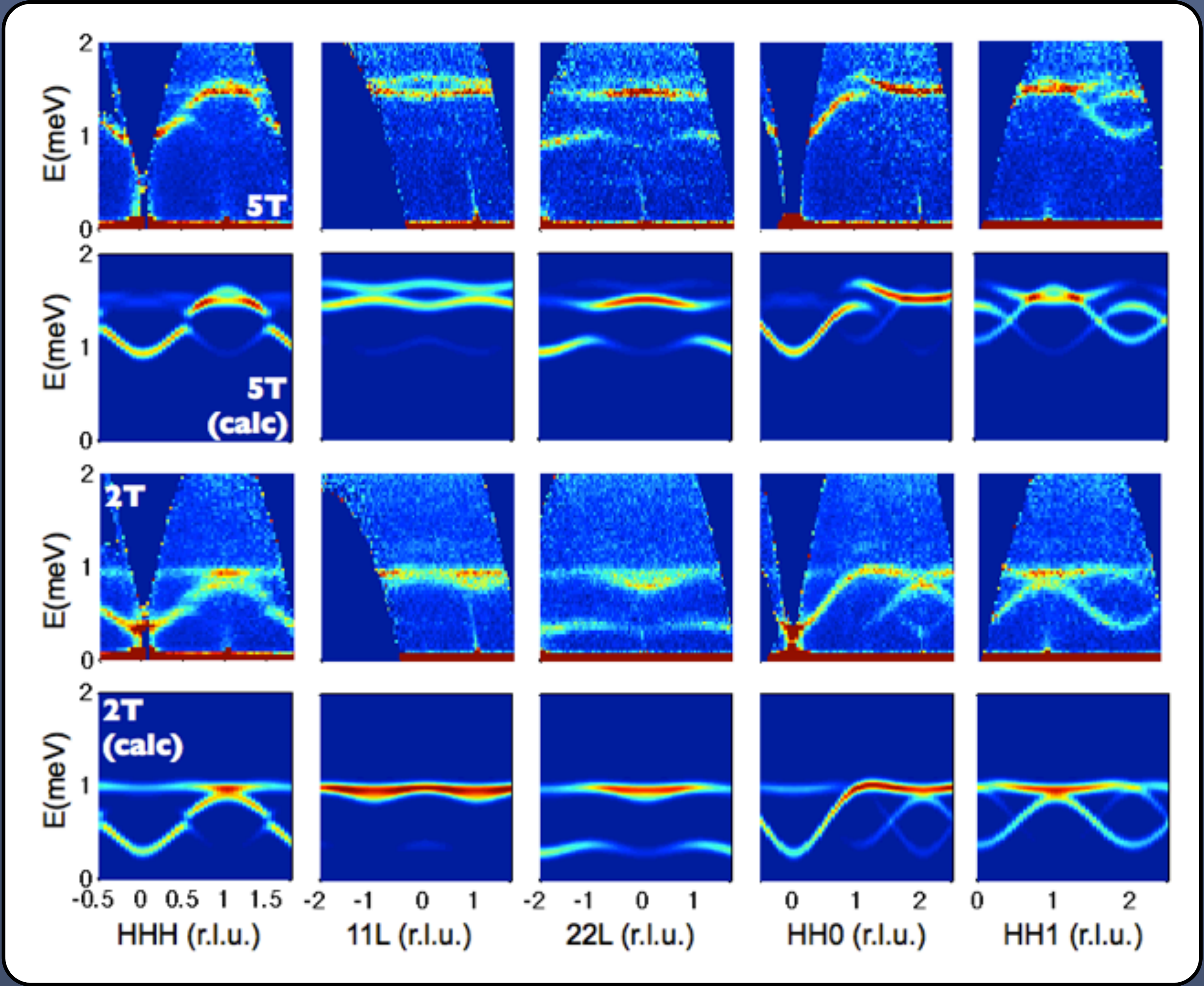
“Quantum Spin Ice” Physics Determined from High Field Spin Waves in $Yb_2Ti_2O_7$



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Collaborators

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Carl Adams
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Paul Scherrer Institut

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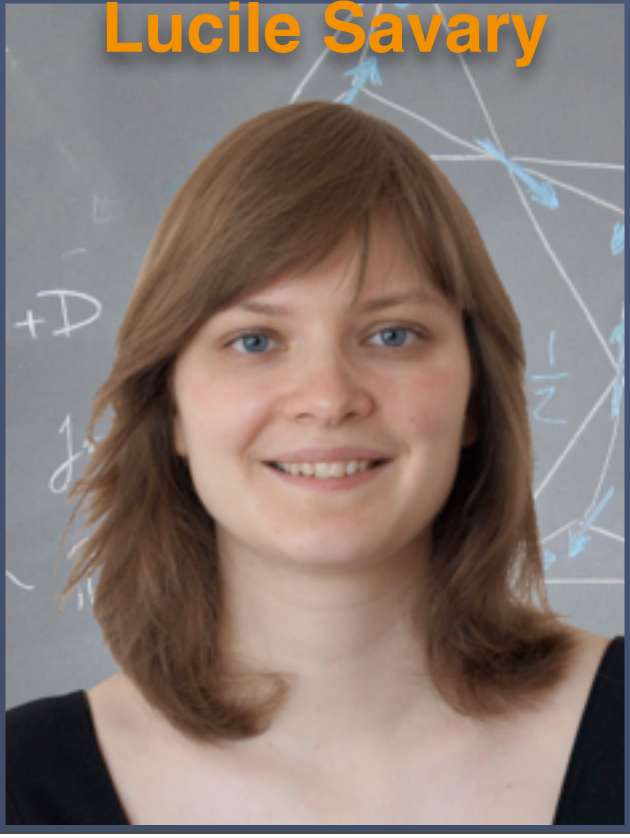
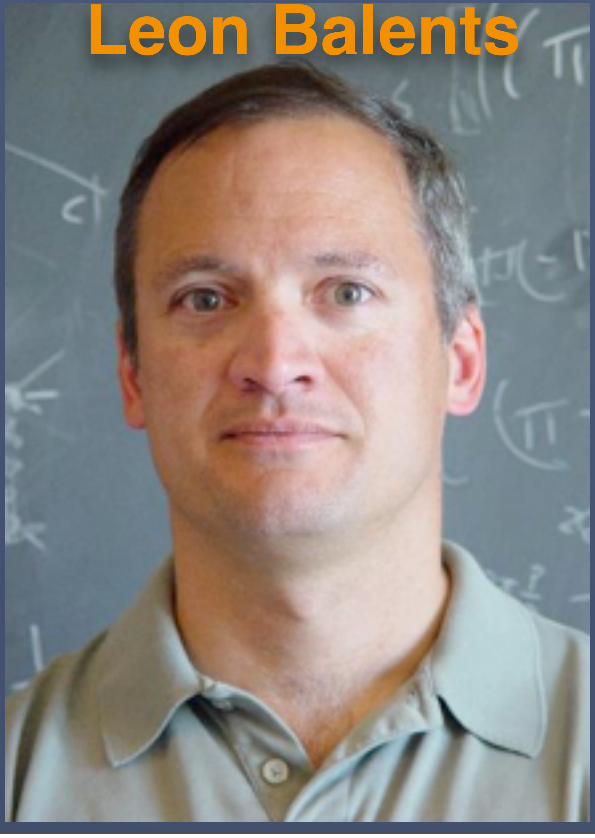
Los Alamos

Thomas Proffen



Lucile Savary



Leon Balents

Bruce Gaulin

Outline

Rare Earth Titanate Pyrochlores

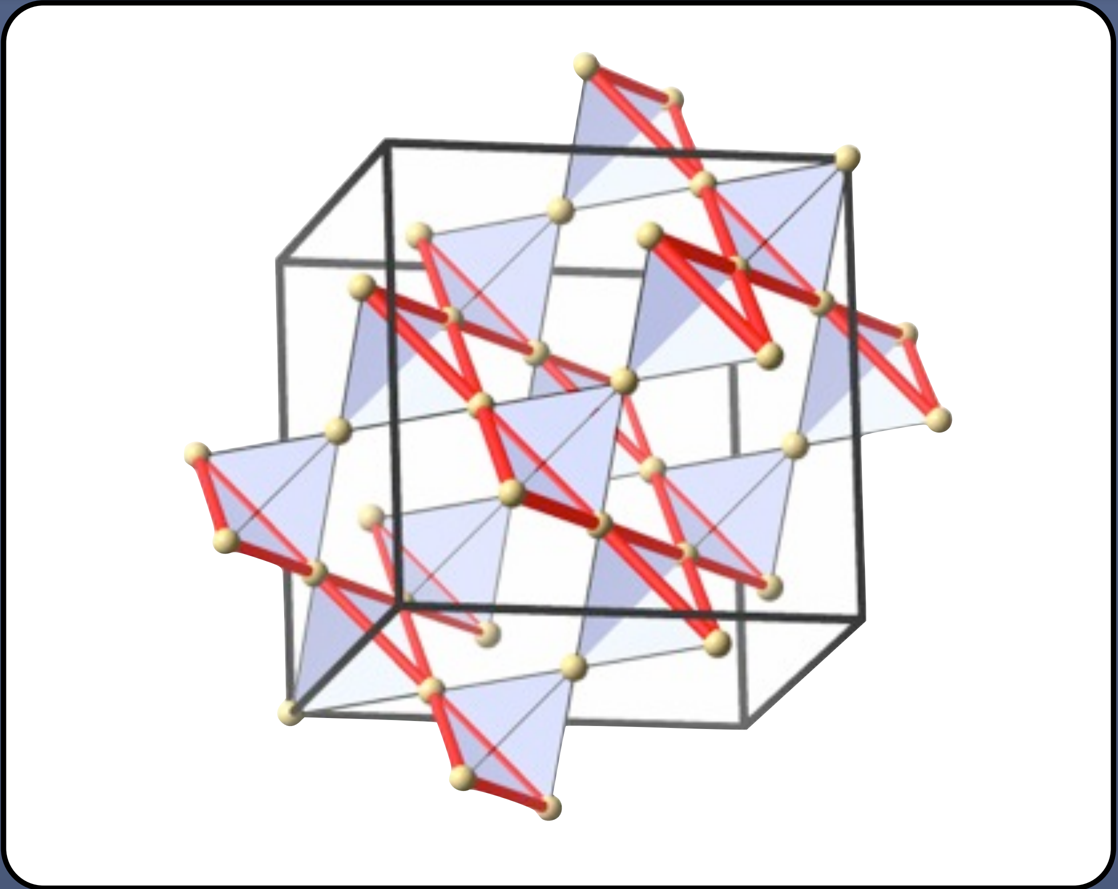
$Yb_2Ti_2O_7$ bulk properties and an “unusual” transition

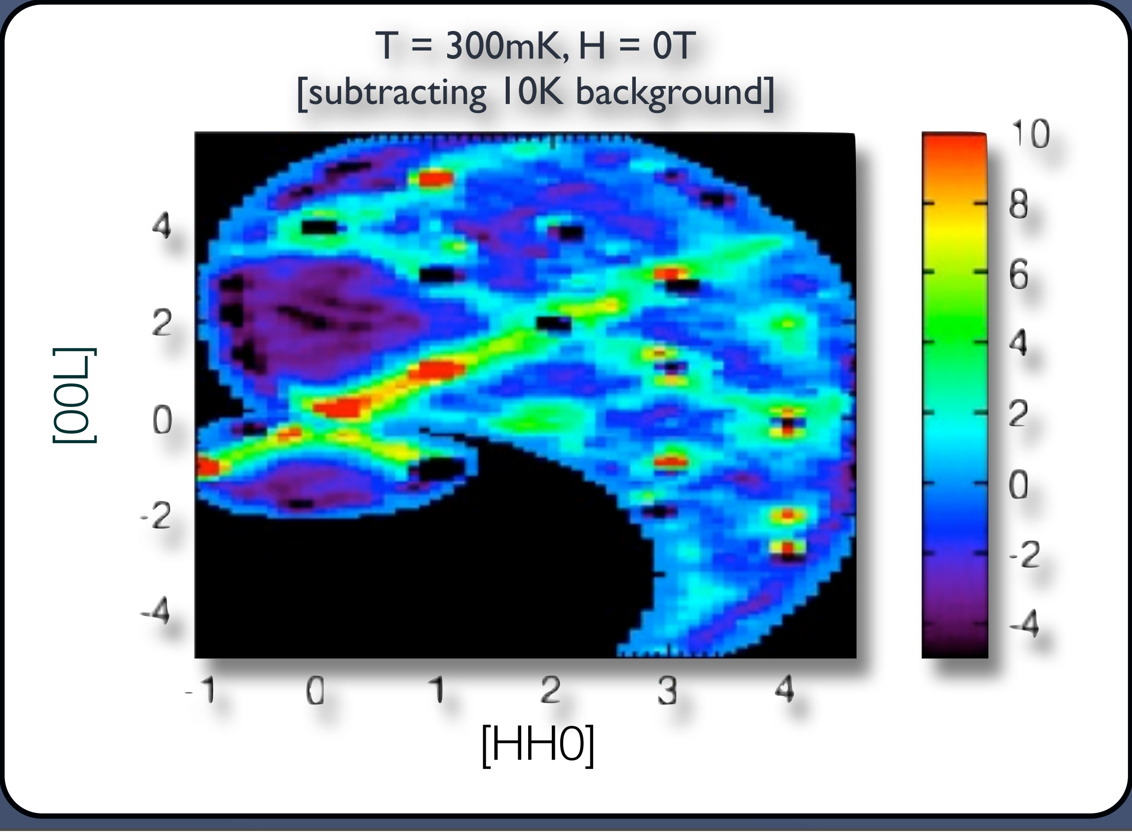
Nature of Spin Correlations

Sensitivity of transition to subtle disorder

Anisotropic Exchange Hamiltonian Determined

$Yb_2Ti_2O_7$ as a Quantum Spin Liquid?





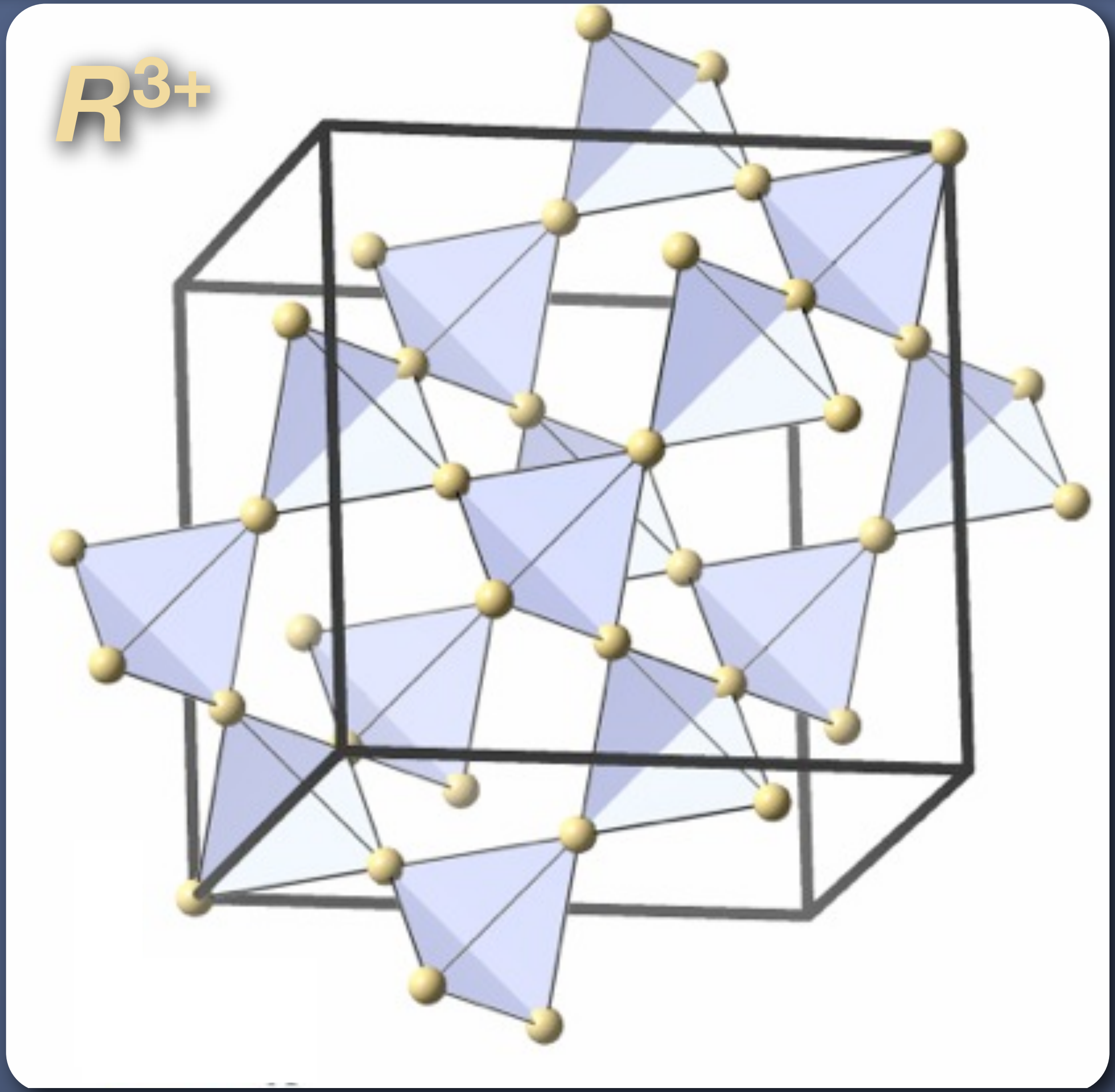
Real Pyrochlores

$R_2Ti_2O_7$

"Rare earth titanates"

Single-ion Anisotropy:
Crystal Field Effects

Exchange Anisotropy:
Spin orbit coupling



$$R^{3+} = \left\{ \begin{array}{l} \mathrm{Ho} \\ \mathrm{Dy} \\ \mathrm{Er} \\ \mathrm{Tb} \\ \mathrm{Yb} \end{array} \right.$$

Ho, Dy → Spin Ice, emergent "Magnetic Monopoles", coulomb phase

Er → Quantum order by disorder

Tb → Spin Liquid

Yb → Low-Dimensional Correlations, Quantum Spin Ice,
Coulomb phase?

Crystal Field Splitting and Effective Spins

$Yb_2Ti_2O_7$

Malkin et al, PHYSICAL REVIEW B **70**, 075112 (2004)

$g_{||}$ = 1.78
$g_{\perp}$ = 4.28

$Ho_2Ti_2O_7$

Malkin et al, PHYSICAL REVIEW B **70**, 075112 (2004)

$g_{||}$ = 19.0
$g_{\perp}$ = 0

At low temperatures, ignore higher levels:
Ground state doublet → effective S = 1/2

Crystal Field Splitting and Effective Spins

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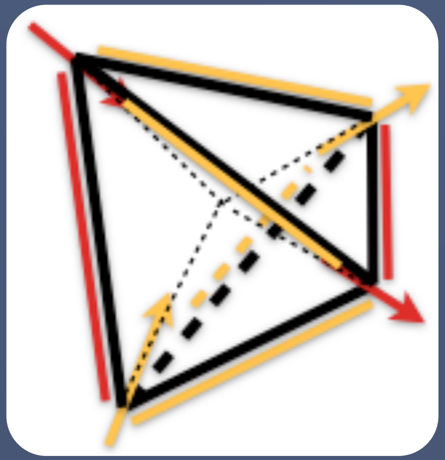

$g_{||} = 19.0$

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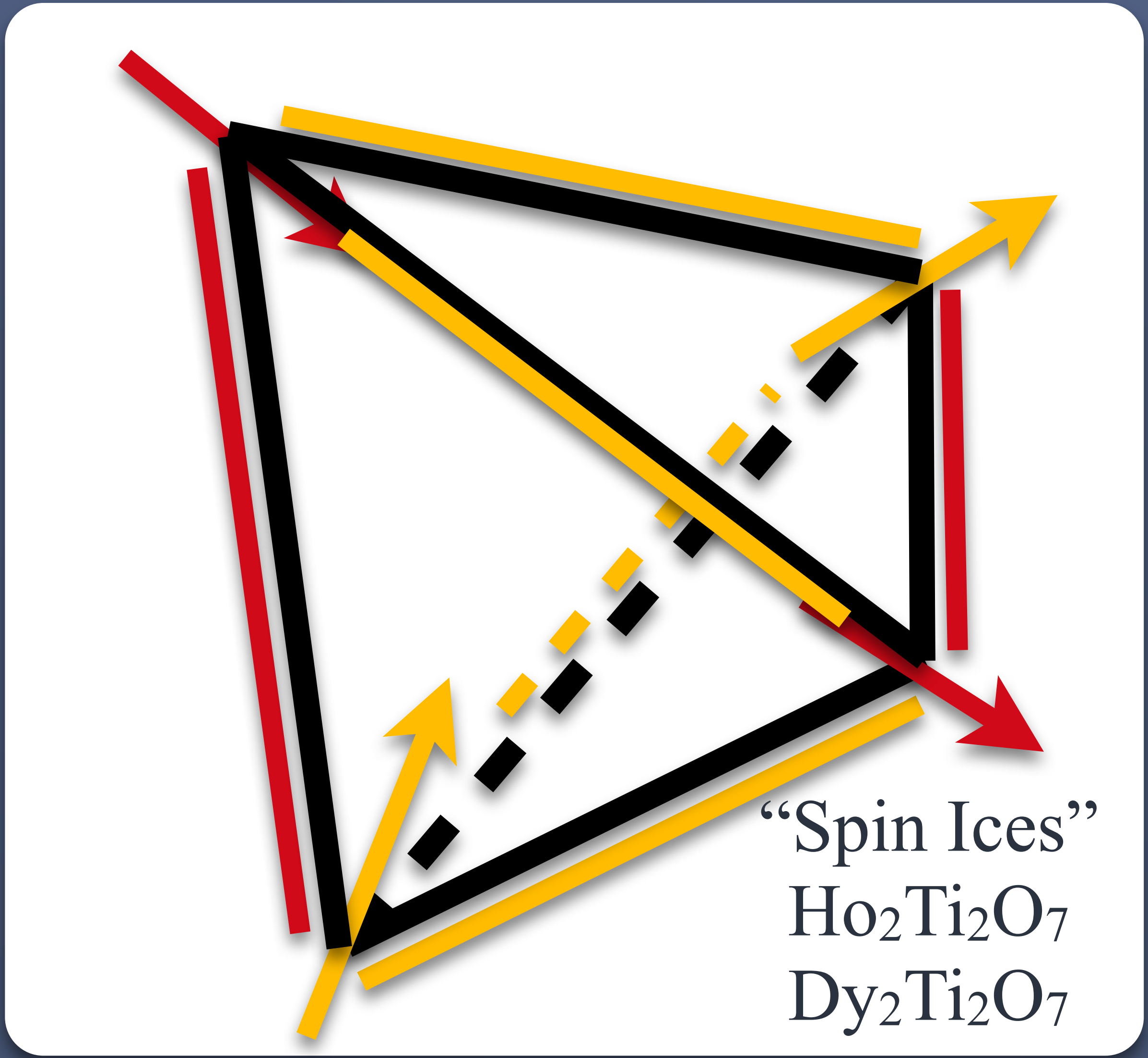
At low temperatures, ignore higher levels:

Ground state doublet → effective $S = 1/2$

Ferromagnetic *Local* Ising Pyrochlore



Ferromagnetic
Easy Axis Anisotropy in Hamiltonian

Local ferromagnetic Ising model maps onto *global* anti-ferromagnetic Ising model.

