Magneto-elasticity in Fragile Magnets

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I. **Introduction:**
   - Multiferroic $Ni_3V_2O_8$
   - Spin-Peierls transition $ZnCr_2O_4$

II. **Modulated Kondo screening in $CeCoGe_3$**

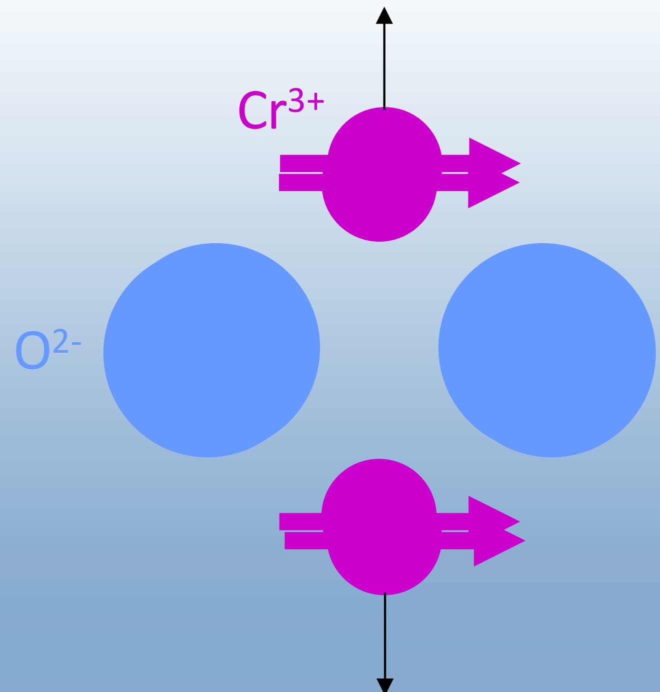
III. **Frustration and its relief in V_2O_3**

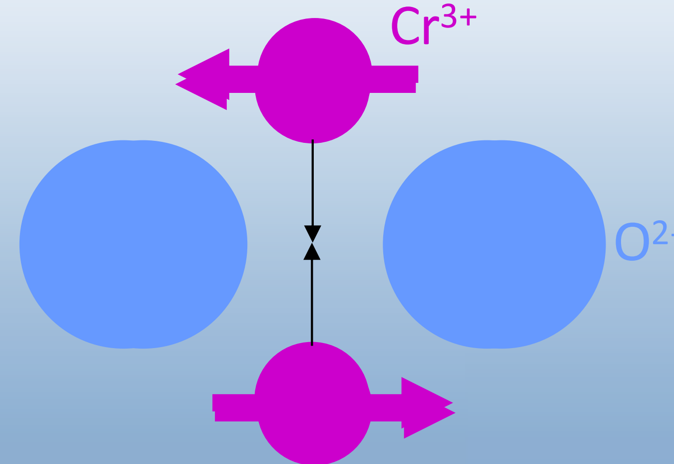
DOE EFRC
DE-SC-0019331

Magneto-striction

$\mathcal{H} = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$ Exchange constants are not actually constant

$$\mathbf{F}_{12} = -\nabla\left(J_{12}\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle\right) = -\hat{\mathbf{r}}_{12} \frac{\partial J_{12}}{\partial r} \langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$$





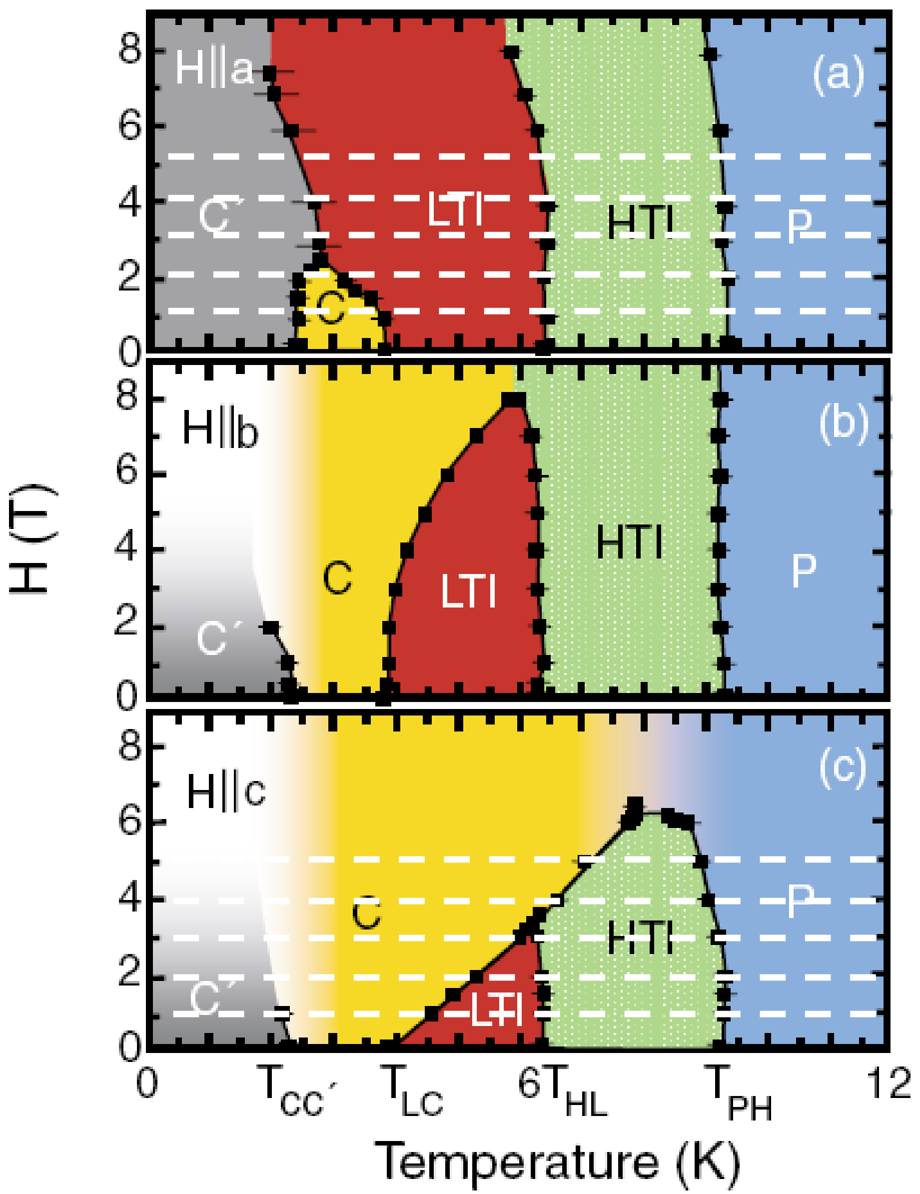
Tchernyshyov et al. PRL (2001) and PRB (2002)

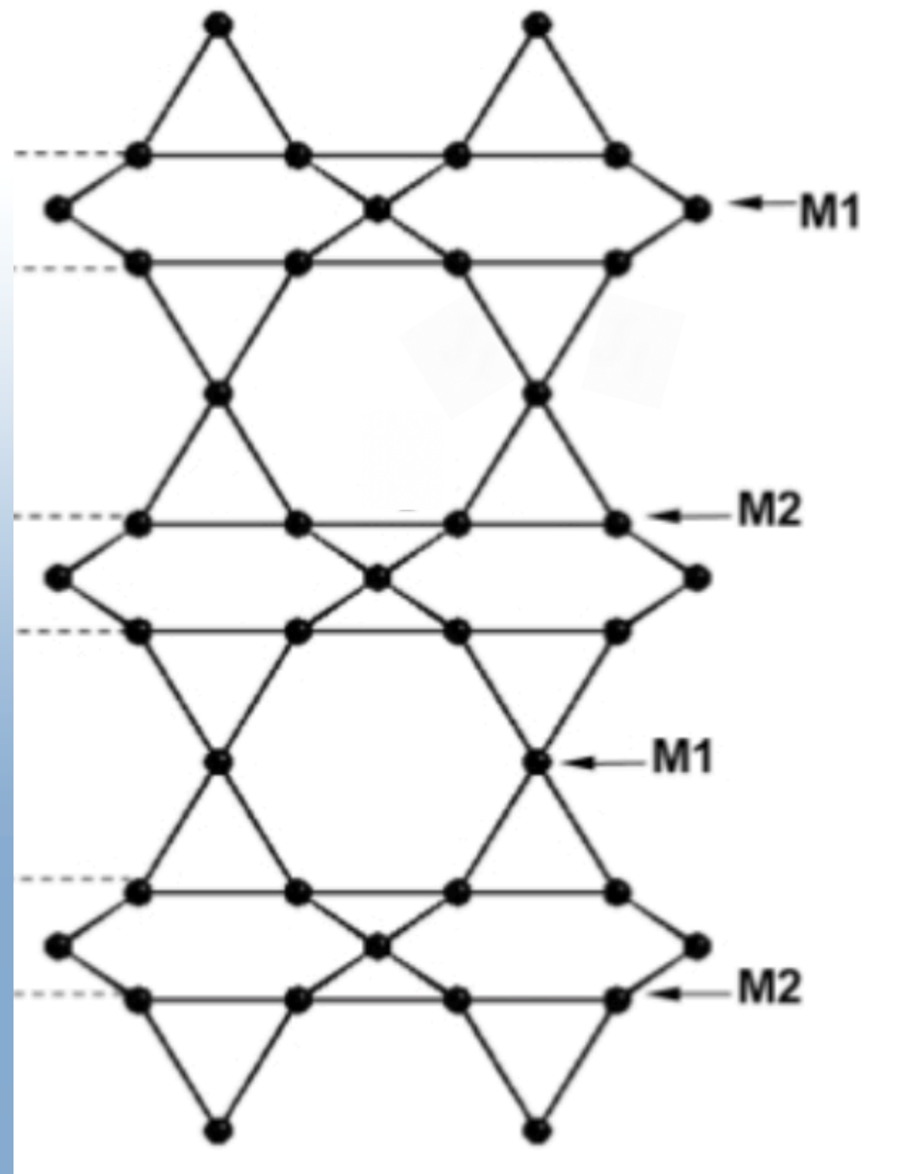
Qualitative impacts when there are competing interactions:

a. Lattice responds to magnetic symmetry breaking

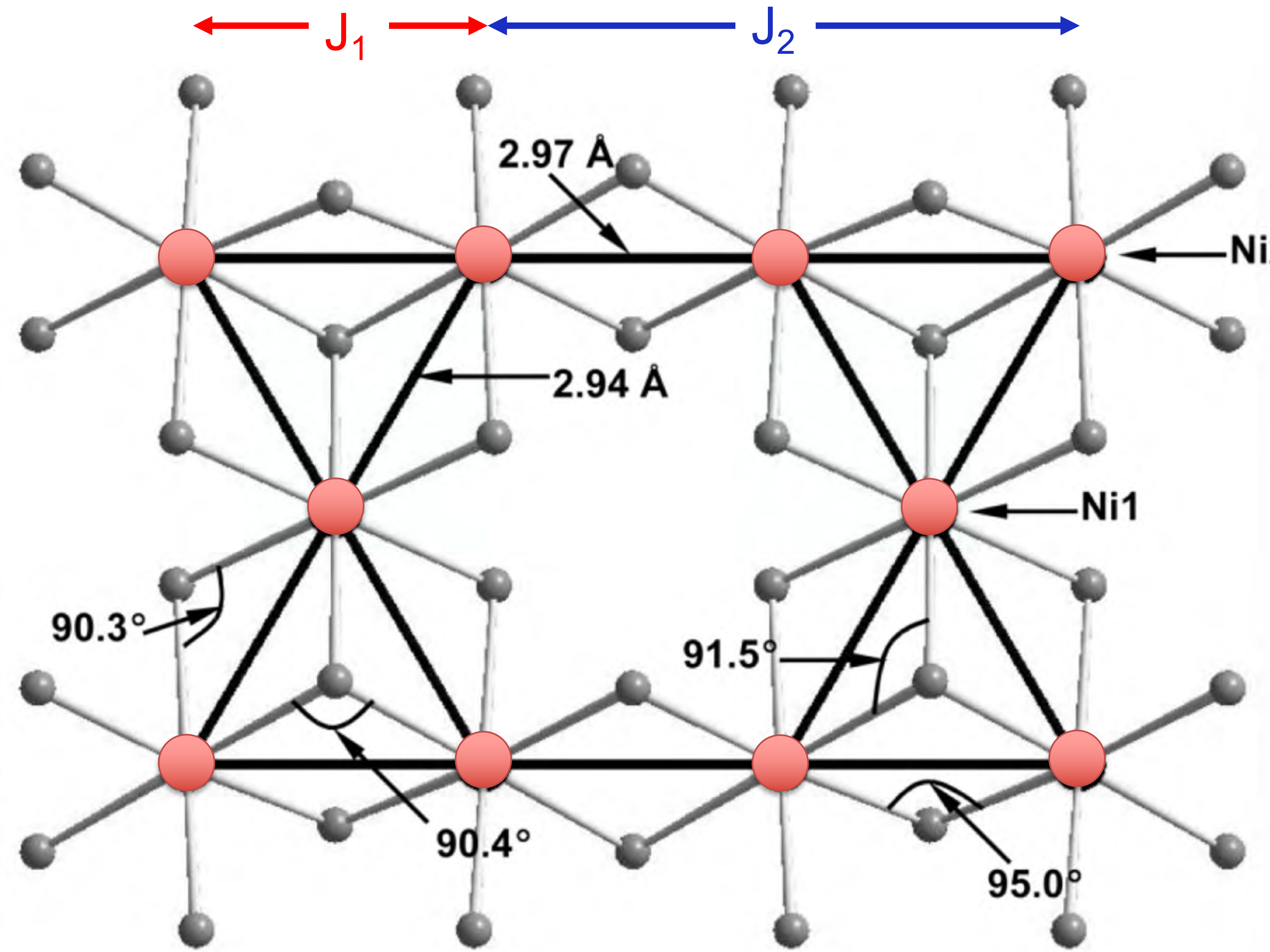
b. Lattice distortion can enable magnetic order by relieving frustration

