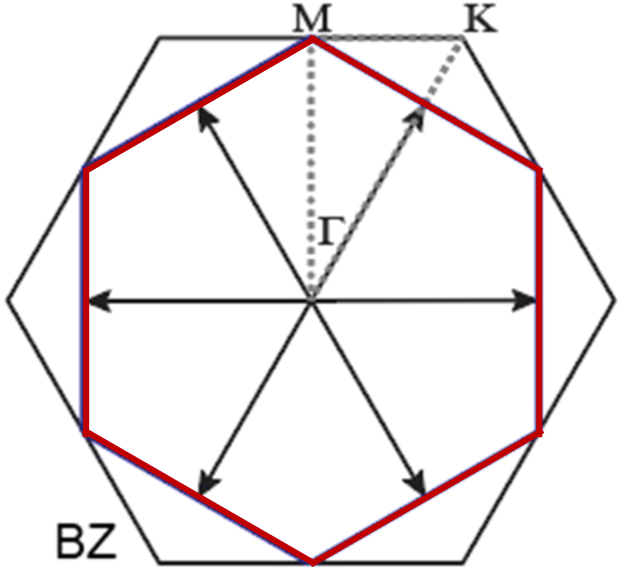


Electronic band structure of CsV_3Sb_5 – **CDW gap**

Fermi surface @ k_z=0 (DFT)

