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Proximal Quantum Spin Liquid in One-Dimensional Spin-1/2 Metal Ti_4MnBi_2

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Acknowledgements

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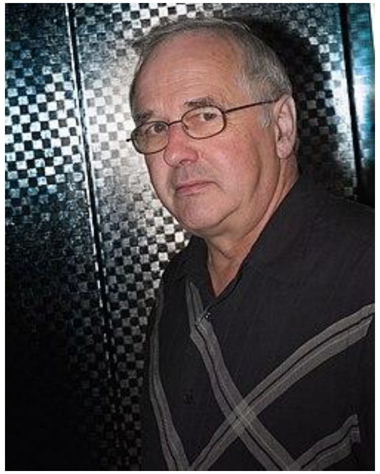

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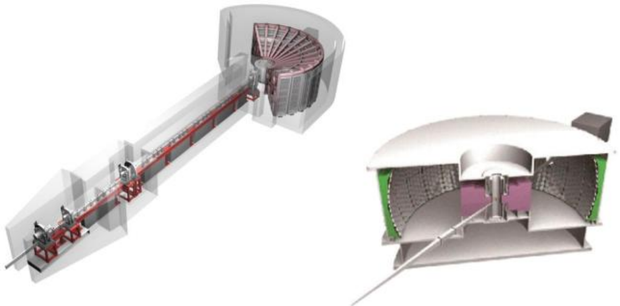
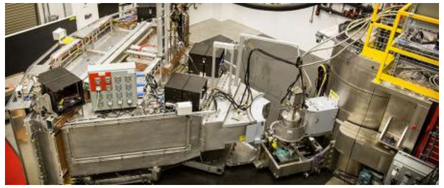


AMATERAS & DNA @ J-PARC



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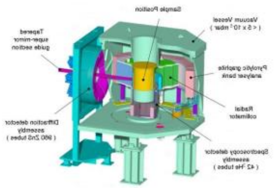


OSIRIS @ ISIS

M20 & M15 @ TRIUMF

Outline

1) Research background

2) Ti_4MnBi_2: A metallic spin S=1/2 J_1-J_2 chain

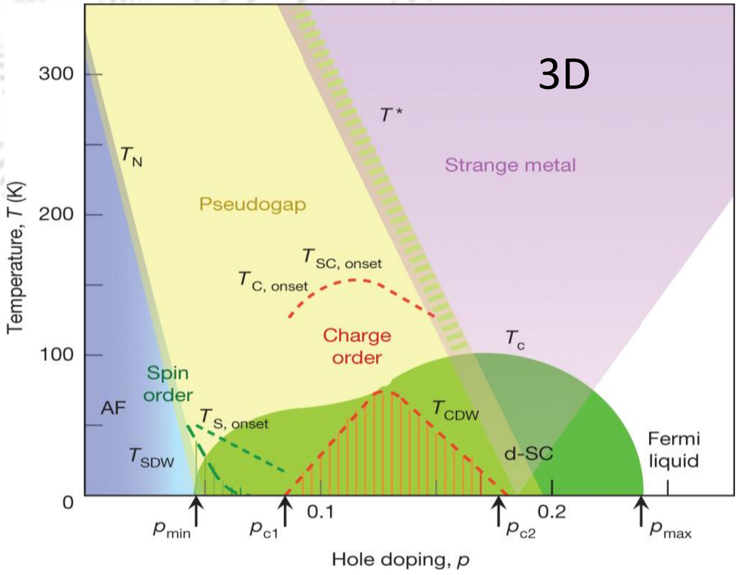
→ INS spin dynamics

3) → µSR spin dynamics

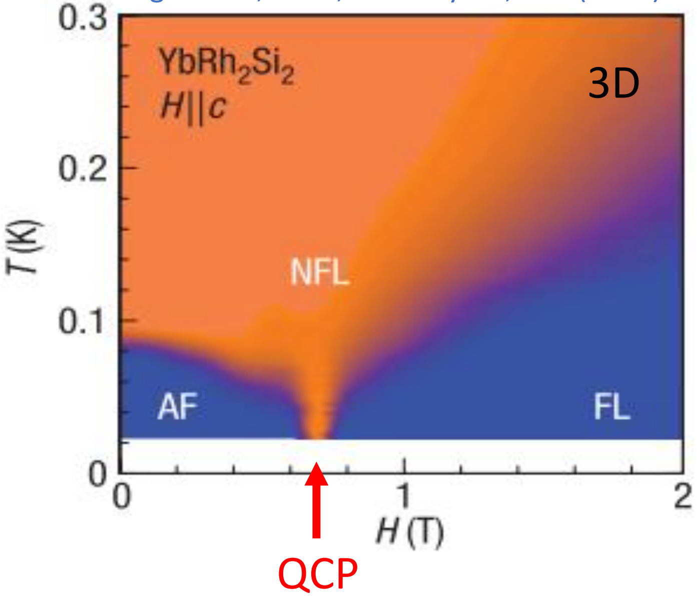
4) Summary

Electronic correlation systems

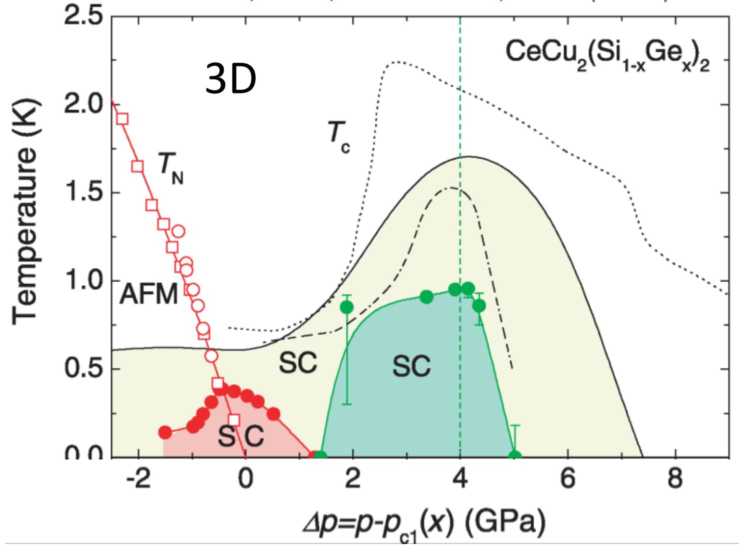
Phase diagram of cuprates.
B. Keimer, *et al.*, Nature **518**, 179 (2015).



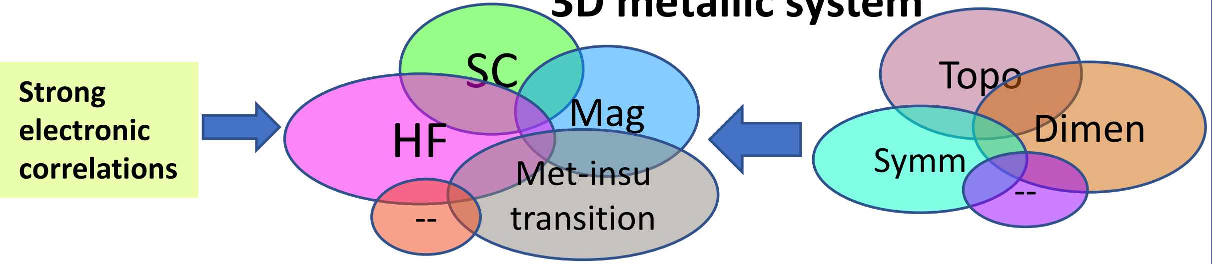
Quantum critical points in heavy fermions.
P. Gegenwart, *et al.*, Nat. Phys. **4**, 186 (2008).



