Hopping frustration-induced flat band and strange metallicity in a kagome metal

Ye, L. *et al.* (2024) 'Hopping Frustration-Induced Flat Band and Strange Metallicity in a Kagome Metal', *Nature Physics*, 20(4), pp. 610–614.

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TITLE BREAKDOWN

KAGOME METAL

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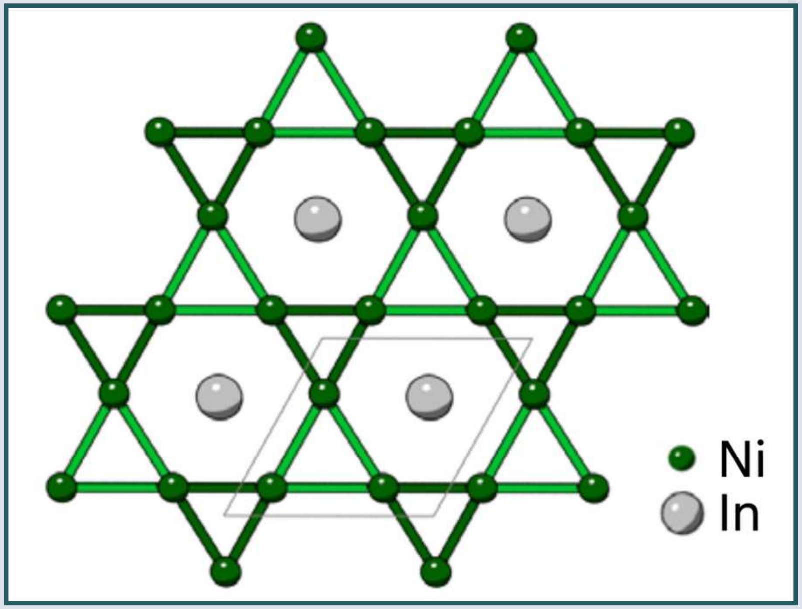


- Any metal with a kagome lattice geometry
  - trihexagonal
  - symmetric
  - periodic
- Ni_3In (trinickle indium)
- Possesses **strange metal** properties

