Frustrated Magnetism in Mott Insulating $(V_{1-x}Cr_x)_2O_3$

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- Collin Broholm
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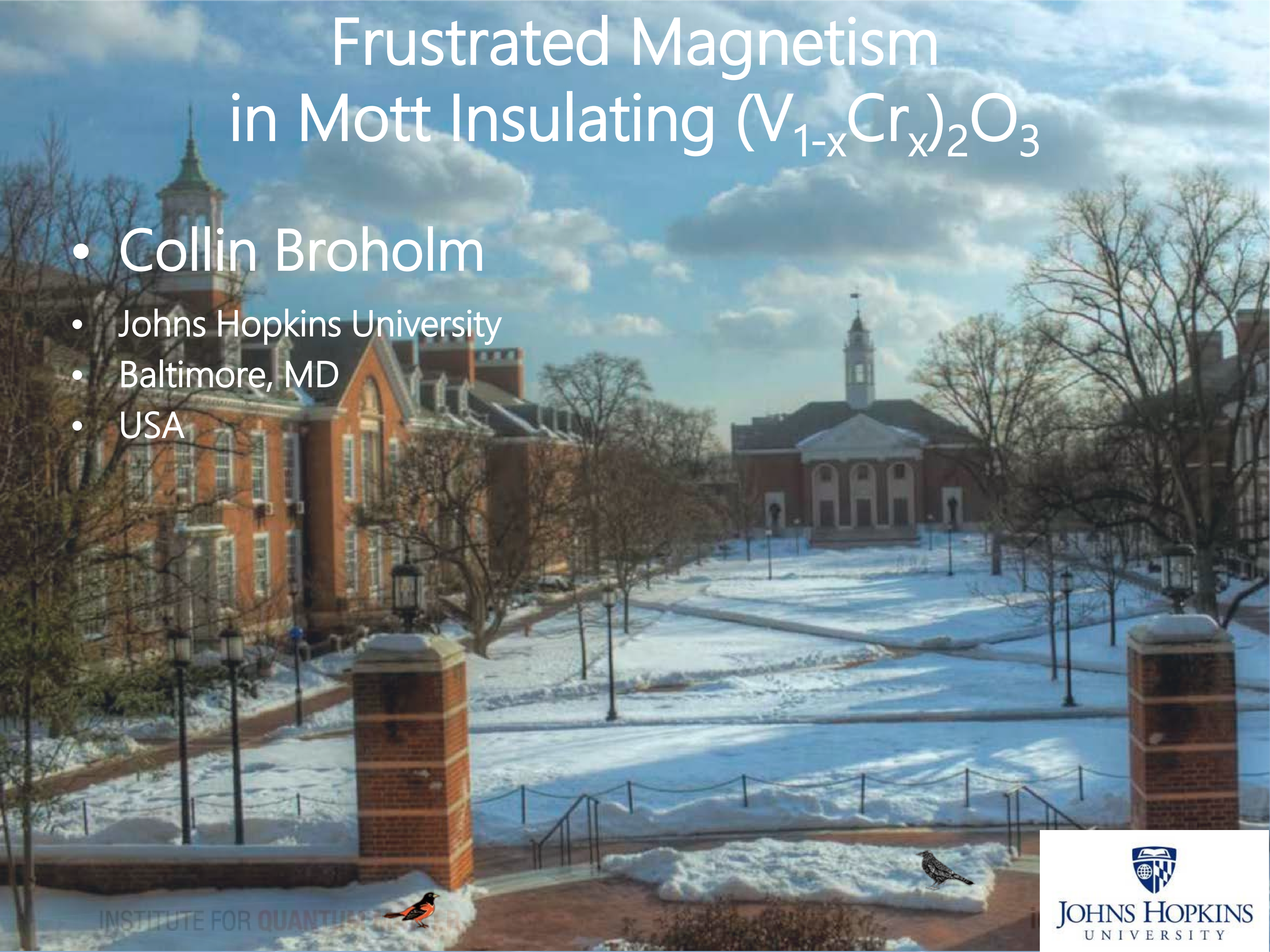

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Outline

- Introduction
  – In search of the Mott transition
- Overcoming frustration in V_2O_3
  – **Insulator:** straining to order
  – **Metal:** Fermi surface nesting
- Conclusions
  – Frustrated magnetism and it's interplay with a lattice instability is key to V_2O_3
  – If lattice instabilities can be avoided, QSL might be expected near Mott transition

Collaborators

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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.


Leiner


Zhang

arXiv:1804.08605v1 [cond-mat.str-el] 23 Apr 2018

GORDON AND BETTY MOORE FOUNDATION

SNS SPALLATION NEUTRON SOURCE

INSTITUTE FOR QUANTUM MATTER

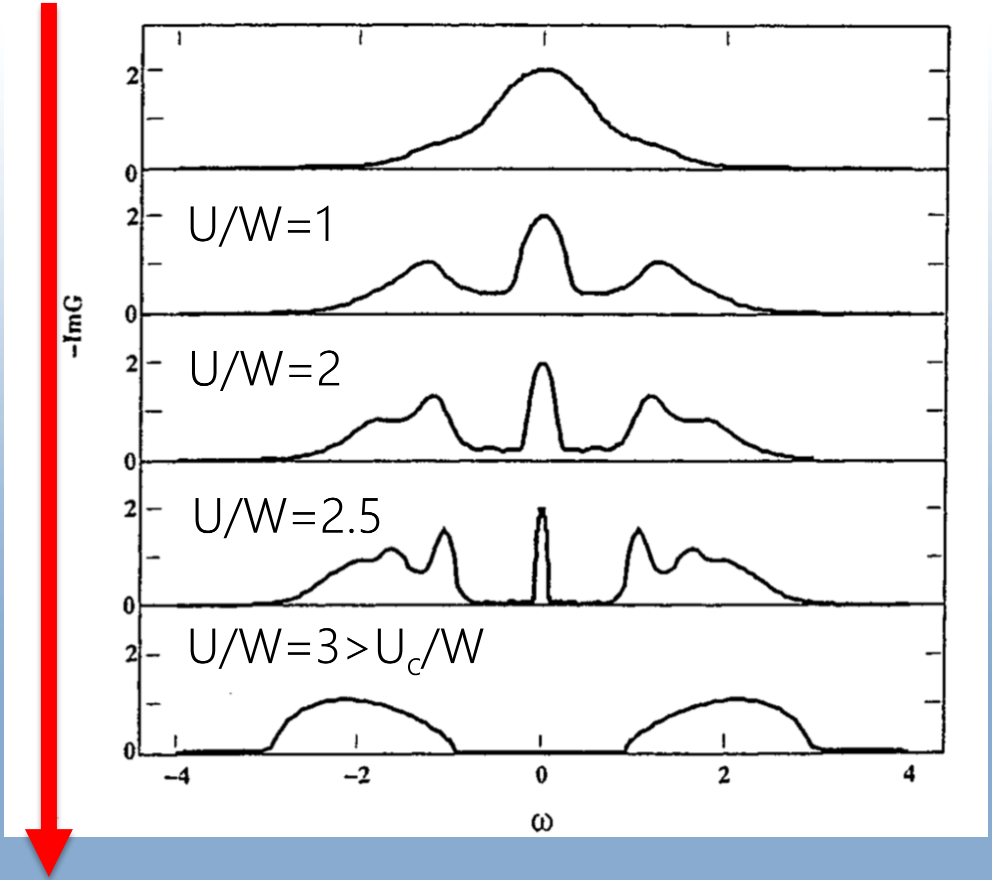
Metal to insulator transitions

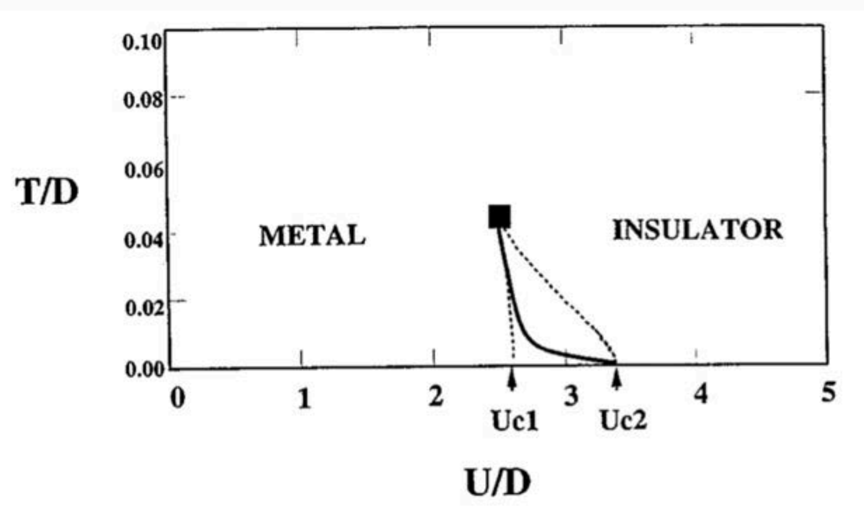
- Band insulator (single electron)
  - Filled and empty bands carry no current
- Slater insulator (single electron)
  - Unit cell doubling yields band insulator
- Charge transfer insulator
  - Ligand states involved in conduction
  - Parent to Cu-O superconductivity
- Mott insulator
  - Charge localization from e-e repulsion in 1/2 filled band
  - Correlation induced upper and lower Hubbard band

Rare and interesting

Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions

Antoine Georges, Gabriel Kotliar, Werner Krauth, Marcelo J. Rozenberg





This DMFT does not describe interacting spins so there is NO magnetic ordering. Just the self consistent single site Mott transition

Reviews of Modern Physics, Vol. 68, No. 1, January 1996

Magnetism in a Mott Insulator

Fradkin (1991)

Hubbard model

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

Define local moment

$$\vec{S}\,(\vec{r}) = \frac{\hbar}{2} c_\sigma^\dagger(\vec{r}) \vec{\tau}_{\sigma\sigma'} c_{\sigma'}(\vec{r})$$