Emergent SC phase in Ce-based metals.
H. Q. Yuan, *et al.*, Science **302**, 2104 (2003).



3D metallic system



➢ **Stability of magnetic order**
→ Competition of interactions
→ Electron delocalization
→ **Spin diso (QSL)**

➢ **Is there an analogous instability in 1D systems?**

→ **lack of correlated metallic spin chains**

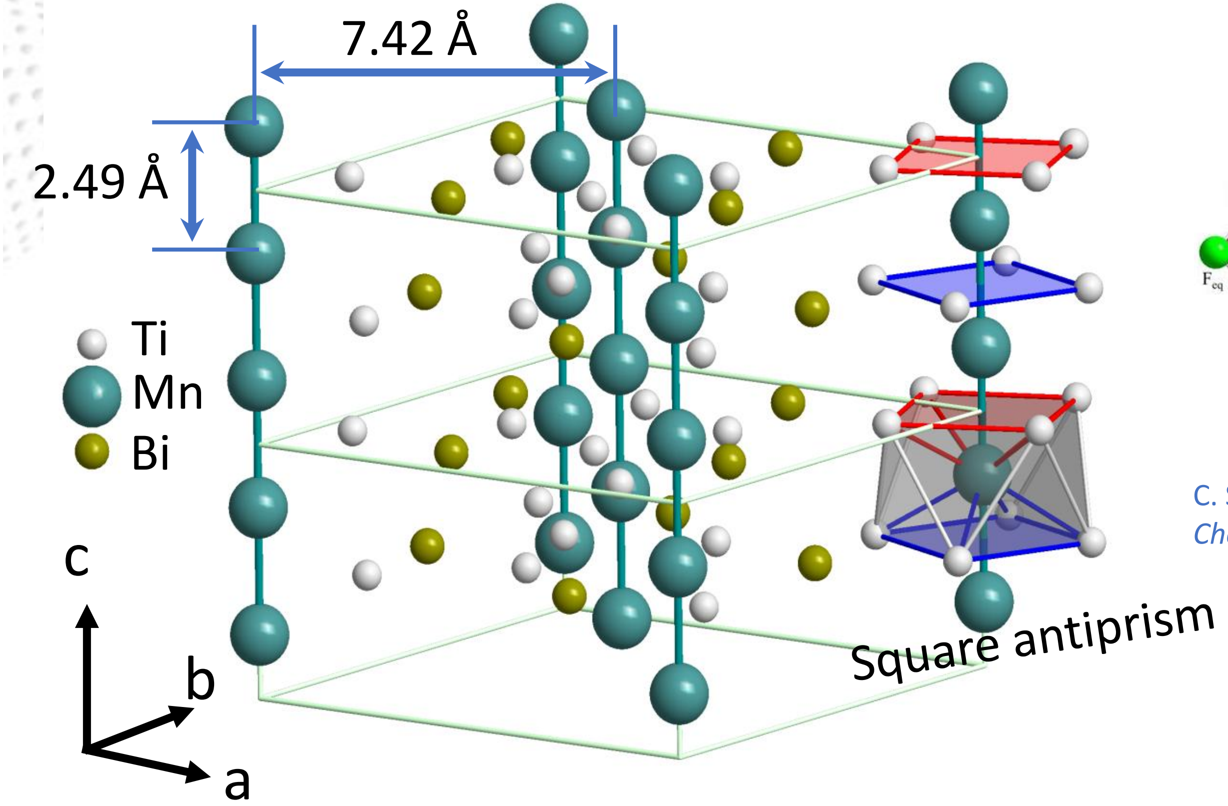
➢ Advantages of studying 1D systems:

❖ Hamiltonian is simpler → computational controllable, precise

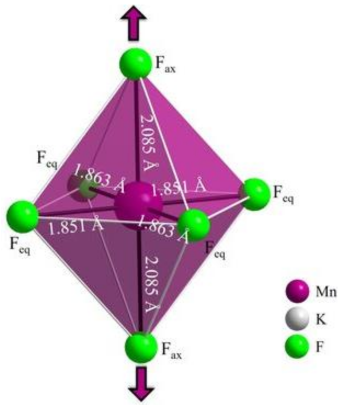
❖ Robustness of 1D characteristics → more accurate Exp vs Theo

Is Ti_4MnBi_2 a S-1/2 AF chain?

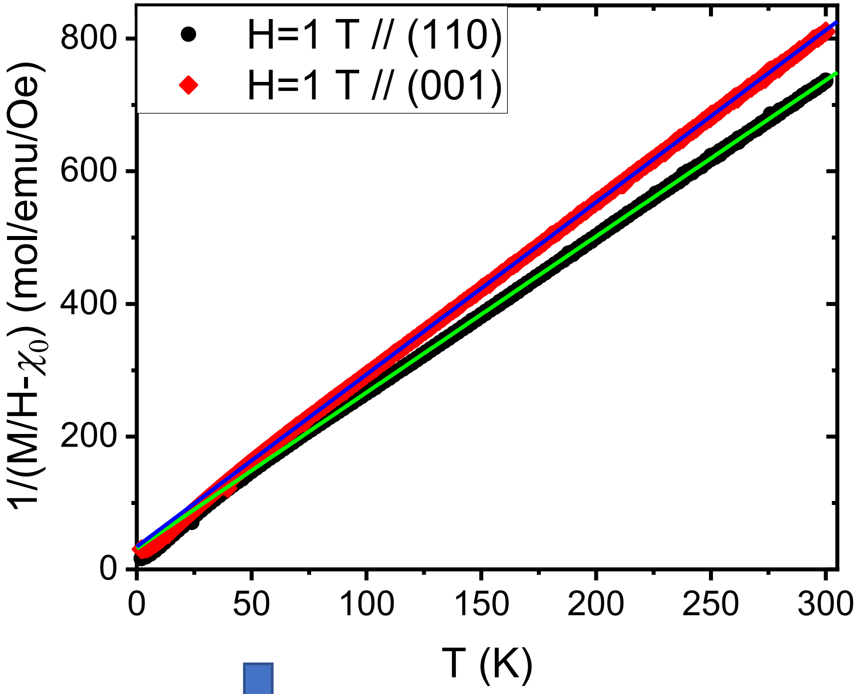
Tetragonal *I*4/*mcm* (No.140)



Octahedral
Mn S=5/2



C. Stoll, *et al.*,
Chem.- Eur. J. **27**, 9801 (2021)



Curie-Weiss fitting

	θ_{CW} (K)	$\mu_{eff} = \sqrt{8C}$ (μ_B/Mn)
H // (110)	**-13.3(2)**	**1.843(2)**
H // (001)	**-13.2(2)**	**1.756(2)**

The small spacing of 2.49(1) Å would ordinarily lead to itinerant magnetism, so, surprisingly, Curie-Weiss fitting gives spin *S* = ½.