Frustrated!

$$H=\frac{D}{2}\sum_{K,\kappa}(\hat{\mathbf{d}}_\kappa\cdot\mathbf{S}_{K,\kappa})^2+J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j$$

$$\updownarrow$$

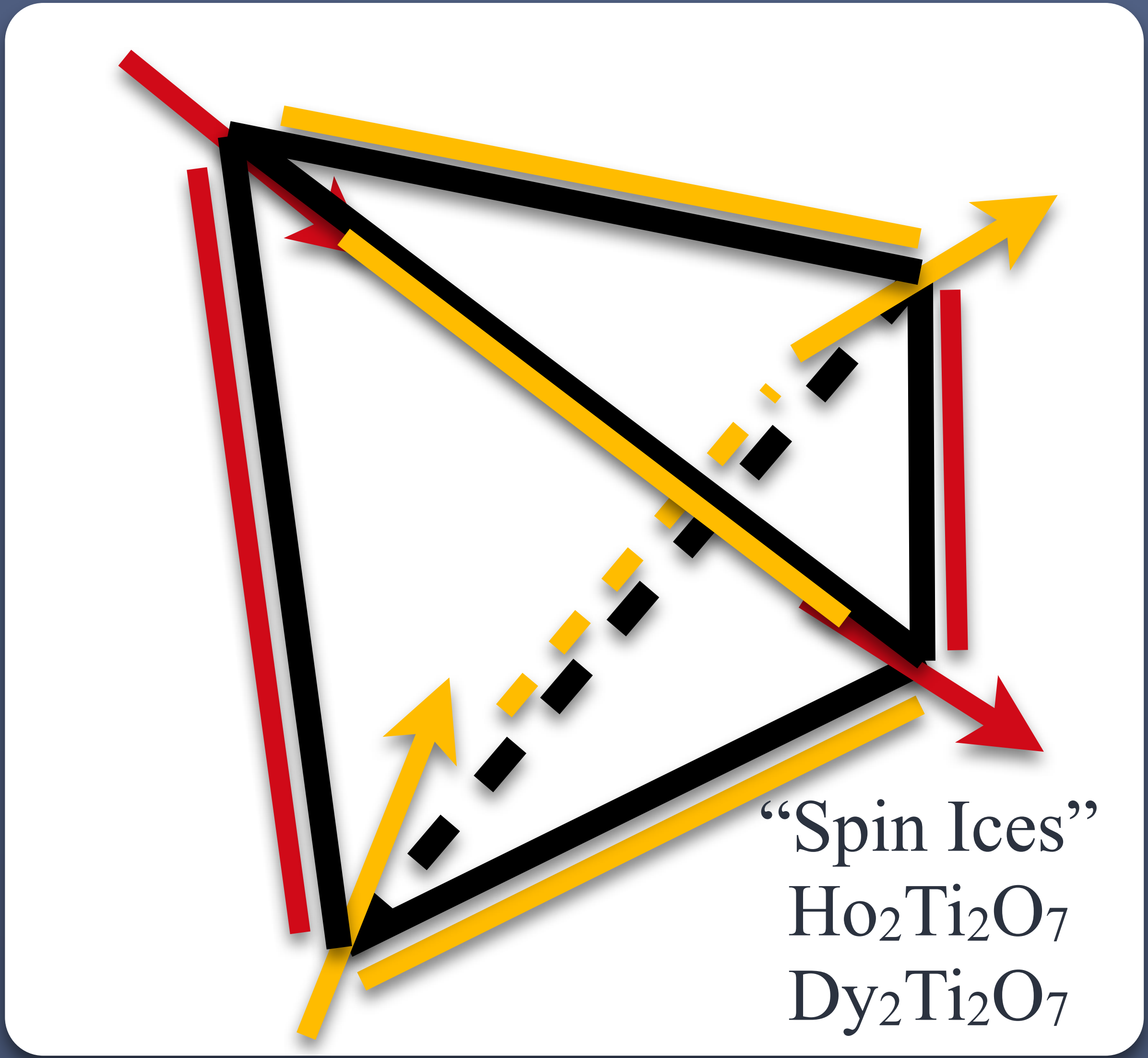
$$H=DN-\frac{J}{3}\sum_{\langle i,j\rangle}T_iT_j$$

R. Moessner, Physical Review B 57, 5587 (1998).

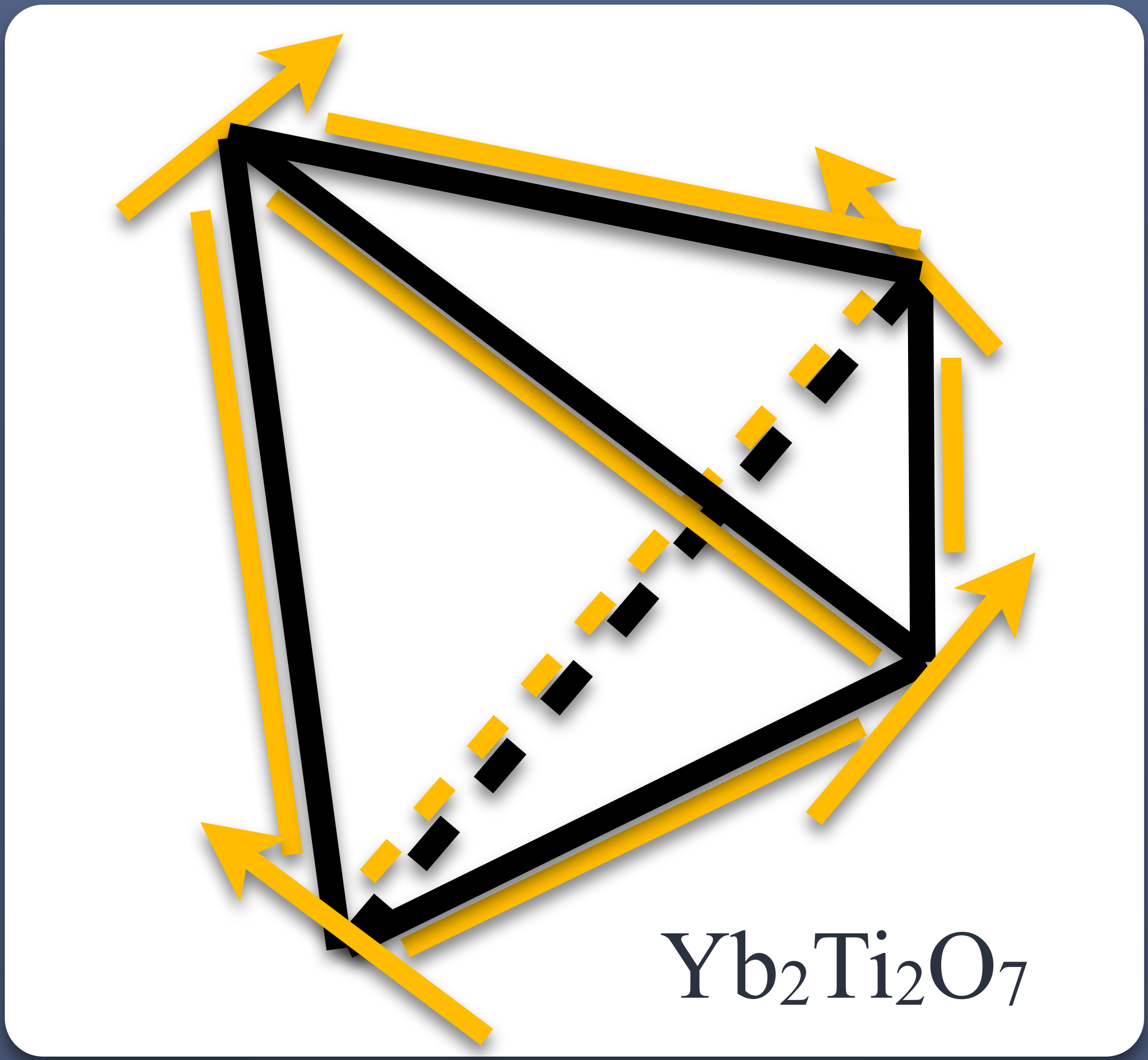
D is the strength of anisotropy

T_i is an Ising variable: +1 or -1 for spin pointing in or out

Two Ferromagnetic Cases


“Spin Ices”
$Ho_2Ti_2O_7$
$Dy_2Ti_2O_7$

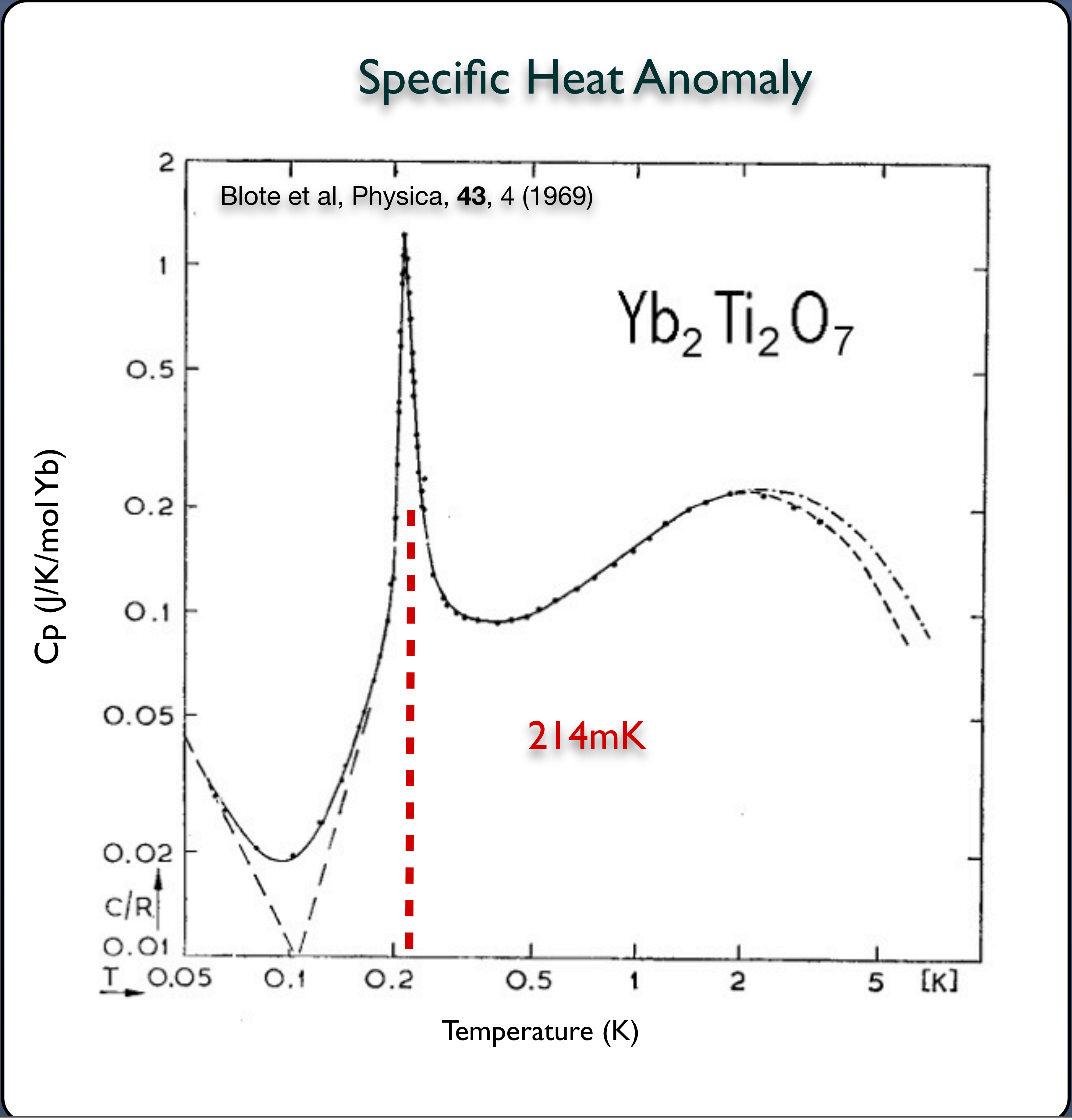
Ferromagnetic
Easy Axis Anisotropy in Hamiltonian

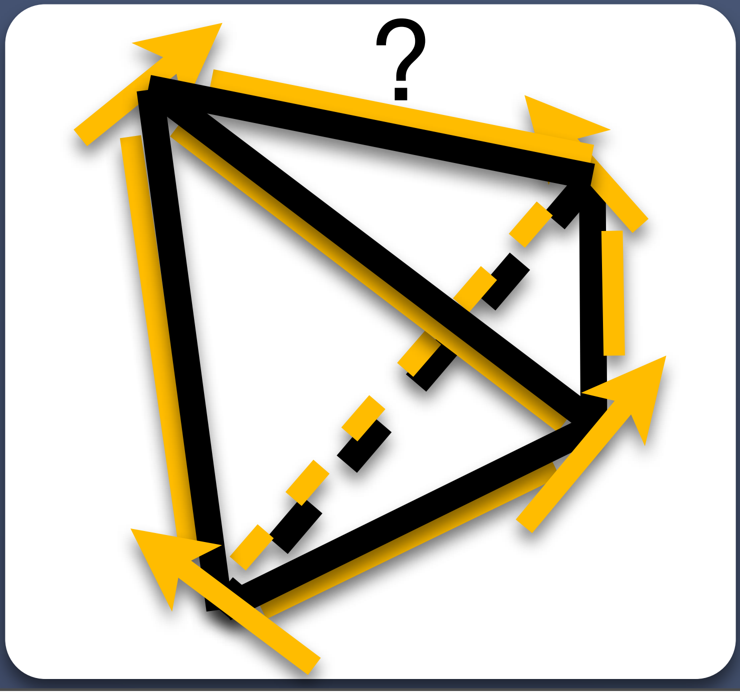

$Yb_2Ti_2O_7$

Ferromagnetic
Easy-Plane (XY) anisotropy

- ➡ $\theta_{cw} \approx [400mK, 800mK]$
- ➡ $g_{xy} = 4.3, \; g_z = 1.8$

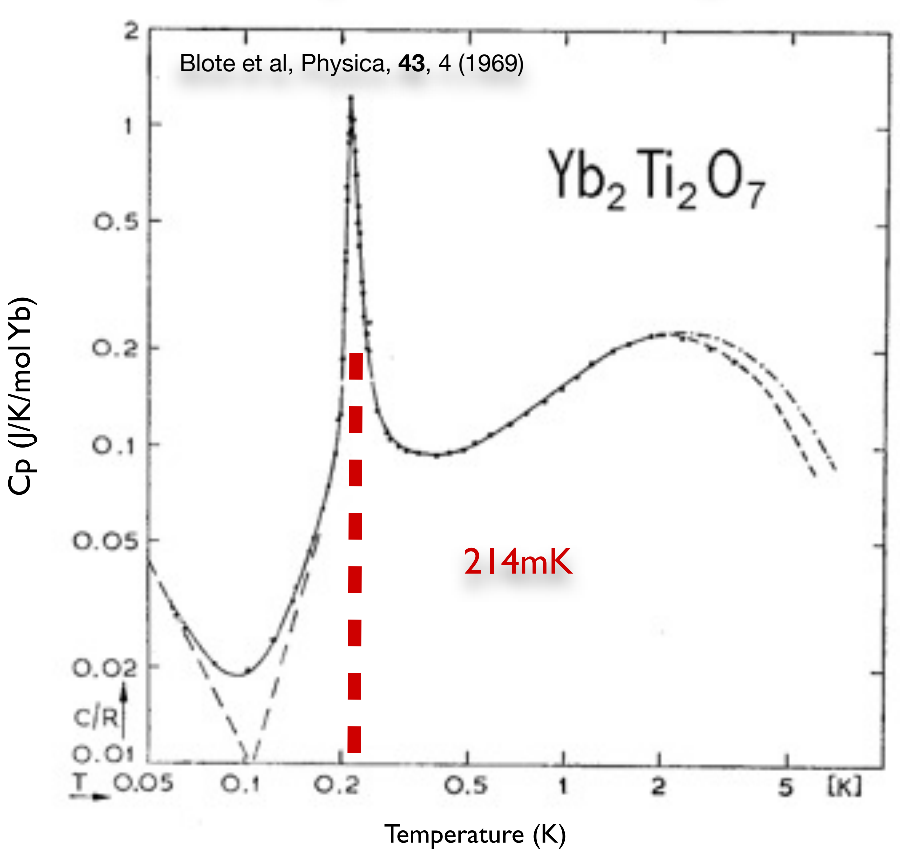
Does $Yb_2Ti_2O_7$ Order?





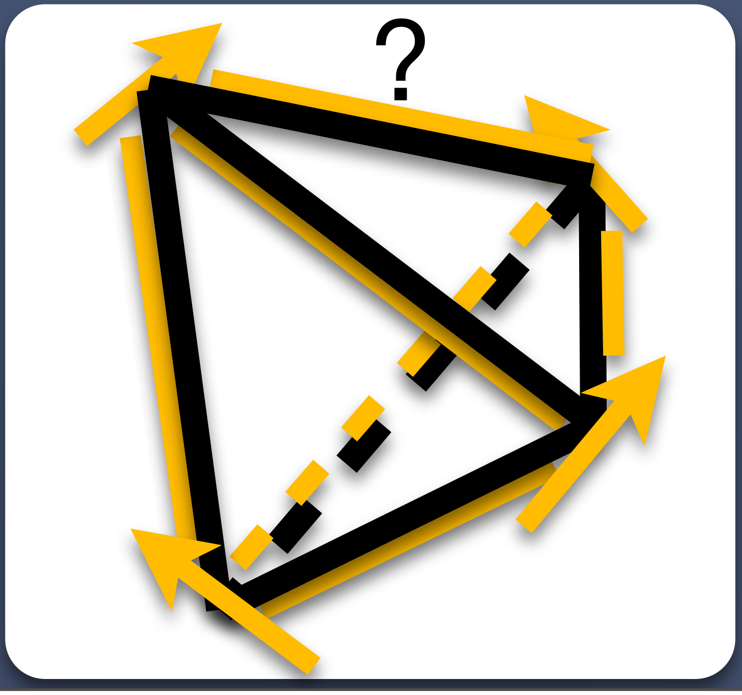
Does $Yb_2Ti_2O_7$ Order?

Specific Heat Anomaly



Blote et al, Physica, **43**, 4 (1969)

214mK



Does $Yb_2Ti_2O_7$ Order?

