PDW Workshop
KITP, UC Santa Barbara
Tuesday May 17th, 2022

Experiments on kagome CDW/Superconducting Materials

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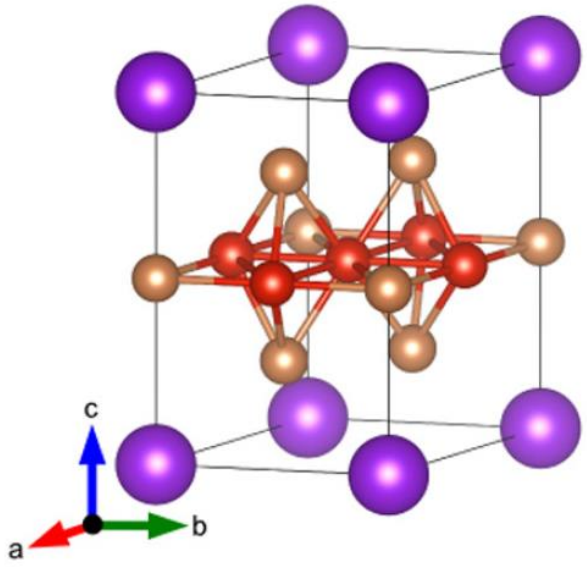
UC SANTA BARBARA Quantum Foundry

DMR-1906325

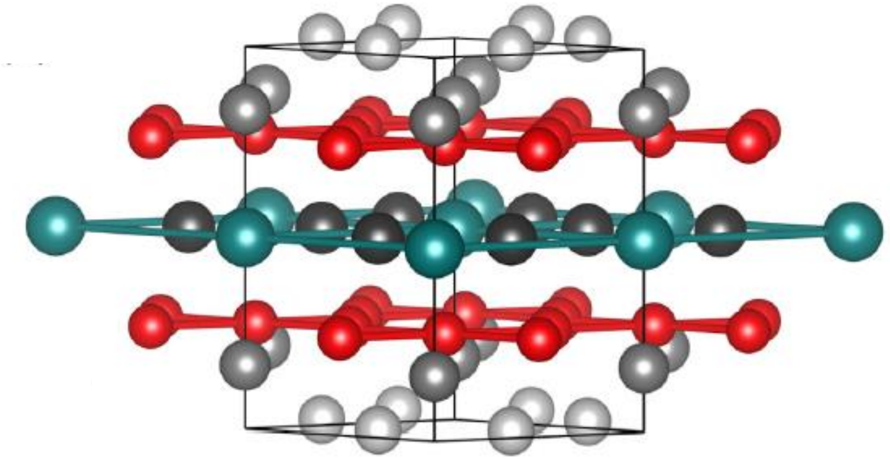
Overview

- Motivation for kagome metals
- New kagome systems AV_3Sb_5 (A=K, Rb, Cs)
  - CDW order
  - Superconductivity
  - Intertwined CDW and SC order
- Other recent materials/candidates
  - New series of RV_6Sn_6 systems (R=Y, Gd-Yb)
  - Other classes
- Prospects

AV_3Sb_5

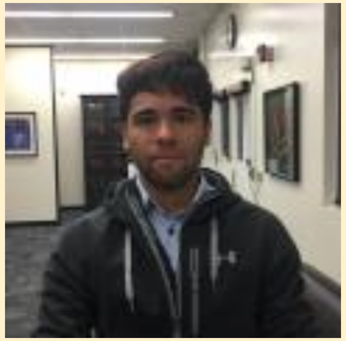


RV_6Sn_6



Collaborators

Brenden Ortiz



Sam Teicher

Yuzki Oey

Farnaz K.

Linus Kautszch

Ganesh Pokharel

UCSB: Leon Balents, Ram Seshadri, John Harter

BROWN: Vesna Mitrovic

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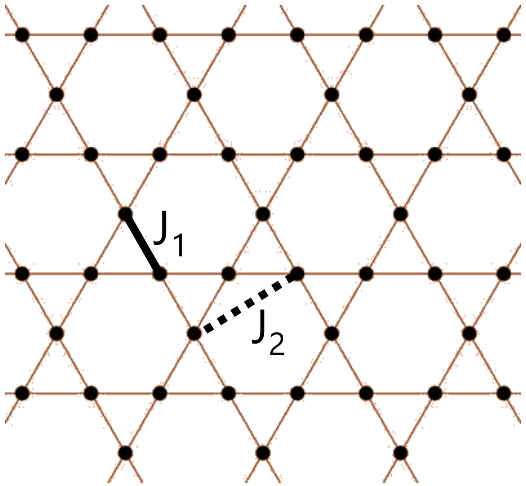
Rutgers: Girsh Blumberg

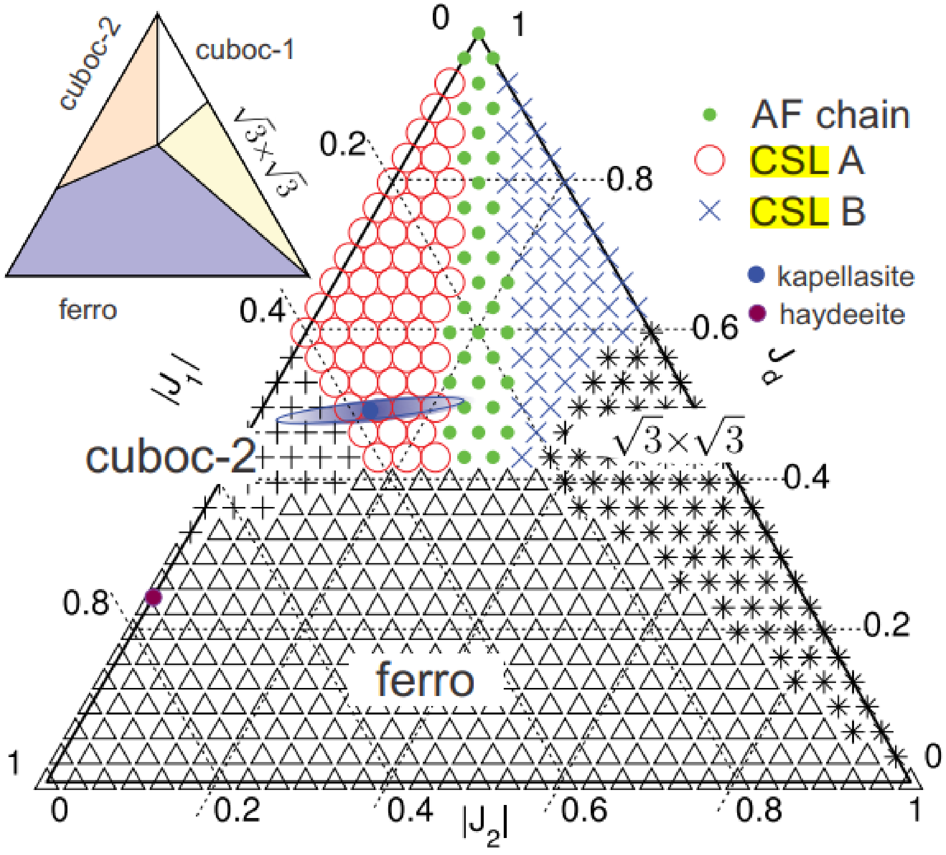
Penn UNIVERSITY of PENNSYLVANIA: Liang Wu

Argonne NATIONAL LABORATORY: Zahir Islam

Kagome lattice as promising structural motif



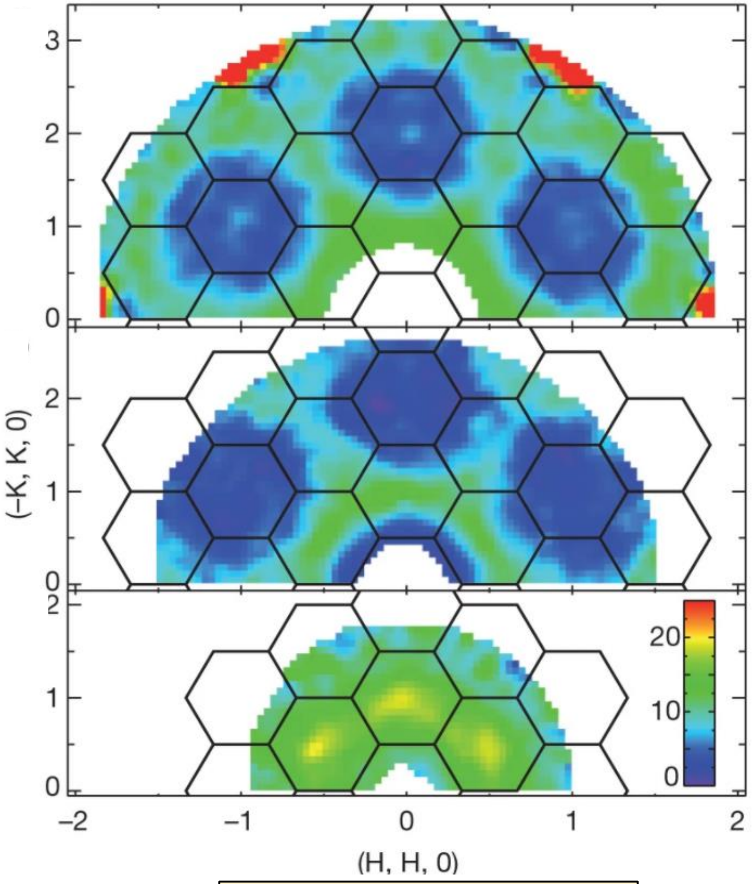
Bieri et al., PRB (2015)



$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Diversity of noncoplanar and spin liquid states

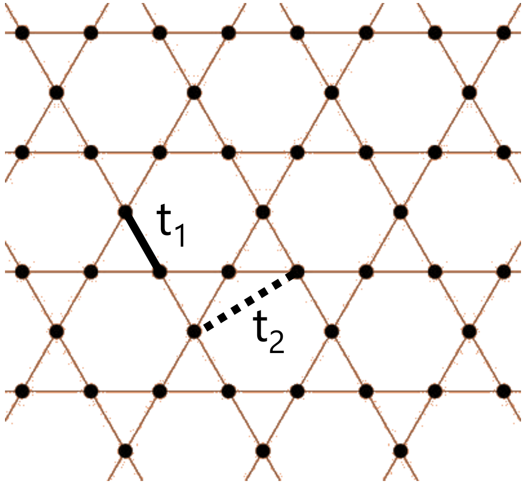
Han et al., Nature (2012)



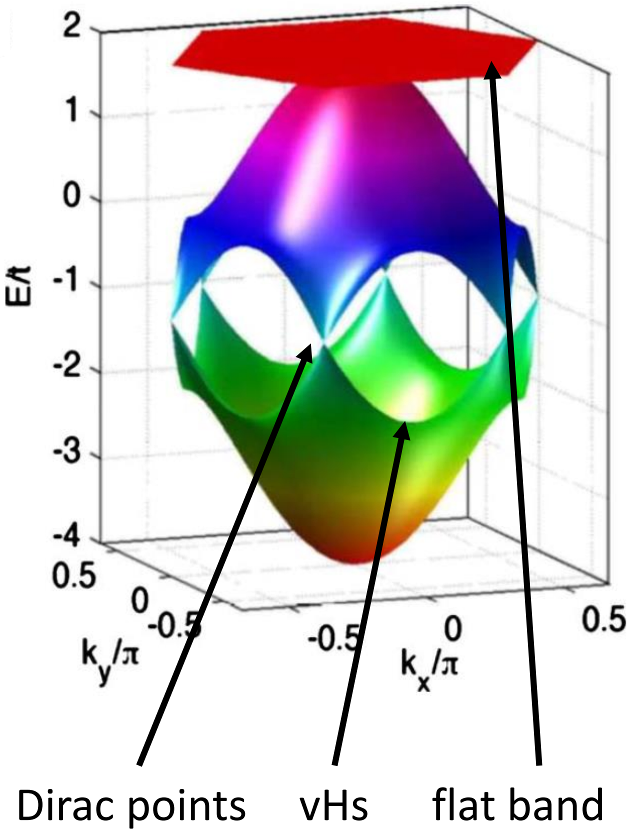
$ZnCu_3(OD)_6Cl_2$

Fractionalized spin excitations
Quantum spin liquid candidate

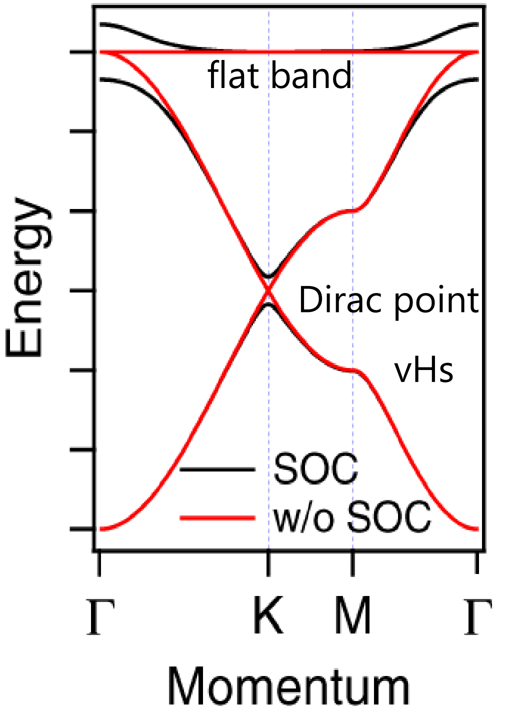
Kagome lattice band structure



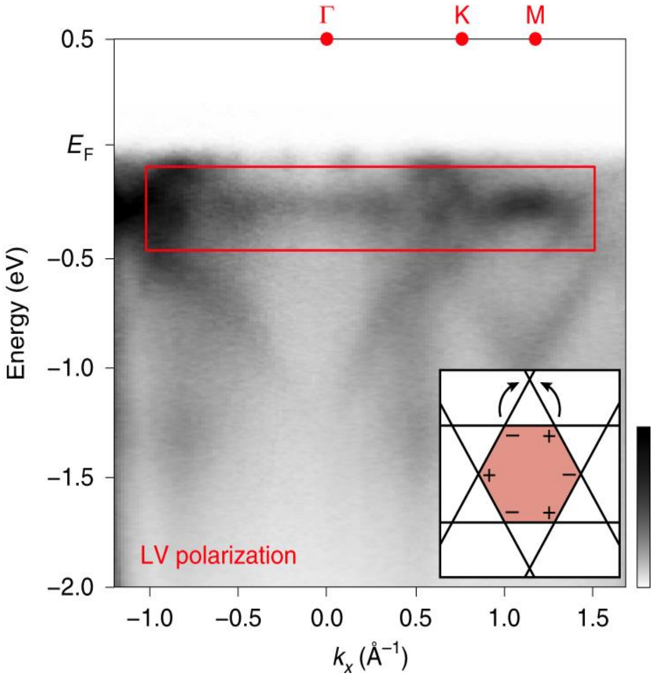
O'Brian et al., Phys. Rev. B (2010)



Liu et al., Nature Comm. (2020)



Kang et al., Nature Mat. (2020)



$$H = -t\sum_{\langle i,j\rangle}(c_i^\dagger c_j + \mathrm{H.c.}) + V\sum_{\langle i,j\rangle} n_i n_j$$

Examples in:

Fe_3Sn_2: FM Chern insulator (Ye et al., Nat. 2018)

FeSn : FM 2D Dirac (Kang et al., Nat. Mat. 2020)

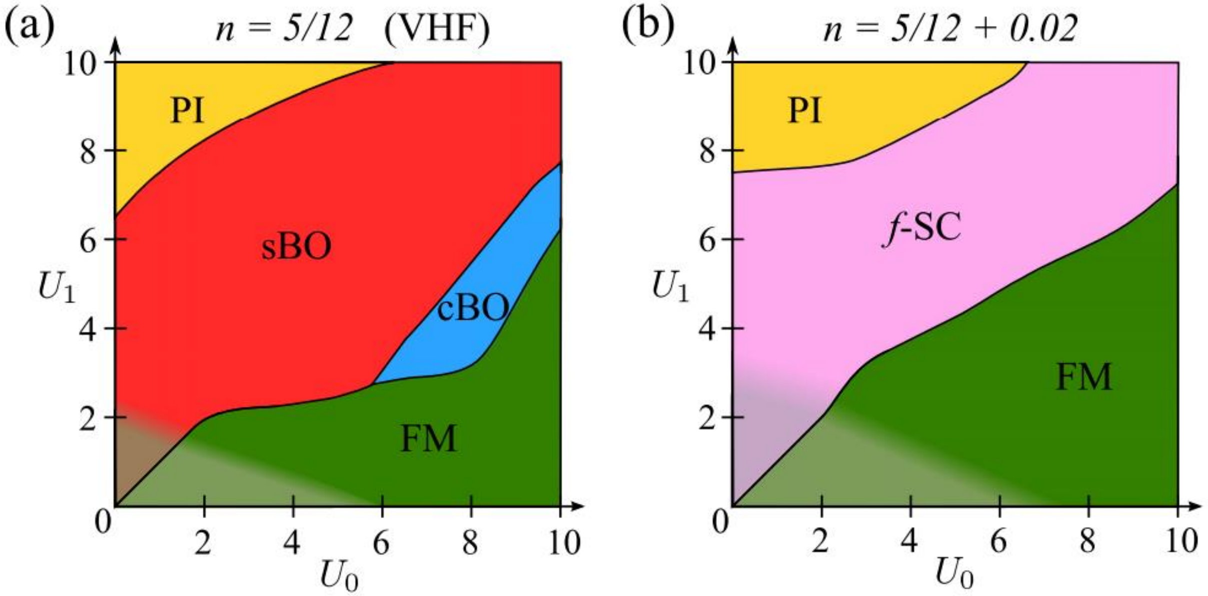
$Co_3Sn_2S_2$: Magnetic Weyl (Liu et al., Nat. Phys. 2018)

CoSn: Dirac (Liu et al., Nat. Comm. 2020)

$TbMn_6Sn_6$: QAH, Chern gap (Yin et al., Nature 2020)

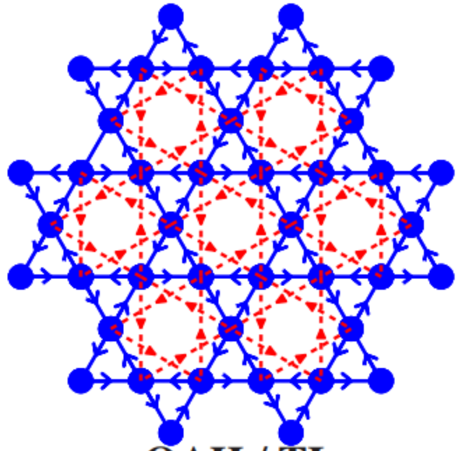
Electronic instabilities on kagome lattice

Kiesel et al., Phys. Rev. Lett. (2013)

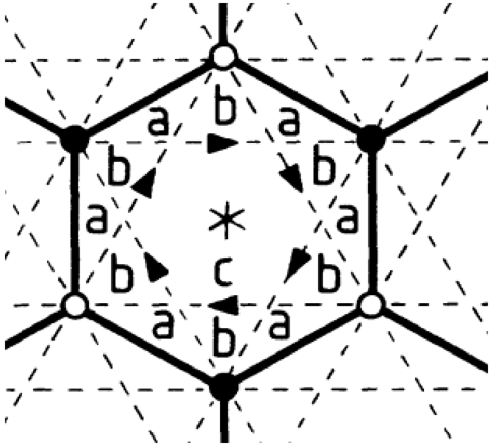


J. Wen et al., Phys. Rev. B (2010)

Haldane et al., PRL (1988)



QAH / TI

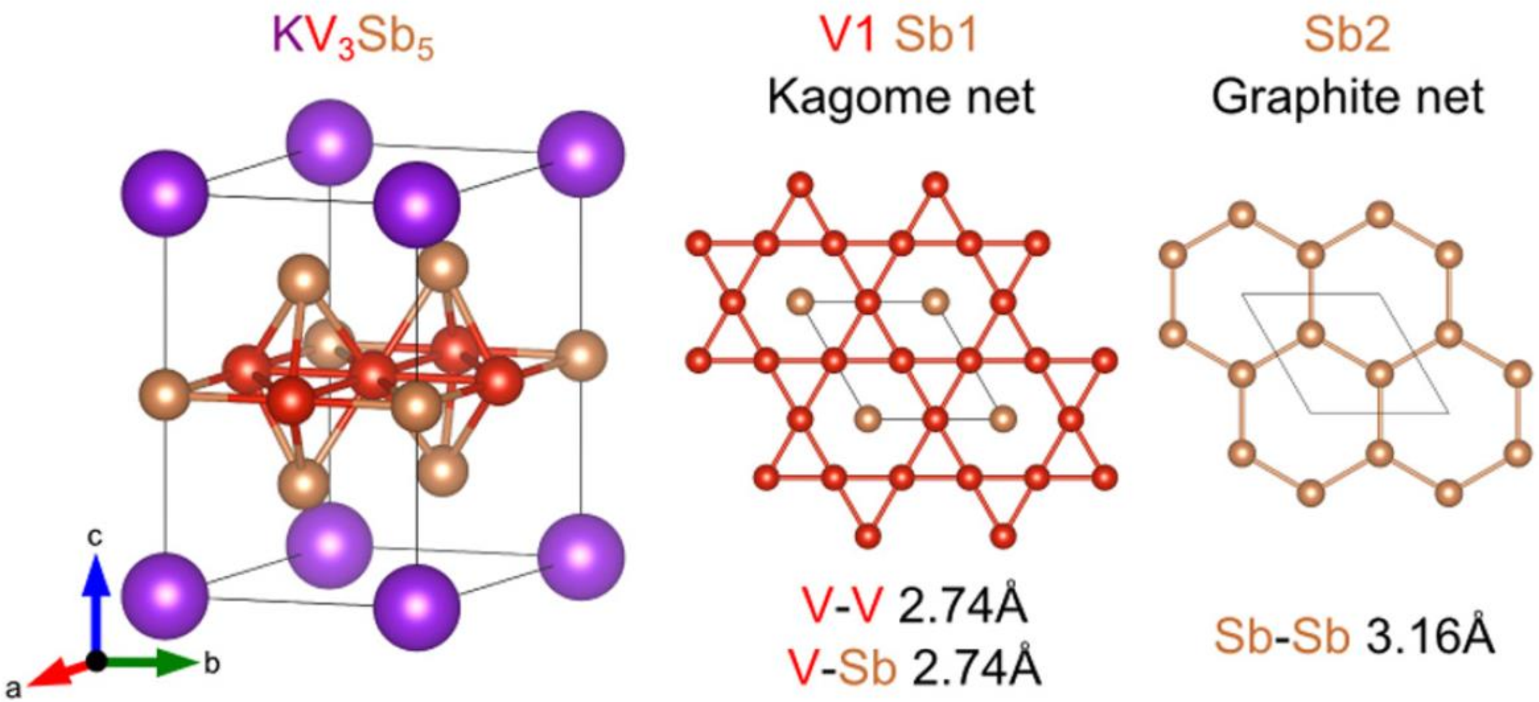


- Variety of interaction-driven instabilities predicted at different fillings
  - Charge density wave order
  - Bond density wave states
  - Chiral spin density waves
  - Superconductivity
- Saddles points at select fillings give rise to van Hove singularities (e.g. 5/4 electrons per band)
  - Wan-sheng Wang et al., Phys. Rev. B (2013)
  - Kiesel et al., Phys. Rev. Lett. (2013)
- Sublattice interference amplifies influence of U_1

AV_3Sb_5 (A=K, Cs, Rb)

Kagome lattice of AV_3Sb_5 (A=K, Rb, Cs)

Ortiz et al., Physical Review Materials (2019)



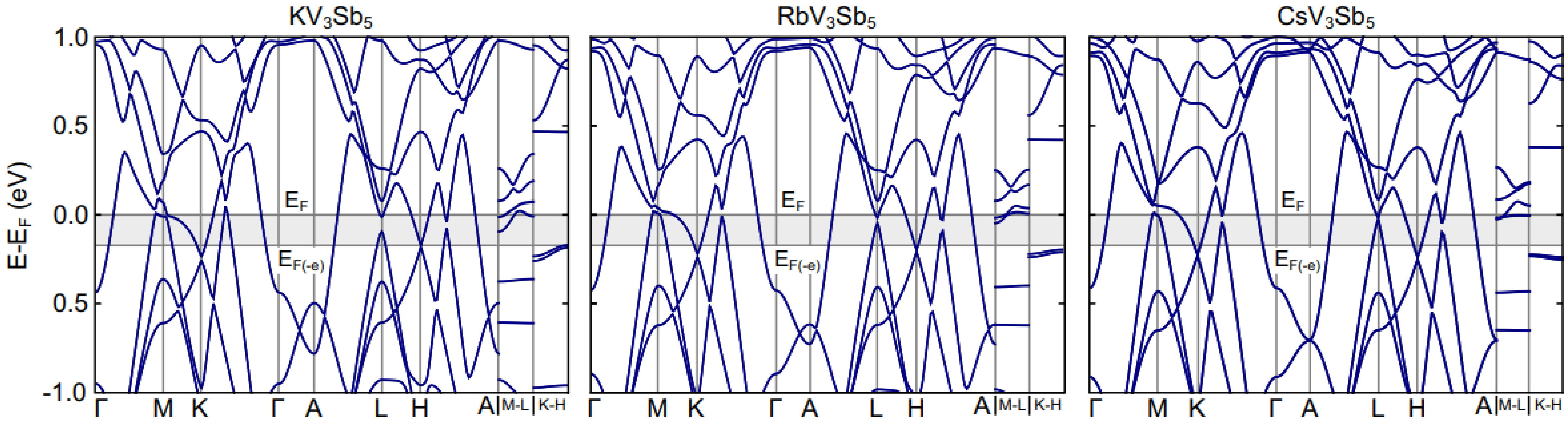
V

Vanadium metal: V-V 2.6 Å

- New phase found in ternary phase diagram of A-V-Sb
- Layered, exfoliable material with perfect (P6/mmm) Kagome nets of V-ions
- V-V distances are small (~2.75 Å), suggesting V-ions are nonmagnetic