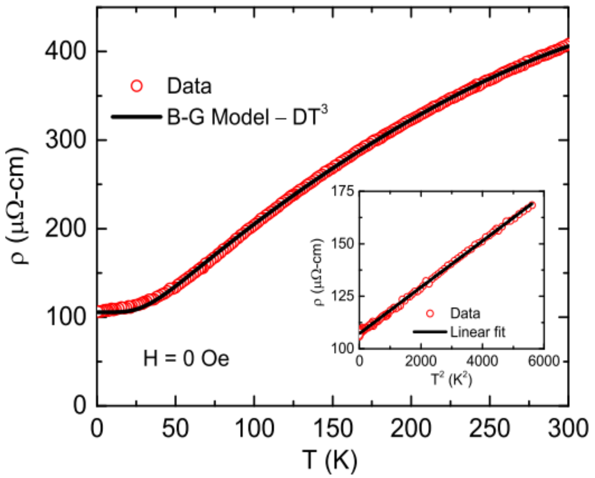
Xiyang Li*, *et al.*, Nature Materials **24,** 716–721 (2025).

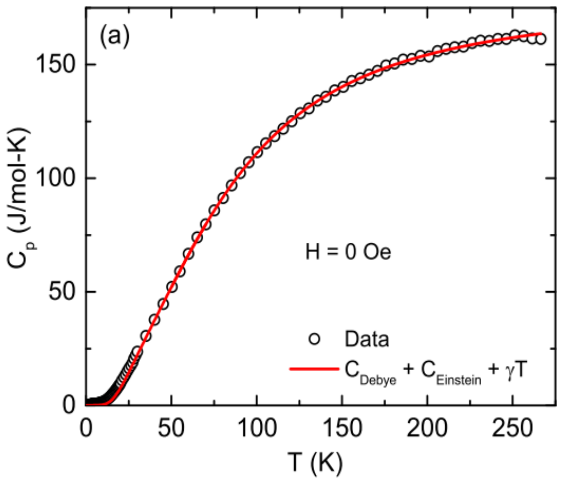
A. Pandey, *et al*. Phys. Rev. B **102**, 014406 (2020).

Ti_4MnBi_2 is a correlated metal

Electrical resistivity and C_P fitting in Ti_4MnBi_2.

A. Pandey, *et al.*, Phys. Rev. B **102**, 014406 (2020).



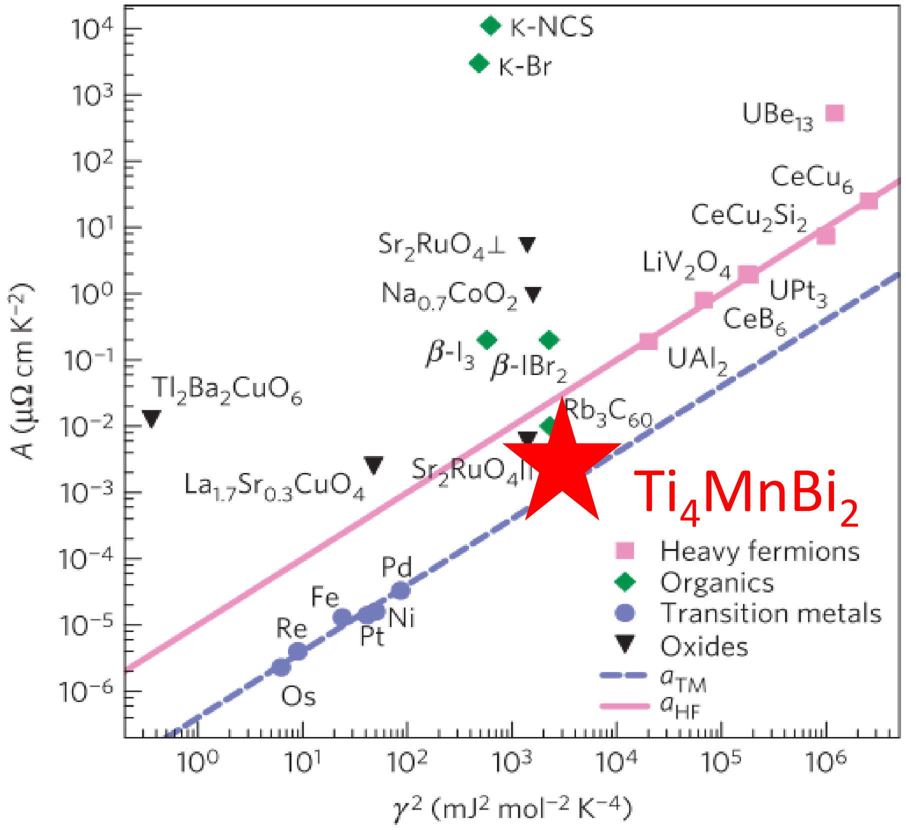


$\rho(T) \sim AT^2$ (A=1.1*10^{-3} μΩ-cm/K^2)

$C \sim \gamma T$ (γ=57 mJ/mol-K^2)

Kadowaki-Woods plots.

A. Jacko, *et al.*, Nat. Phys. **5**, 422 (2009).



✓ Ti_4MnBi_2 is an example of a metallic compound with moderate to strong electronic correlations.

Small spin moment, S-1/2

Low-dimensional, 1D

→ Strong quantum fluctuation → QSL

We have a spin-1/2 metallic compound, Ti_4MnBi_2, with electronic correlations.

Is it really 1D?

Is it QSL?

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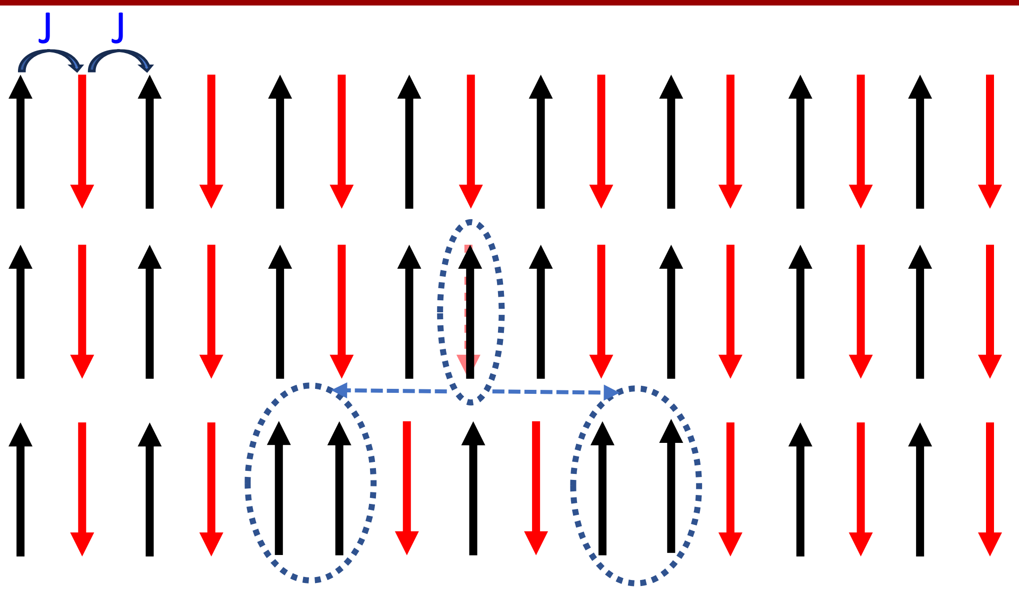
Fractionalized excitations in S=1/2 AF chain: Spinons



