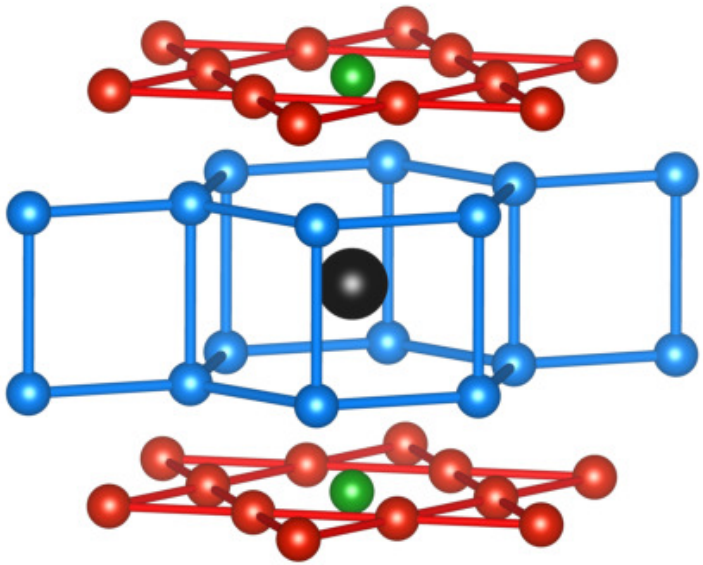
The world of kagome

Alexander Tsirlin

Felix Bloch Institute for Solid-State Physics



UNIVERSITÄT LEIPZIG

Antrittsvorlesung
June 13, 2023

Condensed matter

- Soft matter
- Hard condensed matter (solid-state)

Peter Debye Institute for Soft Matter Physics ›

Felix Bloch Institute for Solid State Physics ›

Institute for Geography ›

Institute for Meteorology ›

Institute of Geophysics and Geology ›

Institute of Theoretical Physics ›

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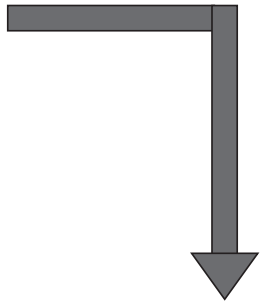
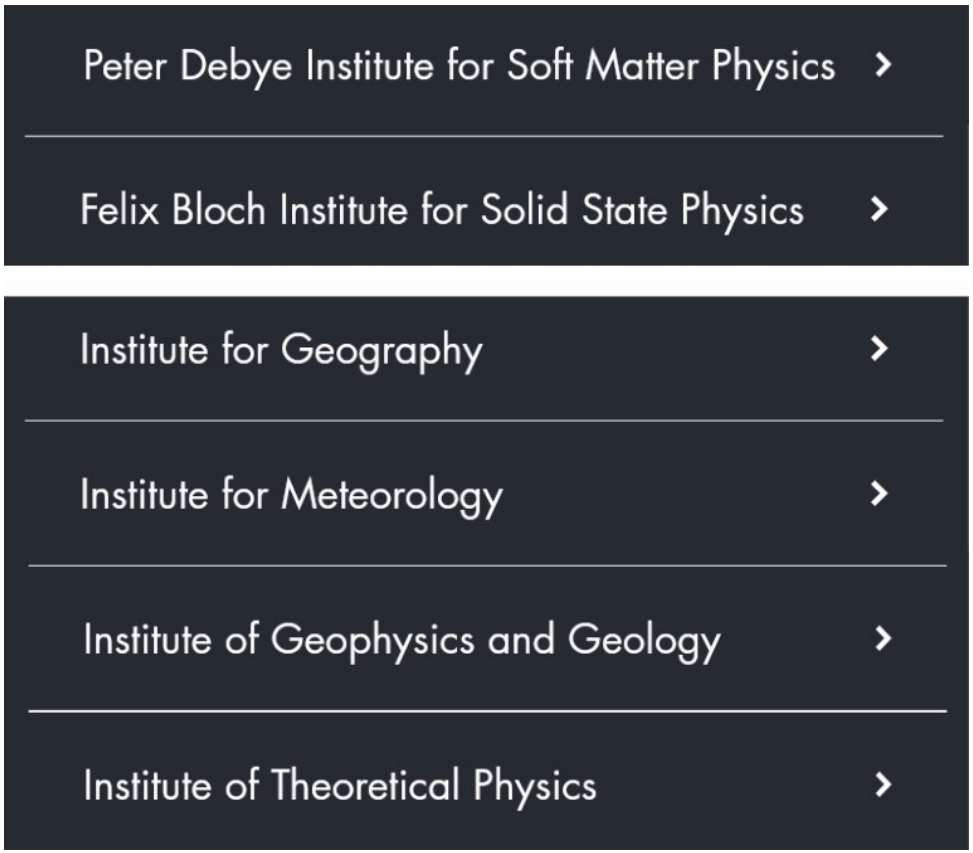


- glasses
- thin films / heterostructures
- ultracold atoms
- quantum dots
- crystals



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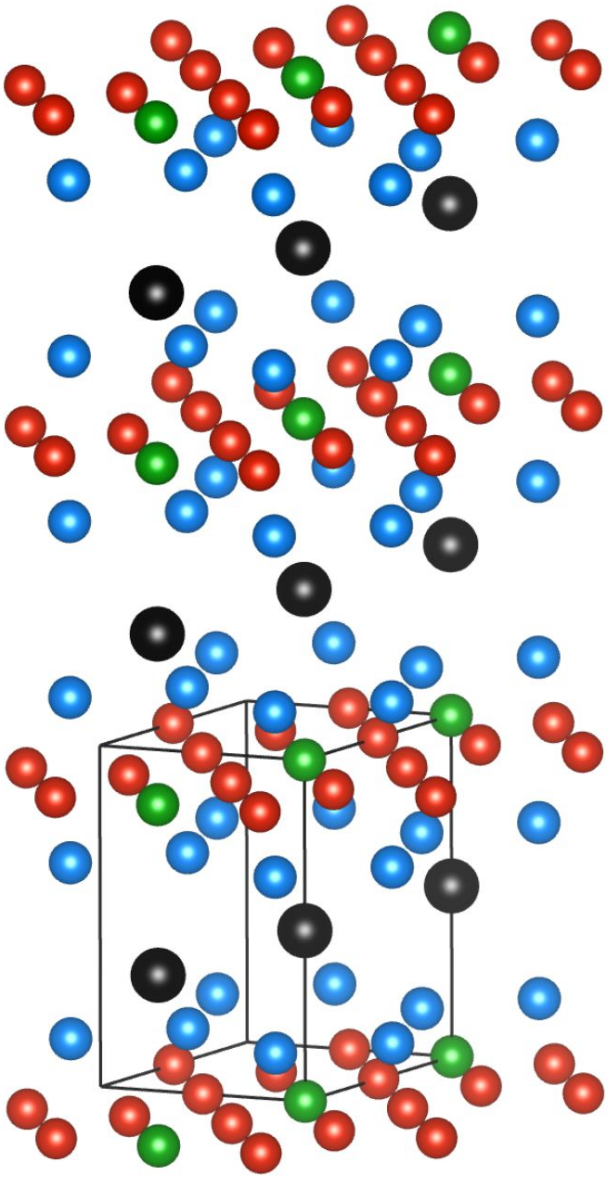
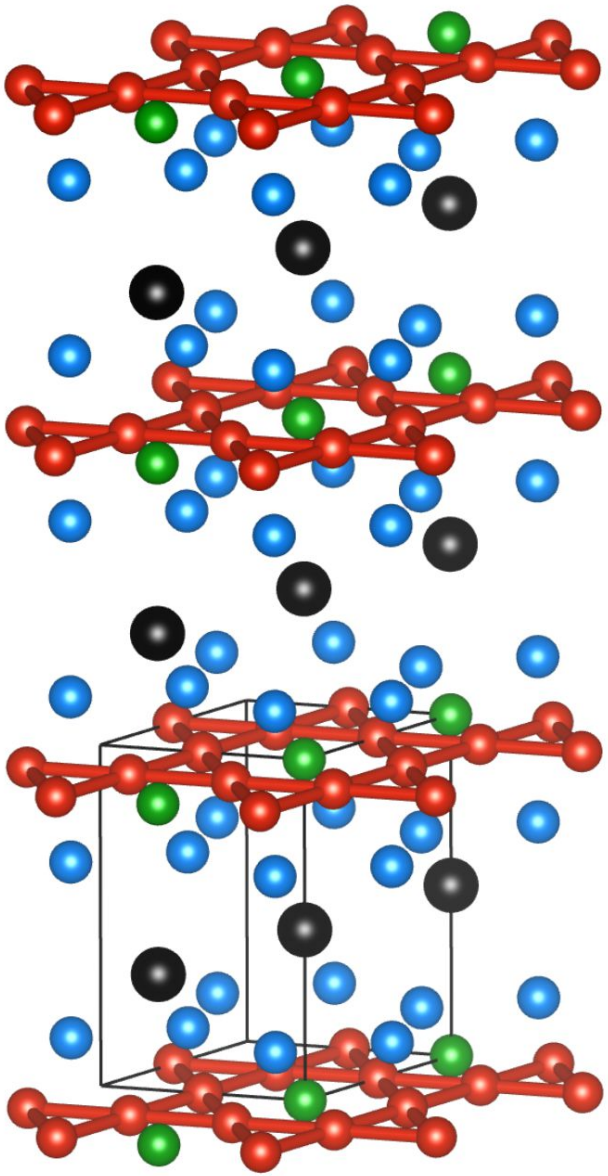
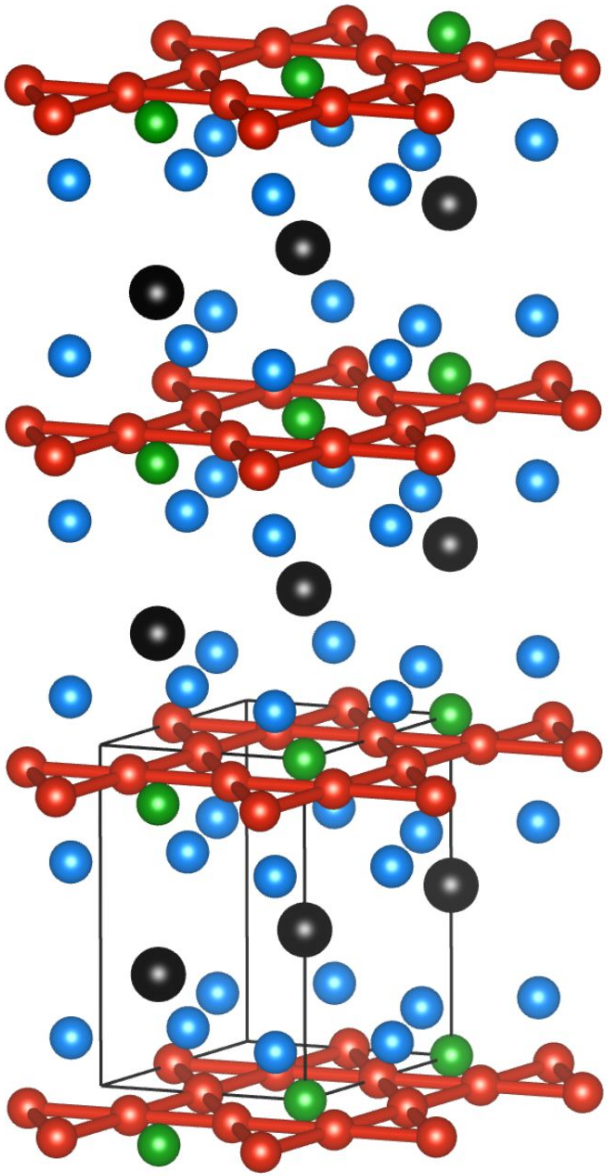
- glasses
- thin films / heterostructures
- ultracold atoms
- quantum dots
- **crystals**

Structural motif

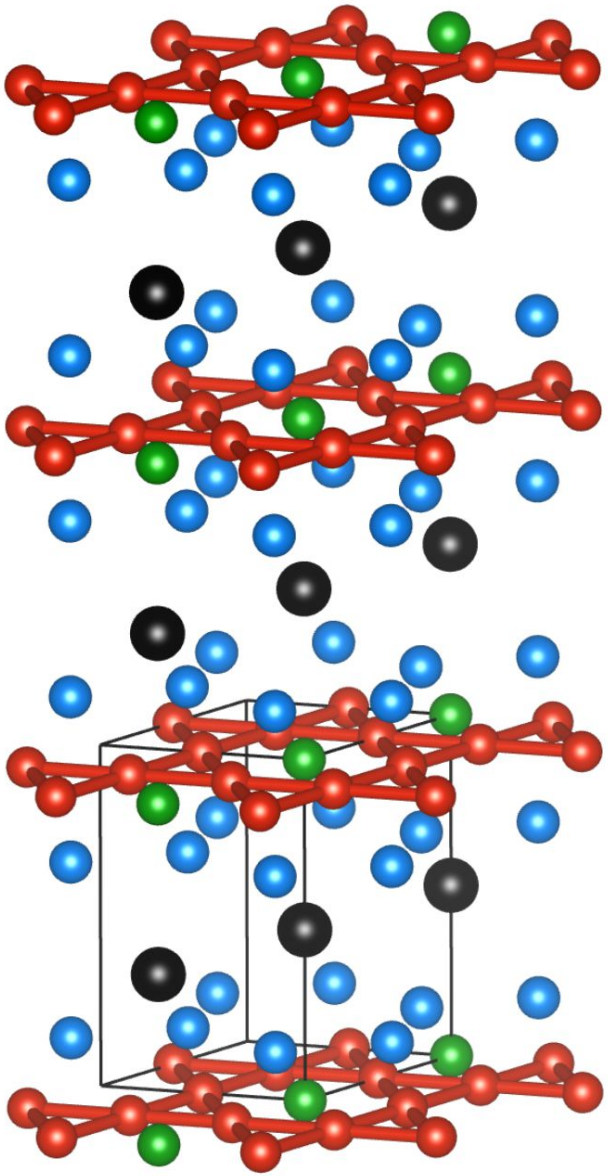


Structural motif





1D solvable,
but limited physics



1D solvable,
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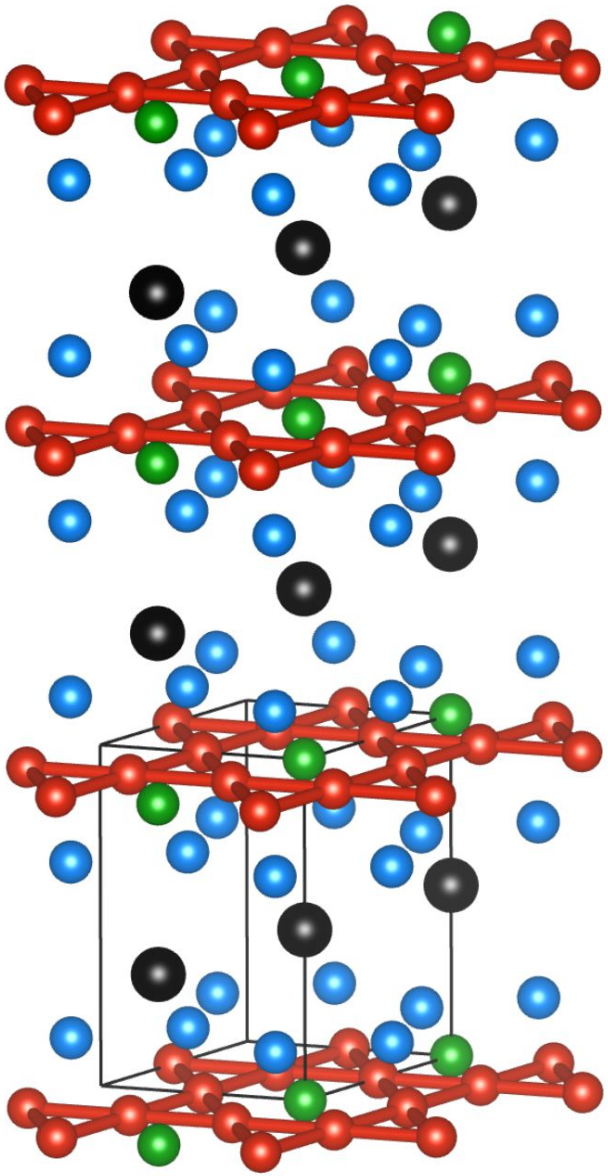
3D typically unsolvable
for quantum models

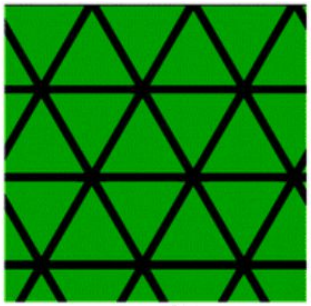


1D solvable,
but limited physics

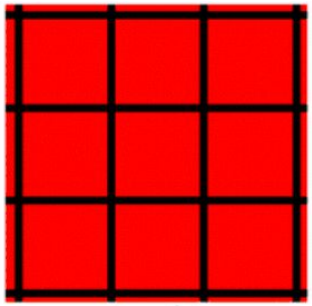
2D *quantum Hall effect,*
high-T_c superconductivity...

3D typically unsolvable
for quantum models

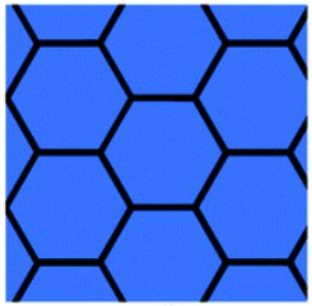
Archimedean lattices



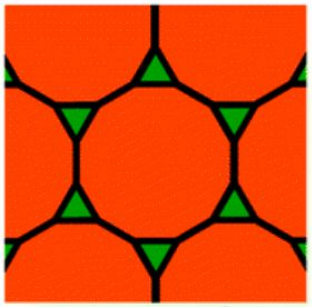
(3^6)



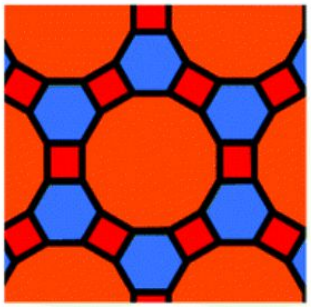
(4^4)



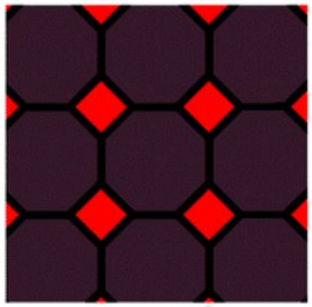
(6^3)



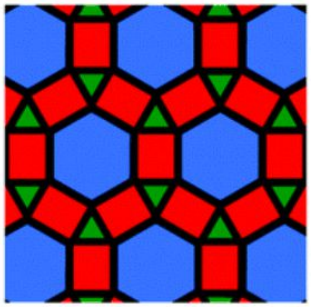
$(3, 12^2)$



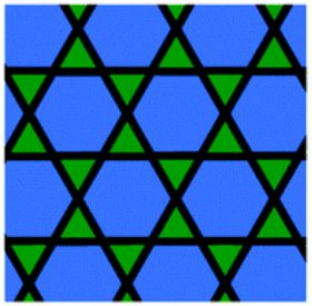
$(4, 6, 12)$



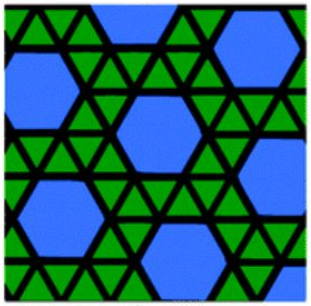
$(4, 8^2)$



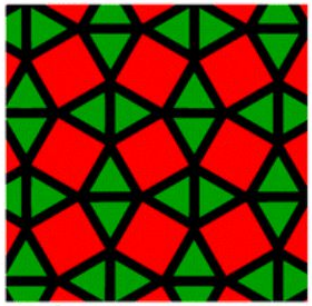
$(3, 4, 6, 4)$



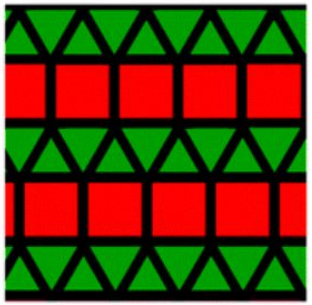
$(3, 6, 3, 6)$



$(3^4, 6)$



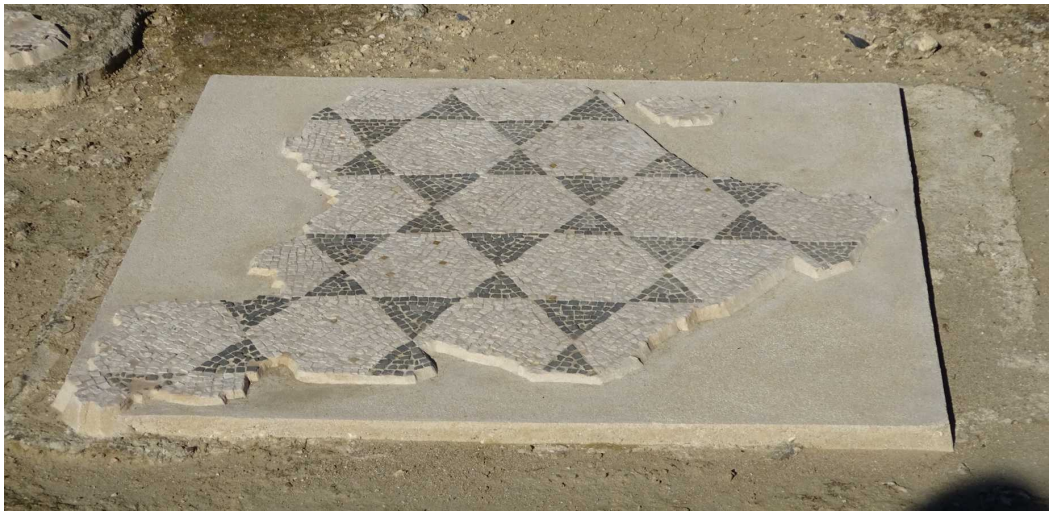
$(3^2, 4, 3, 4)$



$(3^3, 4^2)$

Phys. Chem. Chem. Phys. 21, 22344 (2019)