Half filling strong coupling limit: Heisenberg model

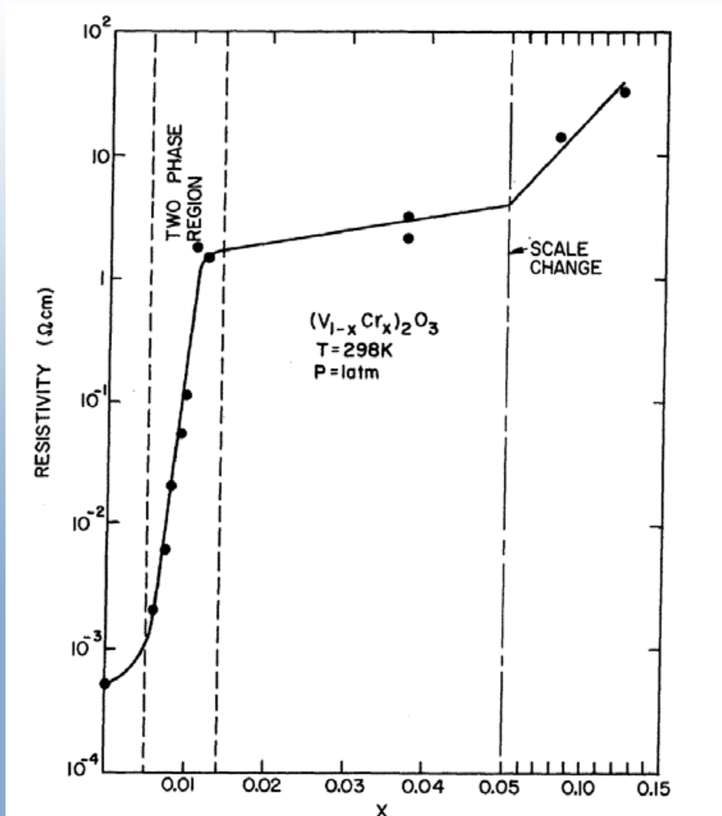
$$H_0' = \frac{2t^2}{|U|} \sum_{\langle \vec{r}, \vec{r}\,' \rangle} \vec{S}(\vec{r}) \cdot \vec{S}(\vec{r}\,')$$

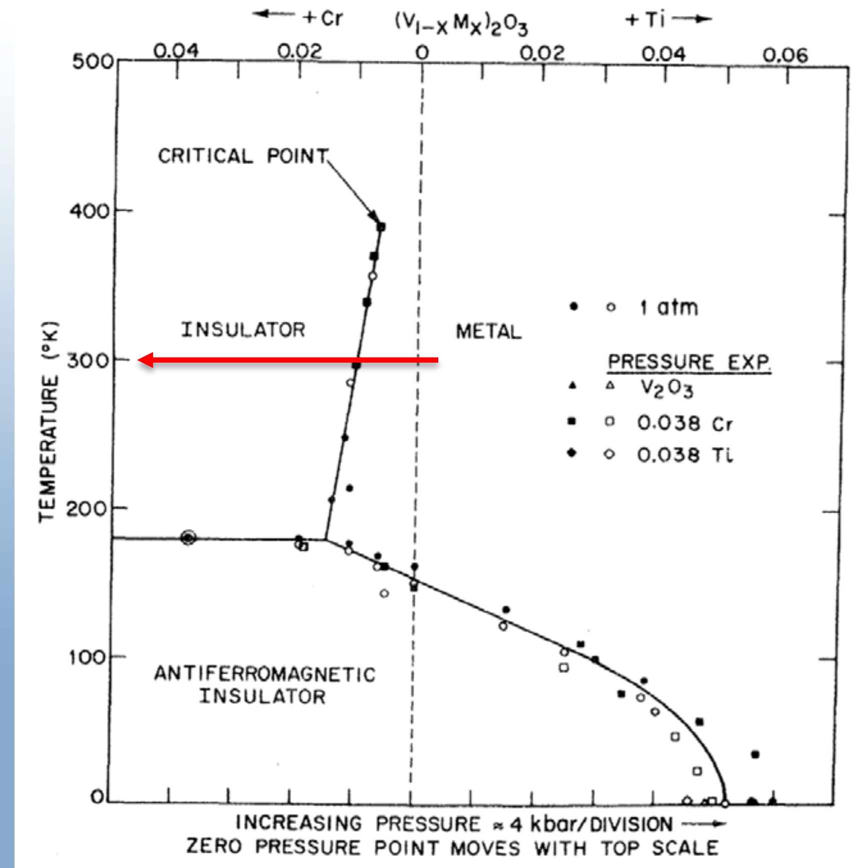
A spin liquid retains aspects of the Fermi-liquid though charge is localized

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

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

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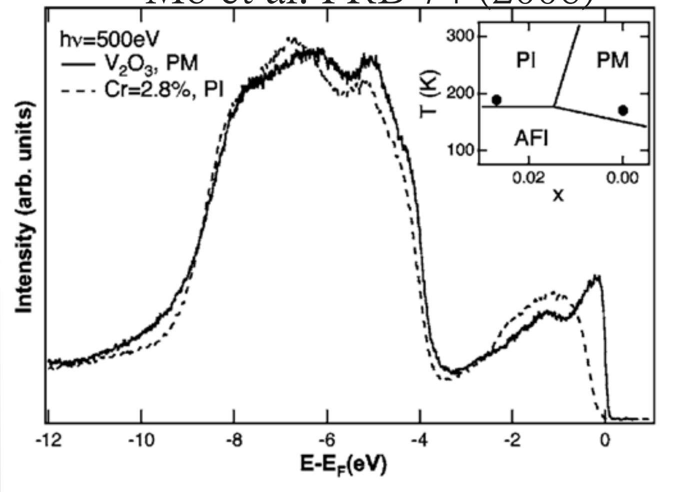
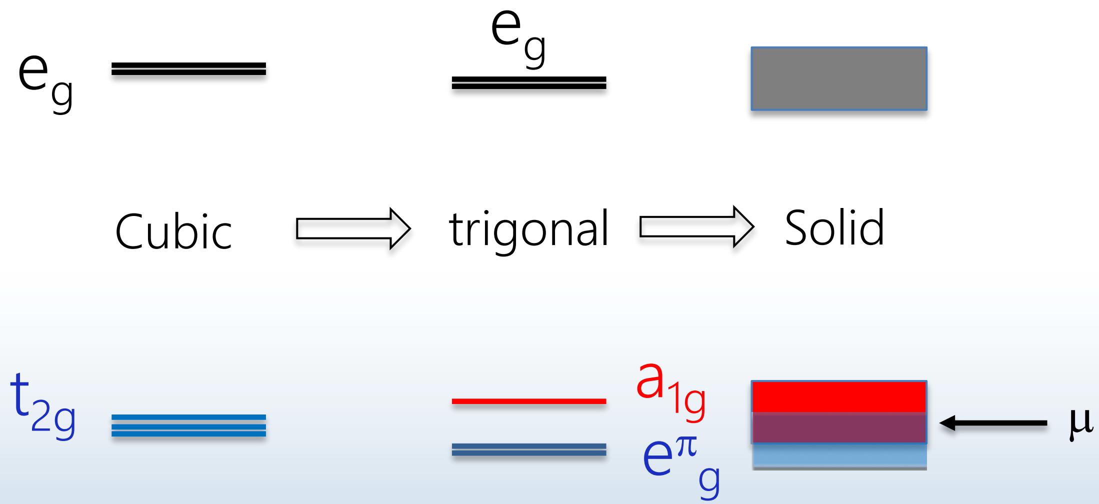
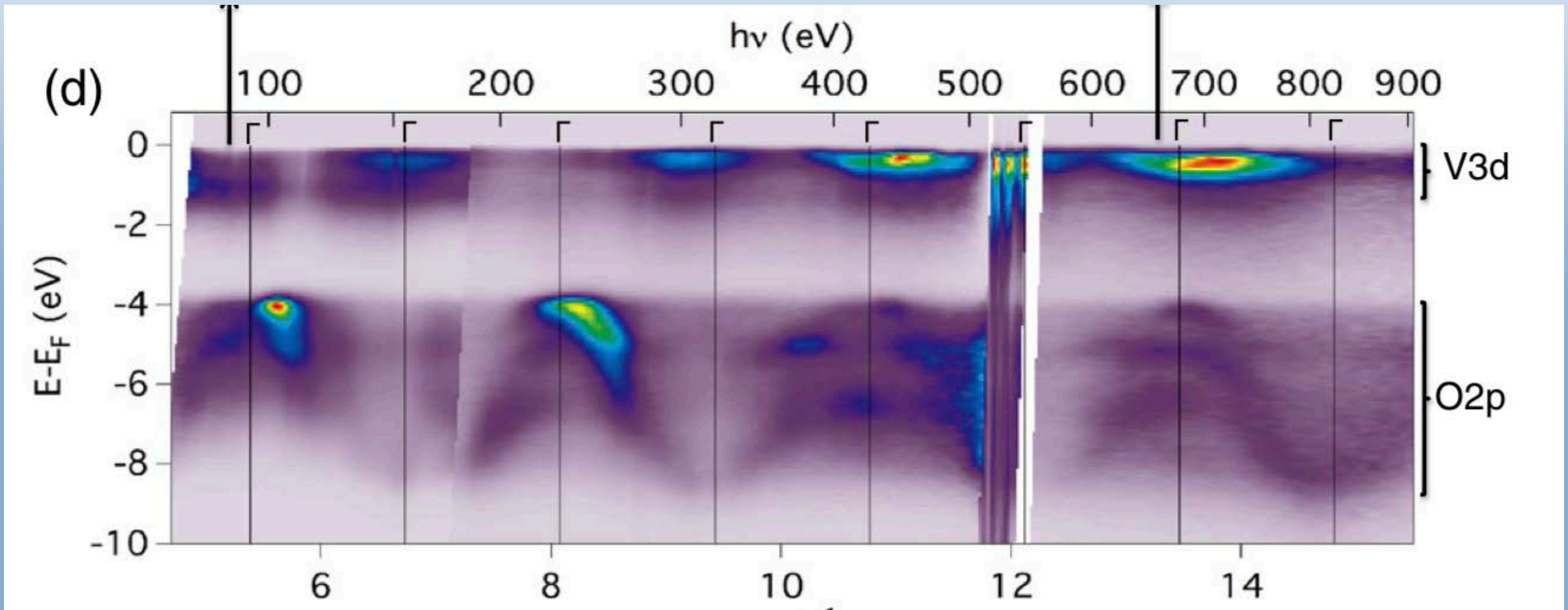
Photoemission: Mott insulator

Mo et al. PRB 74 (2006)