Electronic structure of AV_3Sb_5

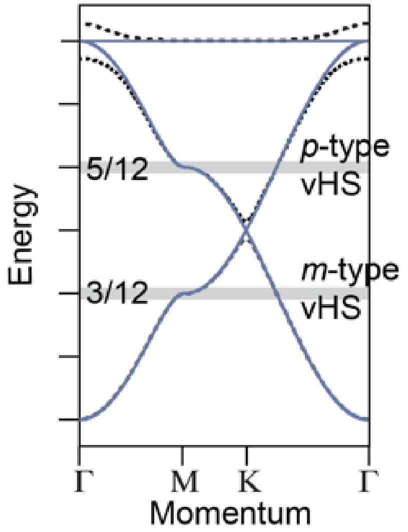
Ortiz et al., Physical Review Materials (2019)

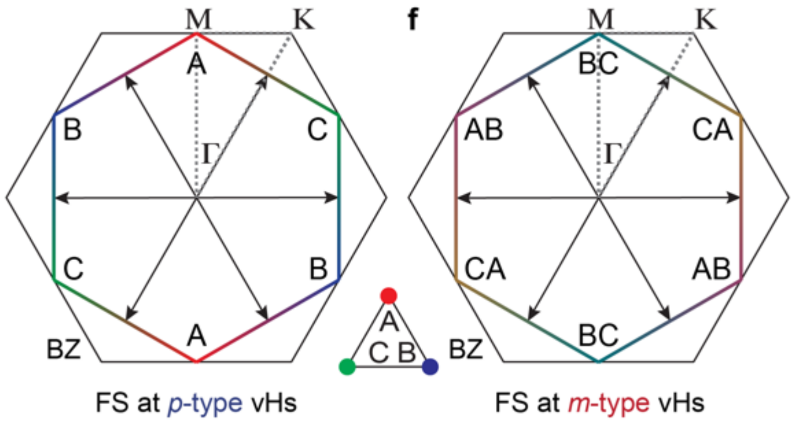


- Initial DFT modeling shows Fermi level close to saddle points at M
- Electronic structure similar across the AV_3Sb_5 series

vHs in multiband CsV_3Sb_5

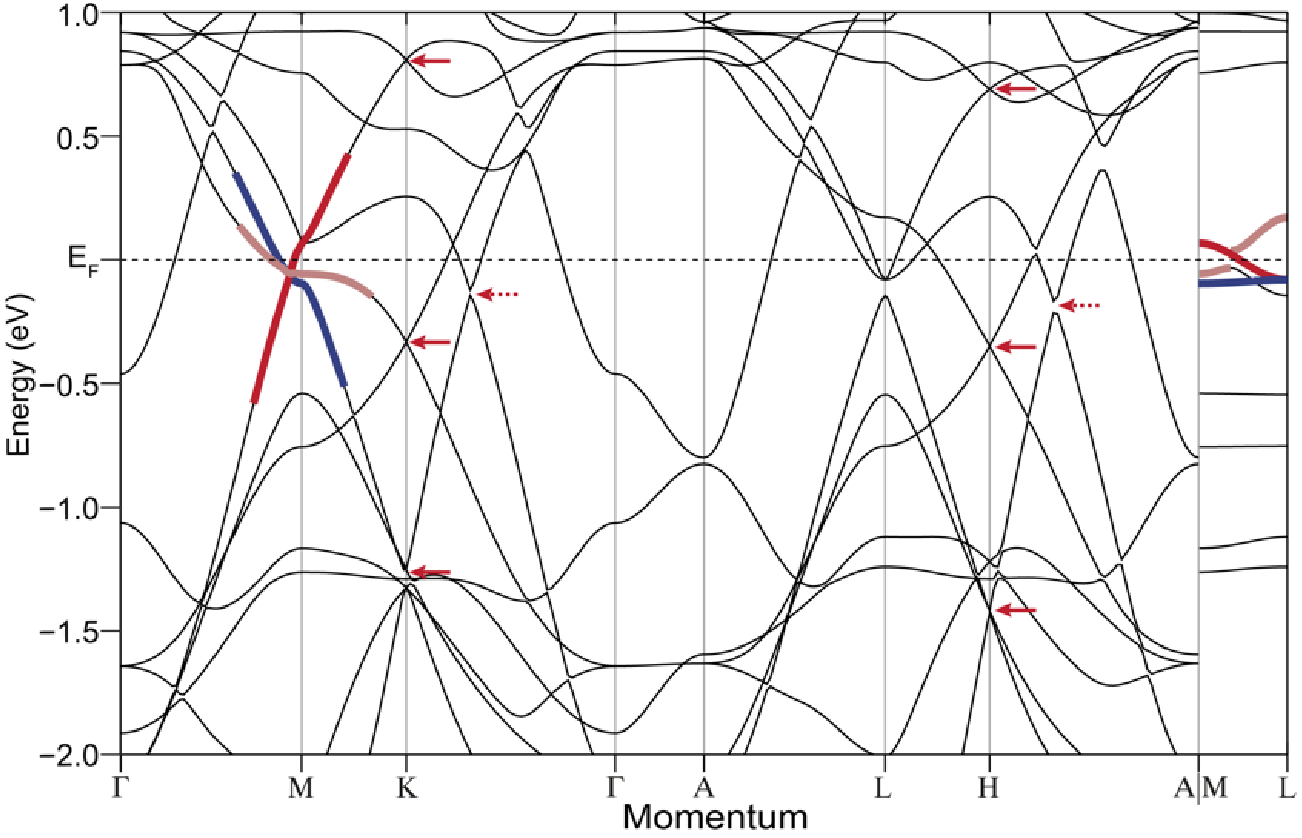
Single orbital picture





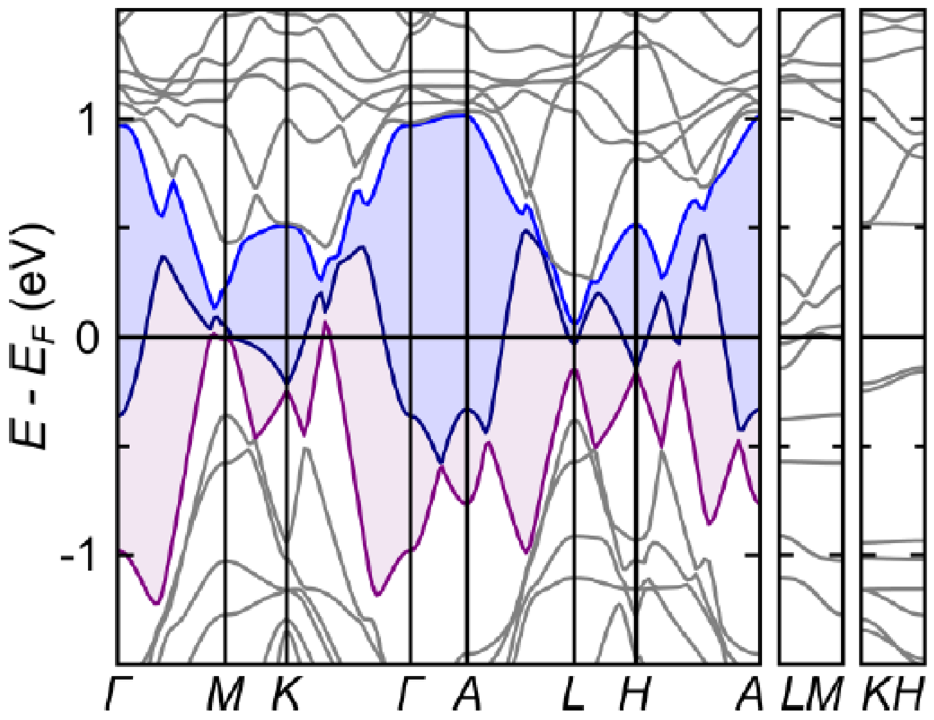
Mingu Kang et al., Nat. Phys. (2022)

DFT analysis of multiorbital CsV_3Sb_5



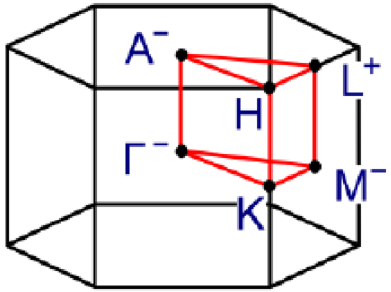
- Three vHs close to E_F
  - *p*-type (d_{xy}/d_{x2-y2}) + *m*-type (d_{xz}/d_{yz}) just below
  - *p*-type (d_{xz}/d_{yz}) a bit lower
- Electronic structure similar across the AV_3Sb_5 series

Topological classification: Z2 metal

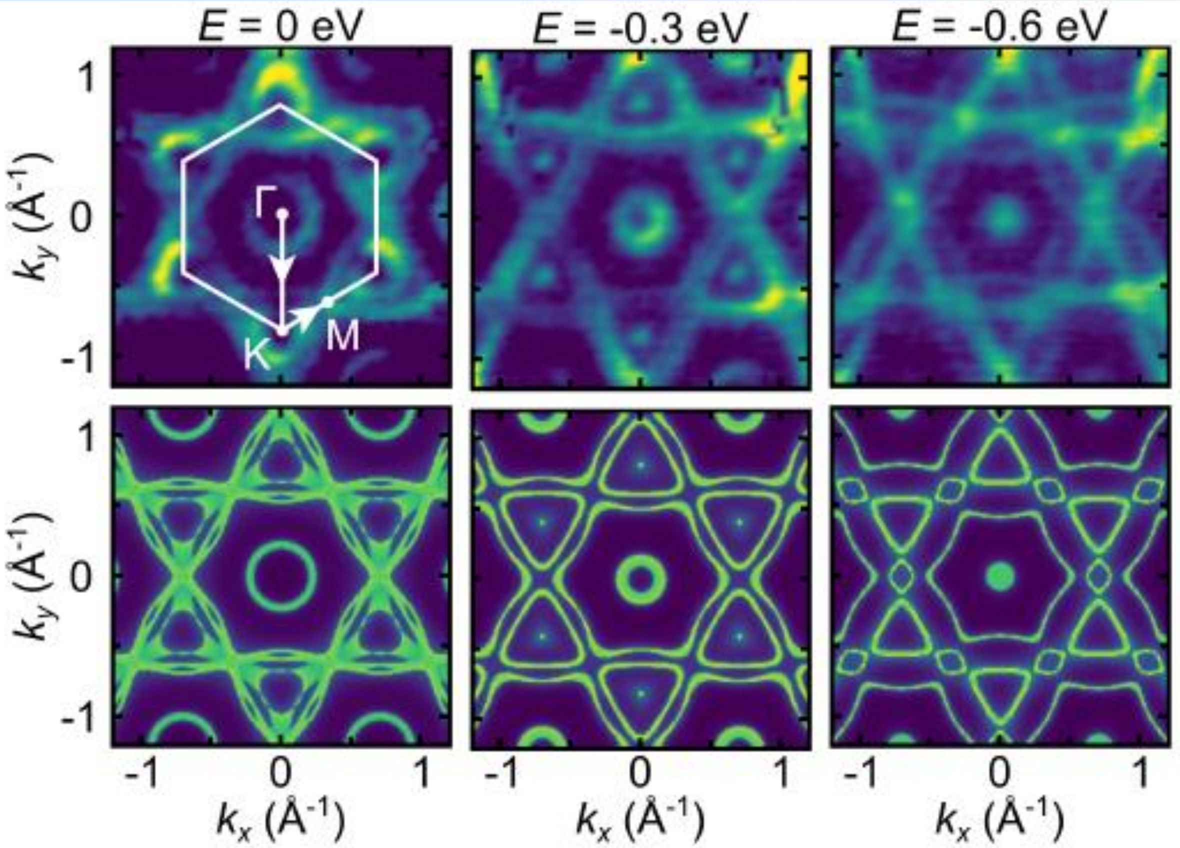


Parity Products

Band	δ_Γ	δ_A	δ_L	δ_M
75	-1	+1	-1	+1
73	-1	-1	+1	-1
71	+1	-1	-1	-1



Ortiz et al., Phys. Rev. Lett. (2020)



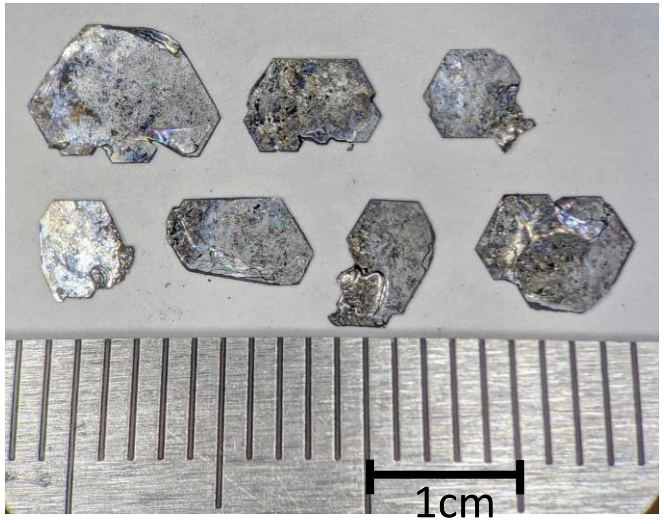
Normal state band structure categorized as Z2 topological metal

Surface states reasonably close to E_F

Good agreement between DFT and observed band structure

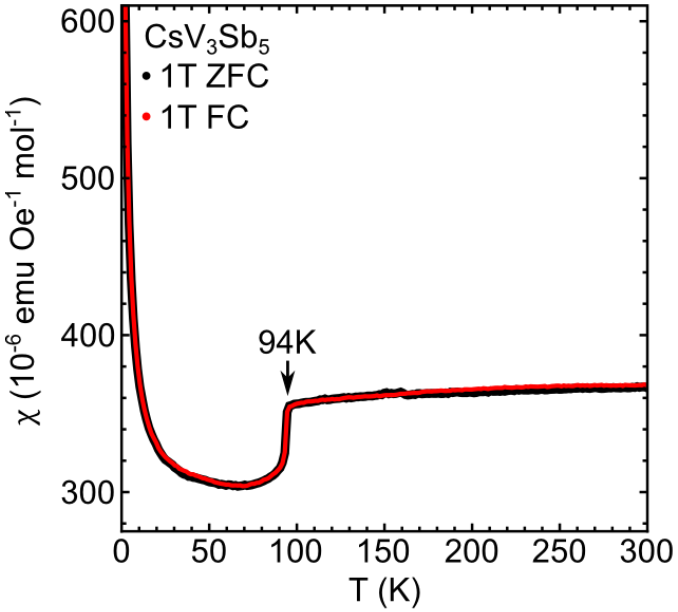
CDW order in AV_3Sb_5 (A=K, Cs, Rb)

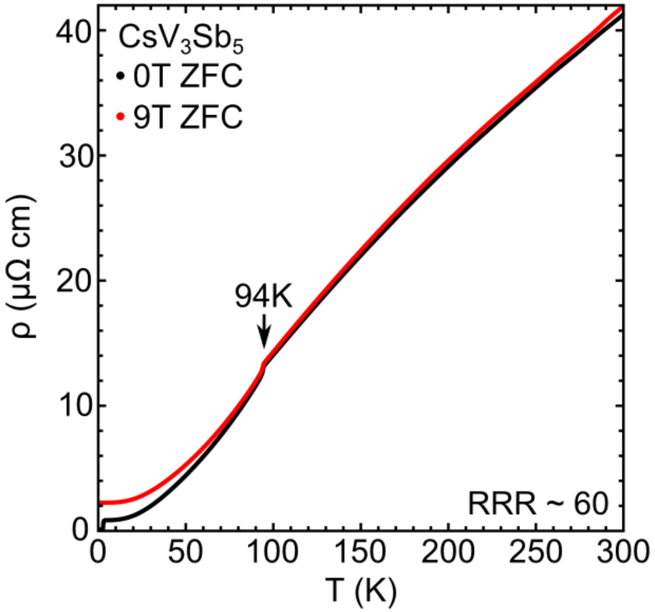
High temperature phase transition in AV_3Sb_5

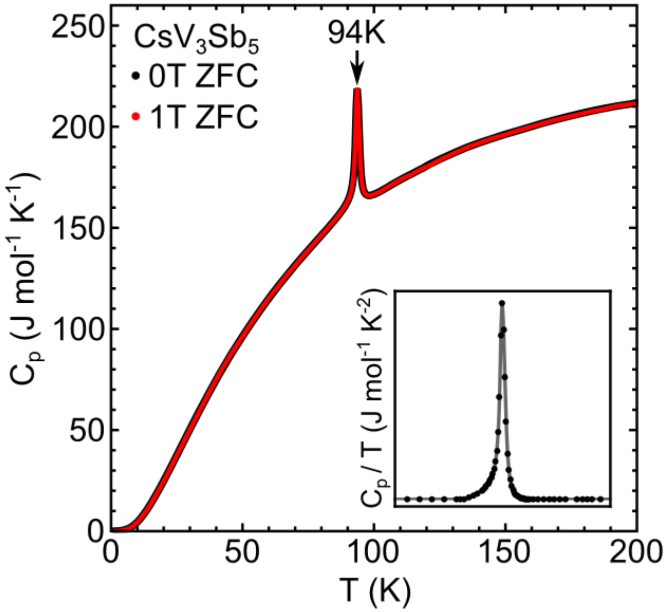


- Quasi-2D electron transport
- High-temperature Pauli paramagnetism
- *T** anomalies in χ(T), ρ(T), C_P(T)
- Strong MR turns on below *T**

Ortiz et al., Phys. Rev. Lett. (2020)

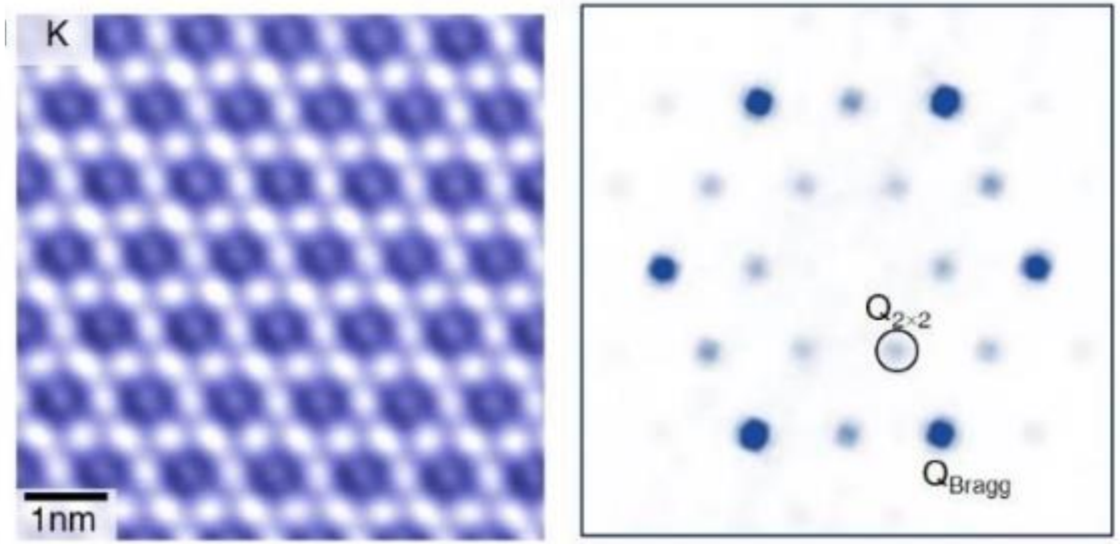


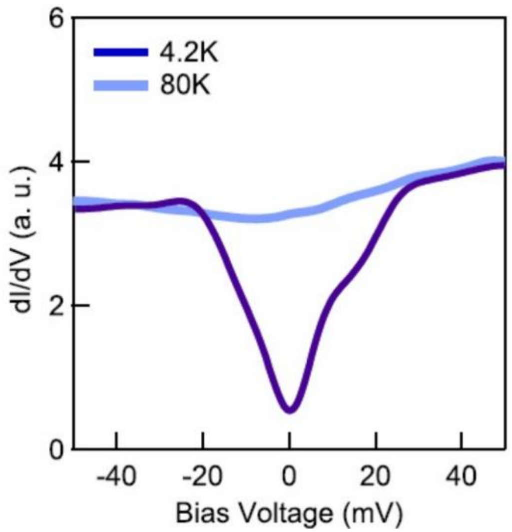




CDW state in AV_3Sb_5

Yu-Xiao Jiang et al, Nature Materials (2021)



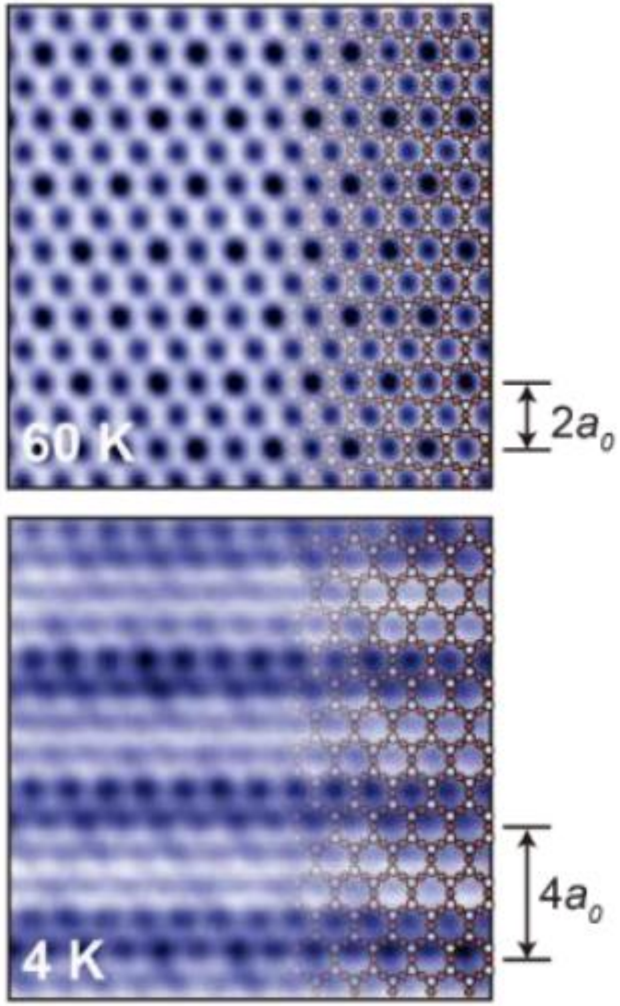


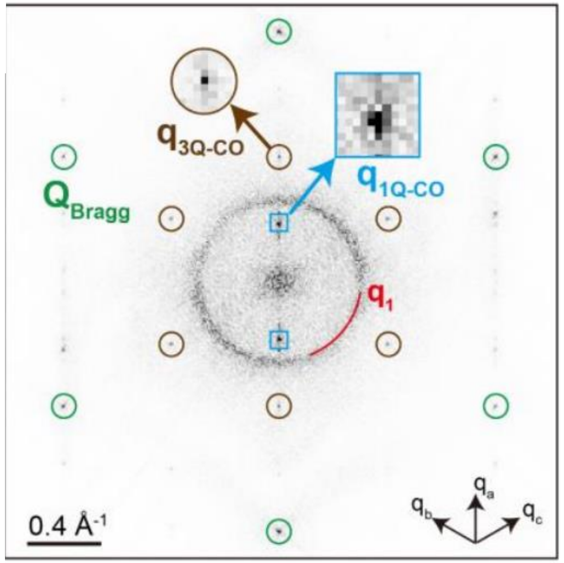
KV_3Sb_5

3**Q** CDW ordering

2x2 reconstruction in ab-plane

He Zhao et al, Nature (2021)