Ground state at T=0

Flip one spin cost 2J, ΔS=1

Spin flip propagate to 2 directions, so spinon S=1/2.

des Cloizeaux-Pearson (1962)

Spinon energy: $E_S=\pi J|\sin Q|$
(AF spin wave)

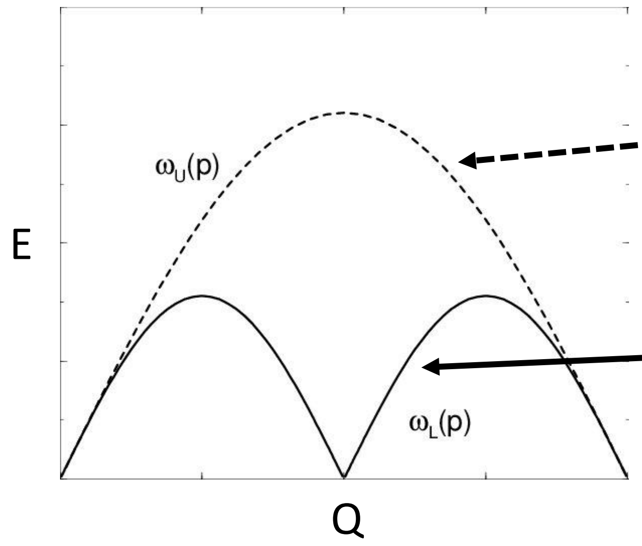
Spinons: $Q=Q_1+Q_2$

$E(Q)= E_S(Q_1)+ E_S(Q_2)$

$$E(Q)= 2\pi J\left|\frac{\sin Q}{2}\right|\left|\cos\left(\frac{Q_1-Q_2}{2}\right)\right|$$

AF Heisenberg Hamiltonian:

$$H = 2J\sum_{i,j} S_i S_j$$



Upper bound: $Q_1=Q_2=Q/2$

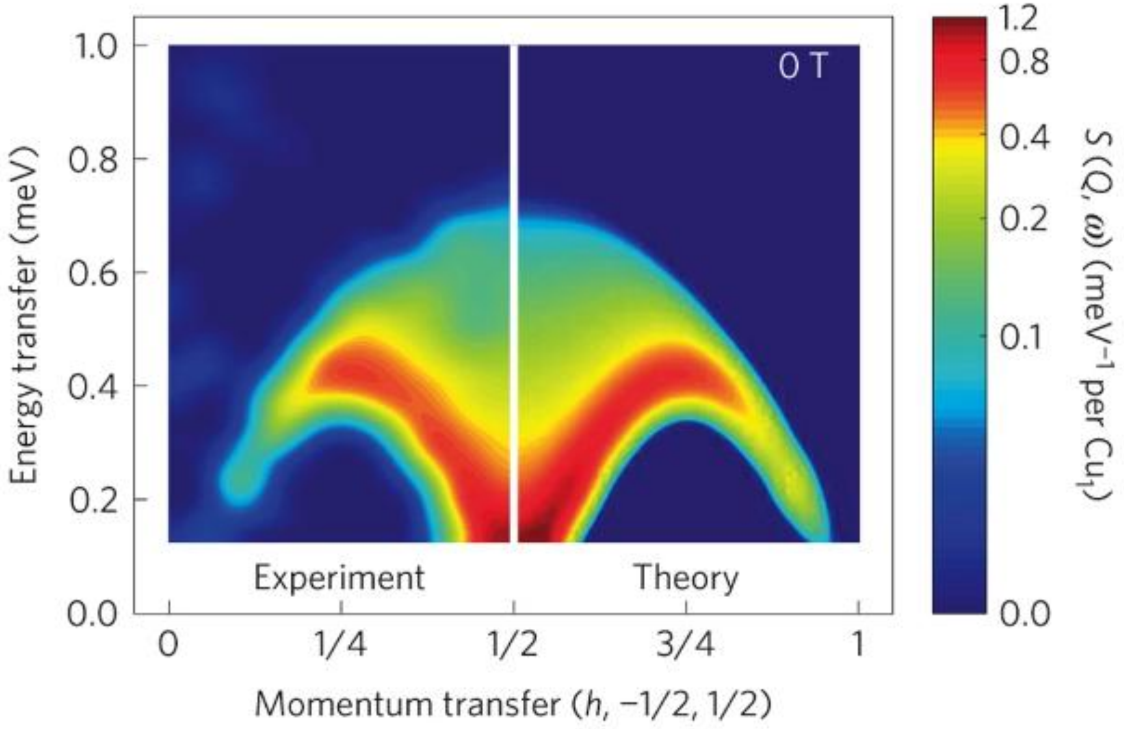
$E(Q)= 2\pi J\left|\sin(\frac{Q}{2})\right|$