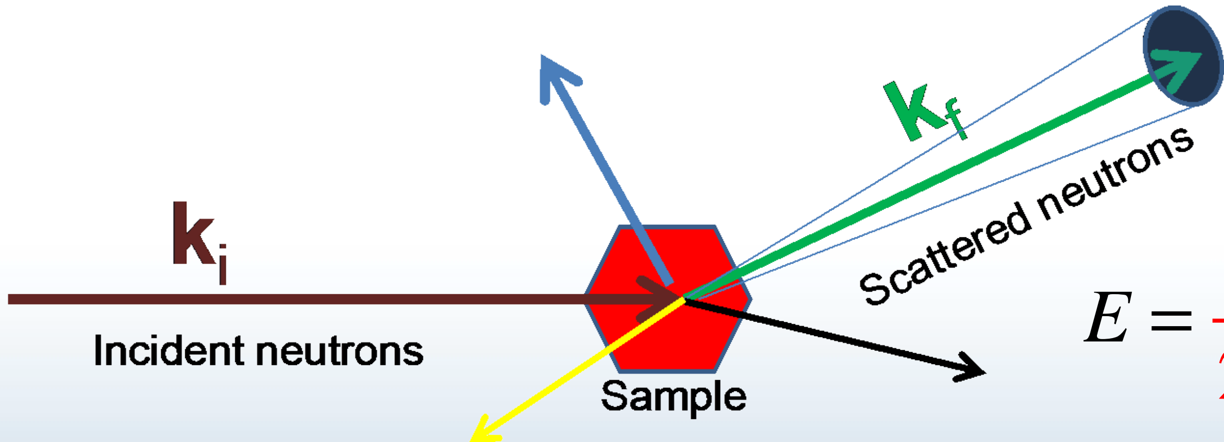






I. L. Vechio et al. PRL 117, 166401 (2016)

Neutron Scattering



$$E = \frac{\hbar^2}{2m} k^2$$

$$= 2.072\ \text{meV}\text{Å}^2 k^2$$

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\textit{Rate of neutrons into } d\Omega \textit{ and } dE_f}{\Phi \times d\Omega \times dE_f}$$

$$V_M(\mathbf{r}) = -\mu_N \cdot \mathbf{H}$$

$$\sigma \sim \left(\gamma \frac{e^2}{m_e c^2}\right)^2 = 0.2916 \text{ barn}$$

n-matter Interactions:

- Weak (Born limit)
- Energy independent
- Well characterized
- similar strengths

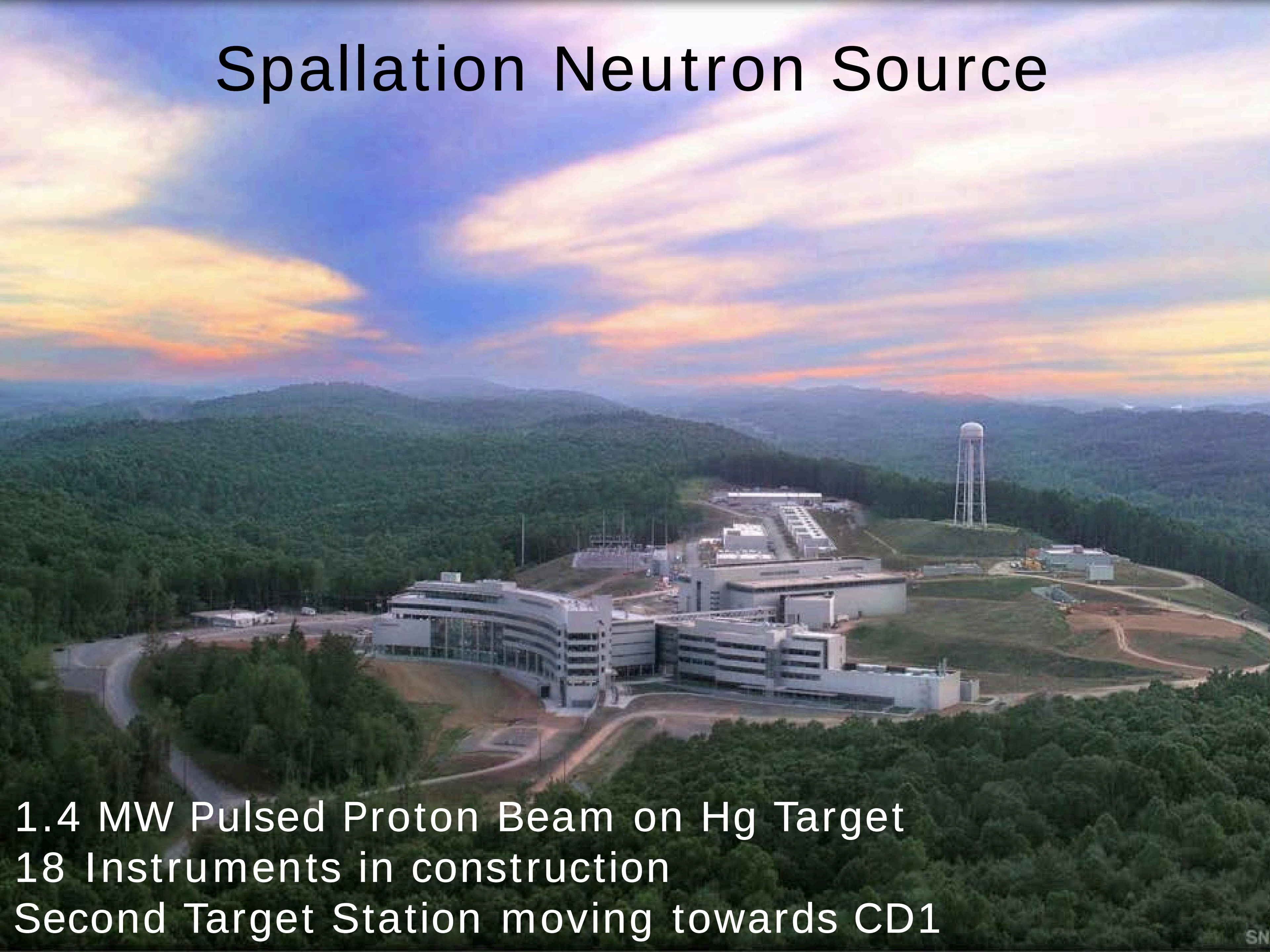
$$V_N(\mathbf{r}) = \frac{2\pi\hbar^2}{m} b\delta(\mathbf{r})$$

$$\sigma = 4\pi b^2 \sim 1 \text{ barn}$$

$$\mathcal{S}^{\alpha\beta}(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t} \frac{1}{N}\sum_{\mathbf{RR'}} e^{i\mathbf{Q}\cdot(\mathbf{R}-\mathbf{R'})} \left\langle S^{\alpha}_{\mathbf{R}}(0) S^{\beta}_{\mathbf{R'}}(t)\right\rangle$$

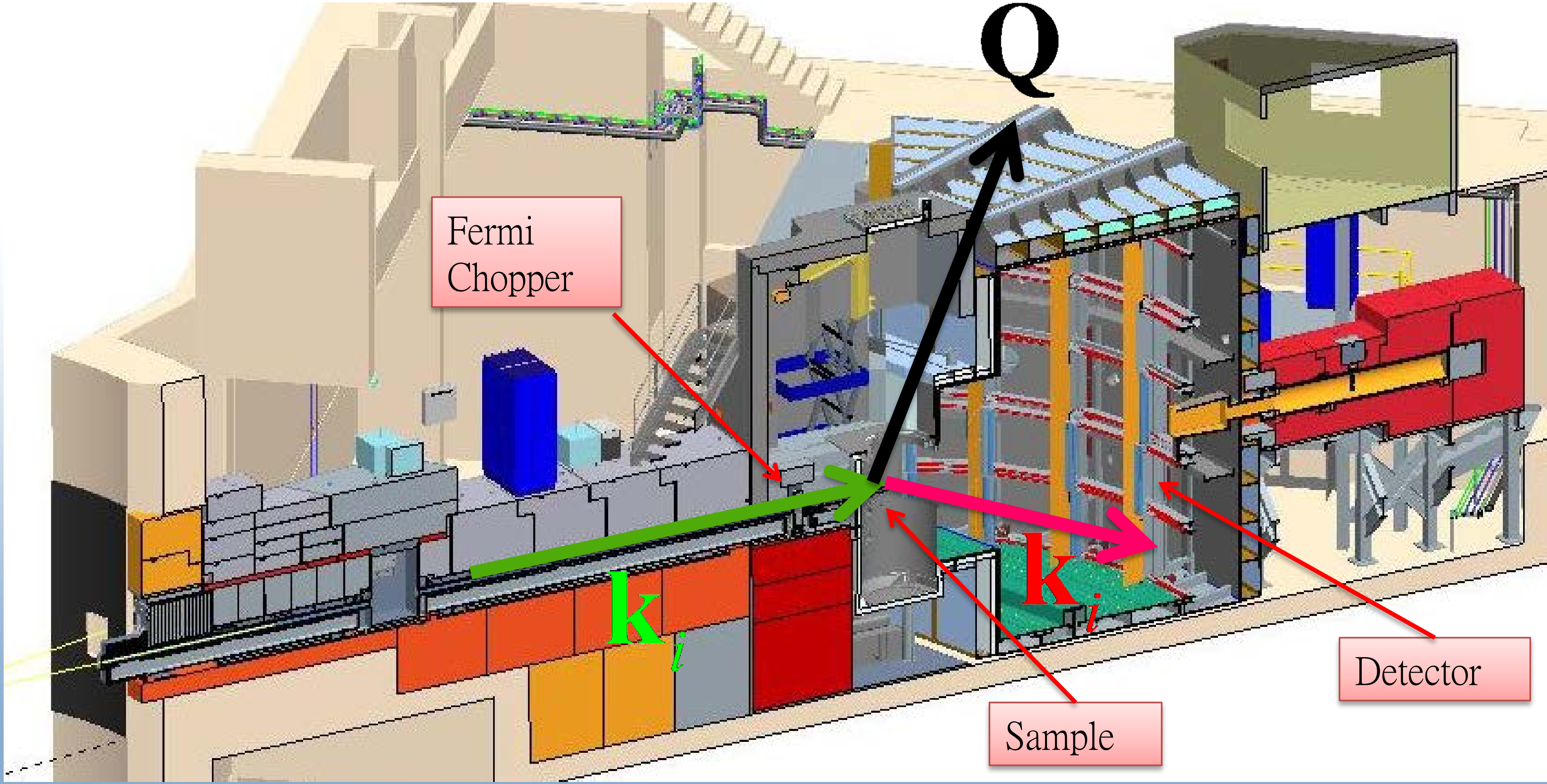
$$\mathcal{S}(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t} \frac{1}{N} \left\langle \rho_{\mathbf{Q}}(0) \rho_{-\mathbf{Q}}(t)\right\rangle$$