CsV_3Sb_5

3**Q** CDW ordering

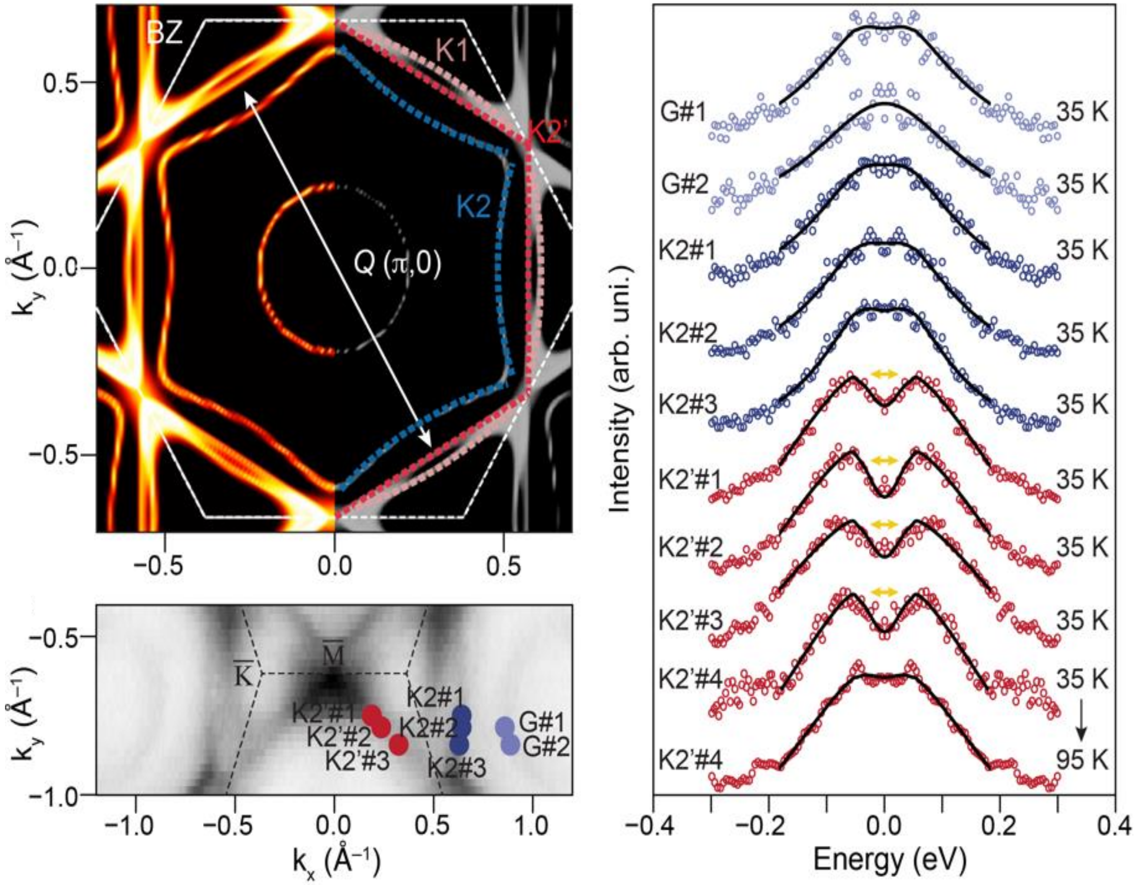
+

1D 4a-type ordering

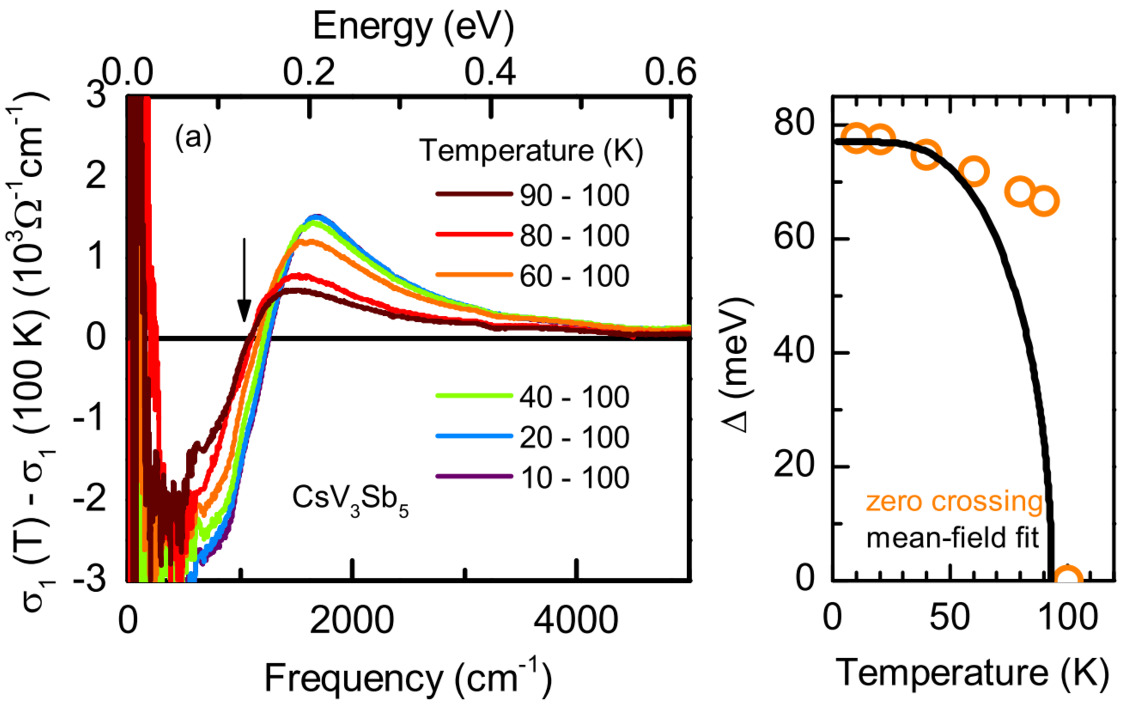
(onset below ~50 K)

Partial gap opening at M-point below *T**

Mingu Kang et al., Nat. Phys. (2022)



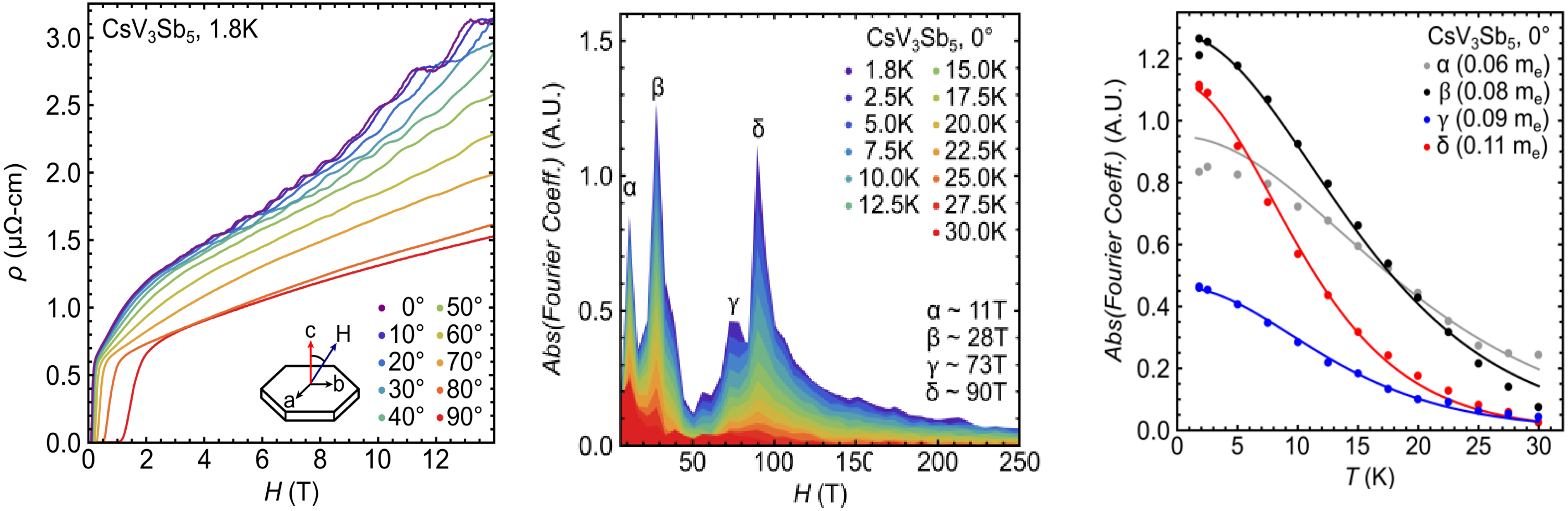
E. Uykur et al., Phys. Rev. B (2021)



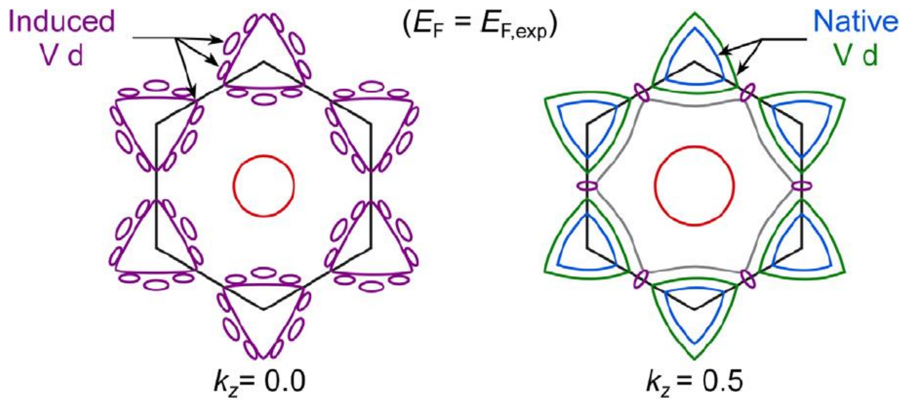
Partial gap opens at M-points, proposed nesting driven by m-type vHs
Nesting alone likely insufficient (Farnaz Kaboudvand et al., APL (2022))

Bulk probe of CDW via quantum oscillations

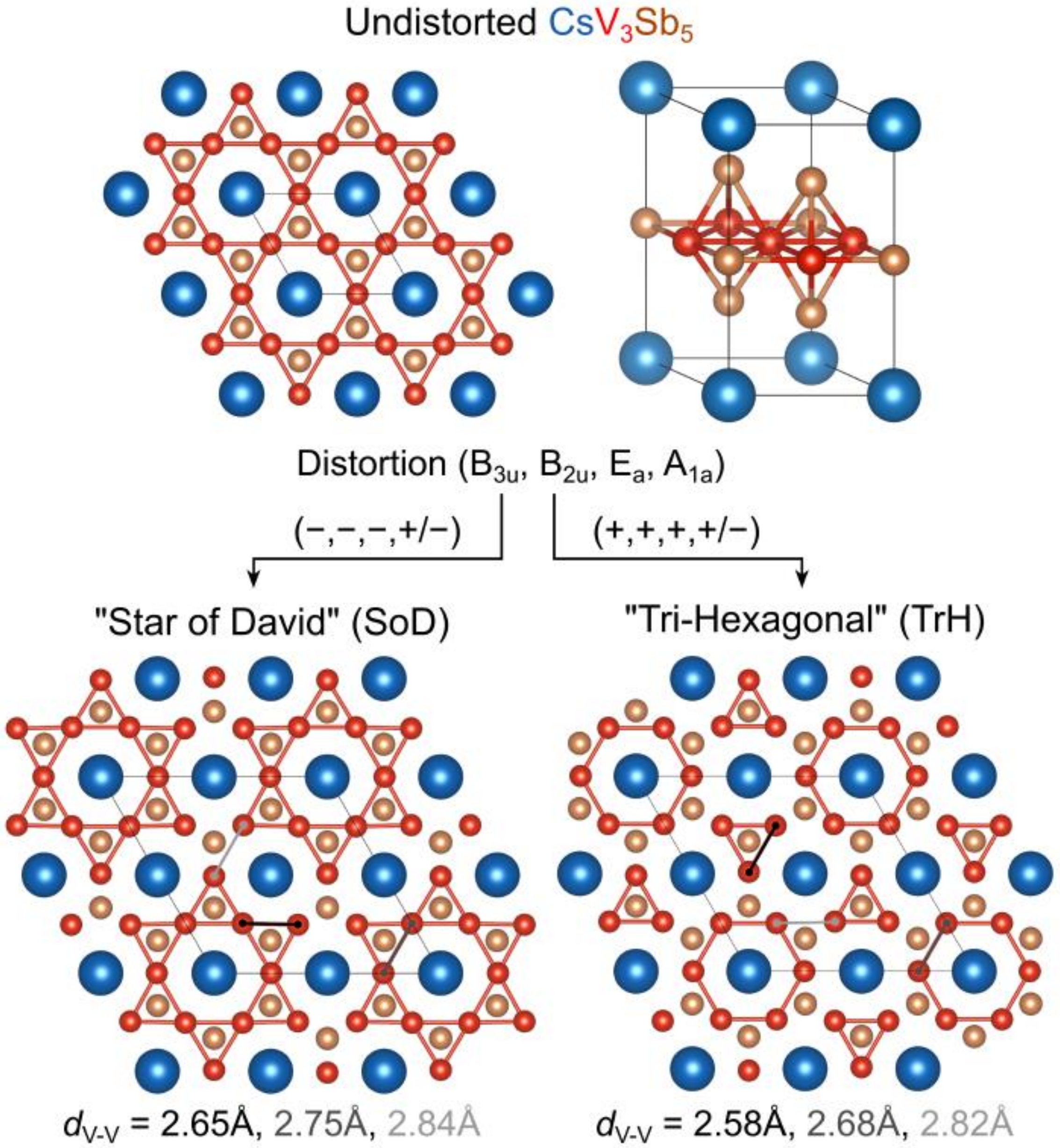
Ortiz et al, Phys. Rev. X (2021)



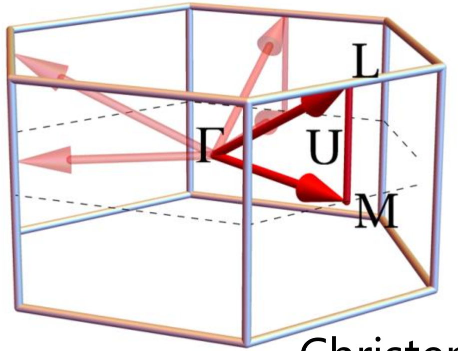
- Reconstruction of V-orbits below CDW
- Light cyclotron masses in new orbits
- New orbits have $\Phi_B = \pi$
  - Fu et al., Phys. Rev. Lett. (2021)
  - Sherstha et al., Phys. Rev. B (2022)



Models for charge density wave state

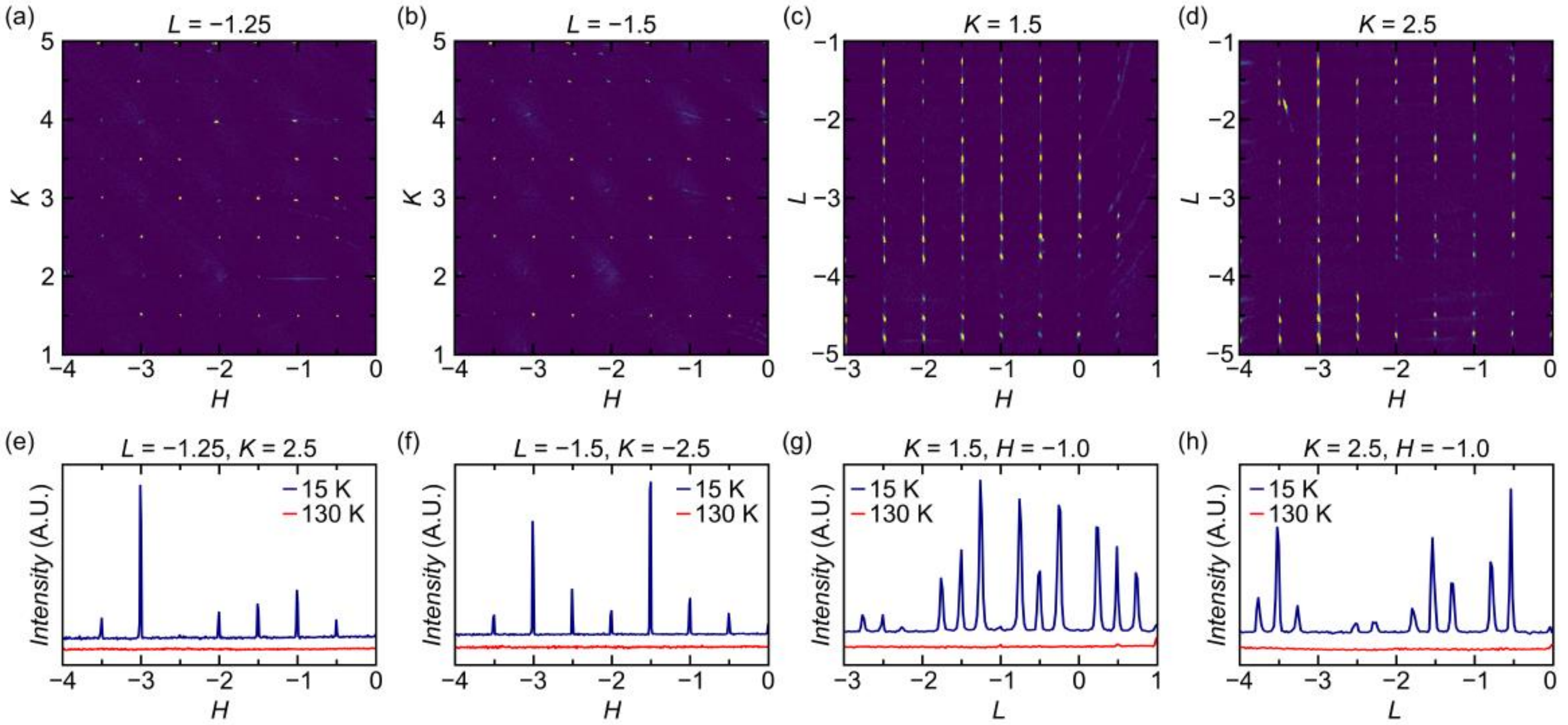


- Two likely distortion modes in kagome plane
  - "Star of David" (*-M, M, M*)
  - "Tri-Hexagonal" (*M, M, M*)
- DFT favors "Tri-Hexagonal"
  - ~10 meV/unit cell below SoD
  - Hengxin et al. PRL (2021)
- Modulation along c-axis can arise from phasing of Q in-plane or mixture of two distortion types



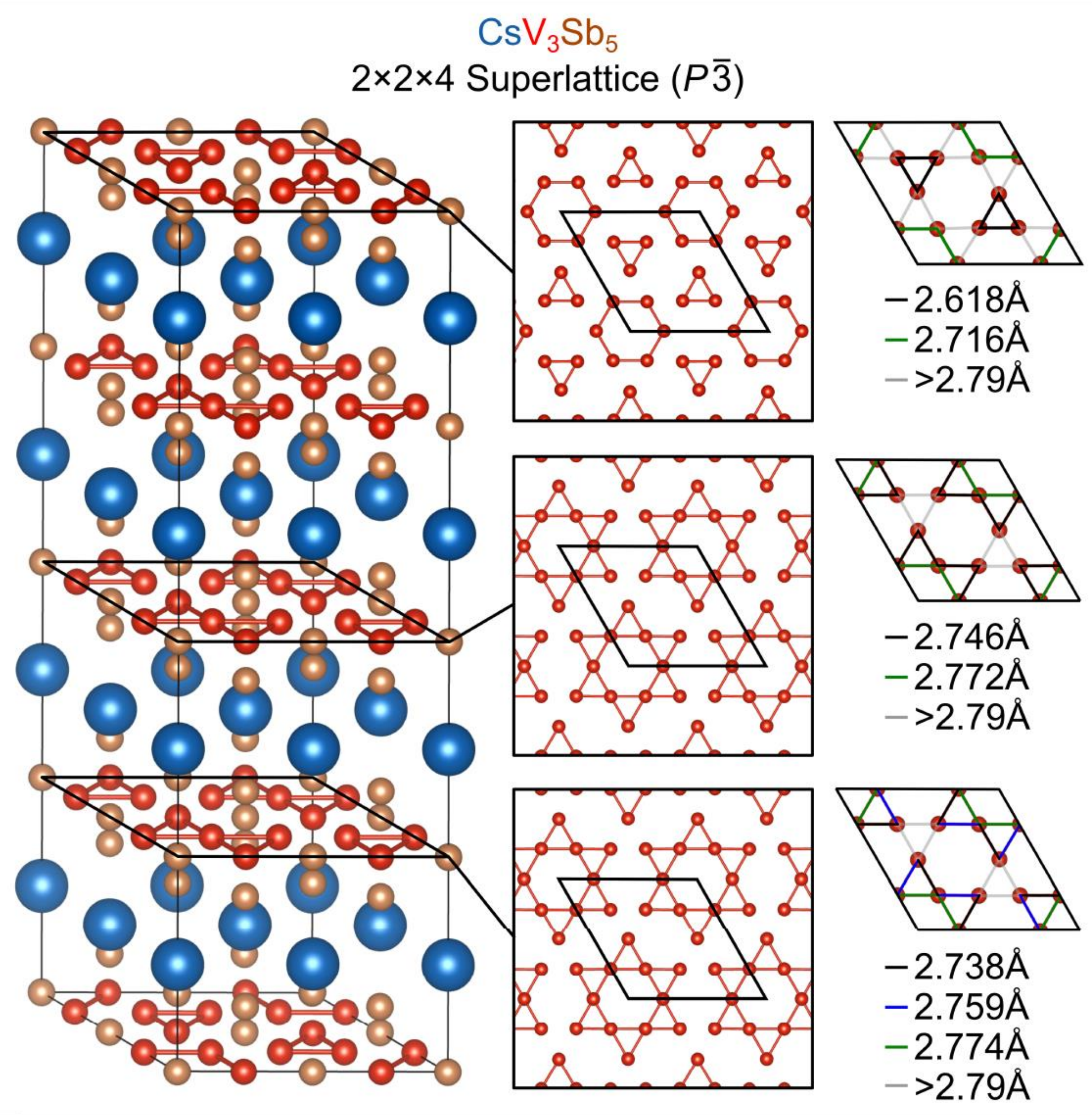
Christensen et al., PRB (2021)

3D CDW-coupled distortion in CsV_3Sb_5



(0.5, 0.5, 0.25)-type peaks consistent with 2x2 in-plane CDW

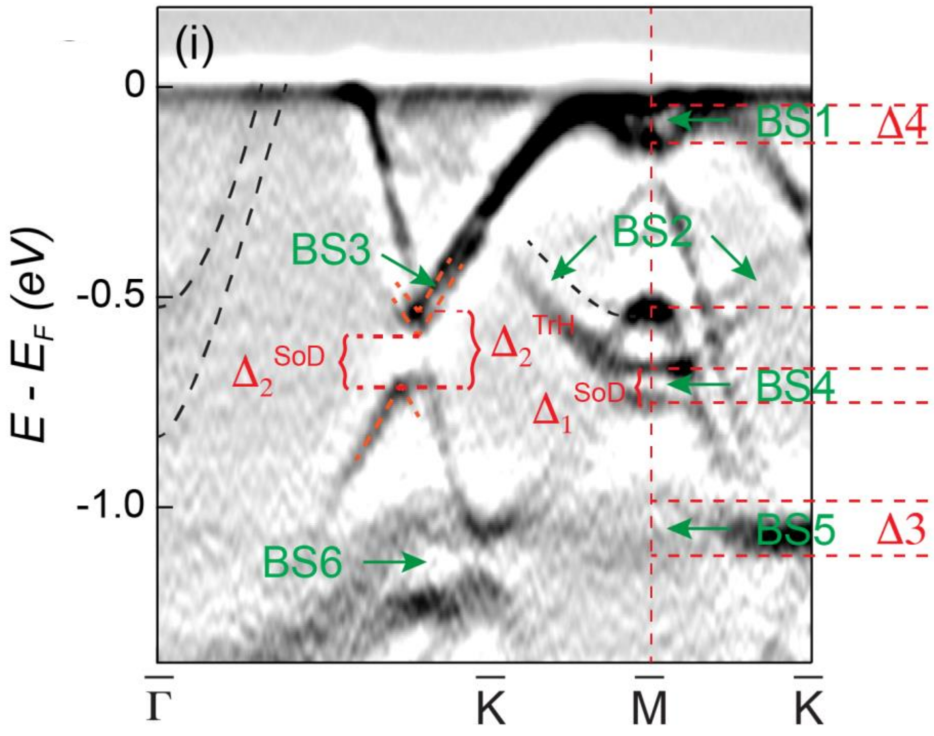
Structure of the CDW state in CsV_3Sb_5



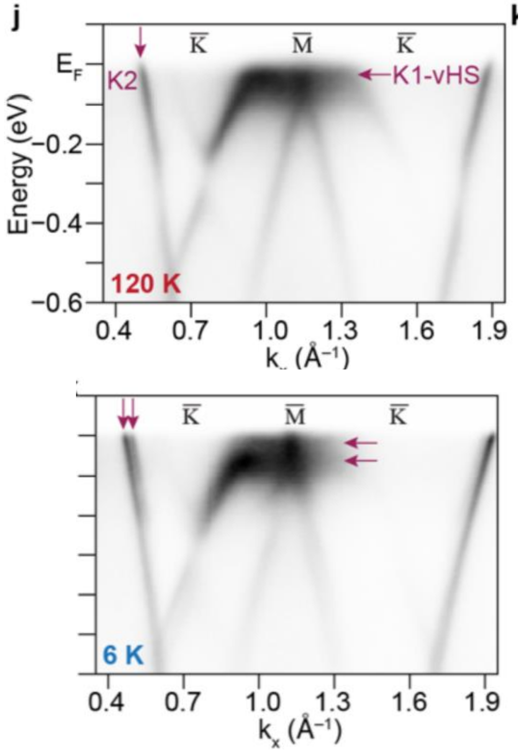
- Inversion symmetry preserved
  - Second harmonic generation data
- Modulation between strongly distorted TrH and weakly distorted SoD layers
- Average structure
  - 2 domains included
  - Likely missing twinning effects due to subtle orthorhombic distortion

Indications of both SoD and TrH in ARPES

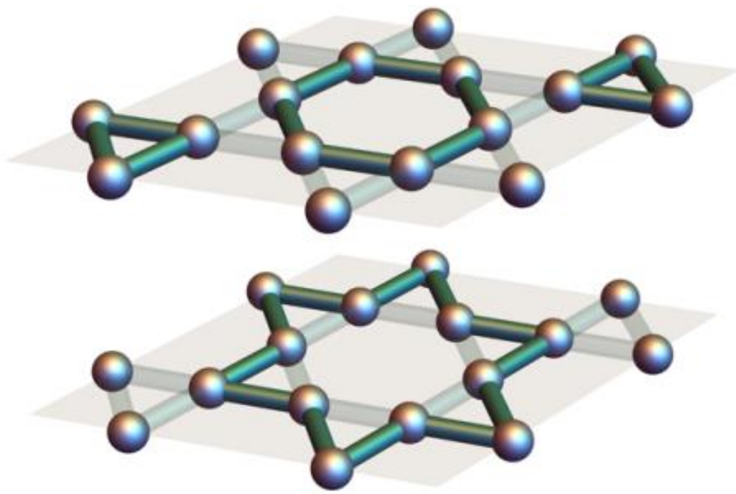
Yong Hu et al., arxiv: 2201.06477



Minggu Kang et al., arxiv:2202.01902



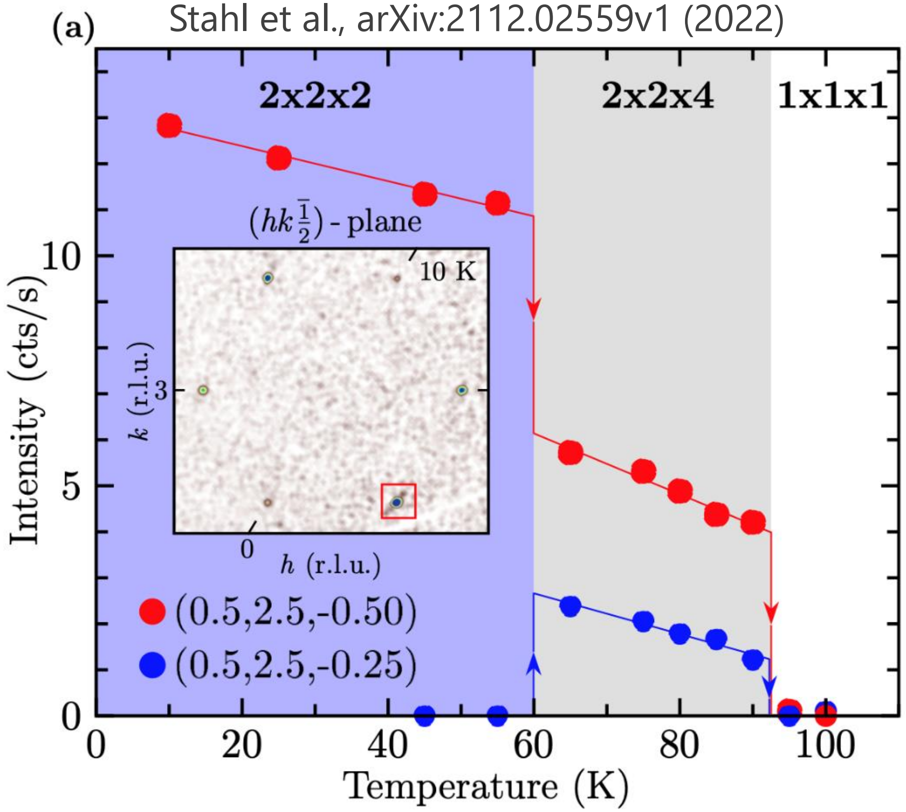
Christensen et al., PRB (2021)