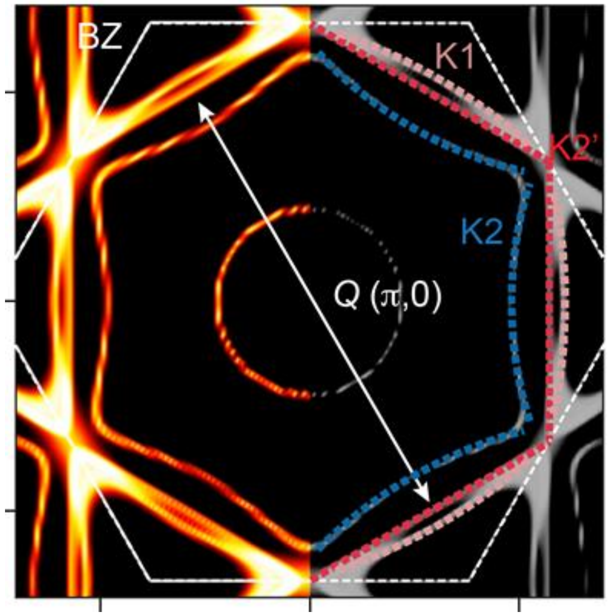


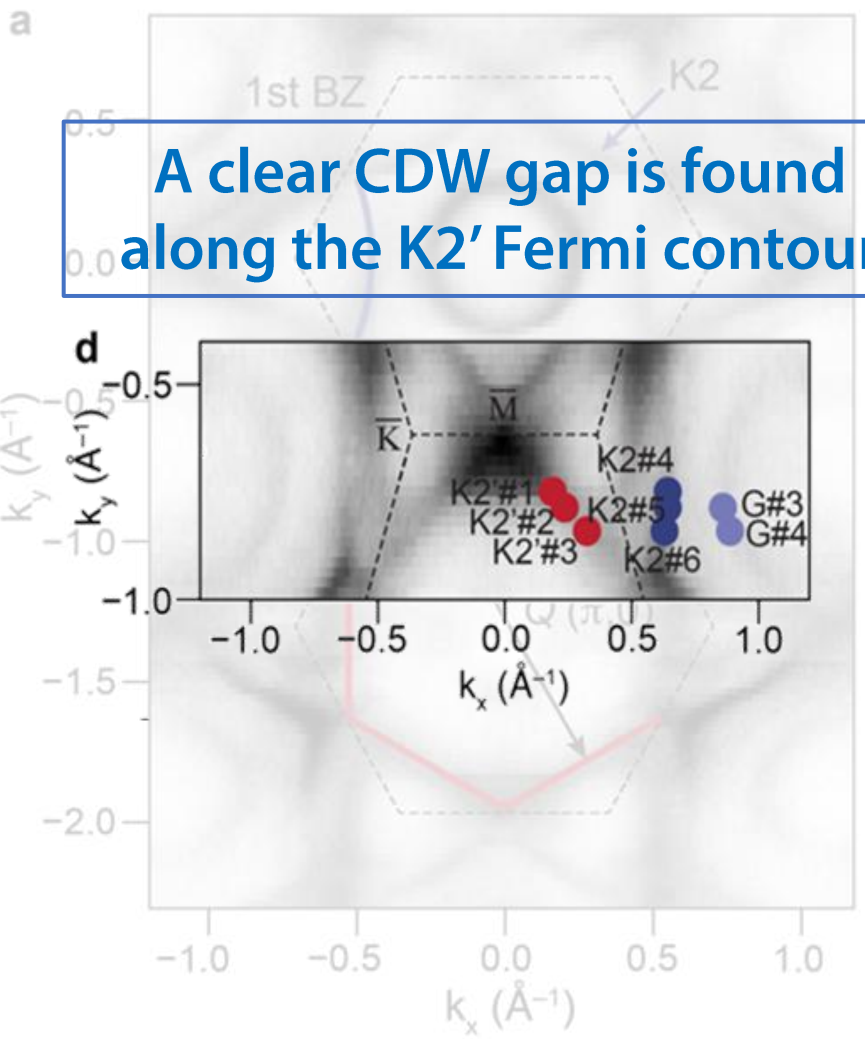




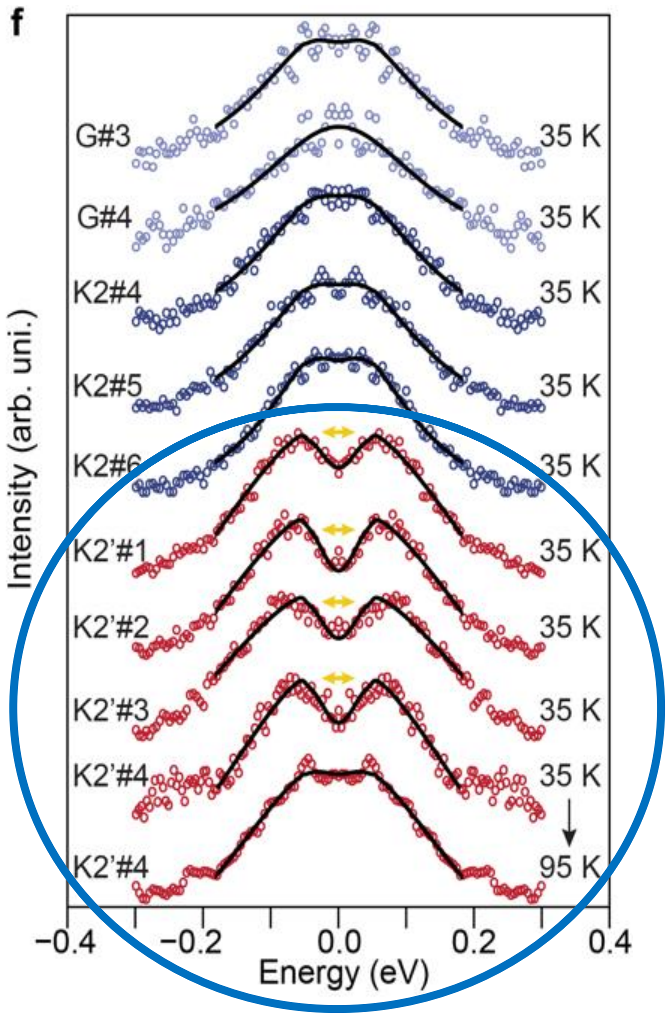
The K2′ band is almost perfectly nested

Electronic band structure of CsV_3Sb_5 – **CDW gap**