Lower bound: $Q_1=Q$, $Q_2=0$
or $Q_1=0$, $Q_2=Q$
$E(Q)= \pi J|\sin Q|$

Spinon in Heisenberg spin-1/2 chains

AF Heisenberg Hamiltonian: $$H = 2J\sum_{i,j} S_i S_j$$

$CuSO_4 \cdot 5D_2O$ $2J = 0.252$ meV

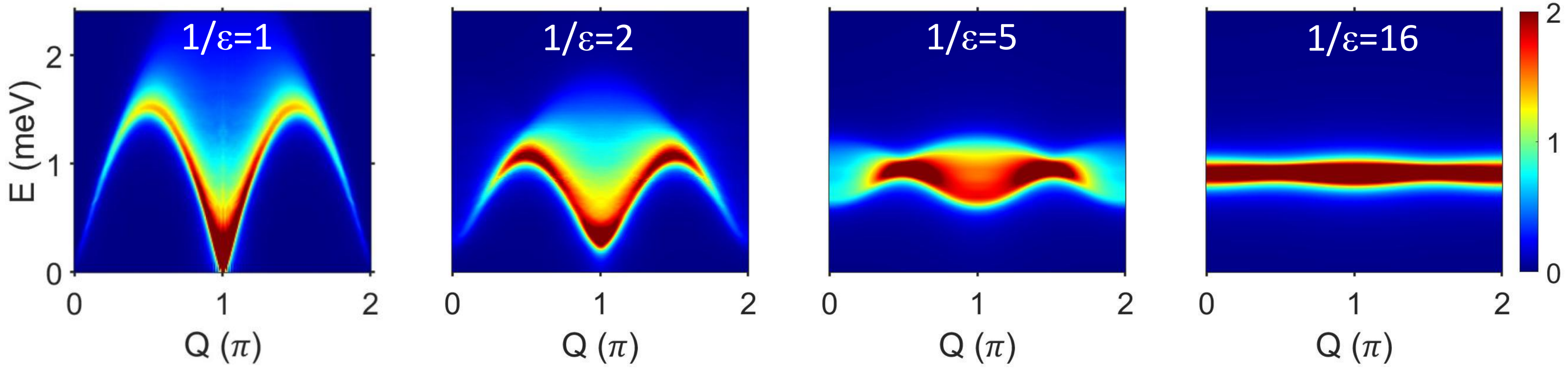


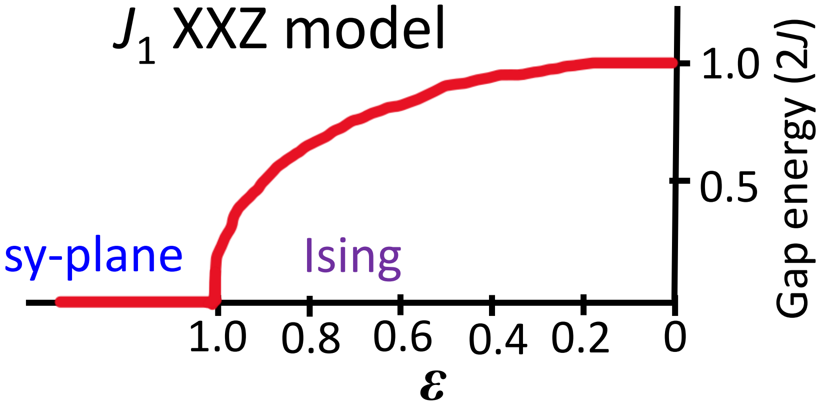
M. Mourigal *et al.*, *Nat Phys* **9**, 435–441 (2013)

Introduce Ising anisotropy in Heisenberg S=1/2 chains

XXZ Hamiltonian: $H = J\sum_i\left[S_i^Z\cdot S_{i+1}^Z + \varepsilon\left(S_i^X\cdot S_{i+1}^X + S_i^Y\cdot S_{i+1}^Y\right)\right]$ Ising-like where ε<1

Transverse $S_{XX}(Q,E)$



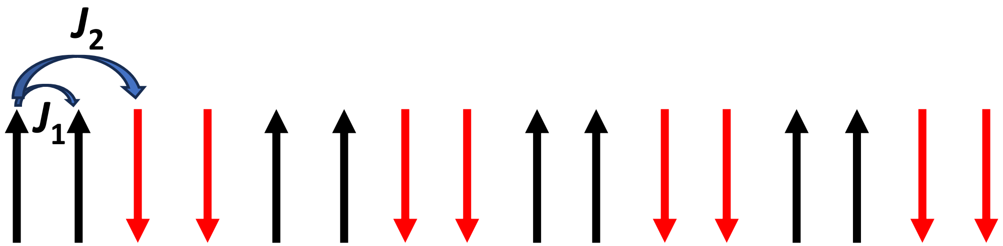


DMRG from A. Nocera. (unpublished)

M. Takahashi, Thermodynamics of One-dimensional Solvable Models, Cambridge (1999)

Introduce J_2 in Ising-like Heisenberg S=1/2 chains

Add second nearest neighbor interaction



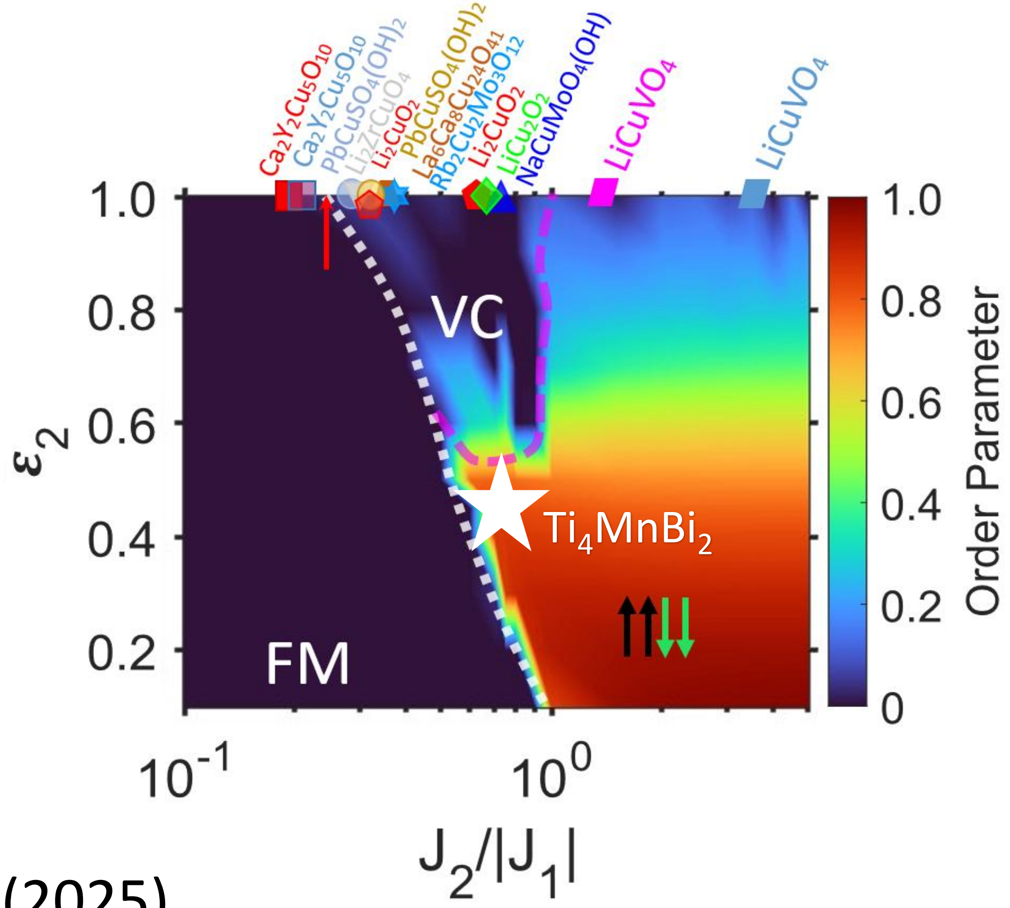
J_1-J_2 XXZ Hamiltonian:

$$H = J_1 \sum_n [S_n^z \cdot S_{n+1}^z + \varepsilon_1 (S_n^x \cdot S_{n+1}^x + S_n^y \cdot S_{n+1}^y)]$$

$$+J_2 \sum_n [S_n^z \cdot S_{n+2}^z + \varepsilon_2 (S_n^x \cdot S_{n+2}^x + S_n^y \cdot S_{n+2}^y)]$$