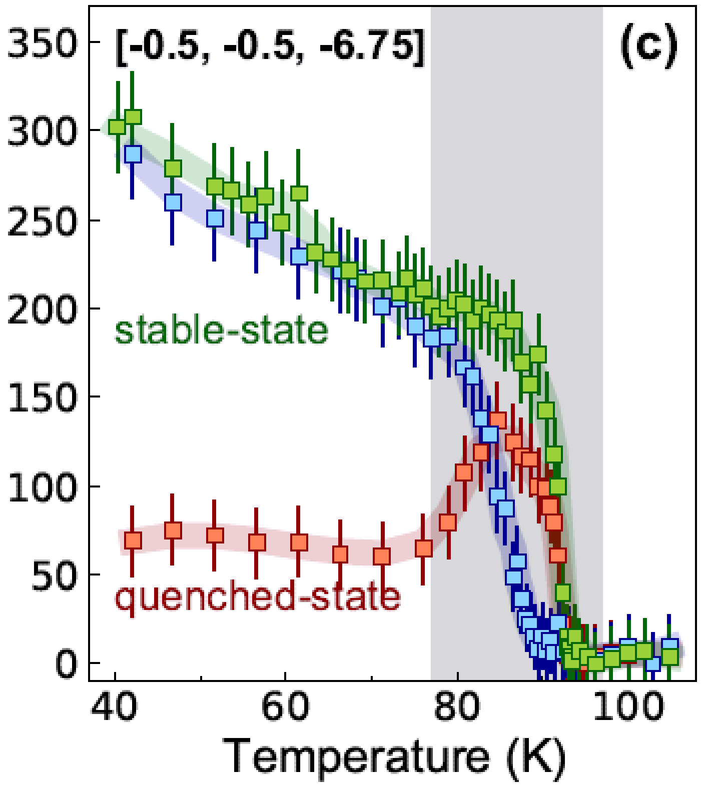
- Photoemission resolves band folding near K and M points
- Folding suggestive of both SoD and TrH models
- Consistent with 3Q=(L,L,L) order (but both are 2x2x2 cells)

Out-of-plane modulation suffers from local minima

Stahl et al., arXiv:2112.02559v1 (2022)



Qian Xiao et al., arXiv (2022)



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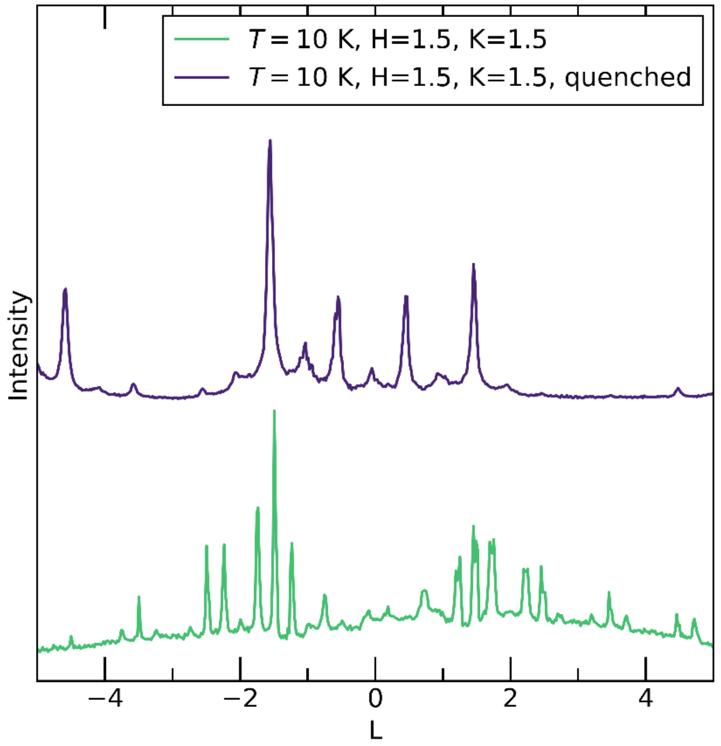
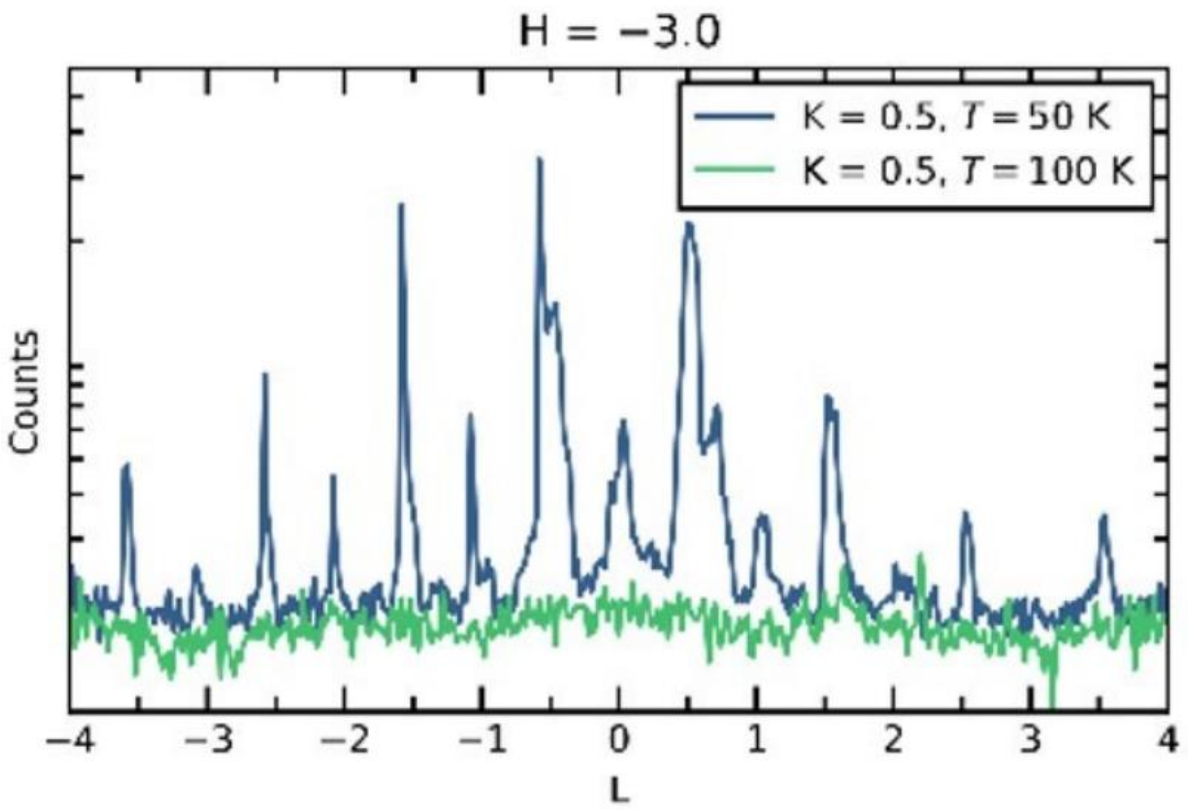


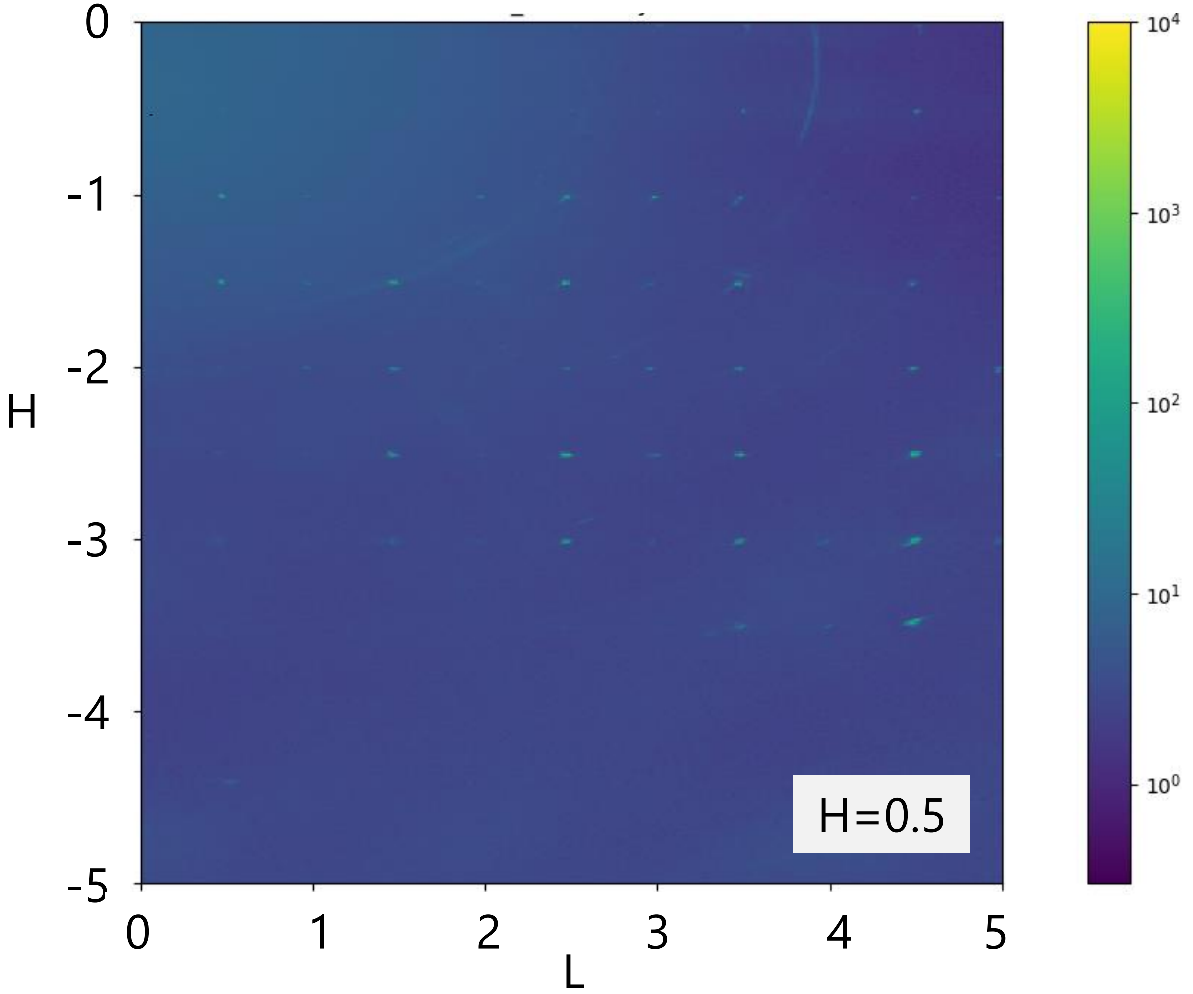
- Others: Q. Chen et al., arXiv (2022) + Haoxiang Li et al., PRX (2021)
- Out-of-plane modulation depends on growth/disorder + thermal history
- Quenching vs slow cooling
- Irreversible changes after thermal cycling

3D CDW-coupled distortion in $(K,Rb)V_3Sb_5$

Yu-Xiao Jiang et al, Nature Materials (2021)



Original data

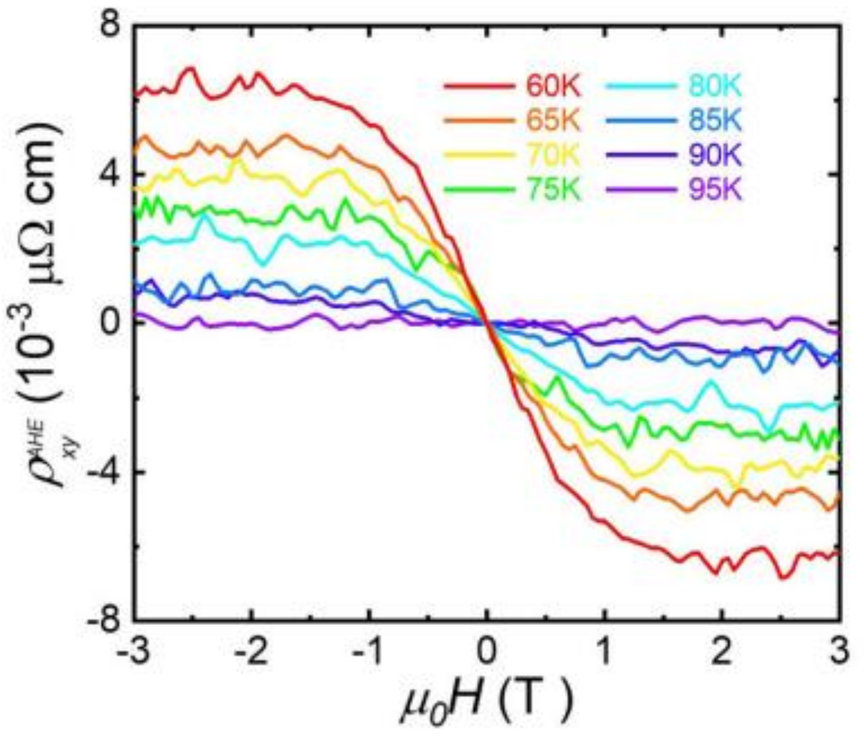


unpublished

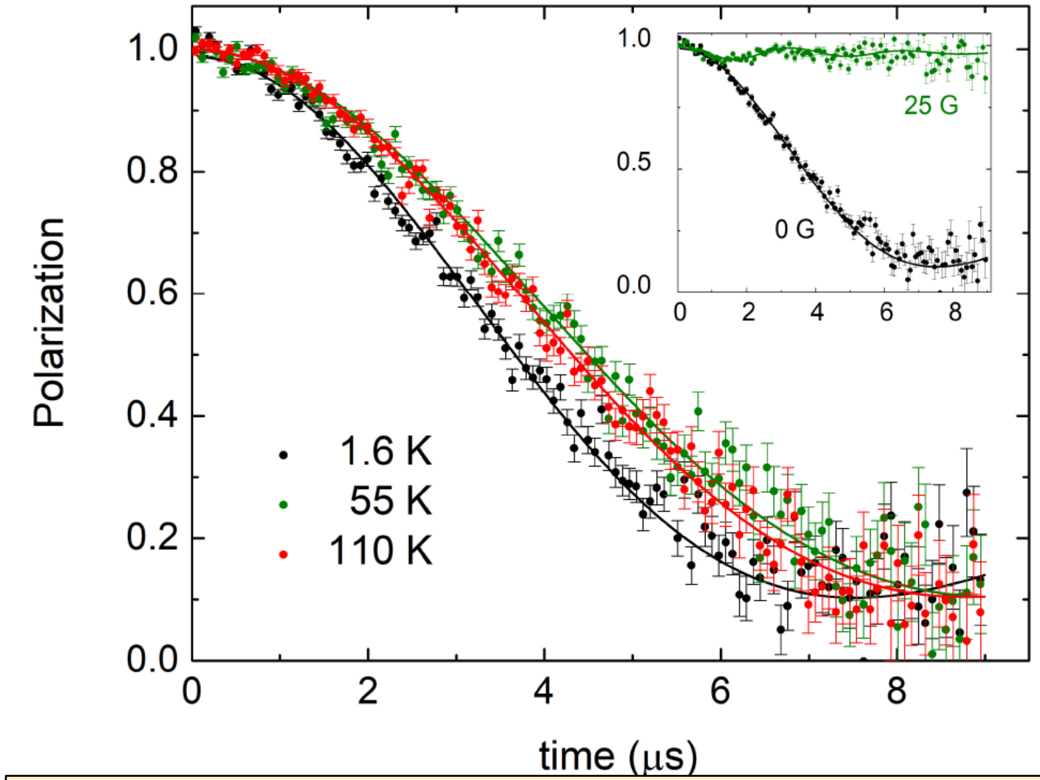
q=(0.5, 0.5, 0.5); same for RbV_3Sb_5

Unconventional behavior in CDW

Yu et al., PRB (2021)



Kenney et al., J. Phys. Cond. Matt. (2021)



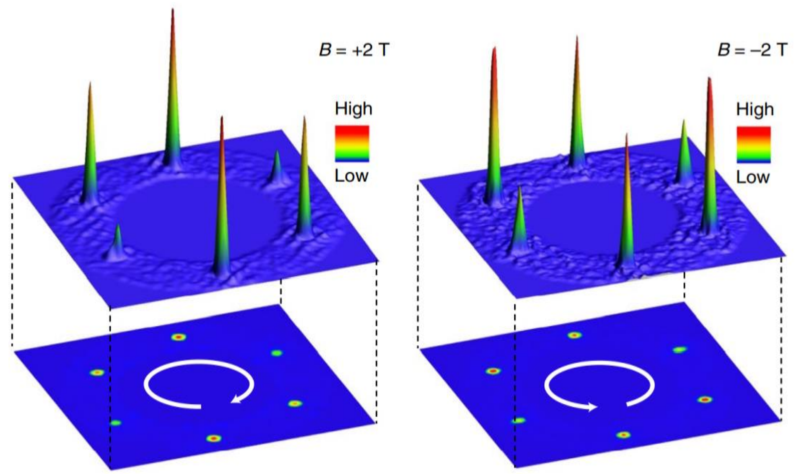
- Extraordinarily large AHE
  - Yang et al., Science Advances (2020)
- AHE appears coincident with CDW

Yu et al., Phys. Rev. B (2021)

- Weak depolarization consistent with nuclear moments
- μsR measurements performed by Mike Graf at Boston College

Hints of TRSB in AV_3Sb_5

STM



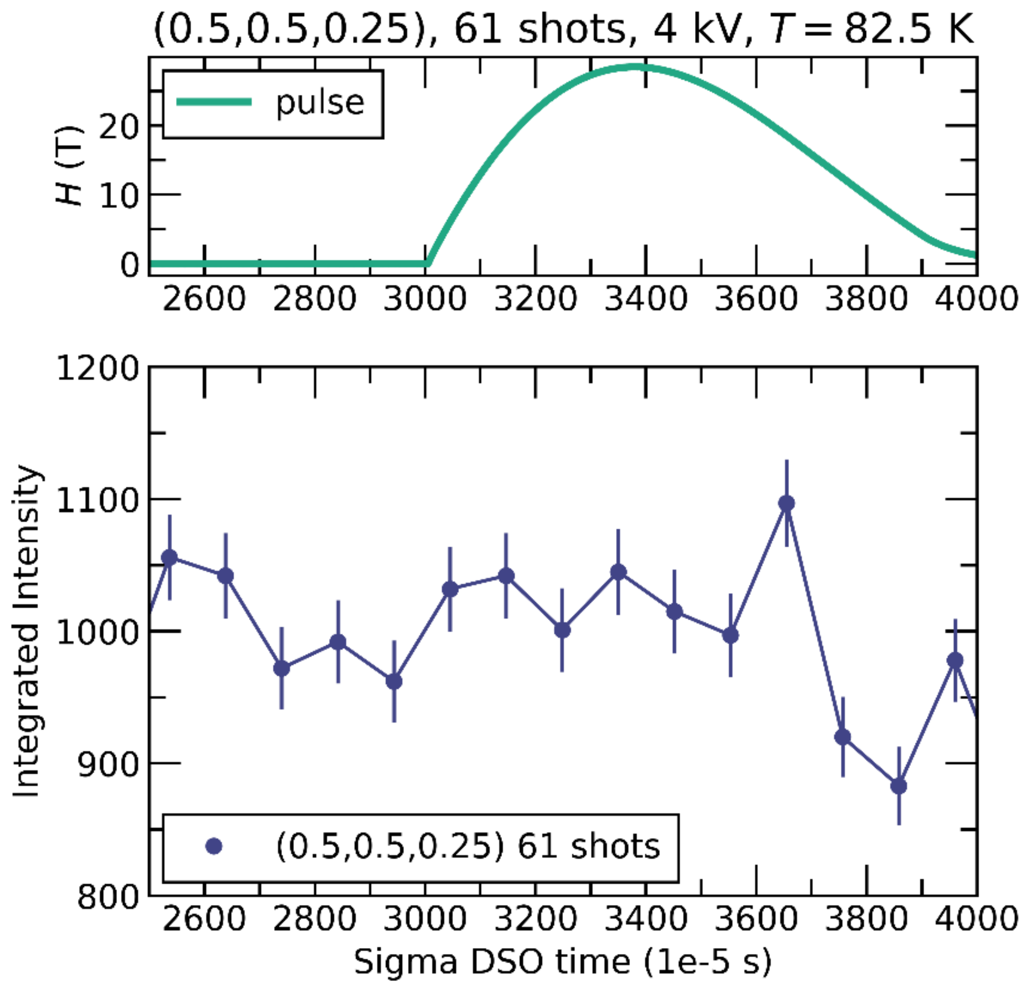
Yu-Xiao Jiang et al, Nature Materials (2021)

Zhiwei Wang et al., Phys. Rev. B. (2021)

Nana Shumiya et al., Phys. Rev. B. (2021)

Not observed in other studies of KV_3Sb_5
(Hong Li et al., Nat. Phys. (2022))