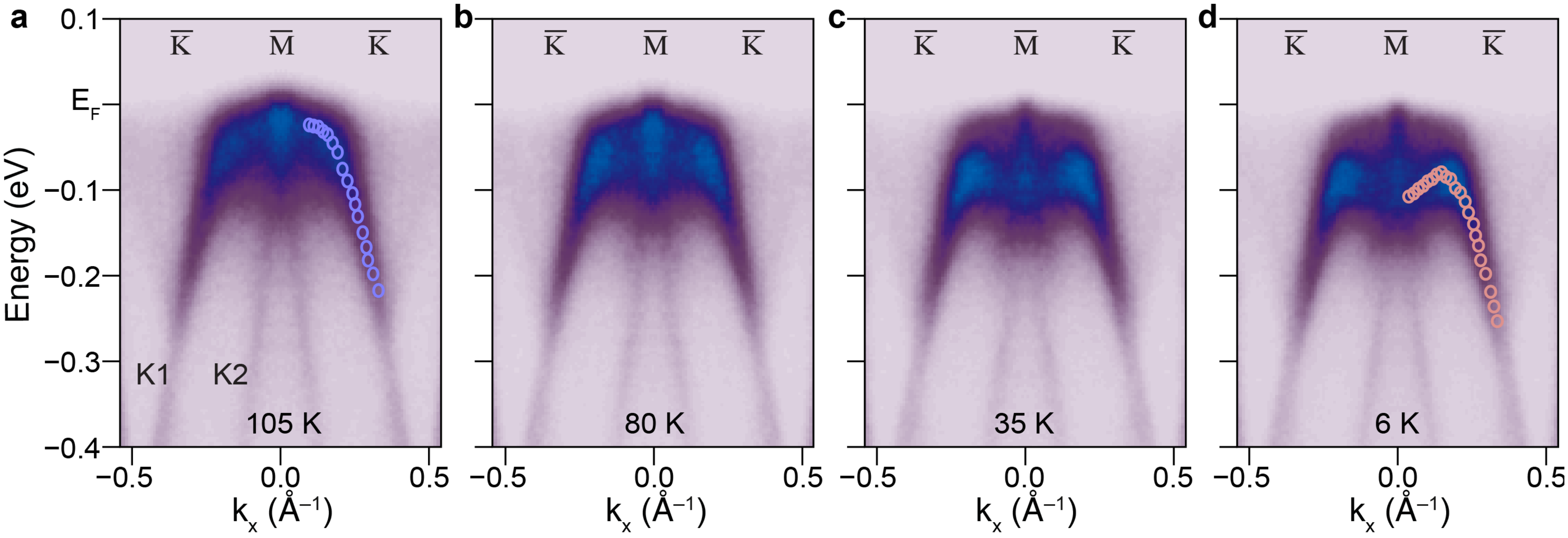




A clear CDW gap is found along the K2' Fermi contour



Electronic band structure of CsV_3Sb_5 – **CDW gap**



The K1 band has its vHs almost precisely at the *M* point,
and is strongly renormalized