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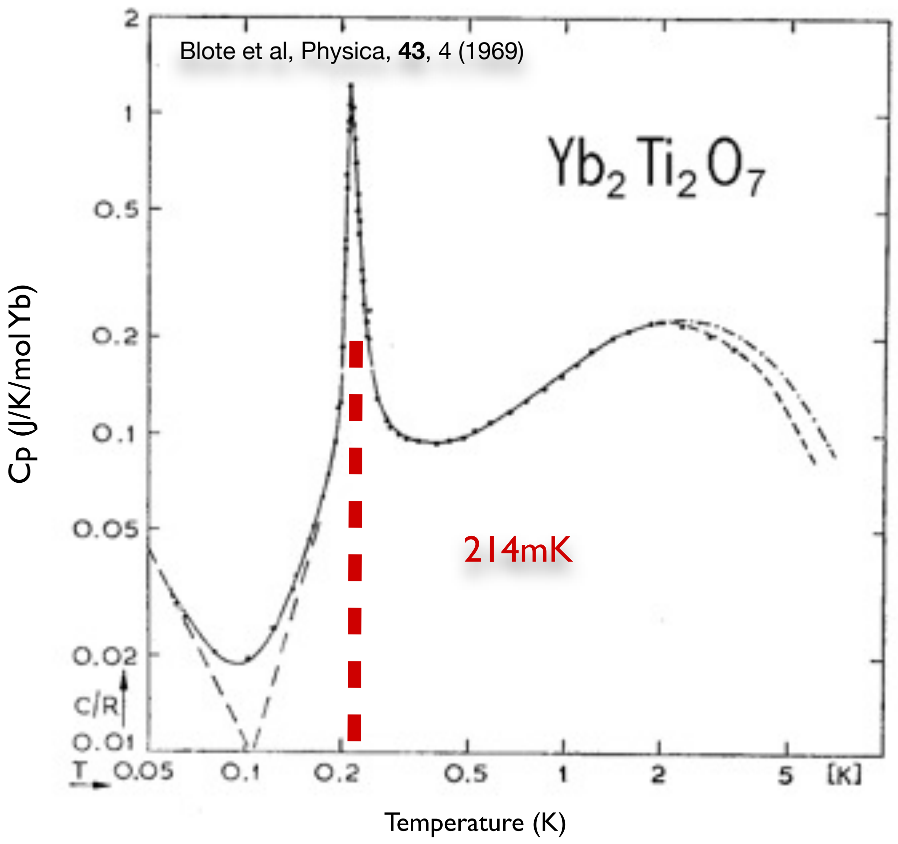

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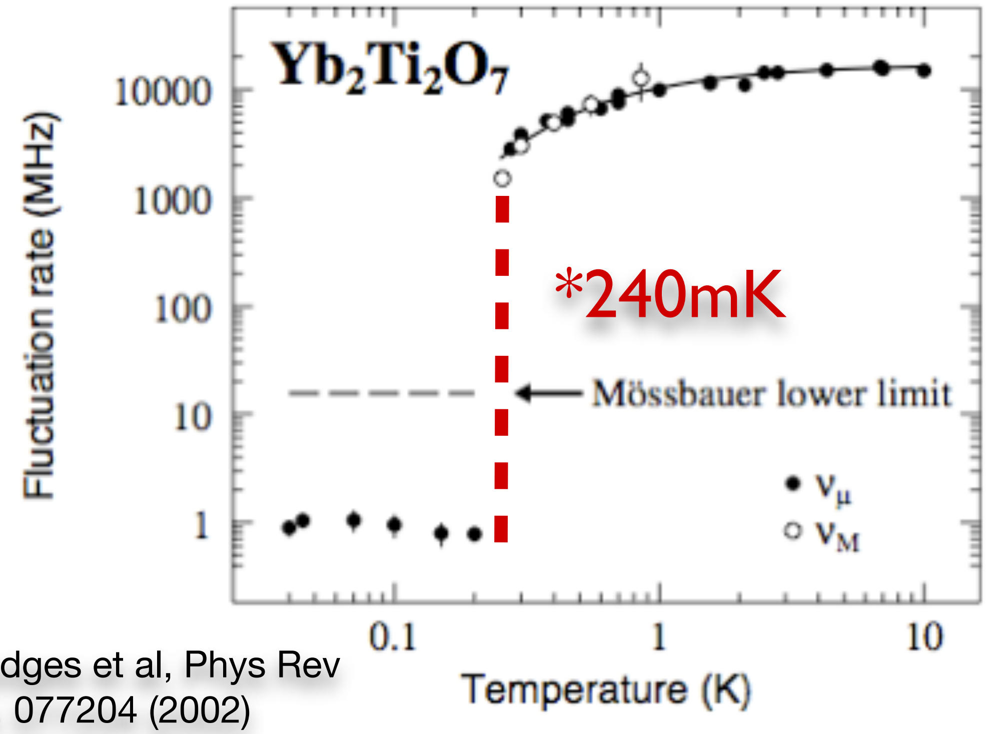
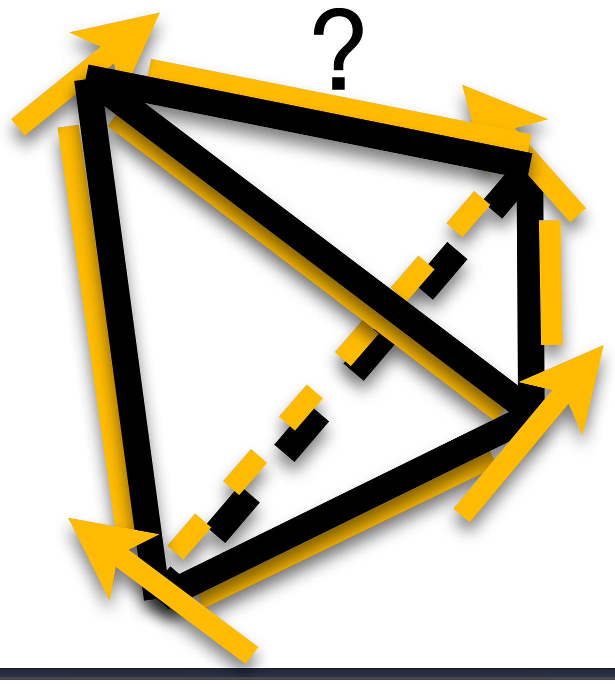
214mK

Drop in Spin Fluctuation Rate



*240mK

J. A. Hodges et al, Phys Rev Lett, **88**, 077204 (2002)



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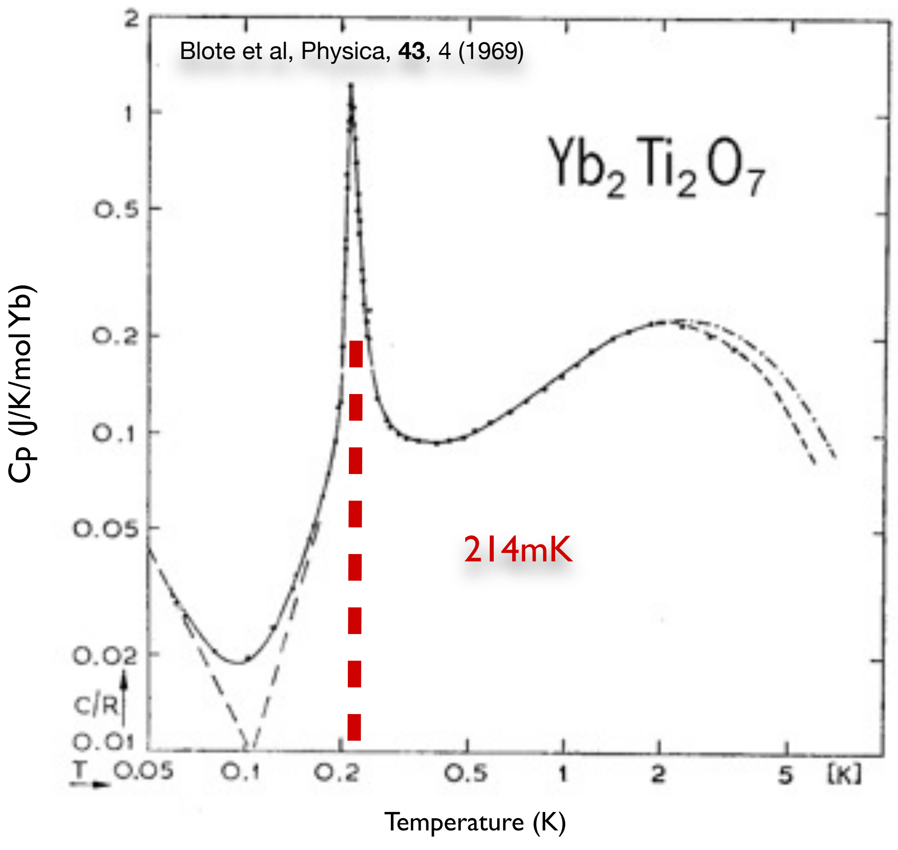

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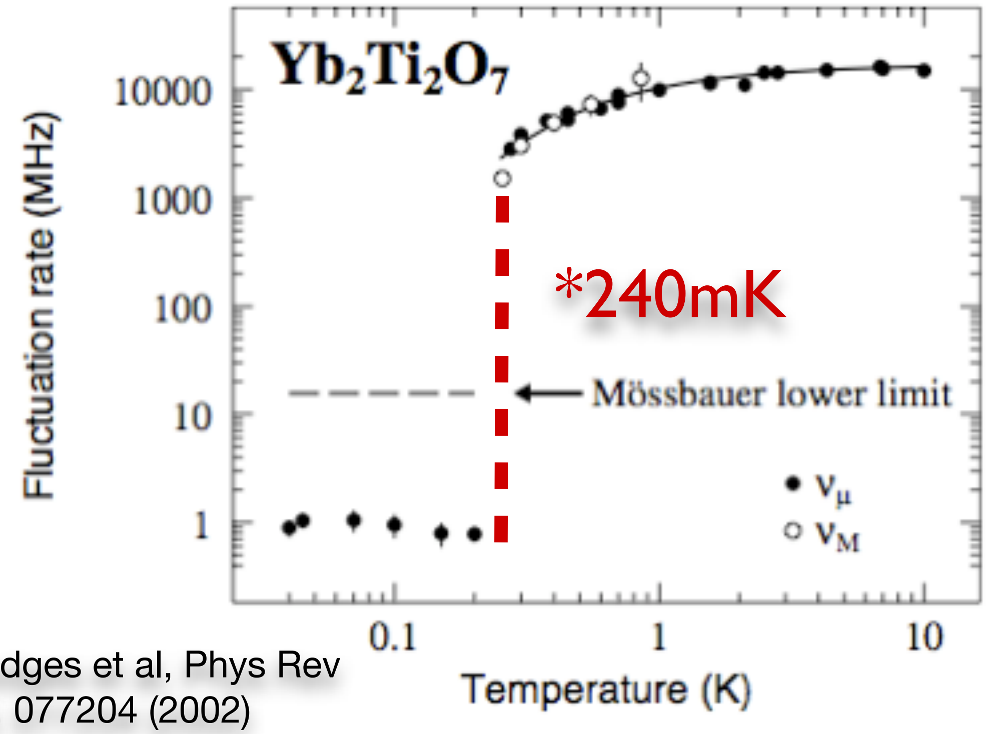
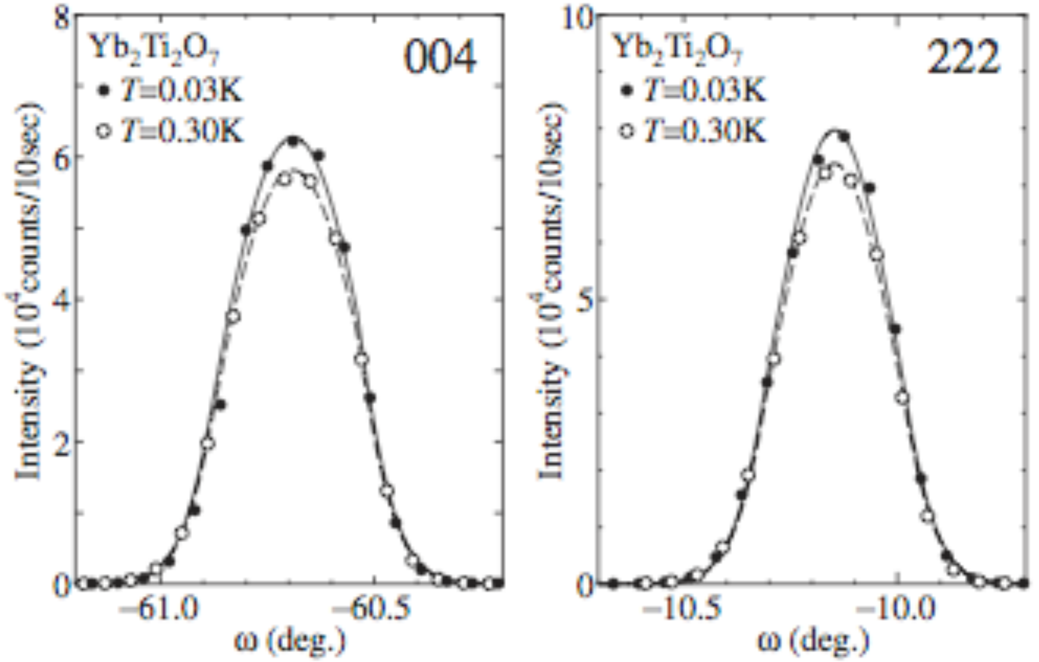


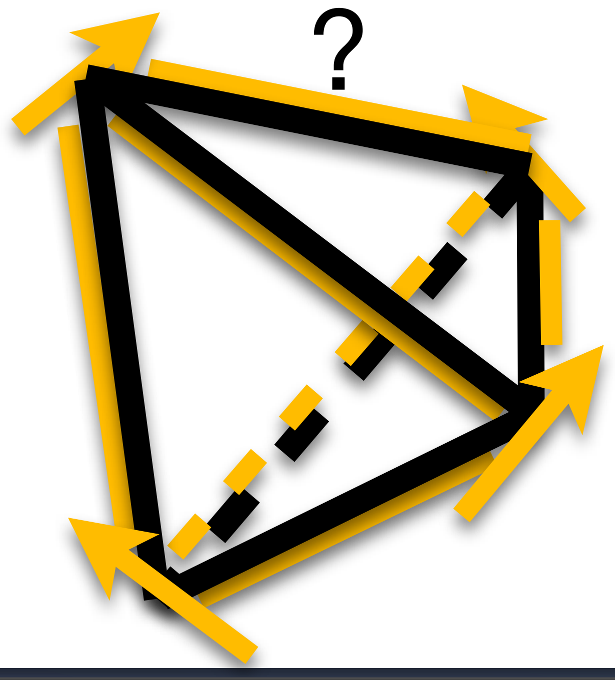
*240mK

J. A. Hodges et al, Phys Rev Lett, **88**, 077204 (2002)

Magnetic scattering at Bragg Peaks



Y. Yasui *et al*, J Phys Soc Jpn, **72**, No. 11 (2003), pp. 3014–3015



Tuesday, November 6, 2012

Time of Flight Neutron Scattering

"Disk Chopper Spectrometer" (DCS)

@ NIST Center for Neutron Research

Single Crystal $Yb_2Ti_2O_7$

Time of Flight Neutron Scattering

"Disk Chopper Spectrometer" (DCS)

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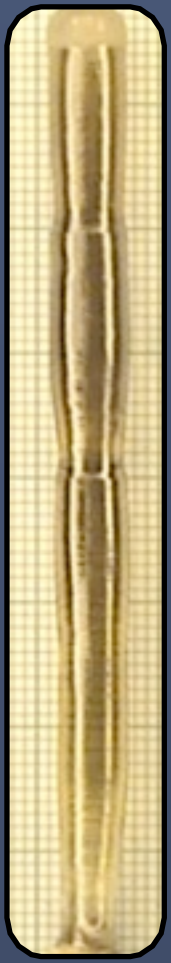
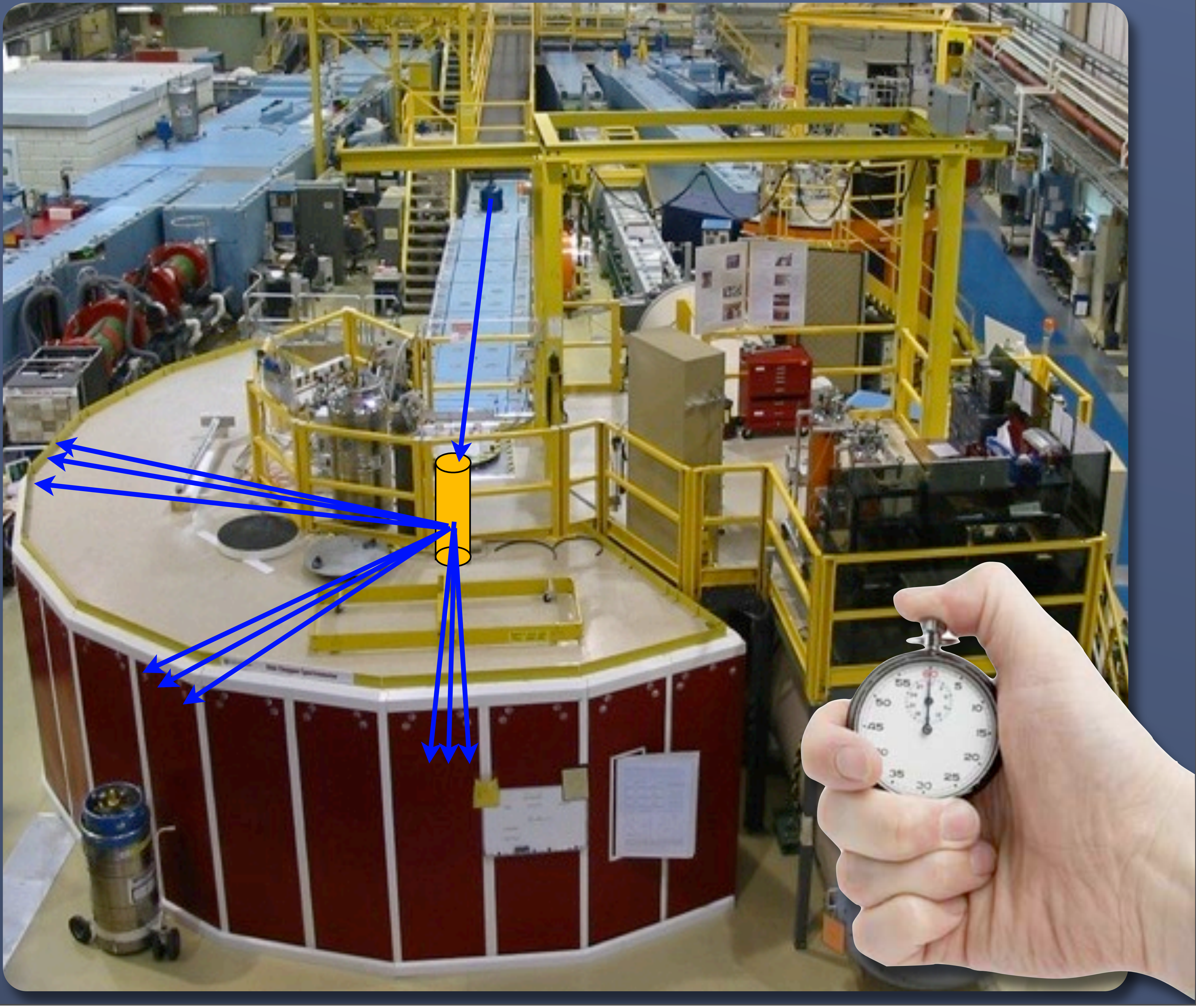
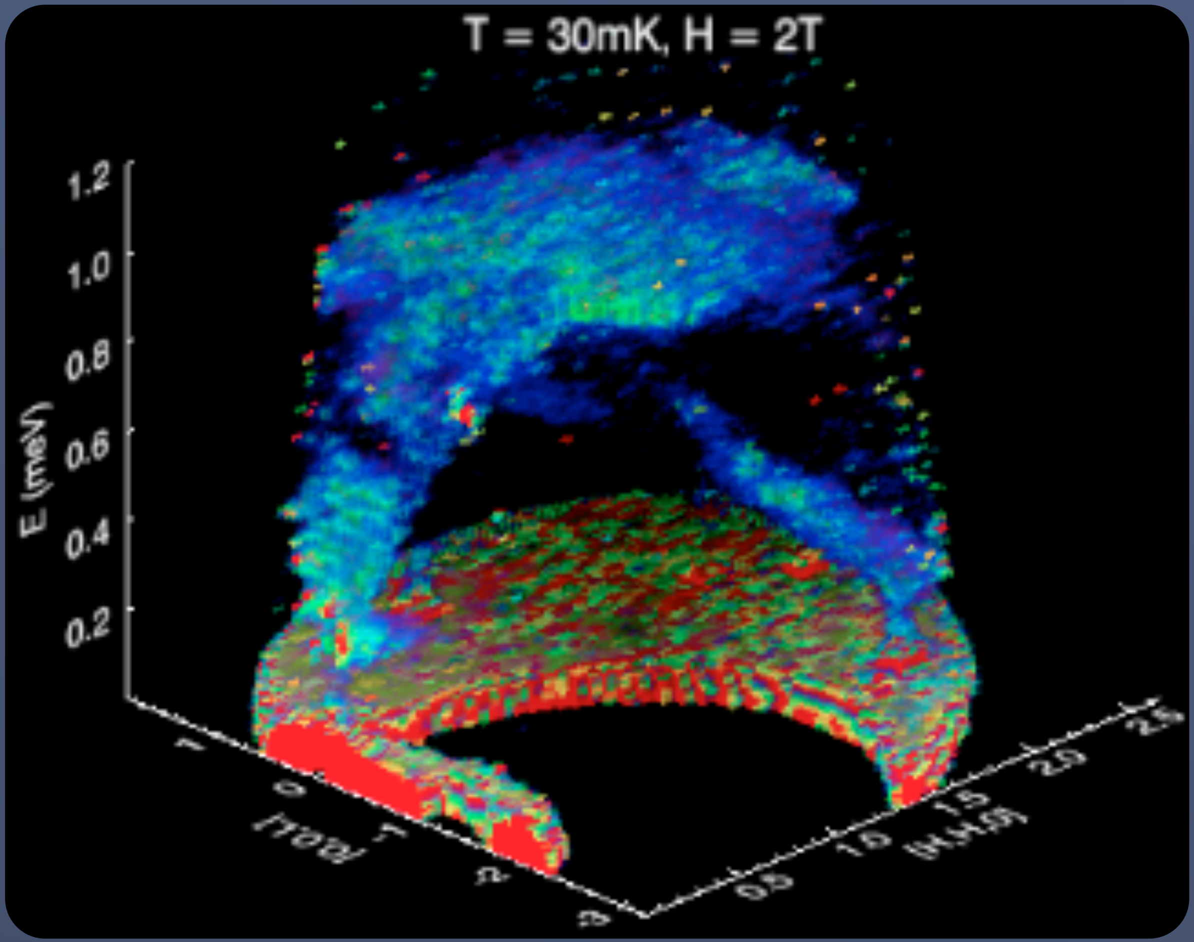