X-ray scattering study of CDW superlattice

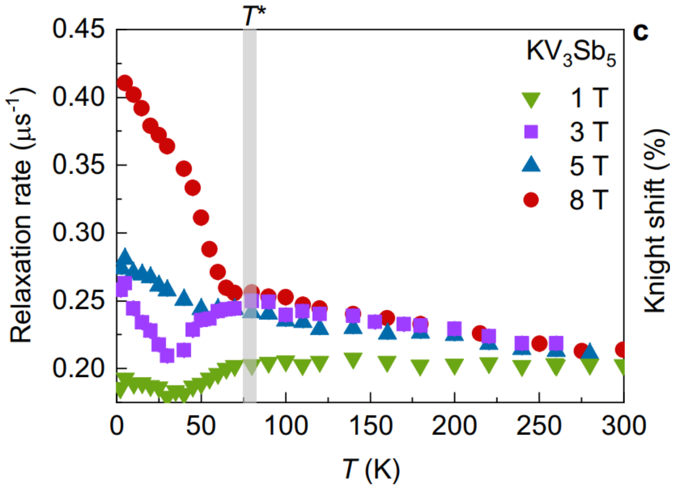


No signature of CDW superlattice coupling to pulsed field
unpublished

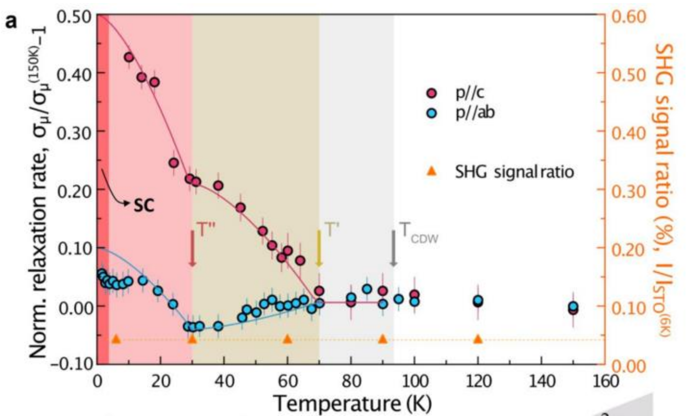
Other hints of TRSB in AV_3Sb_5

μSR studies

C. Mielke III et al., Nature (2022)

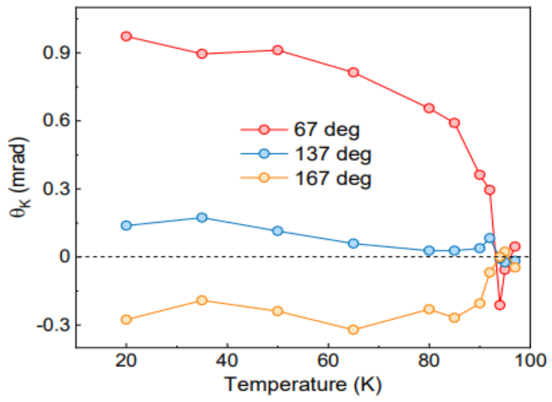


L. Yu et al., arxiv: 2107.10714



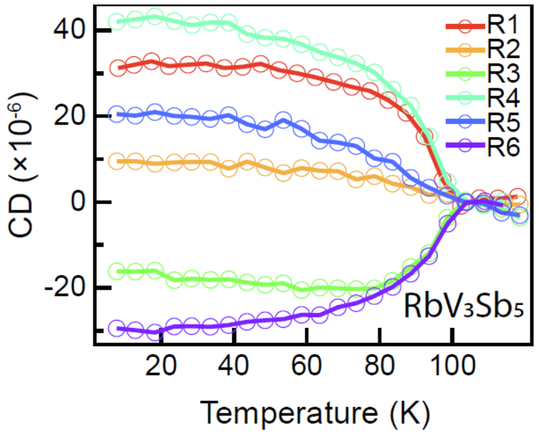
Kerr rotation CsV_3Sb_5

Qiang Wu et al., arXiv:2110.11306v2



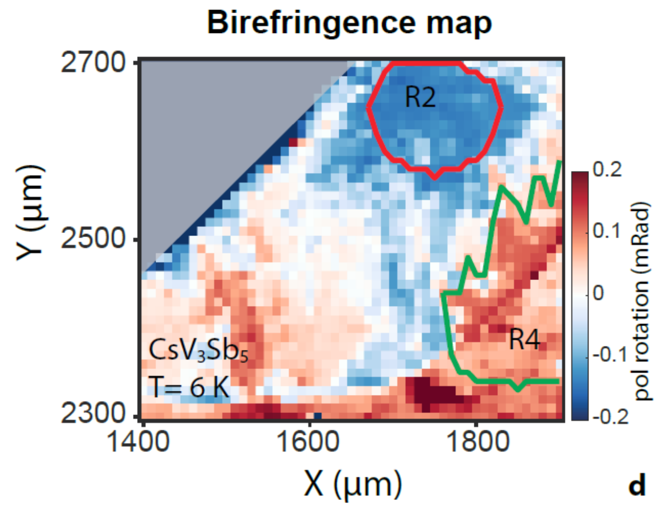
Circular dichroism AV_3Sb_5

Yishuai Xu et al., arXiv:2204.10116

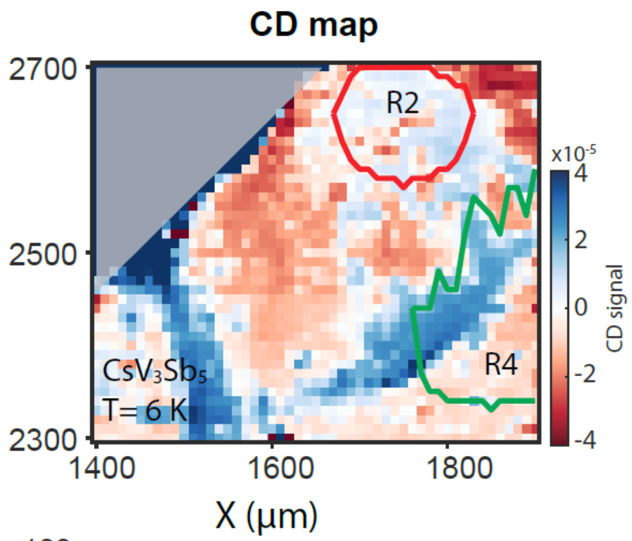


Scanning Kerr rotation

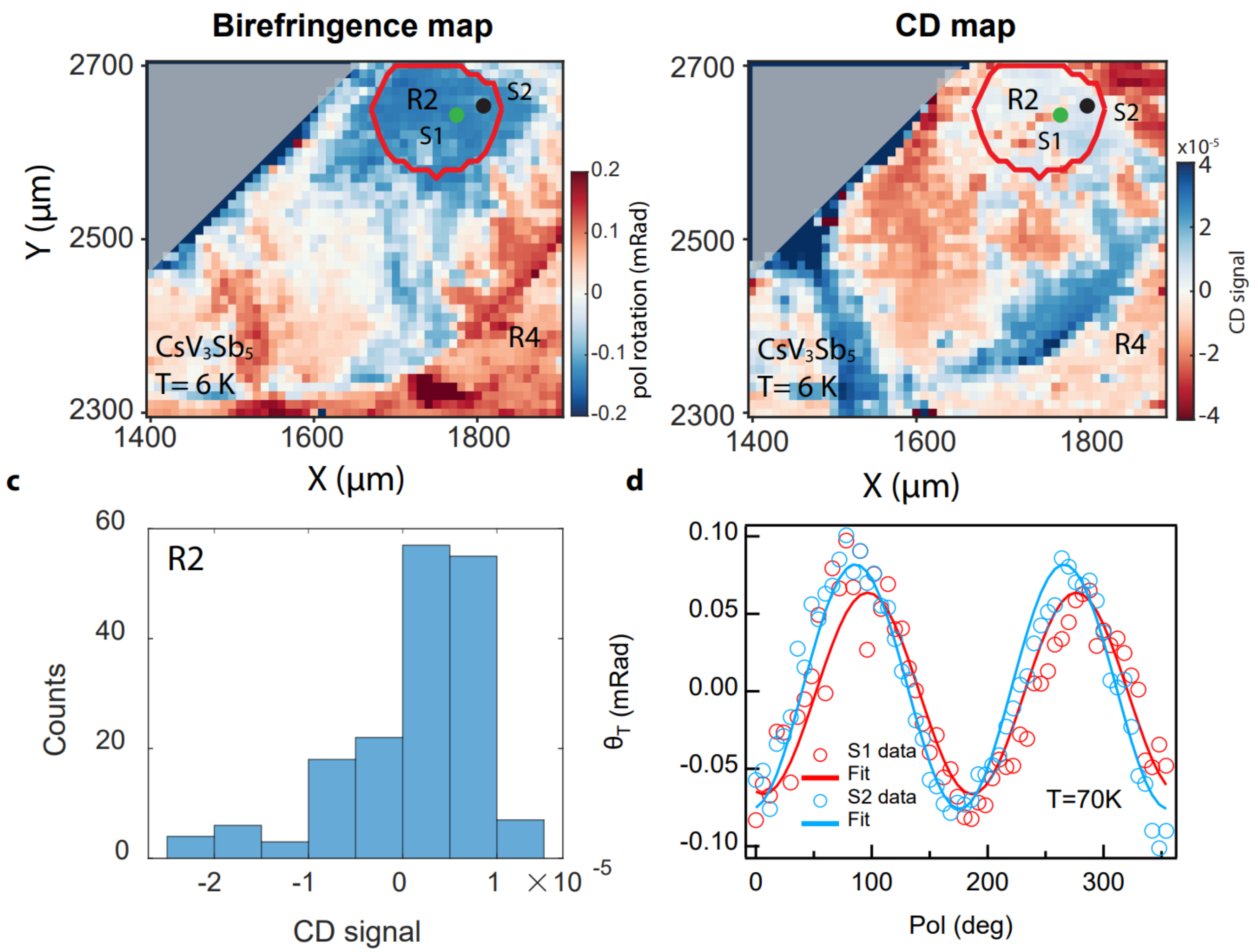
Yishuai Xu et al., arXiv:2204.10116



d



Scanning optical studies cont.

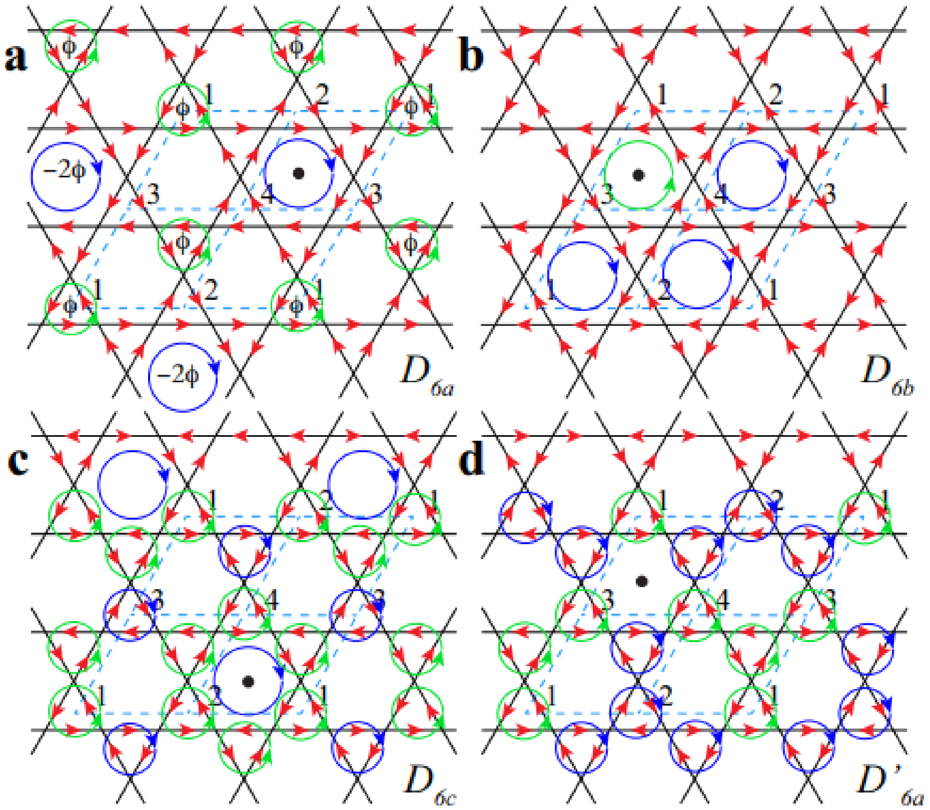


Yishuai Xu et al., arXiv:2204.10116

- CsV_3Sb_5 shows birefringence domains with mixed CD character
- Birefringence domains remain static on thermal cycles
- Some evolution in CD signal upon thermal cycling

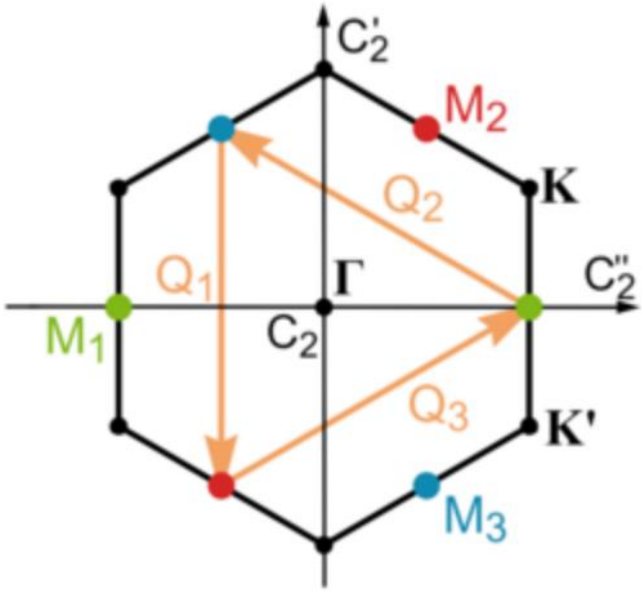
Variety of flux phases predicted

Xilin Feng et al., Phys. Rev. B (2021)



Also:
Lin and Nandkishore Phys. Rev. B. (2021)

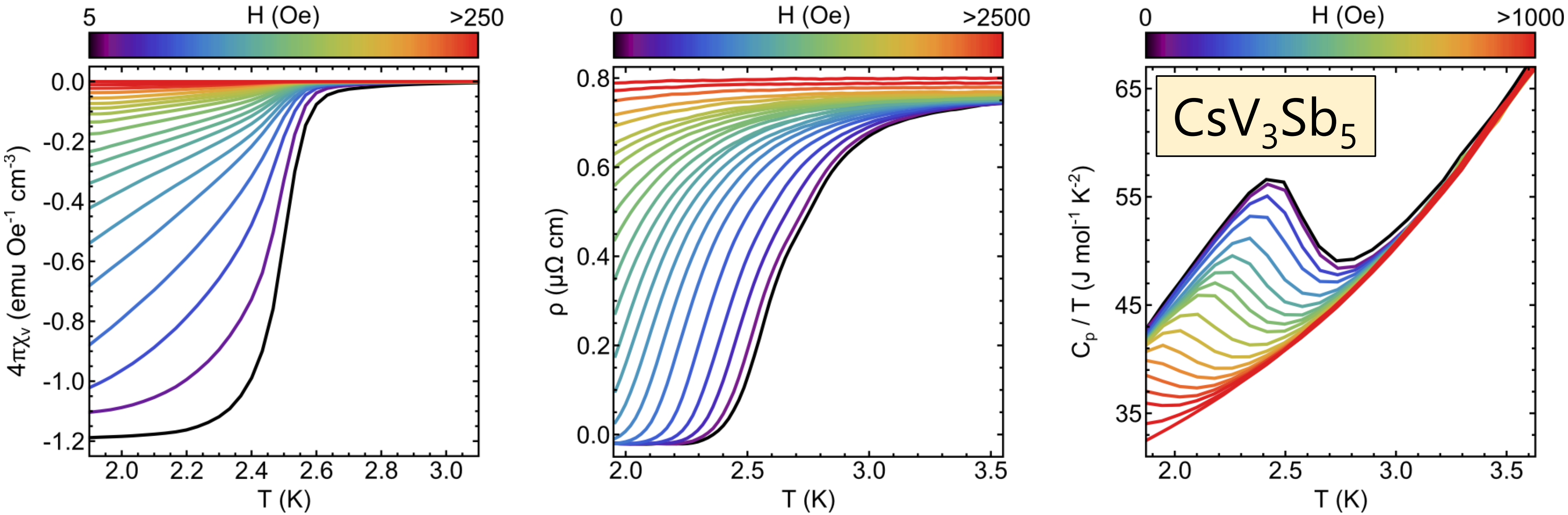
Park, Ye, and Balents., Phys. Rev. B (2021)



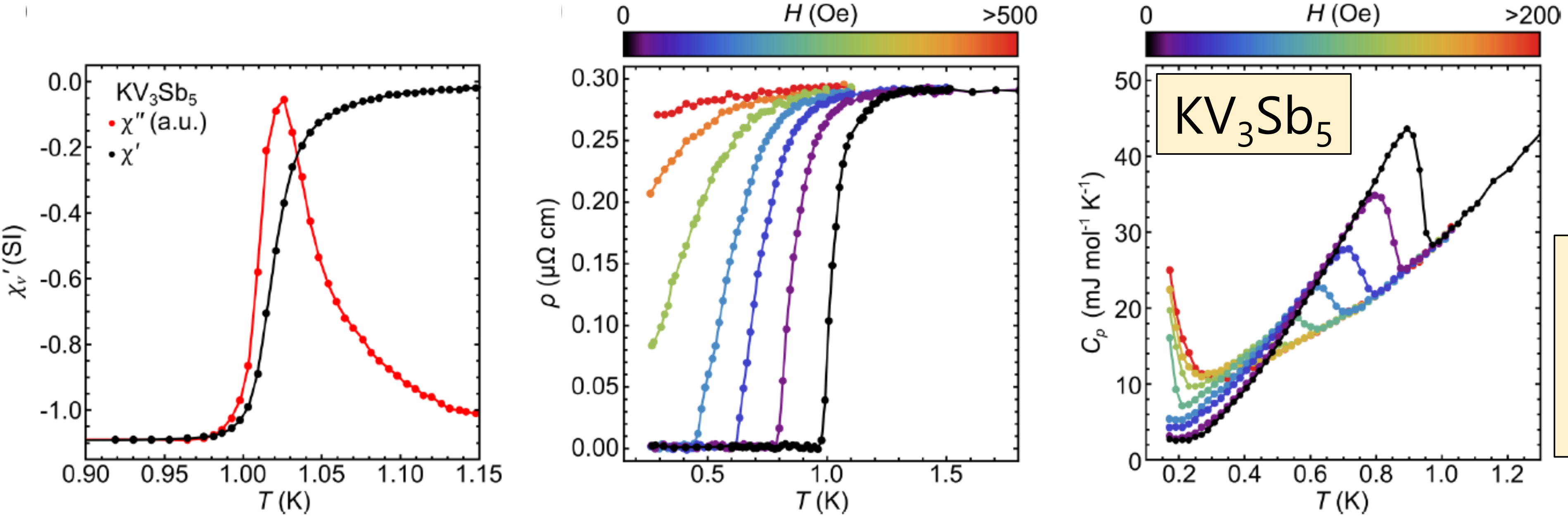
- Chiral flux states
  - Orbital antiferromagnets
- Primary and secondary orders
  - Real and “imaginary” CDW states

SC in AV_3Sb_5 (A=K, Cs, Rb)

Superconductivity in optimized AV_3Sb_5



Ortiz et al., Phys. Rev. Lett. (2020)



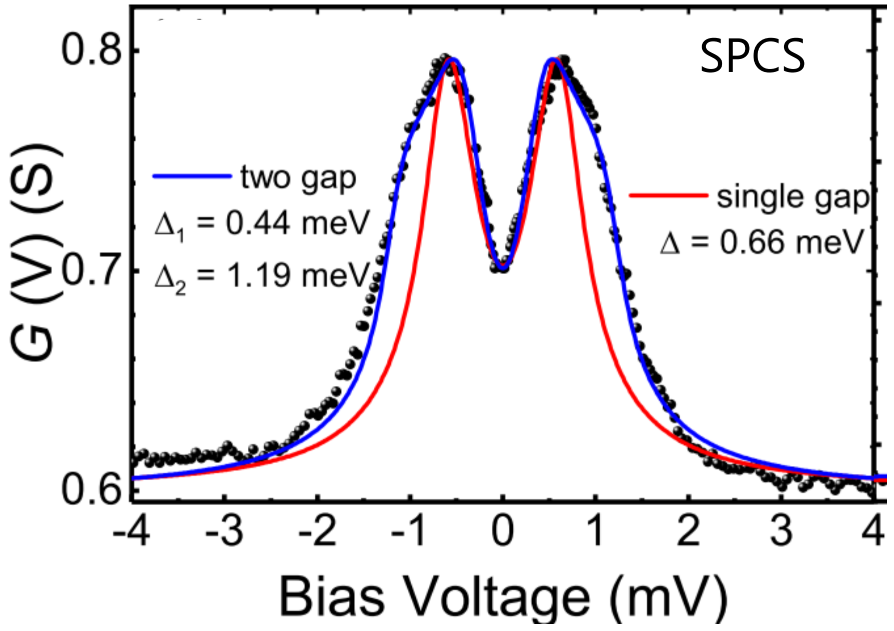
Ortiz et al., Phys. Rev. Mat. (2021)

Also RbV_3Sb_5

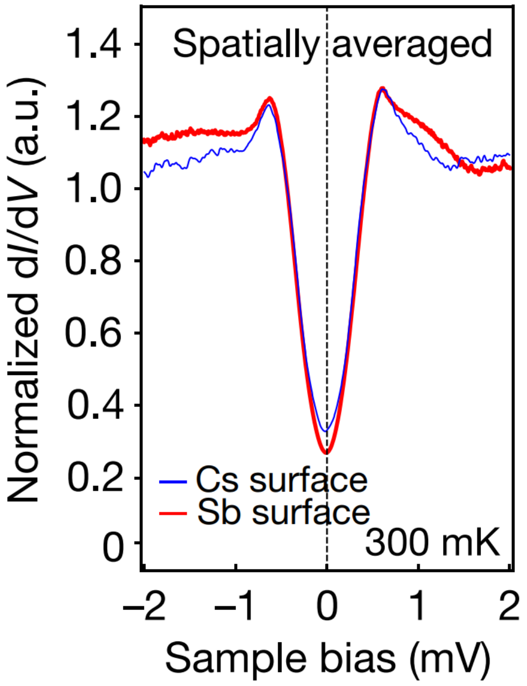
Yin et al., Chin. Phys. Lett. 38, 037403 (2021)

SC state in AV_3Sb_5

Lichang Lin et al., Phys. Rev. B. (2021)



Chen et al., Nature (2021)



- Evidence for multiband, multigap superconductivity
- Isotropic, gap and singlet pairing
  - **TDO measurements**: Weiyin Duan et al., Sci. China Phys. Mech. Astr.. (2021).
  - **NMR measurements**: Chao Mu et al., Chin. Phys. Lett. (2021)

  + others...

Open questions:

Thermal transport
C. C. Zhao et al. arXiv:2102.08356

Little-Parks effect
Jun Ge et al. arXiv:2201.10352

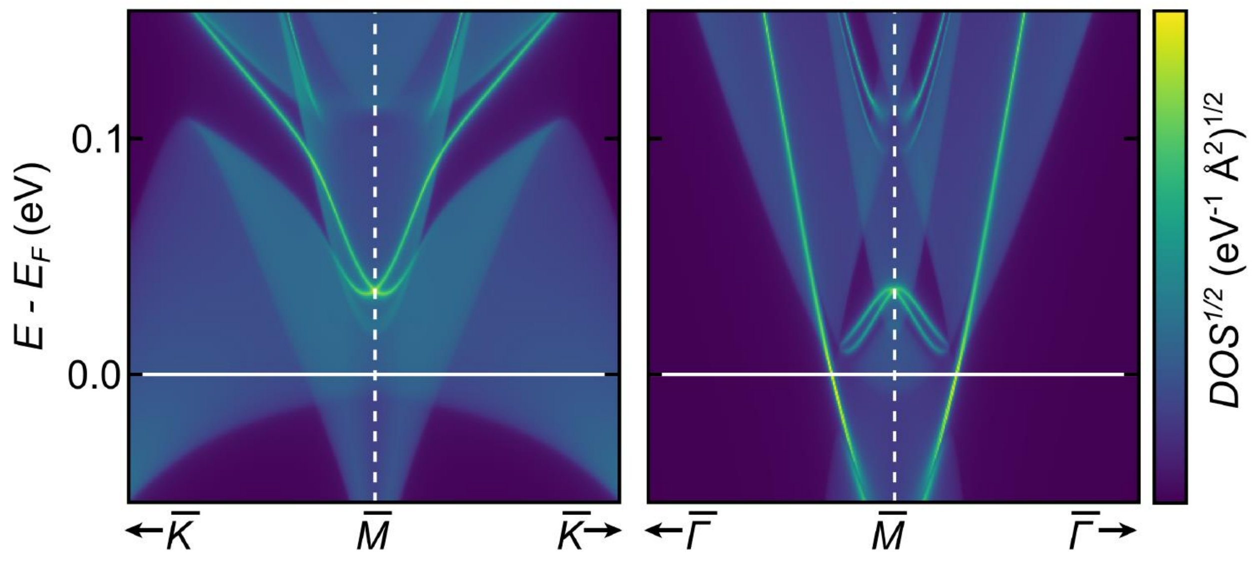
V-shaped gap and PDW instability
Hui Chen et al., Nature (2021).

Nodal SC state, μsR
Z. Guguchia et al., 2202.07713v1

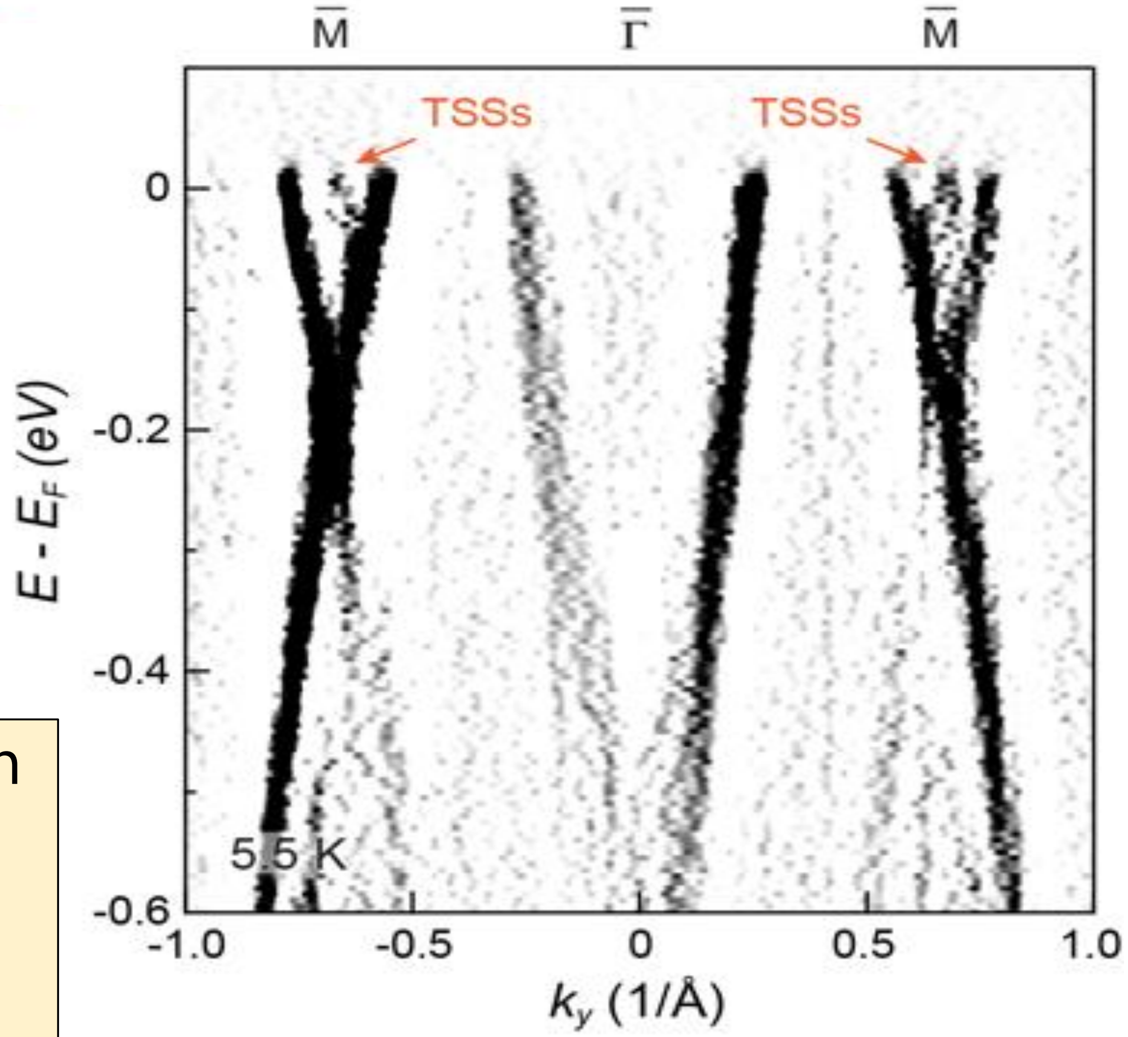
Interplay between CDW and SC order

TSS near E_F and potential coupling to CDW

Ortiz et al., Phys. Rev. Lett. (2020)

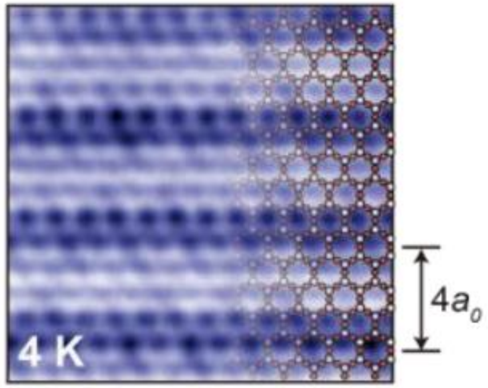


Hong Yu et al., Science Bulletin (2022)



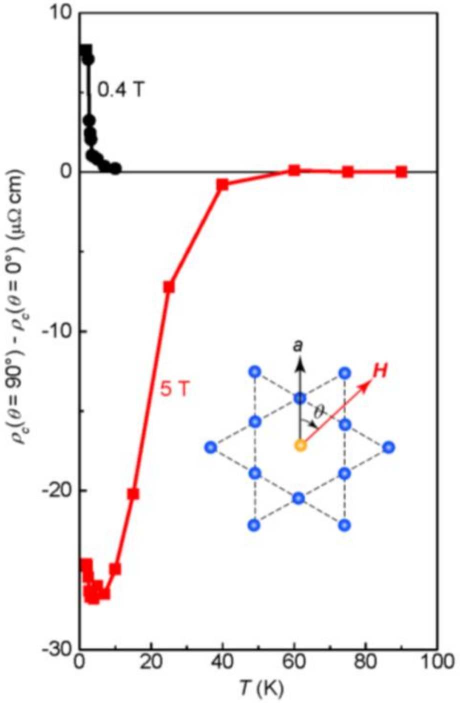
- Topological surface states ~50 meV above E_F in undistorted structure
- ARPES shows TSS pushed down to E_F below CDW
- Suggests TSS participates in conduction at T_c