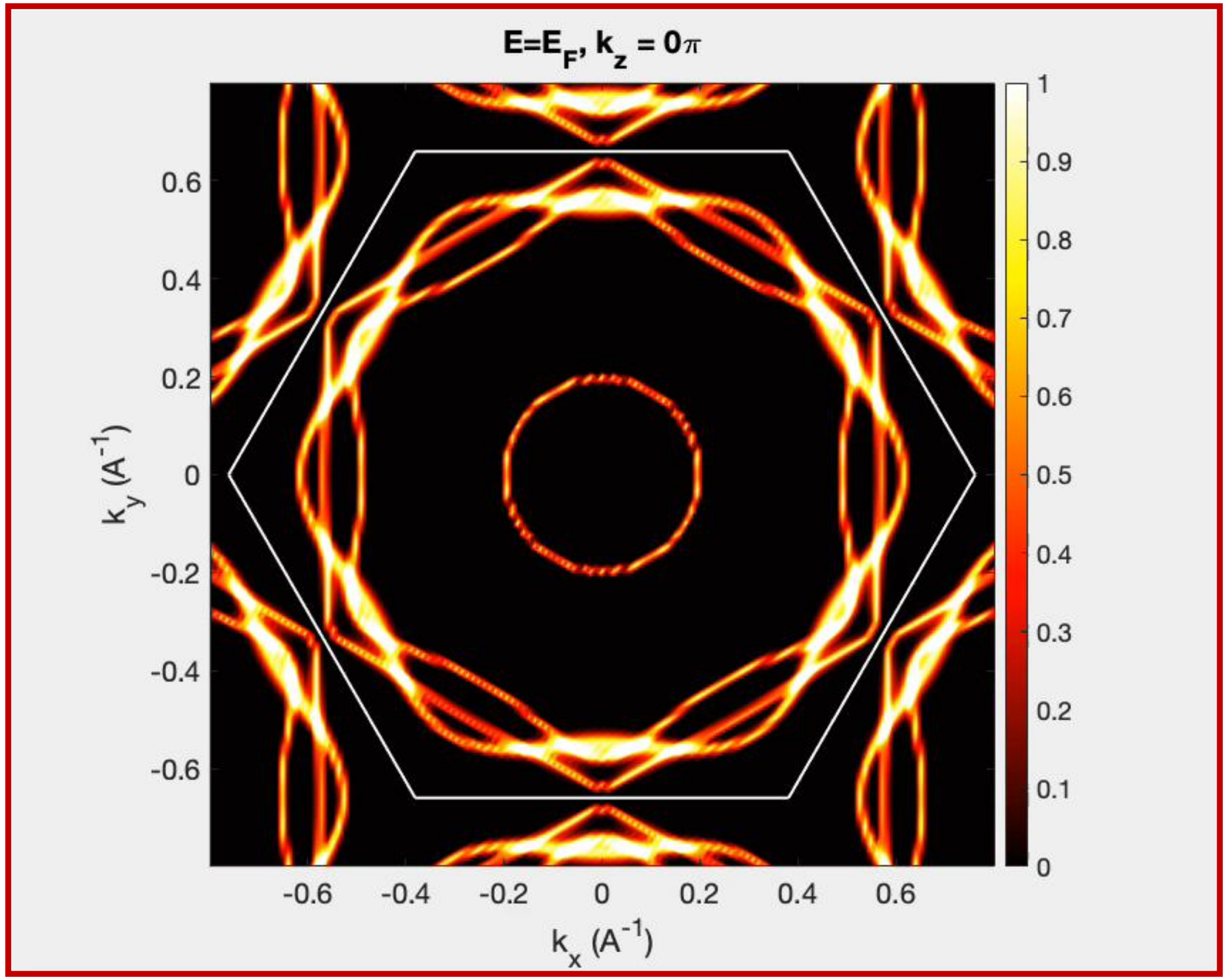
Electronic band structure of CsV_3Sb_5 – **CDW gap**

So…what's making the system unstable toward translational symmetry breaking?

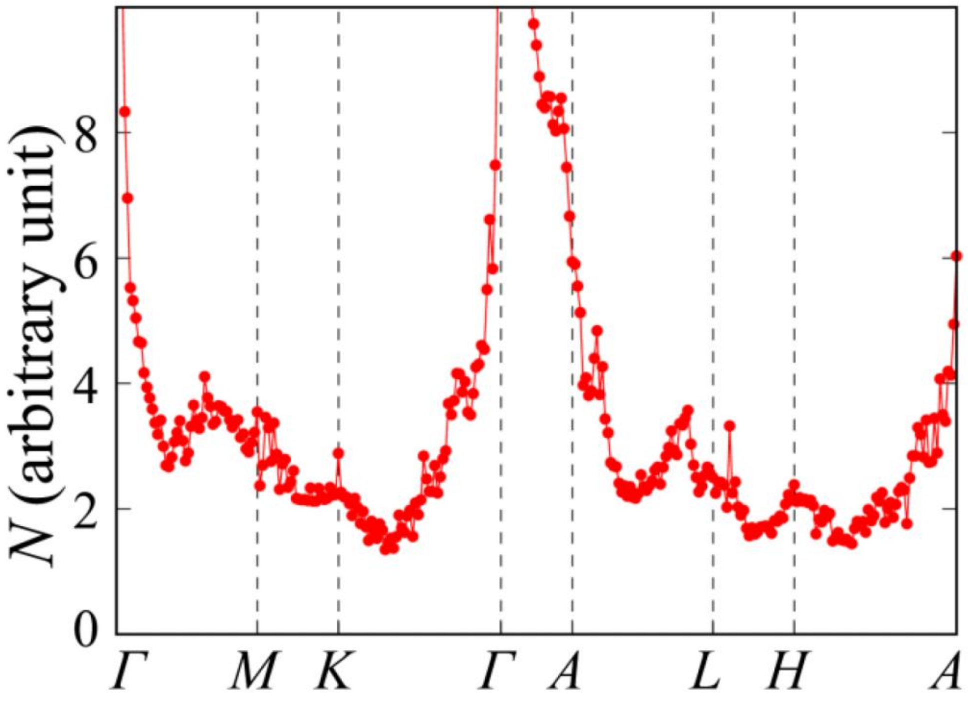
What is the relative role of the high DOS near E_F (van Hove singularity) or the high joint DOS (nesting effects)?