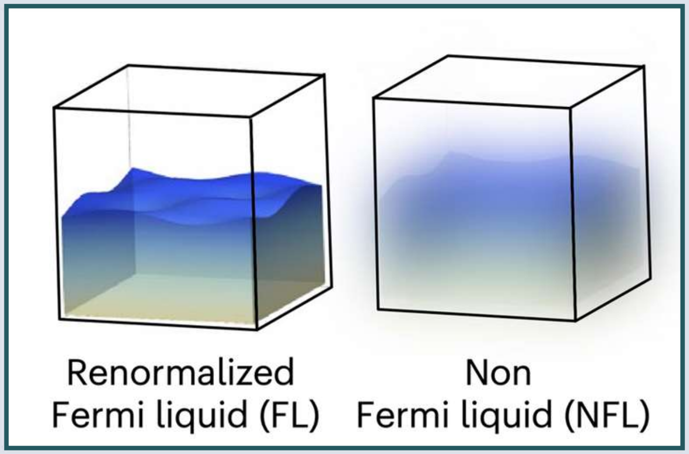
TITLE BREAKDOWN

KAGOME METAL

STRANGE METAL

STRANGE METAL

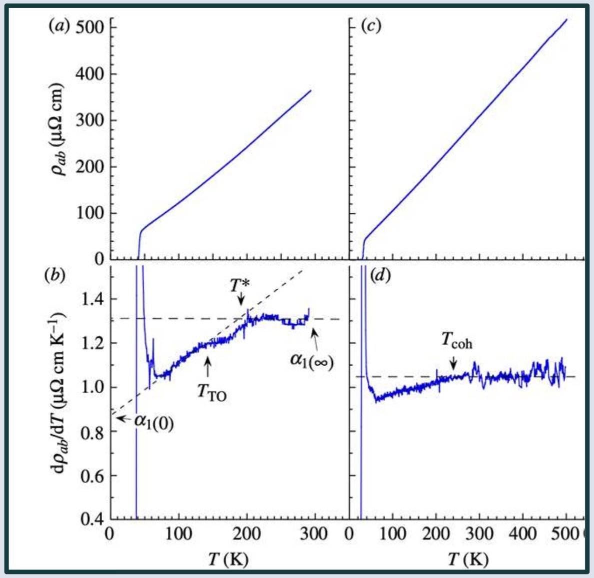
Fermi Liquid Theory



Behaviors

- Quasiparticles no longer resemble free electrons

STRANGE METAL

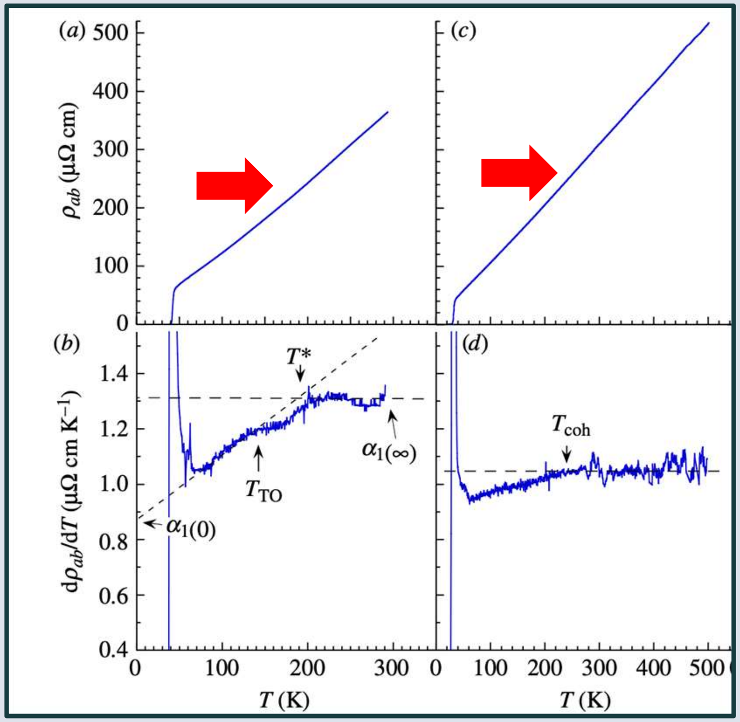


LSCO at different dopings. N. E. Hussey et. al. Phil. Trans. R. Soc. A (2011) 369, 1626–1639

Behaviors

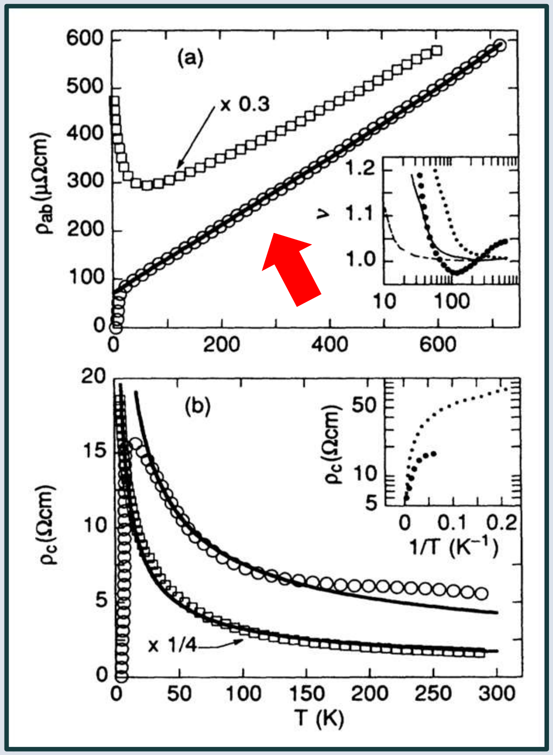
- Quasiparticles no longer resemble free electrons
- Resistivity scales linearly with temperature
- Variety of temperature regimes

STRANGE METAL



Typical resistivity behavior

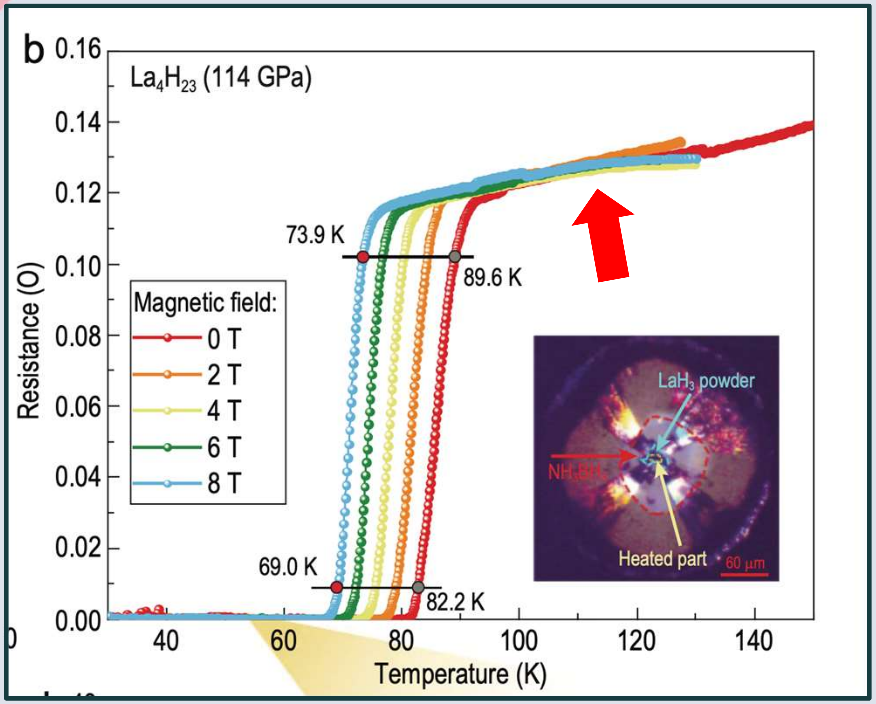
STRANGE METAL



BSCO at different stoichiometries, S. Martin et. al. Phys. Rev. B **41**, 846(R)

Typical resistivity behavior

STRANGE METAL



Hydrides, J. Guo et. al. *National Science Review*, Volume 11, Issue 12, December 2024, nwae149