Staged CDW order

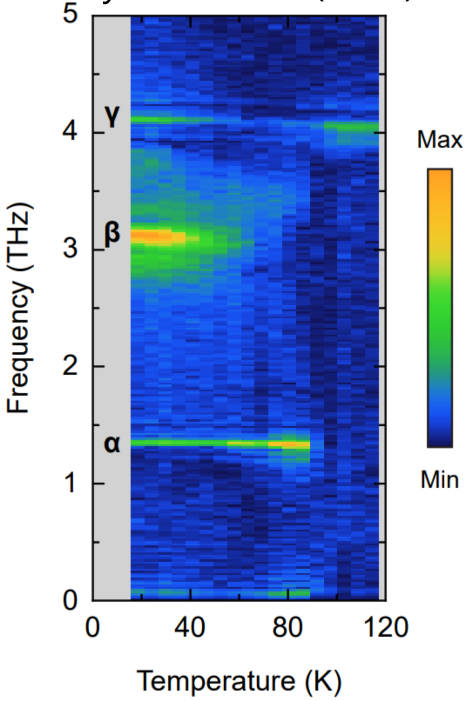


- 1D charge stripes appear below ~60K in CsV_3Sb_5
  - Coexists with 3Q order
- Also observed in RbV_3Sb_5 (rarely in KV_3Sb_5)
- Bulk vs surface effect debated

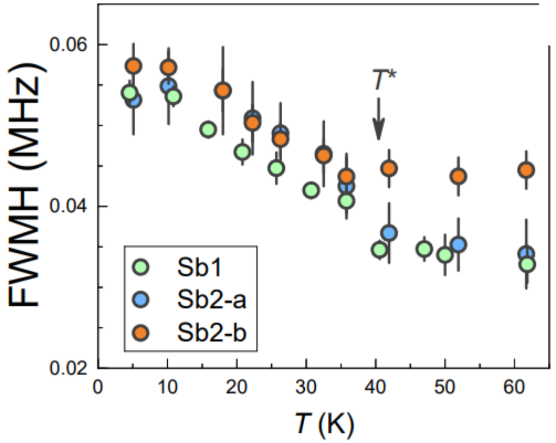
Y. Xiang et al, Nat. Comm. (2021)



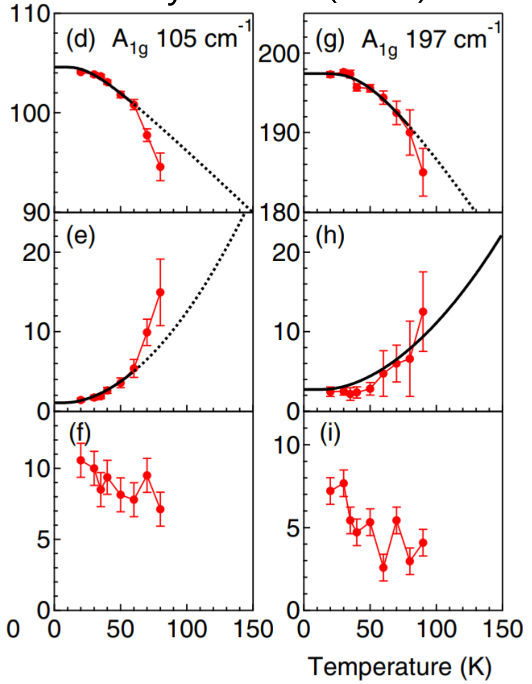
Noah Ratcliff et al,
Phys. Rev. Mat. (2021)



J. Lu et al.,
npj quantum materials (2022)

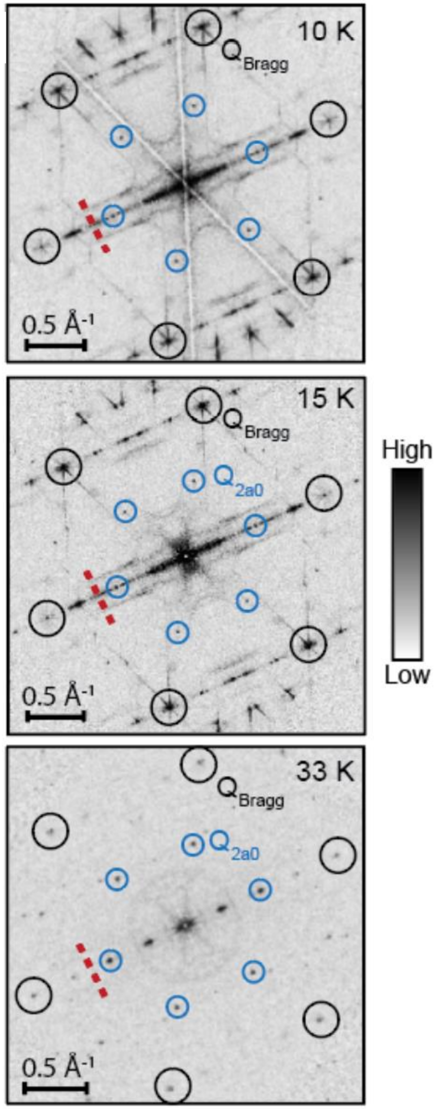


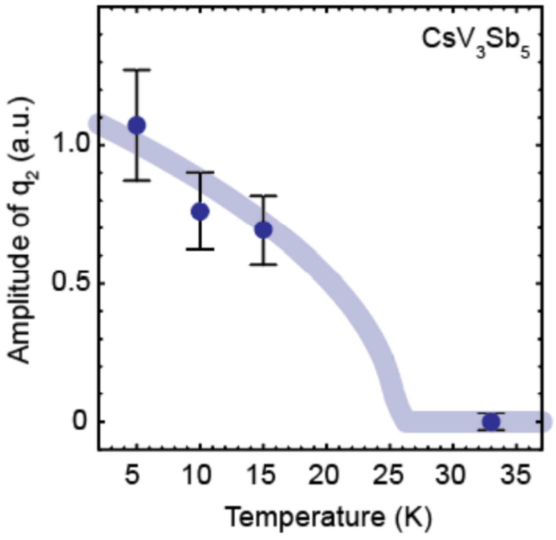
Shangfei Wu et al.,
Phys. Rev. B (2022)

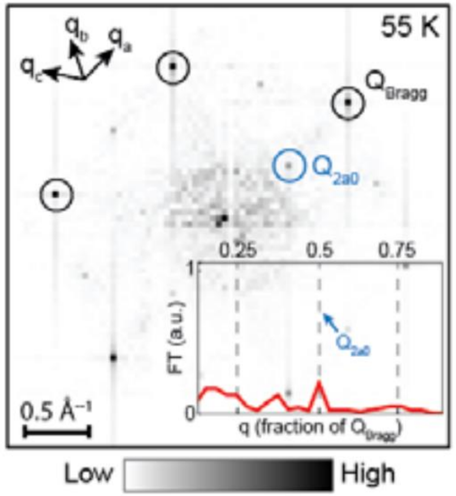


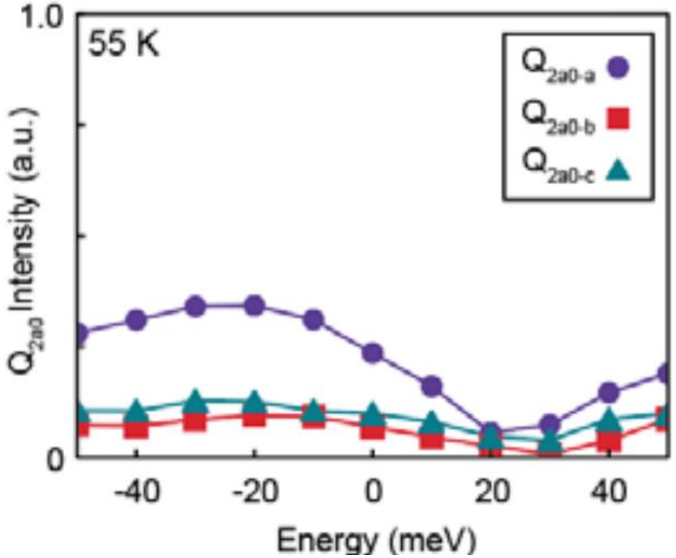
Quasi-1D quasiparticle scattering

Hong Li et al., arXiv:2203.15057







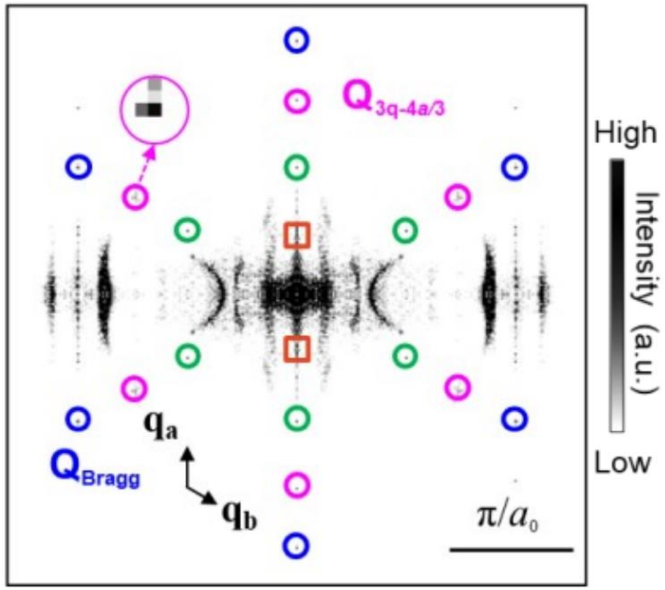


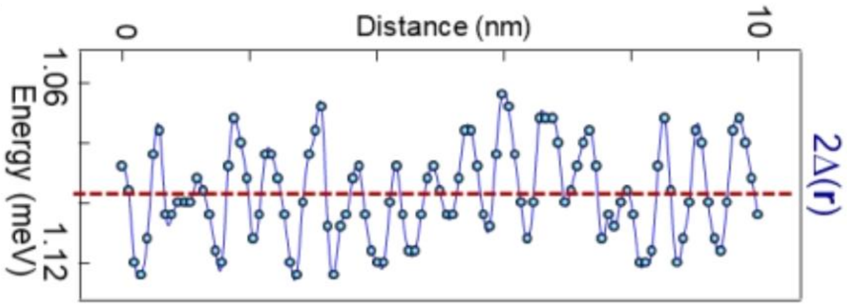
- Unidirectional quasiparticles appear far below CDW
- STM sees quasi-1D quasiparticle interference appear below 30K
- Comes from a state where rotational symmetry is already broken

Hints of PDW order

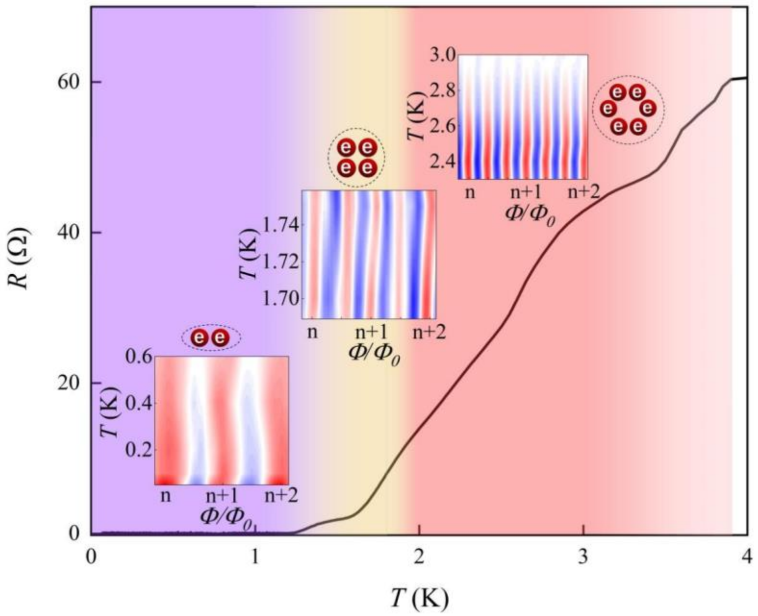
- Superfluid density modulated along wave vector 4a/3
  - Matching new CDW wave vector at low-T
- Little-Parks effect
  - Transition into 4e, 6e pairing states
- Reminiscent of models:
  - D. F. Agterberg et al., Phys. Rev. B 84, 014513 (2011)
  - Zhaoyu Han et al., Phys, Rev, Lett. 125, 167001 (2020)

Hui Chen et al., Nature (2021)





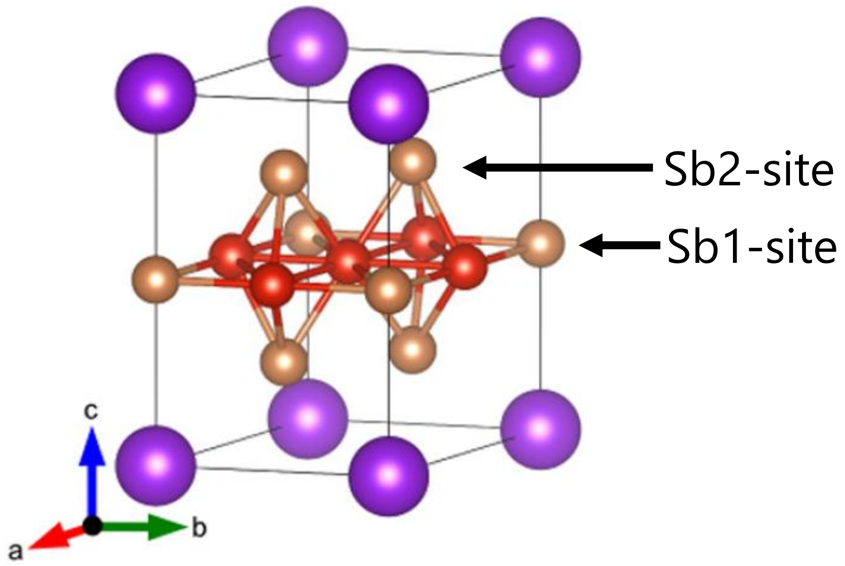
Jun Ge et al., arxiv (2022)

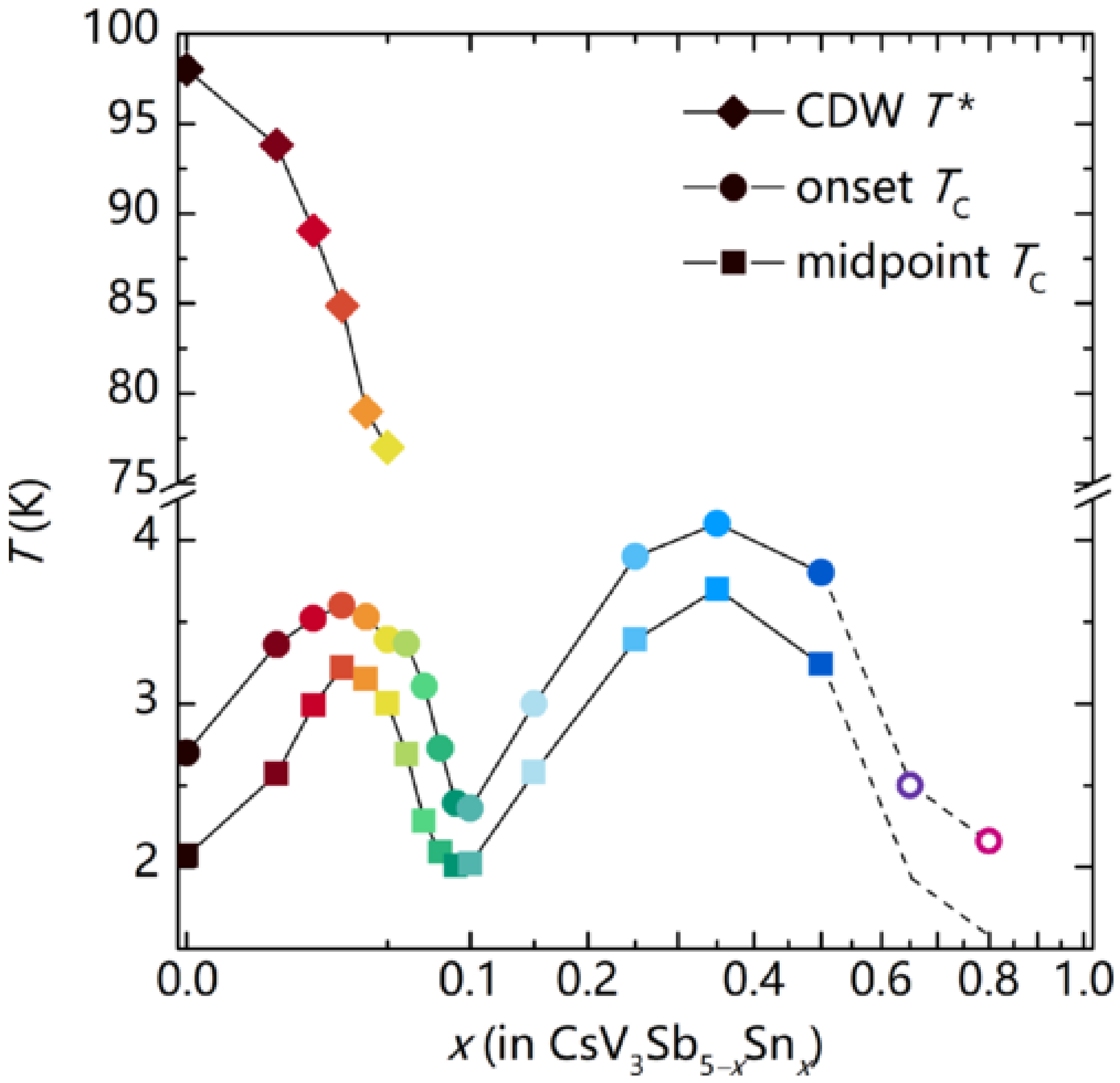


Hole-doping to tune vHs: $CsV_3Sb_{5-x}Sn_x$

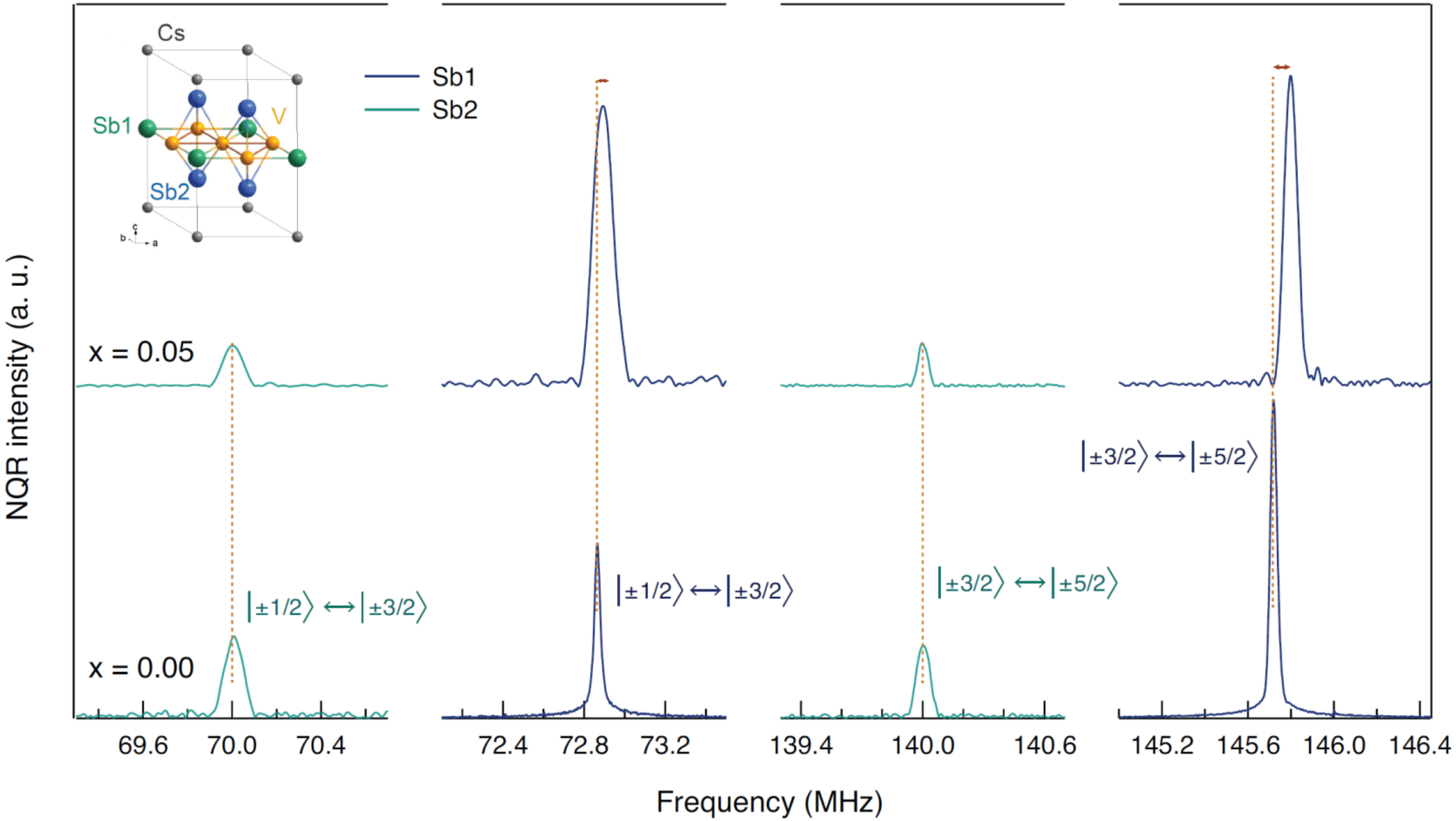
Yuzki Oey et al., Phys. Rev. Mat. (2021)

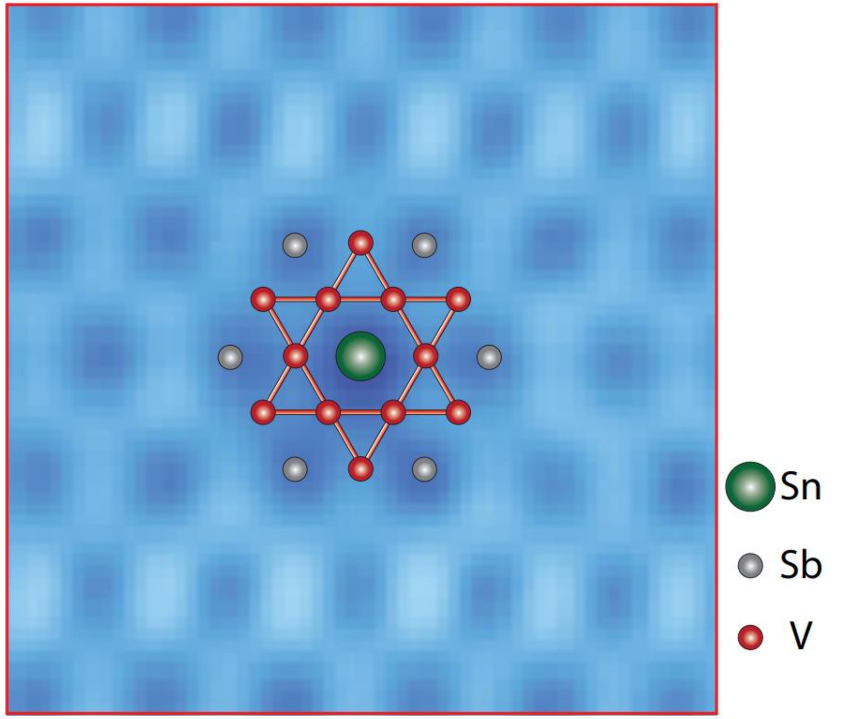
- Sn replaces in-plane Sb1 sites
  - NQR and STM measurements
- Rapidly suppressed the CDW state
  - x=0.06 (0.02 holes/V)
- Two SC domes appear
  - One peak within CDW state