Multiferroic kagome staircase $Ni_3V_2O_8$





Competing Exchange Interactions

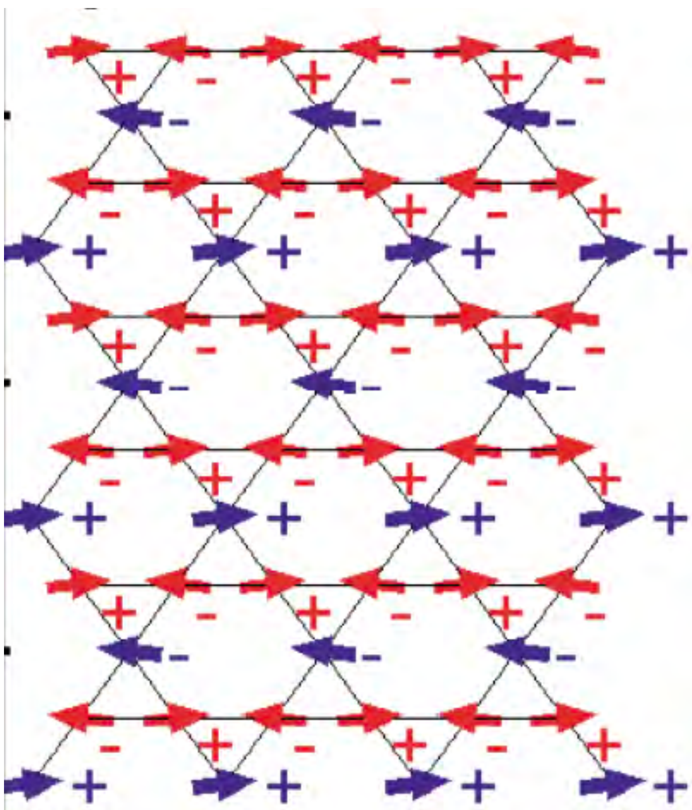


N. Rogado et al (2003)

Modulated magnetic phases

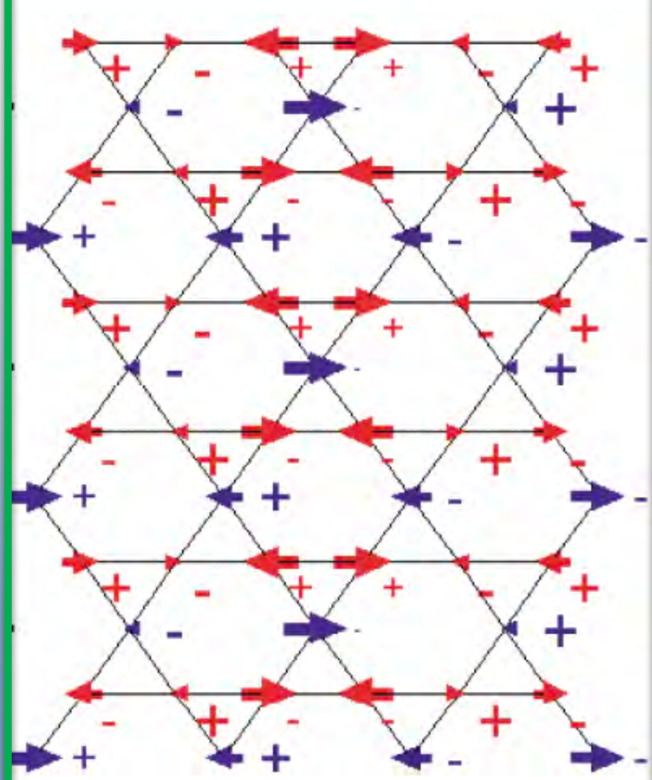
Ferroelectric

Commensurate
Canted FM



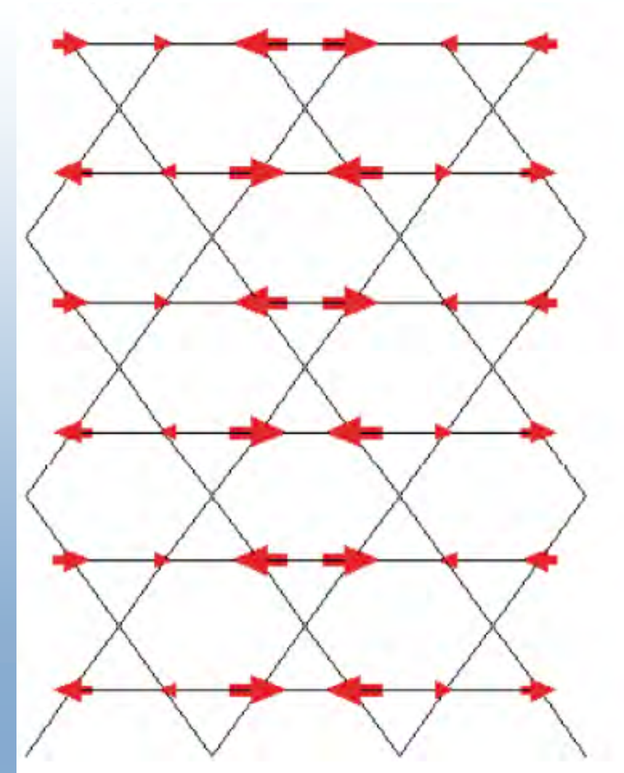
2.2 K < T < 4 K

Incommensurate
Cycloidal



4 K < T < 6.5 K

Incommensurate
amplitude modulated



6.5 K < T < 9.2 K

Lattice responds to magnetic symmetry breaking

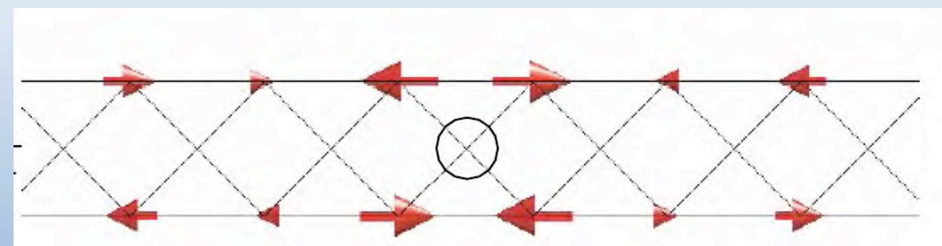
IRREP	1	2_X	$\tilde{m}_y$	$\tilde{m}_z$
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	1	-1
Γ_4	1	-1	-1	1

Tri-linear interaction:

$$V = \sum_{nm\gamma} c_{nm\gamma} \sigma_n(\mathbf{q}) \sigma_m(-\mathbf{q}) P_\gamma$$

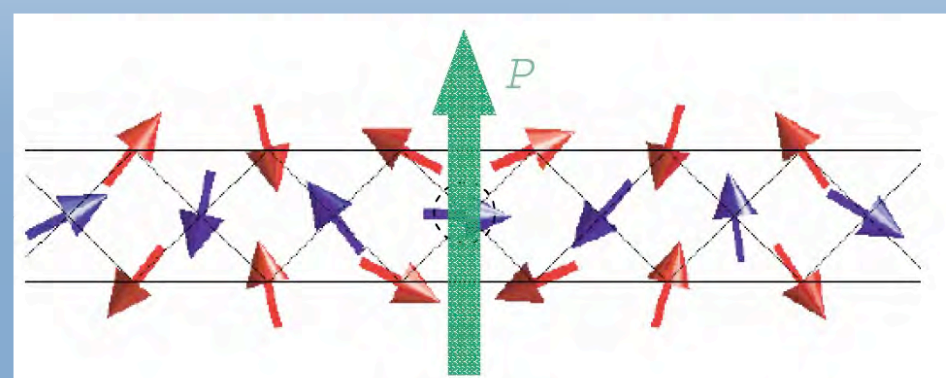
Amplitude modulated (Γ_4)

$$V_{HTI} = \sum_{\gamma} c_{44\gamma} |\sigma_4(\mathbf{q})|^2 P_\gamma \quad \equiv 0$$



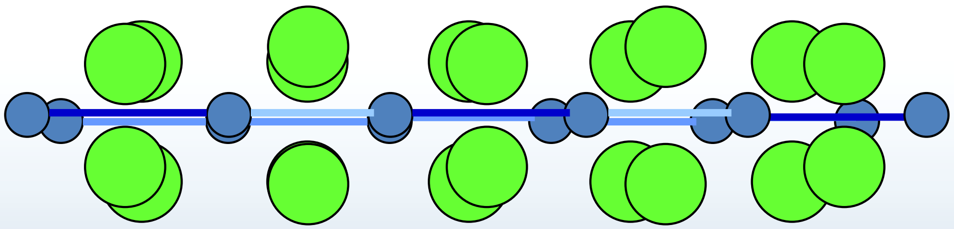
Cycloid state (Γ_4+Γ_1)

$$V_{LTI} = c_{14y}(\sigma_1(\mathbf{q})\sigma_4(-\mathbf{q}) + \sigma_4(\mathbf{q})\sigma_1(-\mathbf{q}))P_y$$

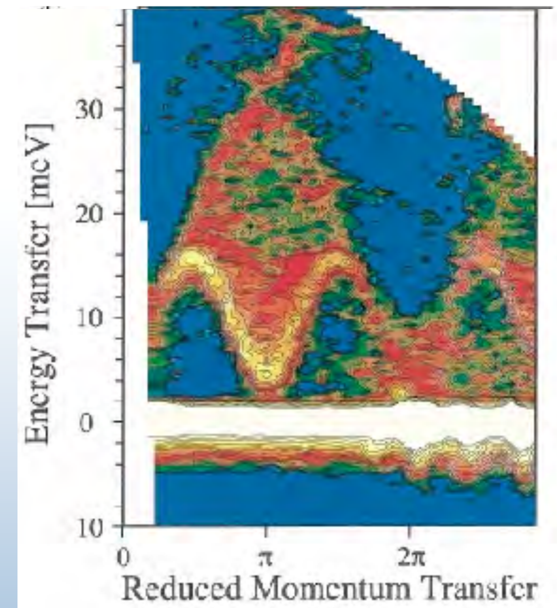


Relieving frustration

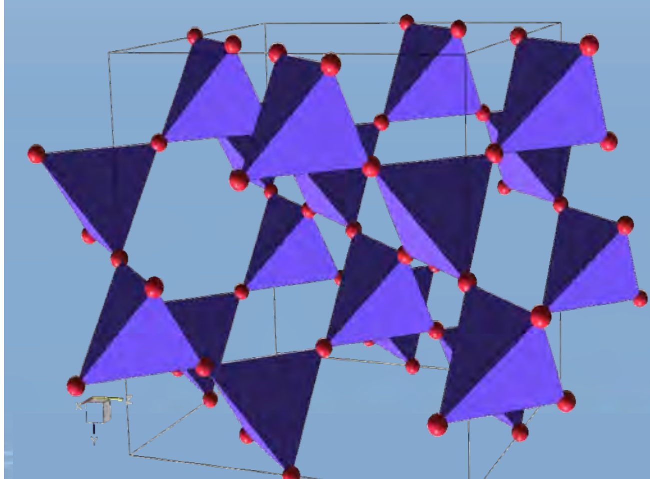
❖ Spin-Peierls transition for AFM spin-1/2 chain

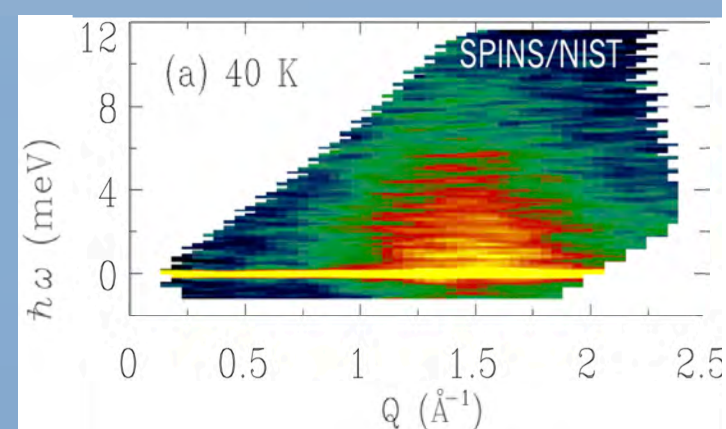


$$H = -\sum_l \left(J\mathbf{S}_{2l} \cdot \mathbf{S}_{2l+1} + J'\mathbf{S}_{2l} \cdot \mathbf{S}_{2l-1} \right)$$



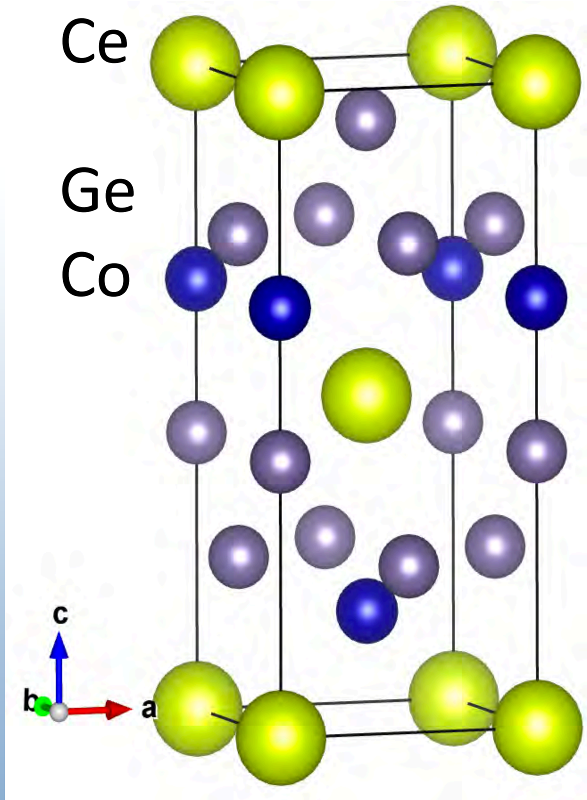
❖ Spin-Peierls-like transition in pyrochlore Antiferromagnets ($ZnCr_2O_4$)

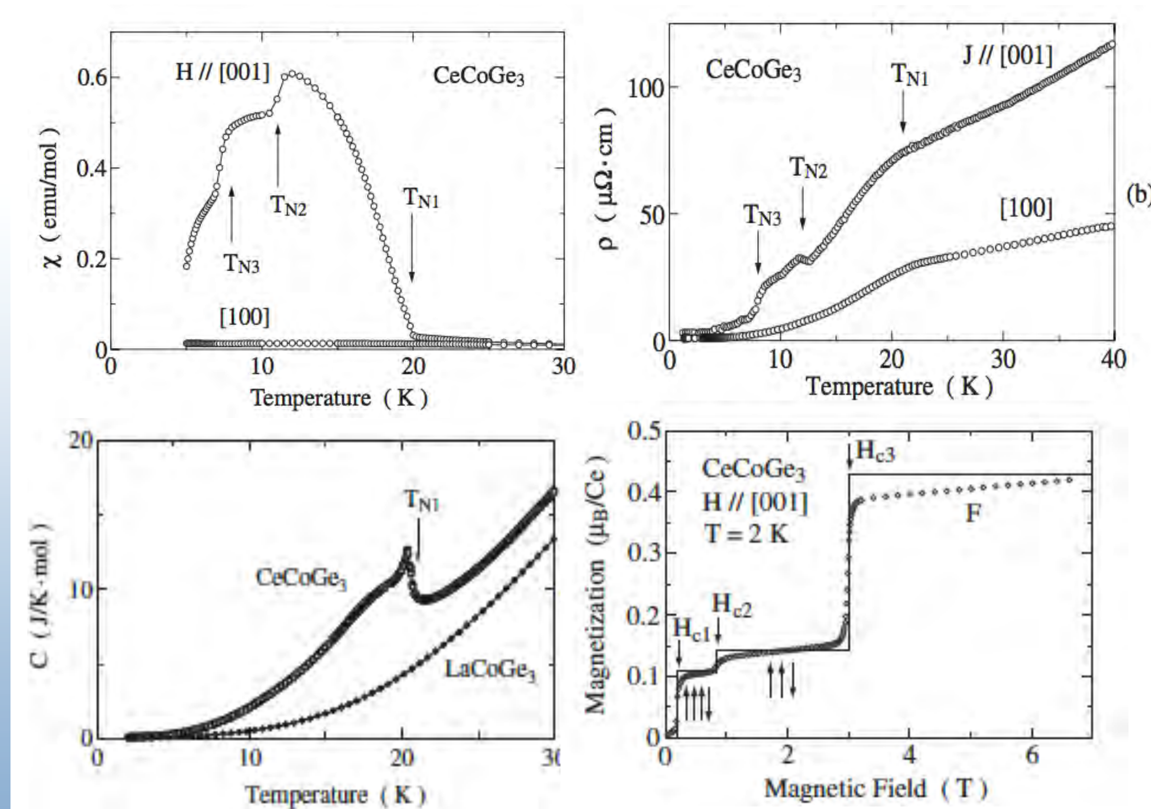




Kondo lattice $CeCoGe_3$

Arumugam Thamizhavel, *et. al.* JPS (2005)





- ❑Non-centro-symmetric tetragonal
- ❑Three thermal phase transitions T_{N1}= 21K, T_{N2}= 12K, T_{N3}= 8K
- ❑[001] easy axis
- ❑Strong coupling of magnetism to transport
- ❑Meta-magnetic transitions

Collaborators: $CeCoGe_3$

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JHU → Berkeley

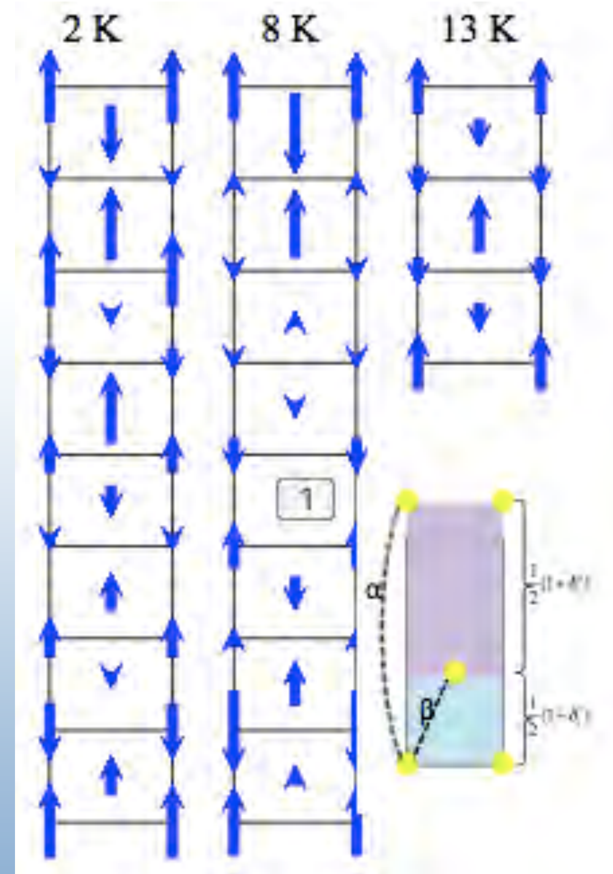
NIST Center for Neutron Research

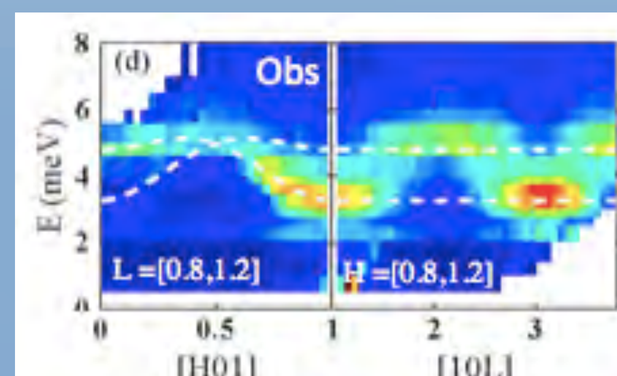
Chris Stock,
University of Edinburgh

Cedomir Petrovic,
Brookhaven National Laboratory

CeCoGe3: Summary

- Ising-like spin-orbital degree of freedom
- Complex sequence of commensurate square-wave structures that extend to eight unit cells
- Intricate spin-lattice order
- Magnons confined within basal plane bi-layers
- Hypothesis: intertwined electronic screening and modulated magnetism





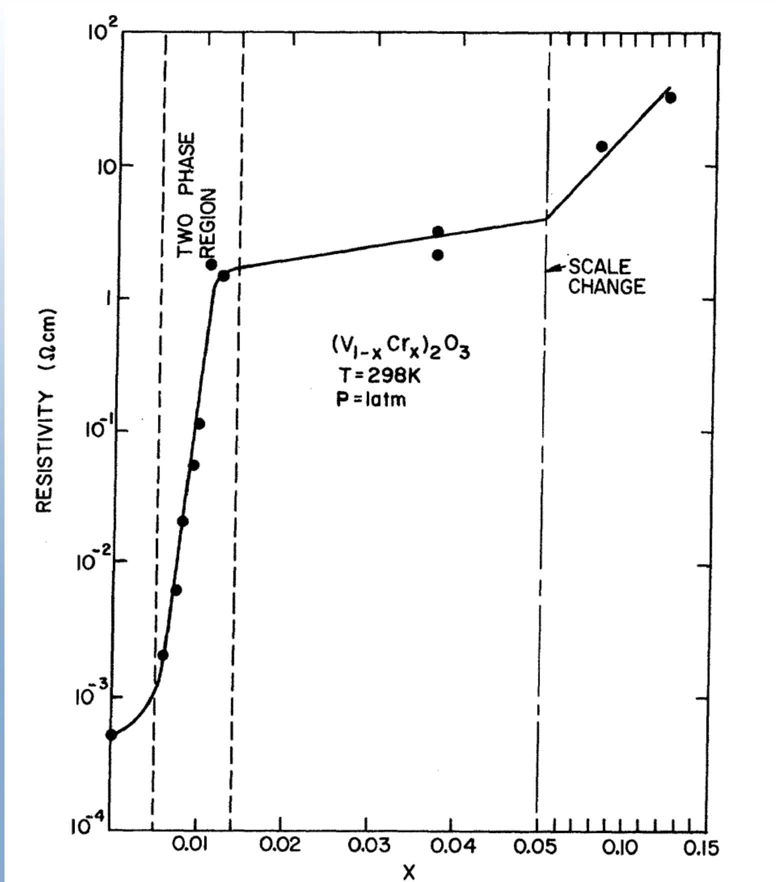
Is a modulated Neel-Kondo phase possible?