Spallation Neutron Source



1.4 MW Pulsed Proton Beam on Hg Target
18 Instruments in construction
Second Target Station moving towards CD1

SEQUOIA Time of Flight Spectrometer (ORNL)



$$t_{\text{chopper}} \rightarrow v_i$$

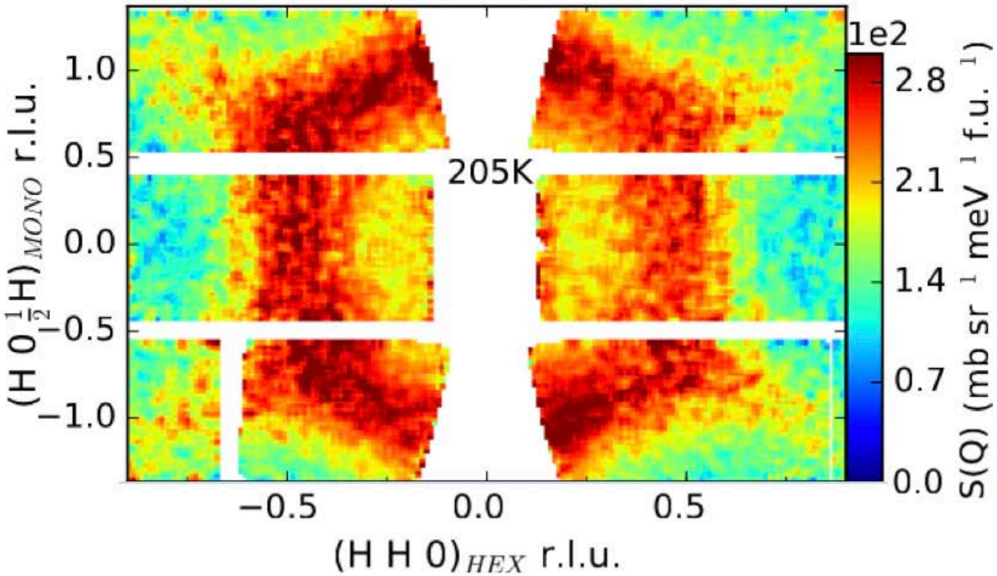
$$t_{\text{detector}} \rightarrow v_f$$

$$\hbar\omega = \frac{1}{2} m\left(v_i^2 - v_f^2\right)$$

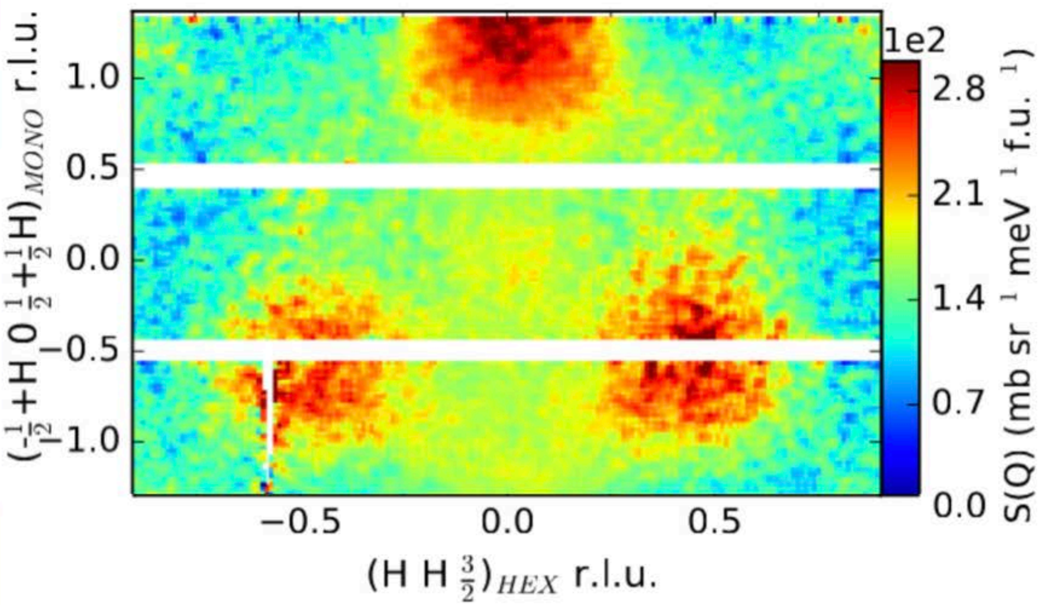
$$\hbar\mathbf{Q} = m\left(\mathbf{v}_i - \mathbf{v}_f\right)$$

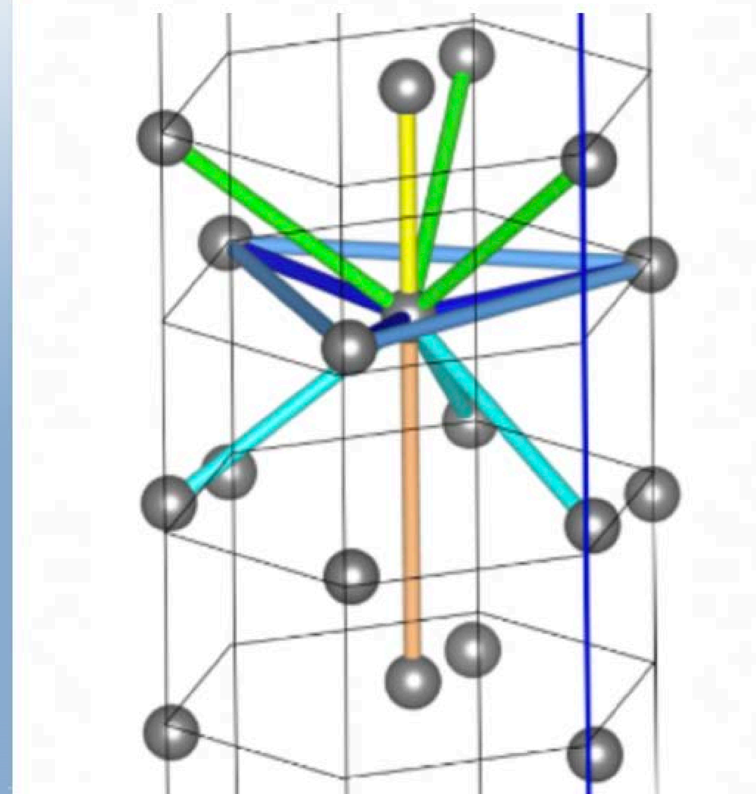
Pixels Galore! (SEQUOIA)

Ultra Short range correlations in PI

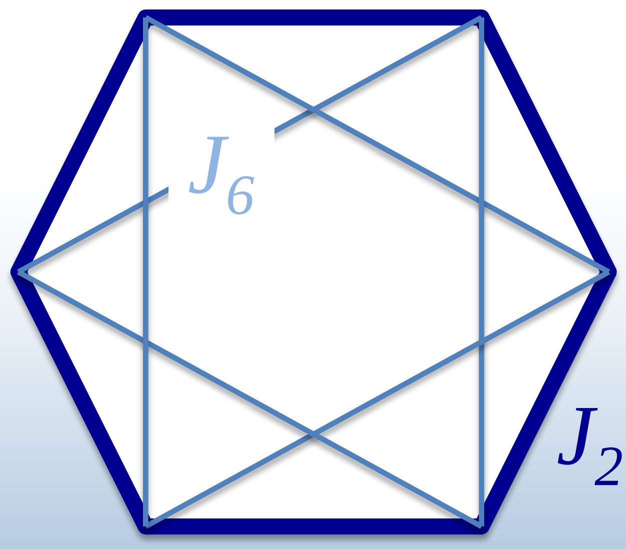


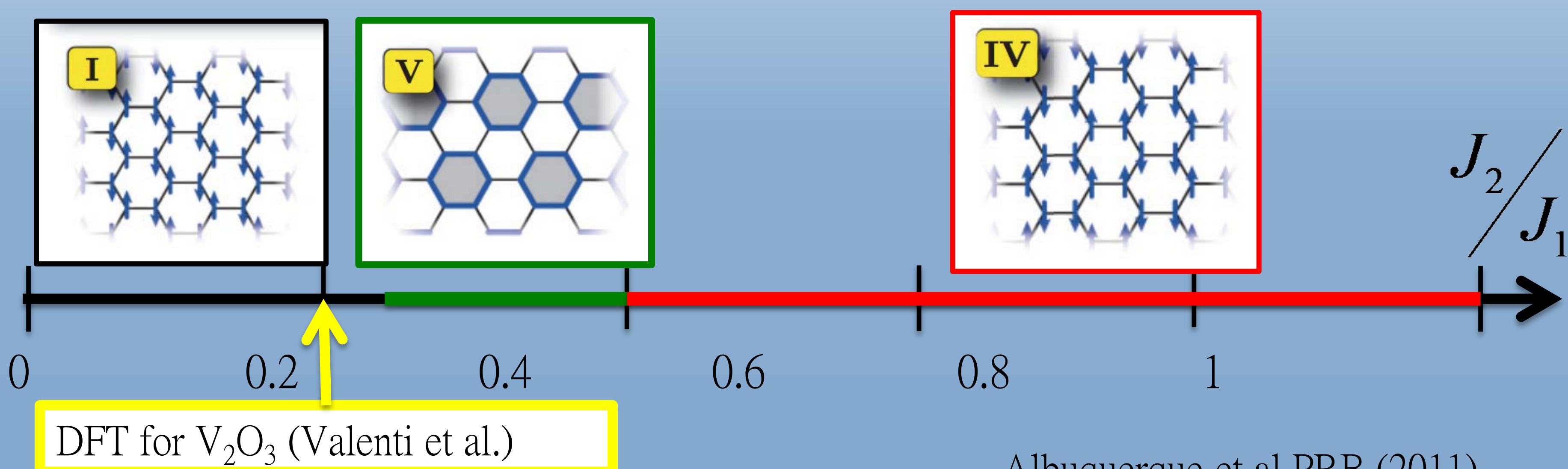
distance (Å)	J_j		DFT (meV)
2.71072	J_1	(yellow)	-0.3(6)
2.87799	J_2	(dark blue)	8.5(3)
3.46255	J_3	(cyan)	0.6(3)
3.68774	J_4	(green)	0.0(2)
4.29734	J_5	(orange)	-1.2(7)
4.94240	J_6	(blue)	1.7(2)





Frustrated Honeycomb AFM



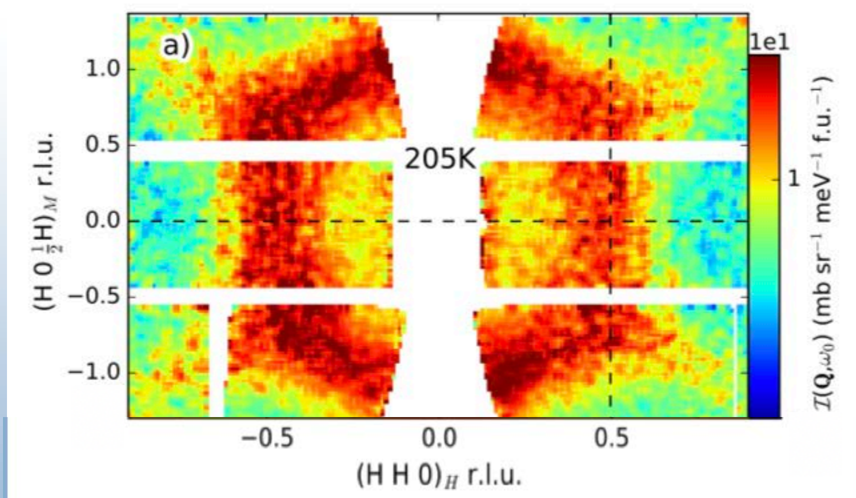


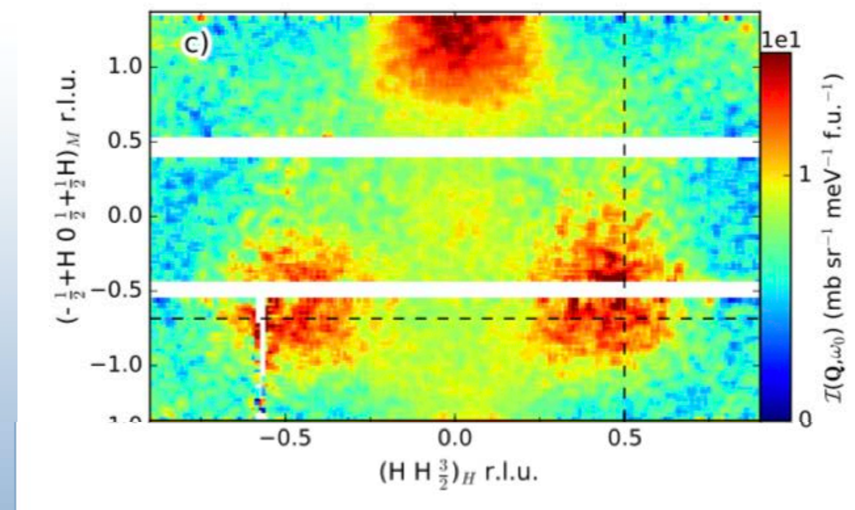
Albuquerque et al PRB (2011)