mosaic at the ruins
of Roman Itálica, Spain



traditional
Japanese basket

mosaic at the ruins
of Roman Itálica, Spain

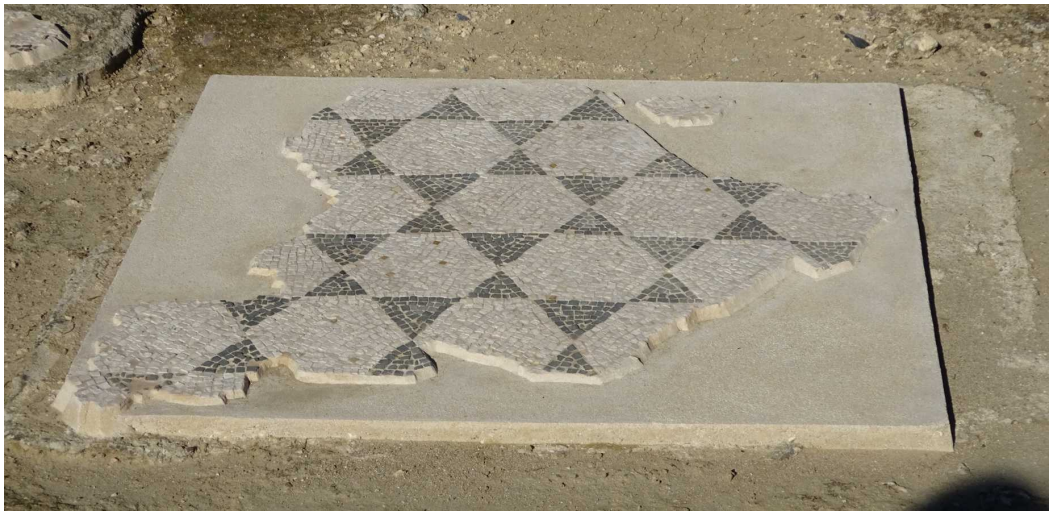
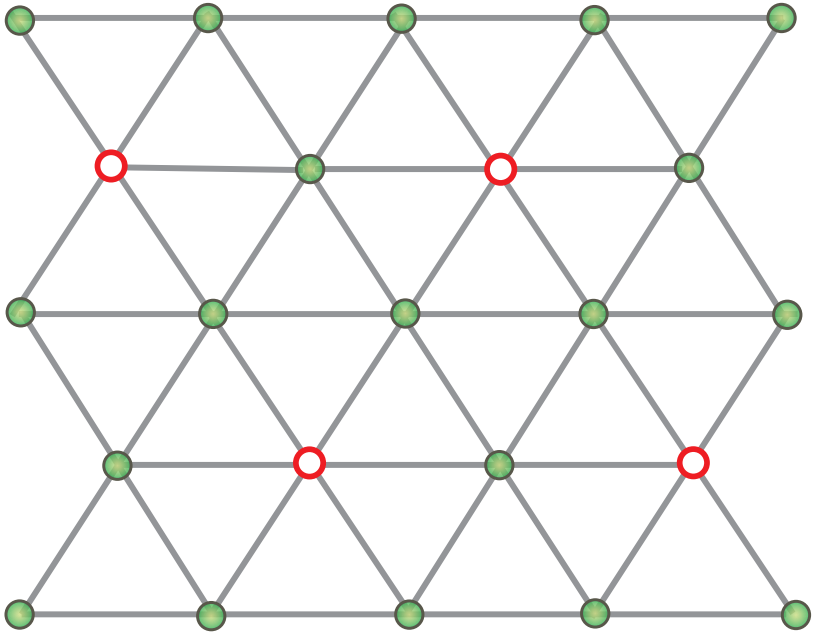
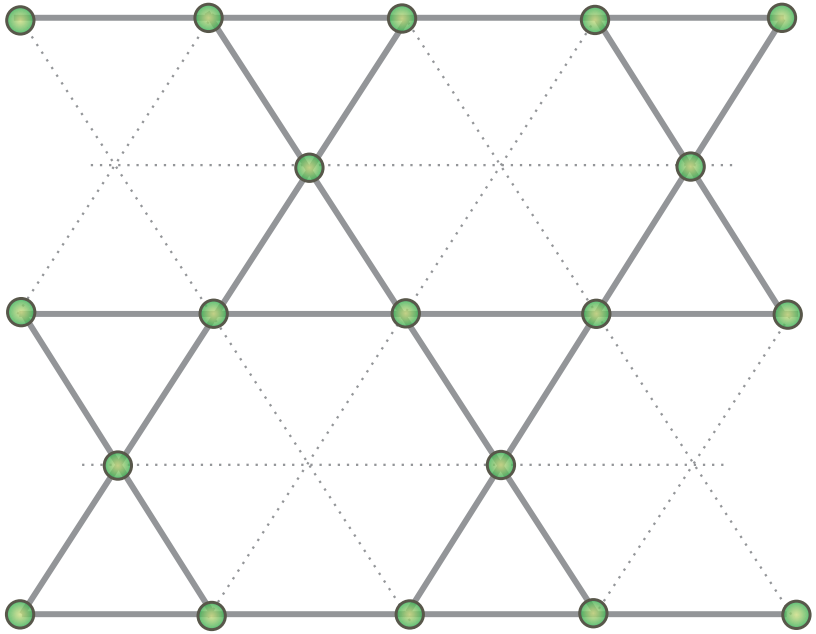


Image credit (basket): Zhu Xiangde

Image source: Wikimedia Commons



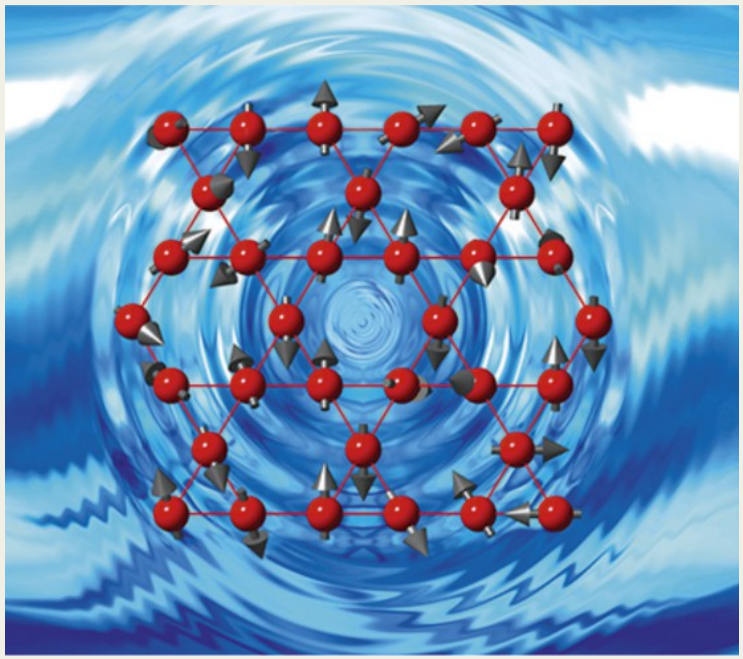


kago – basket

me – eye

Image credit: Robert Izumi (CC-BY-NC)

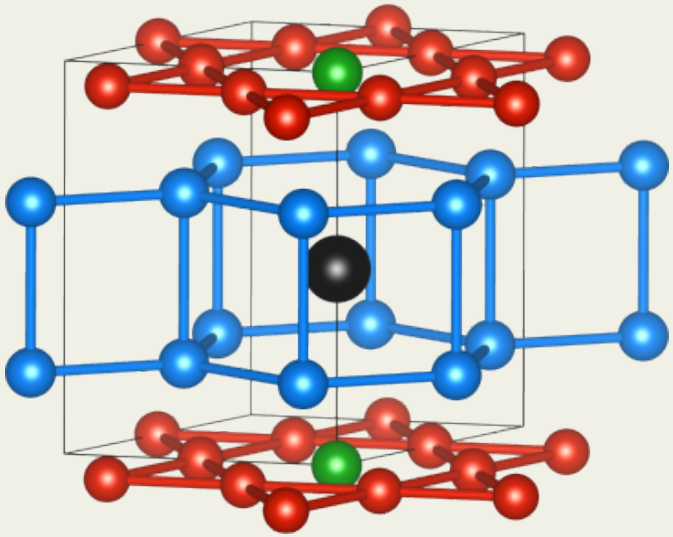
Outline



Magnetic insulators

kagome spin lattice

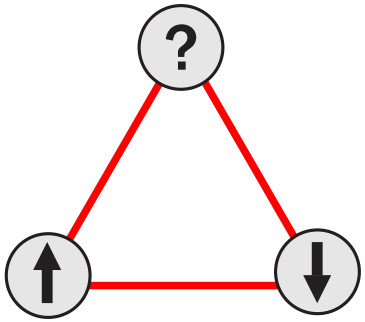
quantum spin liquid

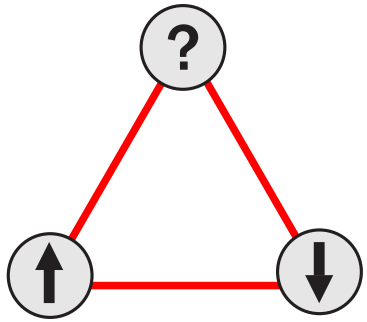


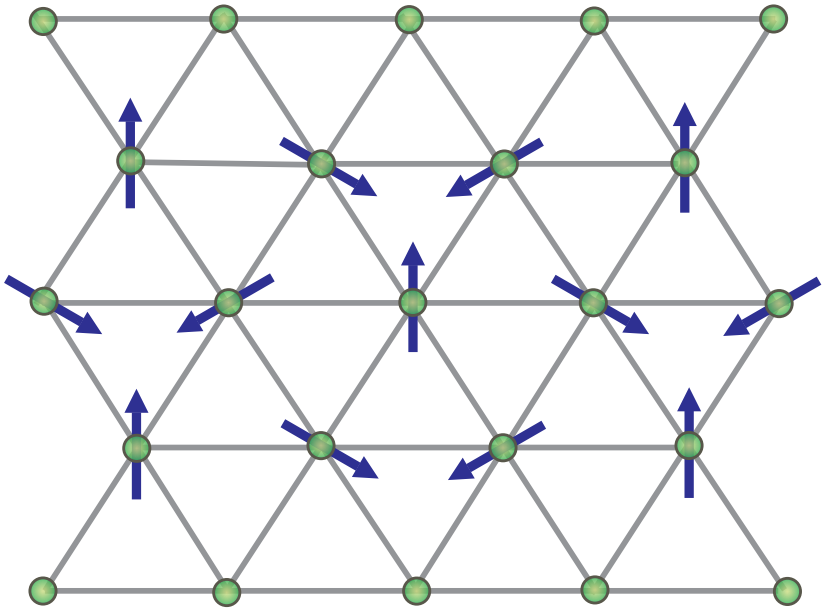
Kagome metals

band topology and nesting

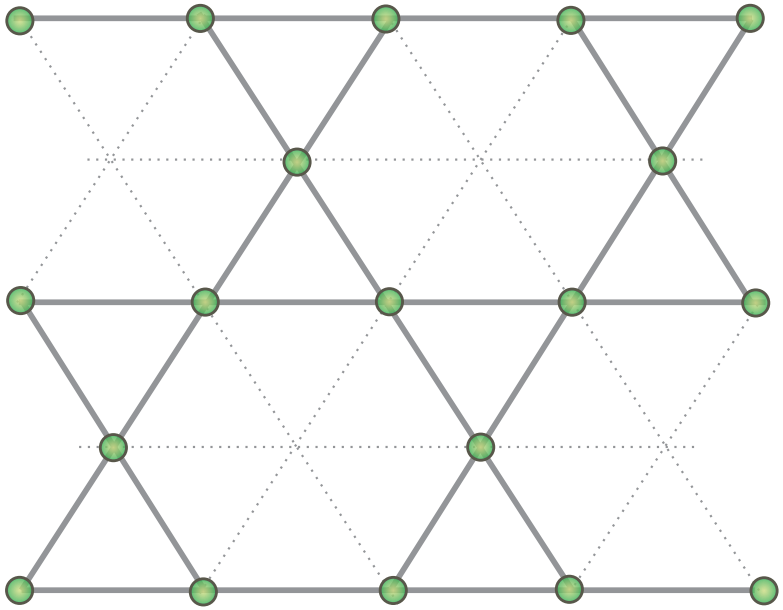
superconductivity







Triangular: 120° order



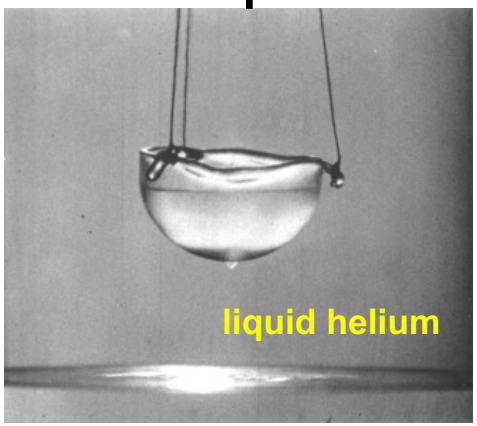
Kagome: no magnetic order

Ordinary liquid

$T < T_{cryst}$

Quantum liquid

$T \rightarrow 0$



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Quantum liquid

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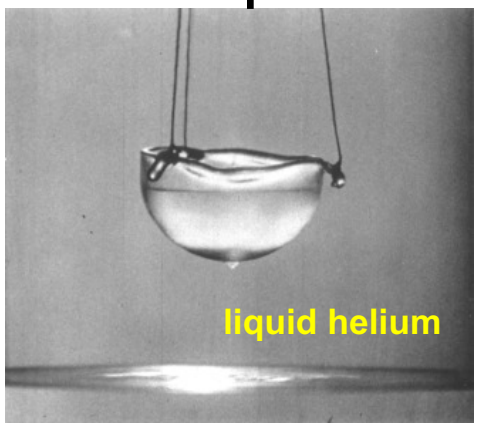
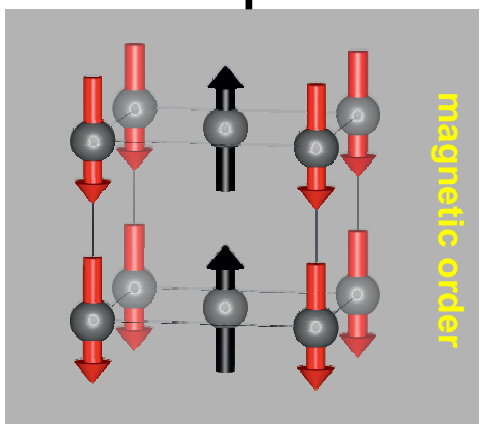


superfluidity

Ordinary magnet

$T < T_N$



Quantum magnet

$T \to 0$

?

entanglement, superconductivity, quantum computing

First attempt: jarosite

Jarosite

$KFe_3(OH)_6(SO_4)_2$

Image credits: Christian Rewitzer (CC-BY-SA)

First attempt: jarosite

Jarosite

$KFe_3(OH)_6(SO_4)_2$

also found on Mars

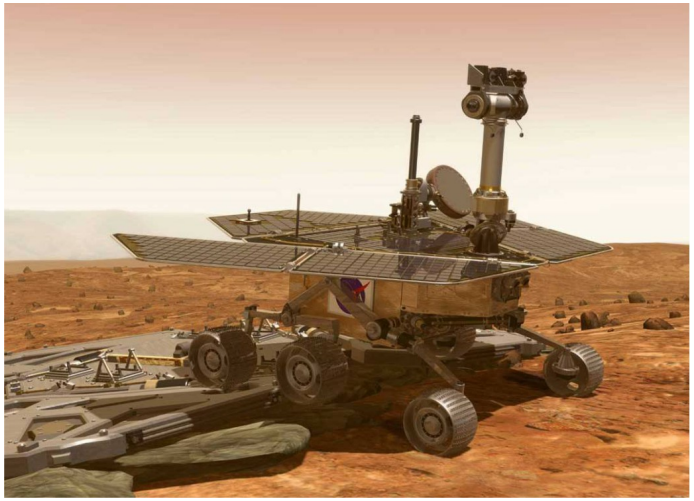


Image credits: Christian Rewitzer (CC-BY-SA) and NASA (public domain)

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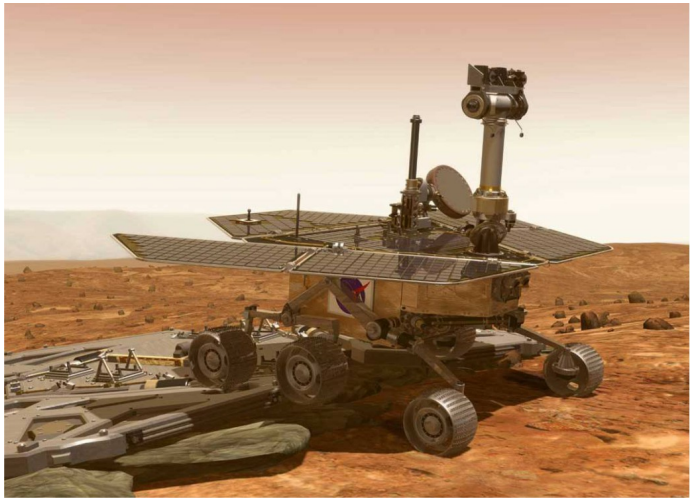
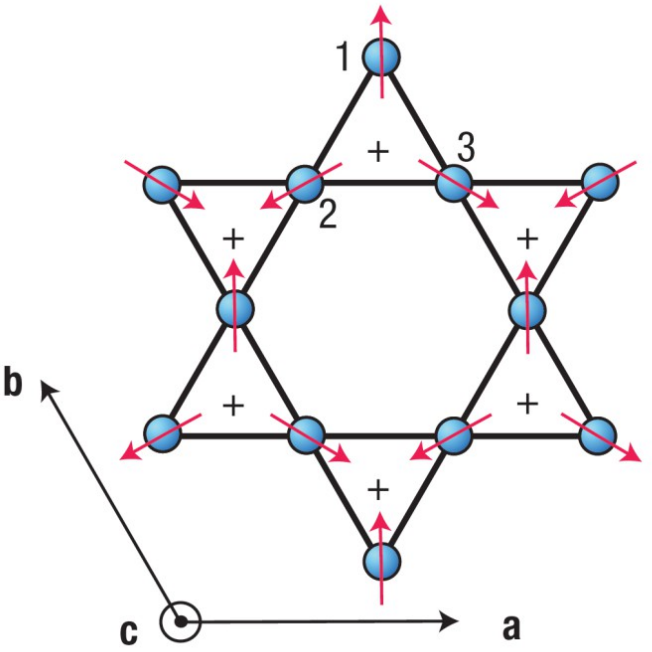




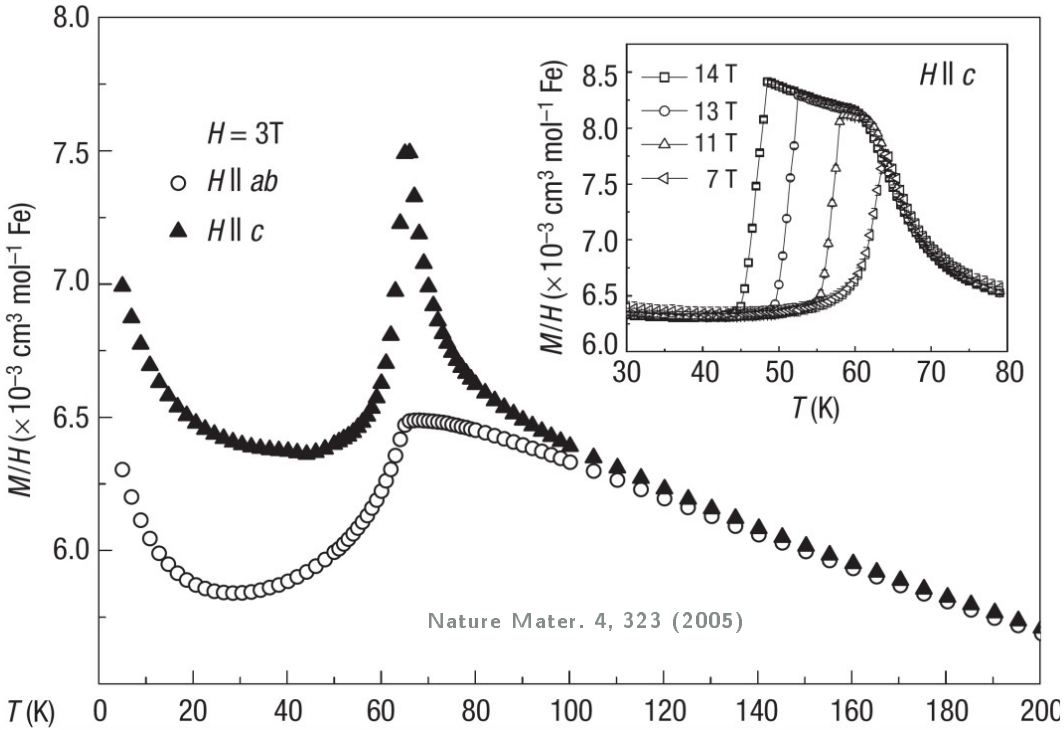
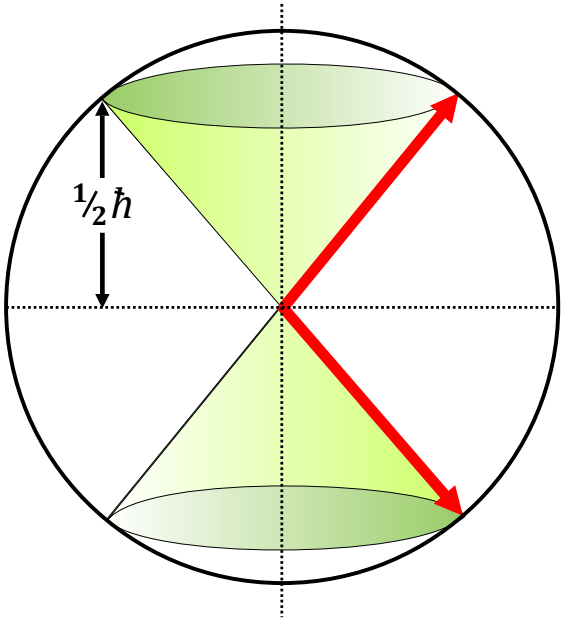
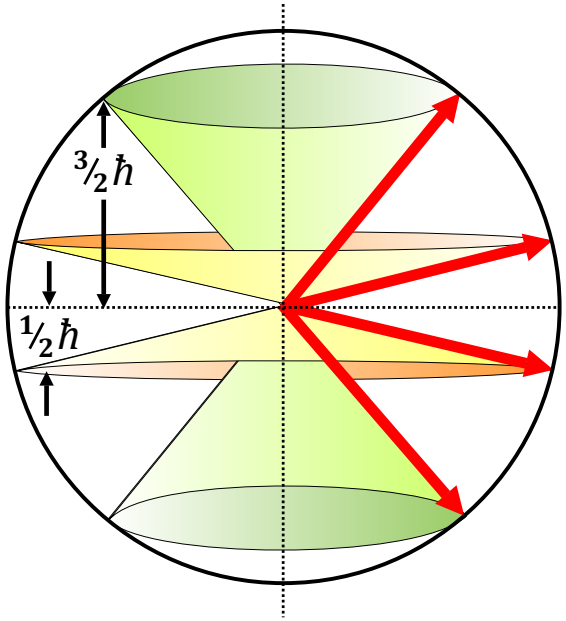