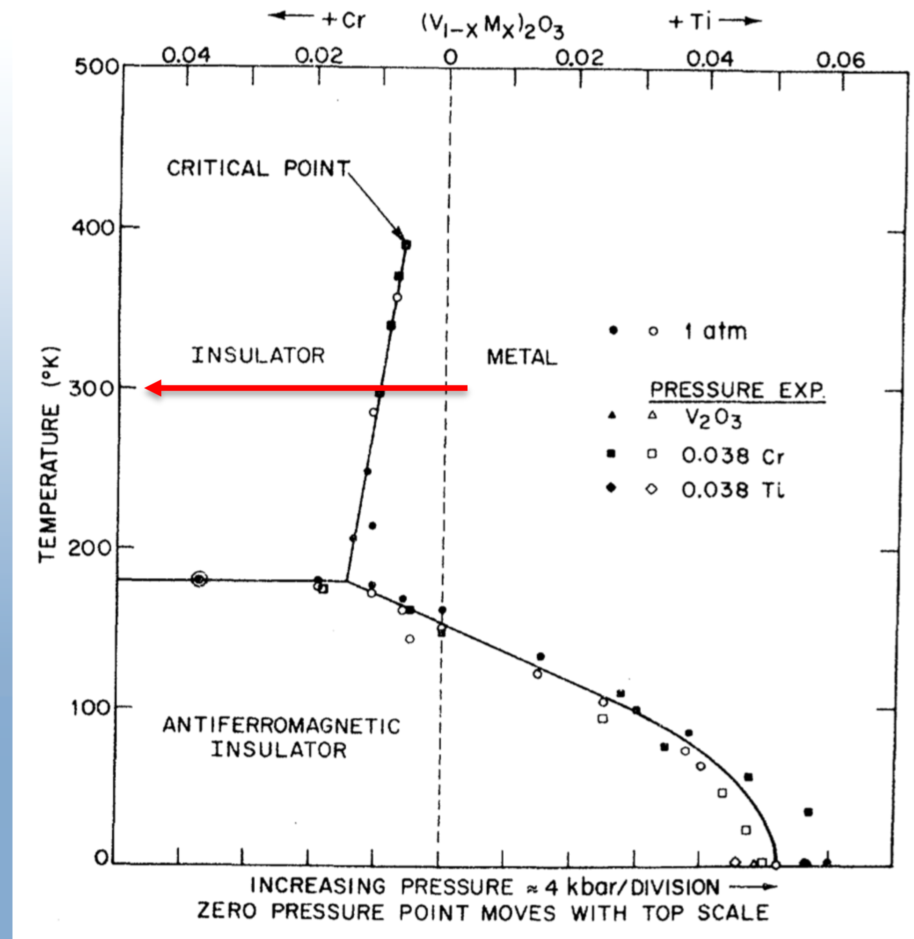
Neel-like Strong Kondo screening Neel-like

Volume 23, Number 24 PHYSICAL REVIEW LETTERS 15 December 1969

MOTT TRANSITION IN Cr-DOPED V_2O_3

D. B. McWhan, T. M. Rice, and J. P. Remeika
Bell Telephone Laboratories, Incorporated, Murray Hill, New Jersey 07974
(Received 8 August 1969)





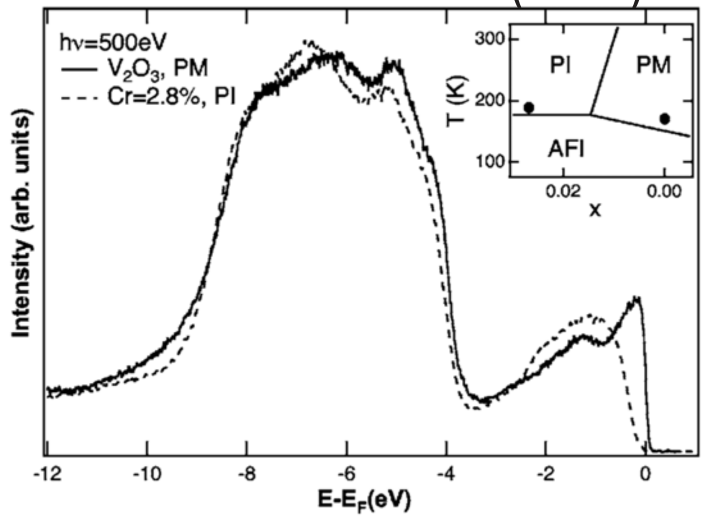
More chromium

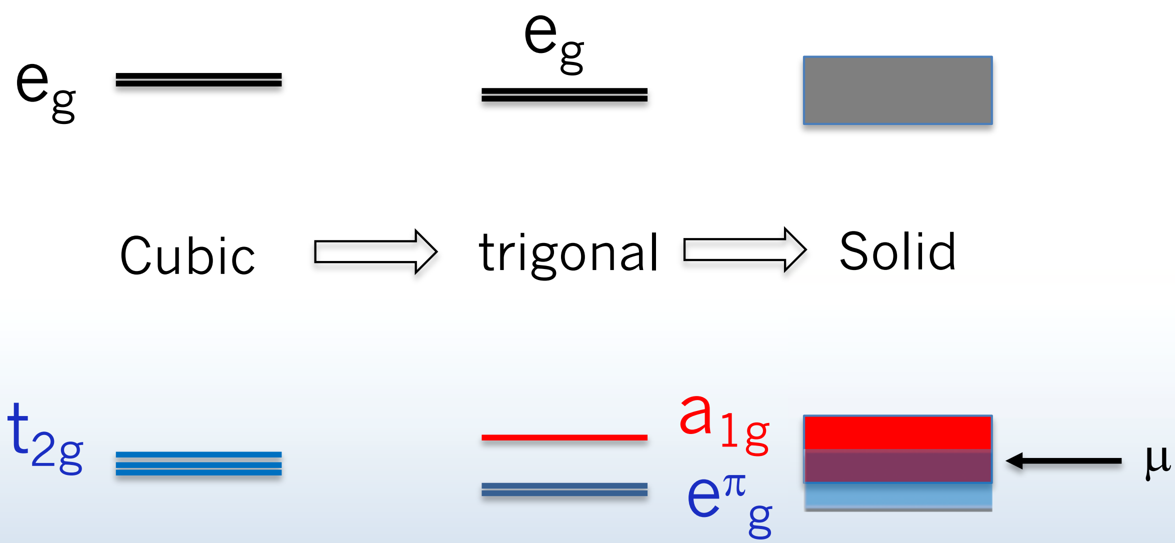
$$H = -t \sum_{\substack{\langle \vec{r},\vec{r}\,'\rangle \\ \sigma=\uparrow,\downarrow}} \left(c^\dagger_\sigma(\vec{r})c_\sigma(\vec{r}\,') + \text{h.c.}\right) + U\sum_{\vec{r}} n_\uparrow(\vec{r})n_\downarrow(\vec{r})$$

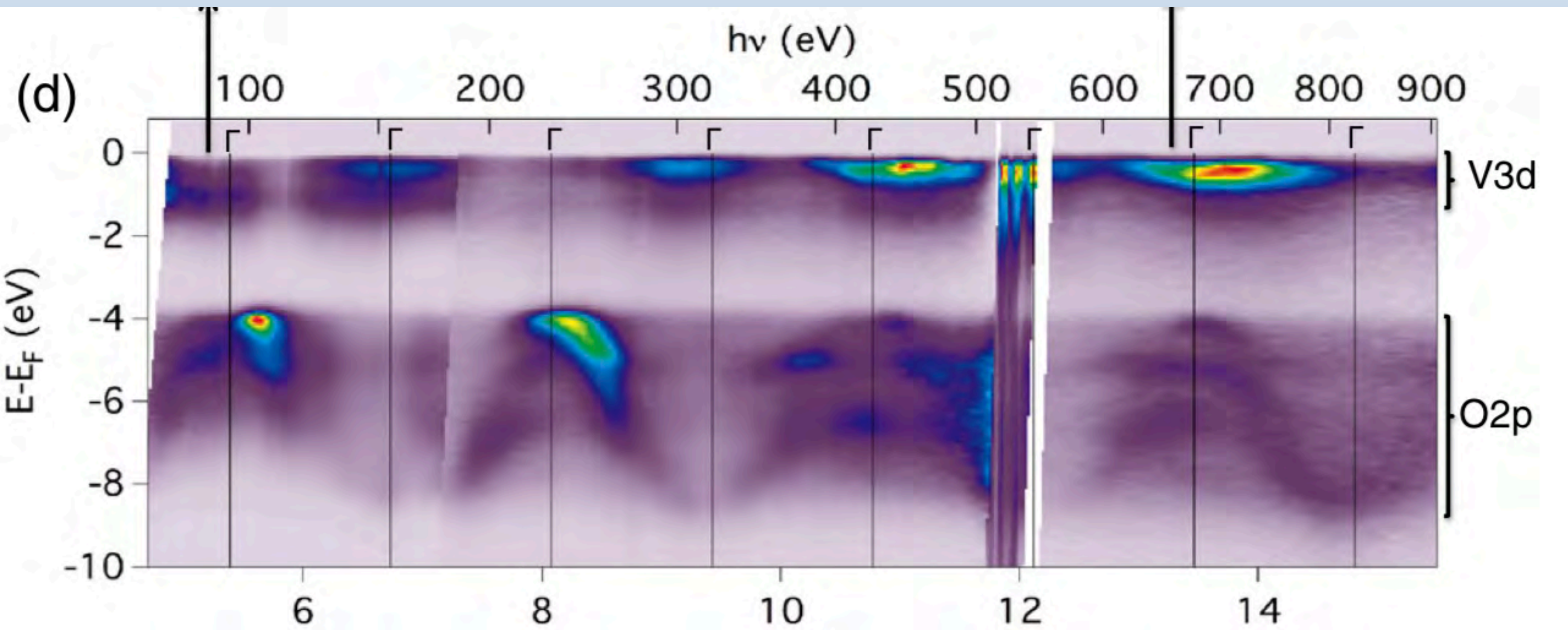
INSTITUTE FOR QUANTUM MATTER

Photoemission: Mott insulator

Mo et al. PRB 74 (2006)







I. L. Vechio et al. PRL 117, 166401 (2016)

Collaborators V_2O_3

J. C. Leiner	CCES and ORNL
H. O. Jeschke	Okayama U and Goethe U.
R. Valenti	Goethe U. Frankfurt
S. Zhang	Johns Hopkins U.
A. T. Savici	ORNL
Jiao Lin	ORNL
M. B. Stone	ORNL
M. D. Lumsden	ORNL
Jiawang Hong	ORNL
O. Delaire	Duke U. and ORNL
Wei Bao	Renmin U.

Phys. Rev. X 9, 011035 (2019).

Leiner

Zhang

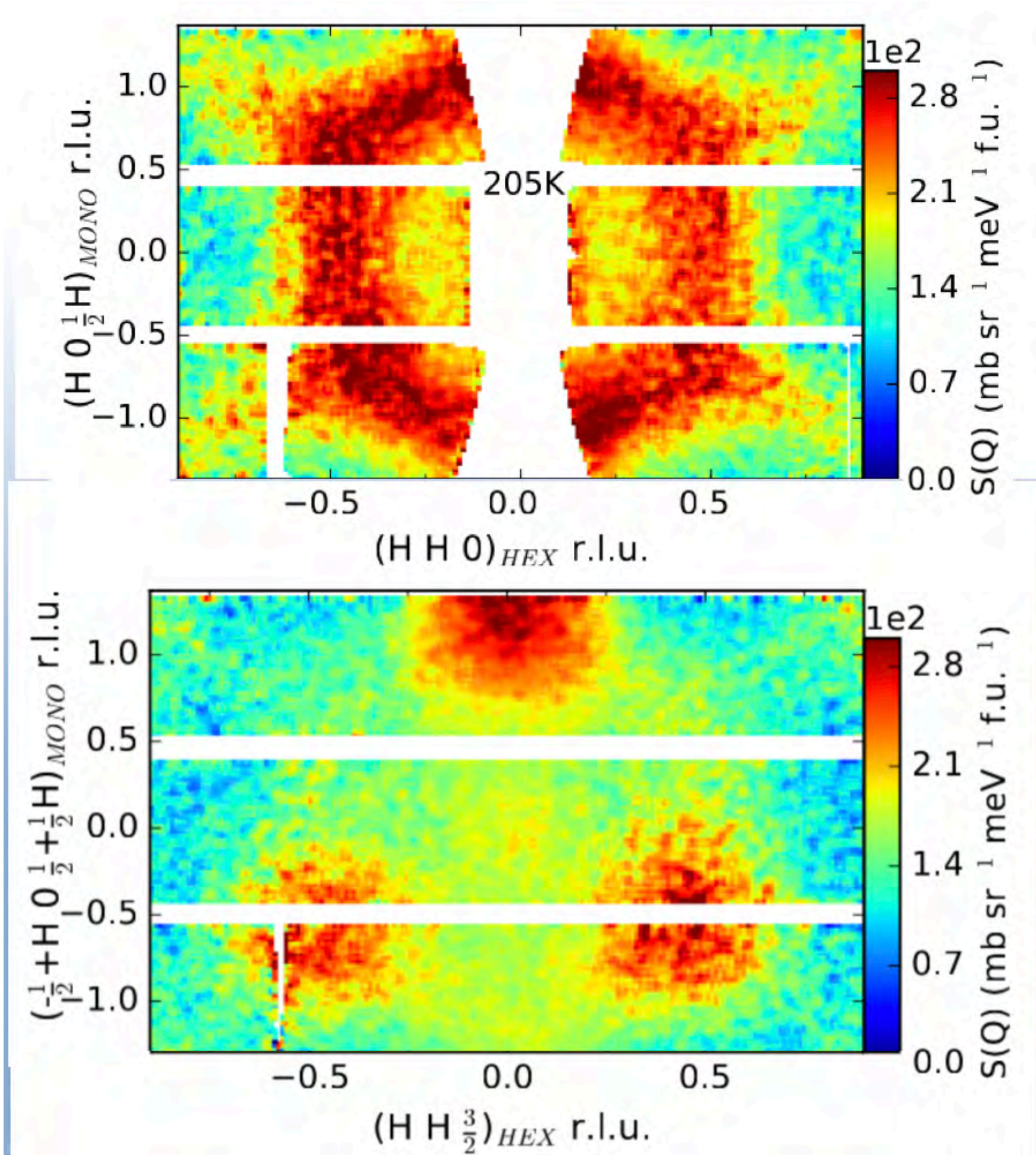
IQM-EFRC Research funded by US DOE-BES DE-SC0019331

GORDON AND BETTY MOORE FOUNDATION

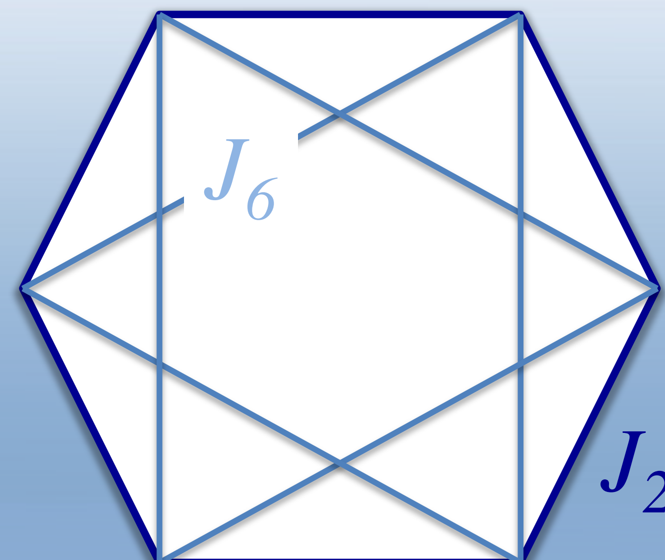
NIST Center for Neutron Research

SNS SPALLATION NEUTRON SOURCE

Ultra Short range correlations in PI



distance (Å)	J_j		DFT (meV)
2.71072	J_1		-0.3(6)
2.87799	J_2		8.5(3)
3.46255	J_3		0.6(3)
3.68774	J_4		0.0(2)
4.29734	J_5		-1.2(7)
4.94240	J_6		1.7(2)