Self consistent Gaussian Approximation

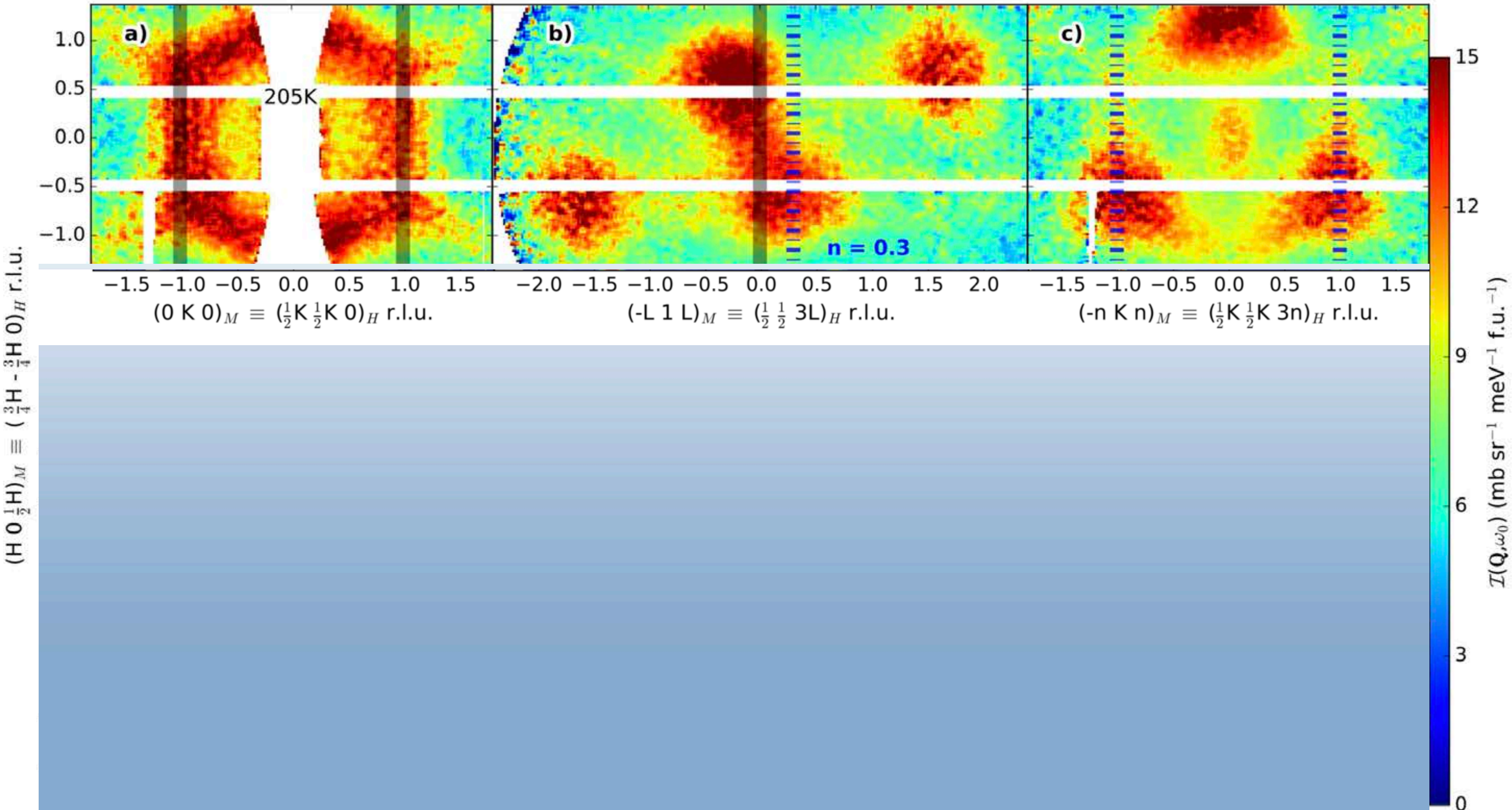
$$\beta E = \frac{1}{2}\sum_{ij}(\beta \sum_{n} J_n A_{ij}^{(n)} + \lambda\delta_{ij})s_i s_j.$$

Include all DFT determined
Exchange interactions (3D)