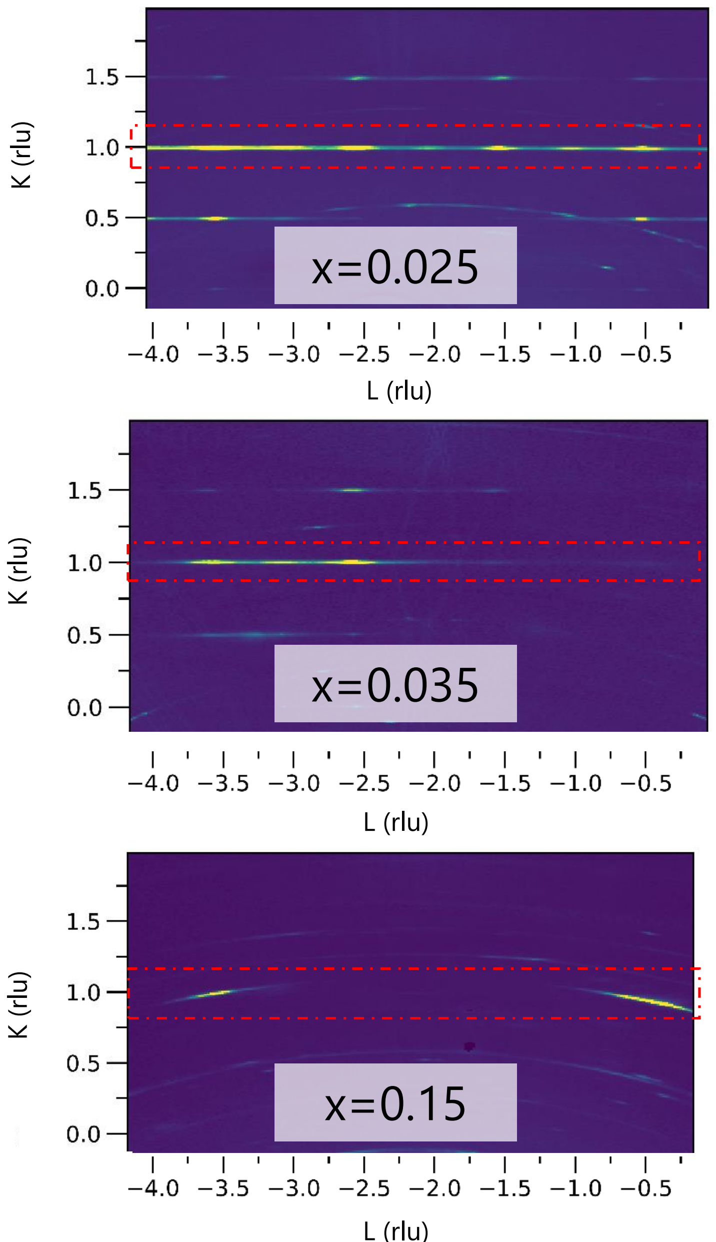
Preferential site substitution

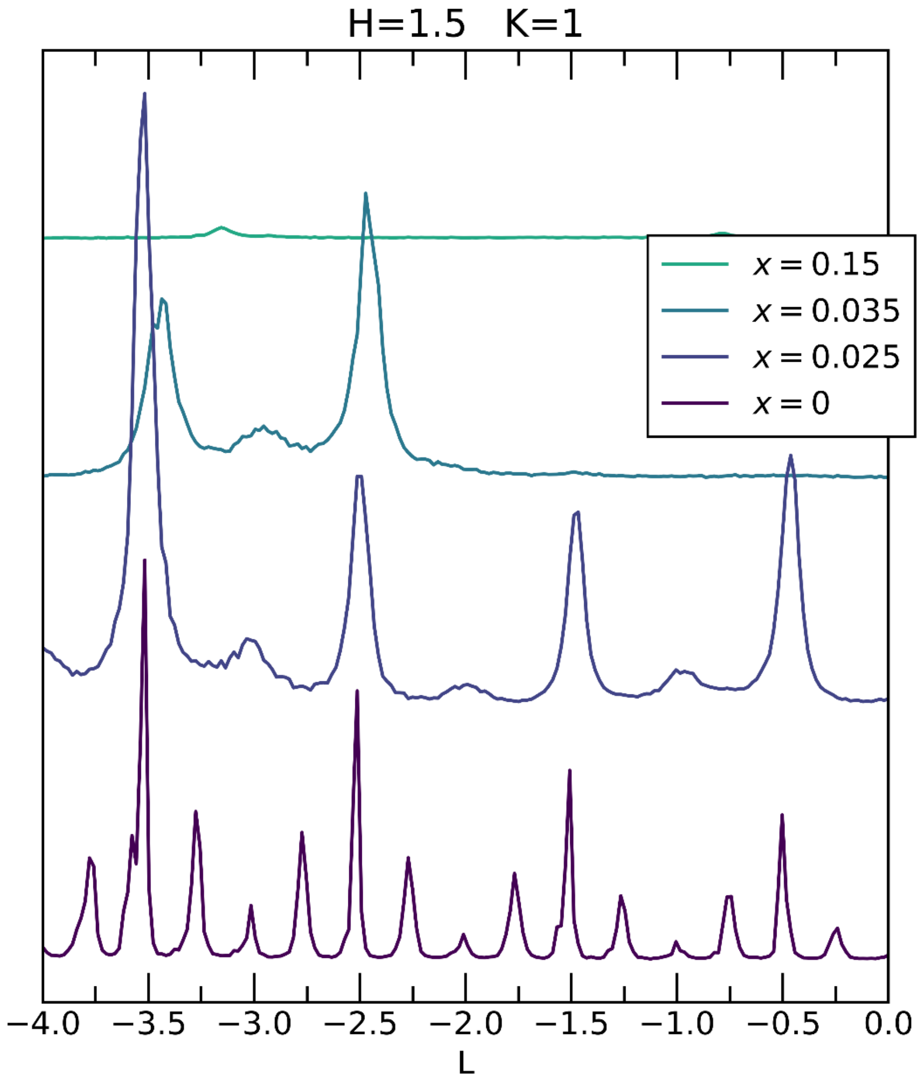




NQR data show shifts at only in-plane Sb site upon Sn-doping
STM identifies Sn atoms in center of kagome net hexagons
DFT suggests a preference for Sn on in-plane site

CDW order in $CsV_3Sb_{5-x}Sn_x$

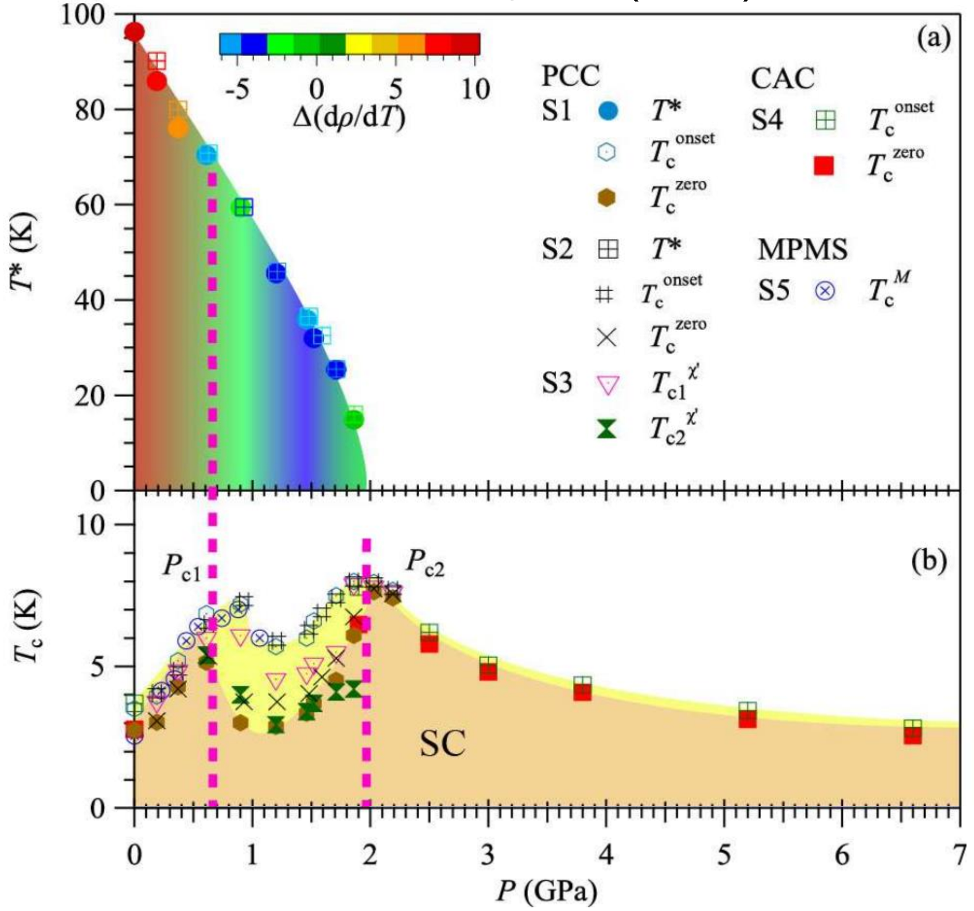




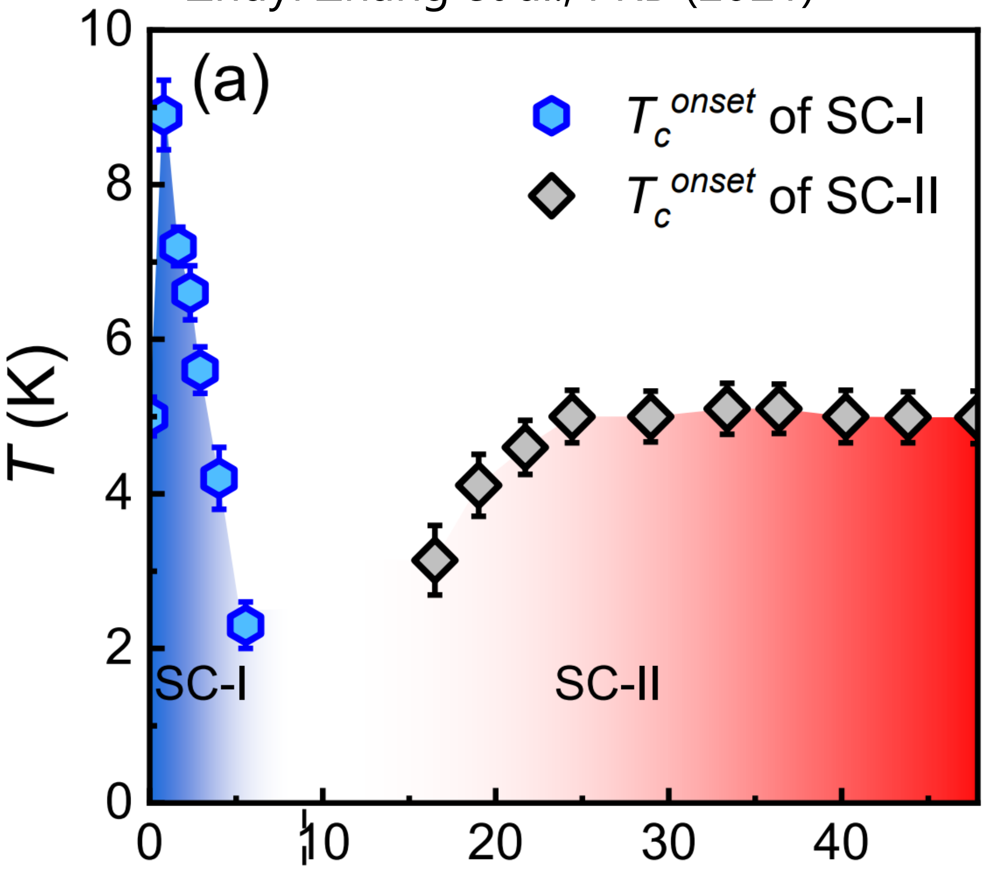
- 2x2x4 order destabilized
  - Highly sensitive to disorder
  - Thermal history
- Switches to short-range 2x2x2
  - Quasi-2D
- CDW correlations vanish by x=0.15

Pressure-T phase diagram of SC

K. Y. Chen et al., PRL (2021)

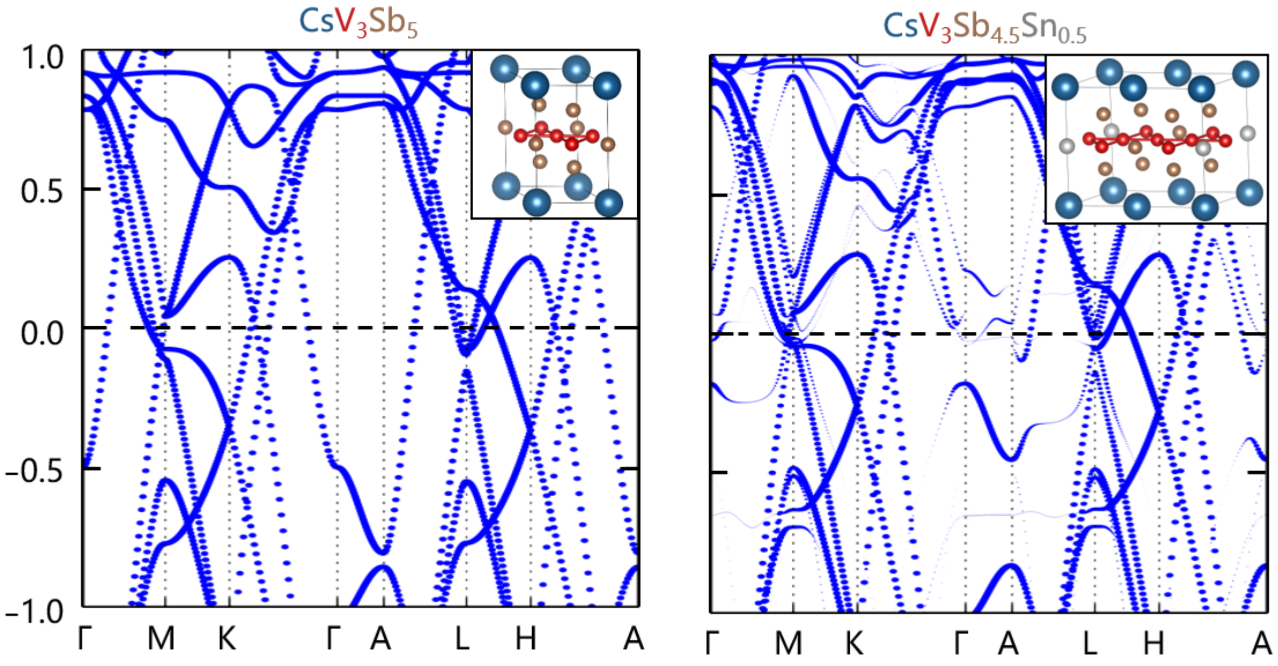


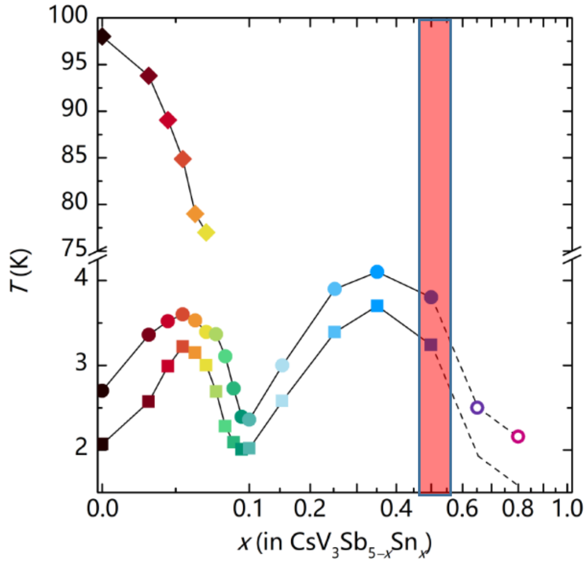
Zhuyi Zhang et al., PRB (2021)



- High-pressure SC-II state universal across AV_3Sb_5
- Low-pressure "double dome" in SC-I state suggestive of phase competition

$CsV_3Sb_{5-x}Sn_x$ vs high-pressure

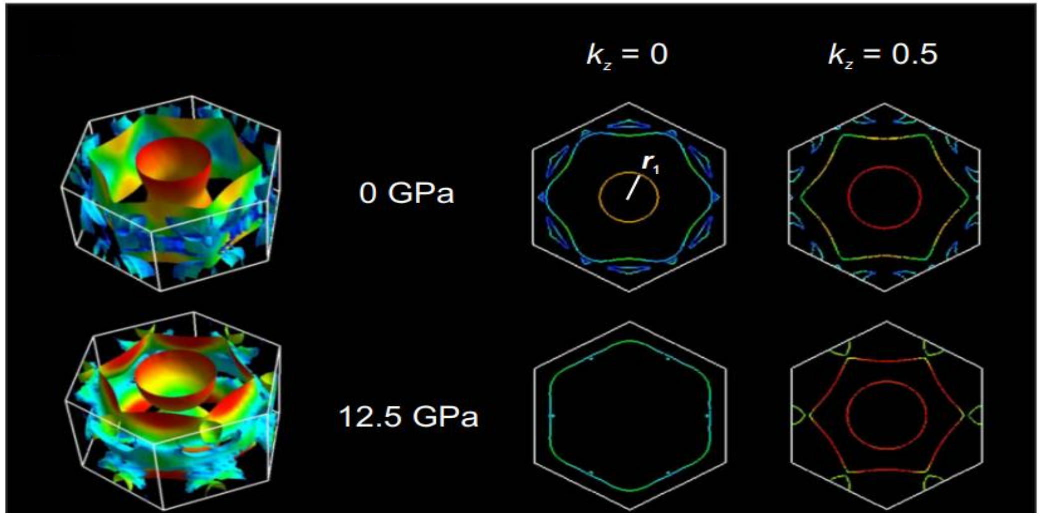




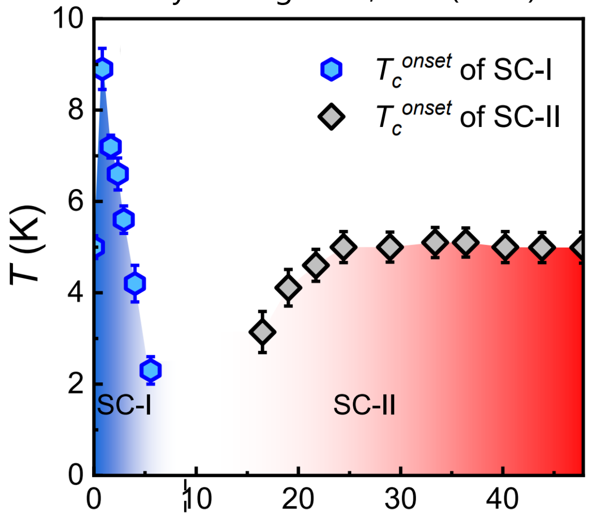
Bulk SC vanishes coincident with Sb p_z electron pocket at x=0.5

Suppression of CDW near x=0.06 an open question

Alexander Tsirlin et al., SciPost Phys. (2021)



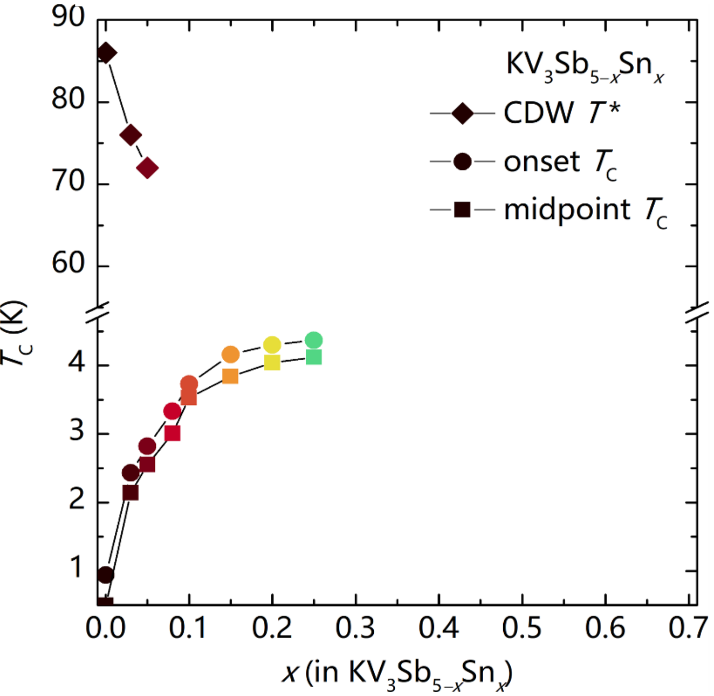
Zhuyi Zhang et al., PRB (2021)

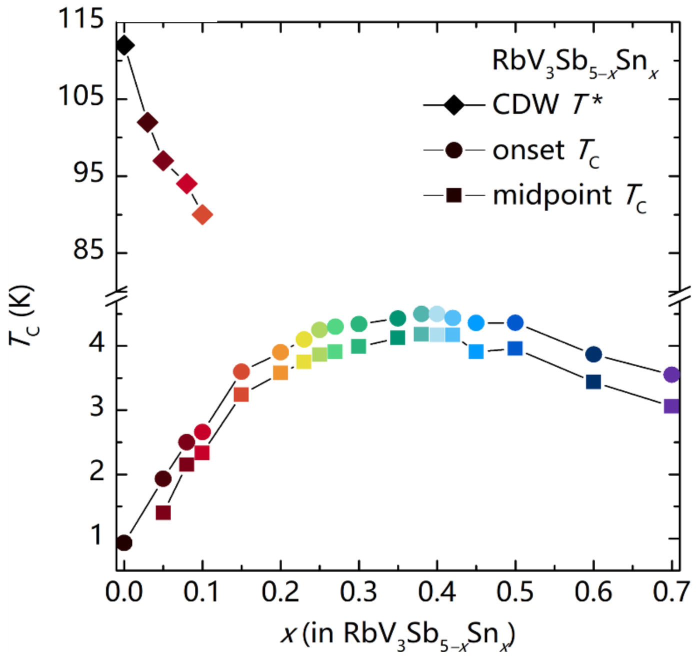


SC vanishes coincident with Sb p_z pocket under pressure

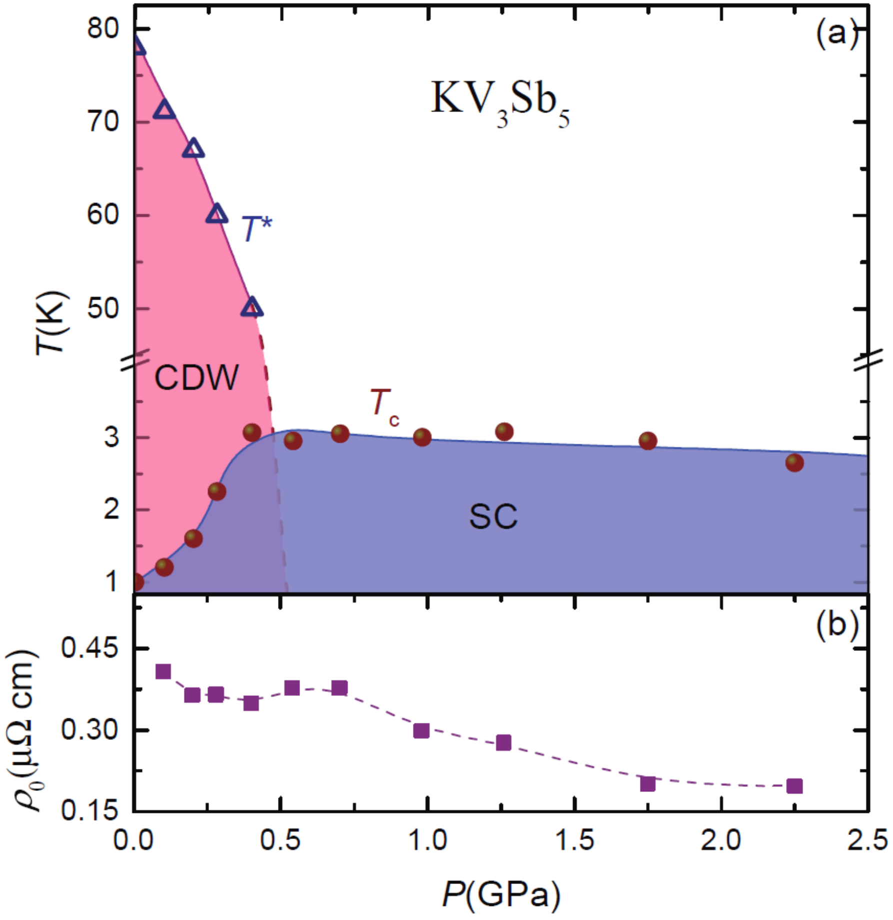
Sn-doping in RbV_3Sb_5 and KV_3Sb_5

Yuzki Oey et al., arxiv:2205.06317





Feng Du et al., Phys. Rev. B (2021)

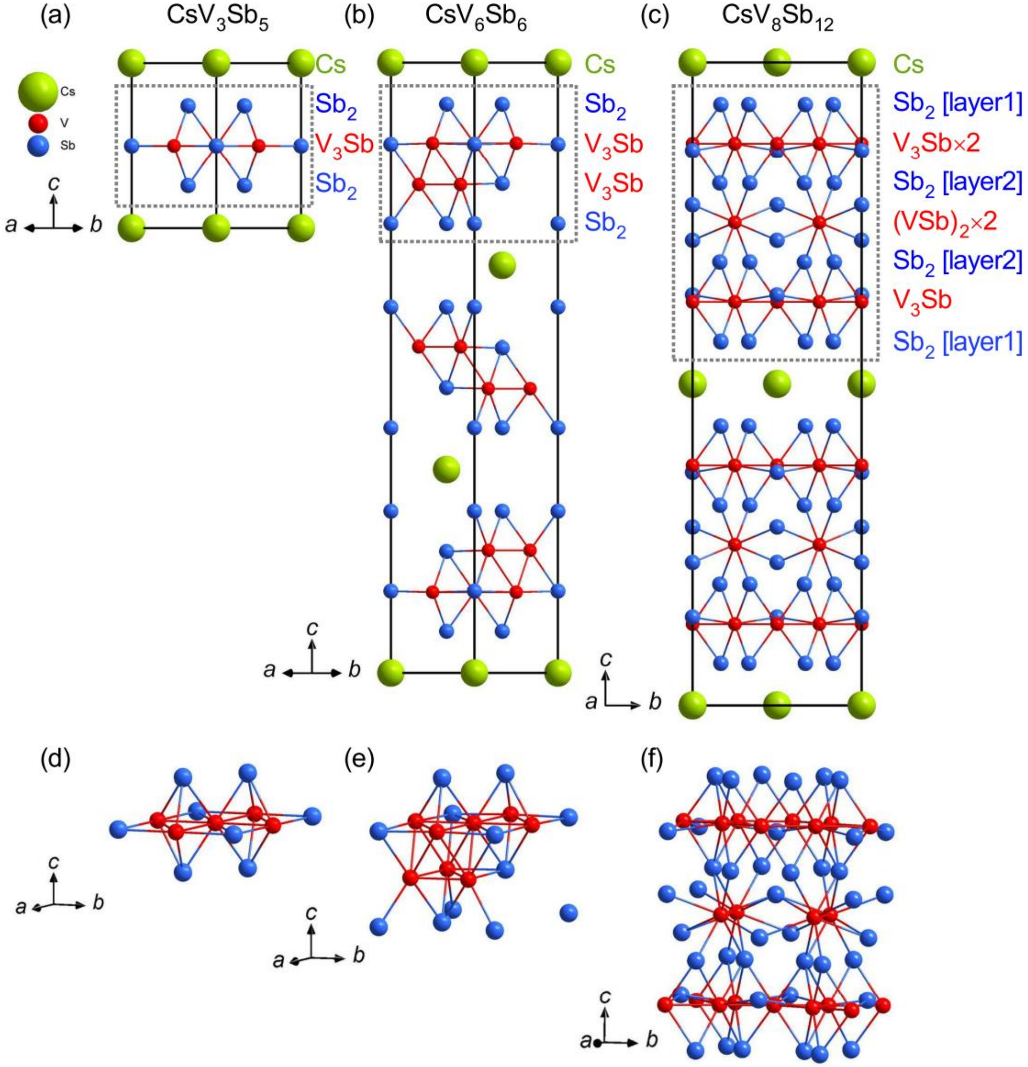


- Only single "dome" observed in hole-doped KV_3Sb_5 and RbV_3Sb_5
- Parallels differences in pressure studies
- Different starting CDW states