Typical resistivity behavior

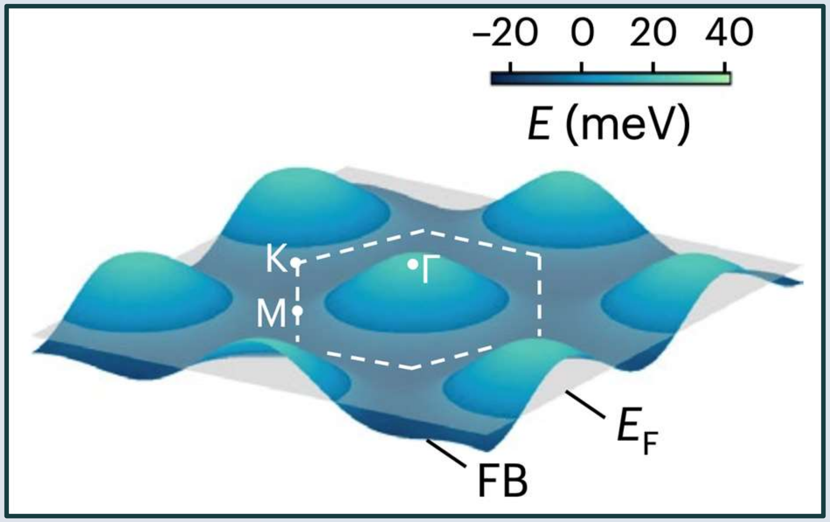
TITLE BREAKDOWN

KAGOME METAL

STRANGE METAL

HOPPING FRUSTRATION

HOPPING FRUSTRATION

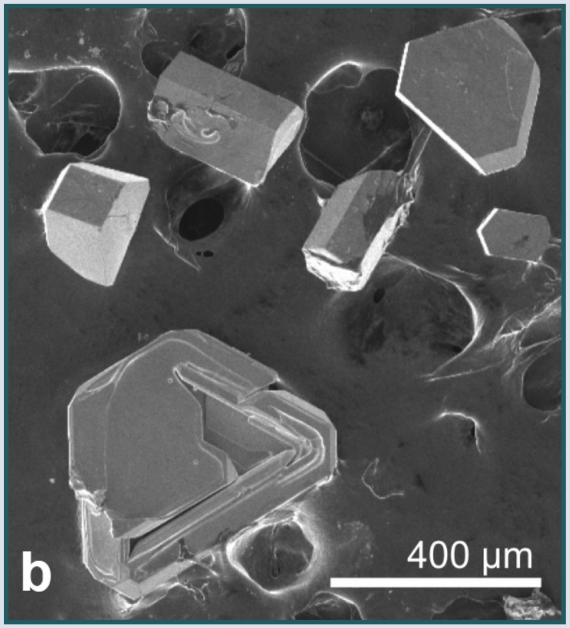


- Lattice of Ni_3In allows for hopping frustration
- Electrons are localized, creating **partially** flat band energy states (highly correlated system)

METHODS

MATERIAL SYNTHESIS

- Ni_3In, Ni_3Sn synthesized with I_2 catalyst
- Cut to 5µm crystals with Ga-ion beam
- Examined with scanning transmission electron microscopy
- Measurements performed at National High Magnetic Field Laboratory (Los Alamos)



Scanning electron microscope image of Ni_3In crystals; Fig. S1 (b) from article's supplementary information

PHYSICAL MEASUREMENTS

C_p Measurements

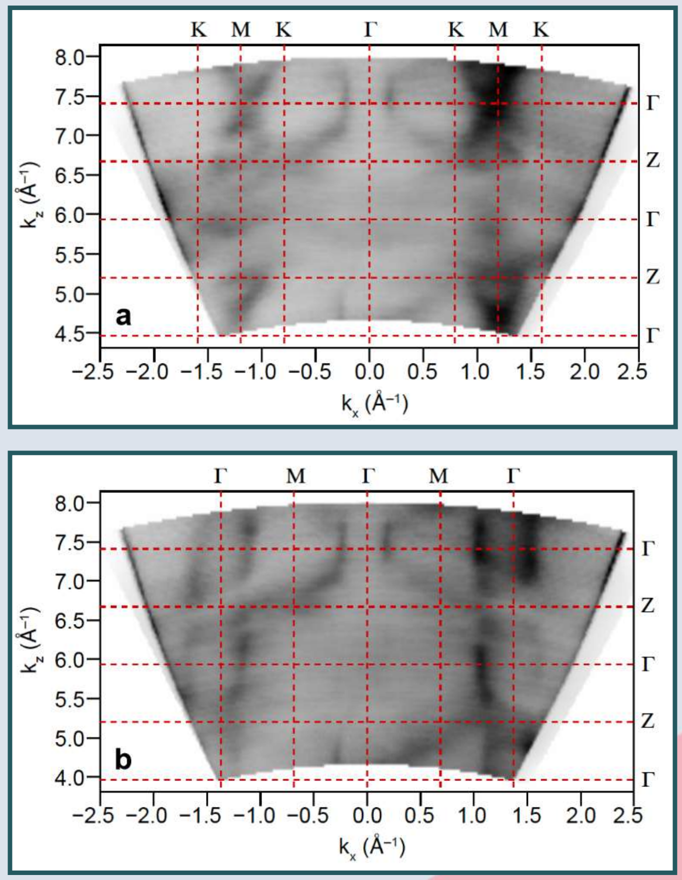
- Crystals sintered together
- Two-relaxation-time method (NMR)
- T_1 (long) → decay of nuclear spin magnetization M_z to thermal equilibrium value
- T_2 (short) → decay of $\mathbf{M} \perp \mathbf{B}$ component to 0