Electronic band structure of CsV_3Sb_5 – $\boldsymbol{k_z}$ **dependence**

A key element is the dimensionality of the band structure.



Lindhard function

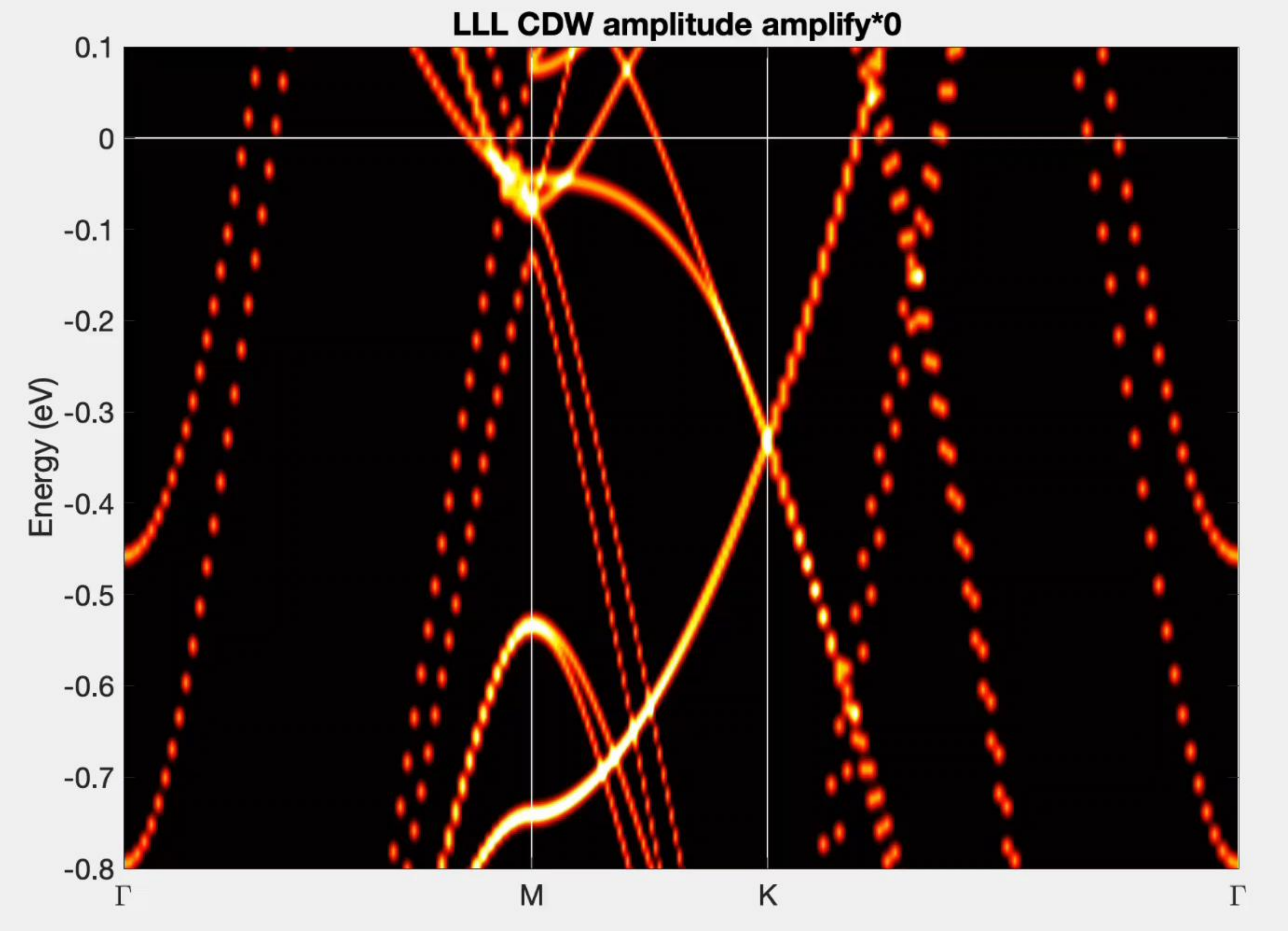


No clear divergence of the electronic susceptibility at the *M* point