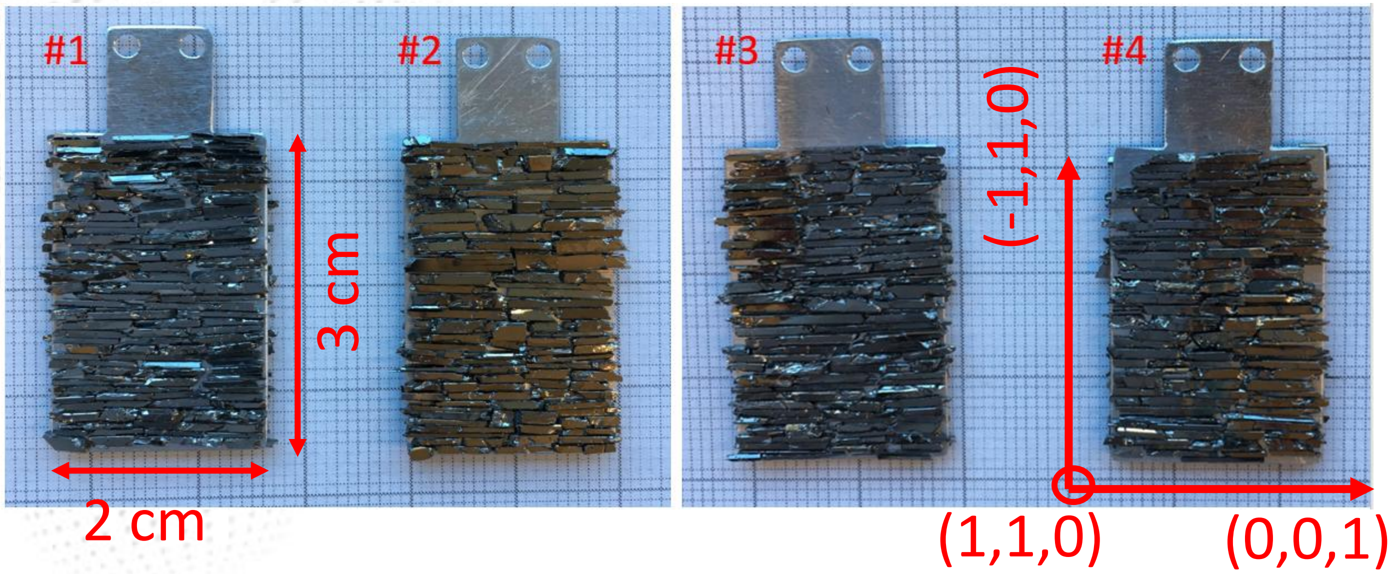
where J_1<0 is FM, and J_2>0 is AFM

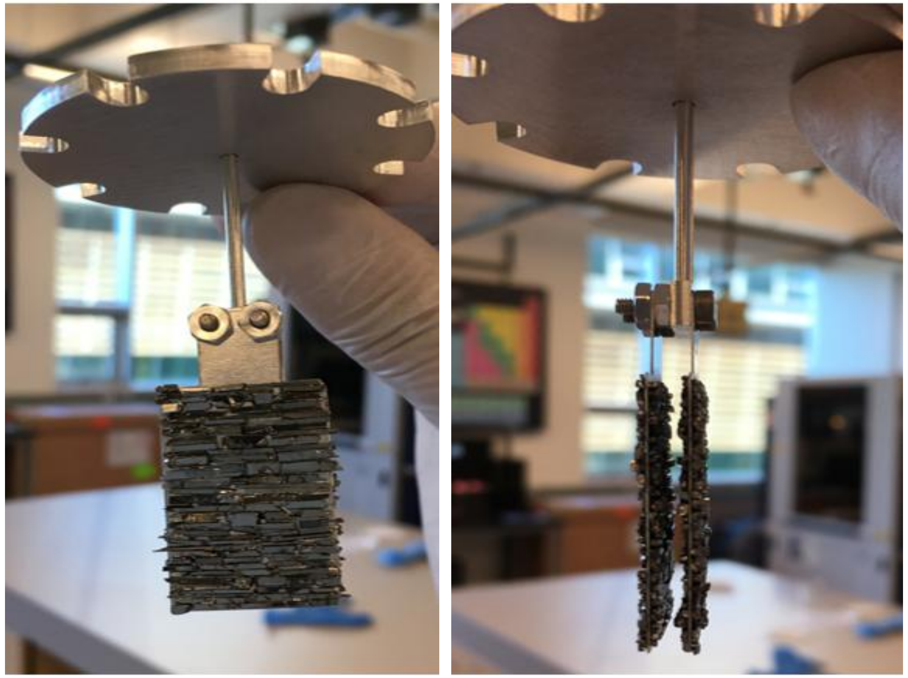
→ Frustrated spin-1/2 XXZ chains



Xiyang Li*, *et al.*, Nature Materials **24**, 716–721 (2025).