Other measurements

- Cryostat for $\rho_{ab}(T)$
- Piston-type pressure cell for $\rho_{ab}(T, P)$
- Vibrating sample magnetometer for $\chi(\mathbf{q})$
- Magnetization measurements at pulsed field facility

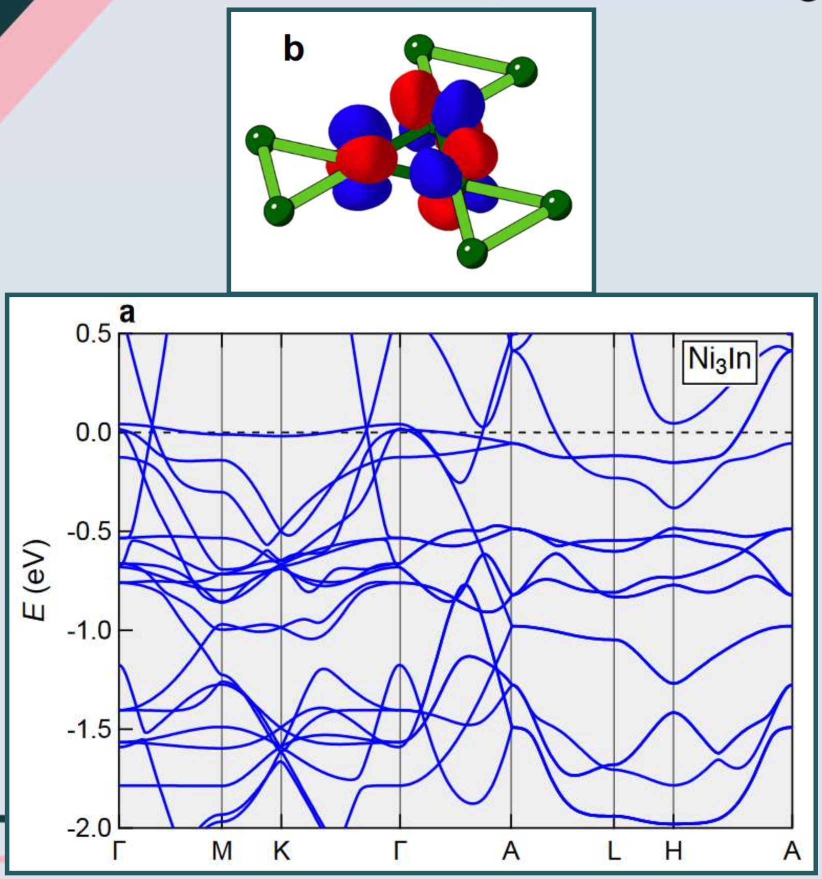
SPECTROSCOPY

- Angle-Resolved Photoemission Spectroscopy (ARPES)
- Used to probe band structure
- Performed at Beamline 7.0.2 (Advanced Light Source)
- Photon energy range 70-230 eV
- Energy resolution: <20 meV
- Momentum resolution: <0.01 Å^{-1}



Ni_3In ARPES measurements along (a) K-M-K-Γ and (b) M-Γ planes; Fig. S8 (a, b) from article's supplementary information

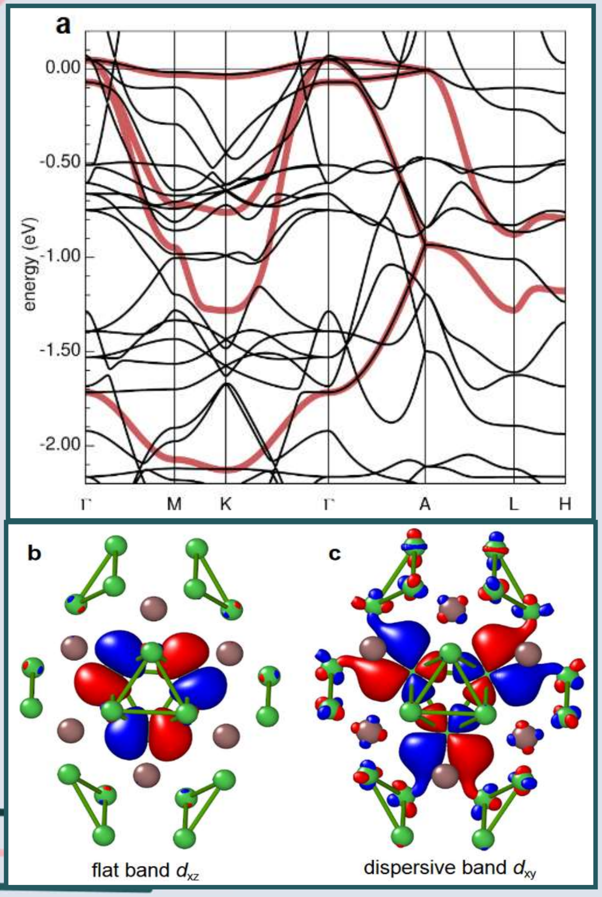
CALCULATIONS



- Ab initio Density Functional Theory (DFT)
- Vienna Ab Initio Simulation Package (VASP)
- PBE Generalized Gradient Approximation (GGA) functional to model exchange-correlation energy
- Reciprocal mesh: 13 x 13 x 11 subdivisions
- Wannier90 code to construct tight-binding Hamiltonian from Ni 3d, 4s, In 5s states