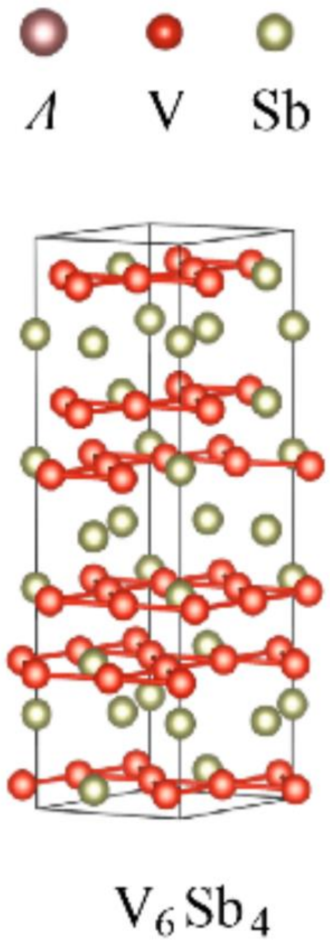
Other potential materials

Other kagome V-Sb families

Qiangwei Yin, Chin. Phys. Lett. (2021)

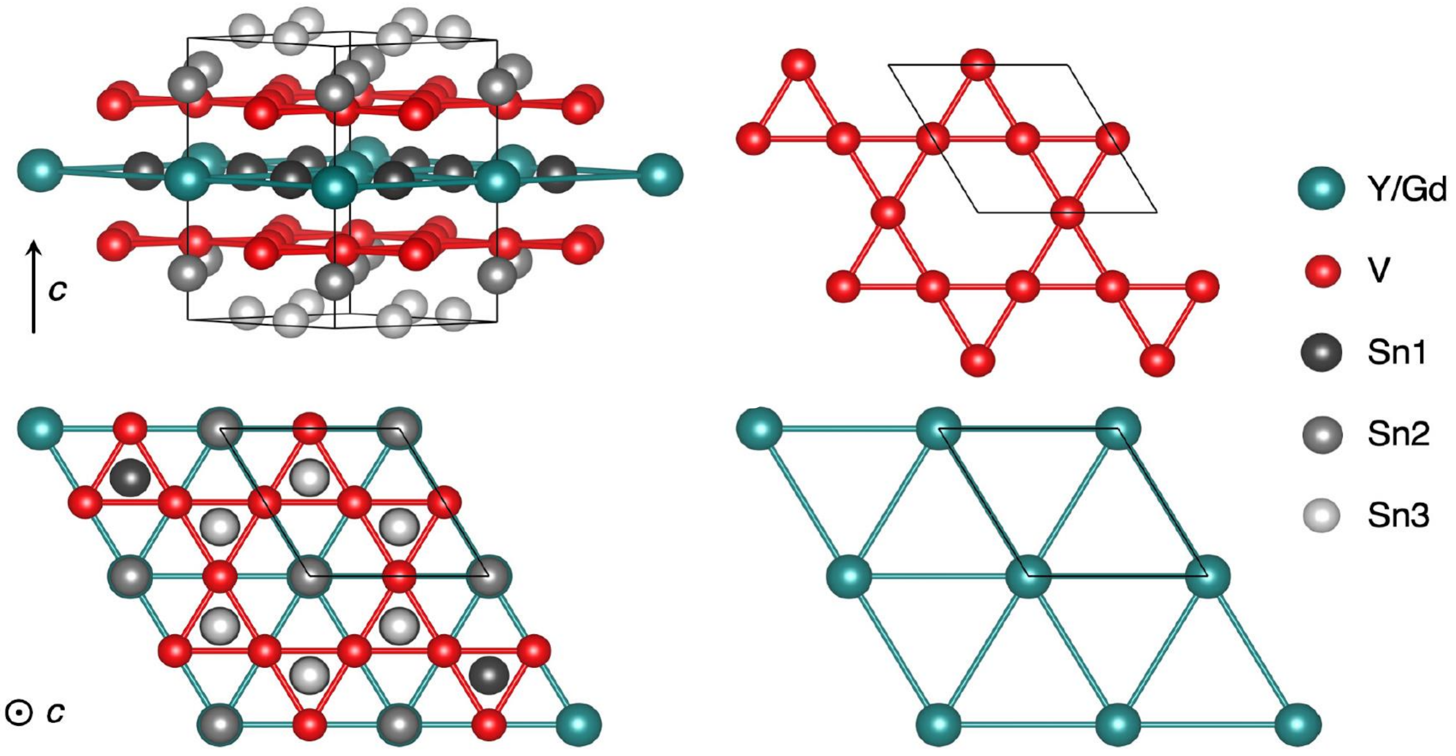


Mengzhu Shi et al., arXiv:2110.09782. (2021)



- No phase transitions under ambient pressure

RV_6Sn_6 structure

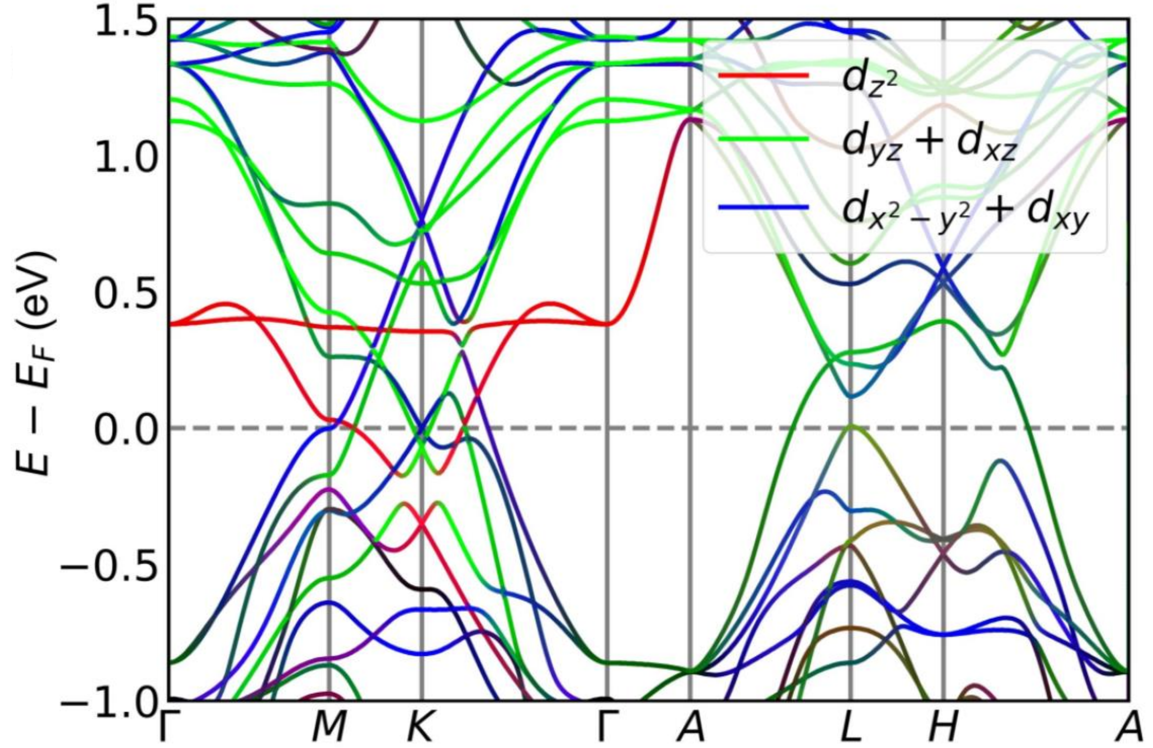


Ganesh Pokharel et al., Phys. Rev. B (2021)

- $MgFe_6Ge_6$ structure type
- P6/mmm space group
- [V_3Sn2][RSn1][V_3Sn2][Sn3]
  - L. Romaka et al. J. All. Comp. (2011)
- Ideal V kagome net
- Triangular lattice of R-site ions
- Affords independent control of R-site magnetism and V-site kagome net

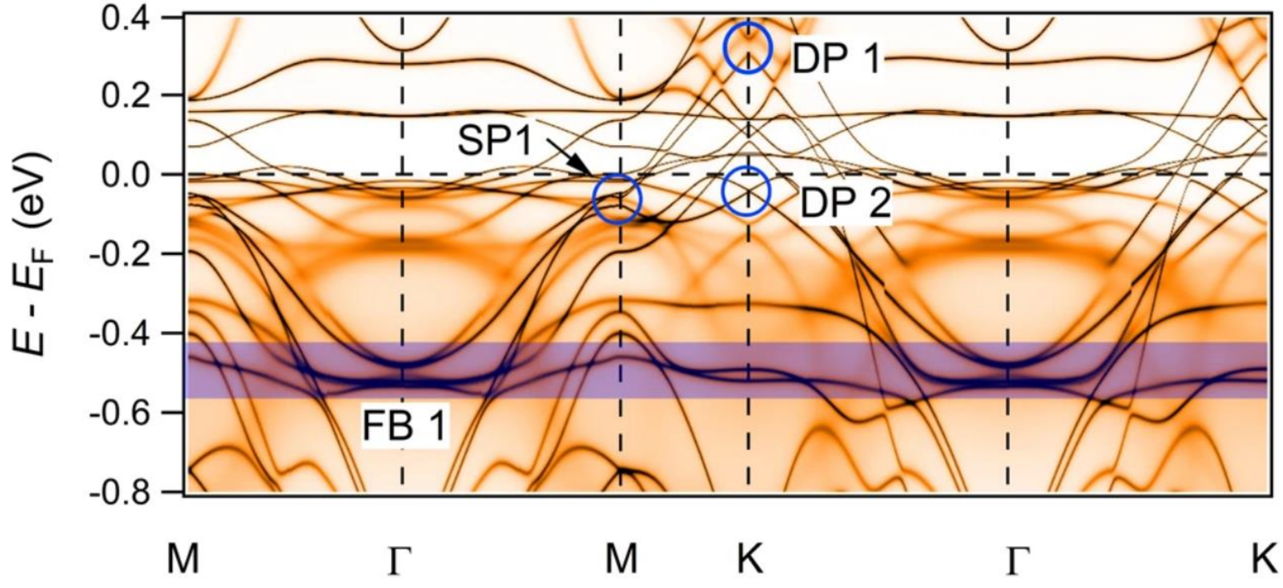
DFT bandstructure of YV_6Sn_6

YV_6Sn_6



Ganesh Pokharel et al., Phys. Rev. B (2021)

YMn_6Sn_6 (DFT + DMFT)

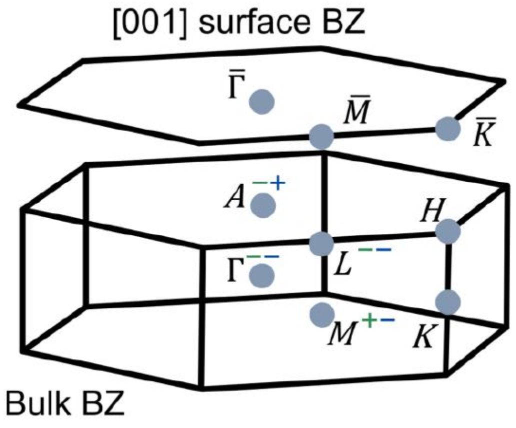


Man Li et al., Nat. Comm. (2021)

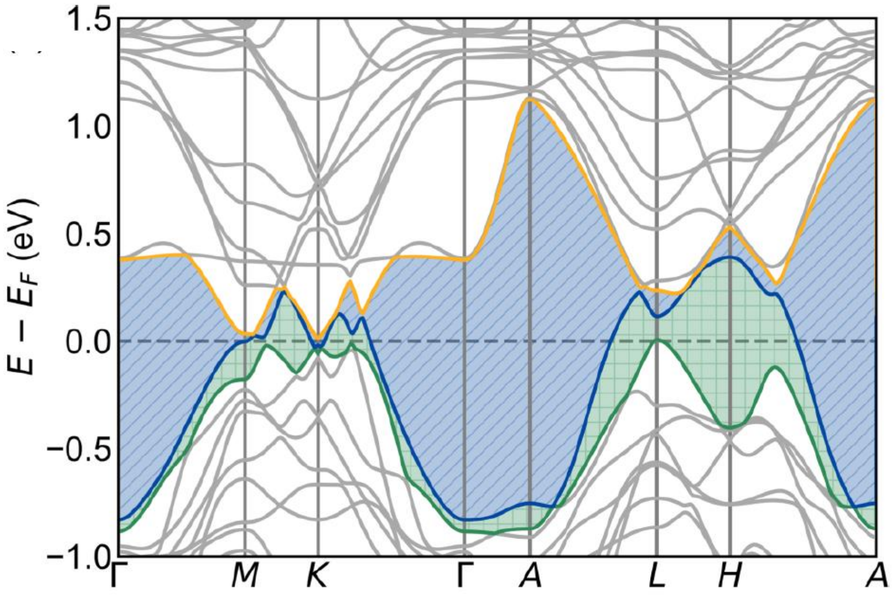
- Flat band above ~0.4 above E_F
- Dirac points at K-point and saddle points at M-point close to E_F

Surface states predicted due to Z2 metal

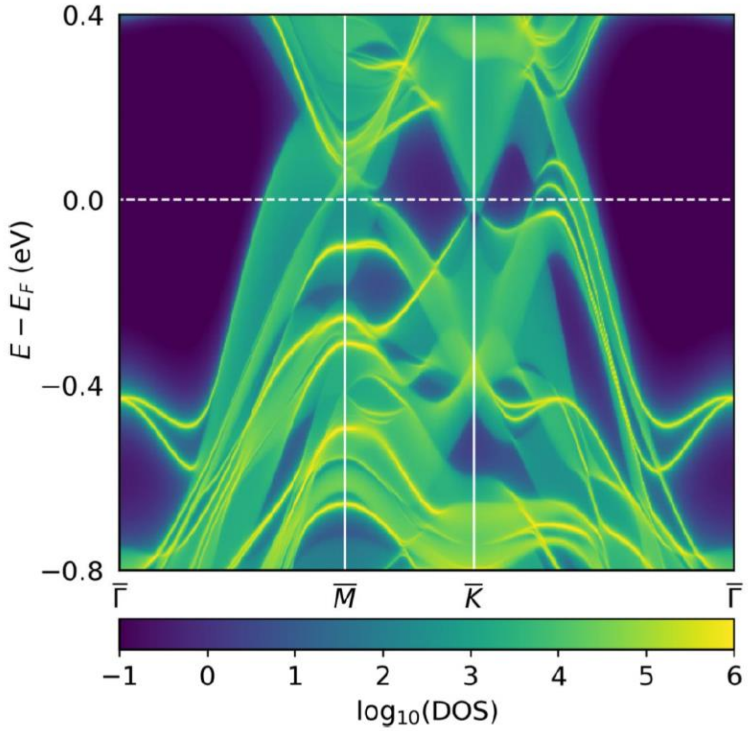
Ganesh Pokharel et al., Phys. Rev. B (2021)



	parity prod.				invariant
band	δ_Γ	δ_M	δ_A	δ_L	$(\mathbb{Z}_2;\nu_1\nu_2\nu_3)$
173	+	+	+	+	(0;000)
171	−	−	+	−	(1;001)
169	−	+	−	−	(1;000)

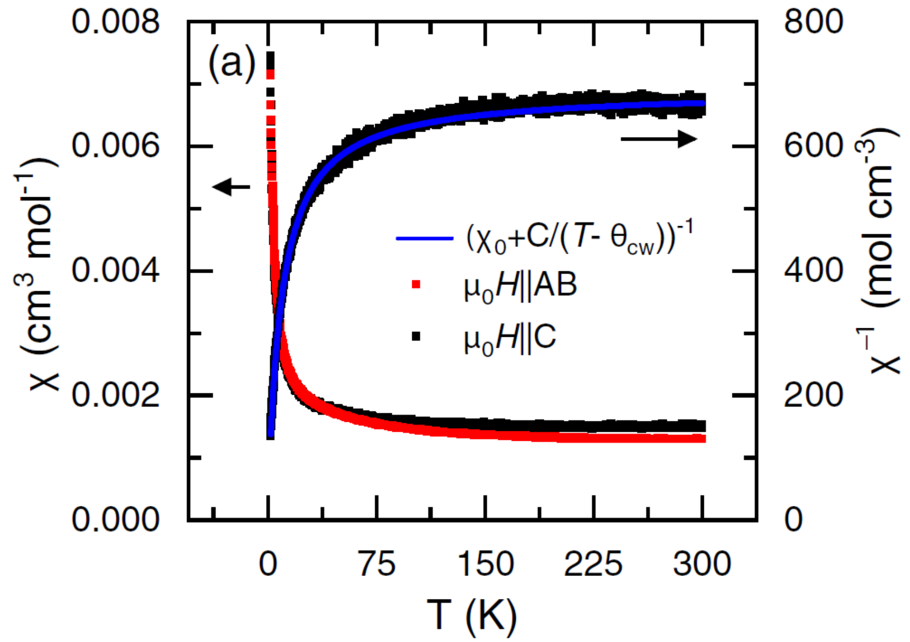


Ganesh Pokharel et al., Phys. Rev. B (2021)
Shutin Peng et al., Phys. Rev. Lett. (2021)



- Qualitative agreement between DFT and ARPES
- Band structure classified as Z2 topological metal
- Surface states predicted near the M- and K-points

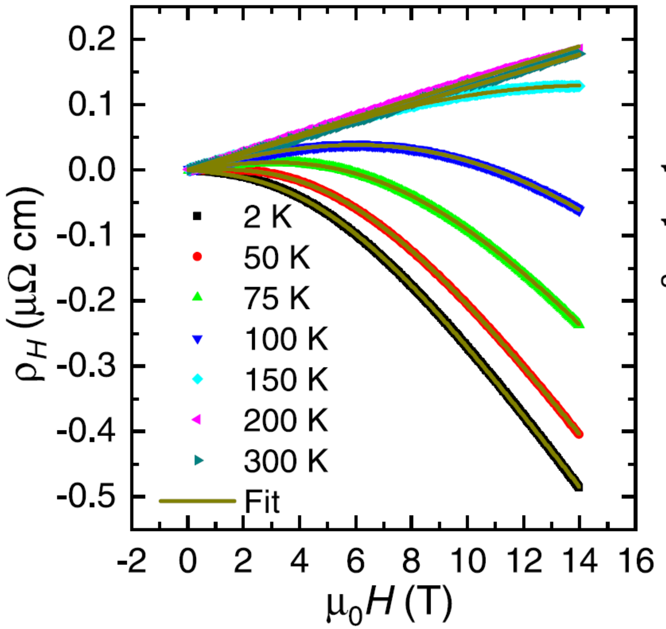
Nonmagnetic Y-166

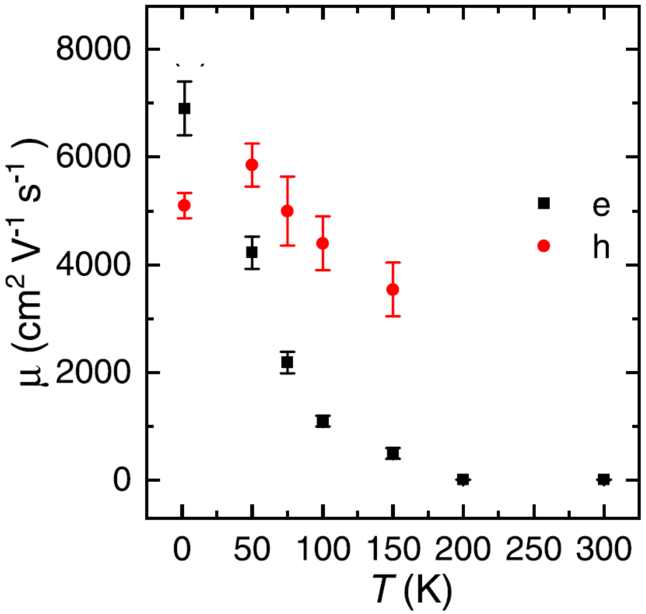


- Local magnetism dominated by weak impurity fraction (~0.3 μ_B/f.u.)
- Confirms nonmagnetic V-lattice (~2.7 Å V-V)

Ganesh Pokharel et al., Phys. Rev. B (2021)

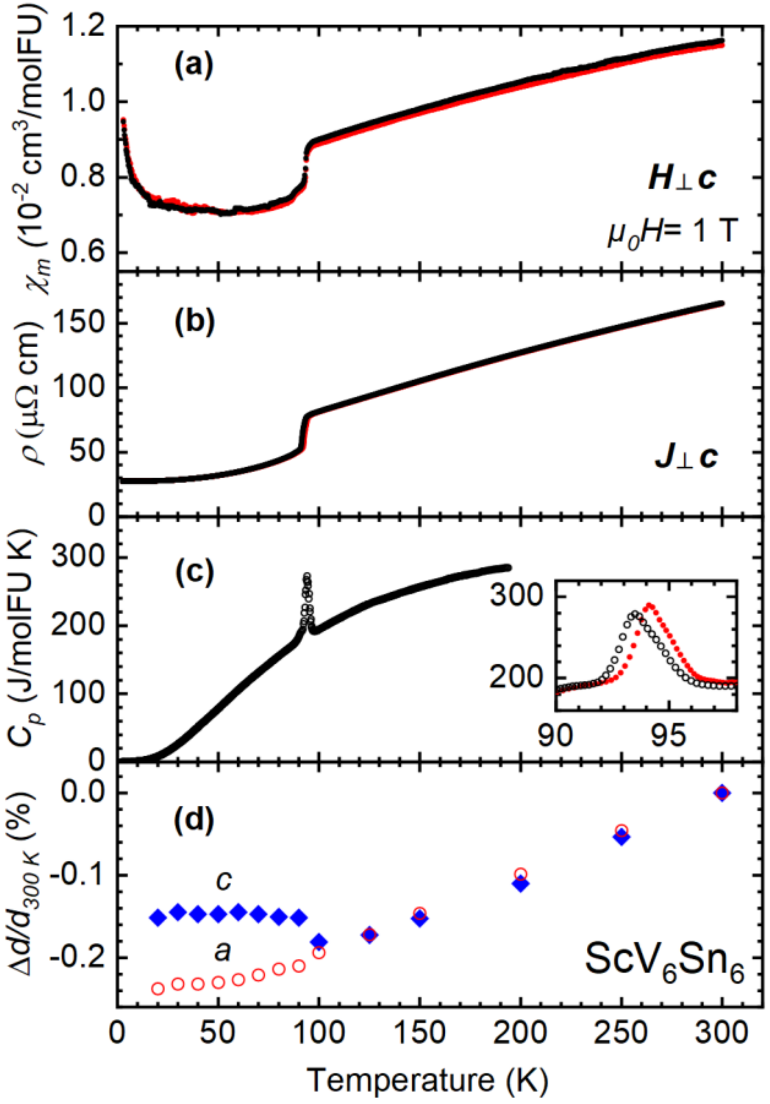
- Multiband transport
  - Parameterized by two-band fits below ~150 K
- High mobility metal

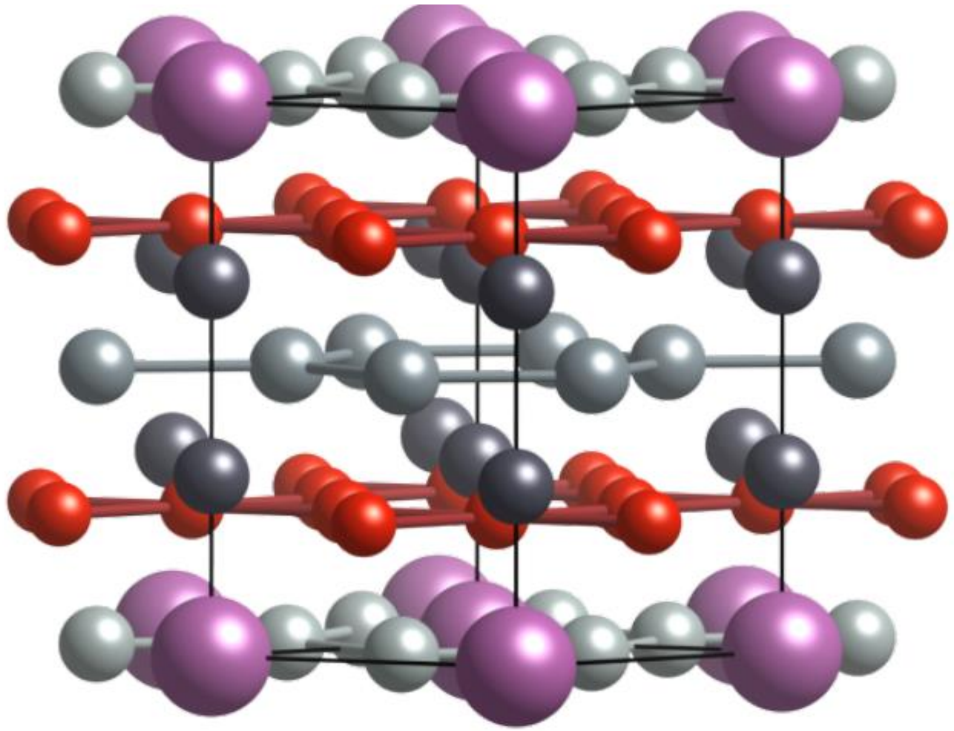




ScV_6Sn_6

Hasitha W. Suriya Arachichige et al., arxiv:2205.04582v1





- Transition near 100 K
- Distortion with q=(1/3, 1/3, 1/3)
- Much larger distortion that 135's

Conclusions

- New classes of kagome metals as platforms for searching for new electronic phases (interplay between correlation effects and topology)
- AV_3Sb_5 (A=K, Cs, Rb)
  - Unconventional CDW state with hints of TRSB
  - CDW order arises from saddle points nested near E_F
  - Multigap SC onsets within the CDW state
  - Unconventional interplay between CDW and SC orders
- Other classes of materials under investigation by community searching for comparable phenomenology
- Exciting new directions and much left to be done

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