Single Crystal $Yb_2Ti_2O_7$



“Time of Flight” data

Can slice through this volume in several directions



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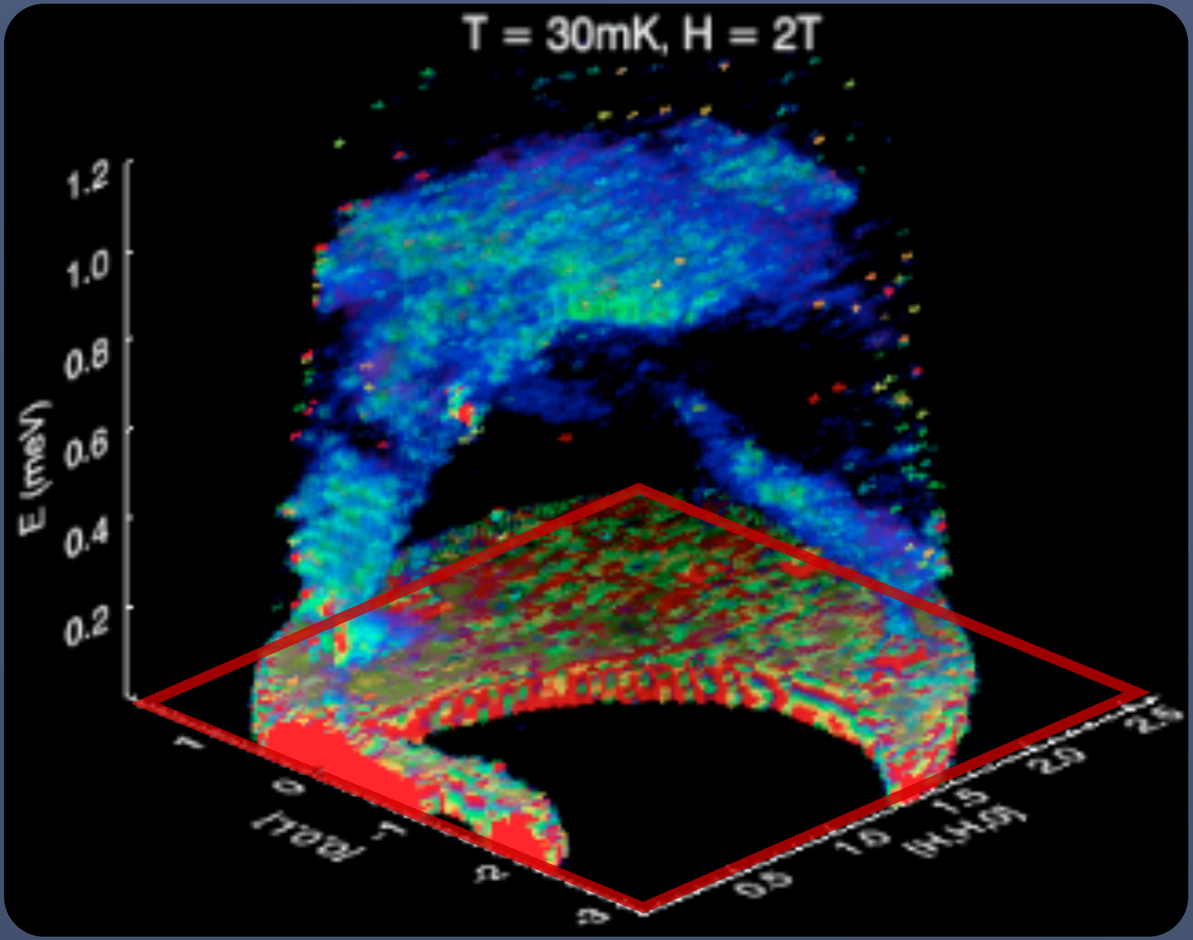

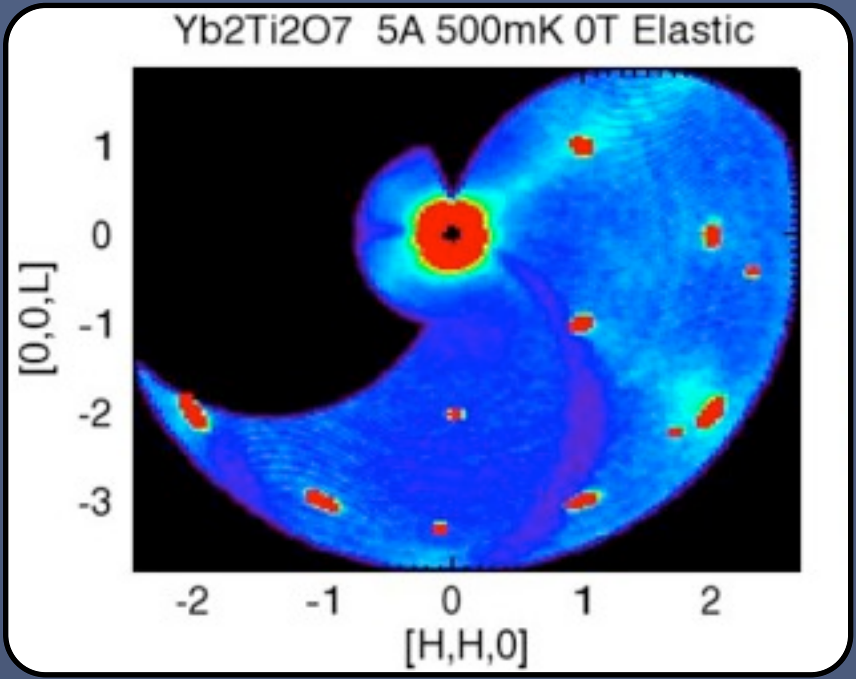

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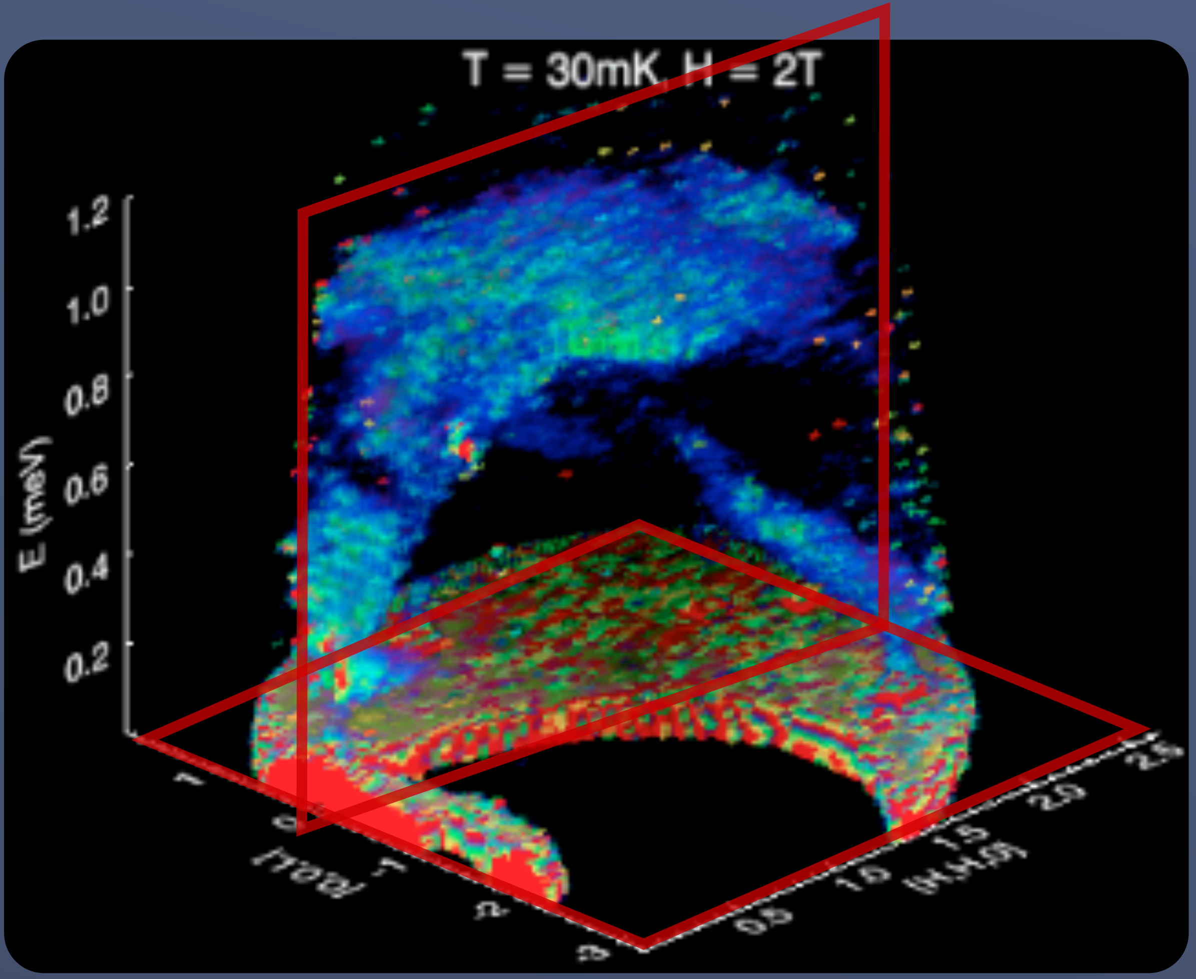
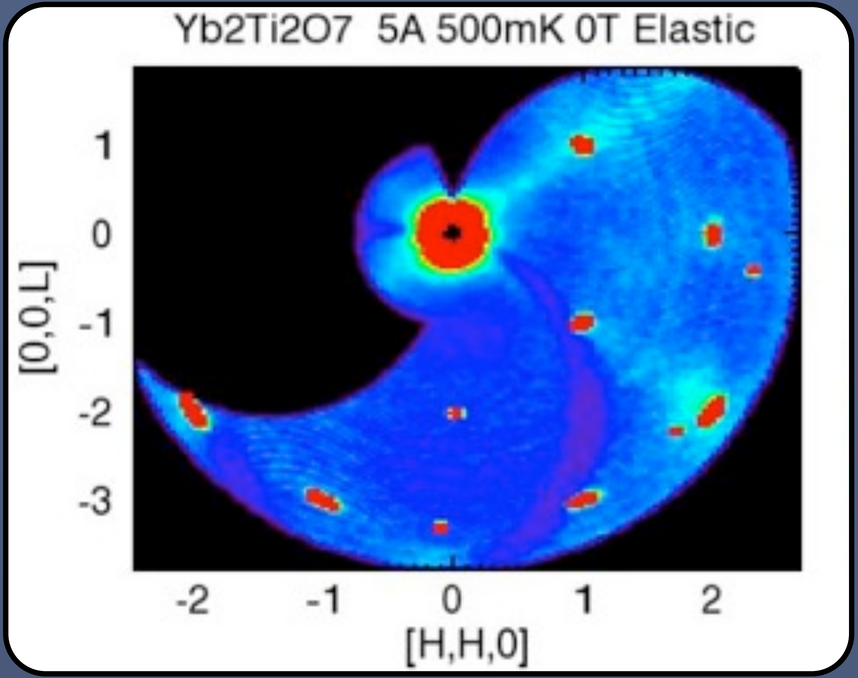
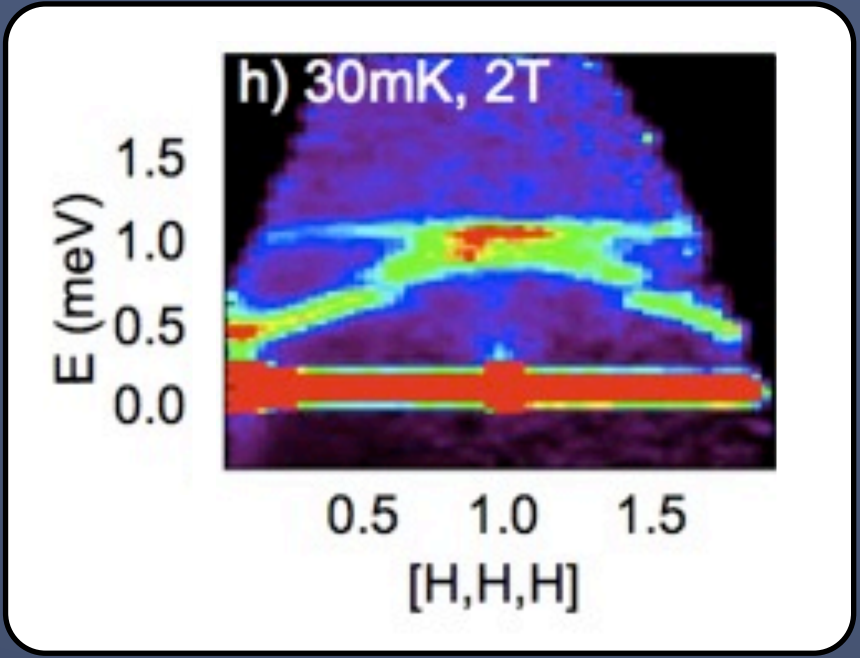
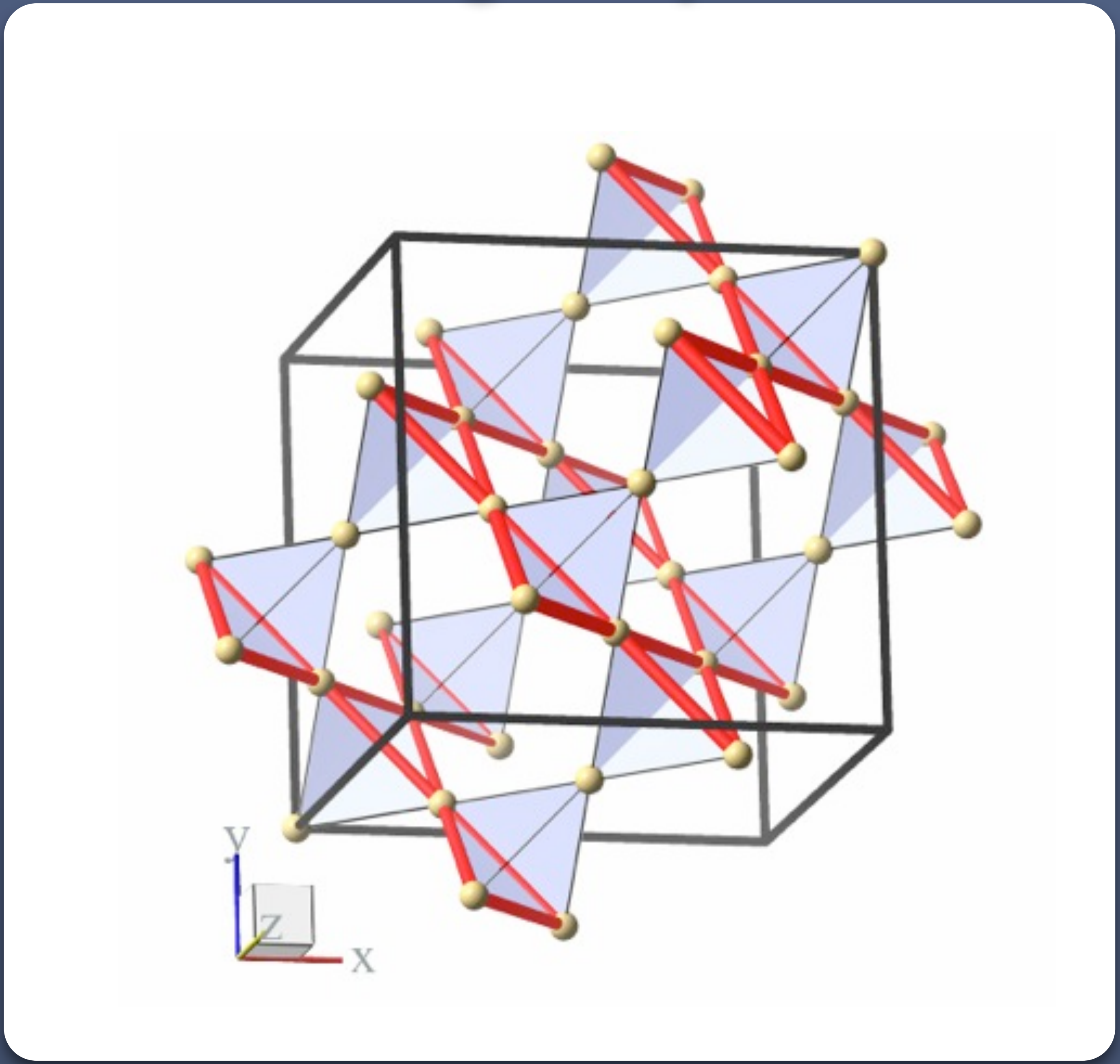