(b) Flat band Wannier wavefunction and (a) DFT band structure for Ni_3In; Fig. S5 (b) and Fig. S11 (a) from article's supplementary information

EFFECTIVE MODEL



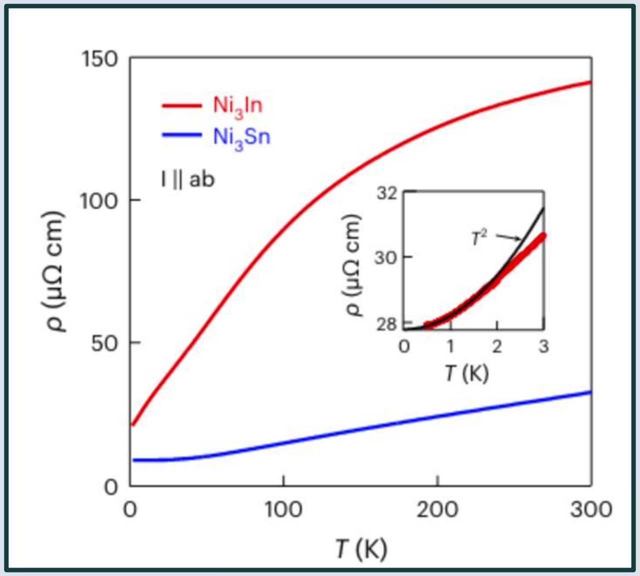
(a) Band structure (red lines), (b) flat band, and (c) dispersive band for four-band model of Ni_3In; Fig. S6 (a-c) from article's supplementary information

- Full-Potential Local-Orbital (FPLO) code used to construct model based on molecular orbitals
- Restricted to dominating Ni d_{xz}, d_{xy} atomic orbital contributions
- Produces four-band model
- Local magnetic susceptibility calculated
- Reciprocal grid of 24 x 24 x 24 subdivisions

RESULTS

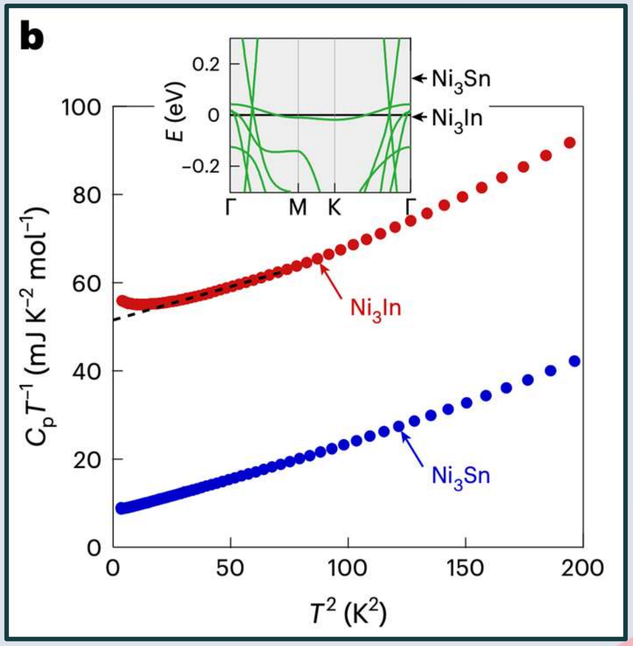
RESISTIVITY

- Resistivity (ρ) exhibits a linear like dependence on T below 100K, when the expected dependence is T^2
- Only at $T < 1.5K \equiv T_{FL}$, does the system show a response of $\rho(T) \propto T^2$ (inset)
- This is indicative of Fermi-Liquid behavior.
- The coefficient of T^2 for Ni_3In (0.25 $\mu\Omega$ cm K^{-2}) is orders of magnitude larger than the upper bound estimated for Ni_3Sn (1×10^{-4} $\mu\Omega$ cm K^{-2})