Image credits: Christian Rewitzer (CC-BY-SA) and NASA (public domain)



S = 1/2



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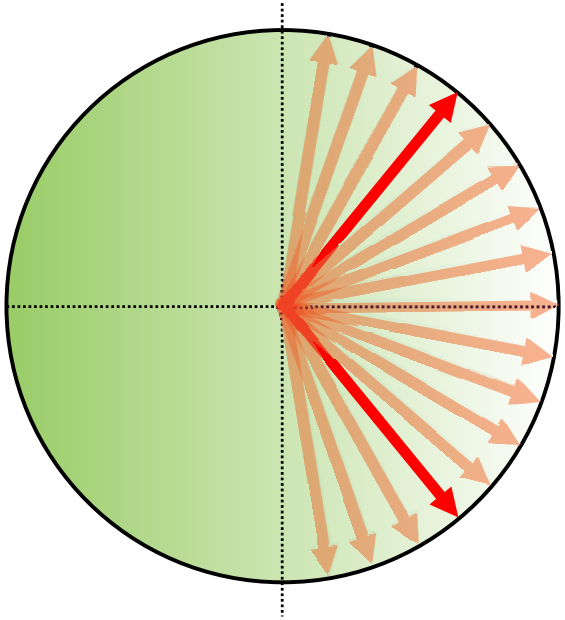
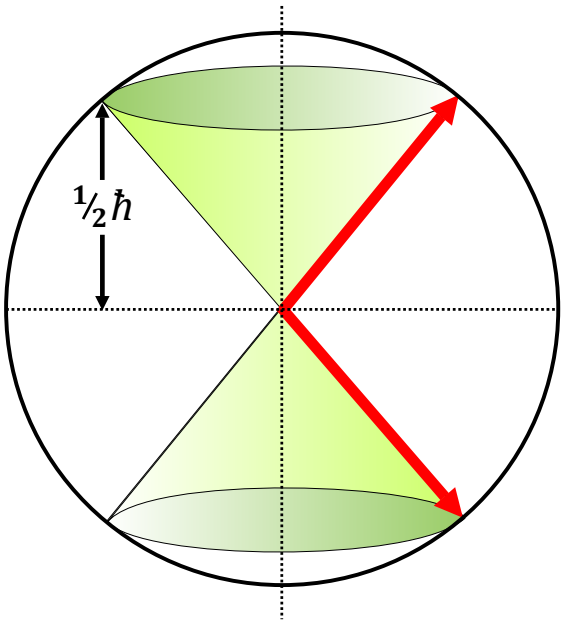


S = ∞



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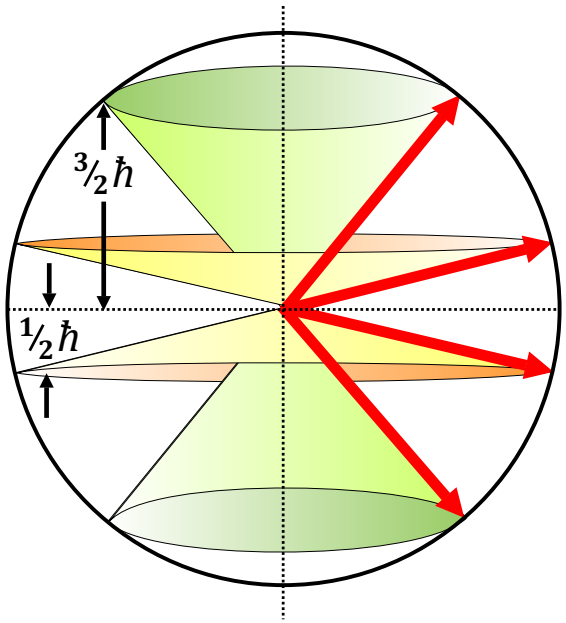
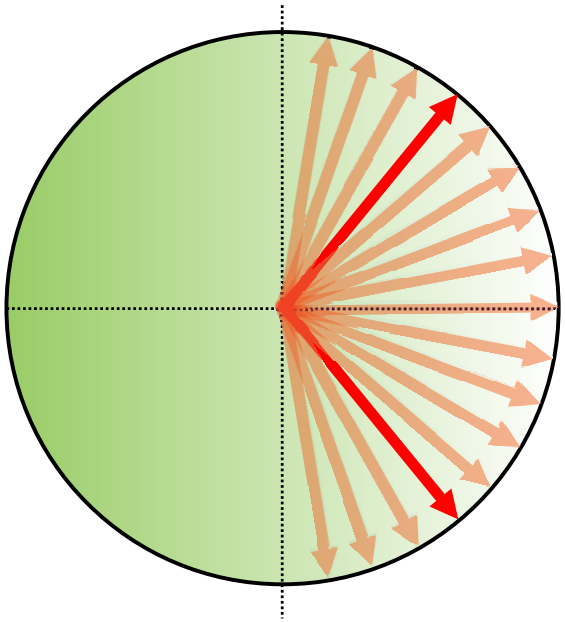


S = 3/2



S = ∞

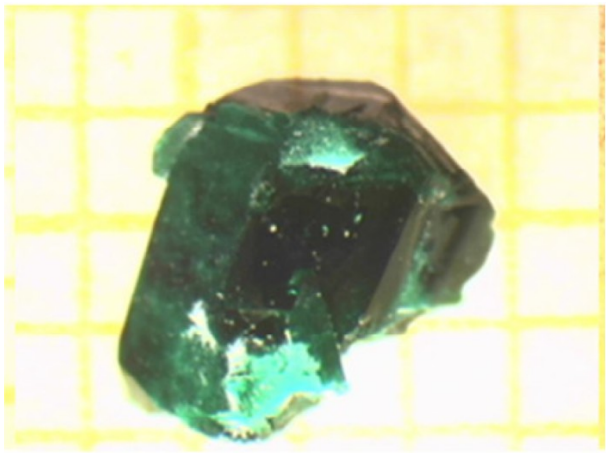
Fe^{3+} ($3d^5$): spin-$\frac{5}{2}$, (almost) classical behavior

Cu^{2+} ($3d^9$): spin-$\frac{1}{2}$, quantum

21	22	23	24	25	26	27	28	29	30
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn

First success: herbertsmithite

natural sample



synthetic sample

Herbertsmithite

$ZnCu_3(OH)_6Cl_2$

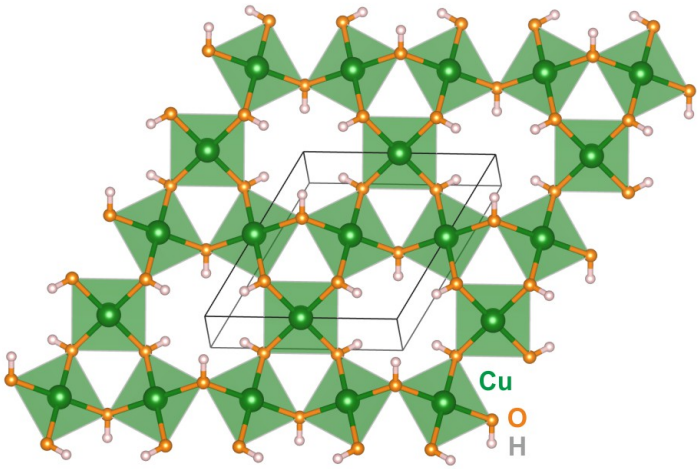
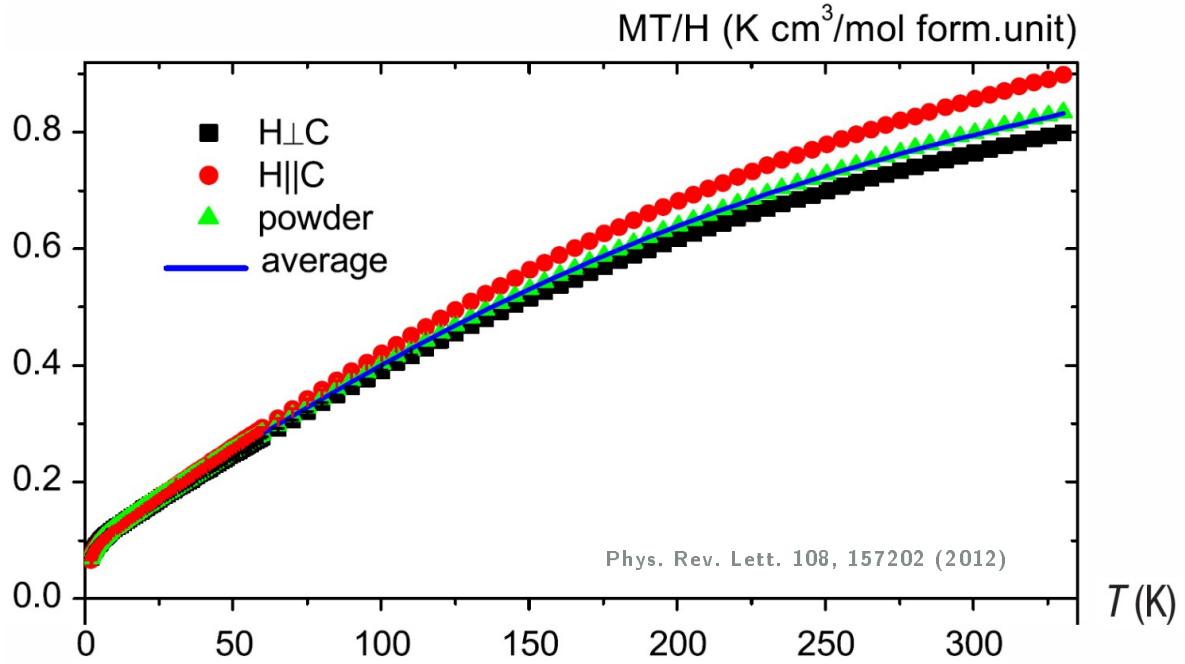


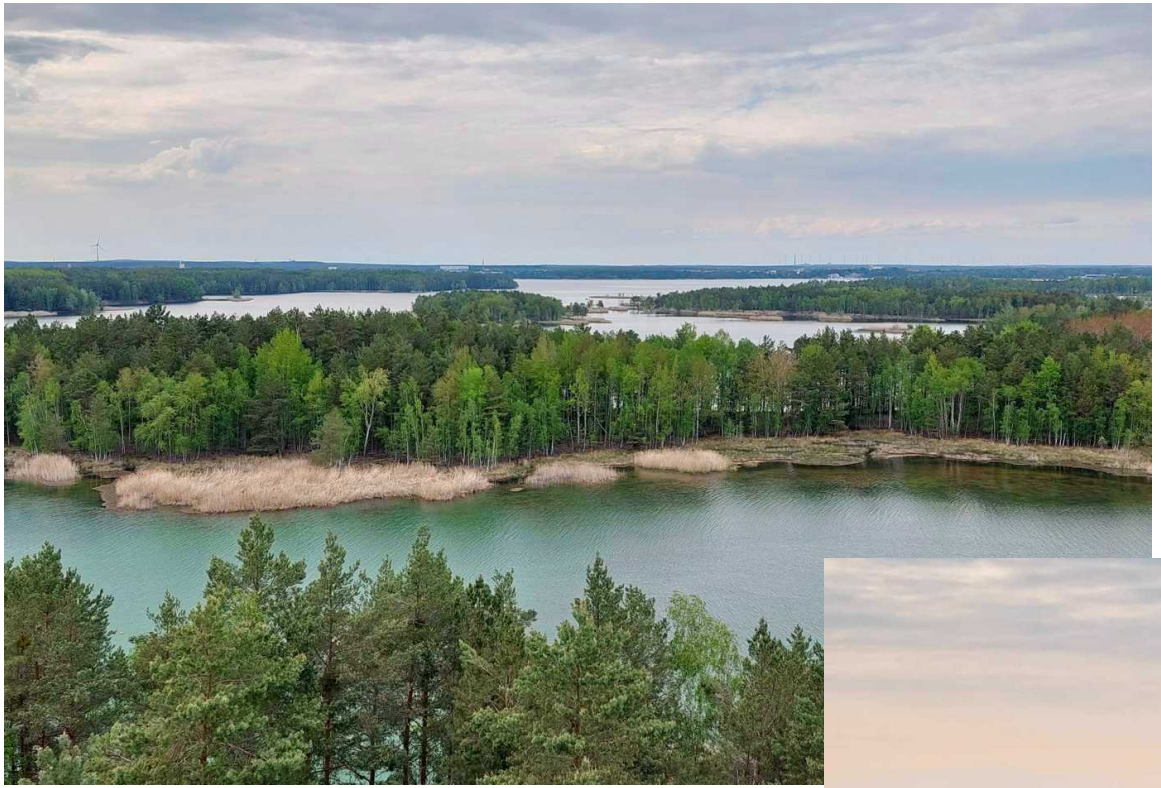
Image credits: Robert M. Lavinsky (CC-BY-SA) and J. Cryst. Growth 531, 125372 (2020)



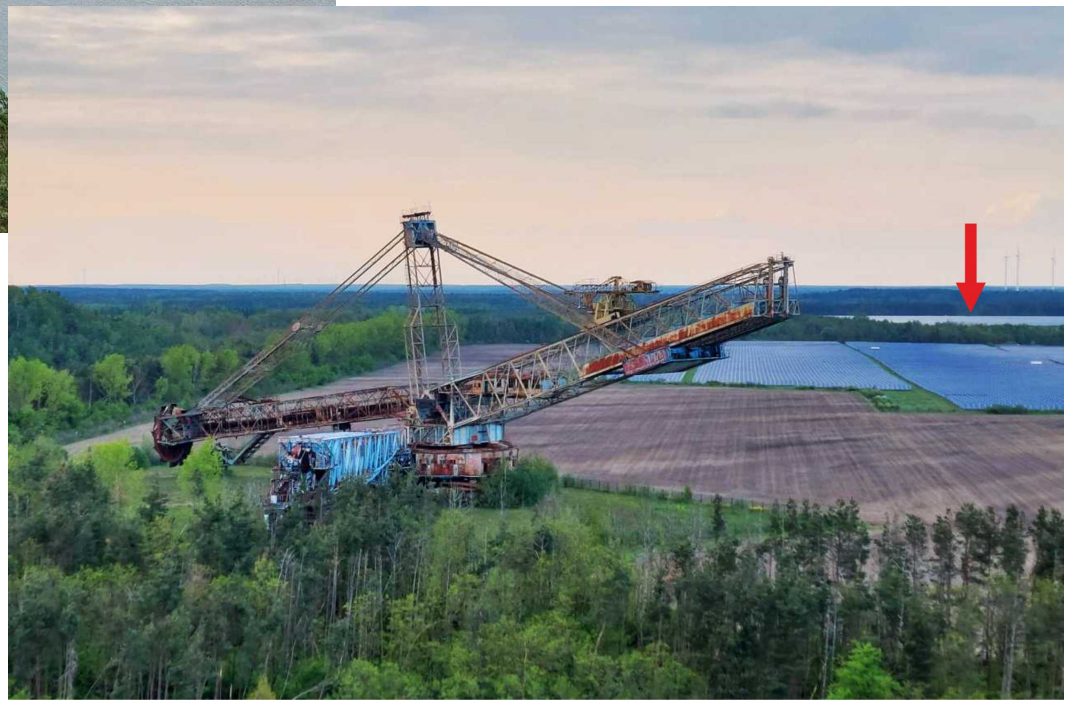
How do we know it is liquid?

Lausitzer Seenland
near Senftenberg

How do we know it is liquid?

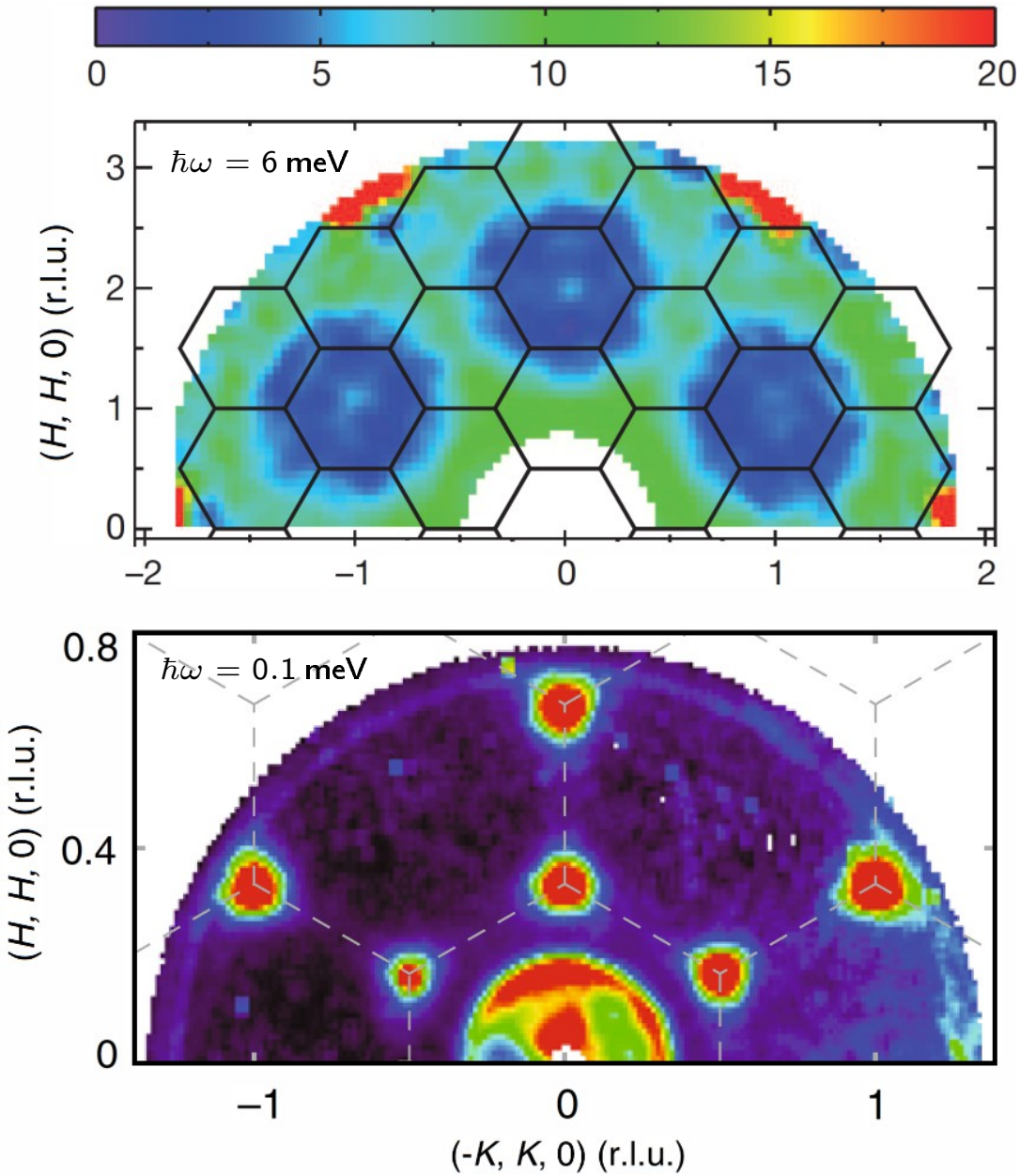


Lausitzer Seenland
near Senftenberg



lake or solar panels?