C. Wang, *et al.*, *PRB* **105**, 045135 (2022)

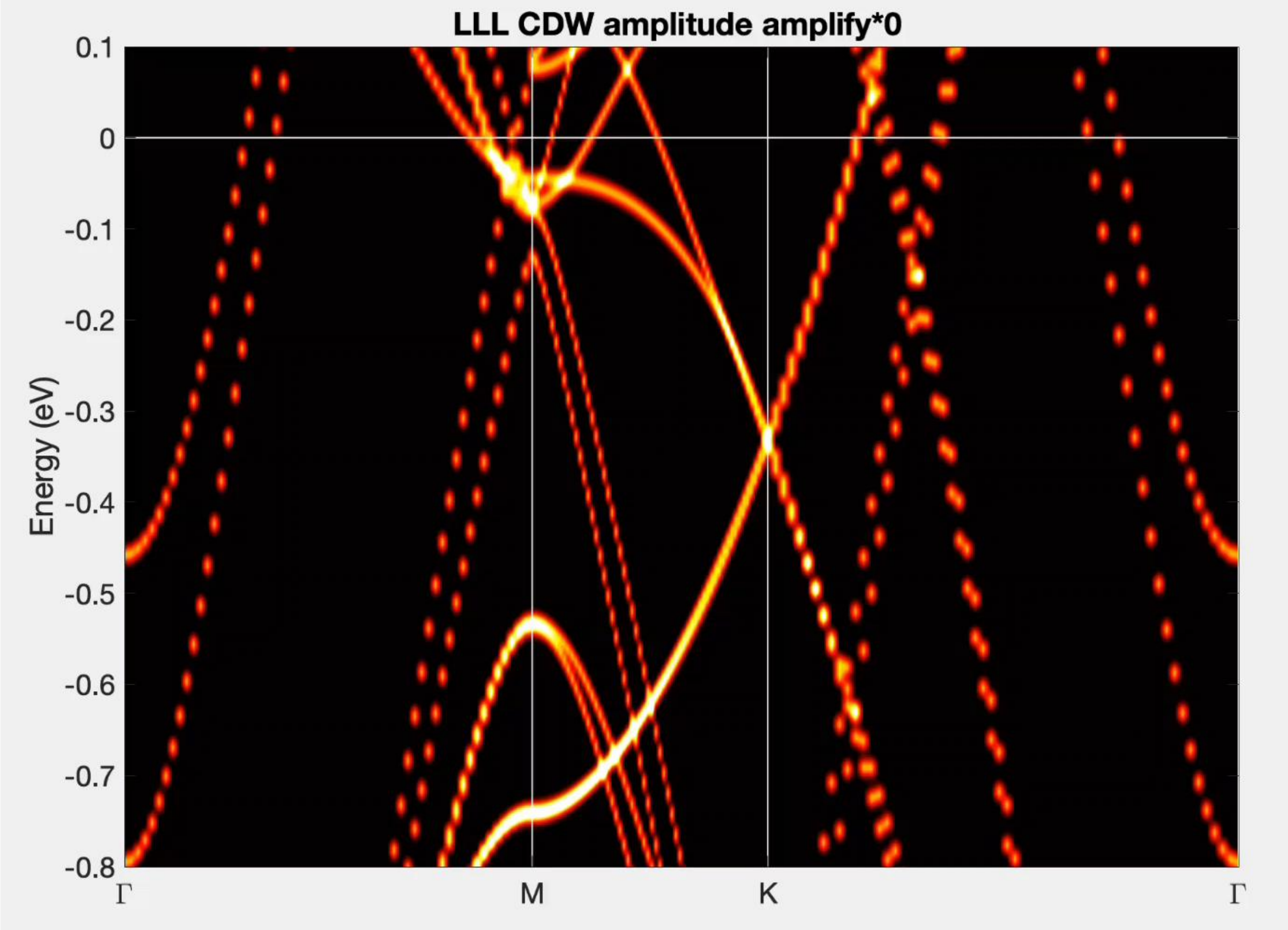
Electronic band structure of CsV_3Sb_5 – **Electron-lattice coupling**

The lattice distortion pushes bands apart by ~ 100 meV and removes the vHs from E_F