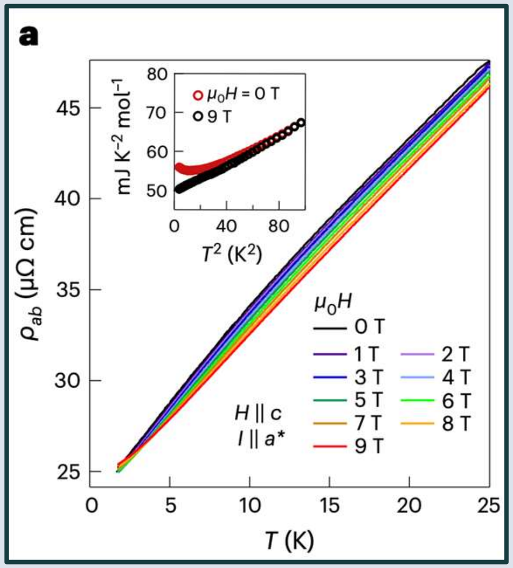
HEAT CAPACITY

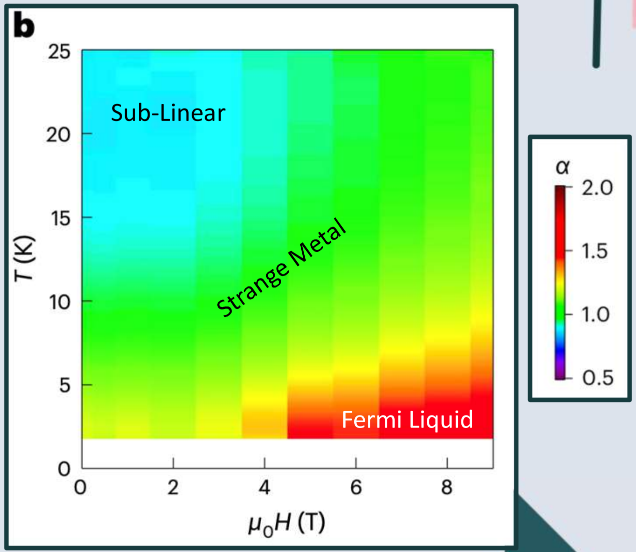
- At low T, a slight upturn is observed, deviating from the expected form $\gamma + \beta T^2$ (where γ is the Sommerfield coefficient and βT^2 is the phonon contribution
- For Ni_3In, $\gamma \approx 51.6$ mJ K^{-2} mol^{-1}, a roughly fivefold increase from 9 mJ K^{-2} mol^{-1} for Ni_3Sn. This is an indication of Heavy Fermion phenomena.
- We can derive a Density of States (DOS) from γ. From the γ values of Ni_3In and Ni_3Sn, we find D = 44 eV^{-1} and 7.6 eV^{-1} per unit cell respectively (inset)
- This result does not agree with the DOS estimated from DFT. We see a nearly threefold increase for Ni_3In (14 eV^{-1}) and only a 50% increase for Ni_3Sn (4.9 eV^{-1})



TUNING

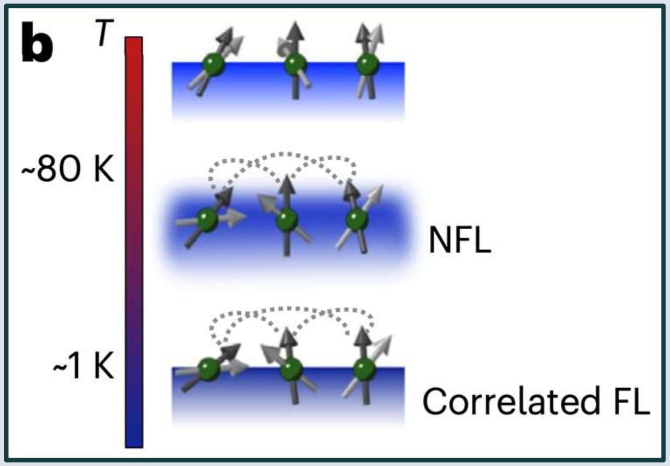
- NFL behavior is suppressed as the magnetic field increases, and the FL behavior is promoted at low temperatures.
- Heat capacity measurements also show a suppression of NFL features with increasing field (inset).
- The evolution of the metallic state in Ni_3In can be seen most clearly in the map of $\alpha(T, H)$