Dynamics of quantum spin liquid



inelastic neutron scattering

Herbertsmithite

spin liquid

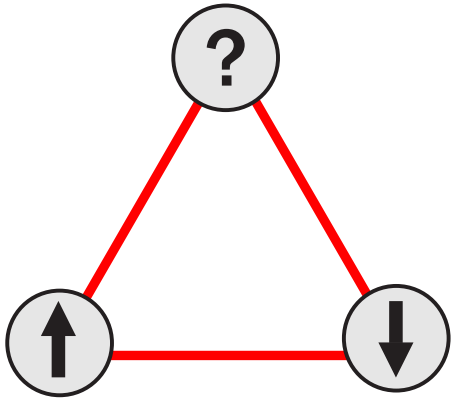
Nature 492, 406 (2012)

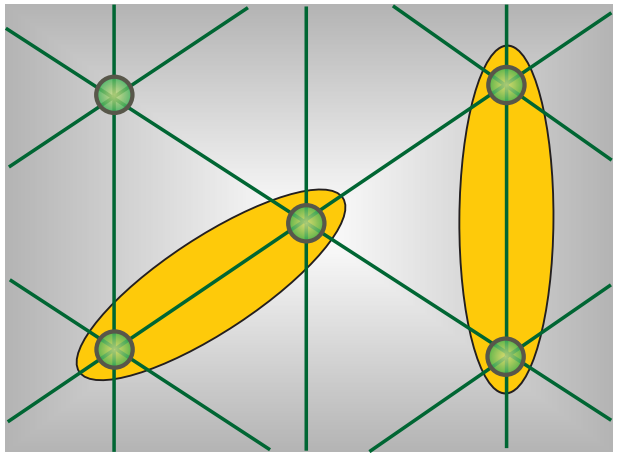
$TmMgGaO_4$

magnetic order

"spin solid"

Nature Comm. 10, 4530 (2019)

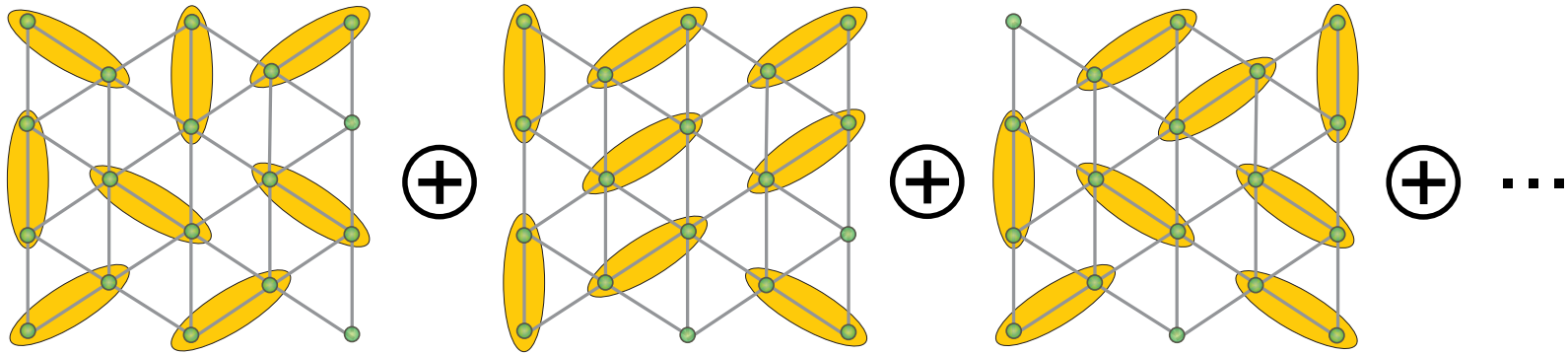




$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

"valence bond"

Excitations of a spin liquid: fractionalization

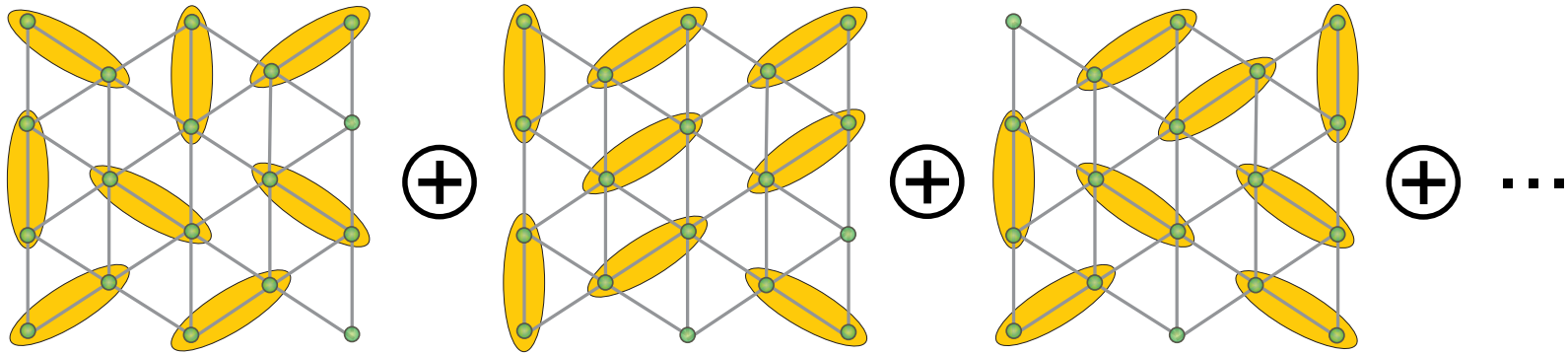
$|\mathrm{RVB}\rangle =$  $\oplus \cdots$

RVB = resonating valence bond

Pauling (1933): benzene molecule

Anderson (1973): triangular magnet

Excitations of a spin liquid: fractionalization

$|\mathrm{RVB}\rangle =$  $\oplus \cdots$

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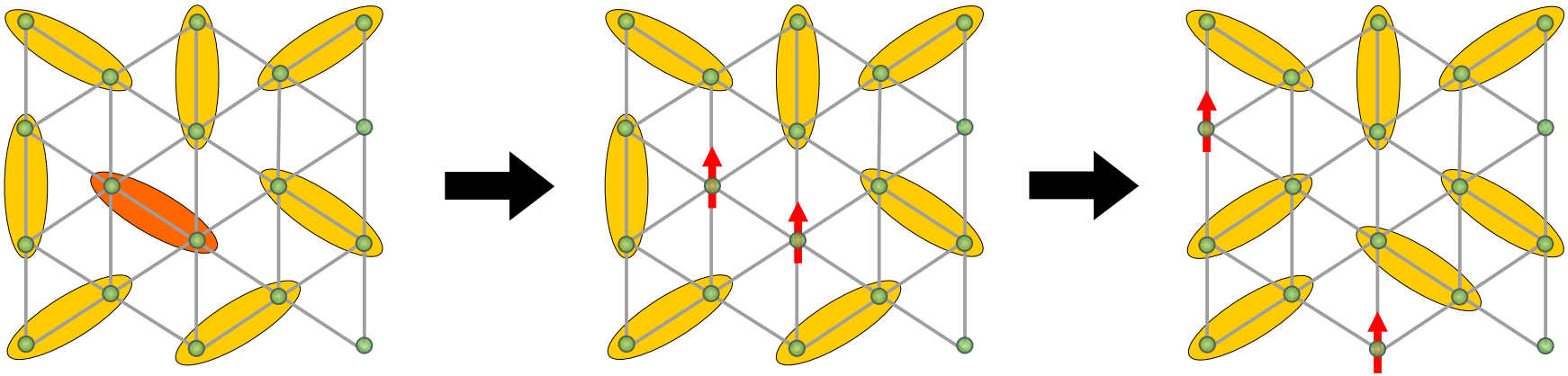
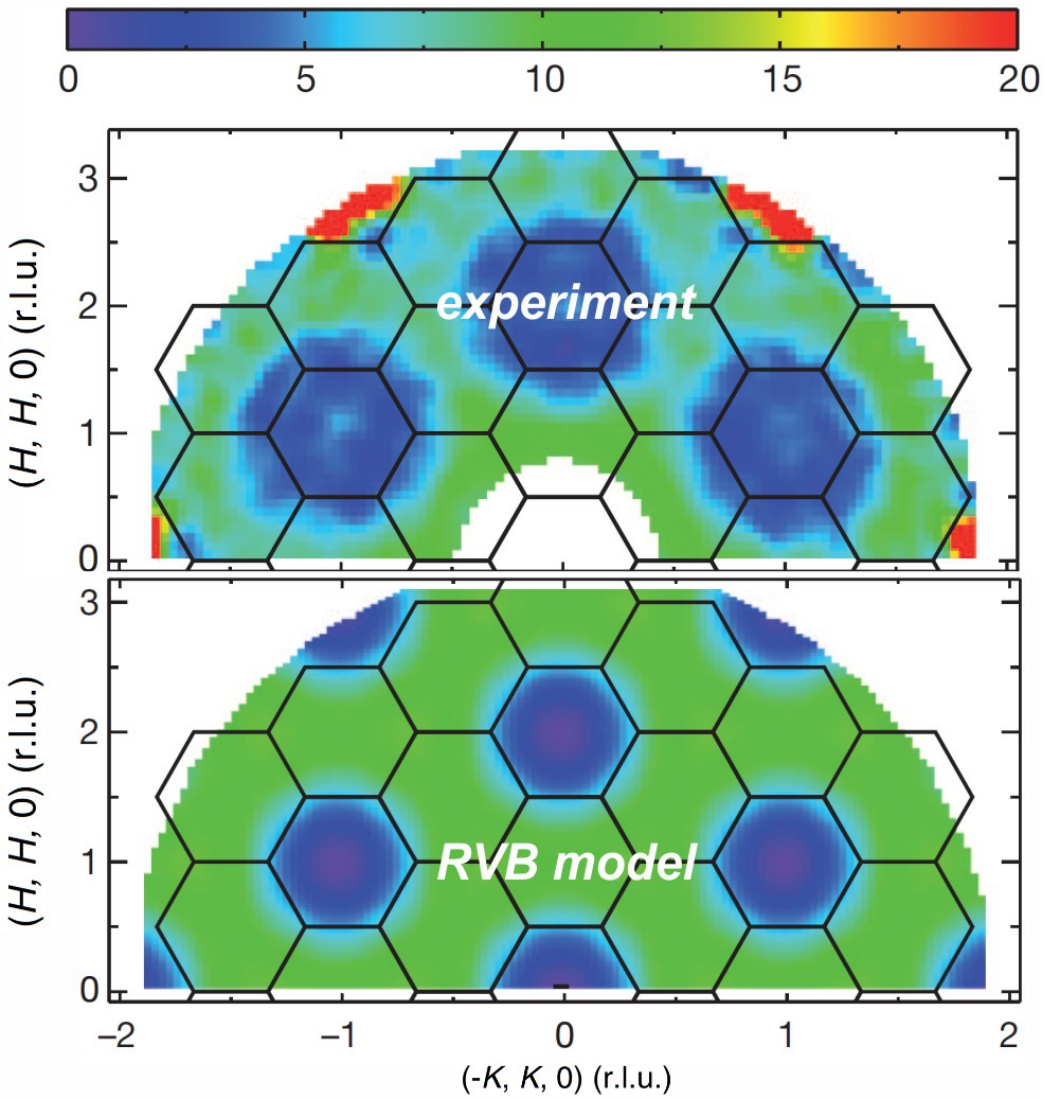
Pauling (1933): benzene molecule

Anderson (1973): triangular magnet



Two spins propagate independently, the $S = 1$ excitation breaks into two spinons

Kagome (herbertsmithite)



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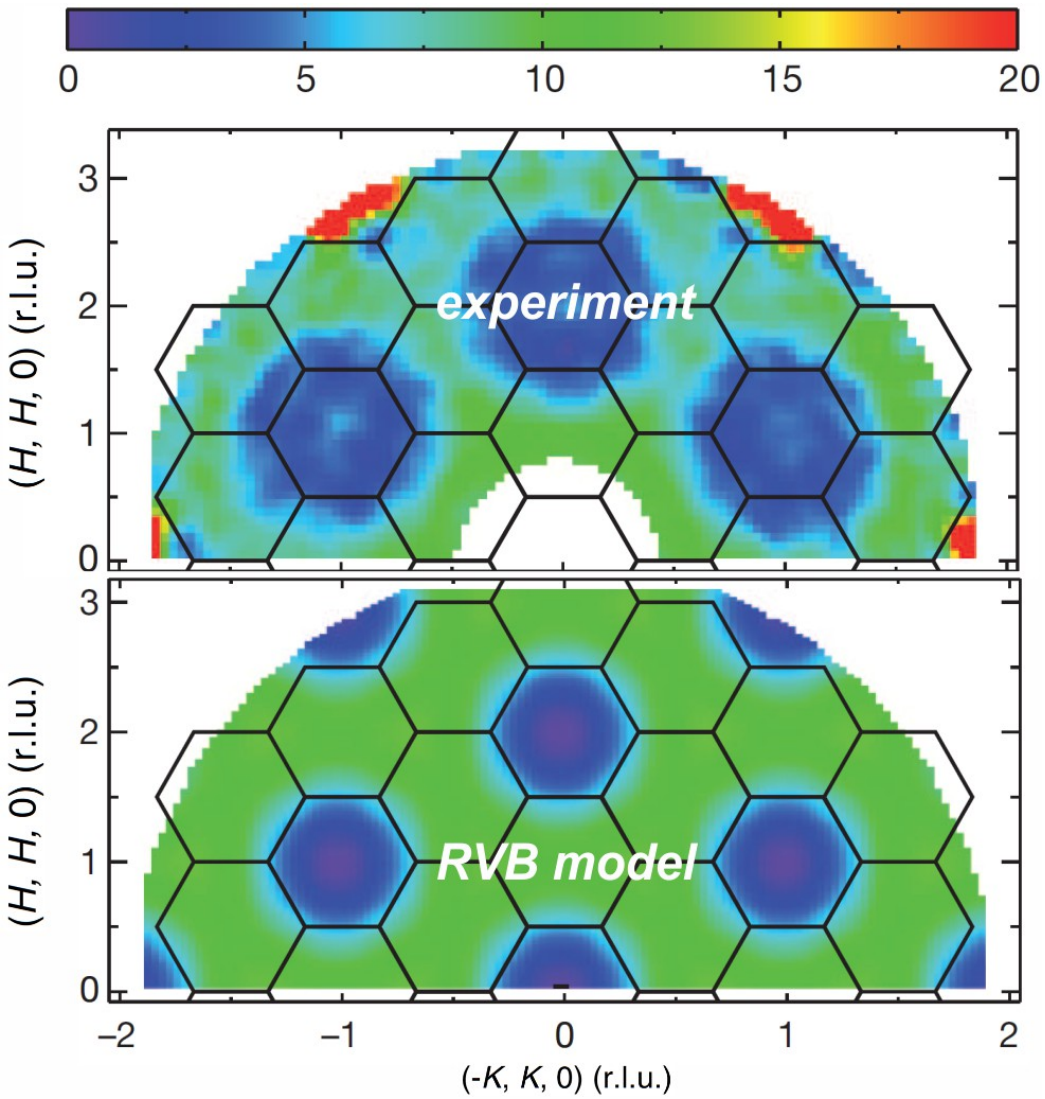
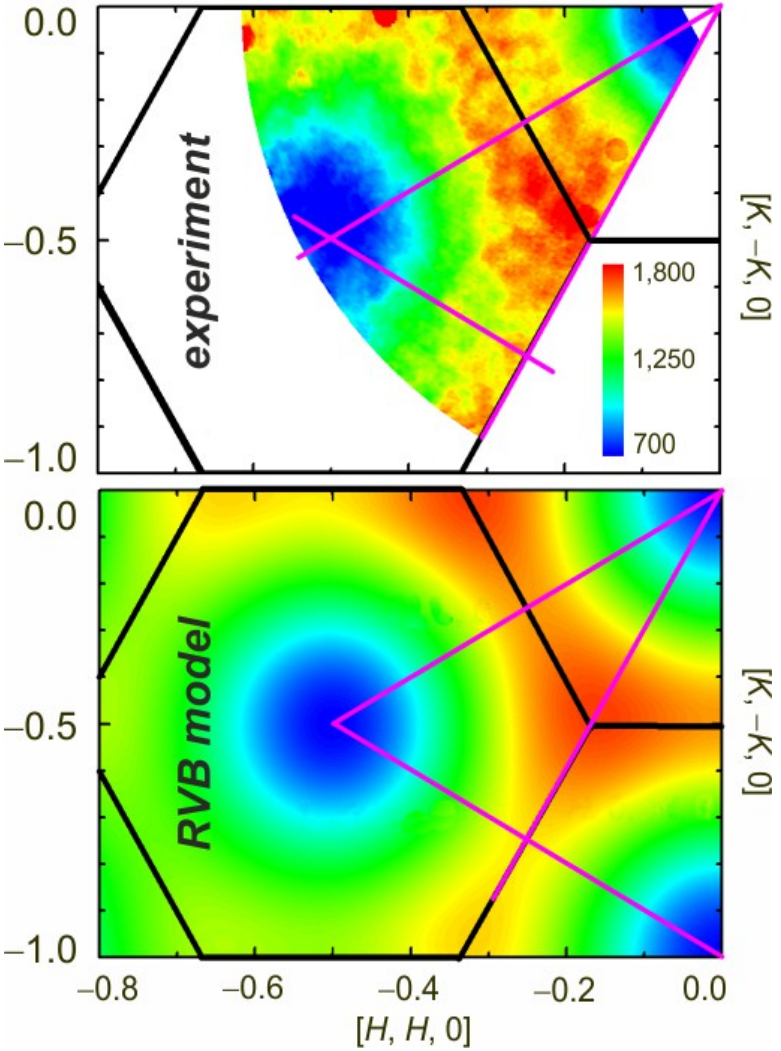
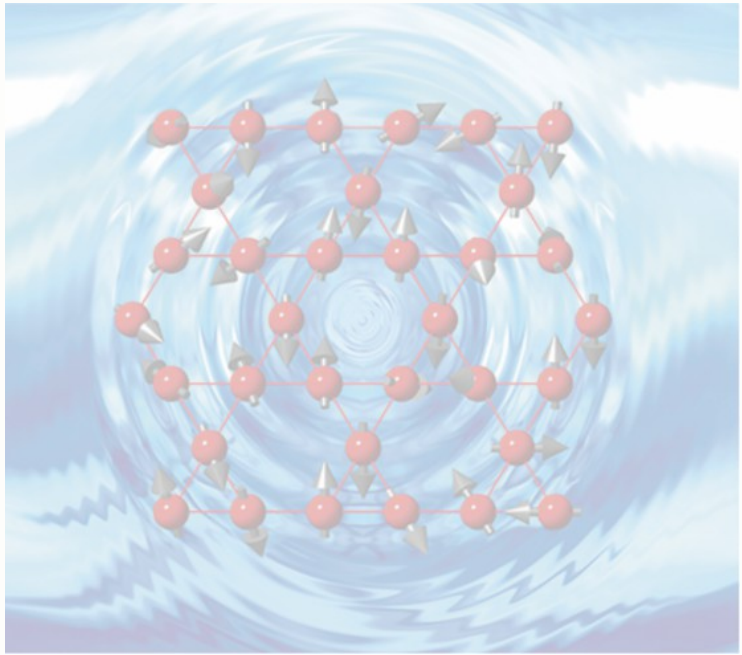


Triangular ($YbMgGaO_4$)

Y. Li, AT *et al.* Nature Comm. (2017)



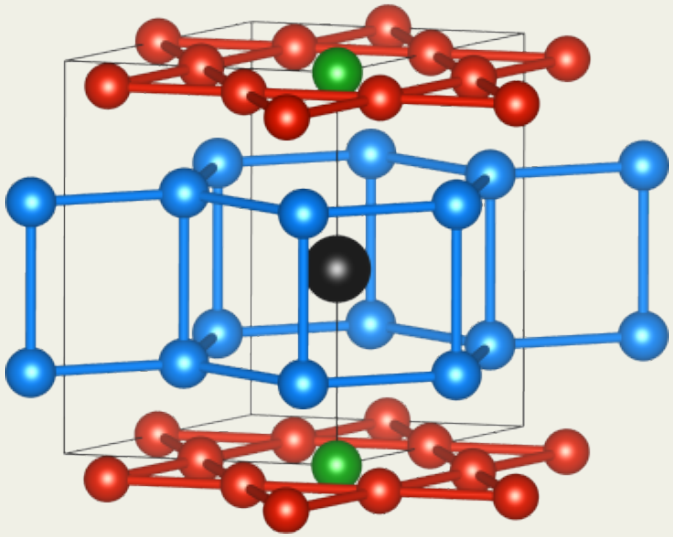
Outline



Magnetic insulators

kagome spin lattice

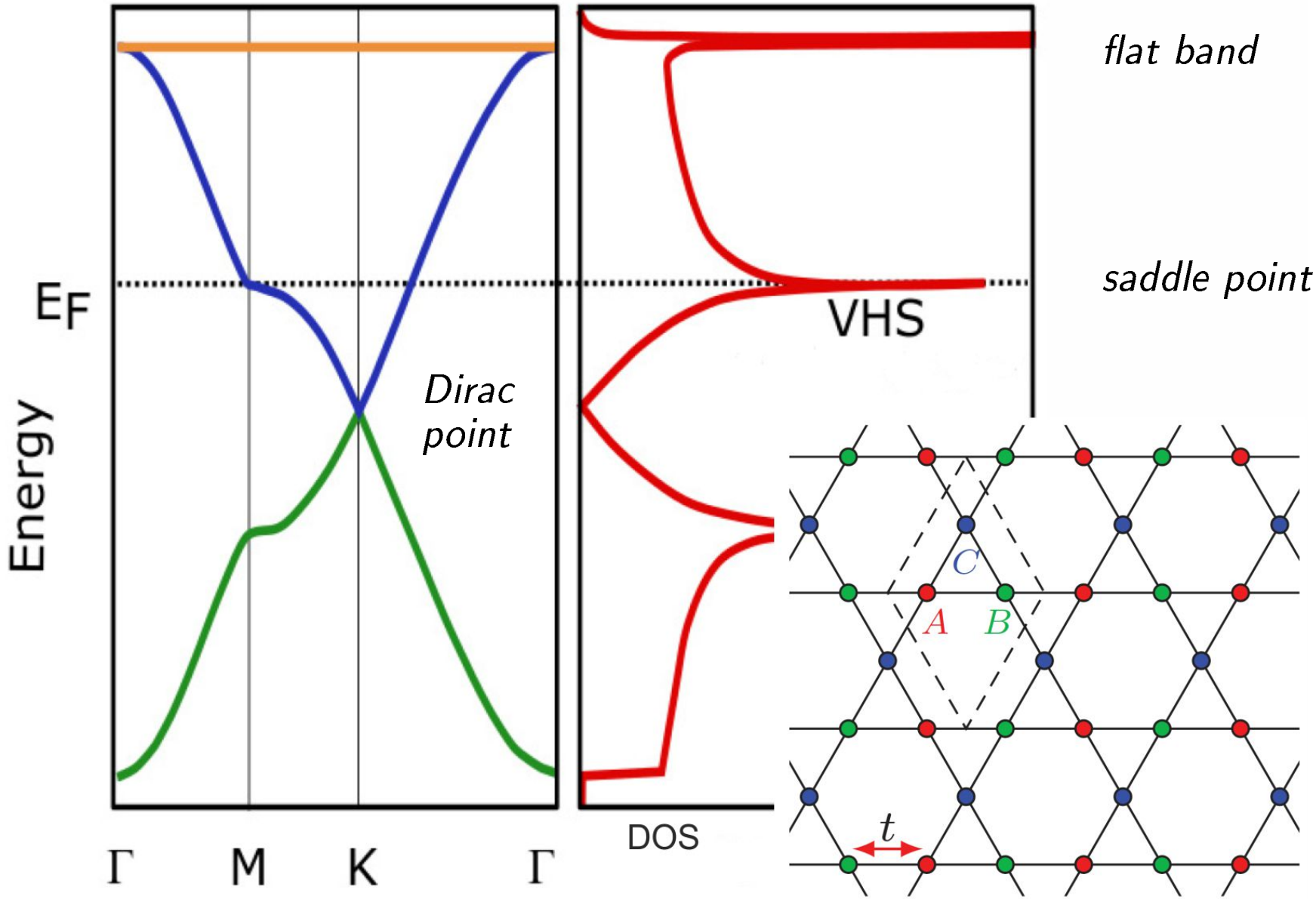
quantum spin liquid



Kagome metals

band topology and nesting

superconductivity


flat band
saddle point
VHS
E_F
Energy
Dirac point
DOS
Γ
M
K
Γ
C
A
B
t

Received 11 Mar 2014 | Accepted 30 May 2014 | Published 1 Jul 2014

DOI: 10.1038/ncomms5261 2014

Theoretical prediction of a strongly correlated Dirac metal

I.I. Mazin[1], Harald O. Jeschke[2], Frank Lechermann[3], Hunpyo Lee[2], Mario Fink[4], Ronny Thomale[4] & Roser Valentí[2]

$ZnCu_3(OH)_6Cl_2$
Mott insulator

replacing Zn^{2+} by Ga^{3+}
should lead to a metal

Nature Comm. 5, 4261 (2014)