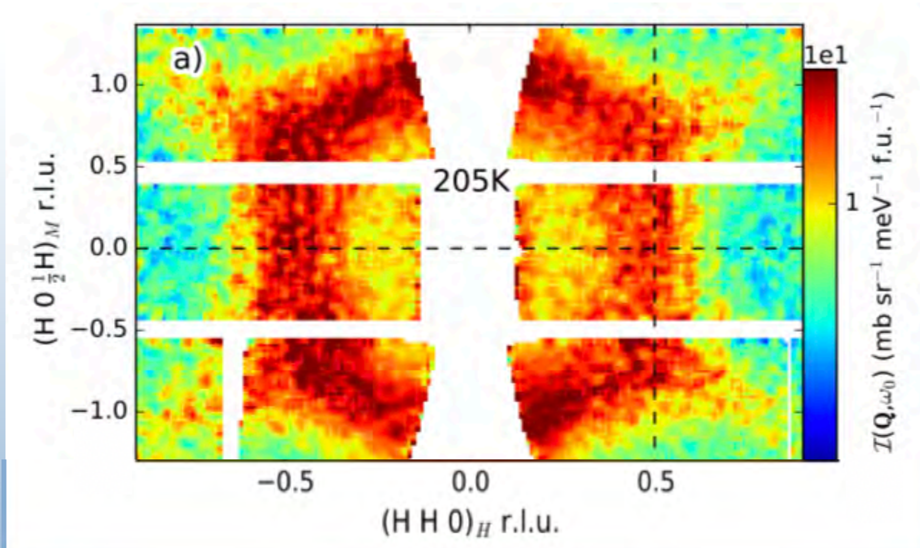


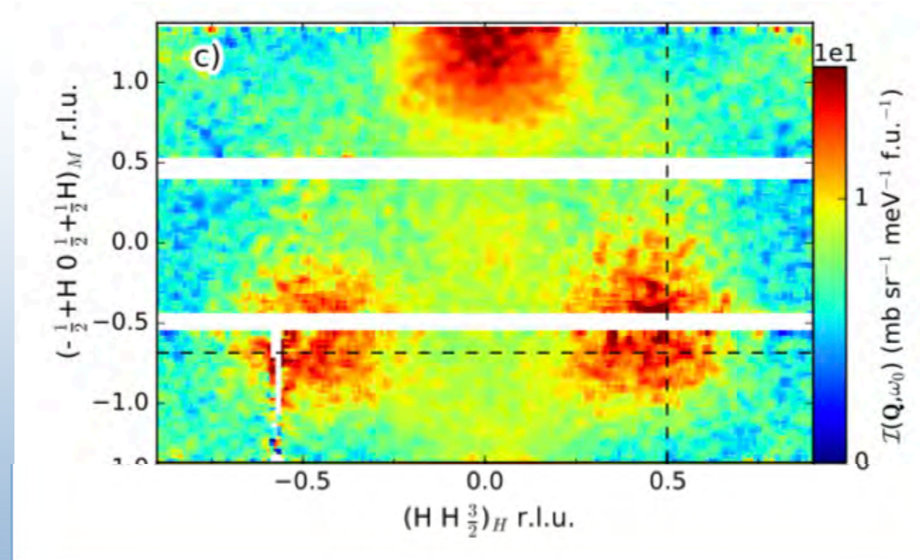
J6/J2=0.2 is in the frustrated regime where neither interaction dominates

Self consistent Gaussian Approximation

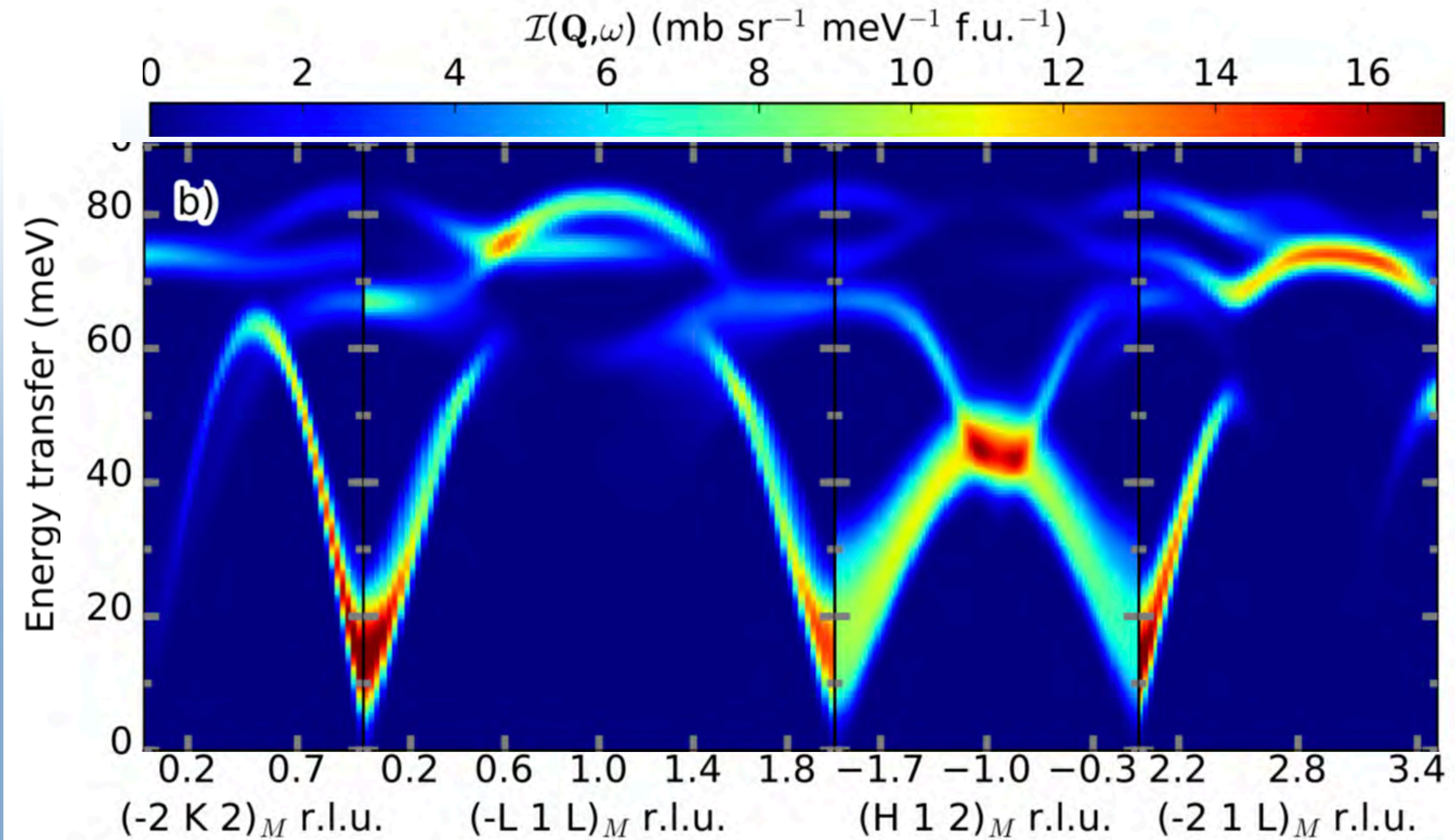
$$\beta E = \frac{1}{2}\sum_{ij}(\beta\sum_{n} J_n A_{ij}^{(n)} + \lambda\delta_{ij})s_i s_j.$$

Include **all** DFT determined Exchange interactions (3D)

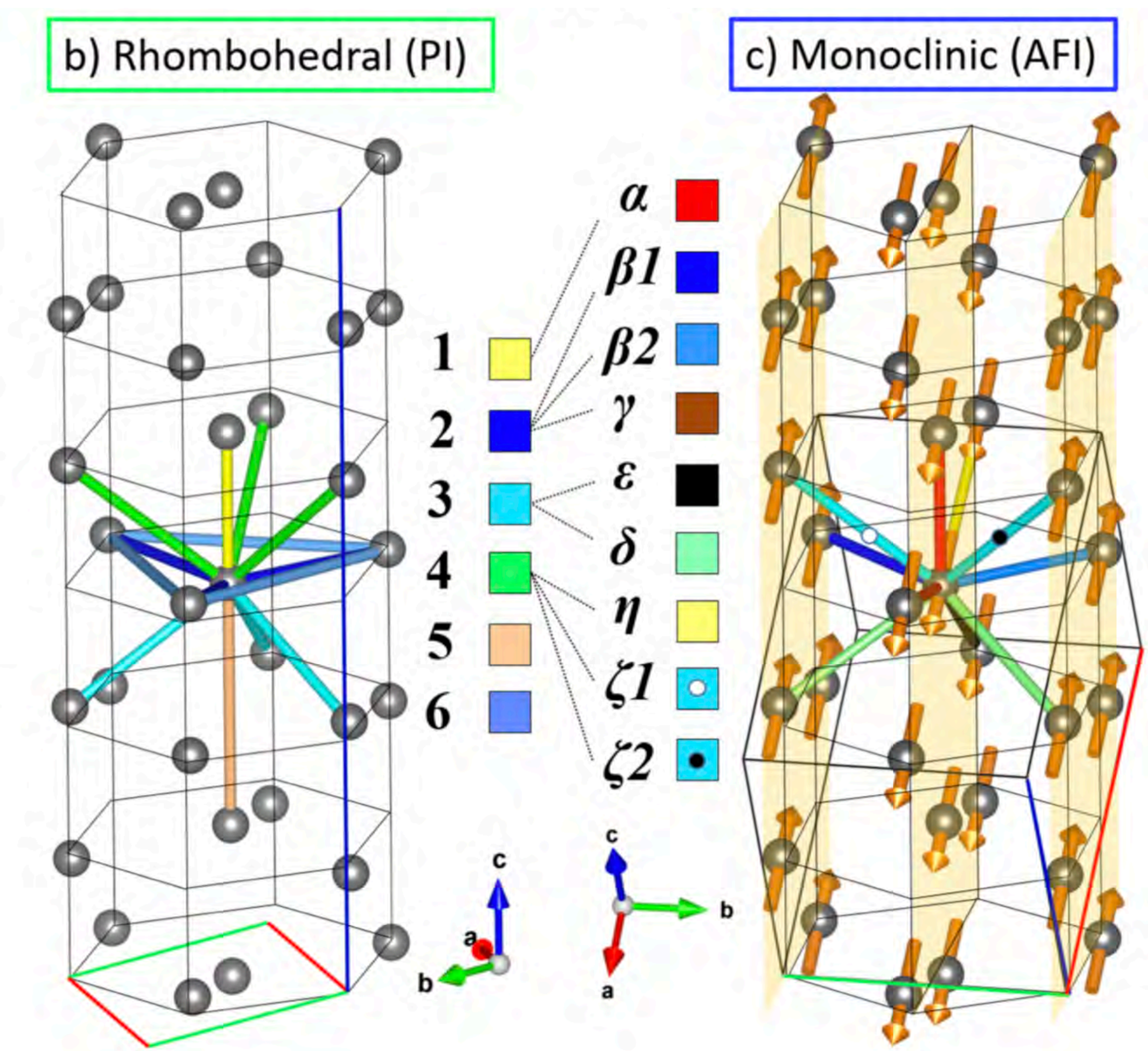




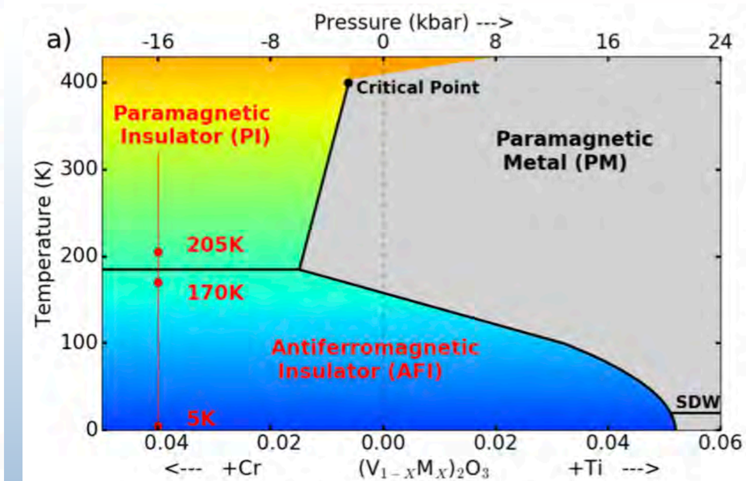
Development of Coherent Magnon



AFI: Frustration relieved!

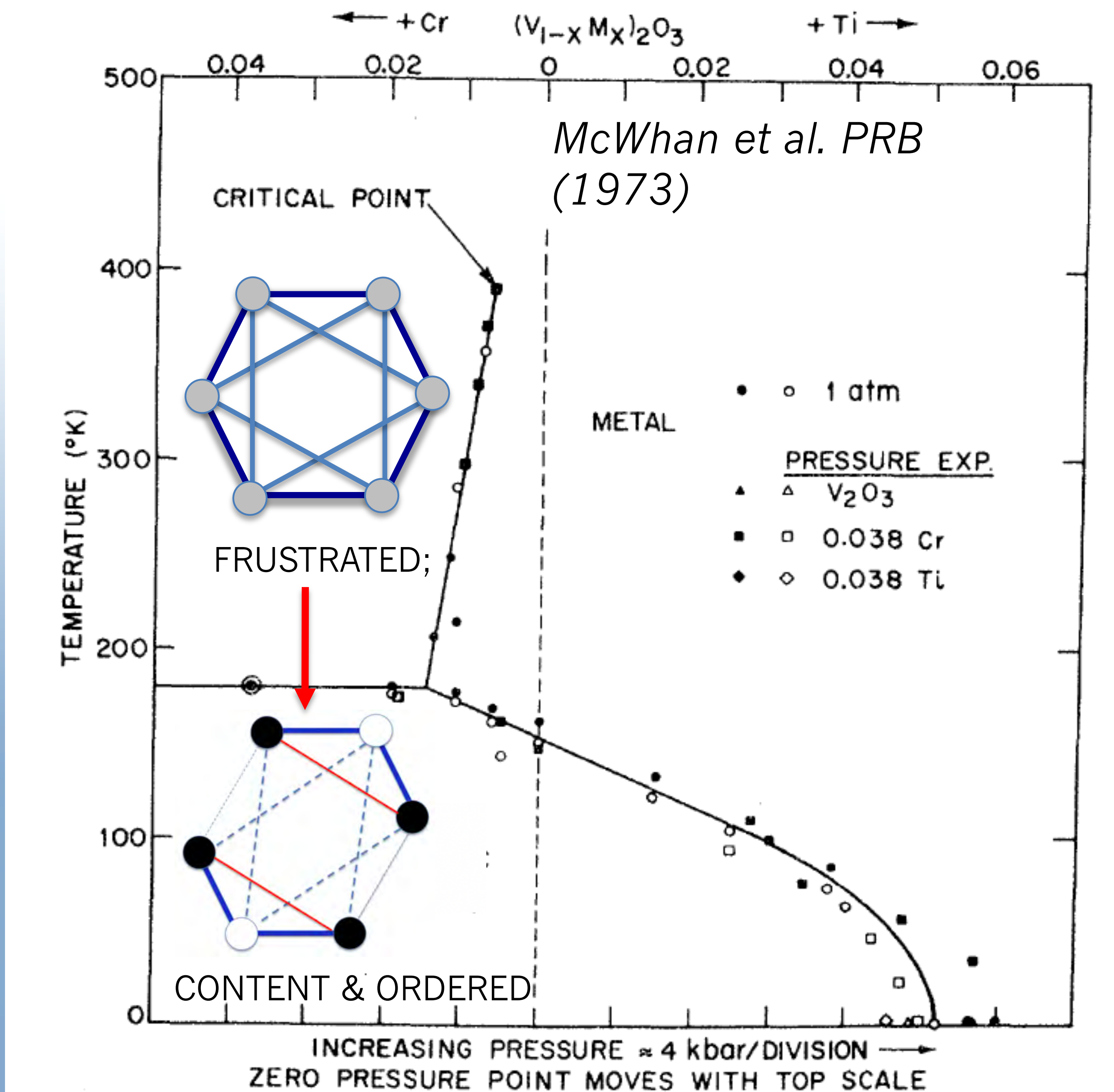


Leiner, Valenti, Jeschke et al.



distance (Å)	J_i (meV)	DFT	Neutron	sgn($\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$)
2.75904	J_α	-1(2)	-6.0(2)	+
2.83083	$J_{\beta 1}$	25(2)	27.7(2)	−
2.91789	$J_{\beta 2}$	9(2)	7.7(2)	−
2.98538	J_γ	3(2)	0.0(2)	+
3.43336	J_ϵ	-9(3)	2.0(2)	−
3.45420	J_δ	4(2)	1.1(2)	−
3.63334	J_η	1(2)	-2.0(2)	+
3.70177	$J_{\zeta 1}$	1(1)	7.1(2)	−
3.76876	$J_{\zeta 2}$	-1(1)	7.1(2)	−
4.22293	J_θ	-4(2)	0	+
4.97765	J_ι	3(1)	0	−
5.00240	J_κ	-1(1)	0	+

Relieving frustration in $(V_{1-x}Cr_x)_2O_3$



Conclusions V_2O_3

- ❖The PI state is frustrated by competing spin interactions on the honeycomb lattice
- ❖The PI to AFI transition is an instability that relieves magnetic frustration
- ❖LDA+U can now produce quantitatively reliable exchange interactions even near the MIT
- ❖Ever closer to “understanding” V_2O_3?