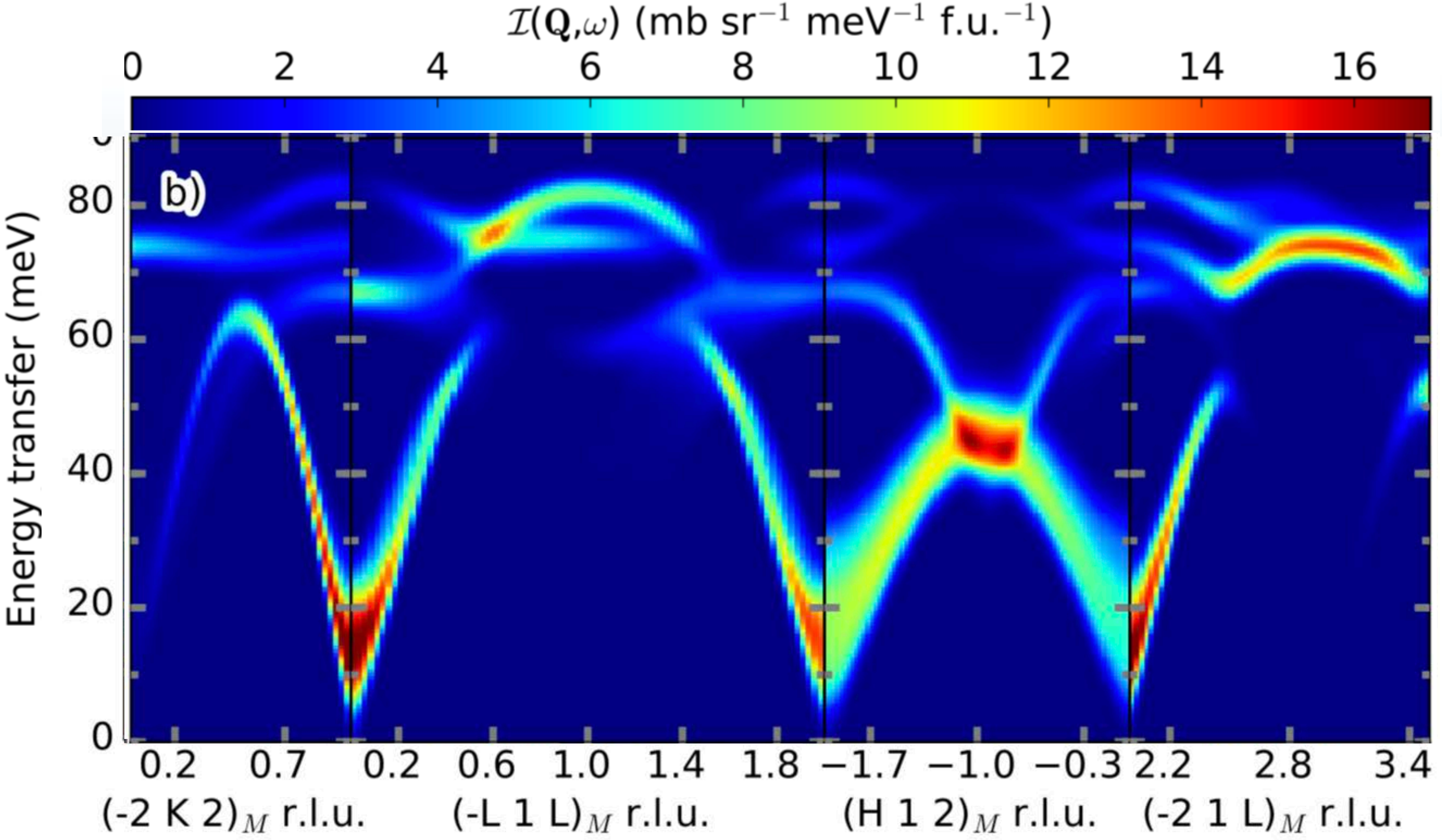




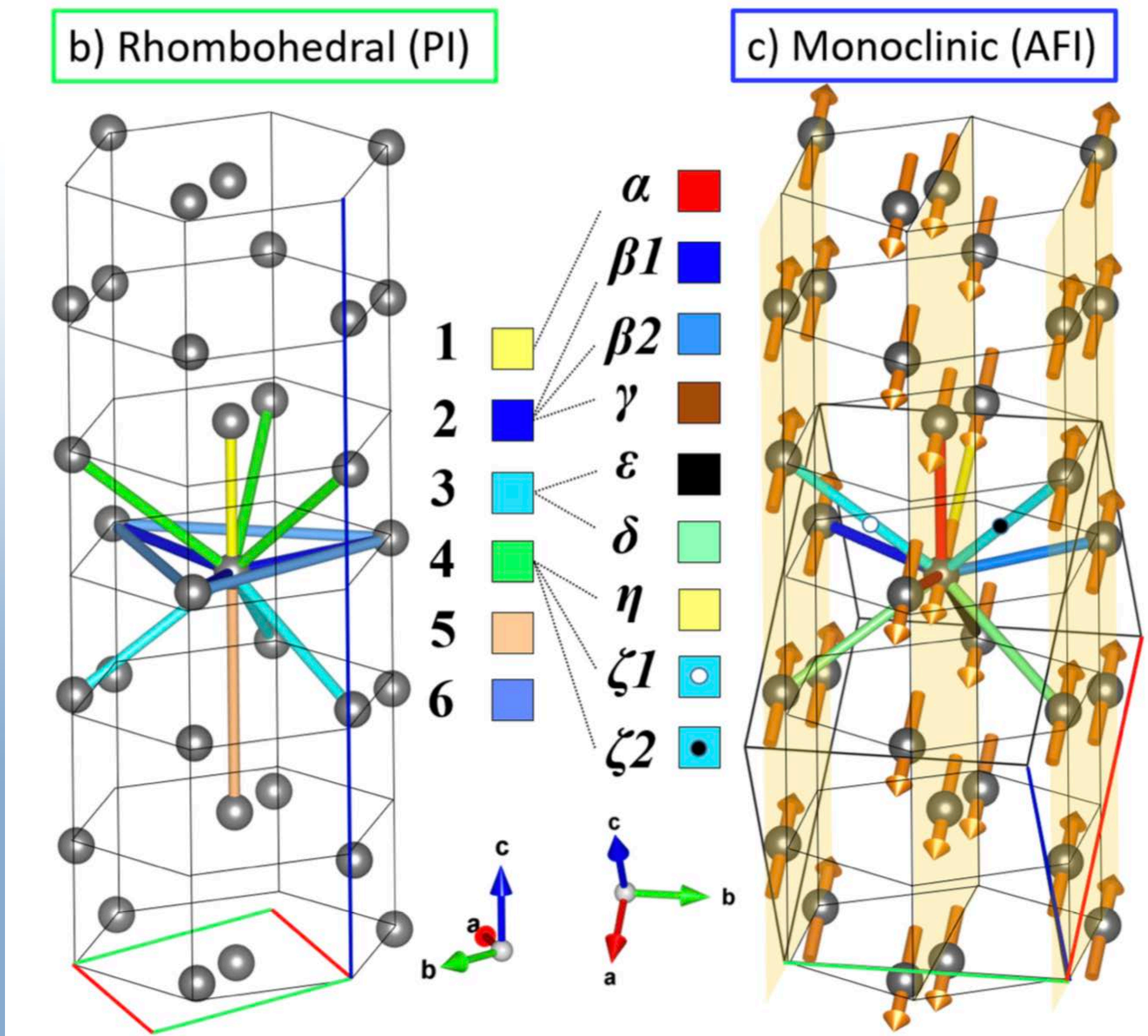
From diffuse to coherent: PI to AFI



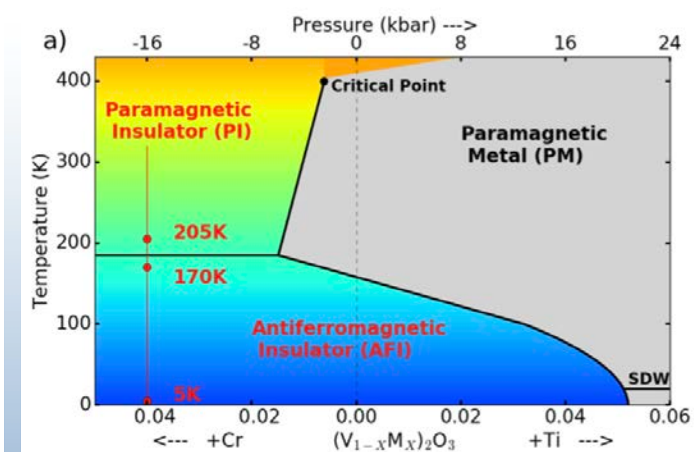
Development of Coherent Magnon



AFI: Frustration relieved!



Leiner, Valenti, Jeschke et al.

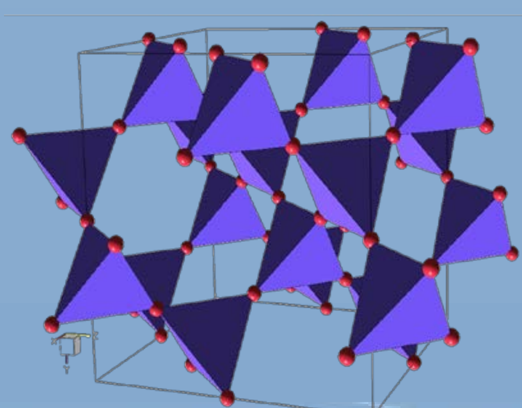


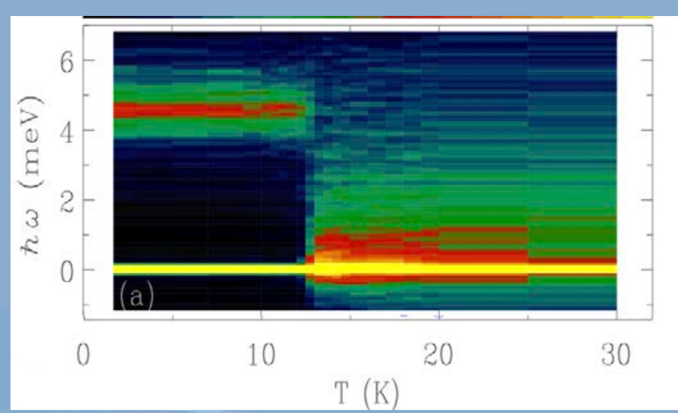
distance (Å)	J_i (meV)	DFT	Neutron	$\mathrm{sgn}(\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle)$
2.75904	J_α	-1(2)	-6.0(2)	+
2.83083	$J_{\beta 1}$	25(2)	27.7(2)	−
2.91789	$J_{\beta 2}$	9(2)	7.7(2)	−
2.98538	J_γ	3(2)	0.0(2)	+
3.43336	J_ϵ	-9(3)	2.0(2)	−
3.45420	J_δ	4(2)	1.1(2)	−
3.63334	J_η	1(2)	-2.0(2)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

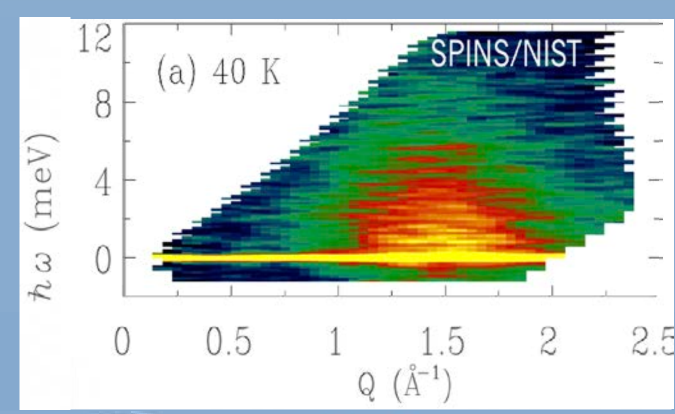
Relieving frustration

$$\mathcal{H} = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

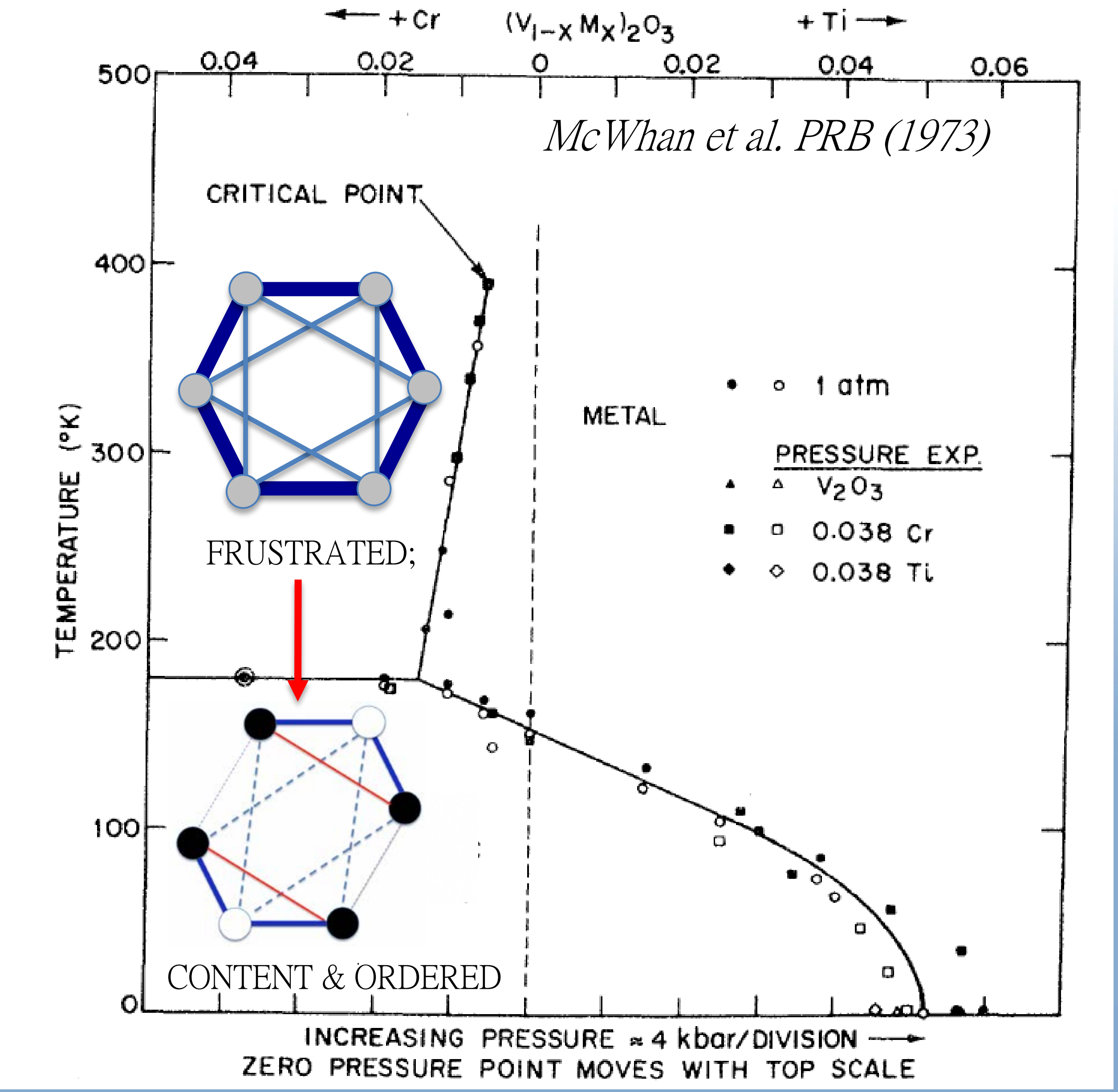
- ❖ J_{ij} typically controlled by quenched degrees of freedom (Born-Oppenheimer-like clamped lattice approximation)
- ❖ The assumption fails when $\mathcal{H}$ yields degenerate manifold of states
- ❖ Then some form of symmetry breaking lifts degeneracy (Lattice, orbital order, charge order):
  - Spin-Peierls transition in CuGeO3
  - Cubic-Tetragonal $ZnCr_2O_4$ spinel
  - Multiferroic phases $Ni_3V_2O_8$