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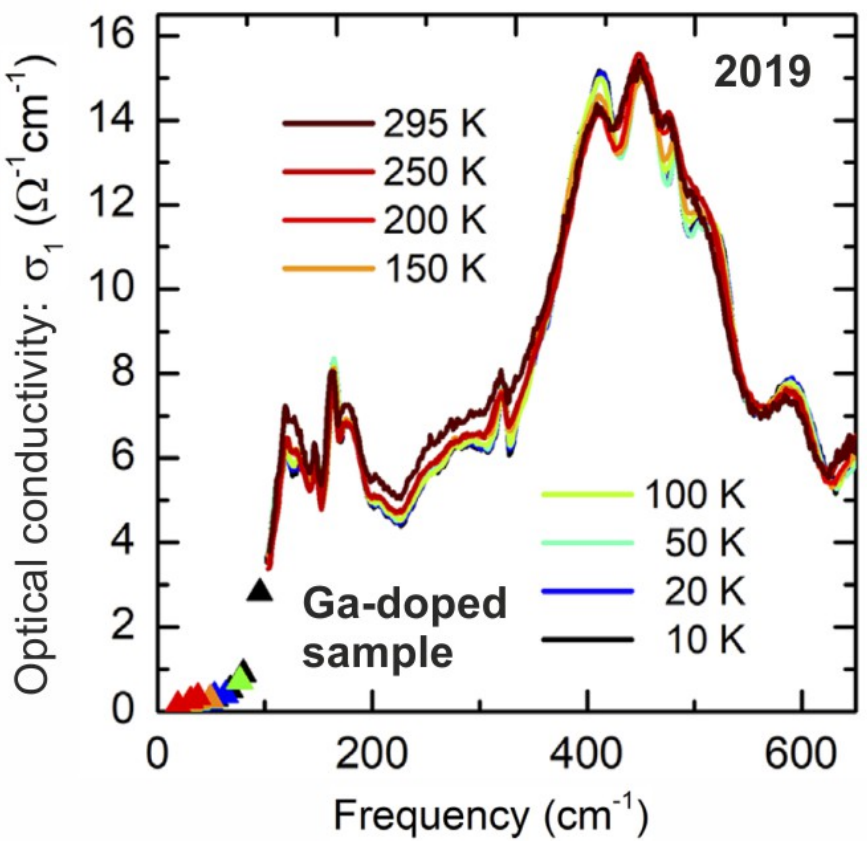
$ZnCu_3(OH)_6Cl_2$
Mott insulator

replacing Zn^{2+} by Ga^{3+}
should lead to a metal

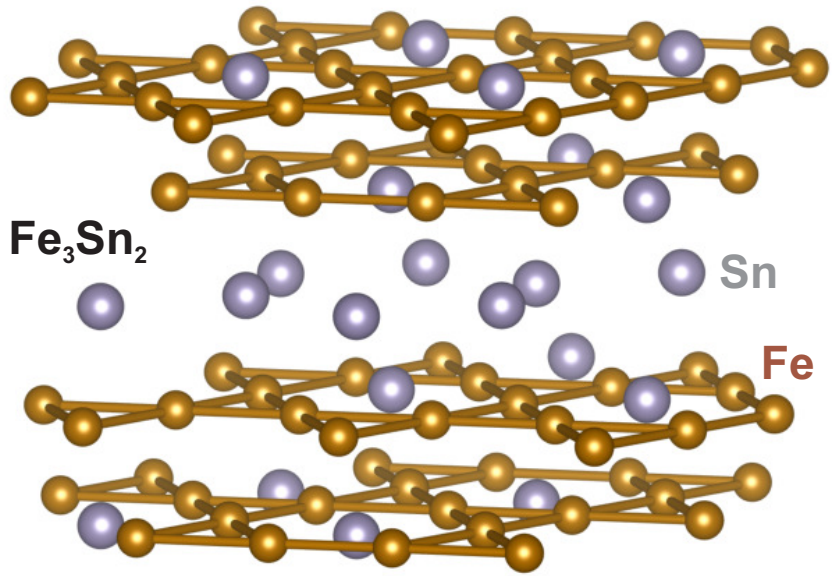
Experiment:
insulating behavior persists

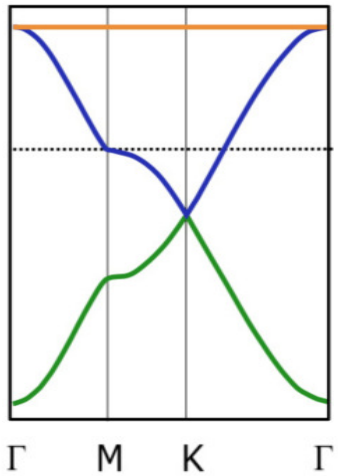


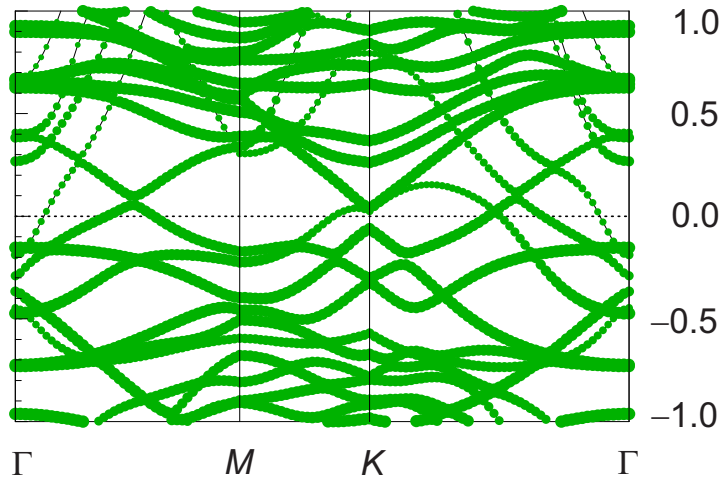
Nature Comm. 5, 4261 (2014), phys. stat. solidi (b) 256, 1800663 (2019)

Finding the right material

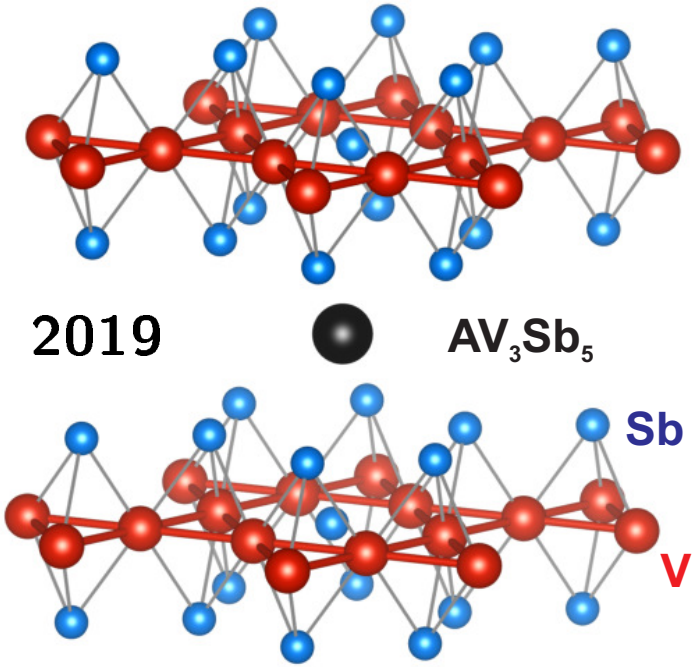
1970's

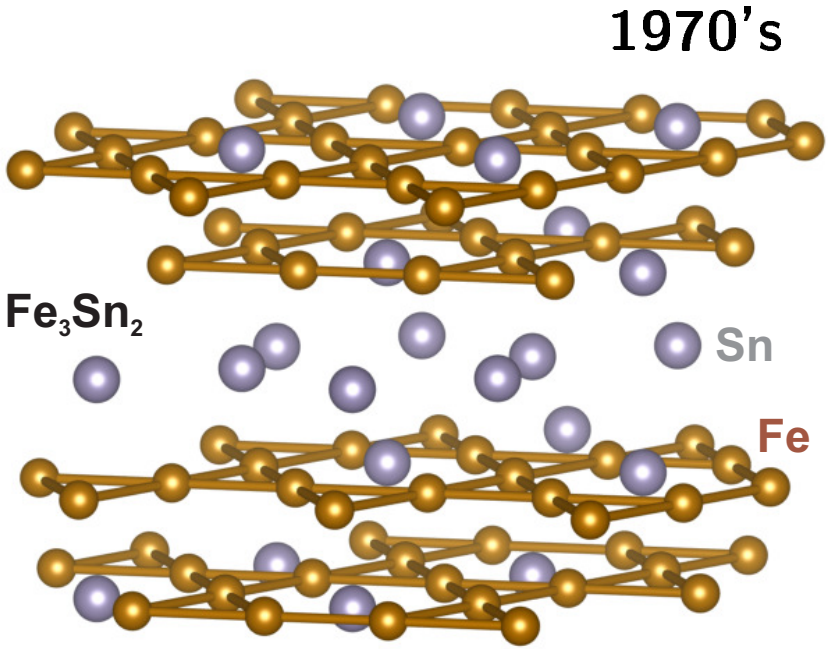


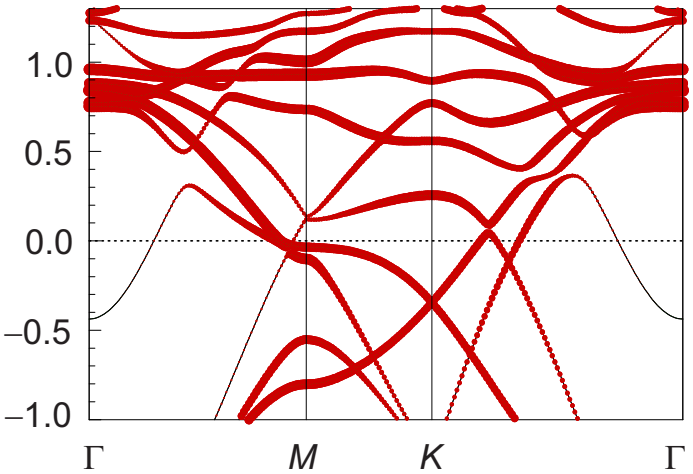


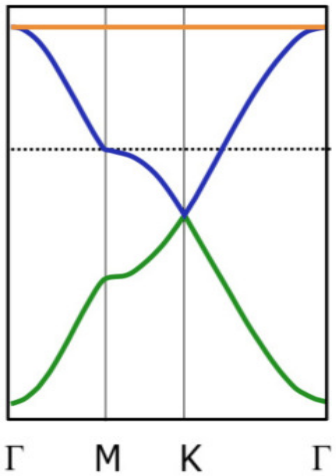


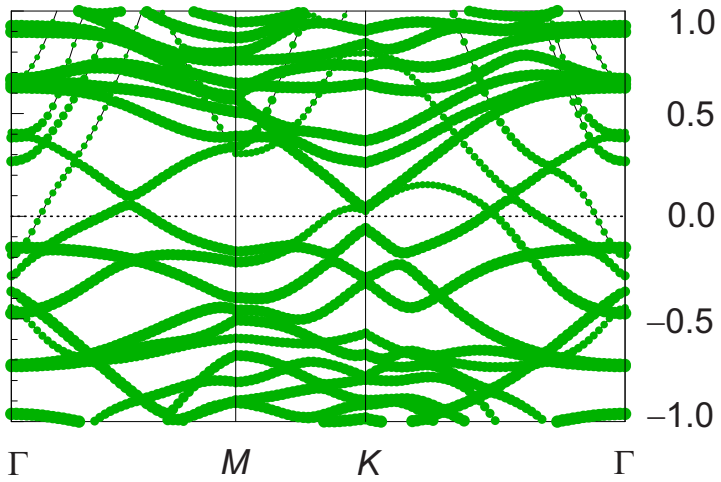
Finding the right material





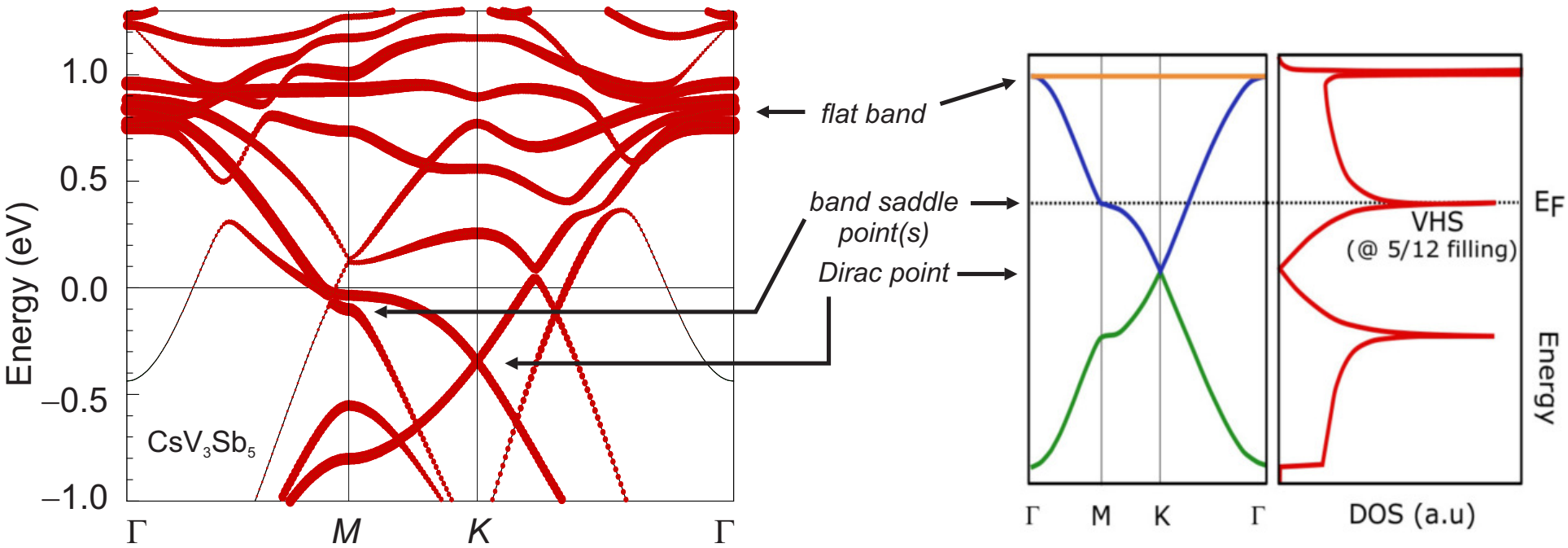






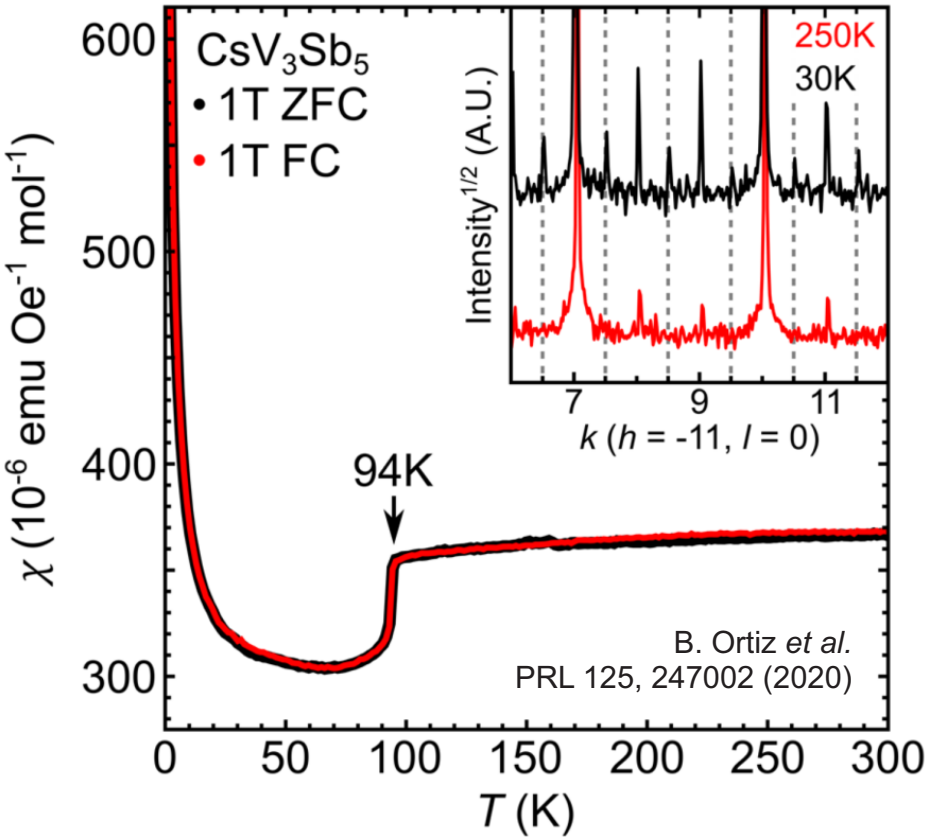
Finding the right material: AV_3Sb_5

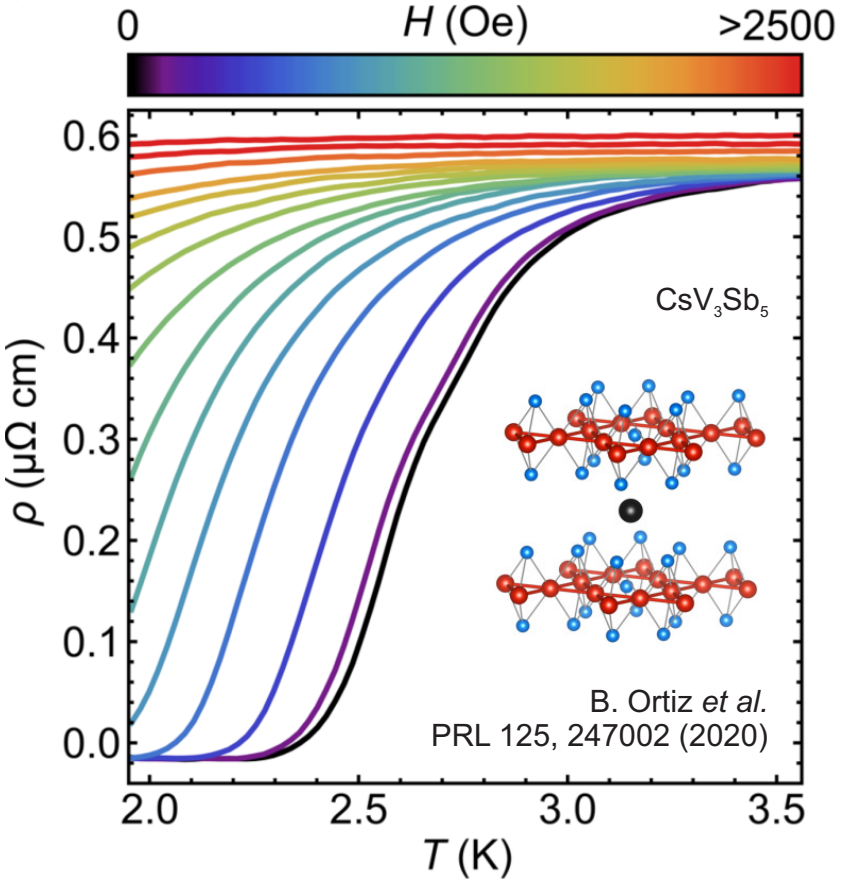
AV_3Sb_5: A = K, Rb, Cs



Band saddle points in the vicinity of the Fermi level

AV_3Sb_5: Main features





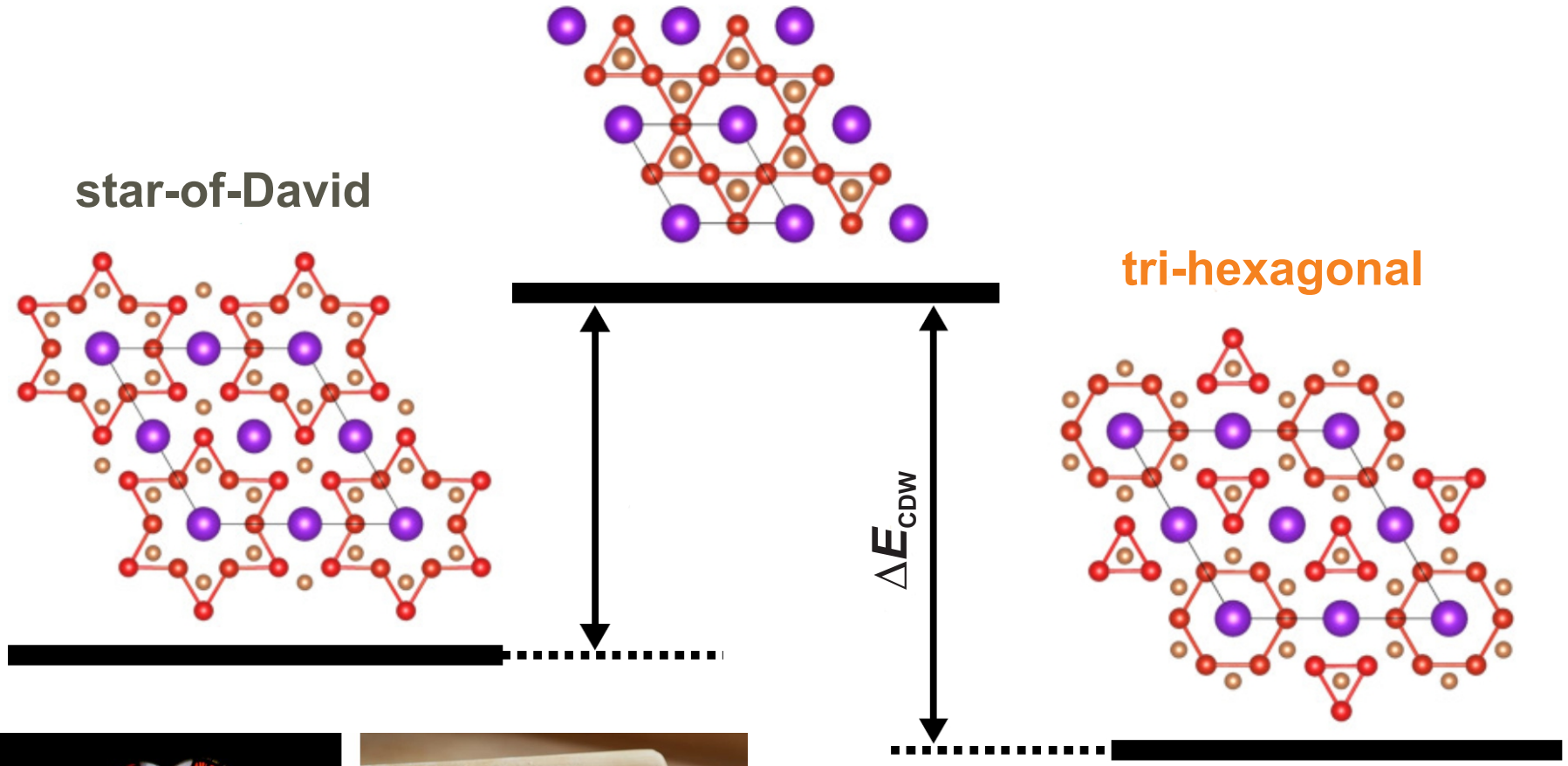
Charge-density-wave transition (94 K)

Superconductivity (around 2.5 K)