Electronic band structure of CsV_3Sb_5 – **Electron-lattice coupling**

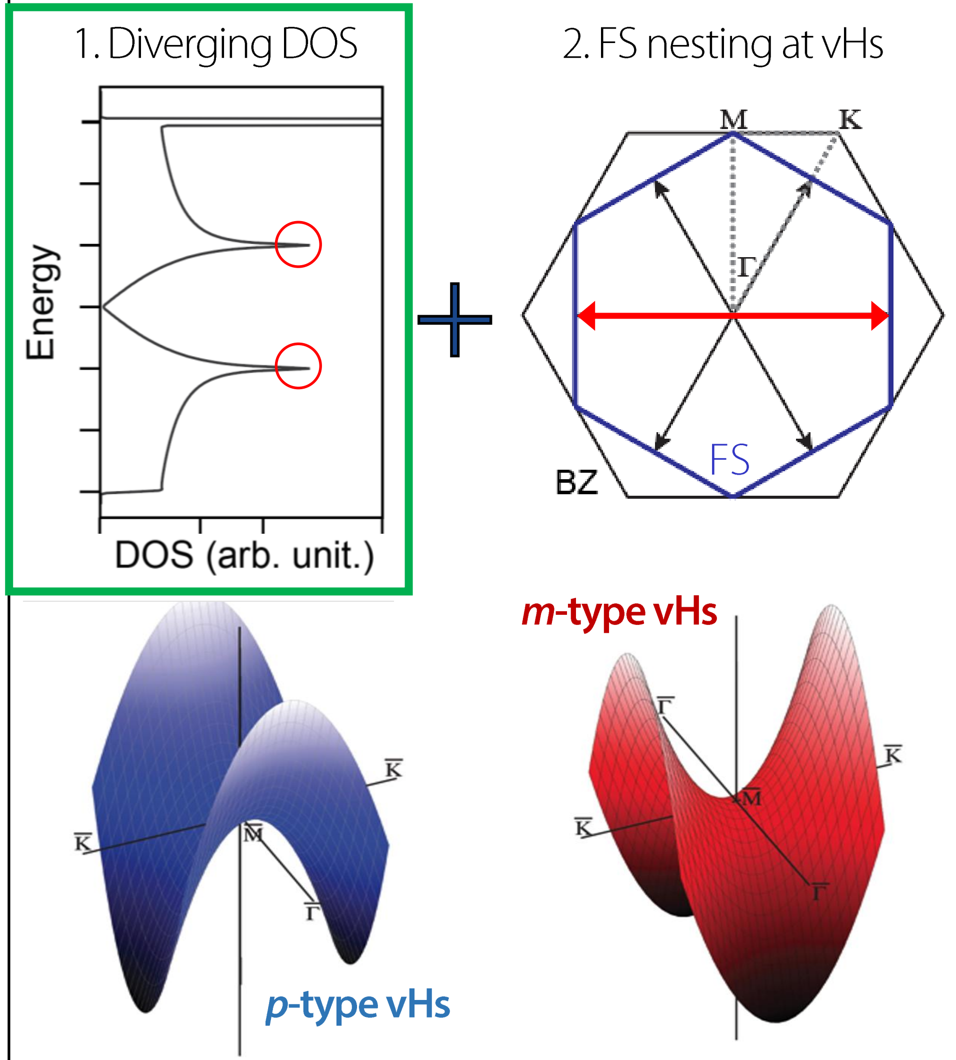
The lattice distortion pushes bands apart by ~ 100 meV and removes the vHs from E_F

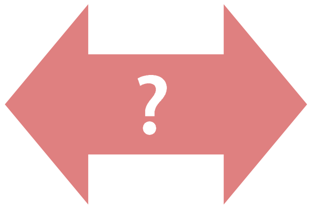


Hallmark of large electron-lattice coupling

Takeaways

Physics of van Hove singularities





Collective electron phases in CsV_3Sb_5

≈ 94 K Chiral charge order
STM: *Nat. Mat.* **20**, 1353-1357 (2021).

≈ 70 K Flux phase (Tr-symmetry breaking)
μSR: *ArXiv:2107.10714* (2021).
μSR: *Nature* (2022).