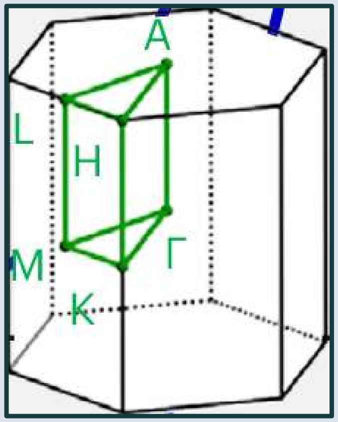
INTERPRETING THE RESULTS

INTERPRETING THE RESULTS: EXPERIMENTAL



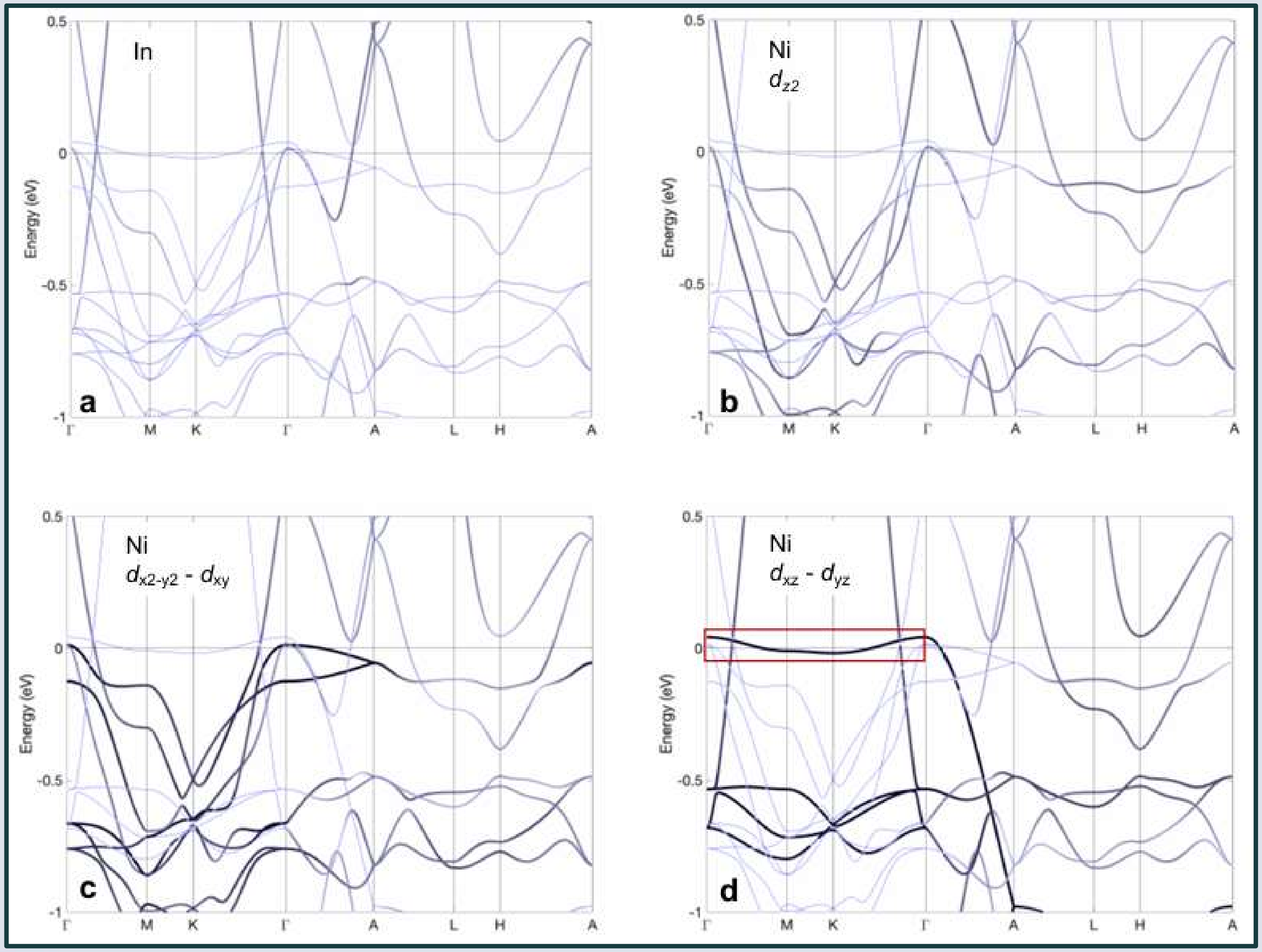
- The Kadowaki-Woods ratio is three orders of magnitude larger than those of elemental transition metals
- Closer to heavy fermion metals and correlated oxides
- Indicates enhanced correlation in the electronic states of Ni_3In

THE DFT FLAT BAND



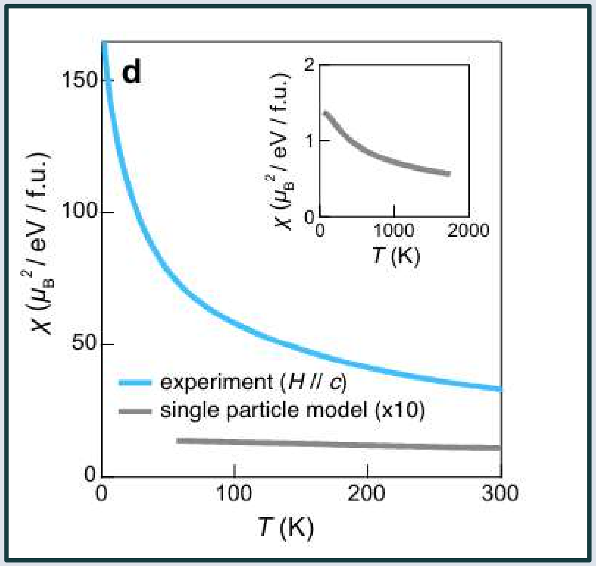
Brillouin Zone for the Kagome Lattice

- From the orbital decomposition of the electronic structure, flat band at the Fermi Level due to the Ni d_{xz}-d_{yz} states
- Band structure has features of the ideal Kagome lattice like symmetry-protected band crossing at near -0.6 eV, with a varying degree of dependence on k_z
- Results from the nature of the underlying d-orbital



In
a
Ni
d_{z2}
b
Ni
d_{x2-y2} - d_{xy}
c
Ni
d_{xz} - d_{yz}
d
Energy (eV)
0.5
0
-0.5
-1
Γ M K Γ A L H A

TIGHT BINDING AND CONSEQUENCES OF THE FLAT BAND



Susceptibility vs Temperature

- The DFT analysis motivates considering Wannier basis states w/. d_{xz} and d_{yz} orbitals (which dominate at the Fermi level)
- Magnetic susceptibility calculation reveals Curie-Weiss behavior (for high T)
- Indicates pre-formation of local magnetic moments, suggestive of emergent heavy fermion behavior