Charge-density wave

normal state

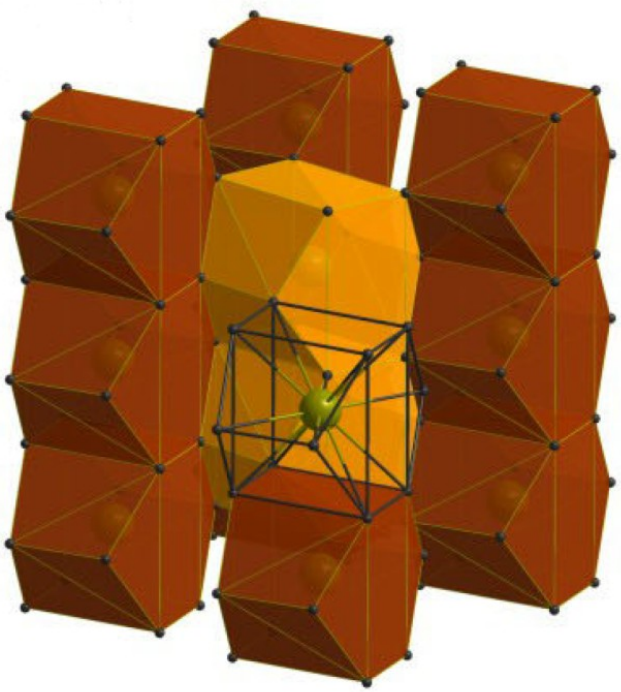
CDW state

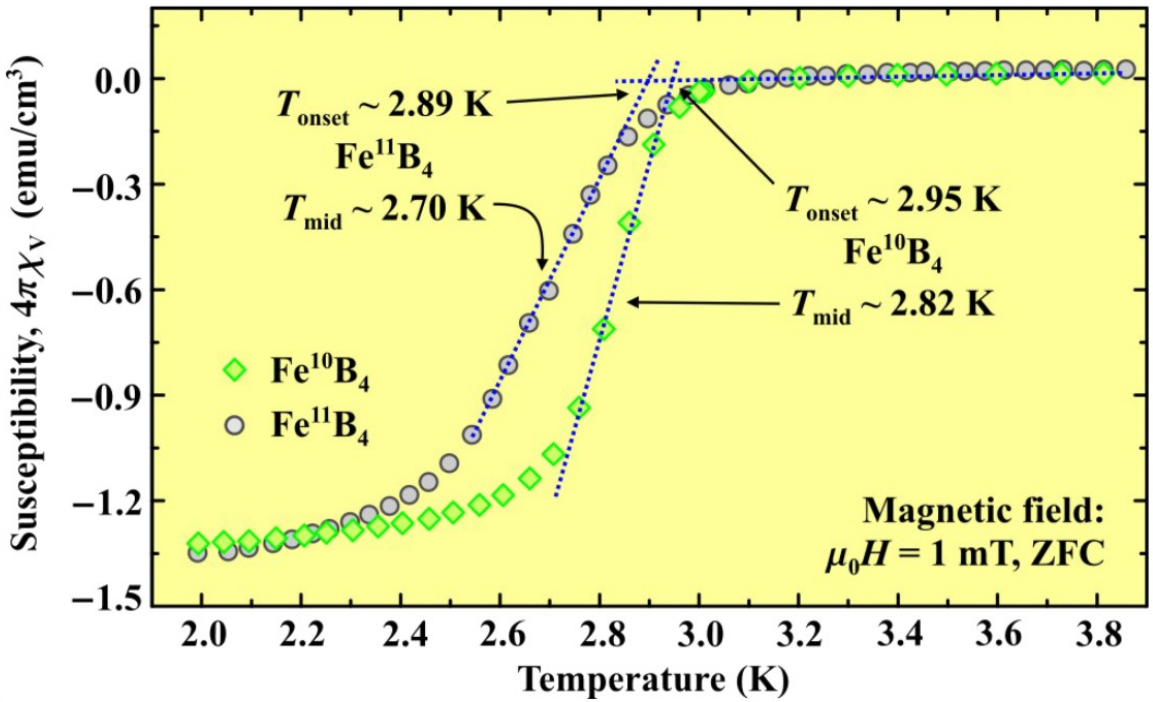


E. Uykur, AT *et al.*
npj Quantum Mater. (2022)

Pairing mechanism: **electron-phonon coupling**

Realistic predictions possible



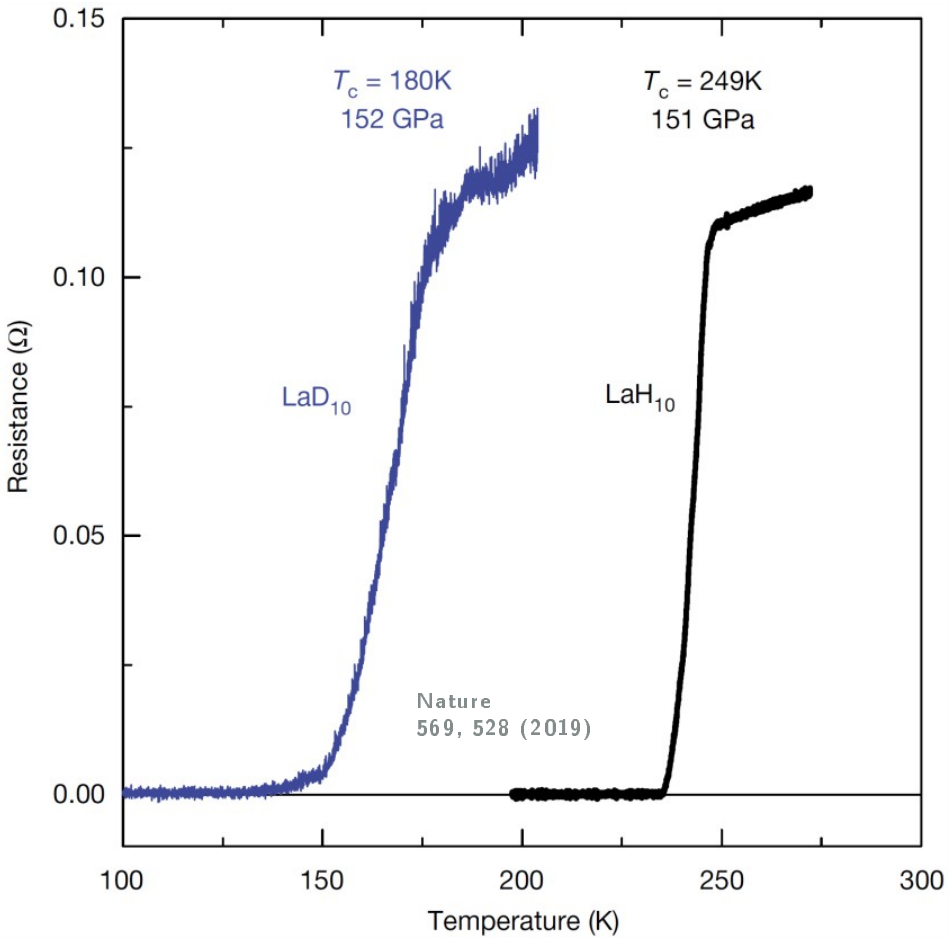


FeB_4, prediction (*ab initio* calculations): 2008

Experimental realization: 2013

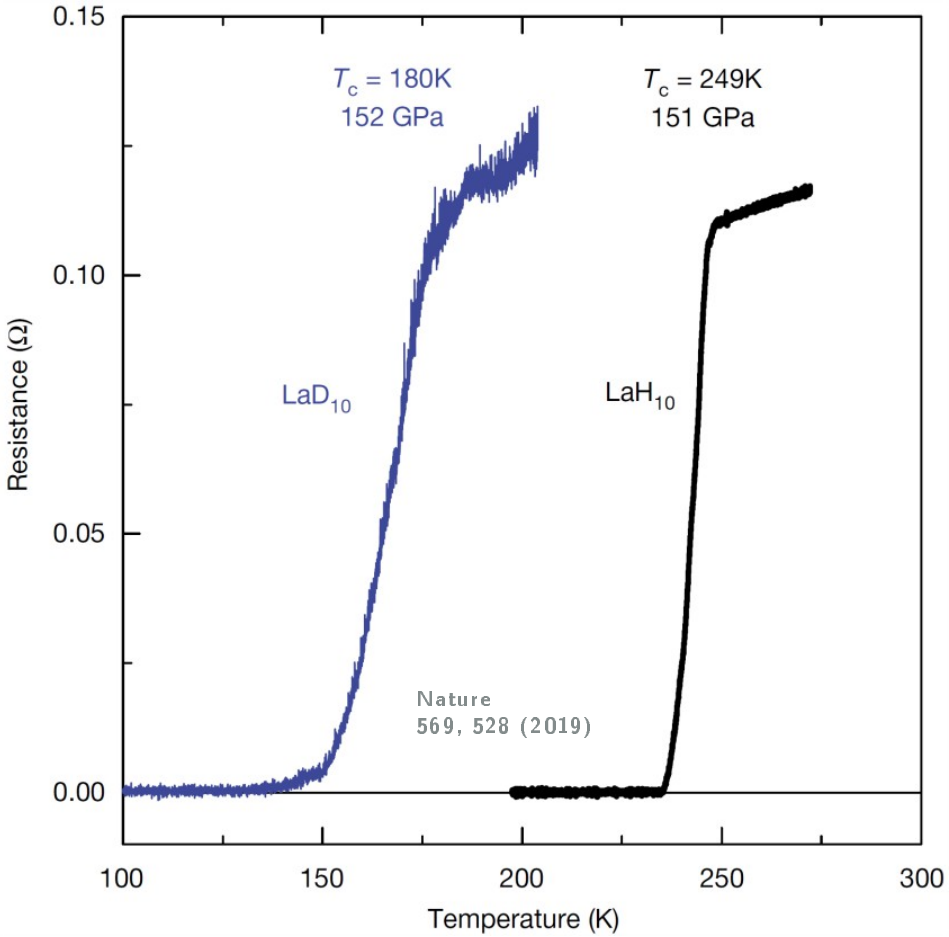
H. Gou, AT *et al.* Phys. Rev. Lett. (2013)

Conventional



typical pressures: 150–250 GPa

Conventional



typical pressures: 150–250 GPa

Unconventional

$YBa_2Cu_3O_{7-\delta}$ (YBCO)

$T_c = 93\,\mathrm{K}$ at $0\,\mathrm{GPa}$

commercial
superconducting cables

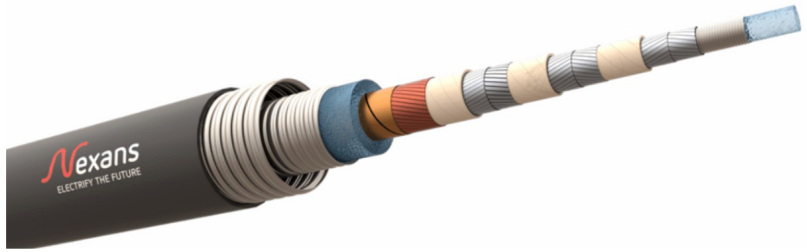
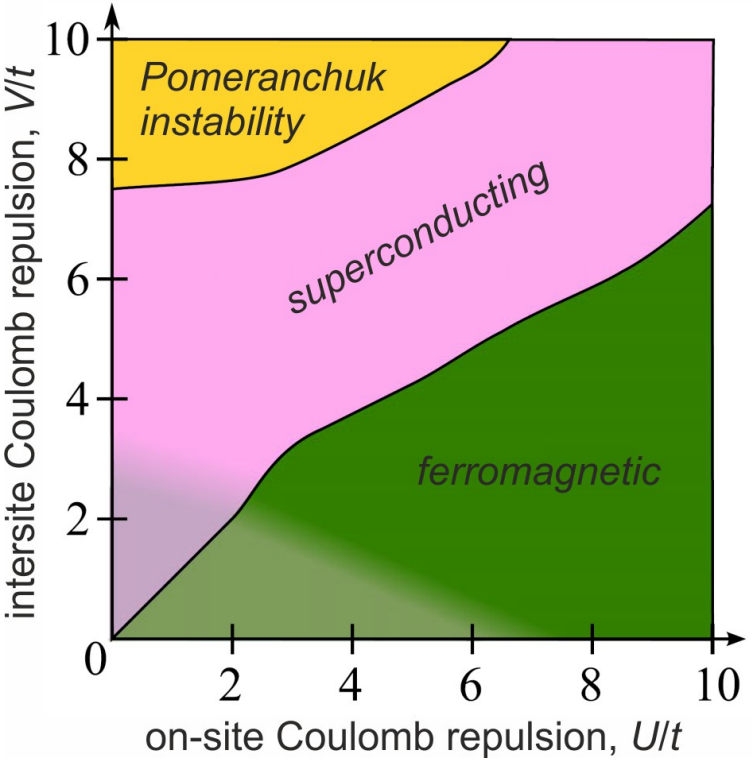
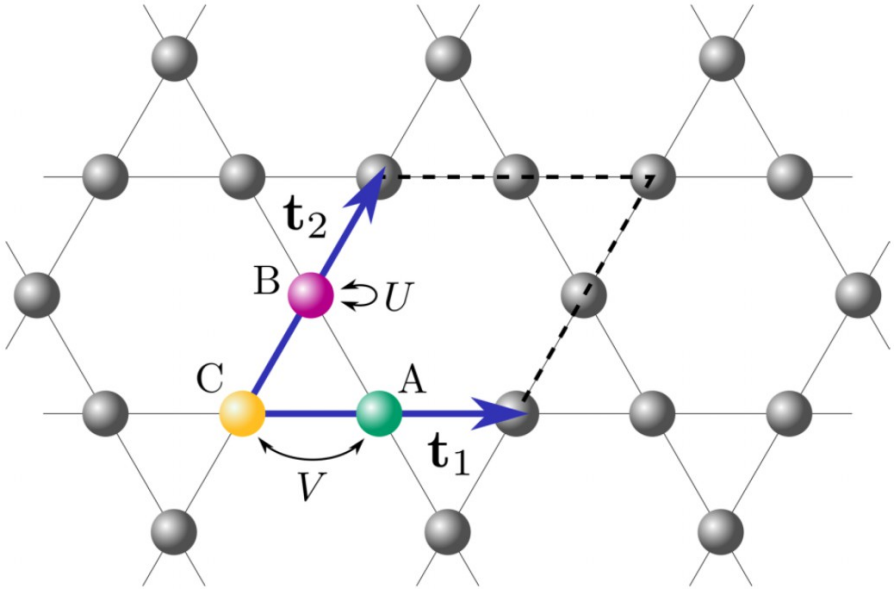
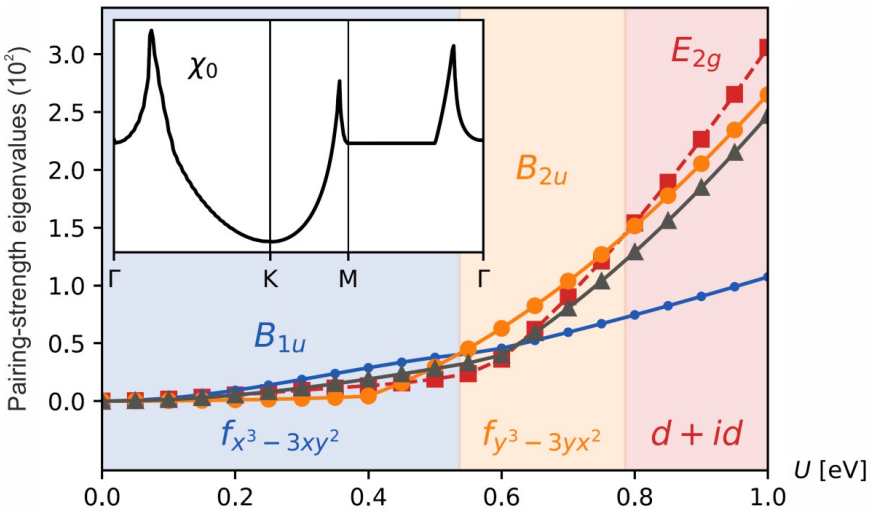


Image credit: Nexans (fair use)

Unconventional superconductivity in kagome

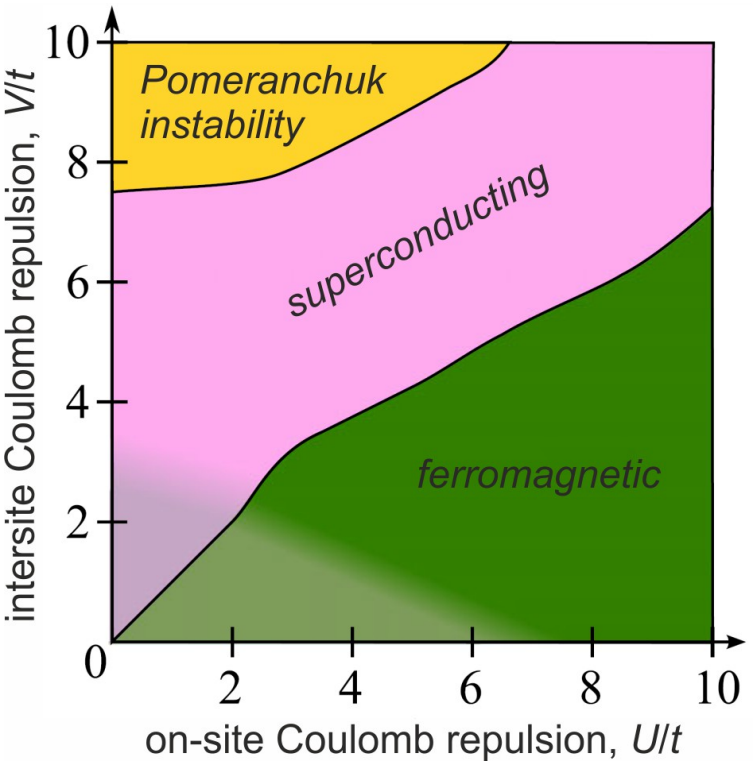


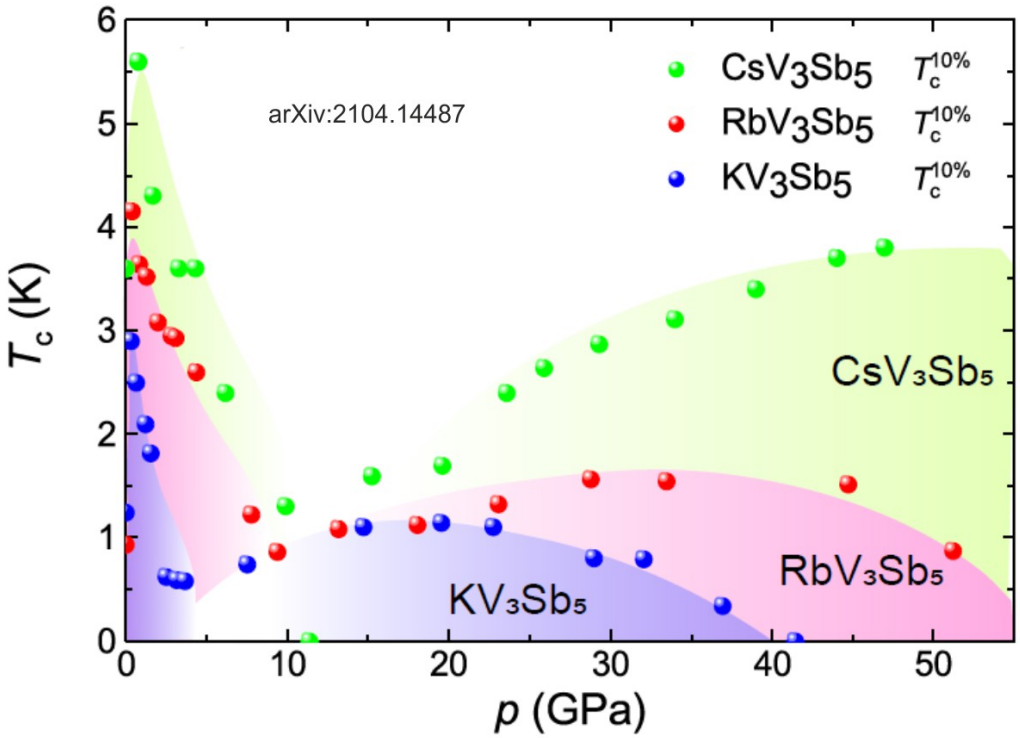


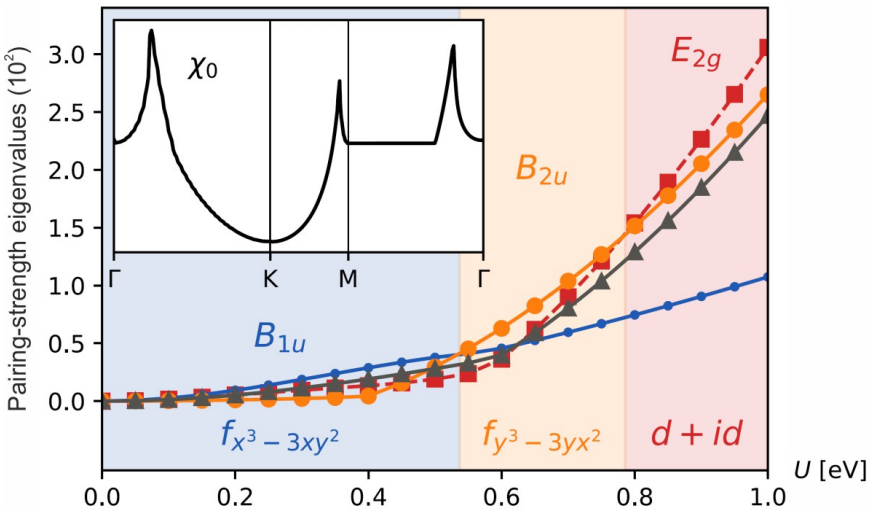


Phys. Rev. B 106, 174514 (2022)
Phys. Rev. Lett. 110, 126405 (2013); Phys. Rev. Lett. 127, 177001 (2021)

Unconventional superconductivity in kagome





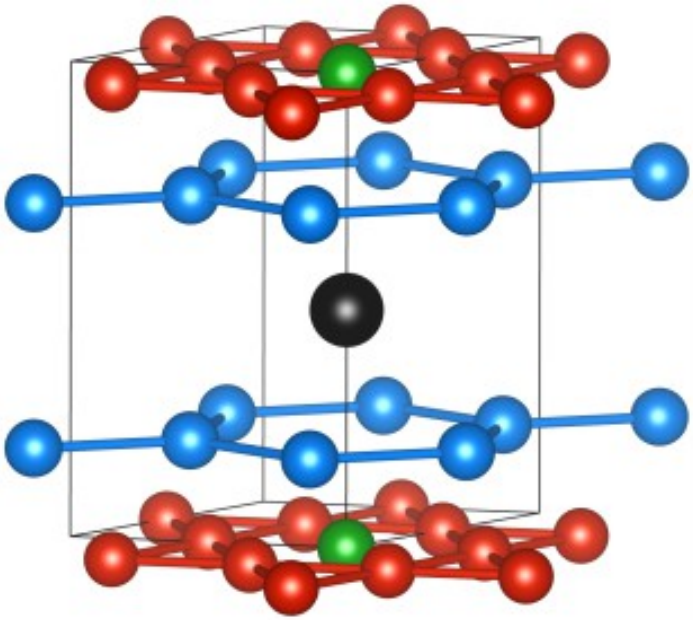


At least two different superconducting phases:

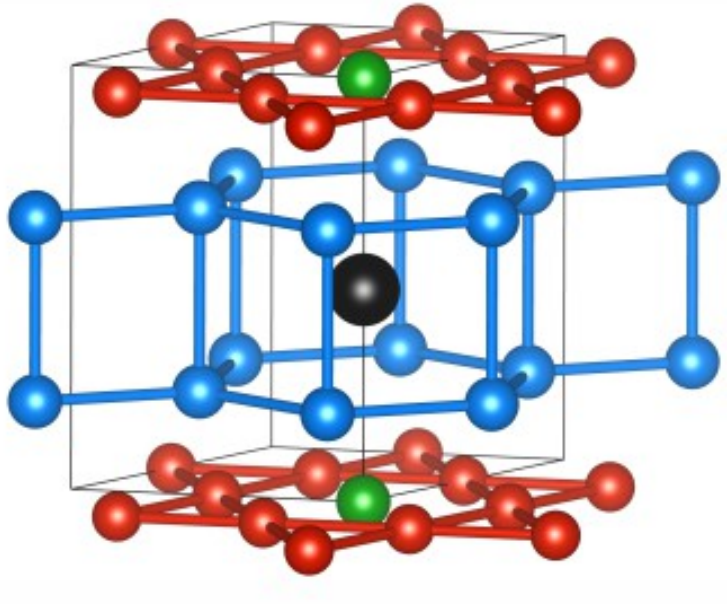
unconventional?