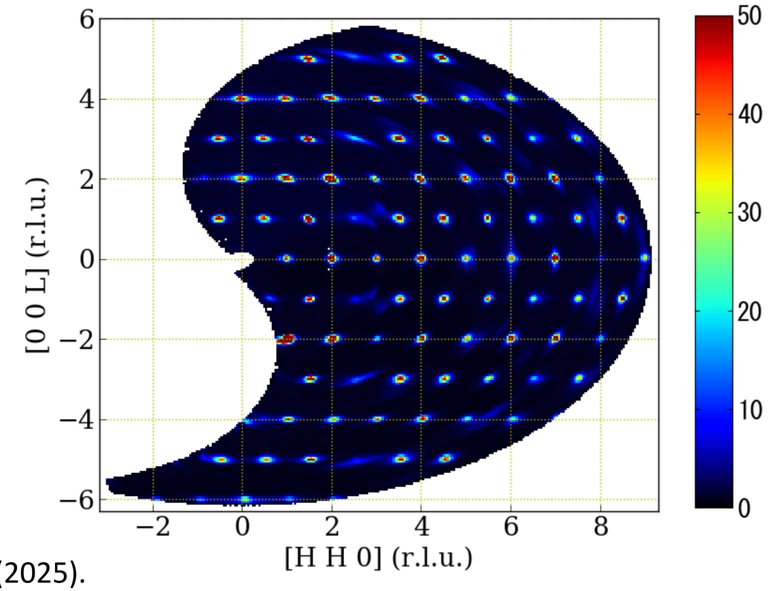
Ti_4MnBi_2 neutron scattering sample

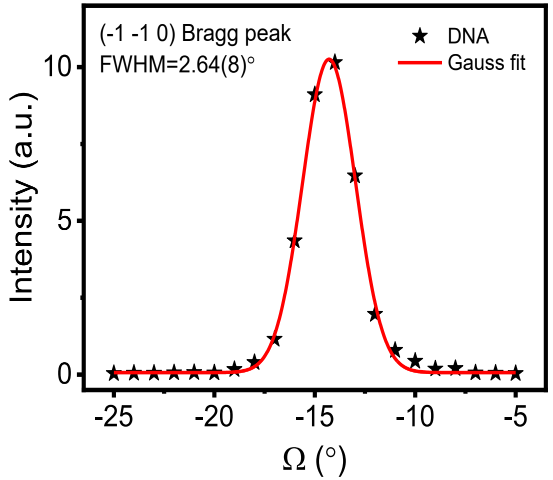




~ 400 single crystals,
Mass: 10.2 g,
0.3 mm Al sheet,
Cytop glue

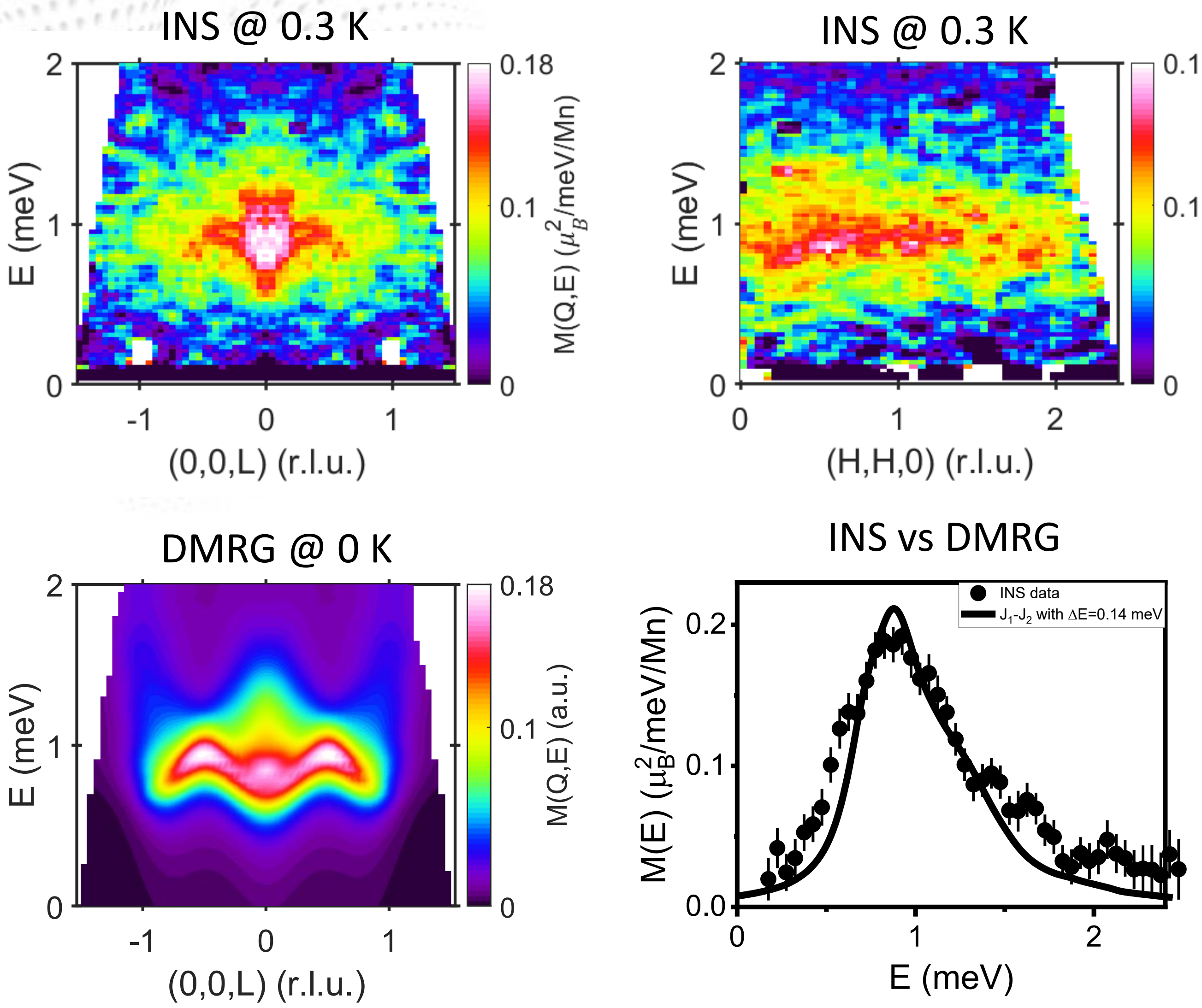
Spent half a year
growing this sample.





Xiyang Li*, *et al.*, Nature Materials **24,** 716–721 (2025).

Ti_4MnBi_2: 1D Ising-like J_1-J_2 model



- ✓ INS established spinon excitations → 1D.

J_1-J_2 XXZ Hamiltonian:

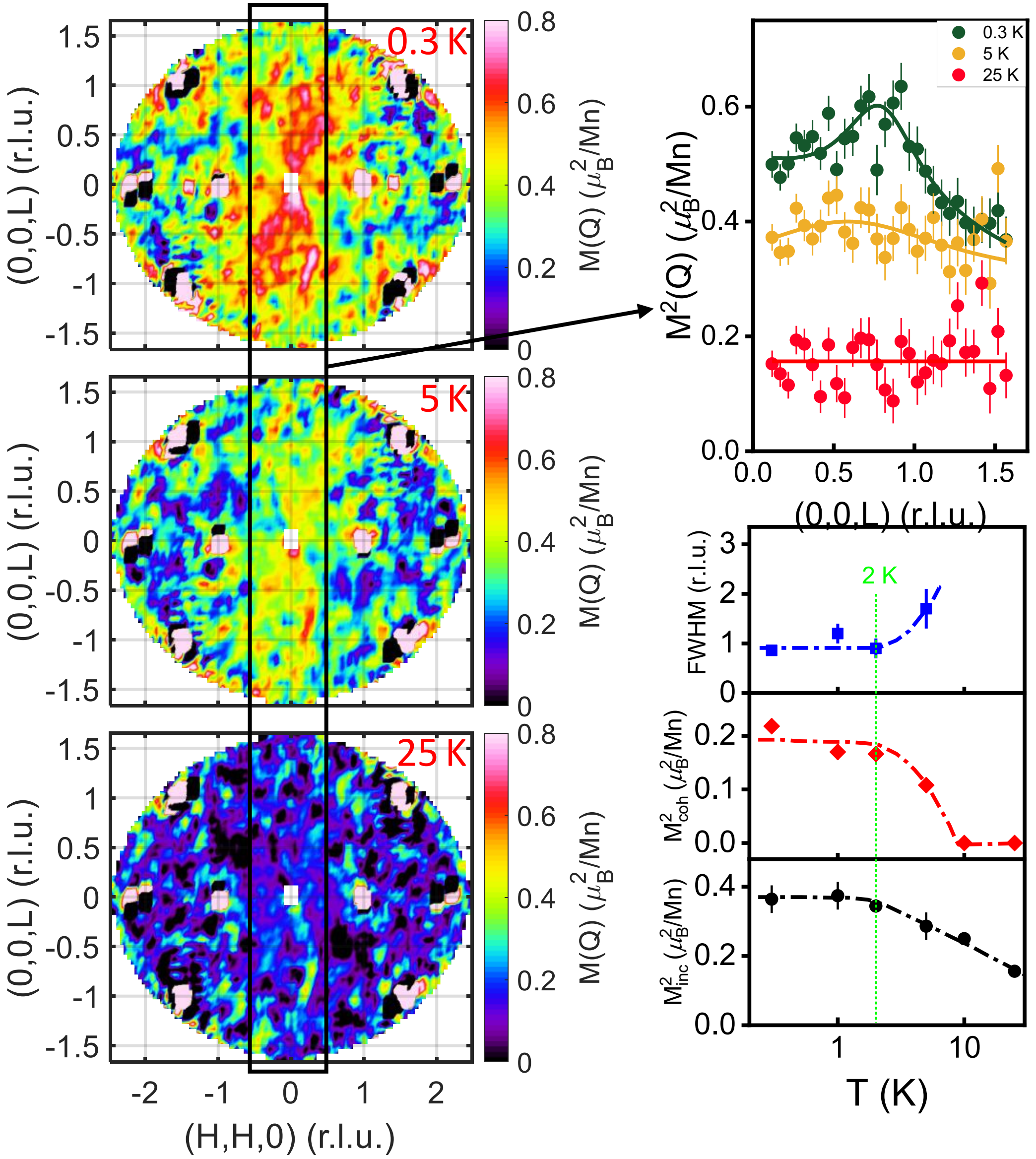
$$H = J_1 \sum_n [S_n^z \cdot S_{n+1}^z + \varepsilon_1 (S_n^x \cdot S_{n+1}^x + S_n^y \cdot S_{n+1}^y)]$$
$$+ J_2 \sum_n [S_n^z \cdot S_{n+2}^z + \varepsilon_2 (S_n^x \cdot S_{n+2}^x + S_n^y \cdot S_{n+2}^y)]$$