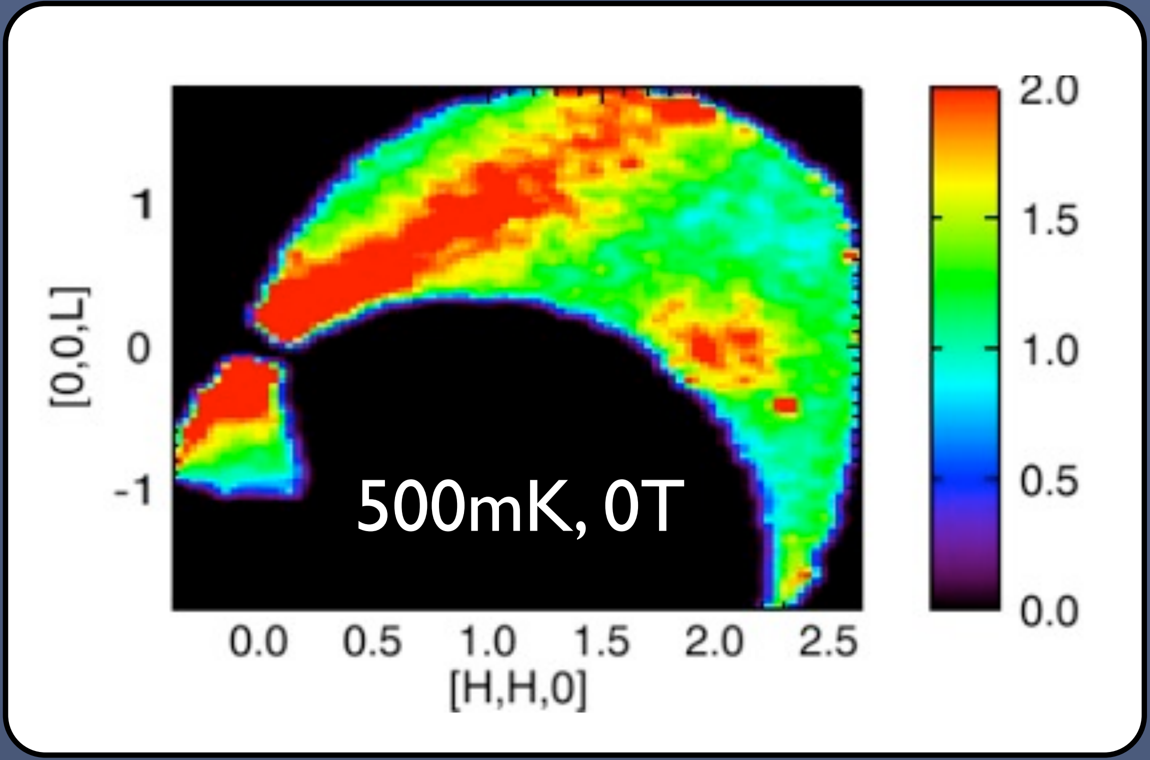


Diffuse “Rods” of Scattering

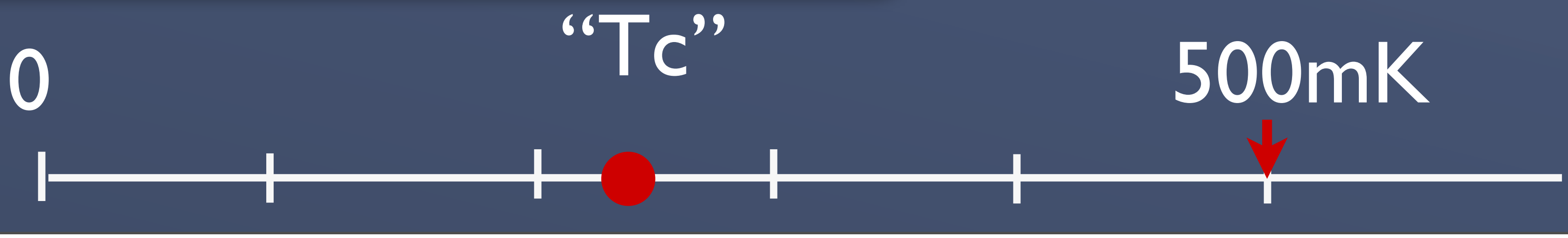
Correlations in 111 “Kagome” planes



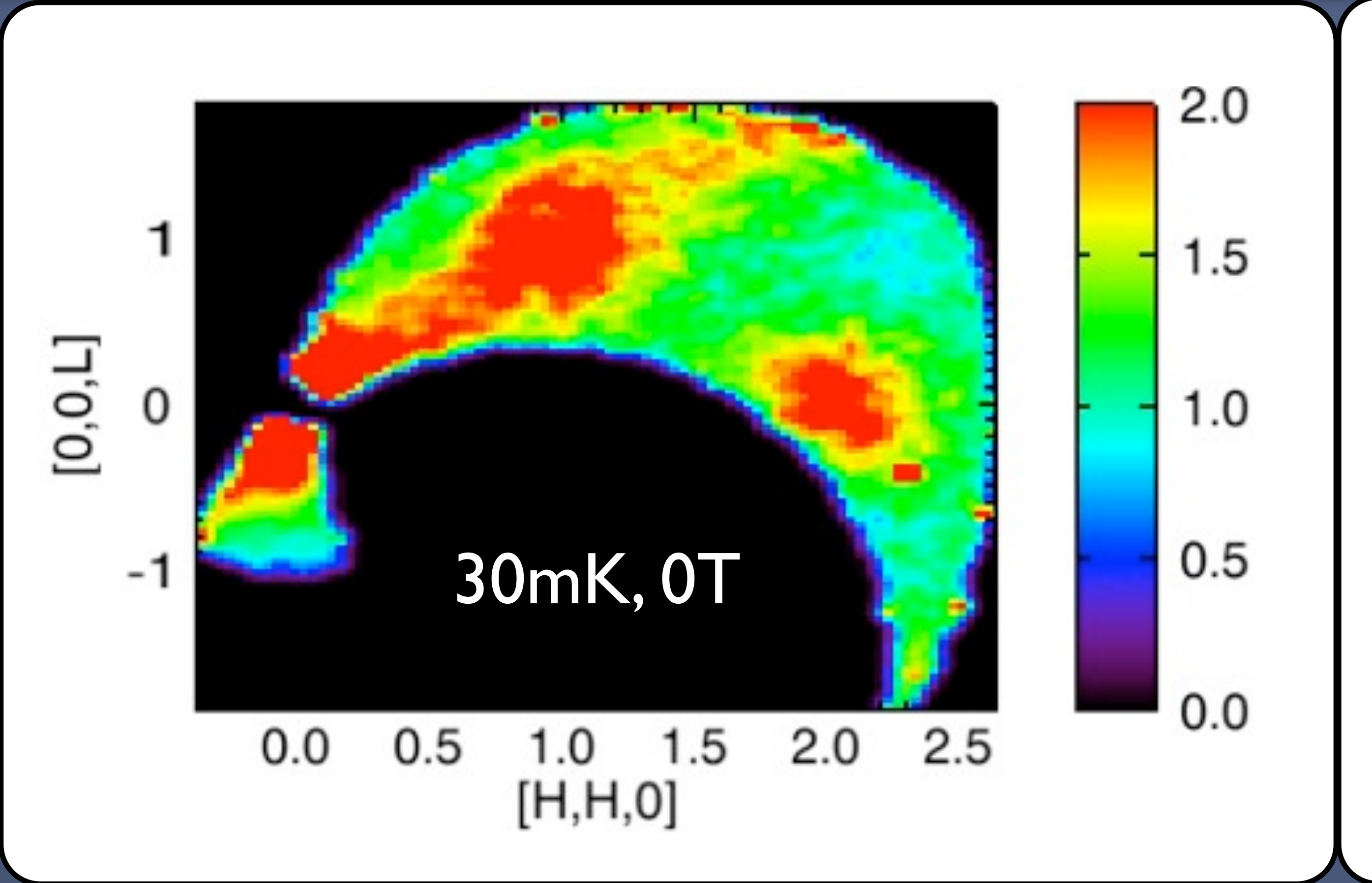
“Rod of scattering” Along 111 direction



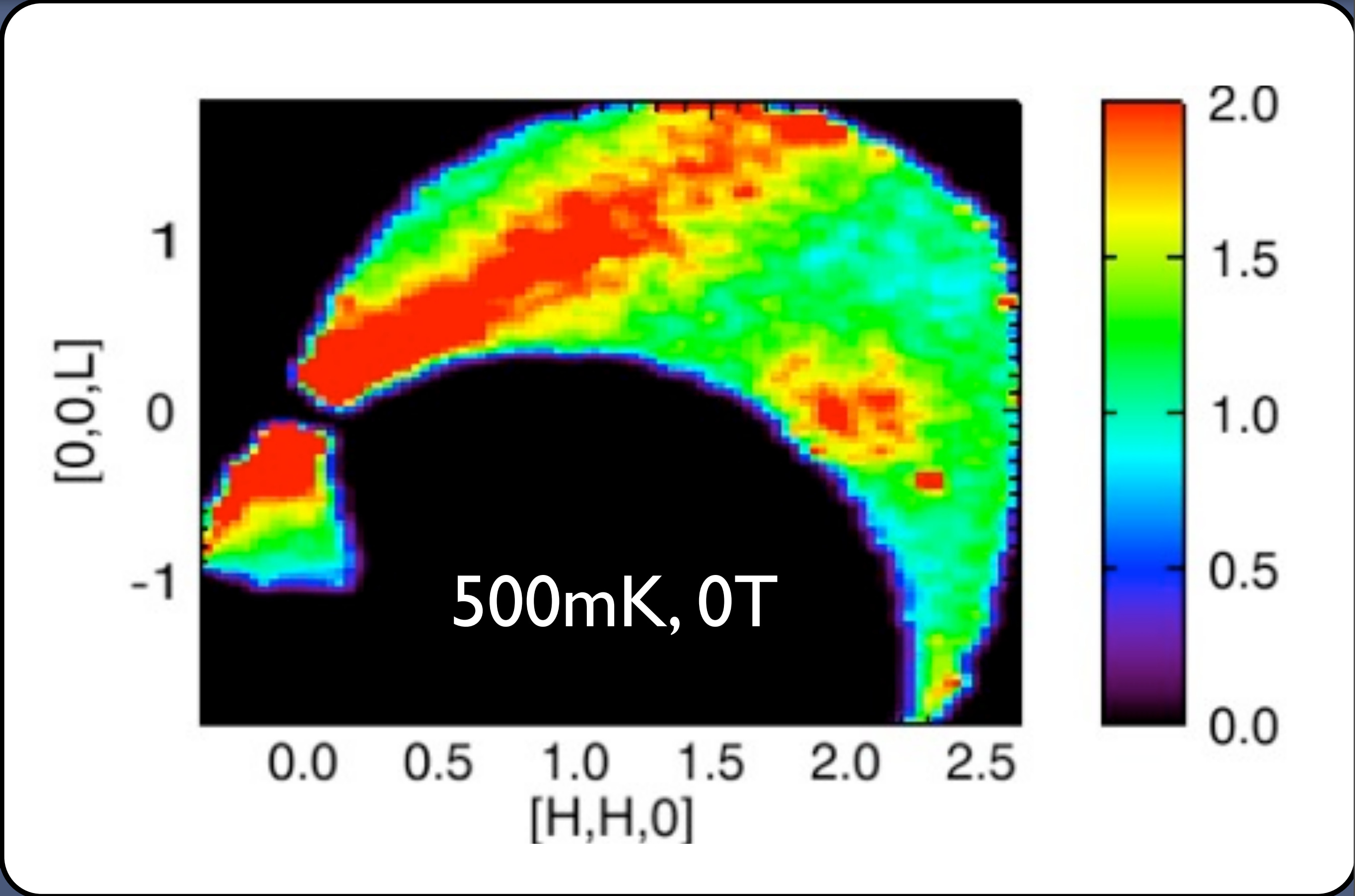
E = [0.1, 0.3] meV (Quasi elastic)



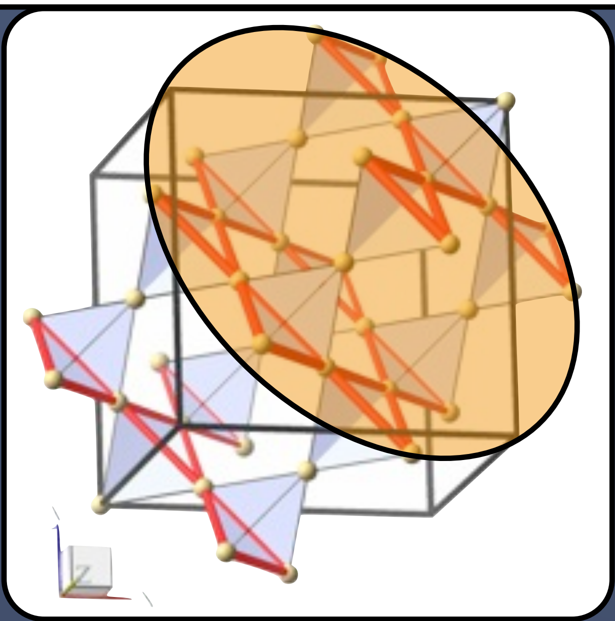
Development of 3D Correlations

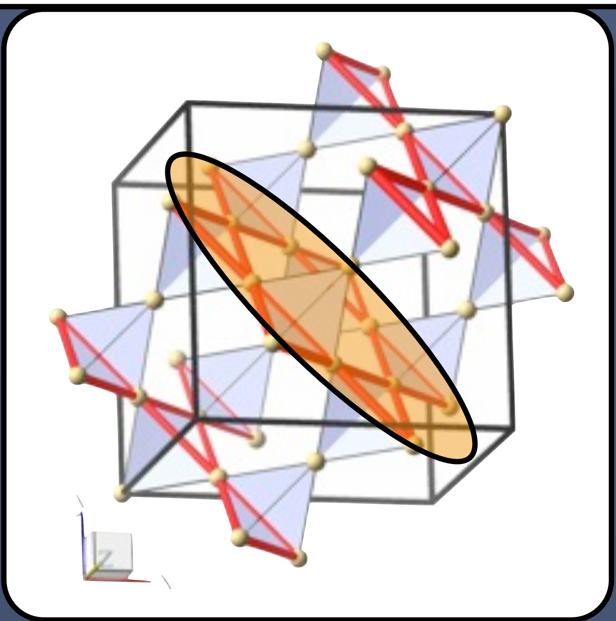


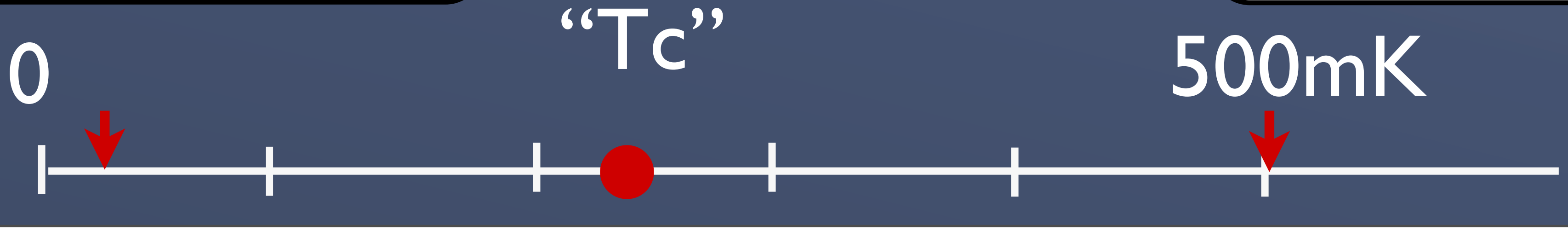
30mK, 0T



500mK, 0T





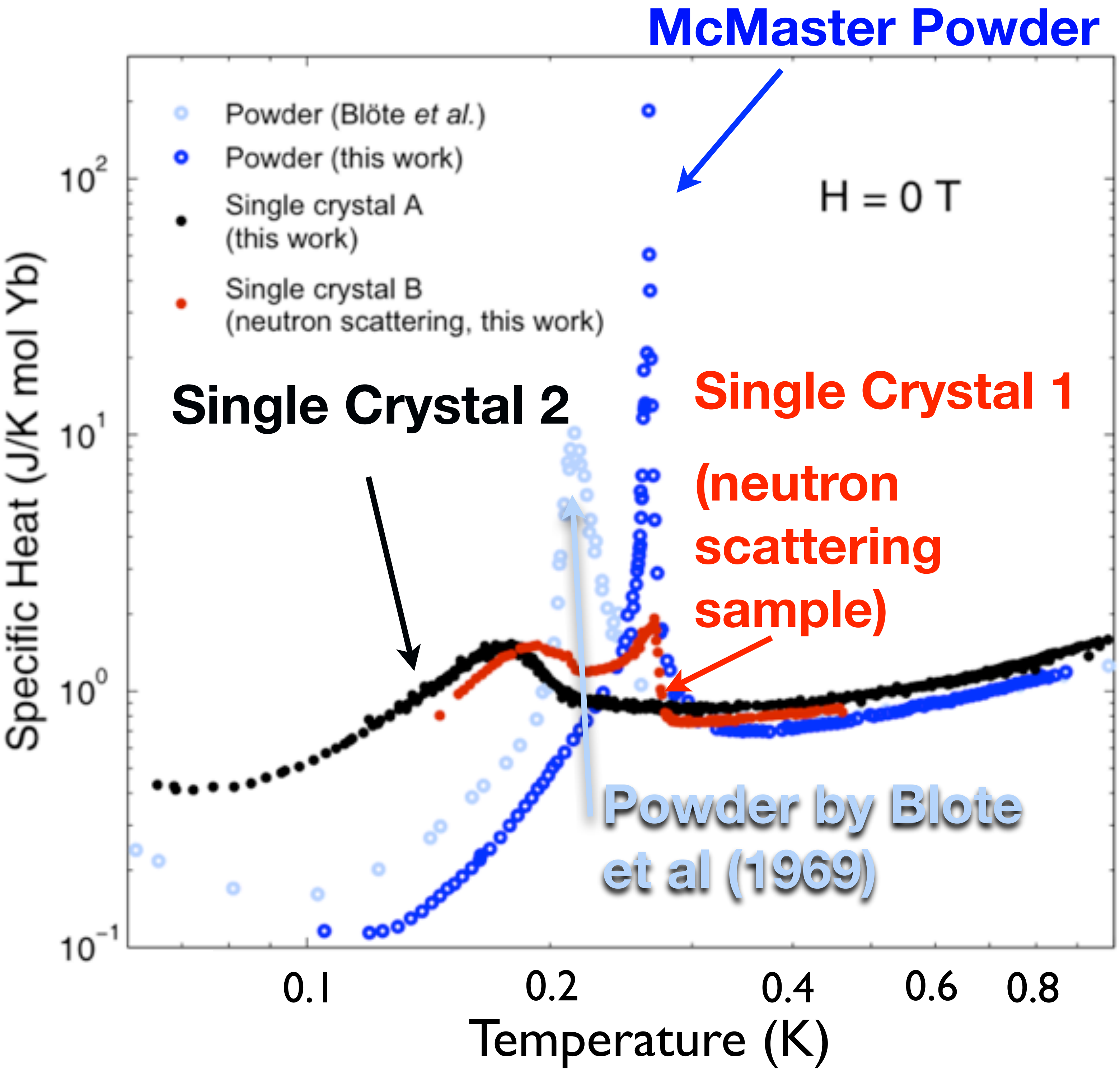


0

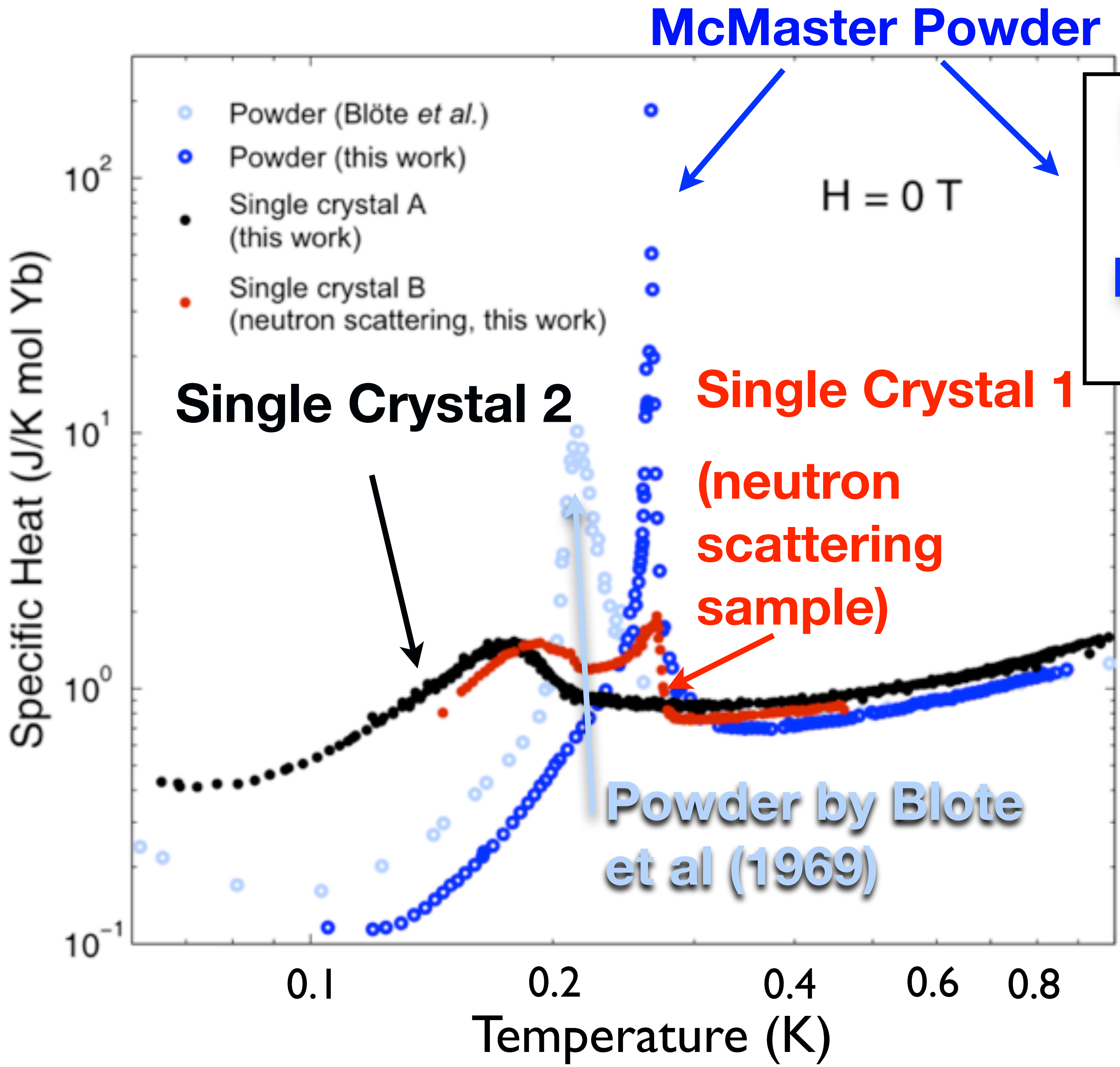
“Tc”

500mK

Sample Dependence of Specific Heat



Sample Dependence of Specific Heat



McMaster Powder

Single Crystal 2

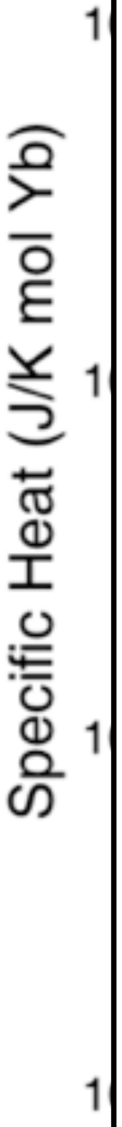
Single Crystal 1

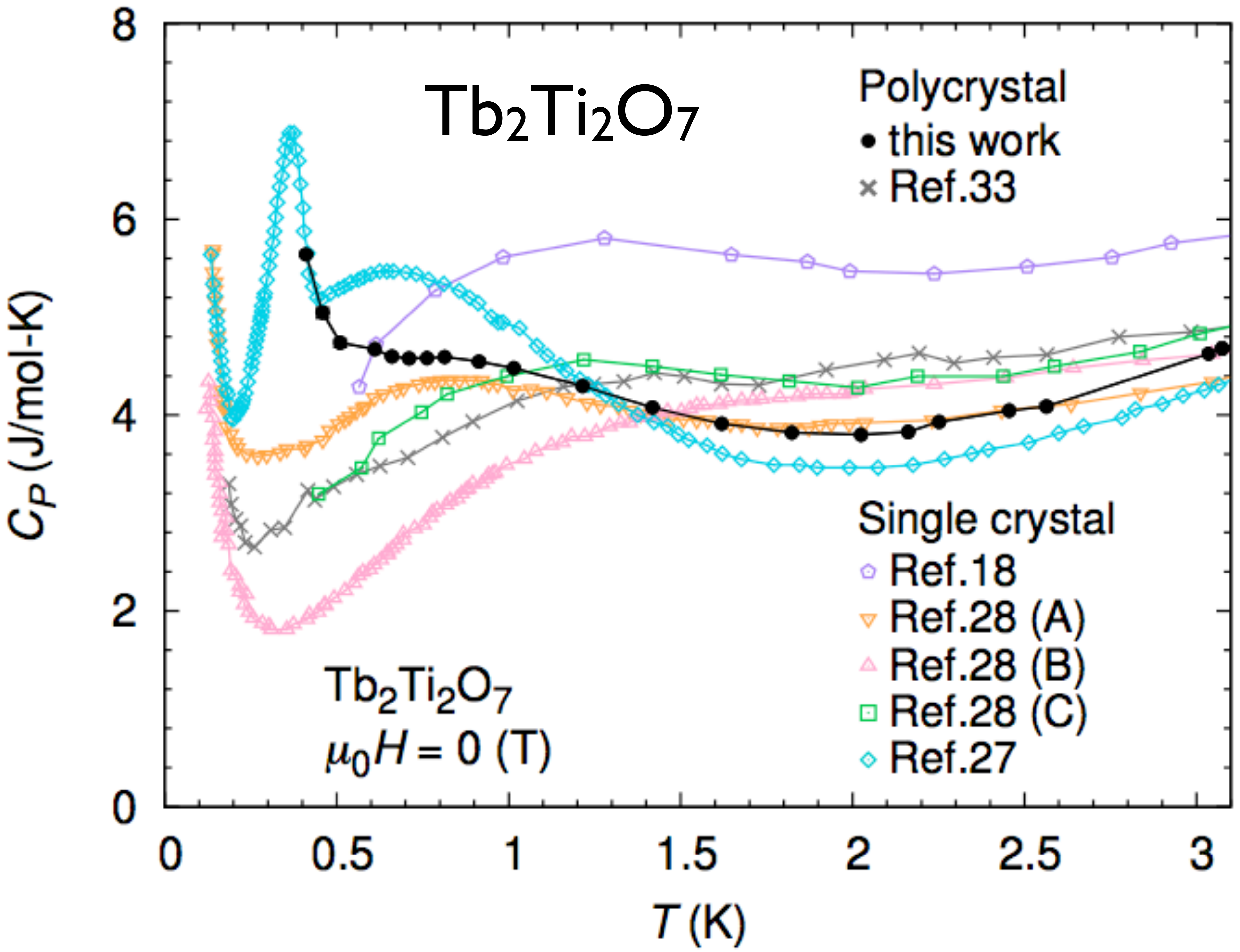
(neutron scattering sample)

Powder by Blote et al (1969)