Phys. Rev. B 106, 174514 (2022)
Phys. Rev. Lett. 110, 126405 (2013); Phys. Rev. Lett. 127, 177001 (2021)

Pressure: 2D–3D crossover



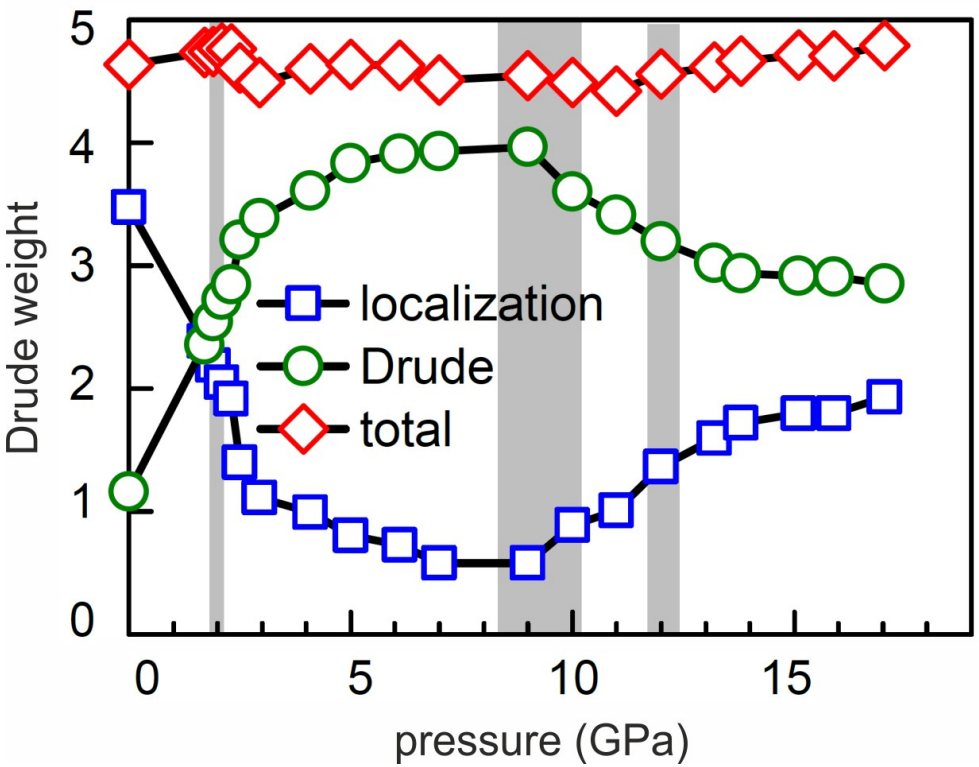
0 GPa



20 GPa

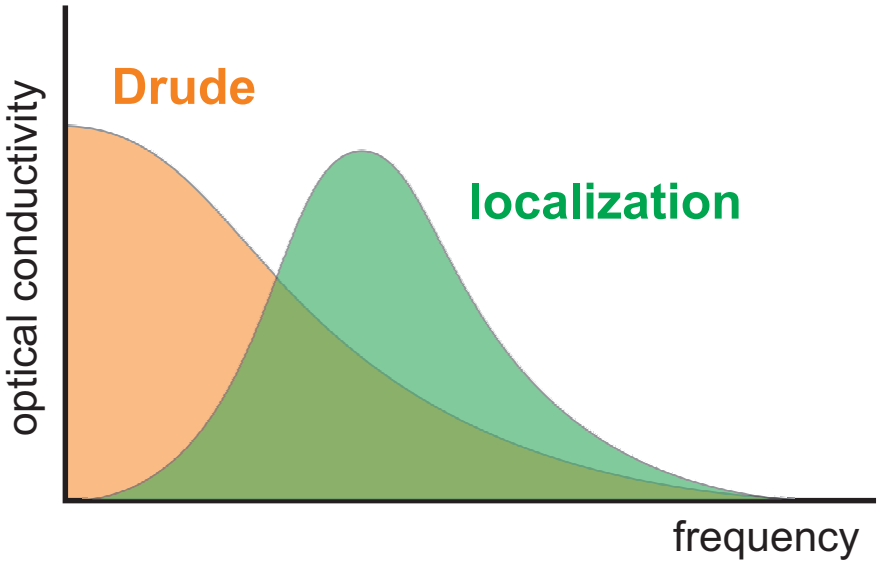
AT, E. Uykur *et al.* SciPost Phys. 12, 049 (2022)

Probe of electron-phonon coupling

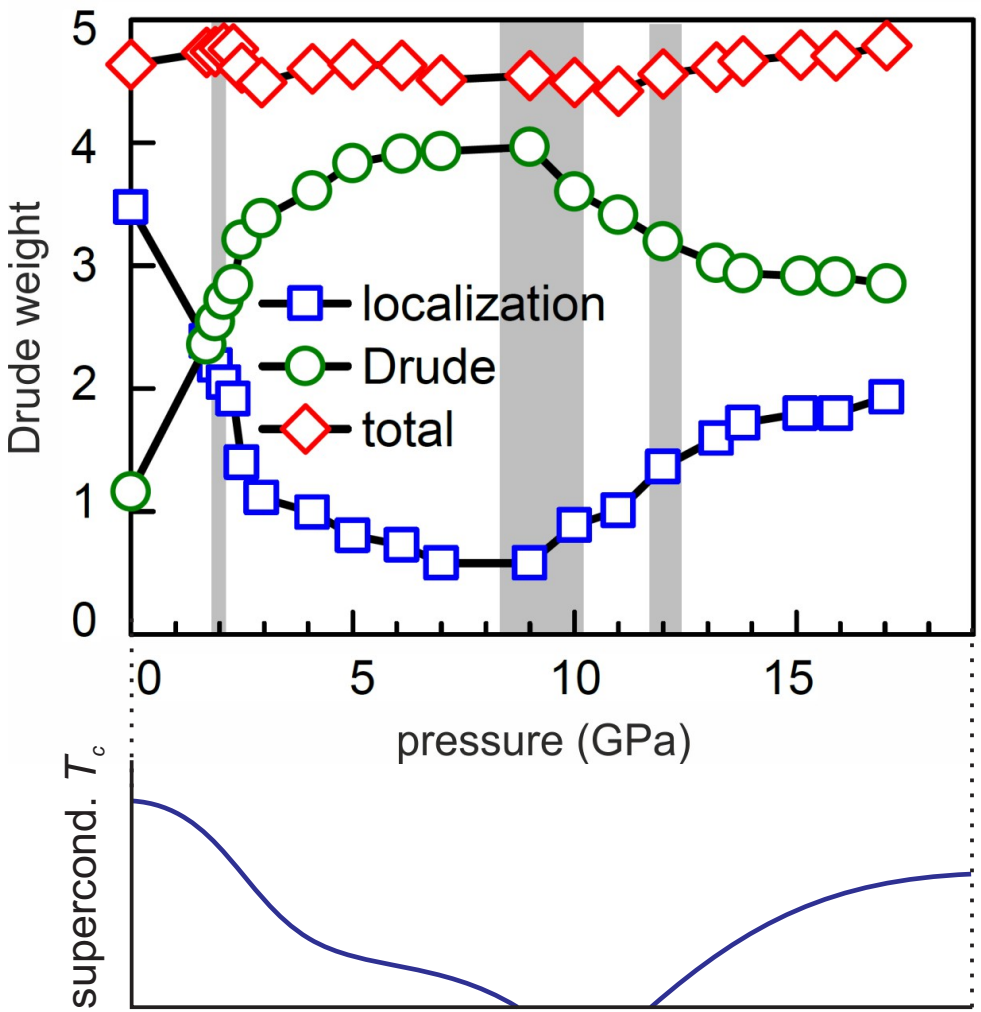


Drude peak: free carriers

Localization peak: carriers damped by e-phonon coupling



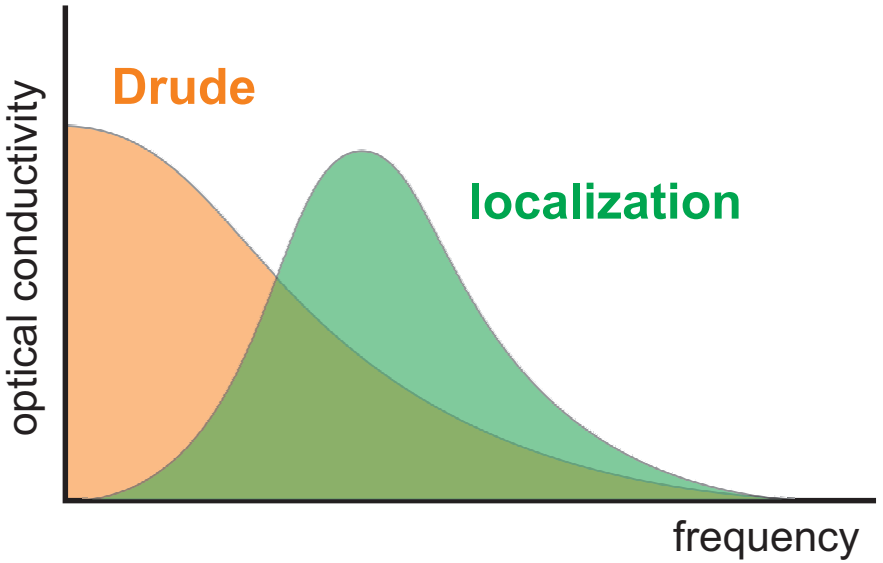
Probe of electron-phonon coupling



Drude peak: free carriers

Localization peak: carriers damped by e-phonon coupling

M. Wenzel, AT *et al.* arXiv:2305.02751



Superconductivity in AV_3Sb_5 is likely conventional

Thank you for your attention!

Food and drinks
will be offered in Aula!

Acknowledgements

Ece Uykur (HZDR)

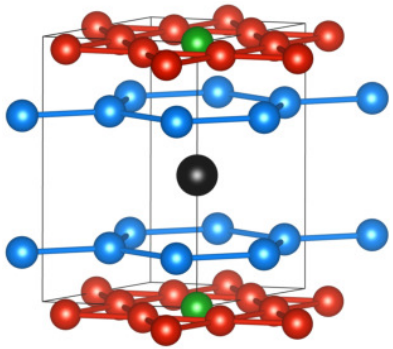
Maxim Wenzel, Martin Dressel (Uni Stuttgart)

ESRF, ISIS, SOLEIL, DFG, AvH Foundation...

Philipp Gegenwart, Yuesheng Li
(Uni Augsburg)

Ioannis Rousochatzakis (Loughborough)

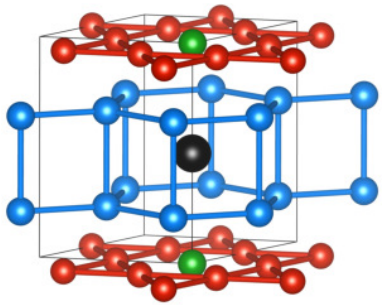
Pressure: 2D–3D crossover

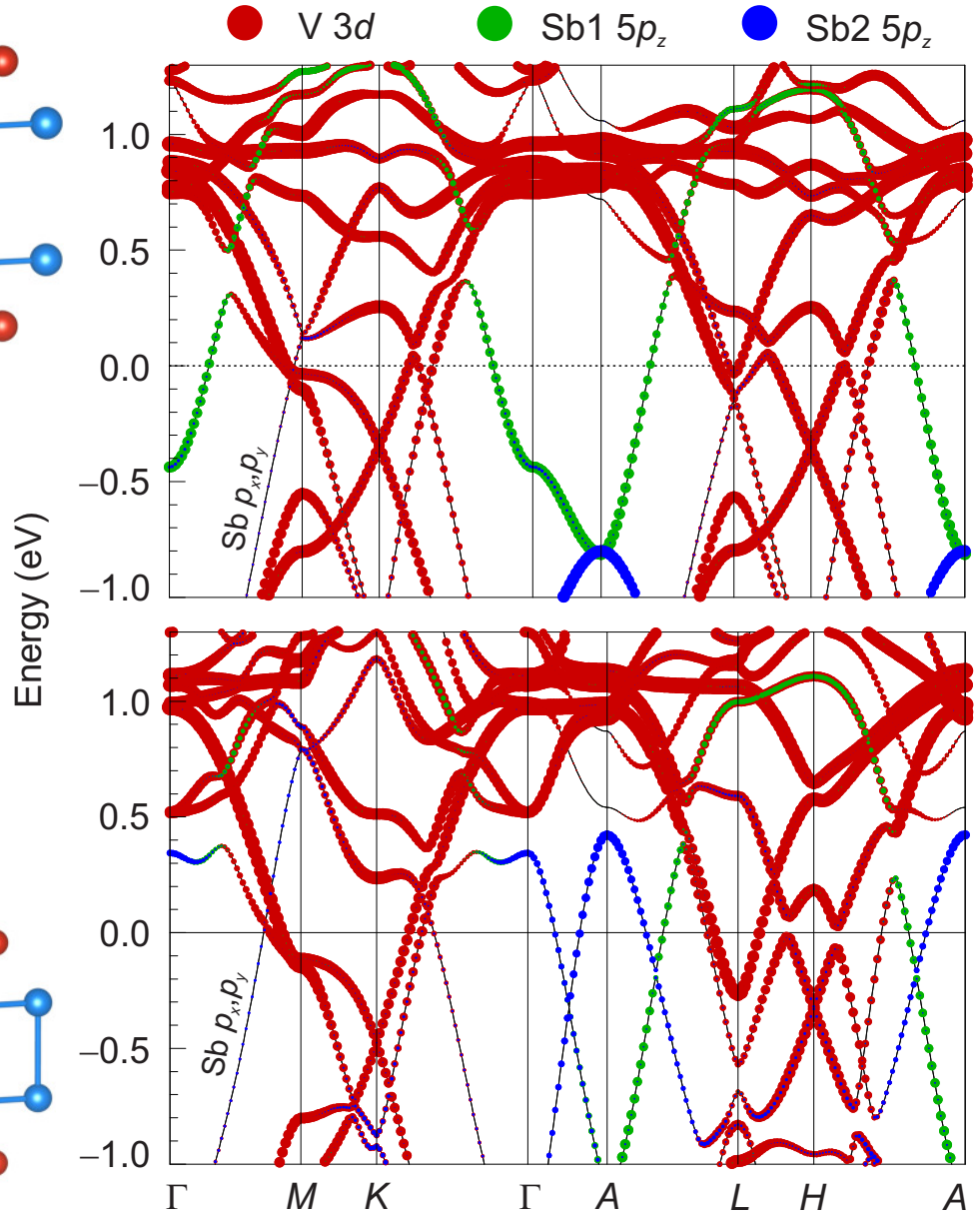


0 GPa

Cs
V
Sb1
Sb2

20 GPa





flat bands (+0.9 eV)

0 GPa

saddle points (–0.07 eV)

linear crossing (–0.35 eV)

flat bands (+1.05 eV)

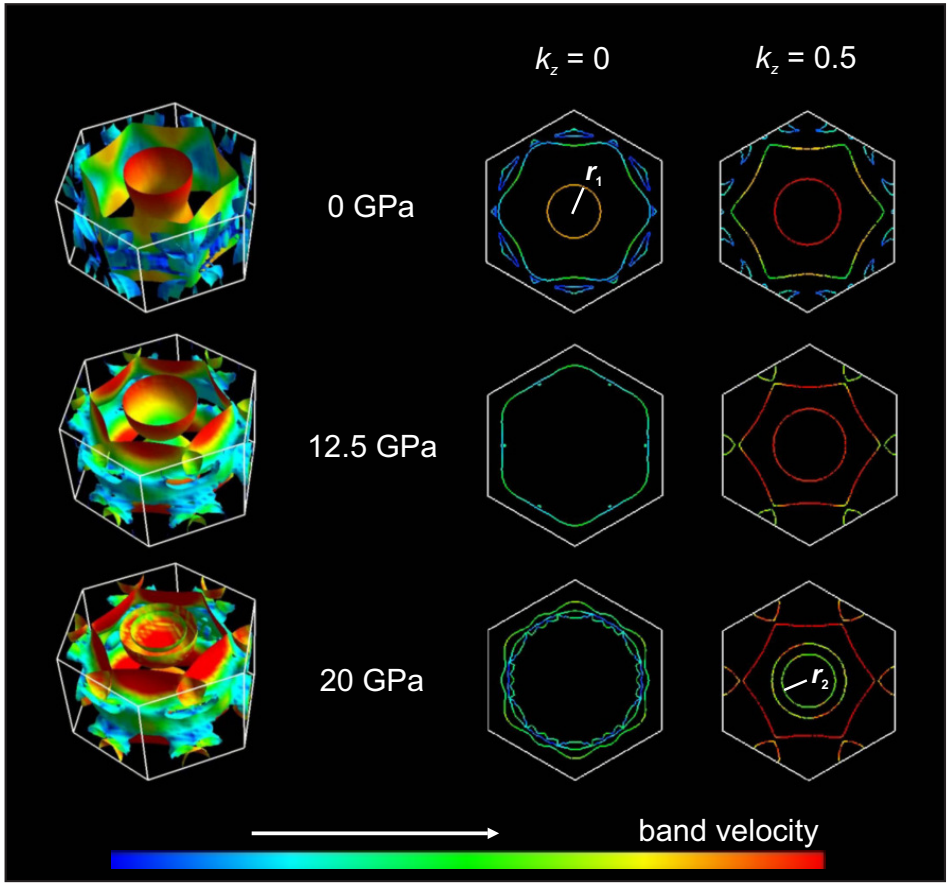
20 GPa

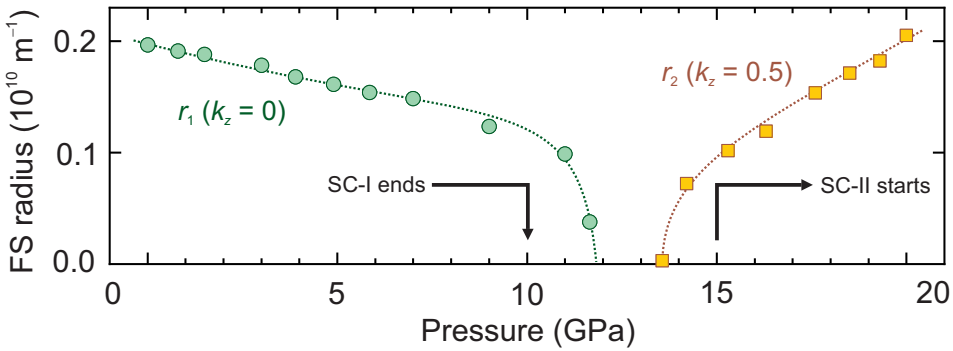
saddle points (–0.12 eV)

linear crossing (–0.5 eV)

AT, E. Uykur *et al.* SciPost Phys. 12, 049 (2022)