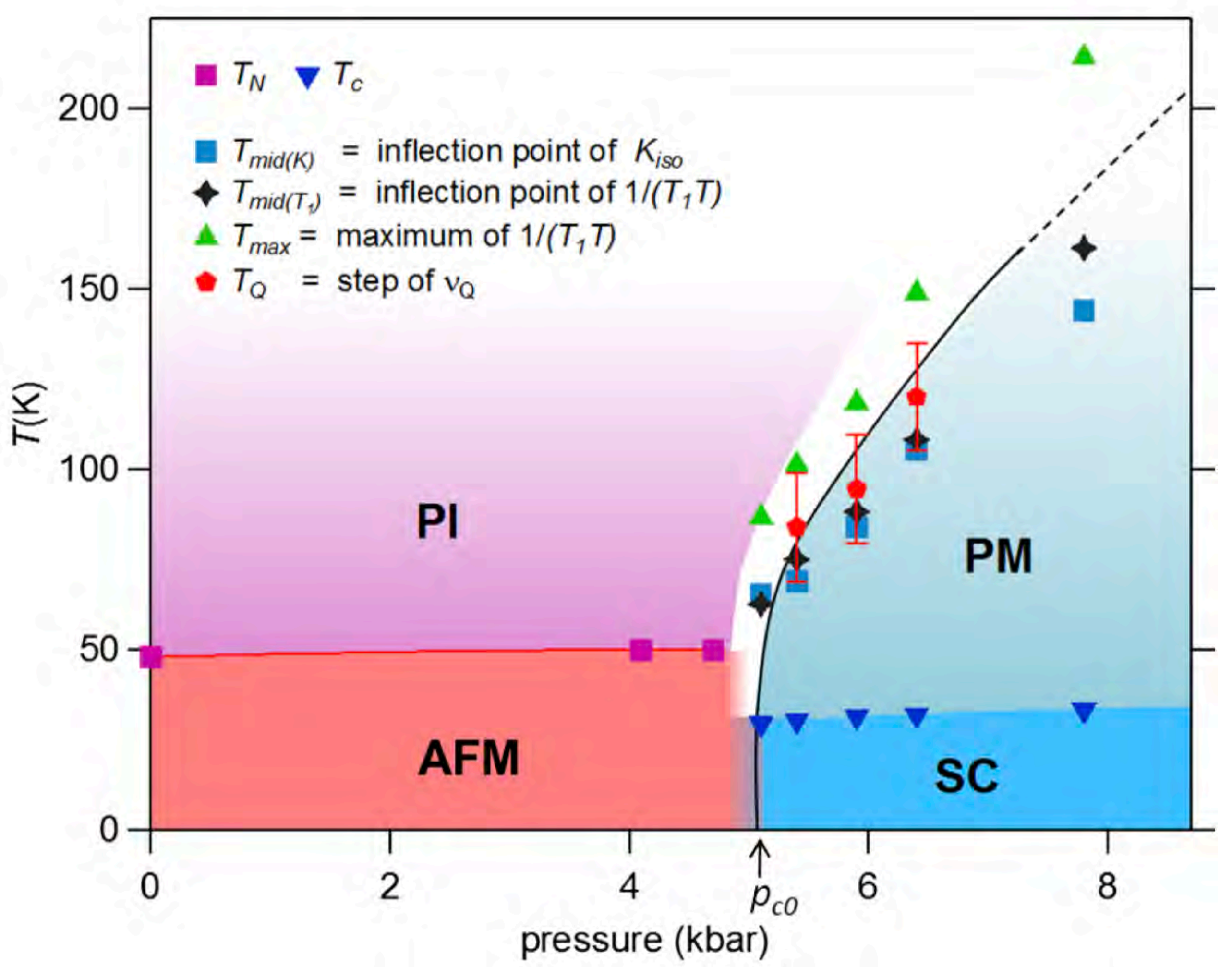
Conclusions

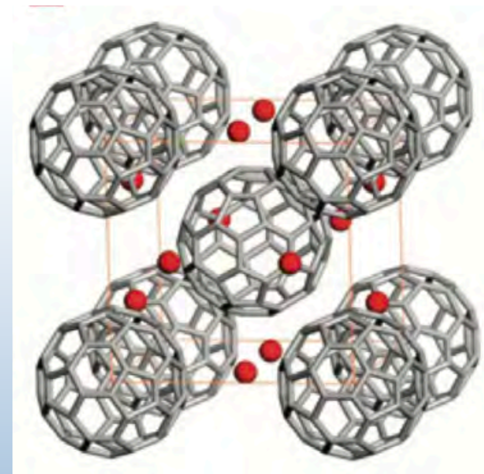
- **V_2O_3**
  - The PI state is frustrated by competing spin interactions on the honeycomb lattice
  - The PI to AFI transition is an instability that relieves magnetic frustration
  - LDA+U can now produce quantitatively reliable exchange interactions even near the MIT
  - Ever closer to “understanding” V_2O_3?

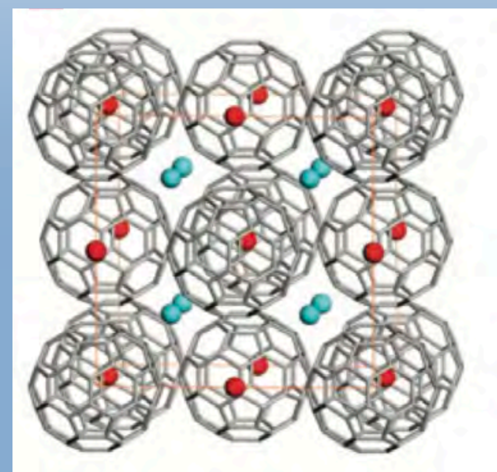
- **The ongoing quest for a QSL:**
  - Proximity to the MIT may be a good indicator
  - Ideas needed to circumvent structural instabilities

Mott Transition in the A15 Phase of Cs_3C_{60}: Absence of a Pseudogap and Charge Order

H. Alloul,[1] P. Wzietek,[1] T. Mito,[1] D. Pontiroli,[2] M. Aramini,[3,2] M. Riccò,[2] J. P. Itie,[4] and E. Elkaim[4]

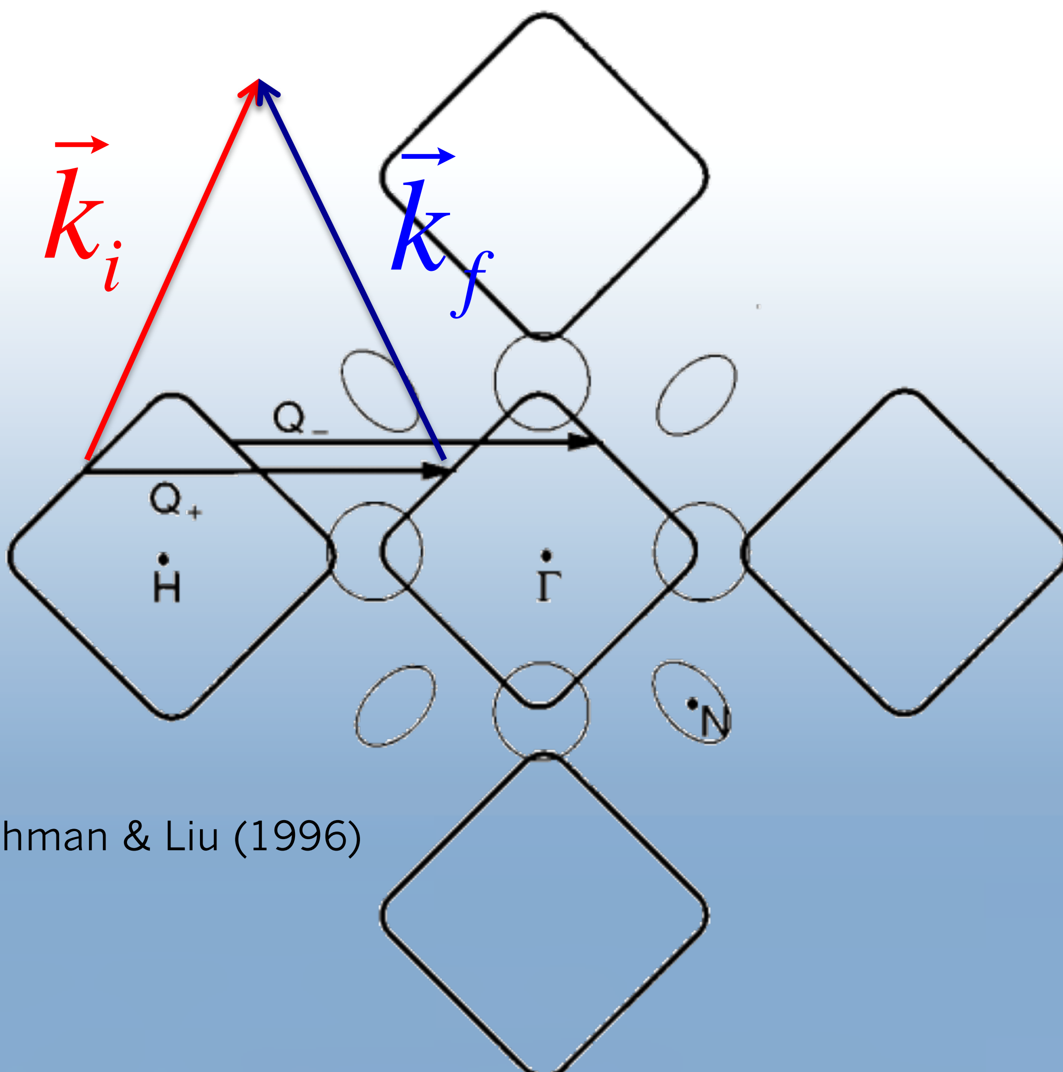






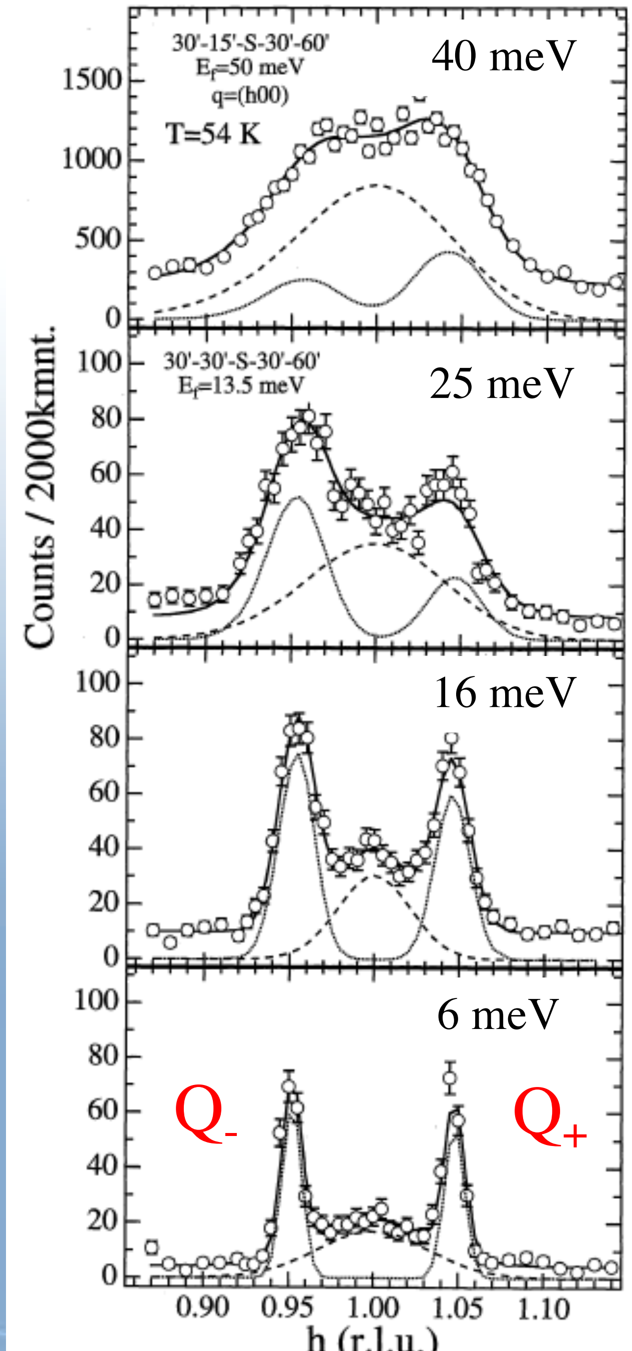
Scattering from band electrons

Chromium Fermi surface



Fishman & Liu (1996)

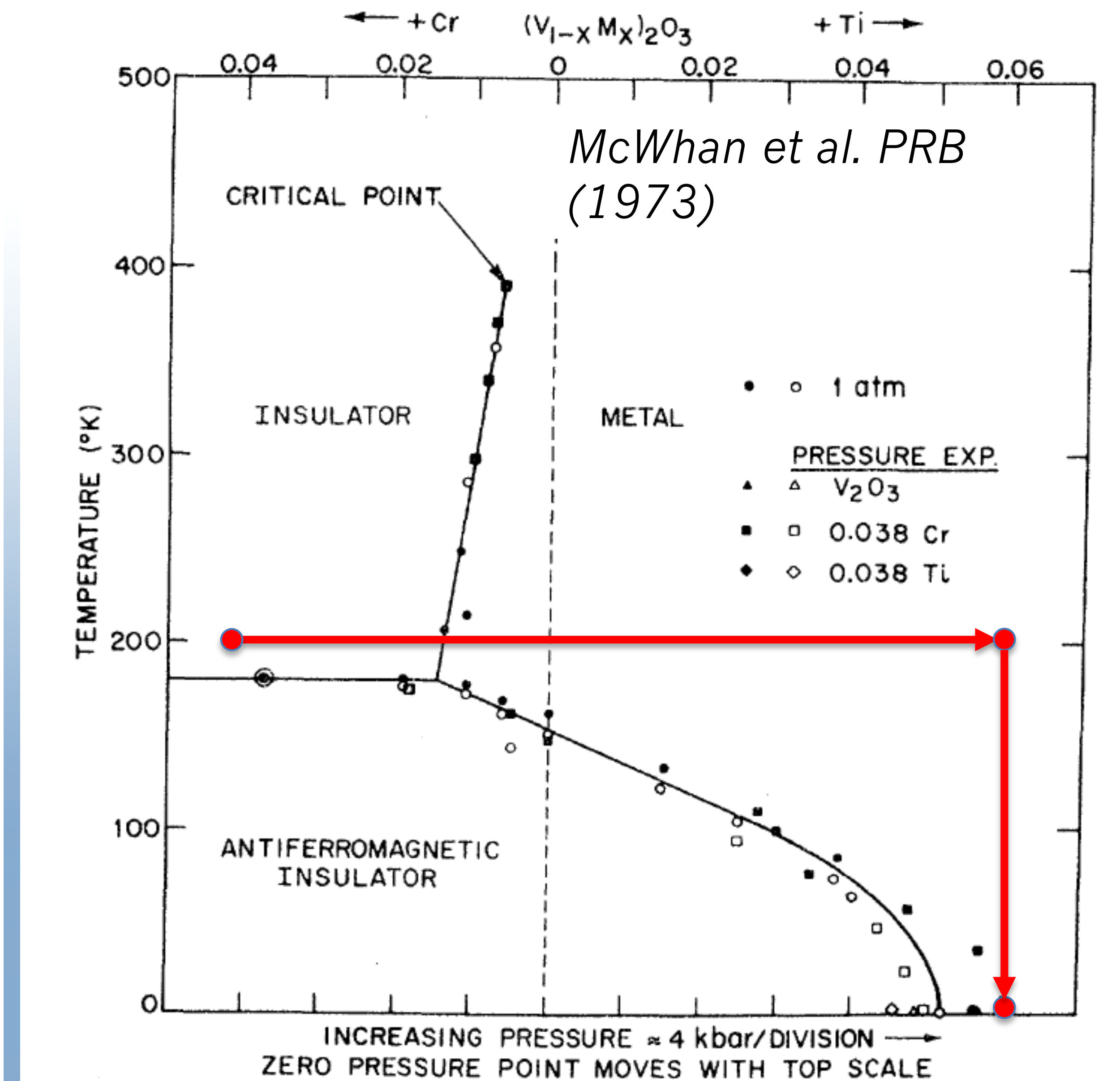
Fukuda et al. (1996)

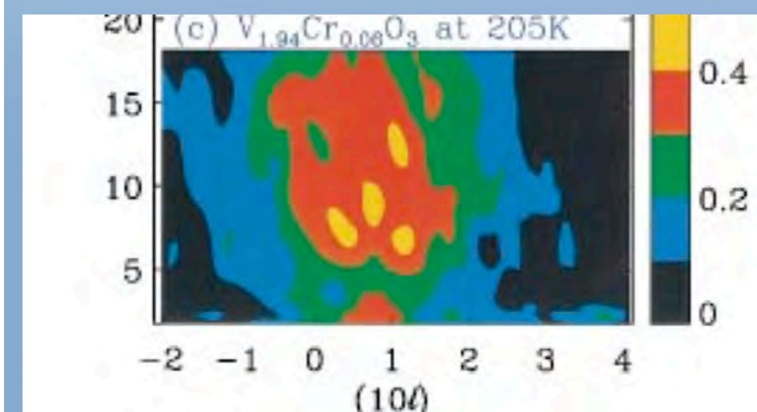


$$\mathcal{S}^{\alpha\beta}(\mathbf{q}\omega) = \frac{1}{1-e^{-\beta\hbar\omega}} \frac{\chi''_{\alpha\beta}(\mathbf{q}\omega)}{(g\mu_B)^2 \pi}$$

$$\chi_0(\mathbf{q}) = \sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k+q}}) - f(\epsilon_{\mathbf{k}})}{\epsilon_{\mathbf{k+q}} - \epsilon_{\mathbf{k}}}$$