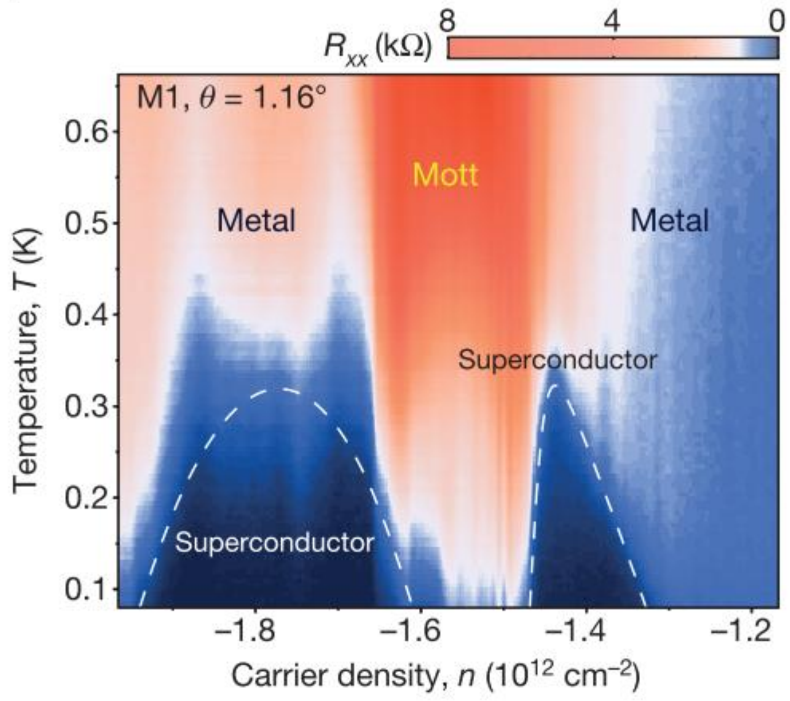
≈ 60 K Uniaxial stripe ordering
STM: *Nature* **599**, 216 (2021).
STM: *Phys. Rev. B* **104,** 035131 (2022).

≈ 35 K Electronic nematicity
STM: *Nat. Phys.* (2022).
Transport: *Nat. Comms.* ***12:****6727 (2021).*
NMR + Strain: *Nature* (2022).

≈ 3 K Superconductivity, Pair density wave
STM: *Nature* **599,** 222-228 (2021).

Outlook – quantum matter phenomena

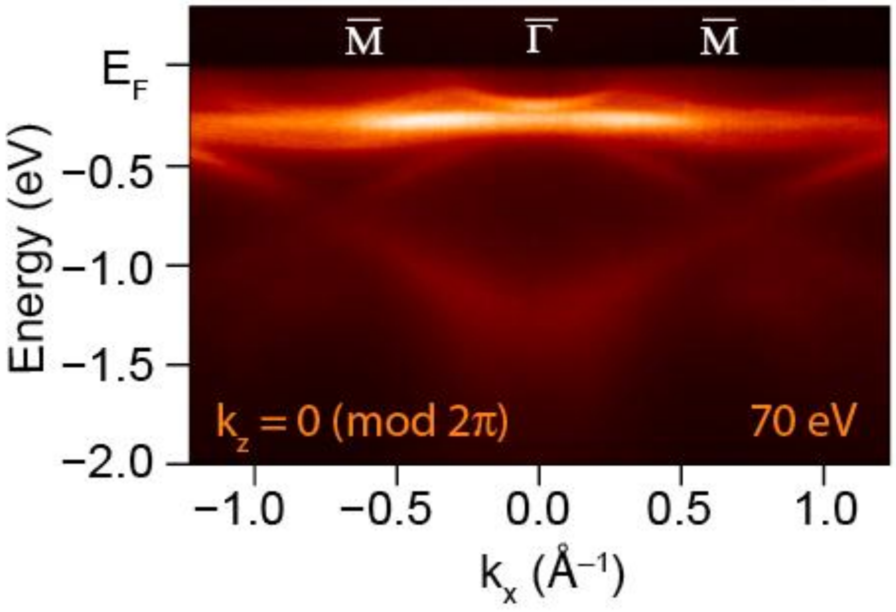
Twisted bilayer graphene



Hosts topology, magnetism, and strong correlation phenomena

Up to temperatures ~ 0.1-1 K

2D kagome network



Hosts topology, magnetism, and strong correlation phenomena

Up to temperature ~ 10-100 K

Questions…?