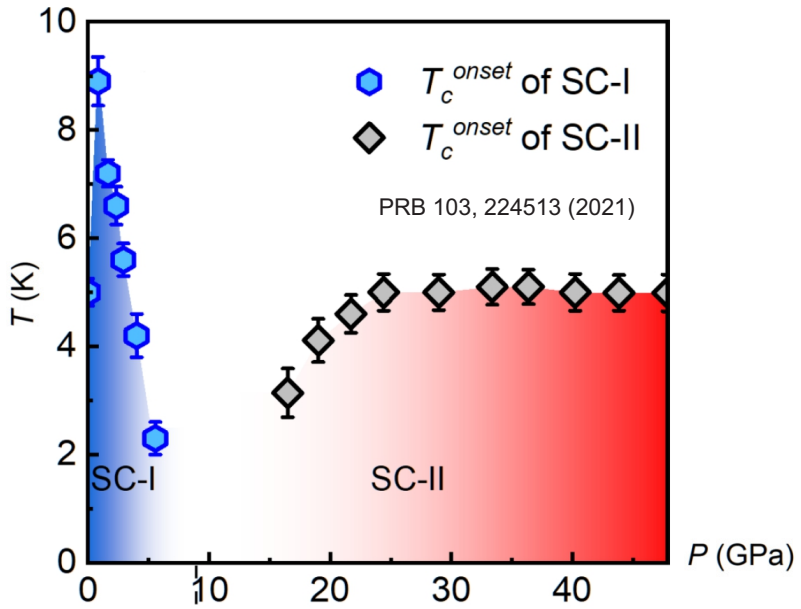
Fermi surface





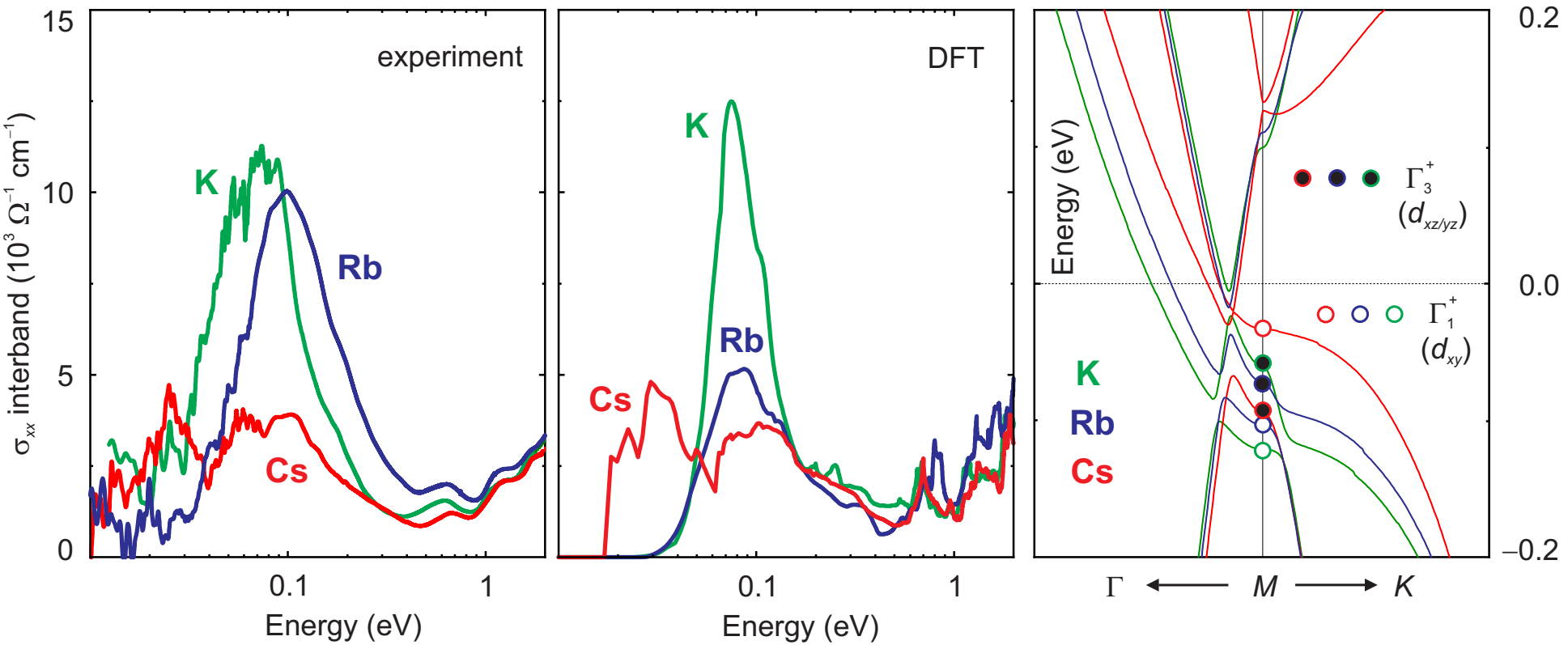
Major reconstruction of the cylindrical Fermi surface (Sb p_z bands)

Correlates with the suppression/re-entrance of superconductivity



AT, E. Uykur *et al.* SciPost Phys. 12, 049 (2022)

Band saddle points

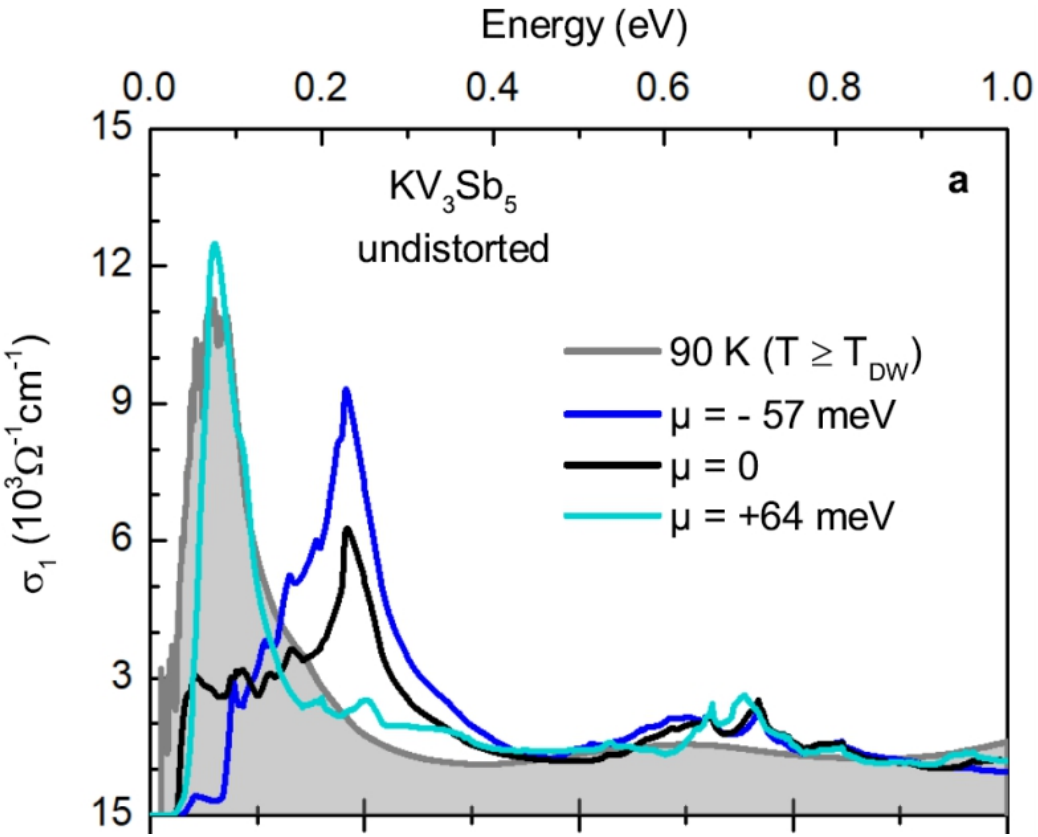


"Inversion" of band saddle points:
Γ_1^+ is above Γ_3^+ in Cs, yet below Γ_3^+ in K and Rb

Can one change the order of band saddle points by pressure?

E. Uykur, AT *et al.* PRB 104, 045130 (2021); npj Quantum Mater. 7, 16 (2022)

Band picture holds, or not?



In KV_3Sb_5
a shift of E_F is required
(renormalization of band energies)

a smaller 41 meV shift in RbV_3Sb_5

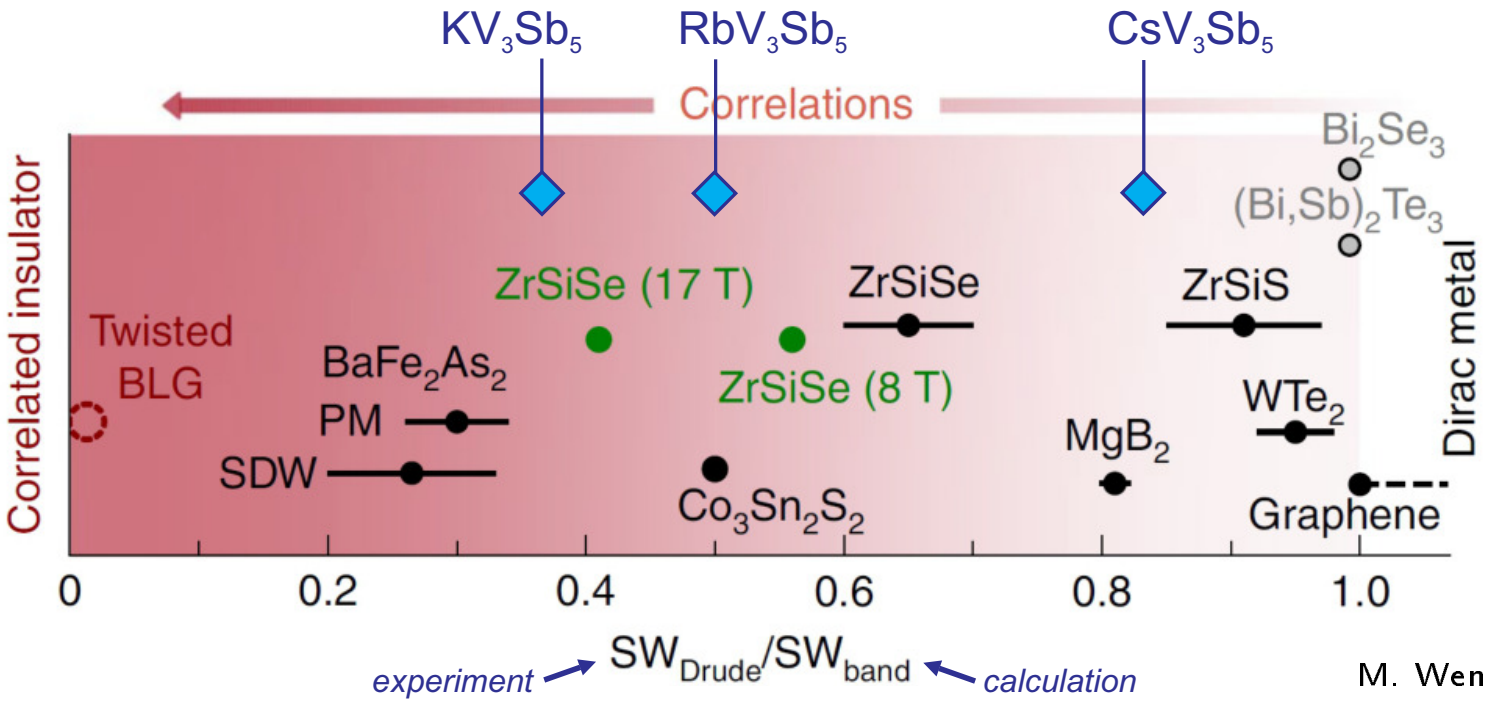
no shift in CsV_3Sb_5

E. Uykur, AT *et al.* npj Quantum Mater. 7, 16 (2022)

LETTERS
https://doi.org/10.1038/s41567-020-0859-z
Nature Phys. 16, 636 (2020)
nature physics
Check for updates

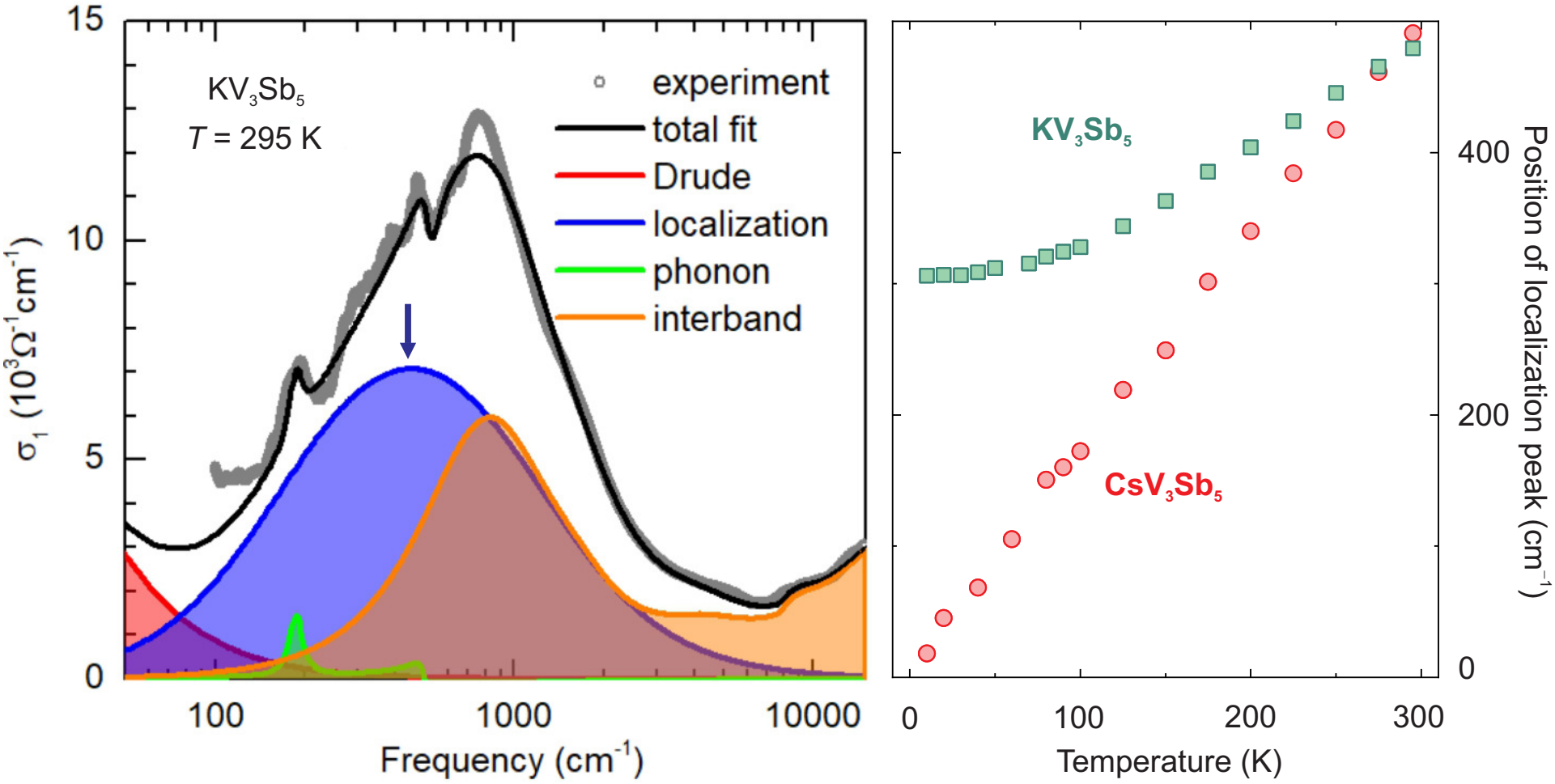
Electronic correlations in nodal-line semimetals

Yinming Shao[1]✉, A. N. Rudenko[2,3], Jin Hu[4], Zhiyuan Sun[1], Yanglin Zhu[5], Seongphill Moon[6,7], A. J. Millis[1,8], Shengjun Yuan[2], A. I. Lichtenstein[9], Dmitry Smirnov[7], Z. Q. Mao[5], M. I. Katsnelson[3] and D. N. Basov[1]✉



M. Wenzel, AT *et al.*
PRB 105, 245123 (2022)

Localization peak

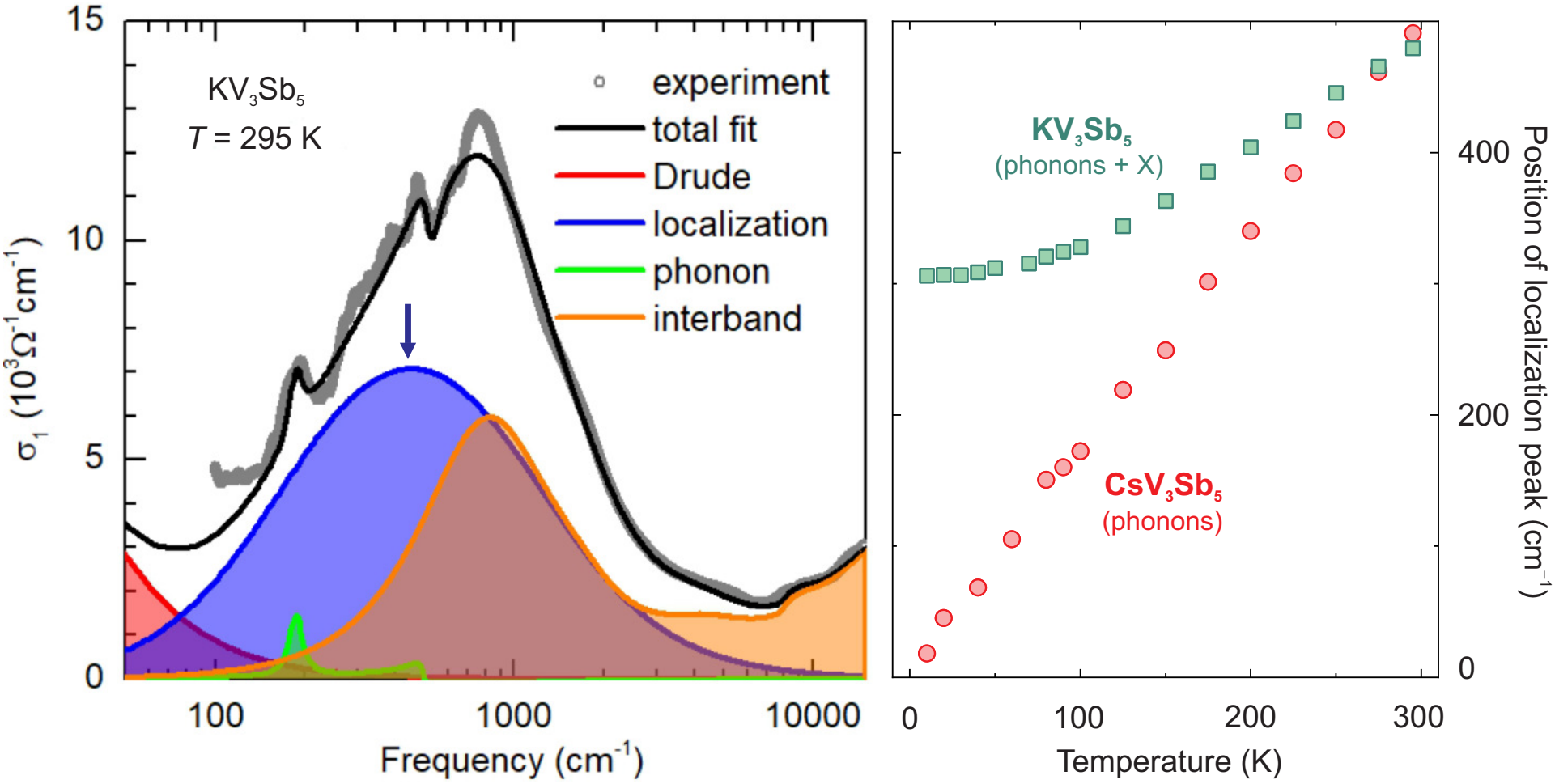


"Displaced Drude peak" – a fingerprint of bad metals

Theory review: [Adv. Funct. Mater. 26, 2292 (2016)] and [SciPost Phys. 3, 025 (2017)]

similar localization peak in the kagome metal Fe_3Sn_2: [PRL 125, 076403 (2020)]

Localization peak

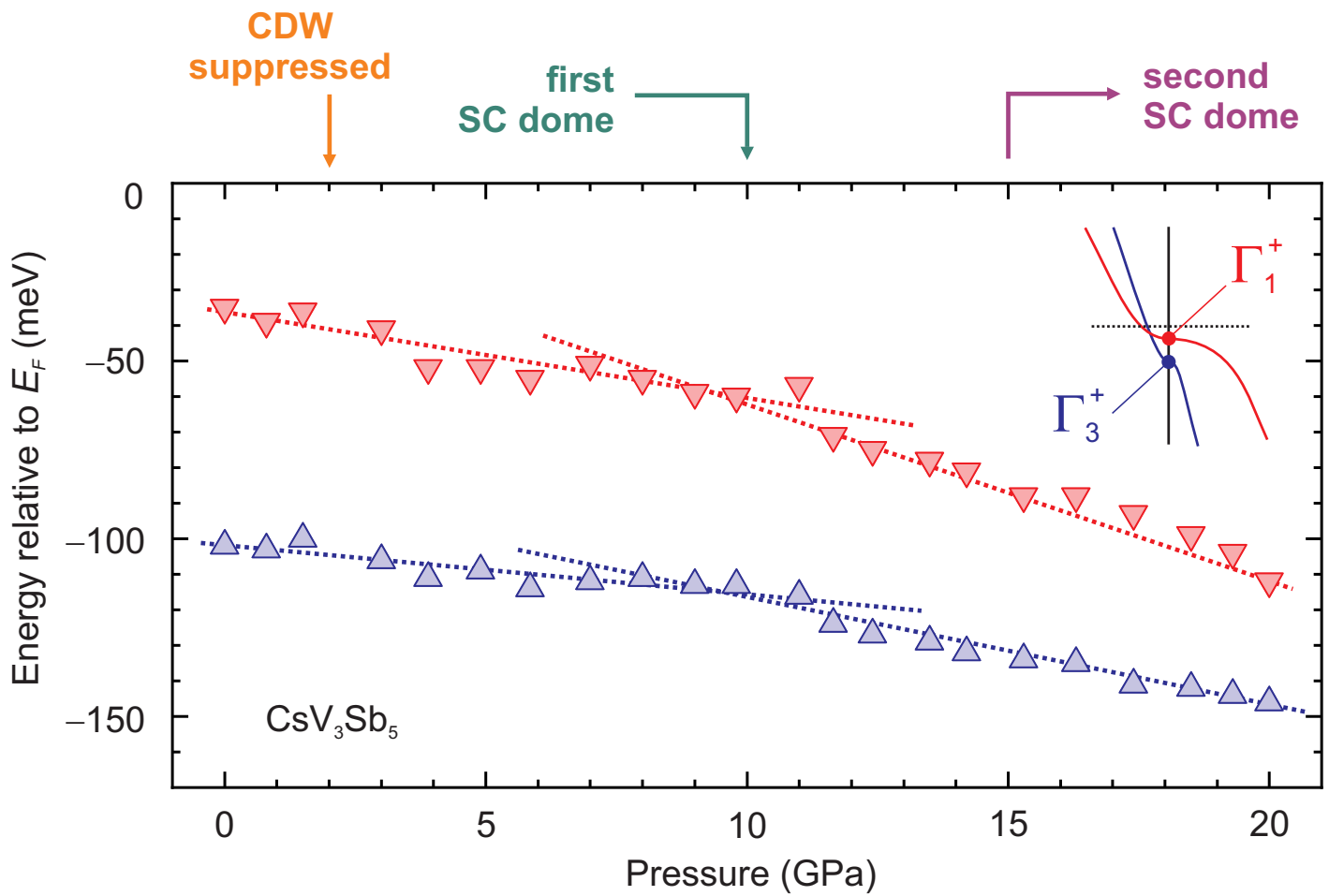


"Displaced Drude peak" – a fingerprint of bad metals

Theory review: [Adv. Funct. Mater. 26, 2292 (2016)] and [SciPost Phys. 3, 025 (2017)]

similar localization peak in the kagome metal Fe_3Sn_2: [PRL 125, 076403 (2020)]

Higher pressures: band saddle points



Pressure has only a minor effect on the band saddle points

Pressurized CsV_3Sb_5 is not the same as KV_3Sb_5!

AT, E. Uykur *et al.* SciPost Phys. 12, 049 (2022)