CITATION ANALYSIS

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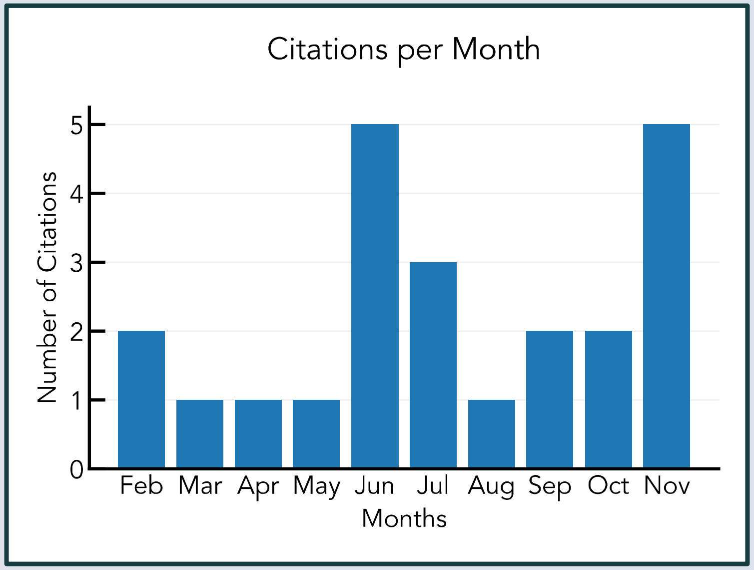
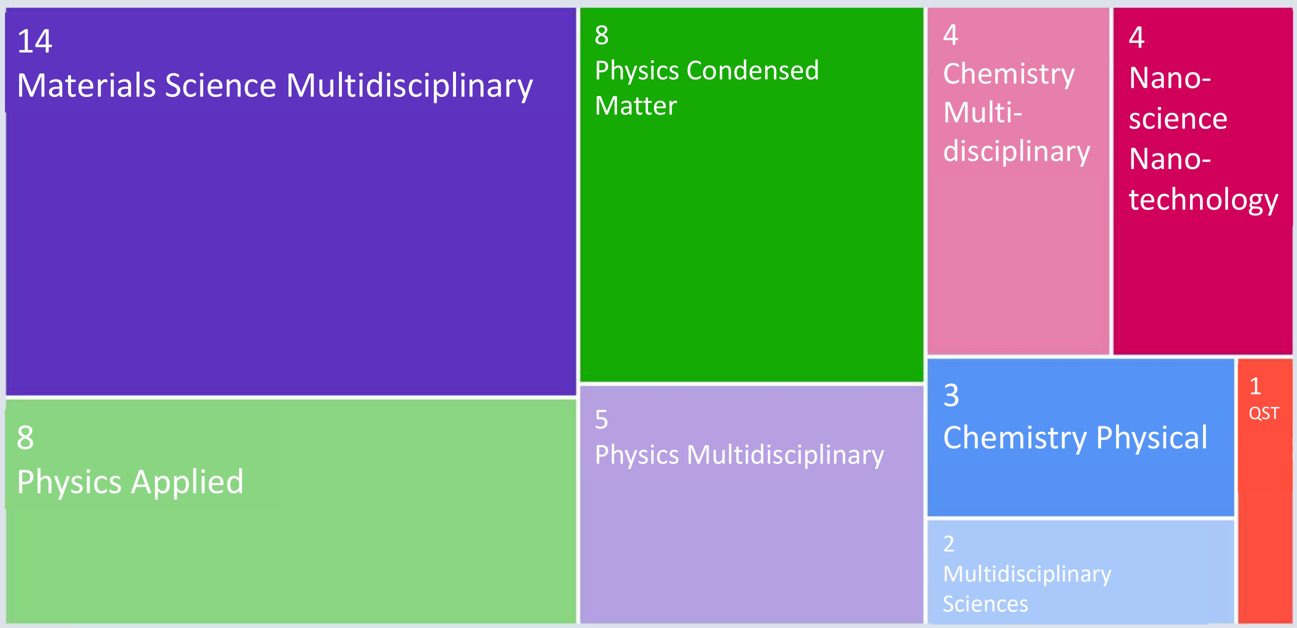


- Paper was published in January 2024
- Has been cited by 23 papers so far

CITATION ANALYSIS



CITATION ANALYSIS

Groups have begun studying kagome metals for correlated electron phenomena

Tuning the flat band with in-plane biaxial strain and the emergence of superconductivity in Ni_3Sn

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(Received 7 February 2024; revised 7 June 2024; accepted 24 June 2024; published 8 July 2024)

https://doi.org/10.1038/s41535-024-00685-9

Interorbital antisymmetric hopping generated flat bands on kagome and pyrochlore Lattices

Keyu Zeng & Ziqiang Wang

Unveiling the Nontrivial Electronic Structures and Fermi Topology of High-Temperature Kagome Ferrimagnet $HoMn_6Sn_6$

Bin Wang, Xiang-Fan Huang, Detong Wu, Huakun Zuo,* Meng Wang, Yusheng Hou,* and Bing Shen*

Cite This: https://doi.org/10.1021/acs.nanolett.4c04411

QUESTIONS?