Upcoming paper: D'Ortenzio, Luke et al.
μSR does NOT show LRO for this sample

Sample Dependence of Specific Heat





Takatsu *et al,* J. Phys.: Condens. Matter 24 (2012) 052201 (4pp)

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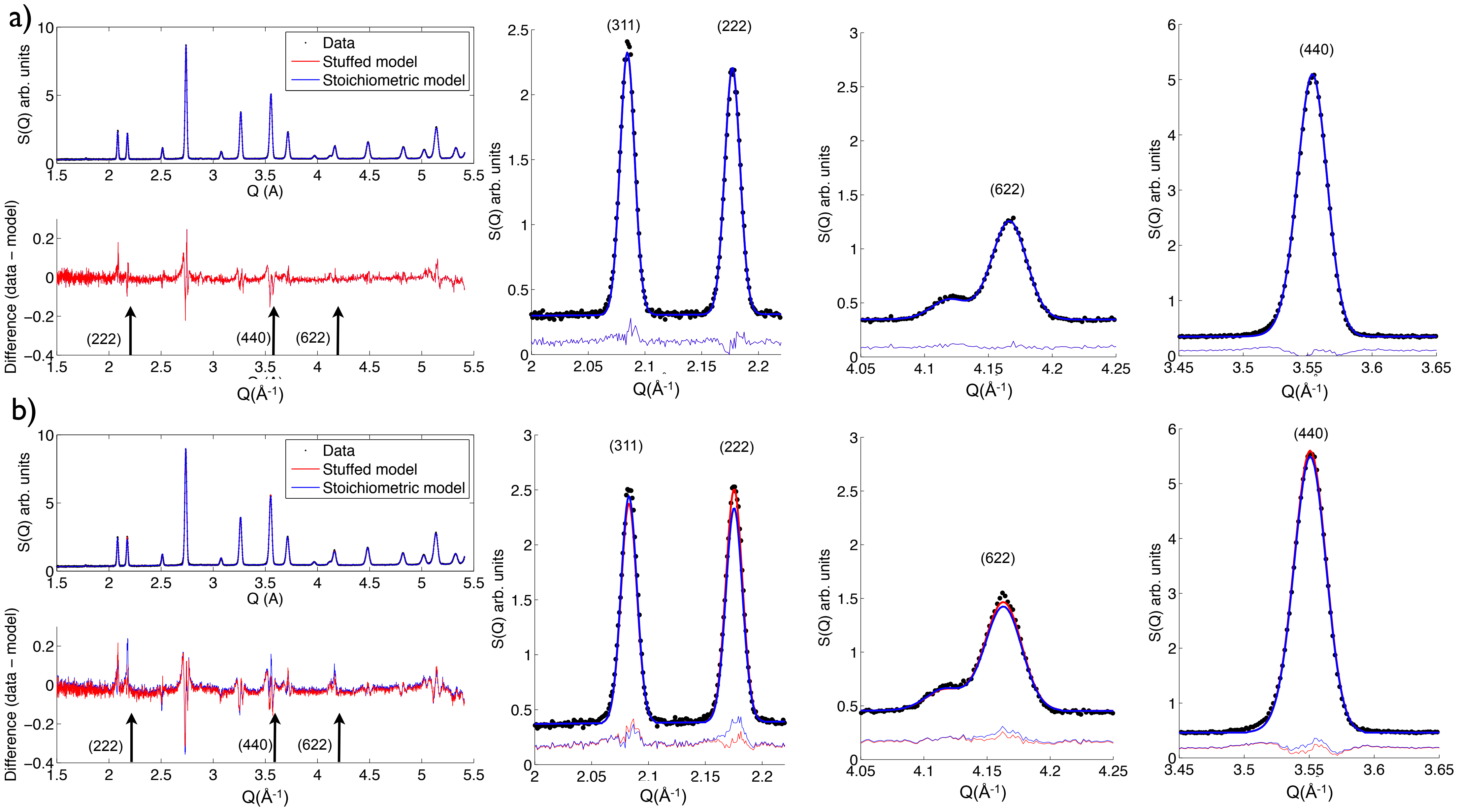
for

Evidence for “stuffing”: Yb on Ti site



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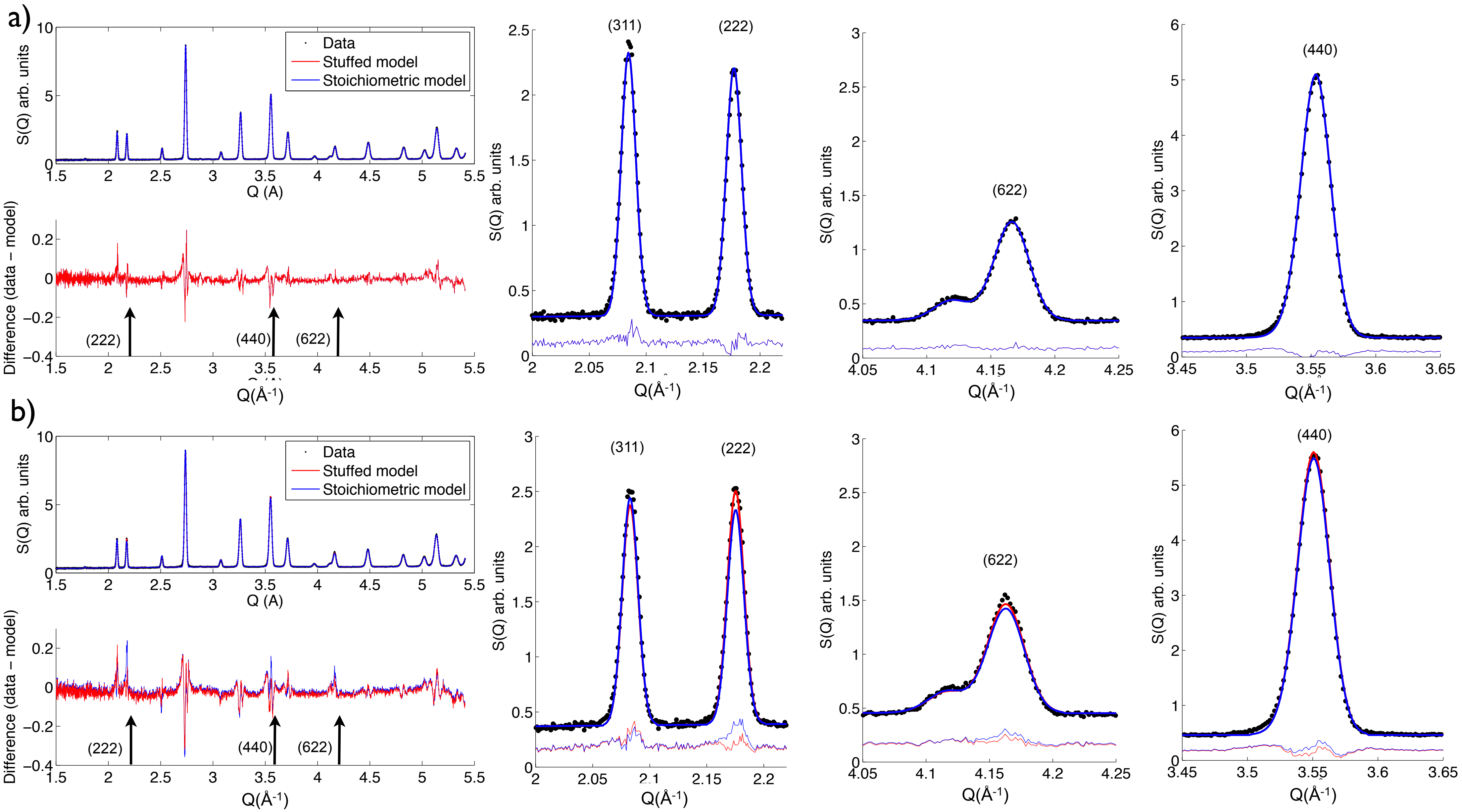
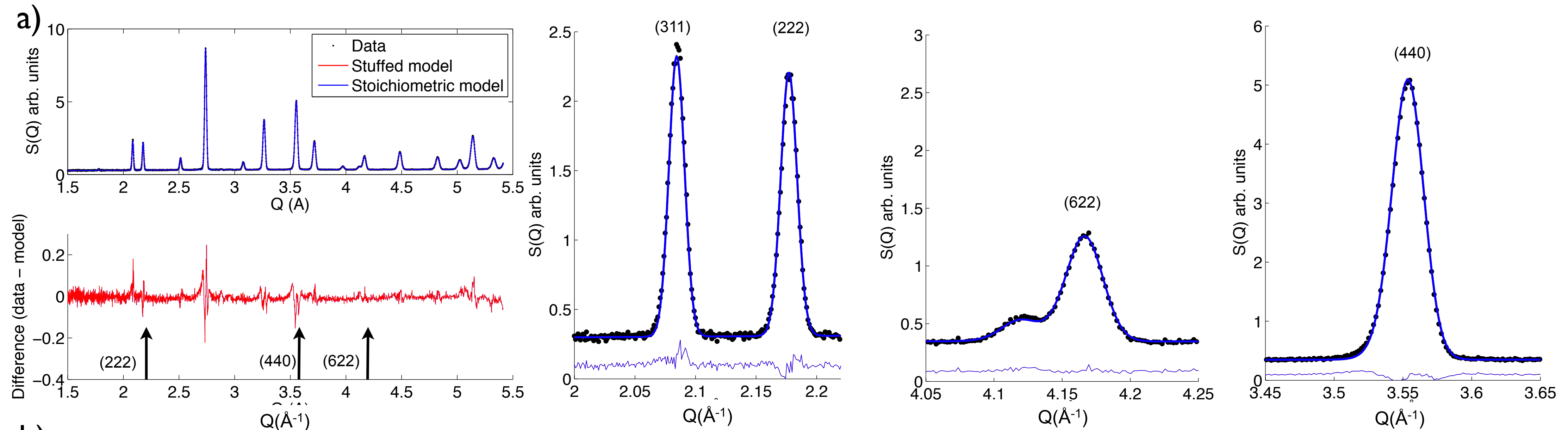
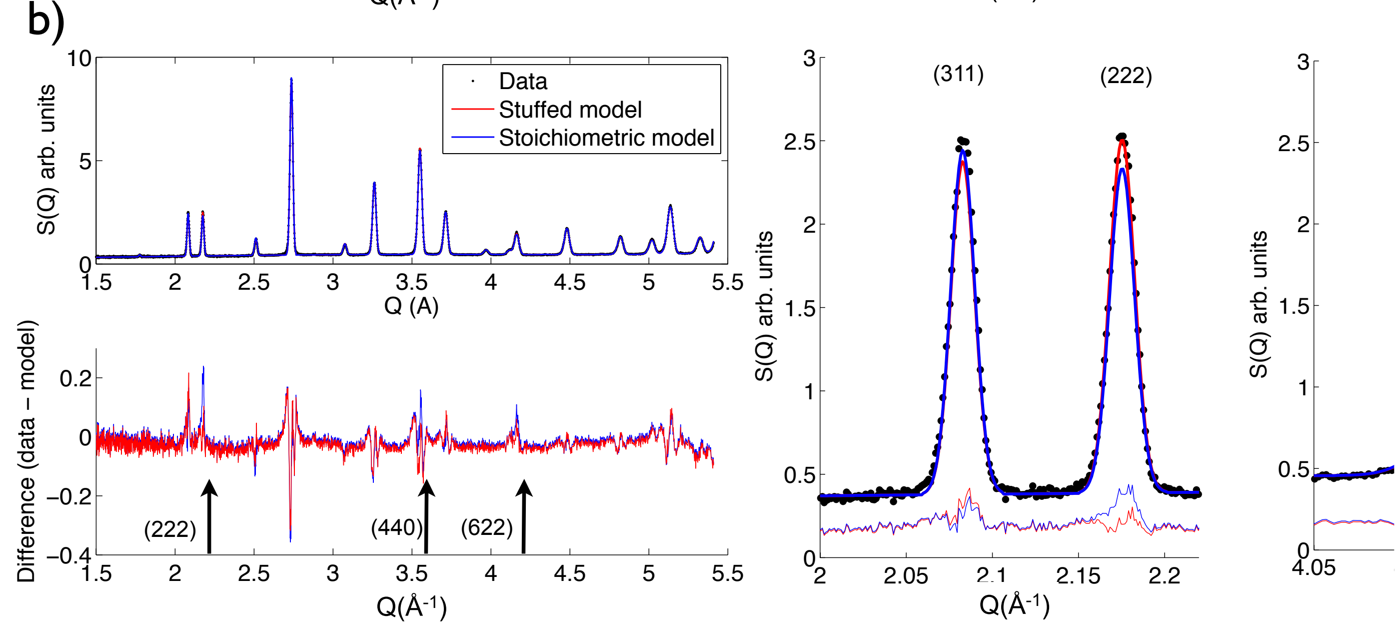
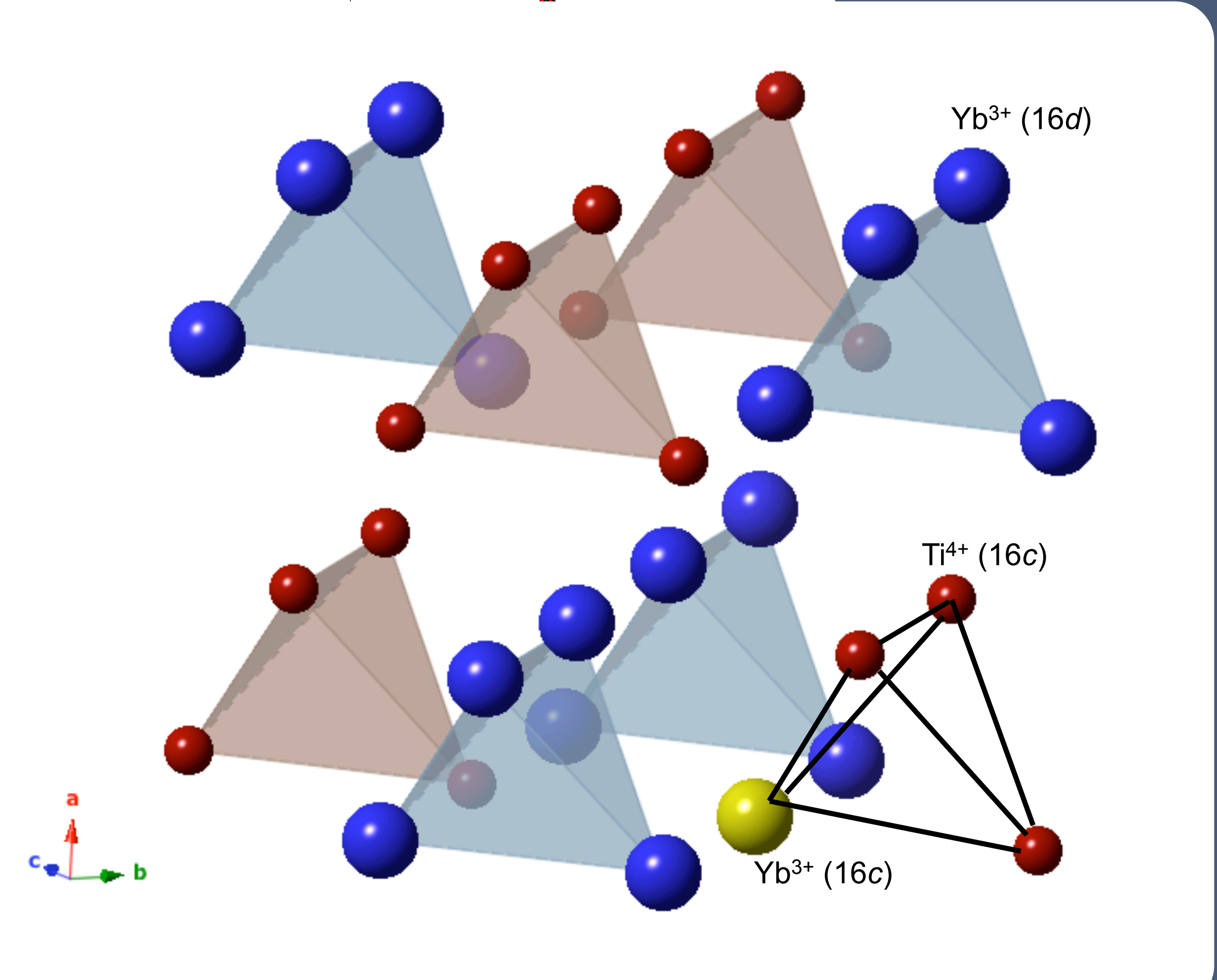


Single crystal sample is best modeled as a stuffed pyrochlore:

Evidence for “stuffing”: Yb on Ti site



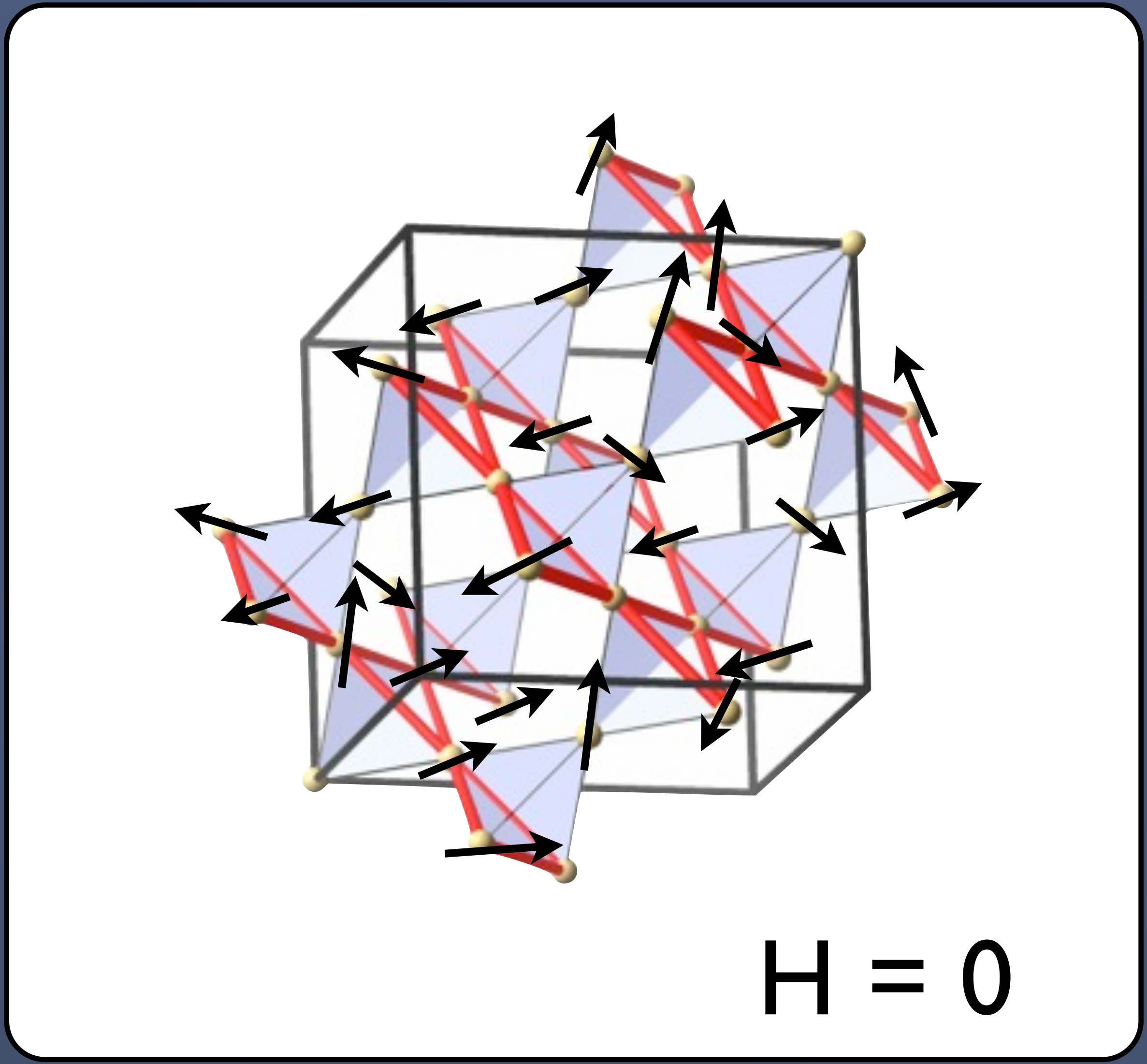




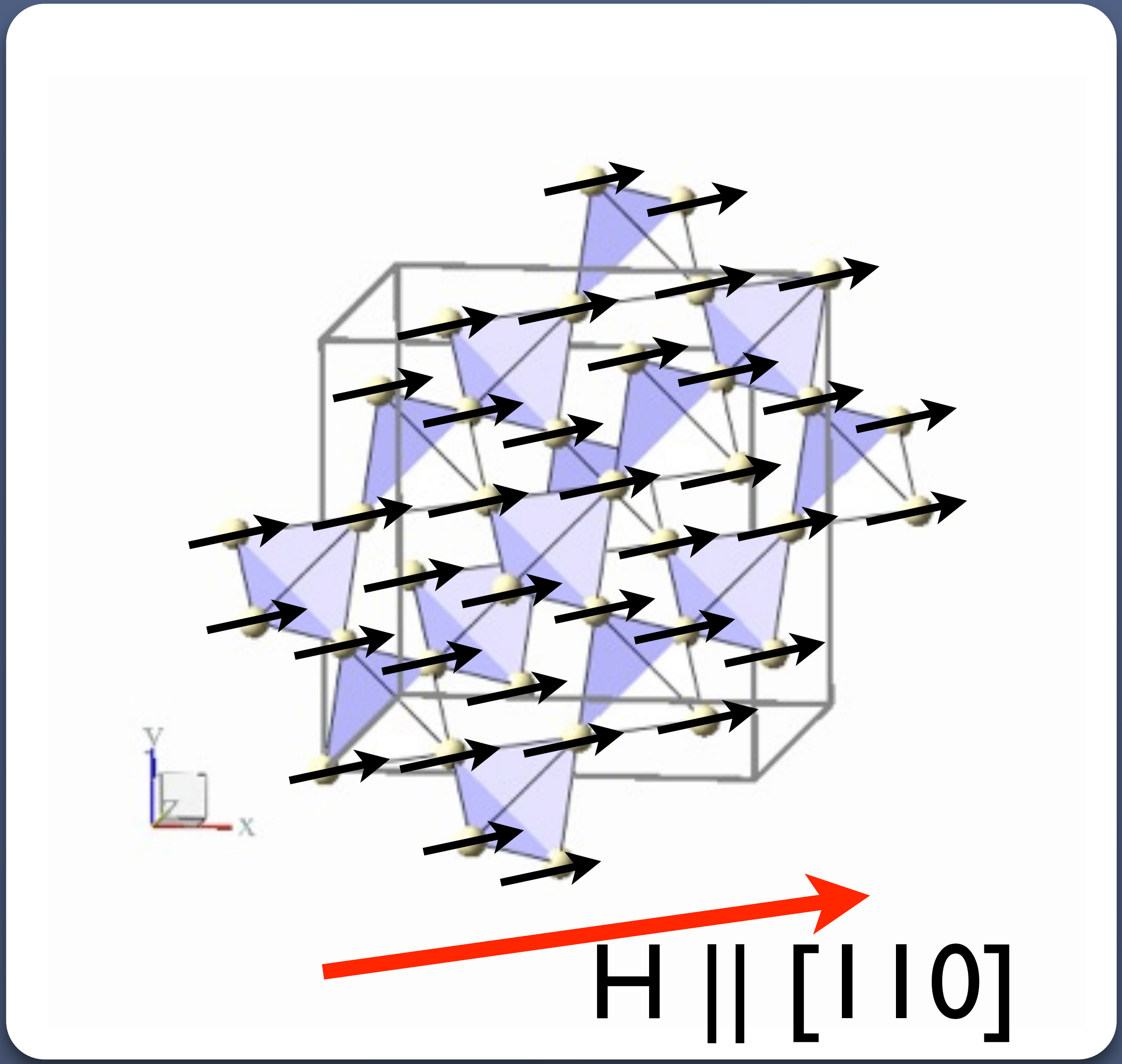
Single crystal sample is best modeled as a stuffed pyrochlore:

2.3% excess Yb on the Ti site

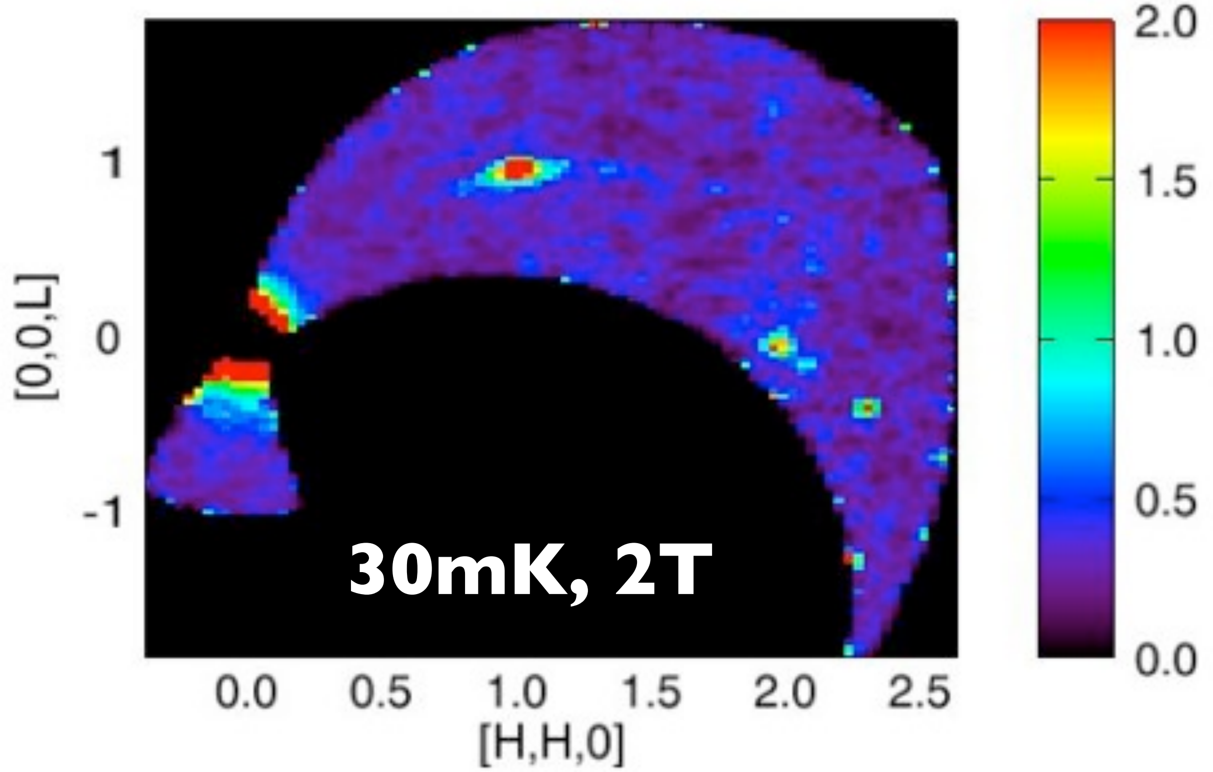
Excitations:
diffuse, continuum-like?



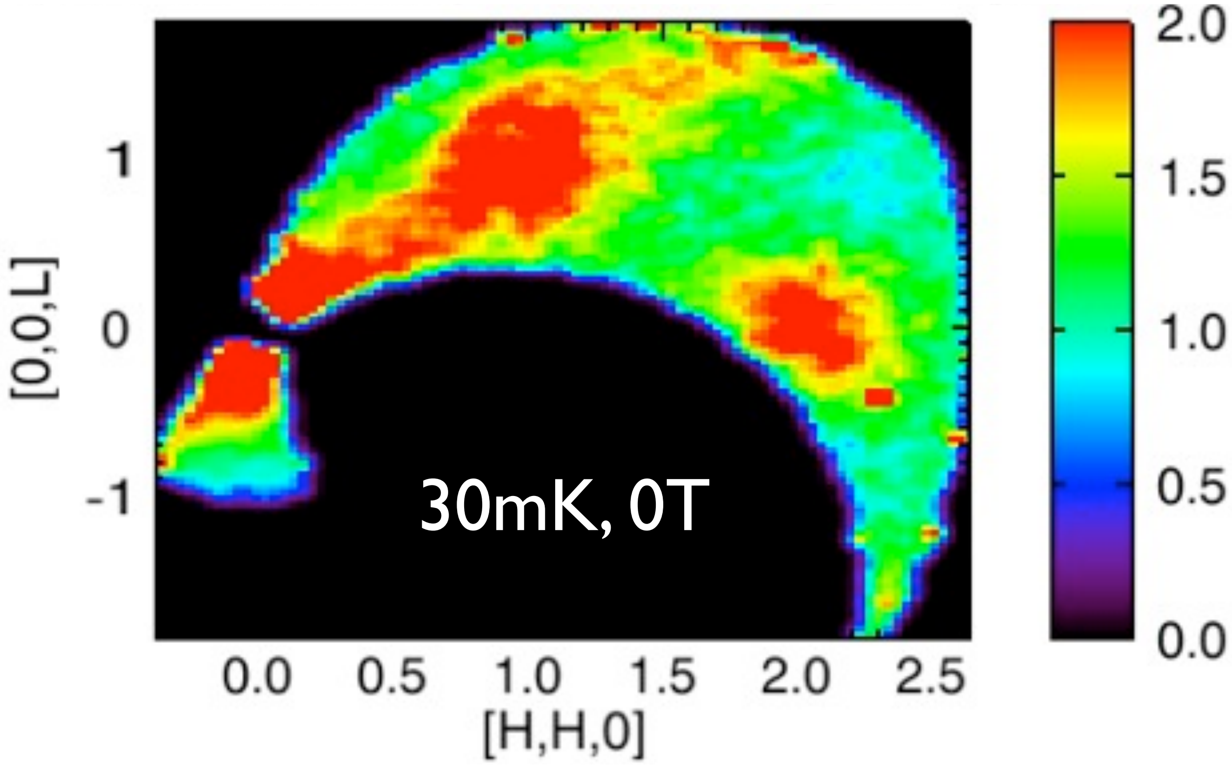
Excitations:
Sharp, conventional magnons

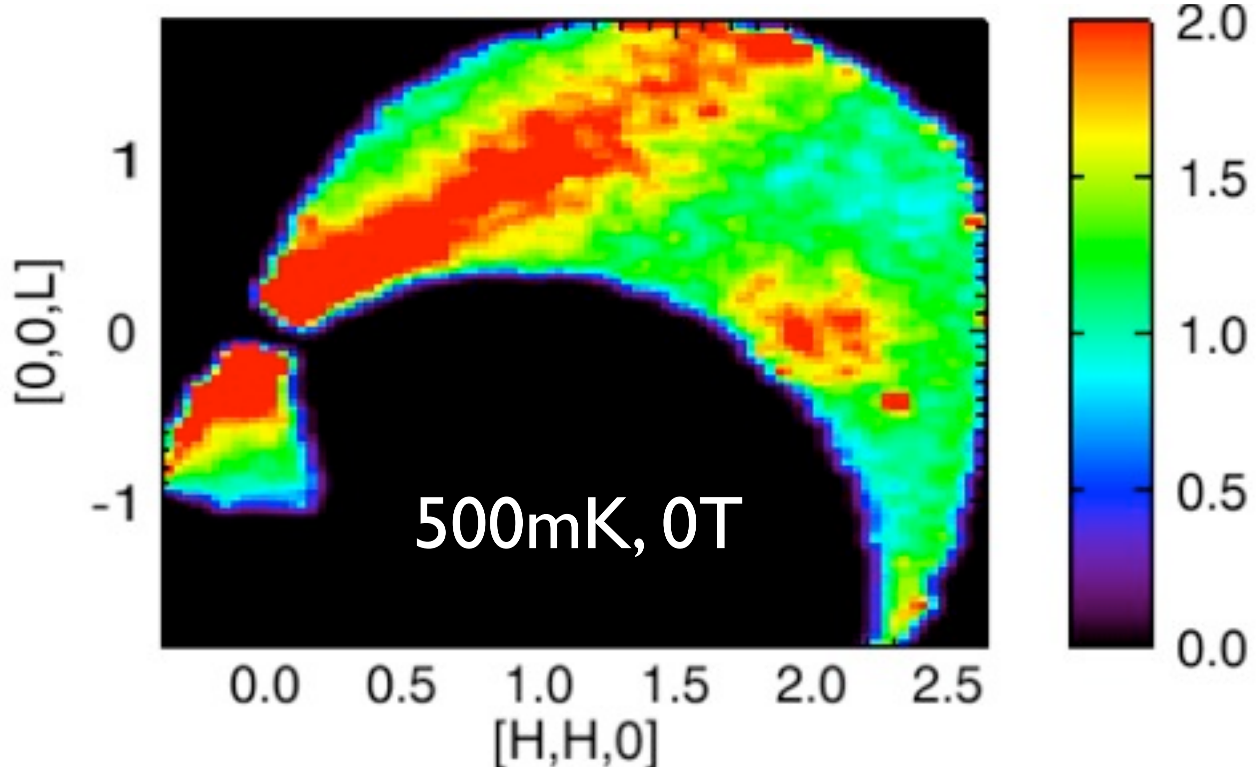


Application of a Field

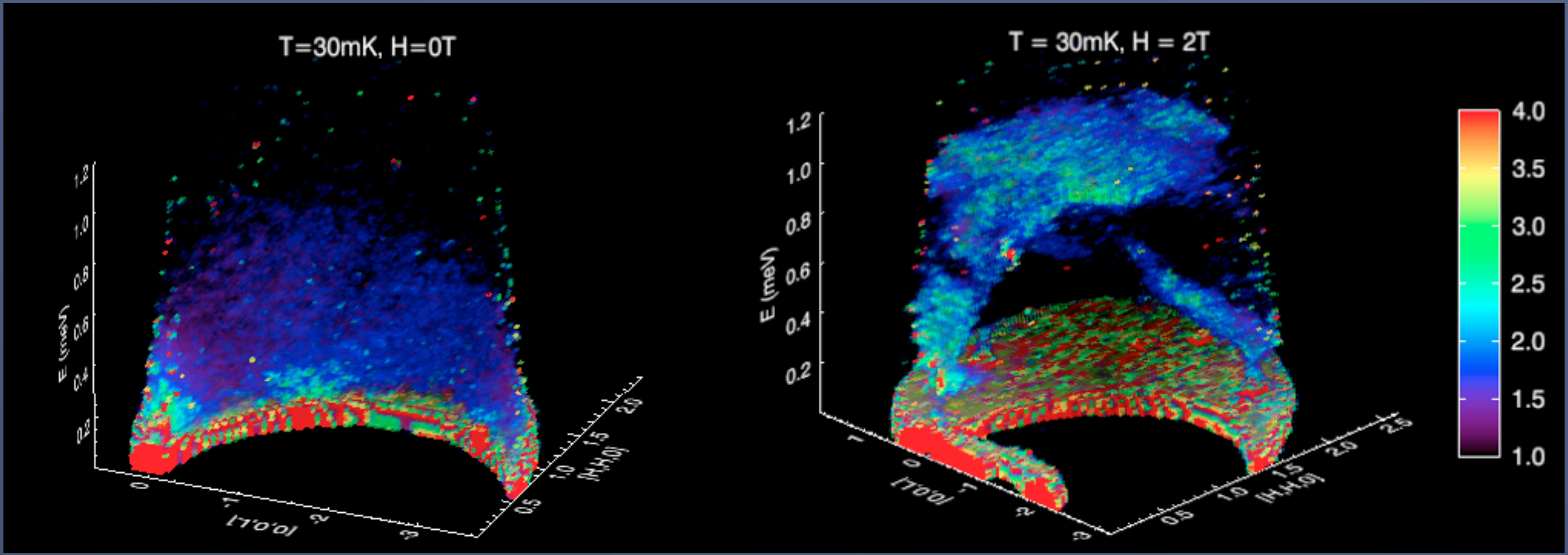


Field removes diffuse scattering





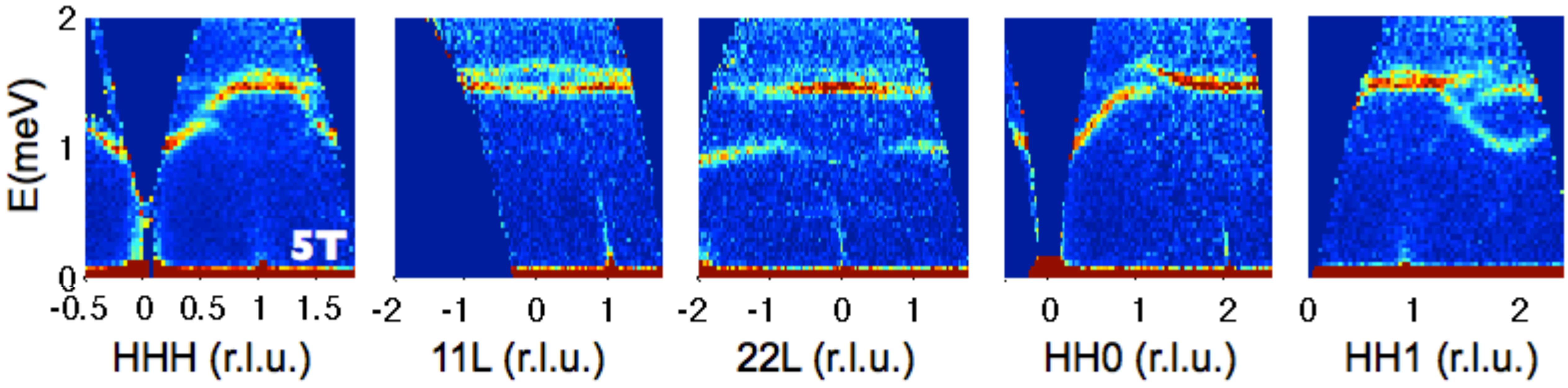
Spin waves from polarized phase

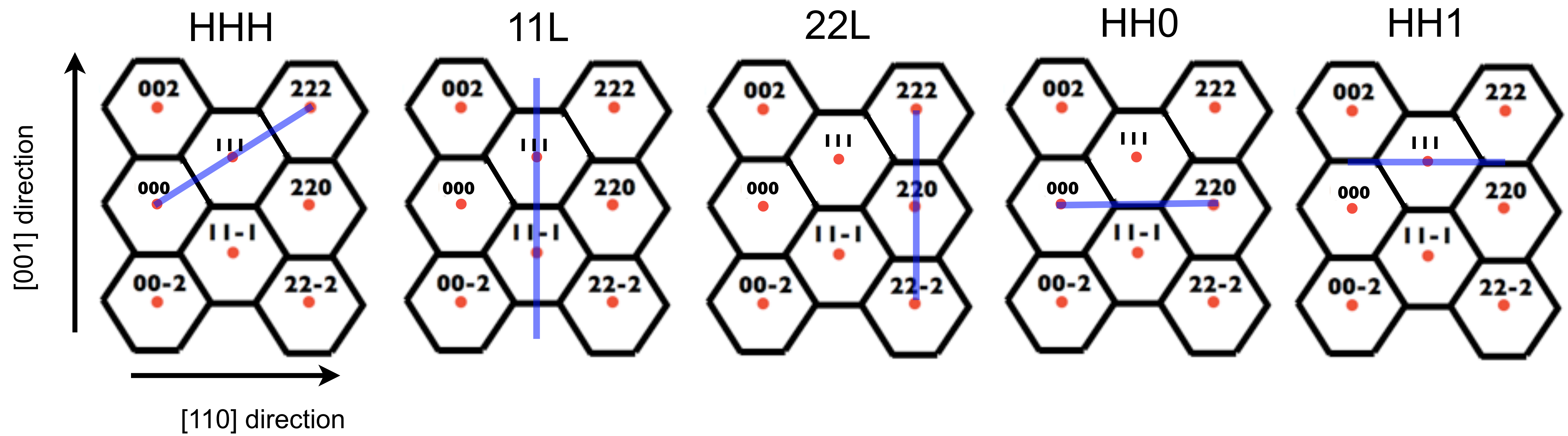


No structure to inelastic scattering

Spin Wave Excitations

Field Induced Order

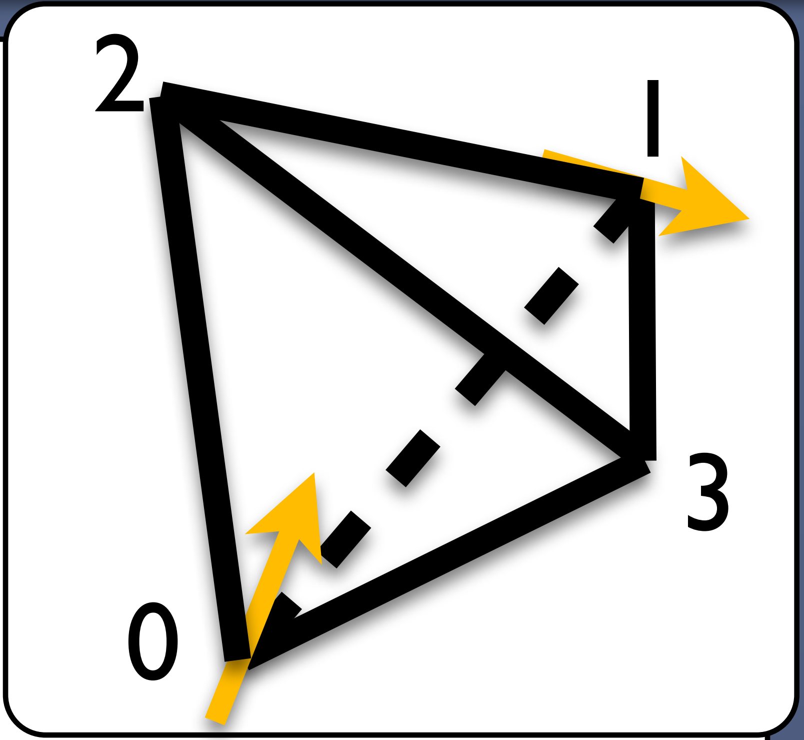




Anisotropic Exchange Model

$$H = \frac{1}{2}\sum_{ij} J_{ij}^{\mu\nu} S_i^{\mu} S_j^{\nu} - \mu_B H^{\mu} \sum_i g_i^{\mu\nu} S_i^{\nu}$$

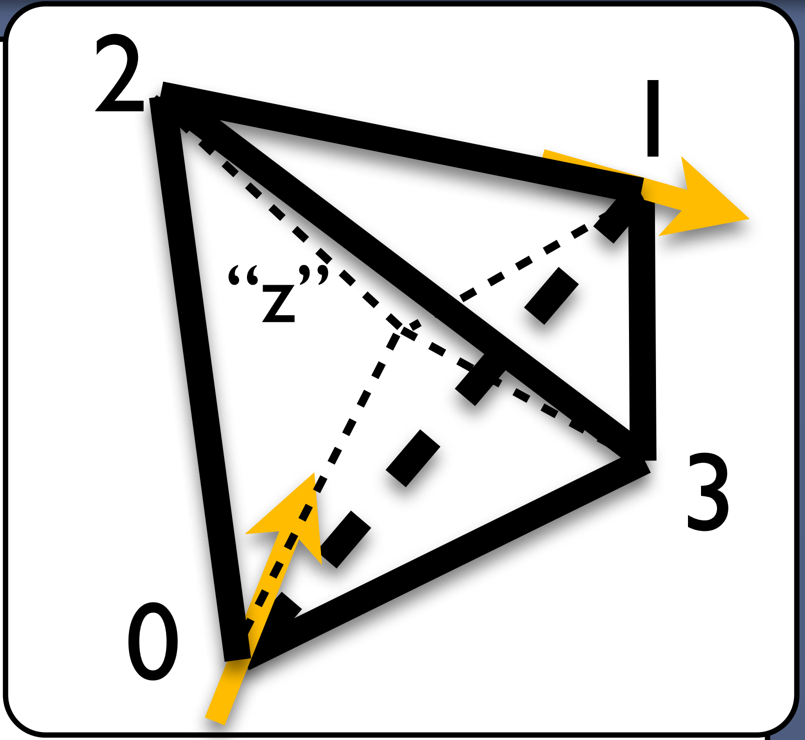
XY anisotropy enters here



$$J_{01} = \begin{pmatrix} J_2 & J_4 & J_4 \\ -J_4 & J_1 & J_3 \\ -J_4 & J_3 & J_1 \end{pmatrix}$$