Spin correlations in different phases of V_2O_3

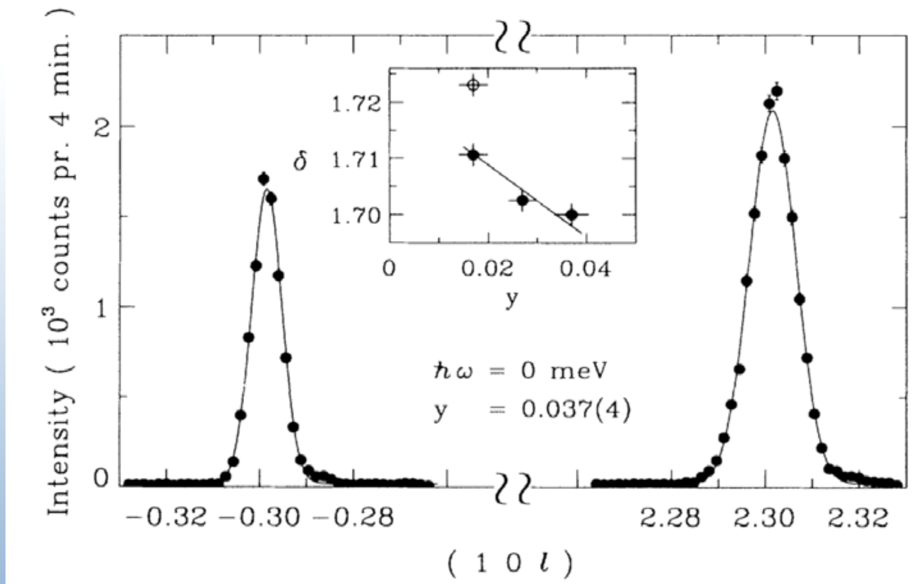


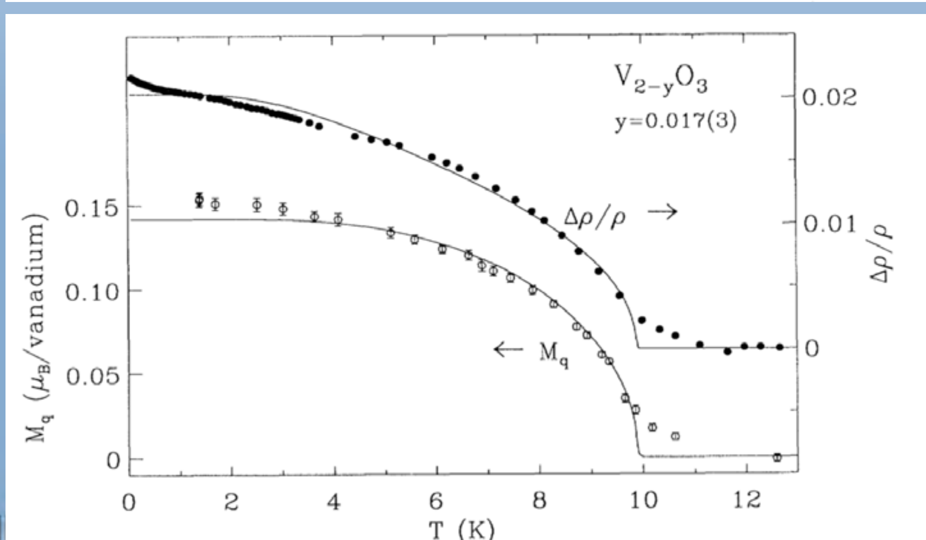


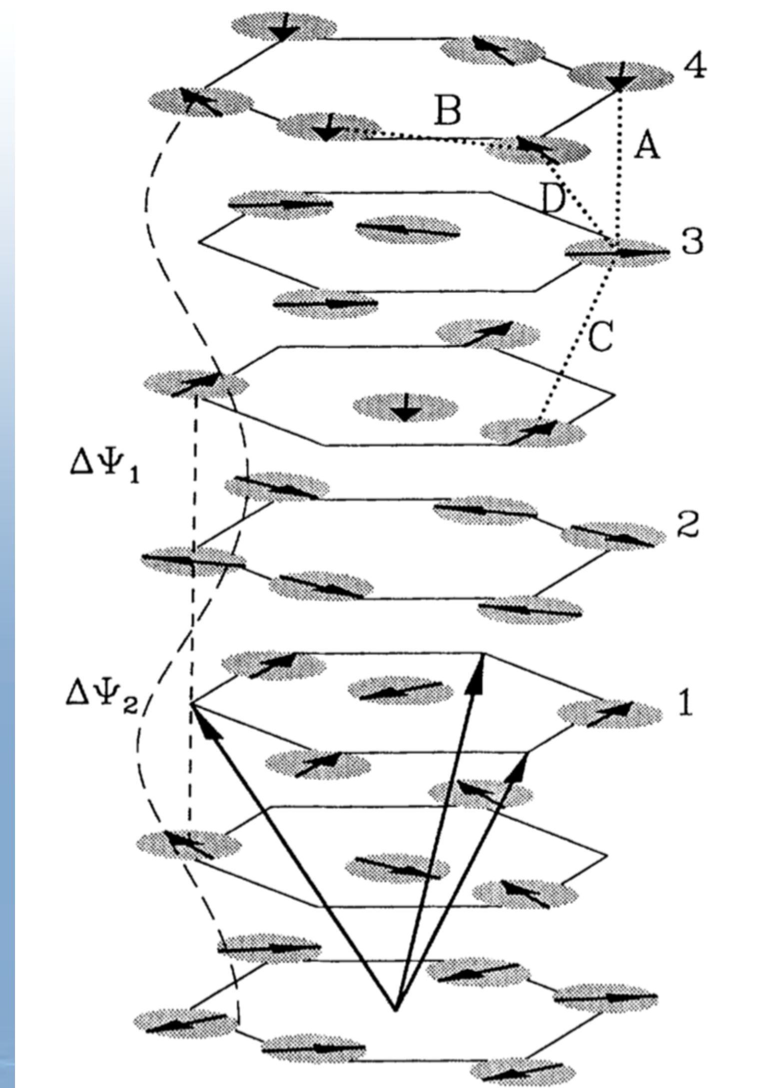
VOLUME 71, NUMBER 5 PHYSICAL REVIEW LETTERS 2 AUGUST 1993

Incommensurate Spin Density Wave in Metallic $V_{2-y}O_3$

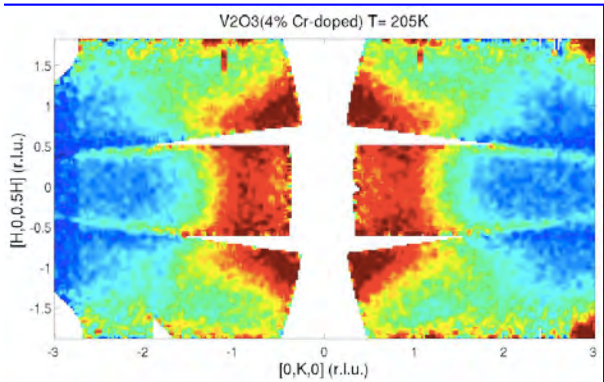
Wei Bao,[1] C. Broholm,[1,2] S. A. Carter,[3] T. F. Rosenbaum,[3] G. Aeppli,[4]
S. F. Trevino,[2,5] P. Metcalf,[6] J. M. Honig,[6] and J. Spalek[6]



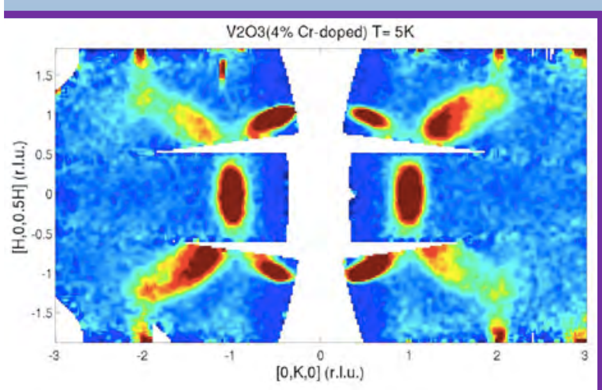


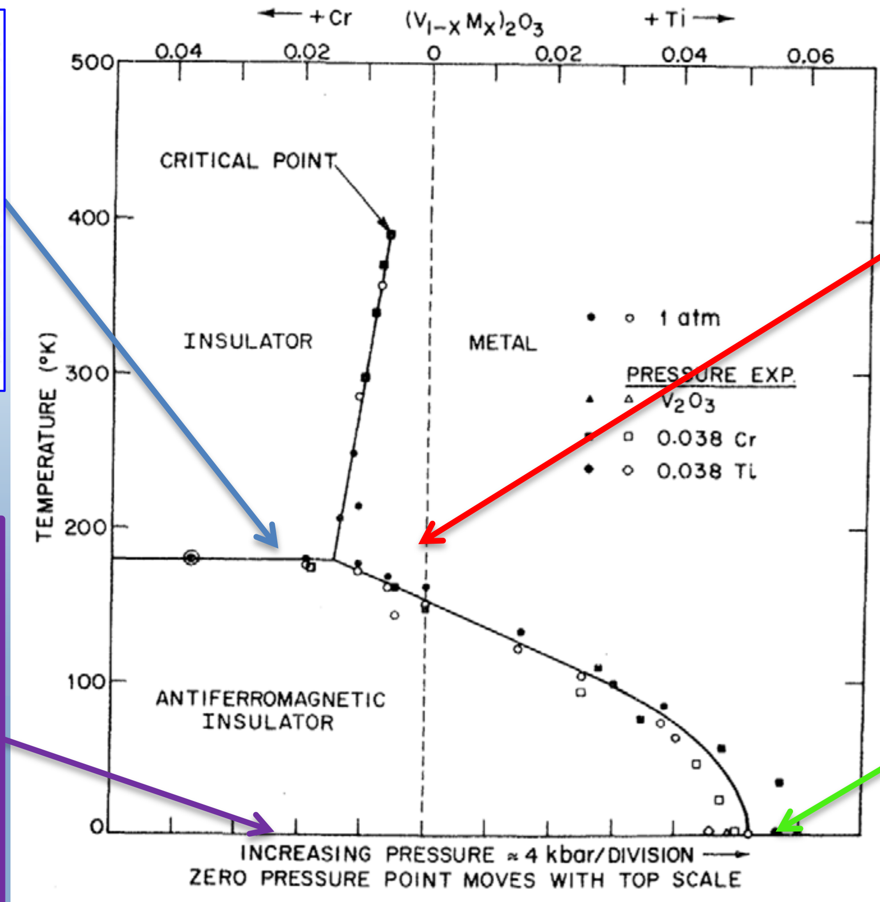


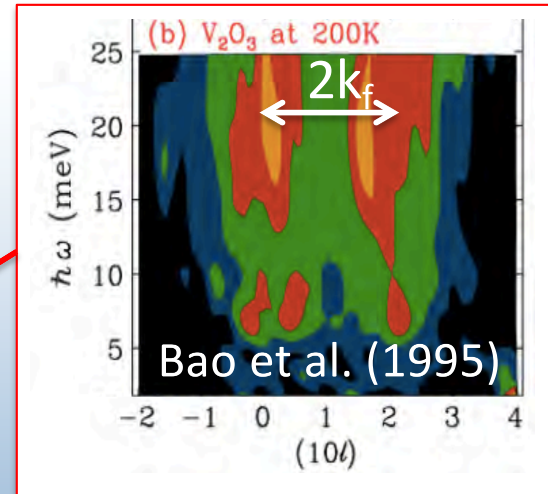
Spin correlations in V_2O_3

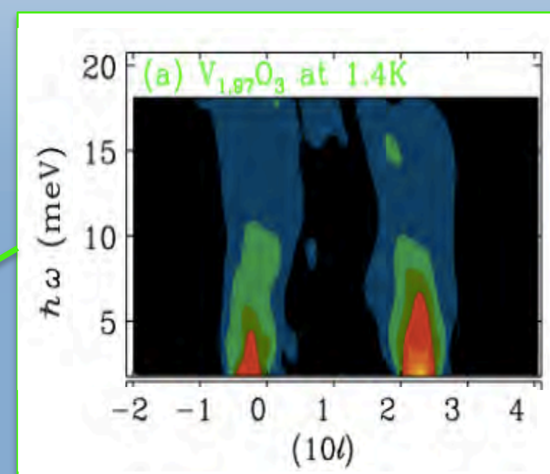


Leiner et al (2018)







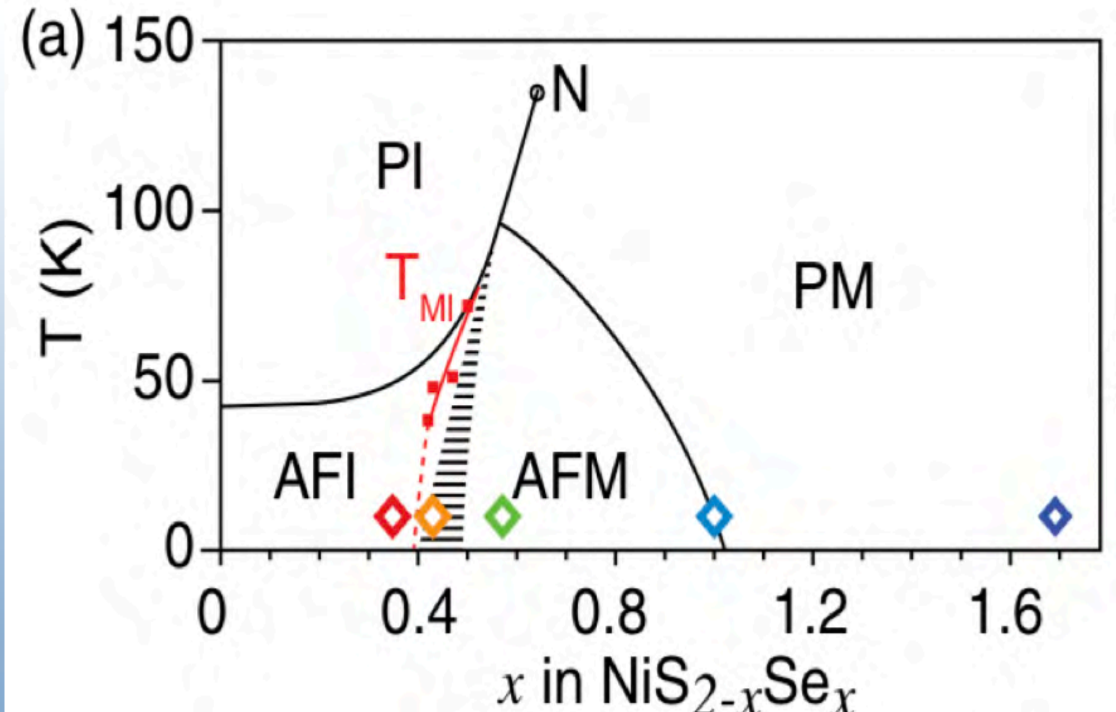


Driven by frustration, the spin-liquid like character of the PI is central to the physics of V2O3

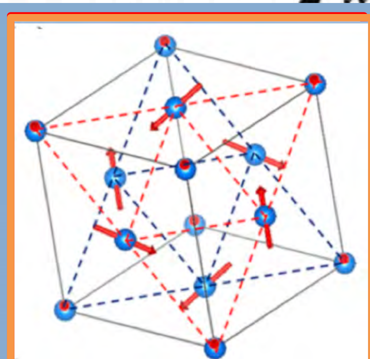
PRL **112,** 087603 (2014) PHYSICAL REVIEW LETTERS week ending 28 FEBRUARY 2014