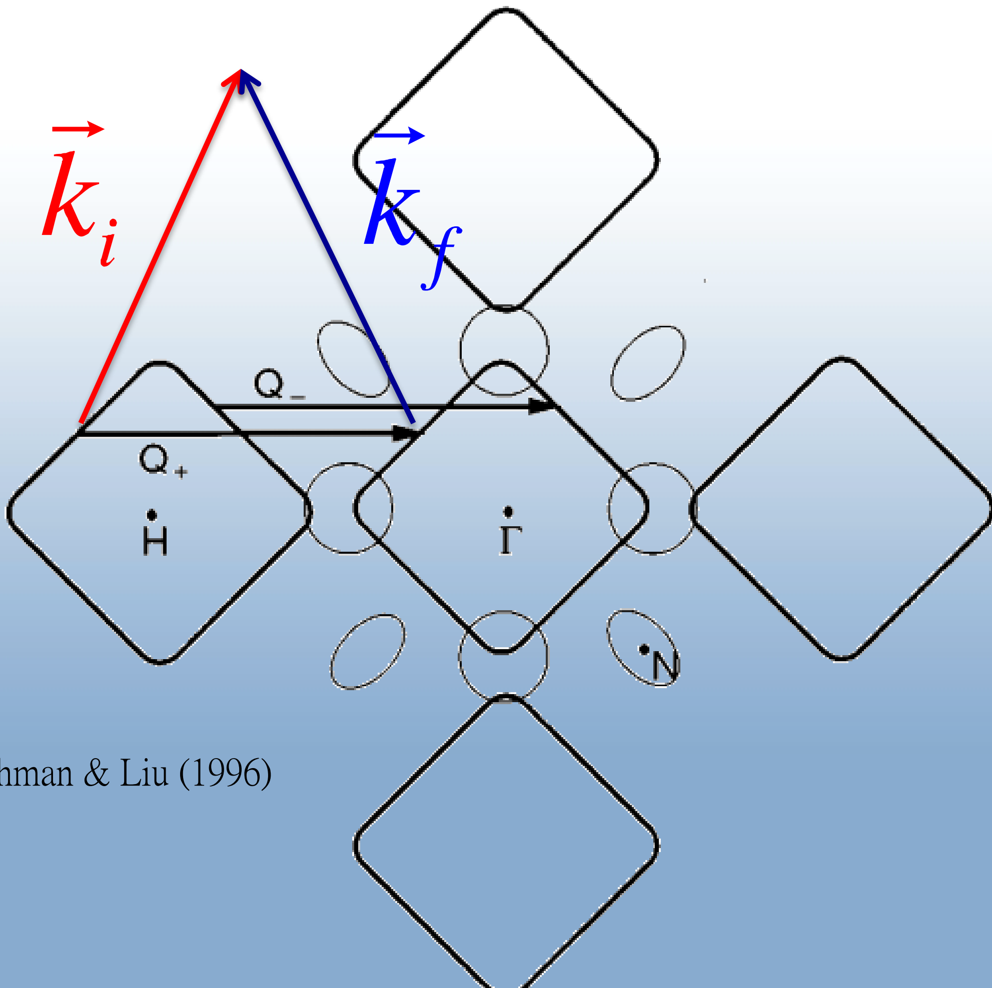


Relieving frustration in $(V_{1-x}Cr_x)_2O_3$



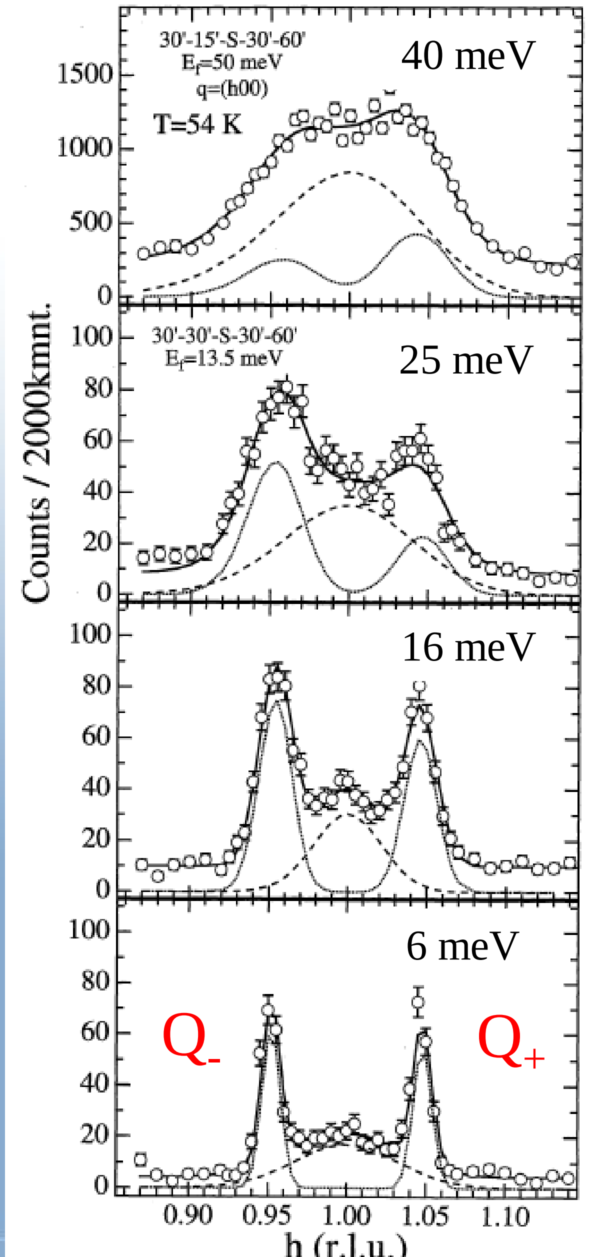
Scattering from band electrons

Chromium Fermi surface



Fishman & Liu (1996)

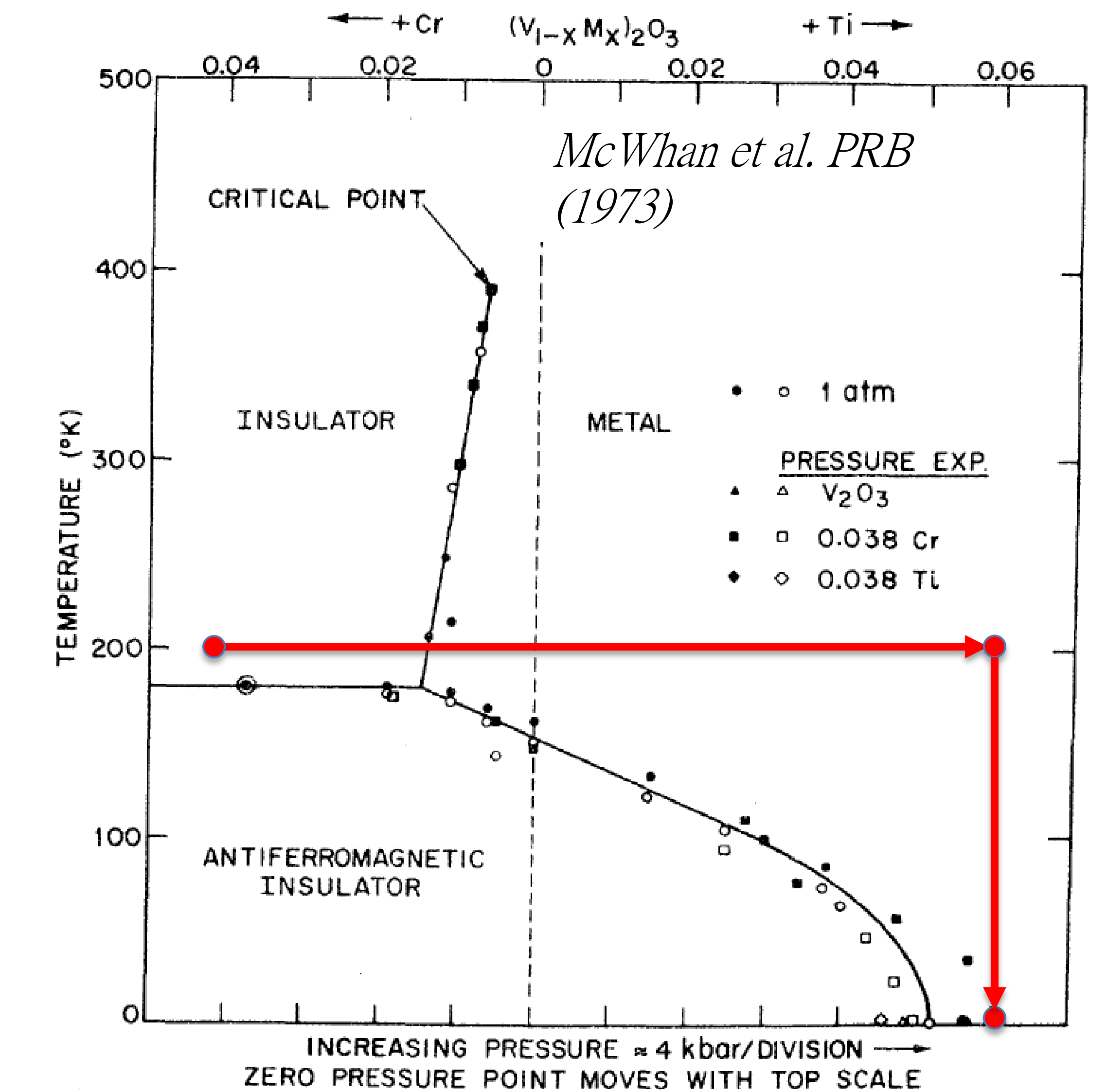
Fukuda et al. (1996)

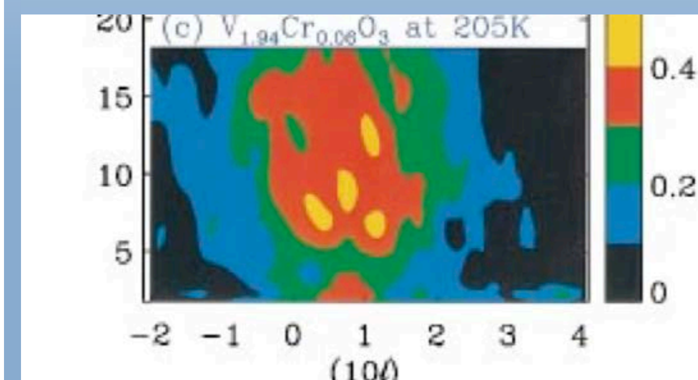


$$\mathcal{S}^{\alpha\beta}(\mathbf{q}\omega)=\frac{1}{1-e^{-\beta\hbar\omega}}\frac{\chi''_{\alpha\beta}(\mathbf{q}\omega)}{(g\mu_B)^2\pi}$$