Fitted parameters:
J_1=-2.8 meV
J_2=2.1 meV
ε_2=0.425

- ✓ Frustrated J_1-J_2 S = 1/2 XXZ chain.

Xiyang Li*, *et al.*, Nature Materials **24,** 716–721 (2025).

Emerging magnetic correlations in Ti_4MnBi_2



- ✓ No long-range magnetic order.
- ✓ Short-range magnetic correlation emerging.
- ✓ The M^2_{coh} and M^2_{inc} increase as T ~ 2 K.
- ✓ FWHM ~ 1 r.l.u. → the spatial correlations never extend significantly beyond the unit cell.

Did we find a QSL candidate?

Xiyang Li*, *et al.*, Nature Materials **24,** 716–721 (2025).

Outline

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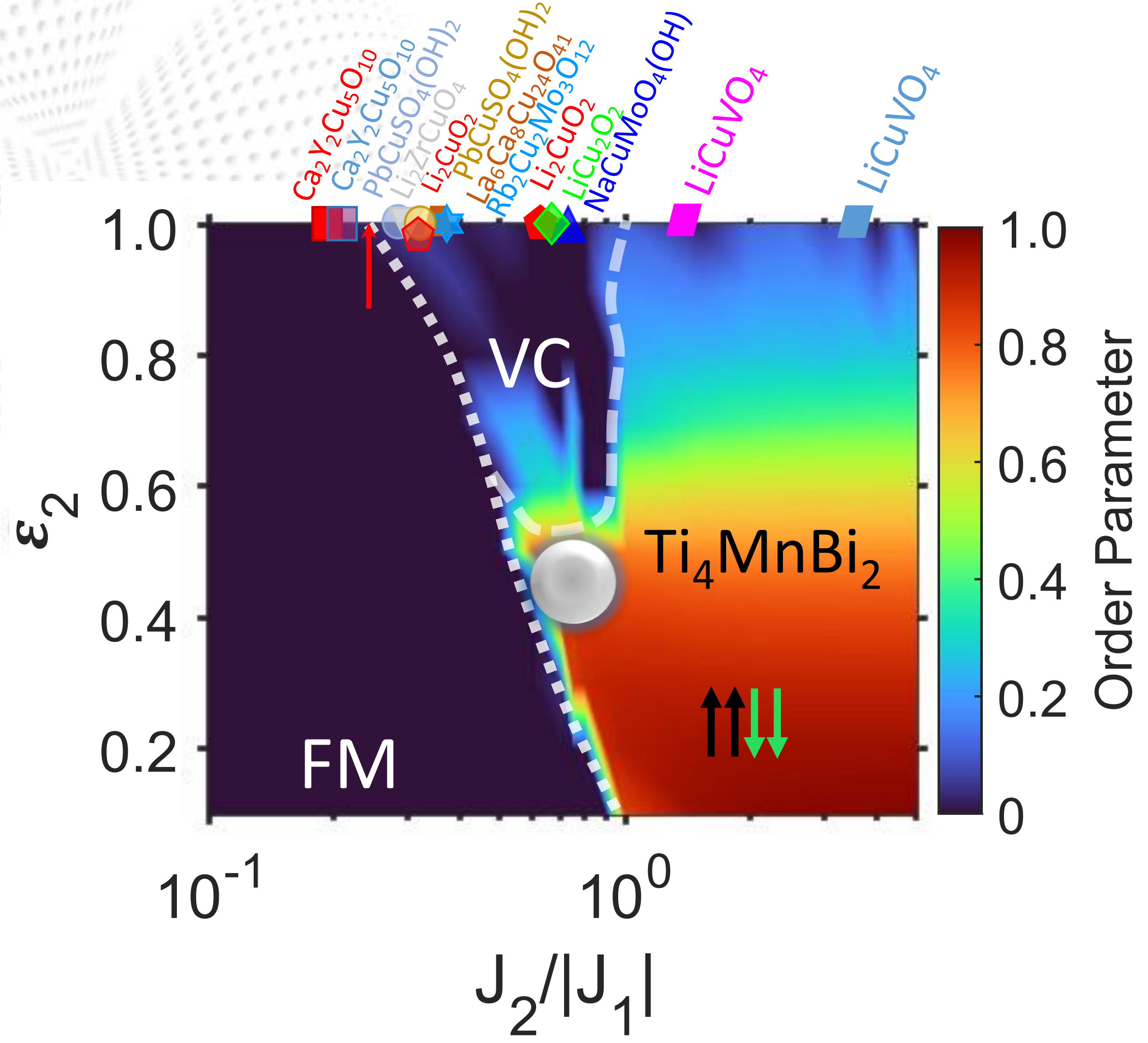
4) Summary

Xiyang Li*, *et al.*, In preparation

Summary



- Ti_4MnBi_2 is inherently frustrated, forming near a quantum critical point separating different temperature $T = 0$ phases of the J_1-J_2 XXZ model.
- Ti_4MnBi_2 is the first metallic spin chain where 3D conduction electrons become strongly correlated due to their coupling to 1D magnetic moments.
- Ti_4MnBi_2 is a QSL candidate.

Xiyang Li*, *et al.*, Nature Materials **24,** 716–721 (2025).

Li Xiyang

北京 海淀

扫一扫上面的二维码图案，加我为朋友。

Thanks for your attention.