4 symmetry allowed exchange terms

Anisotropic Exchange Model



$$H = \frac{1}{2}\sum_{ij} J_{ij}^{\mu\nu} S_i^\mu S_j^\nu - \mu_B H^\mu \sum_i g_i^{\mu\nu} S_i^\nu$$

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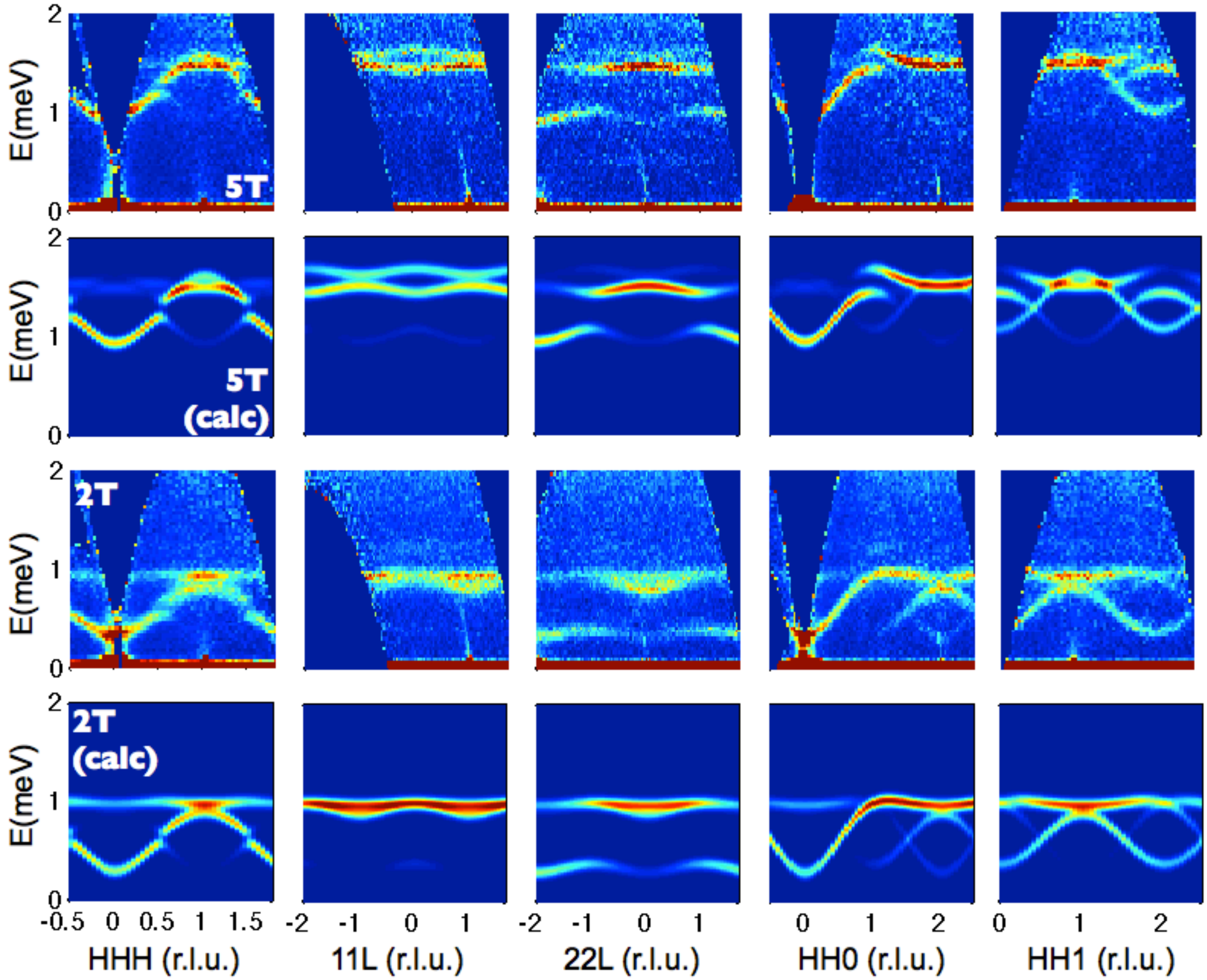
$$J_{01} = \begin{pmatrix} J_2 & J_4 & J_4 \\ -J_4 & J_1 & J_3 \\ -J_4 & J_3 & J_1 \end{pmatrix}$$

4 symmetry allowed exchange terms

$$\begin{aligned} H \;=\; \sum_{\langle ij\rangle} \Big\{ & J_{zz} S_i^z S_j^z - J_\pm (S_i^+ S_j^- + S_i^- S_j^+) + J_{++}\left[\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-\right] \\ & + J_{z\pm}\left[S_i^z(\zeta_{ij} S_j^+ + \zeta_{ij}^* S_j^-) + i \leftrightarrow j\right] \Big\}, \end{aligned}$$



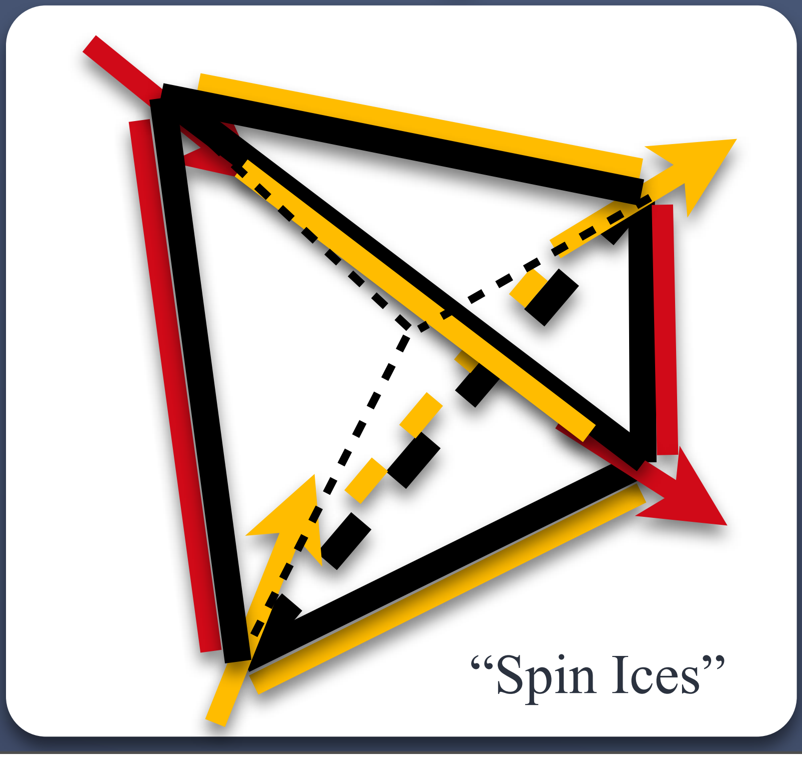
$$J_{zz} = 0.17,\ J_{\pm} = 0.05,\ J_{++} = 0.05,\ J_{z\pm} = -0.14.\quad \text{(meV)}$$

“Quantum Spin Ice”

$$H = \sum_{\langle ij\rangle} \Big\{ J_{zz} S_i^z S_j^z - J_{\pm}(S_i^+ S_j^- + S_i^- S_j^+) + J_{++}\left[\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-\right]$$
$$+ J_{z\pm}\left[S_i^z(\zeta_{ij} S_j^+ + \zeta_{ij}^* S_j^-) + i \leftrightarrow j\right] \Big\},$$

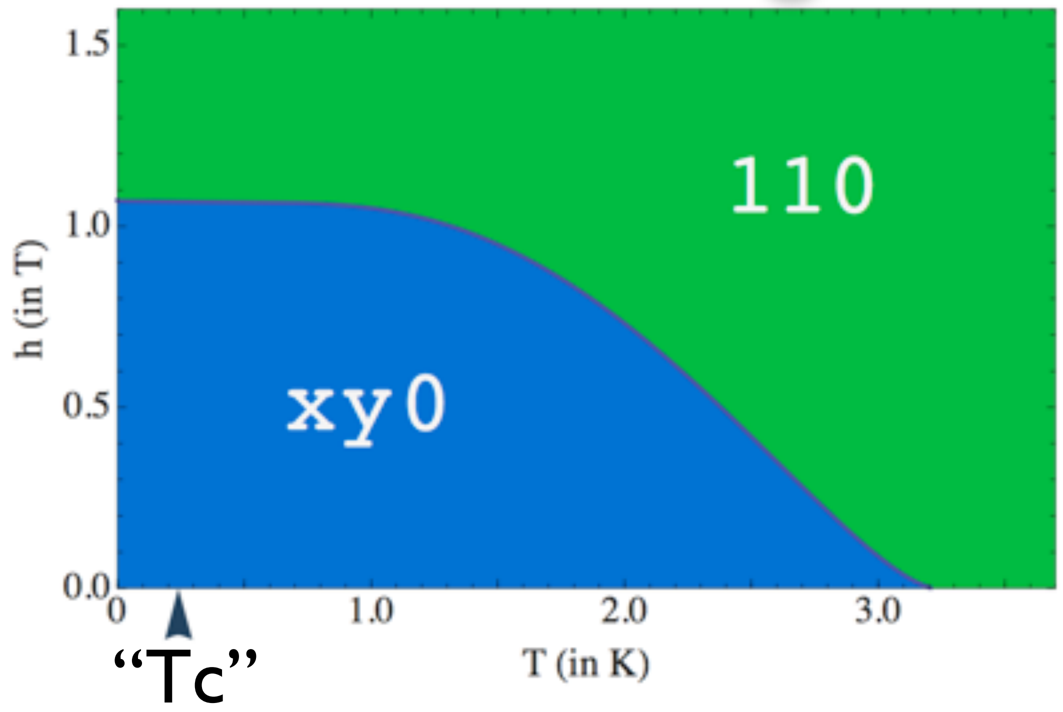
$$J_{zz} = 0.17,\ J_{\pm} = 0.05,\ J_{++} = 0.05,\ J_{z\pm} = -0.14. \quad \text{(meV)}$$

Ferromagnetic “Ising” term

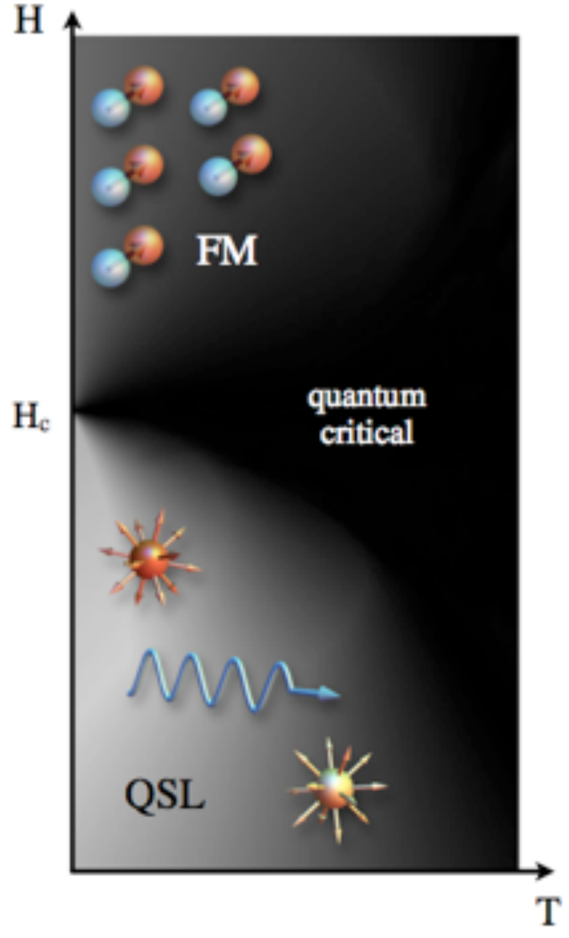


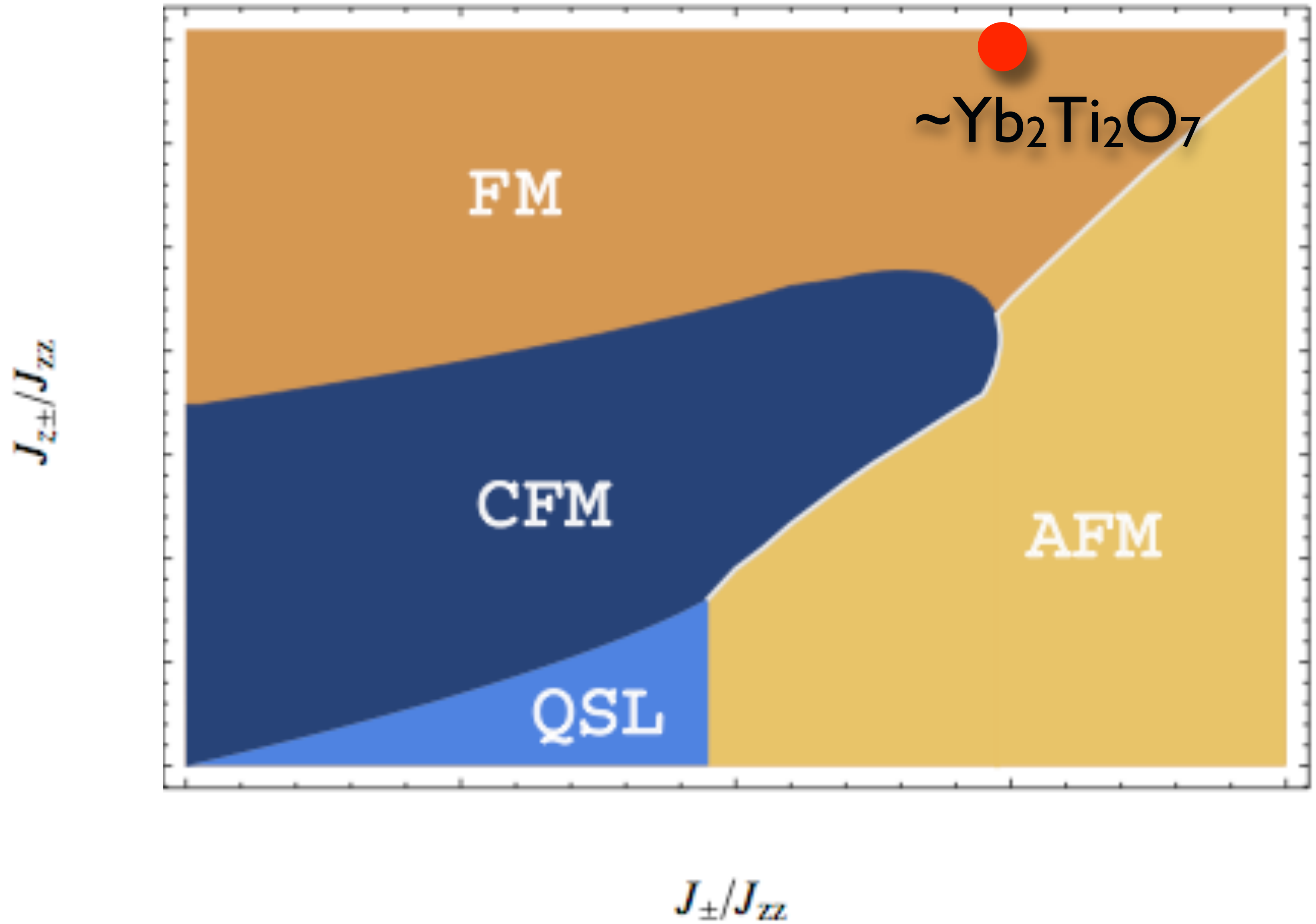
“Spin Ices”

Mean Field Diagram



Coulomb Phase (“U(1) Spin Liquid”)





L. Savary, L. Balents, Phys. Rev. Lett. 108, 037202 (2012)

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FM = Ferromagnet

AFM = Antiferromagnet

CFM = Coulomb Ferromagnet

QSL = U(1) Quantum Spin Liquid

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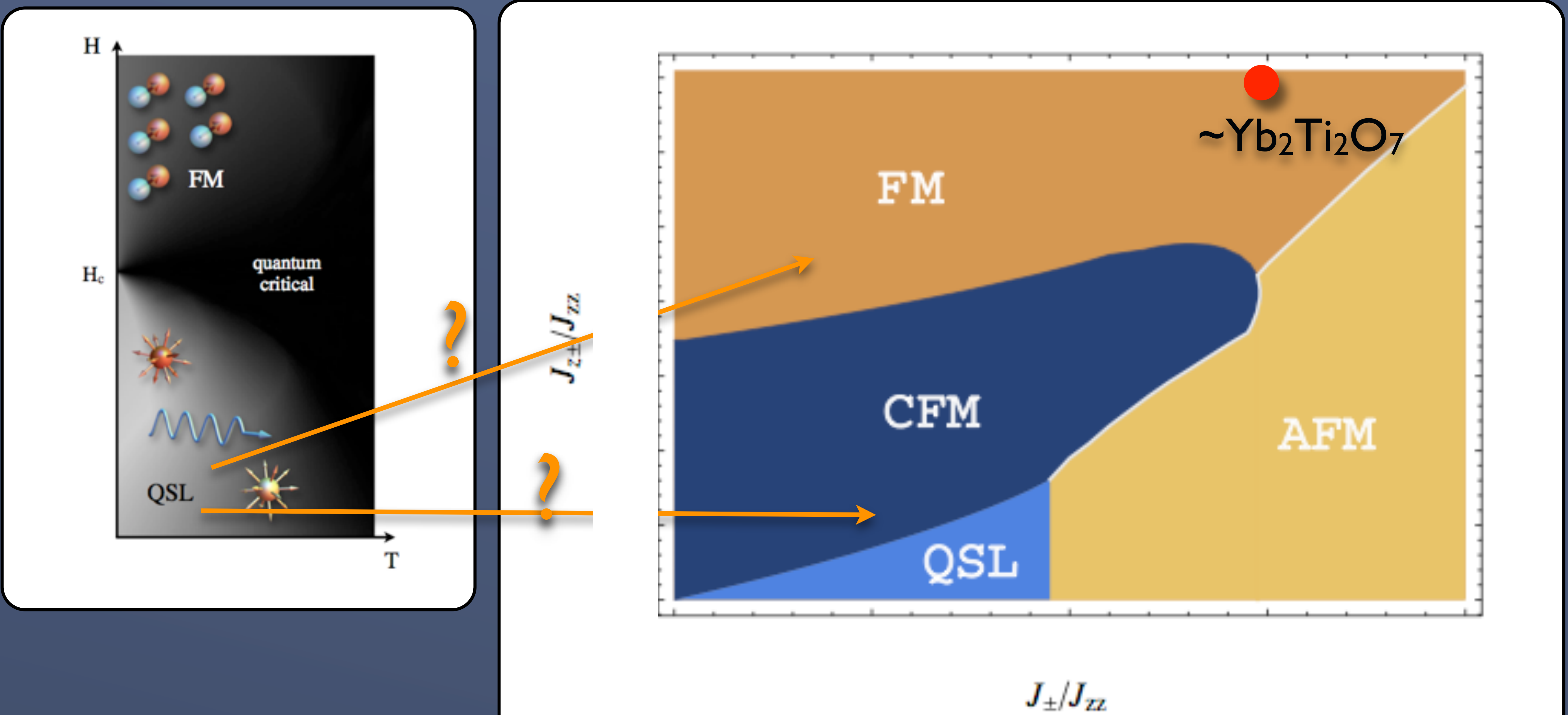

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Conclusions and Remaining Questions

Experimentally observed 2D correlated state above Tc

What are the spin correlations from our Hamiltonian?

Sensitivity of ground state to subtle structural effects

What is the role of stuffing in the magnetic ground state?

High field spin waves show us that $Yb_2Ti_2O_7$ is a Quantum Spin Ice

Exchange is predominantly FM Ising, with quantum fluctuations

Proximity to a Coulomb phase?

Papers

“Two-Dimensional Kagome Correlations and Field Induced Order in the Ferromagnetic XY Pyrochlore $Yb_2Ti_2O_7$”
K.A. Ross, J.P.C. Ruff, C.P. Adams, J.S. Gardner, H.A. Dabkowska, Y. Qiu, J.R.D. Copley, and B.D. Gaulin. Phys. Rev. Lett., **103**, 227202 (2009).

“Dimensional Evolution of Spin Correlations in the Magnetic Pyrochlore, $Yb_2Ti_2O_7$”
K.A. Ross, L.R. Yaraskavitch, M. Laver, J.S. Gardner, J. A. Quilliam, S. Meng, J.B. Kycia, D. K. Singh, H.A. Dabkowska, and B.D. Gaulin. Phys. Rev. B., **84**, 174442 (2011).

“Quantum Excitations in Quantum Spin Ice”
K.A. Ross, L. Savary, B. D. Gaulin, and L. Balents. Phys. Rev. X **1**, 021002 (2011).

“Single crystals of $Yb_2Ti_2O_7$ grown by the Optical Floating Zone technique: naturally "stuffed" pyrochlores?”
K.A. Ross, Th. Proffen, H. Dabkowska, J.A. Quilliam, L.R. Yaraskavitch, J.B. Kycia, and B.D. Gaulin, arXiv:1208.2281 (2012).