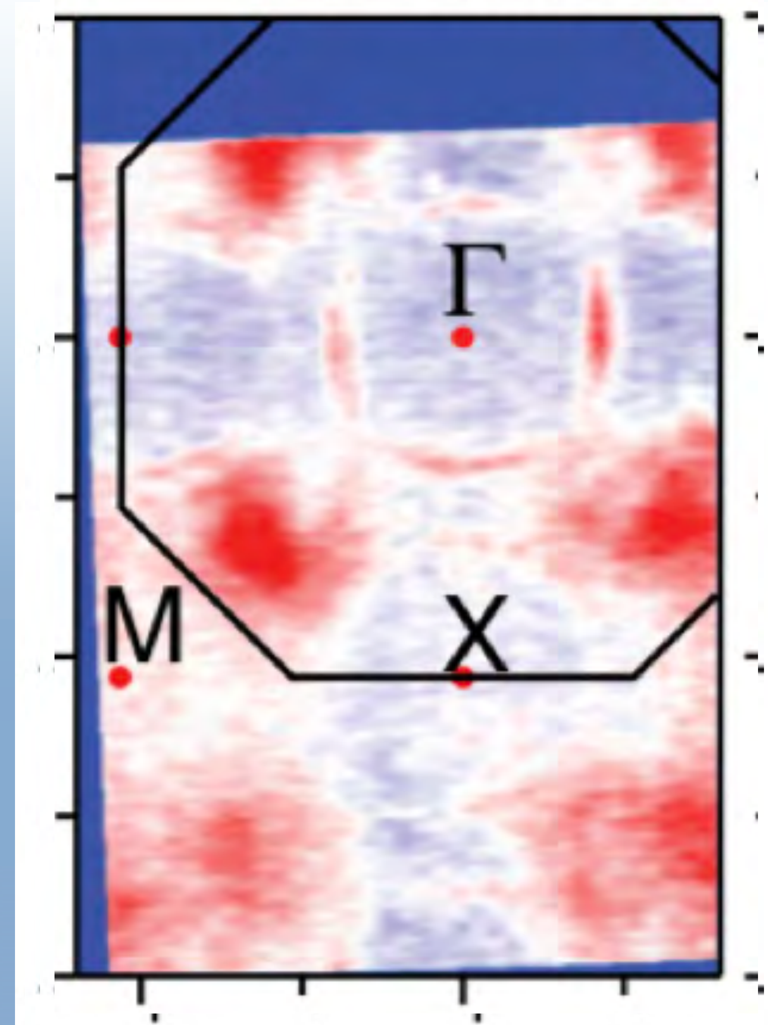
Direct Observation of the Bandwidth Control Mott Transition in the $NiS_{2-x}Se_x$ Multiband System

H. C. Xu,[1] Y. Zhang,[1] M. Xu,[1] R. Peng,[1] X. P. Shen,[1] V. N. Strocov,[2] M. Shi,[2] M. Kobayashi,[2] T. Schmitt,[2] B. P. Xie,[1,*] and D. L. Feng[1,†]



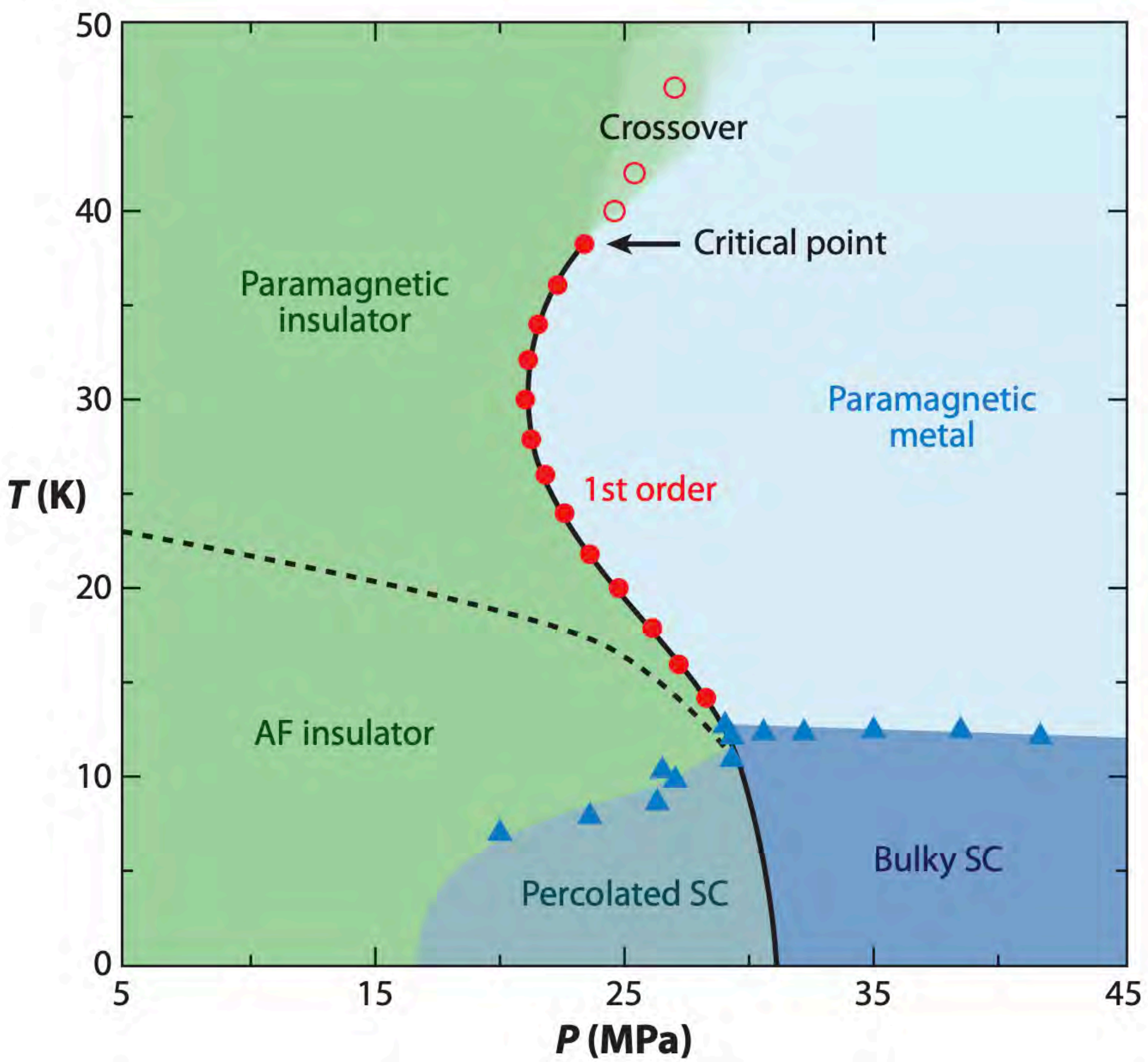
Magnetic Structures by D. Louca et al.

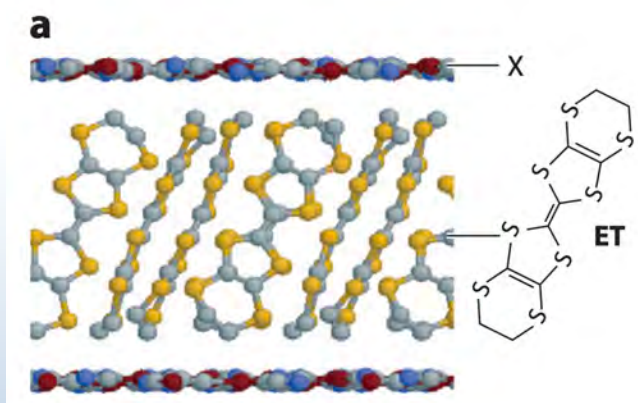


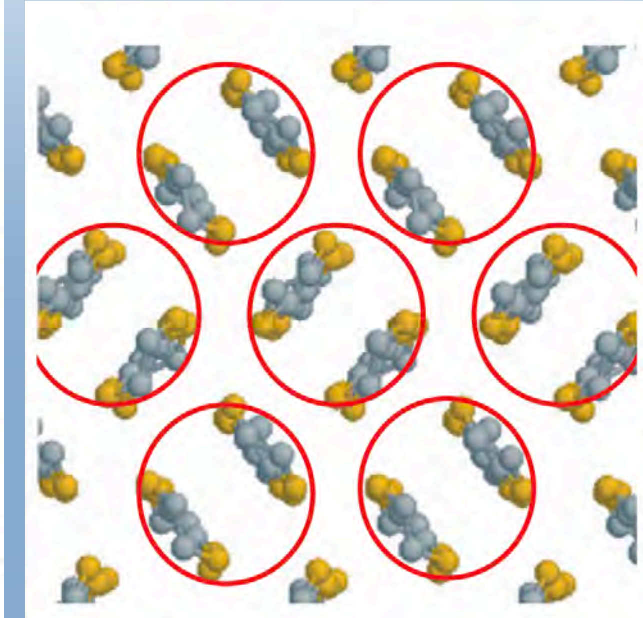


Mott Physics in triangular organic lattices

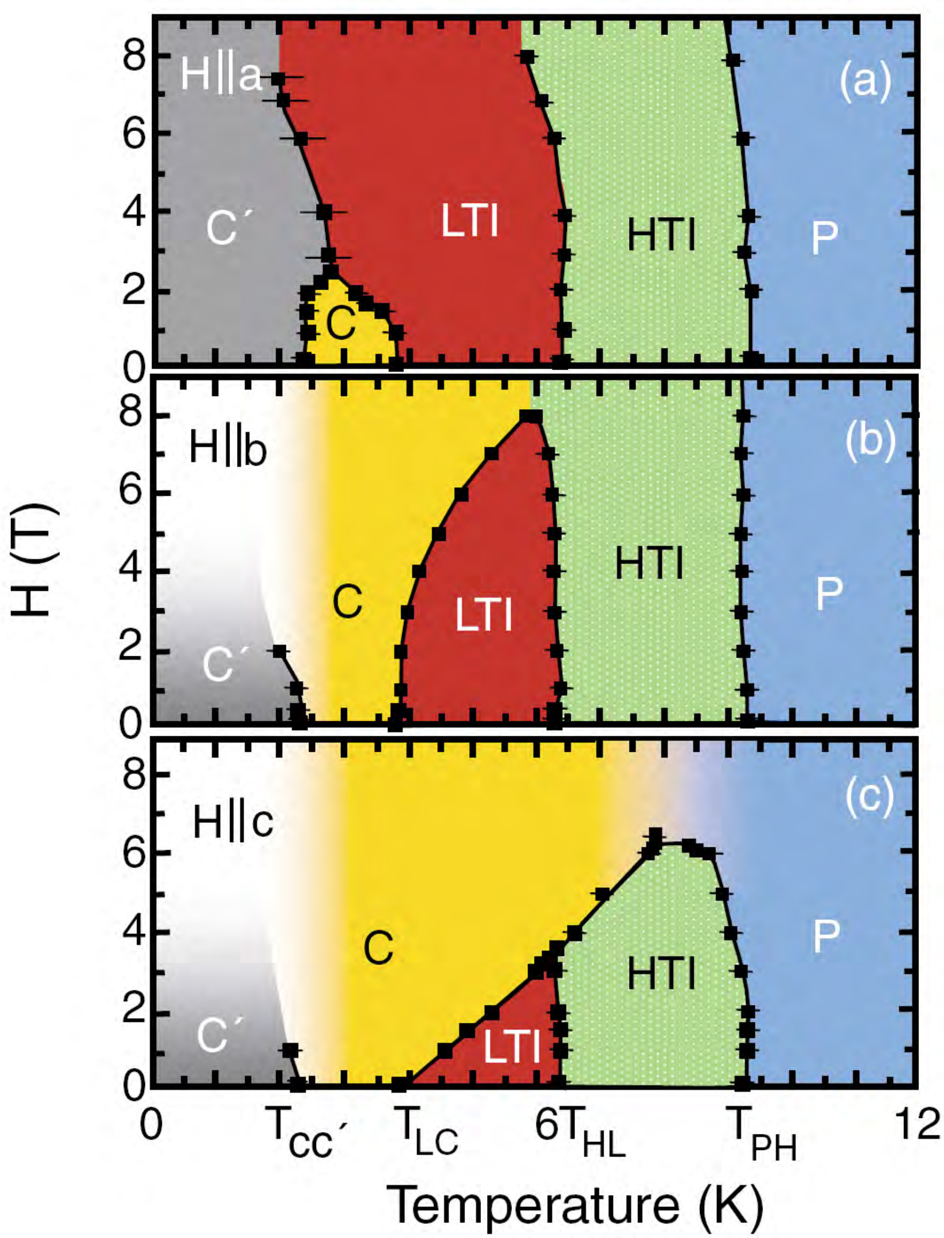
Kazushi Kanoda et al.

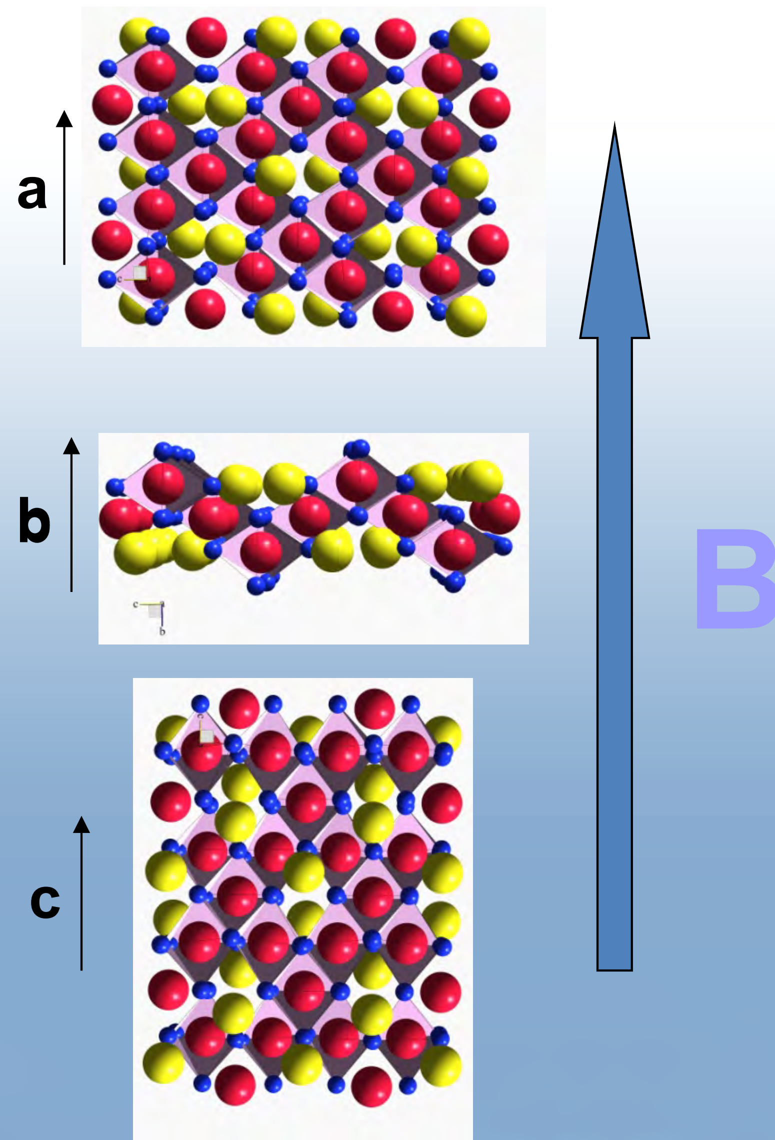






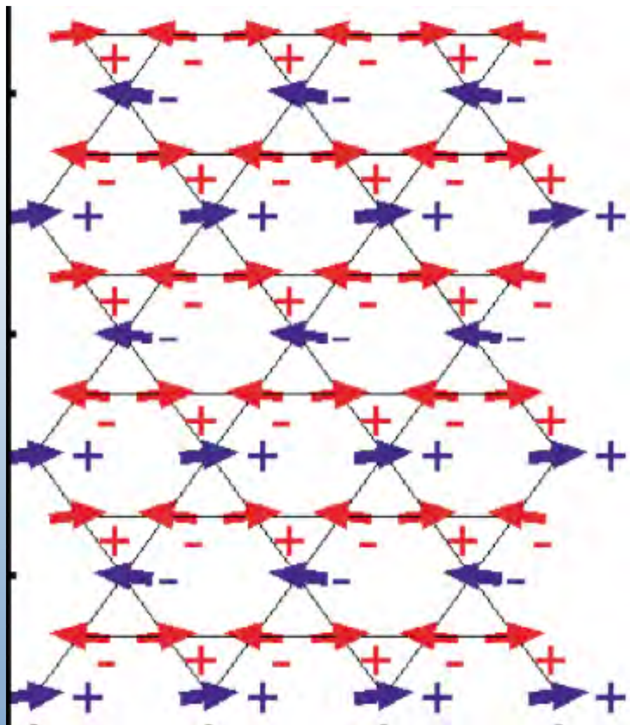
Phases of a kagome staircase





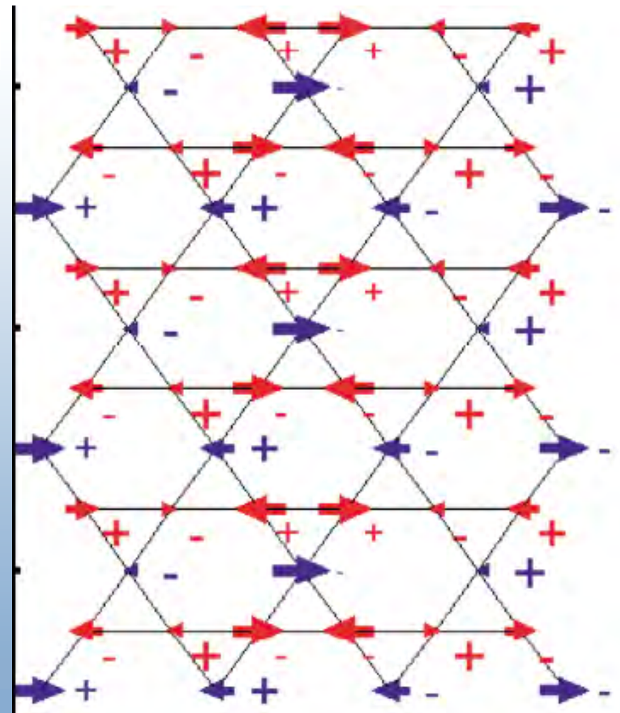
Modulated magnetic phases

2.2 K<T< 4 K



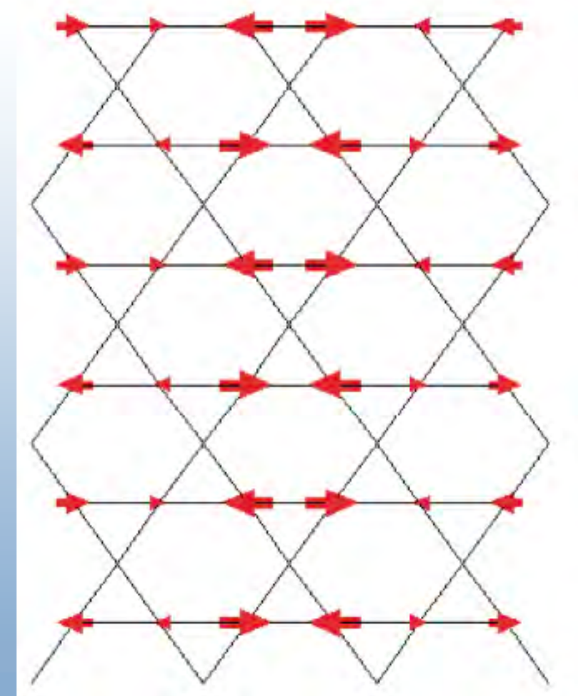
Commensurate
Canted FM

4 K<T< 6.5 K



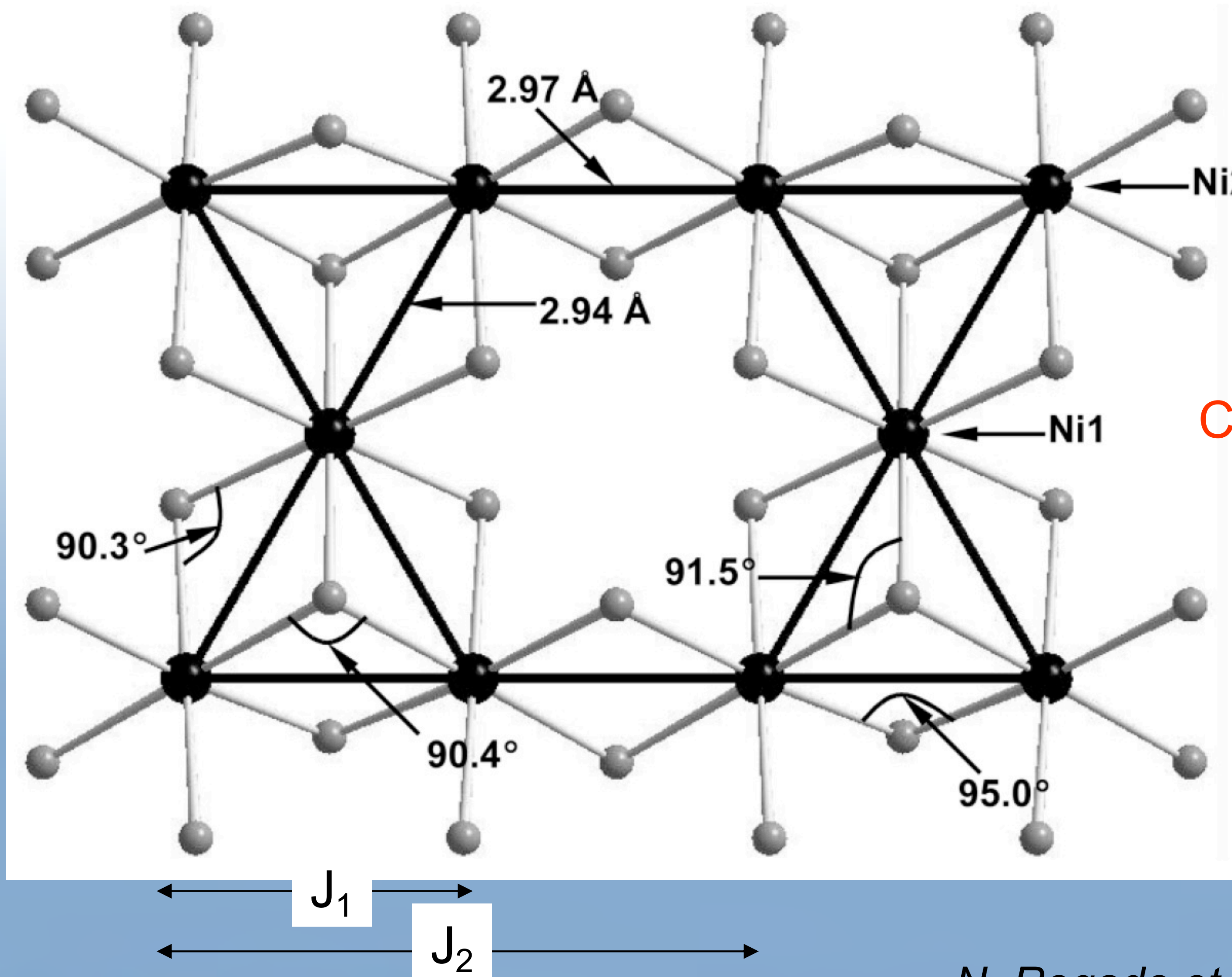
Incommensurate
Cycloidal

6.5 K<T<9.2 K



Incommensurate
amplitude modulated

Exchange Interactions

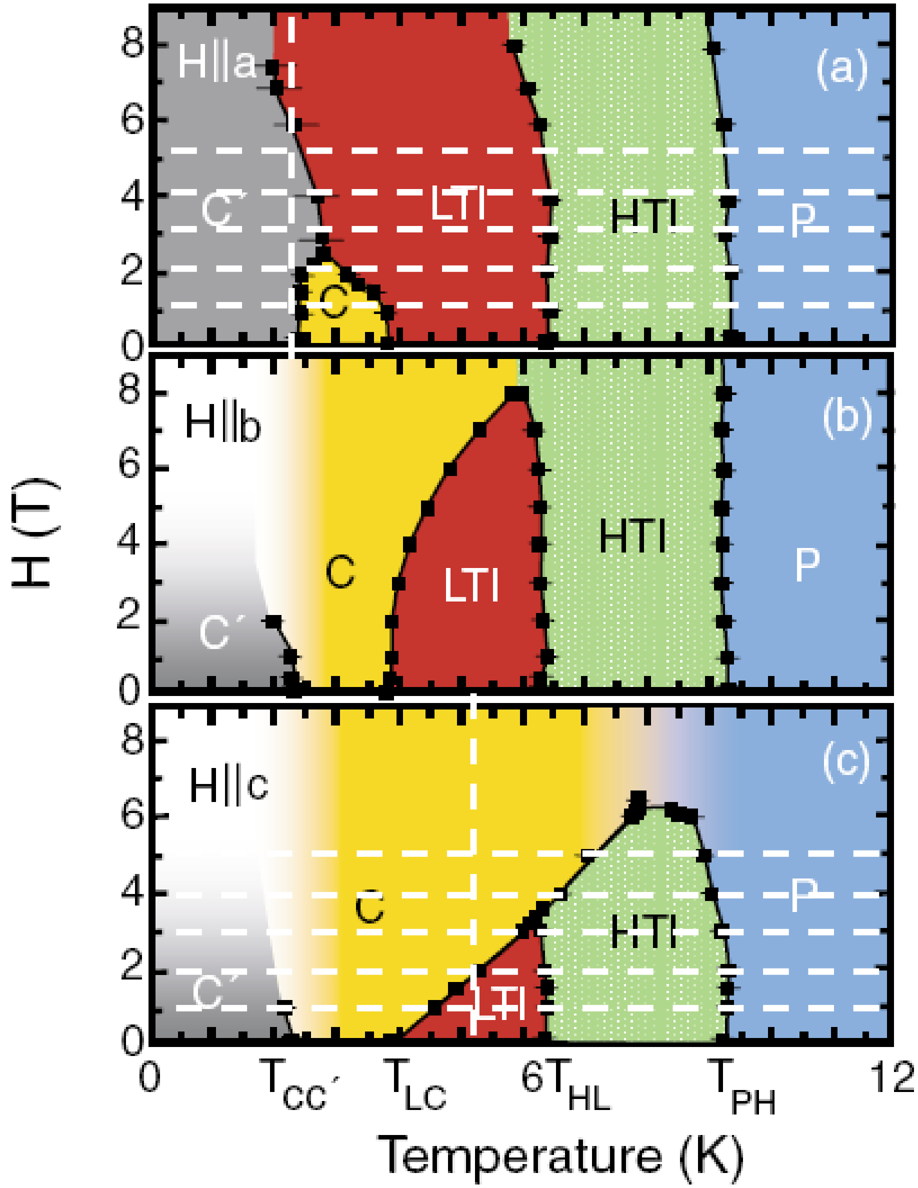


Cross tie spins

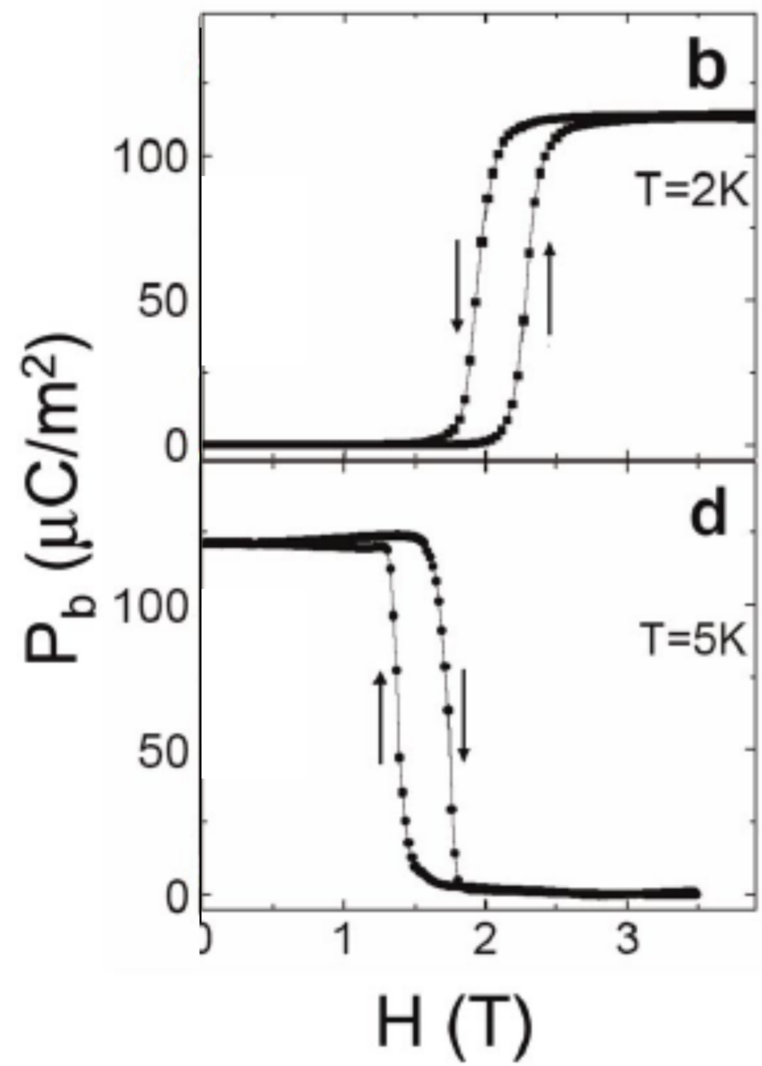
Spine spins

N. Rogado et al (2003)

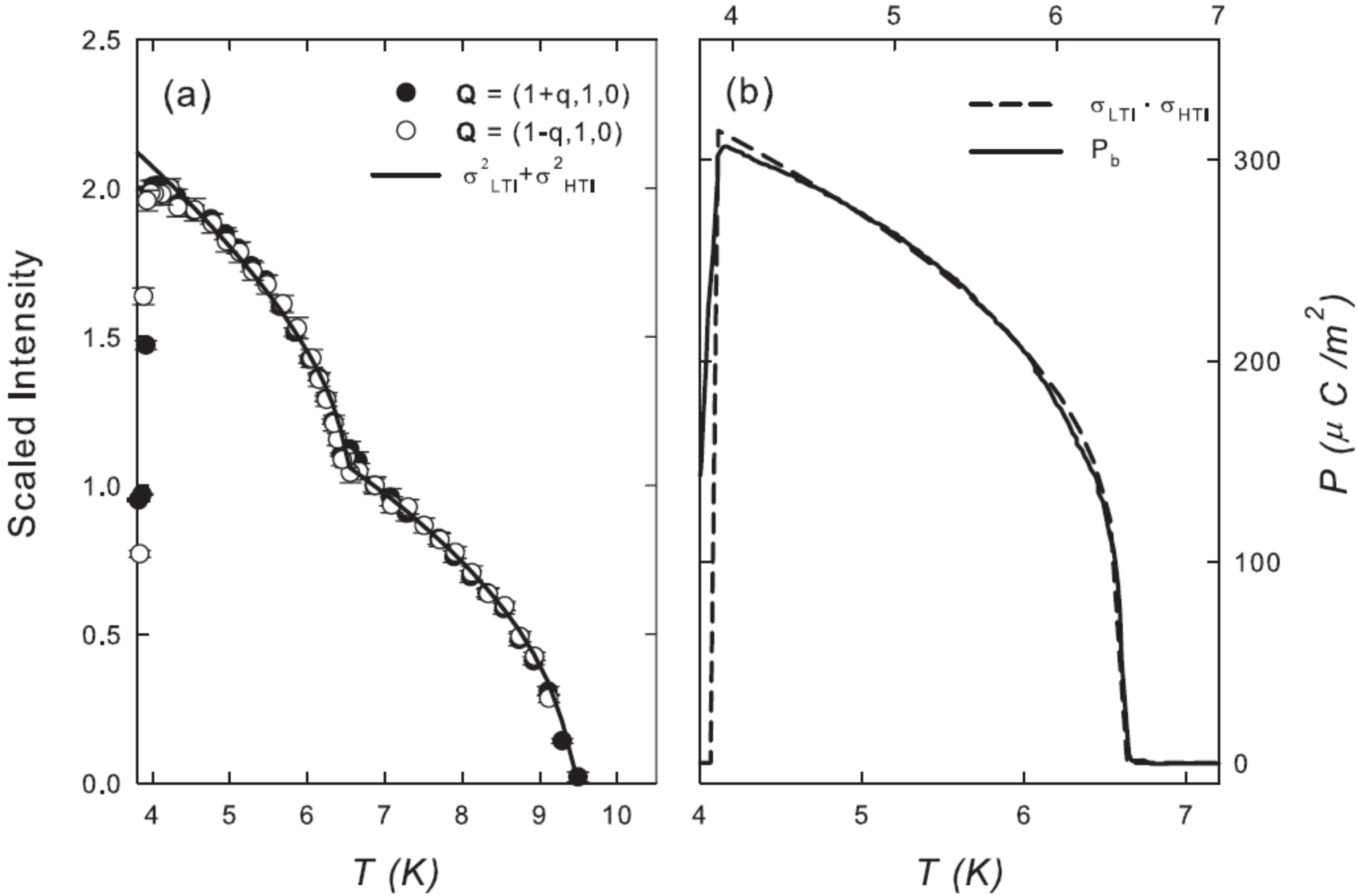
Frustrated Magnetism & Ferroelectricity



Lawes et al (2005)



Tri-linear coupling in $Ni_3V_2O_8$



Landau Theory of Magneto-Electricity

A. B. Harris and Taner Yildirim

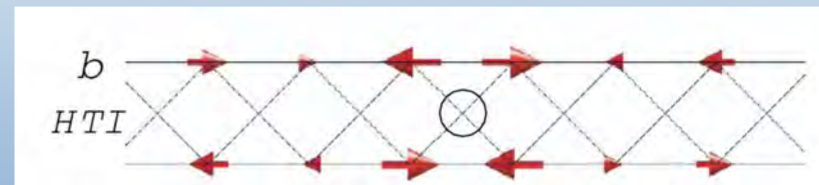
IRREP	1	2_X	$\tilde{m}_y$	$\tilde{m}_z$
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	1	-1
Γ_4	1	-1	-1	1

General case:

$$V = \sum_{nm\gamma} c_{nm\gamma} \sigma_n(\mathbf{q}) \sigma_m(-\mathbf{q}) P_\gamma$$

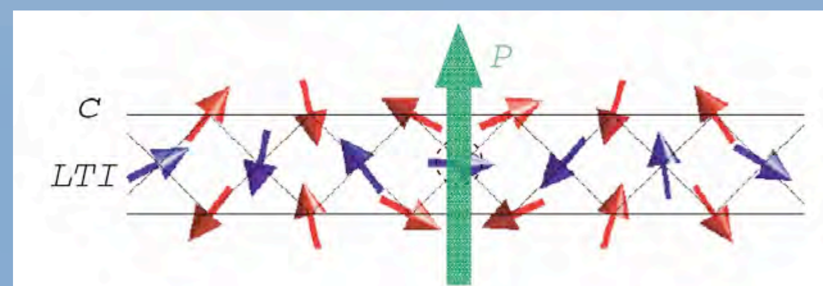
Amplitude modulated (Γ_4)

$$V_{HTI} = \sum_{\gamma} c_{44\gamma} |\sigma_4(\mathbf{q})|^2 P_\gamma \quad \equiv 0$$



Cycloid state (Γ_4+Γ_1)

$$V_{LTI} = c_{14y}(\sigma_1(\mathbf{q})\sigma_4(-\mathbf{q}) + \sigma_4(\mathbf{q})\sigma_1(-\mathbf{q}))P_y$$



Chirality hysteresis in FE state