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

Spin correlations in different phases of V_2O_3

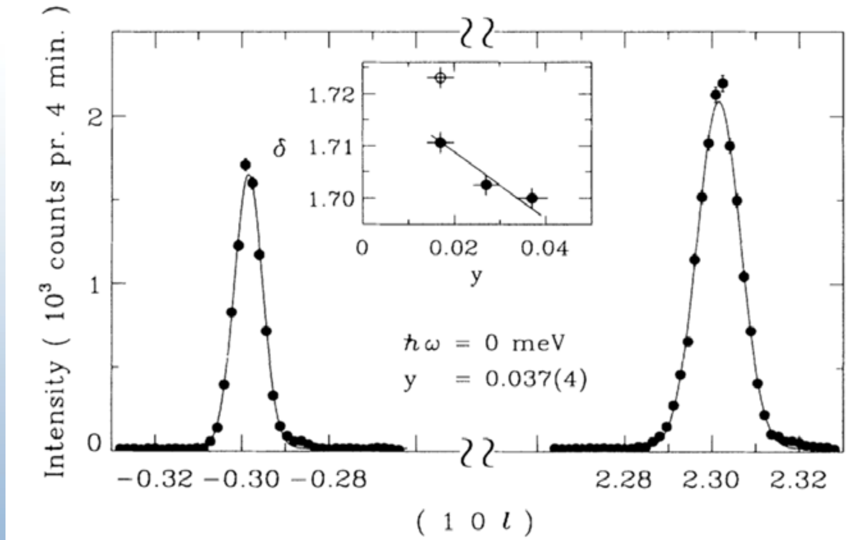


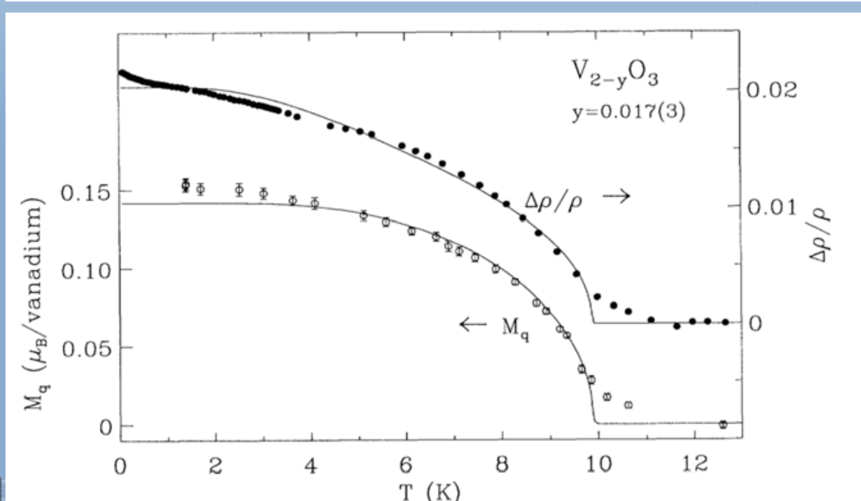


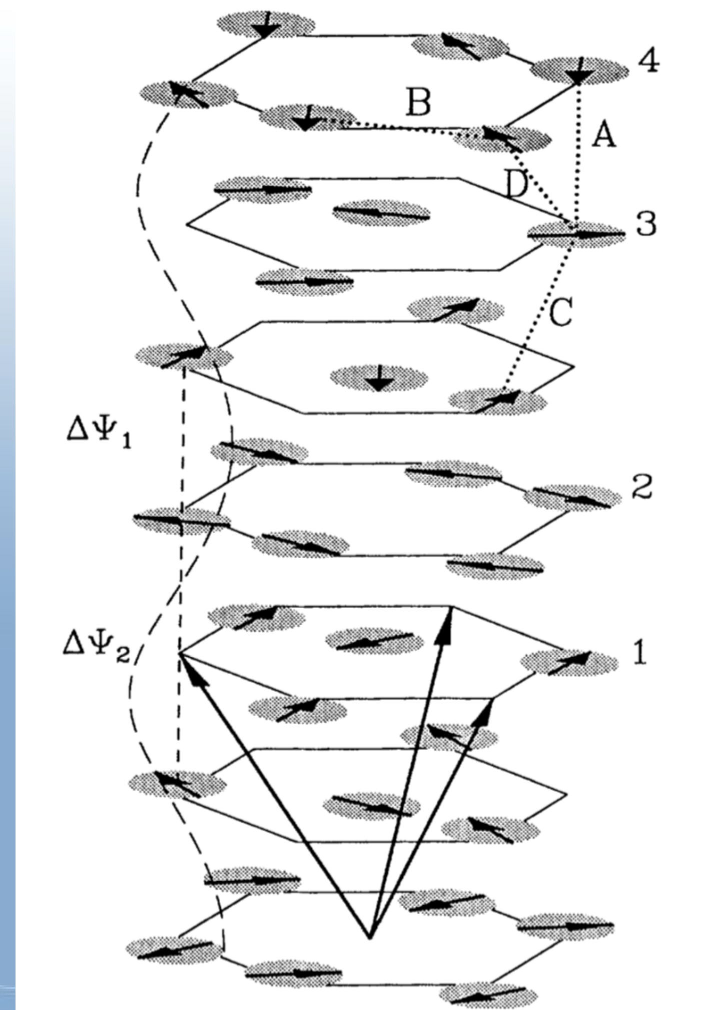
VOLUME 71, NUMBER 5 PHYSICAL REVIEW LETTERS 2 AUGUST 1993

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

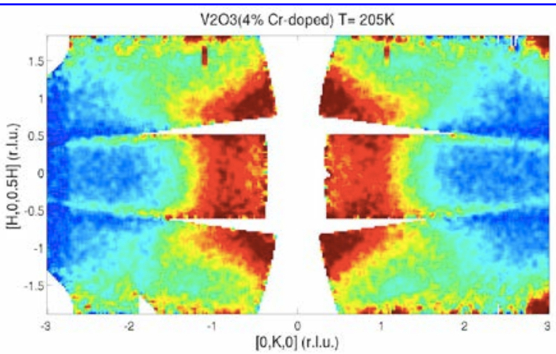
Wei Bao,[1] C. Broholm,[1,2] S. A. Carter,[3] T. F. Rosenbaum,[3] G. Aeppli,[4]
S. F. Trevino,[2,5] P. Metcalf,[6] J. M. Honig,[6] and J. Spalek[6]



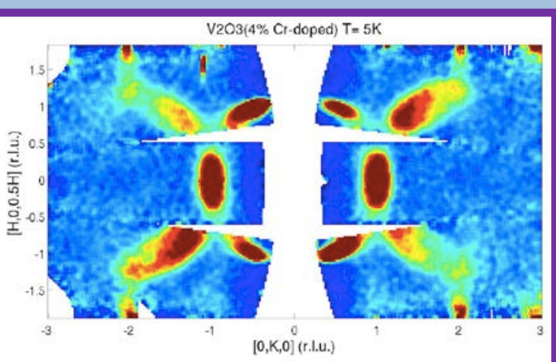


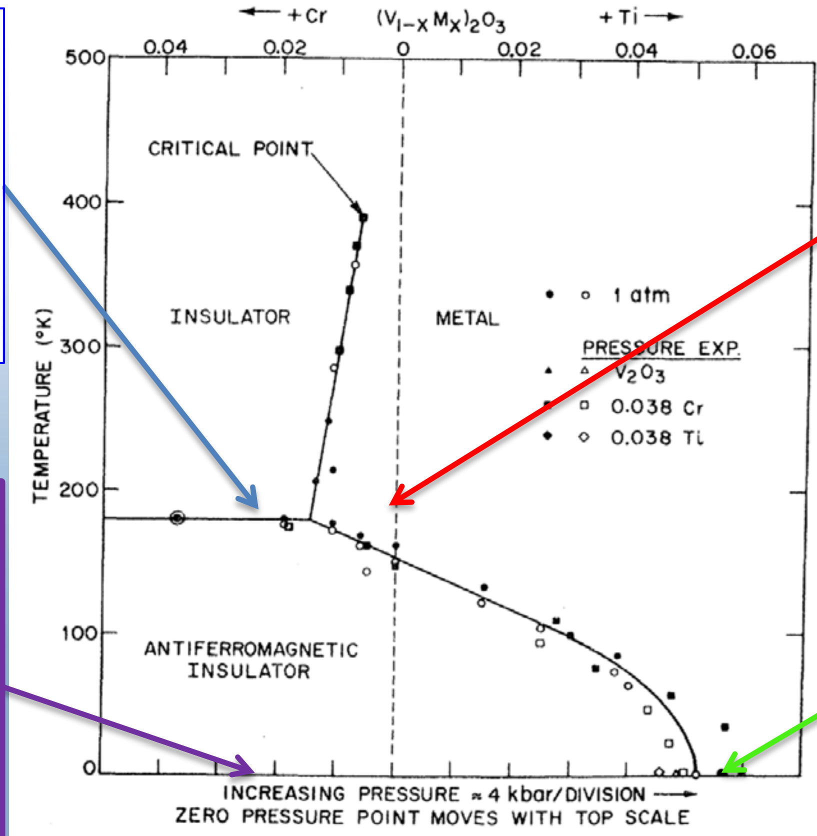


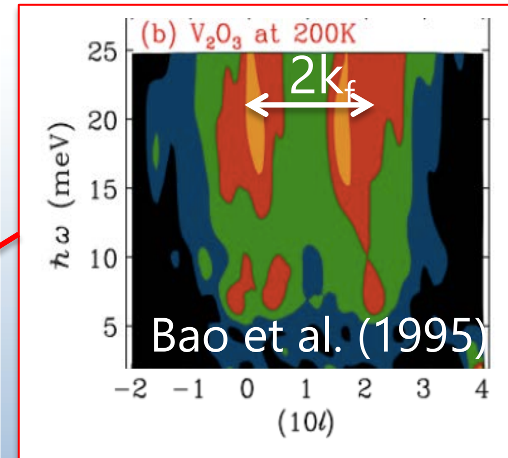
Spin correlations in V_2O_3

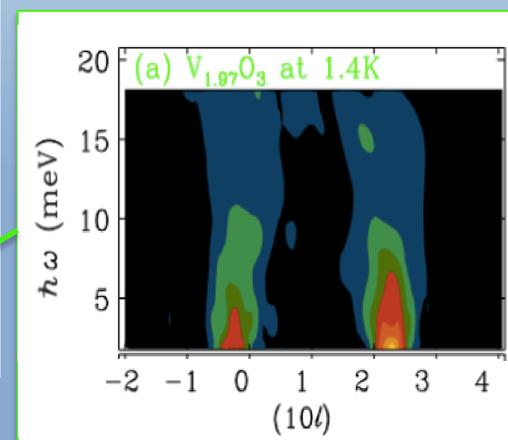


Leiner et al (2018)







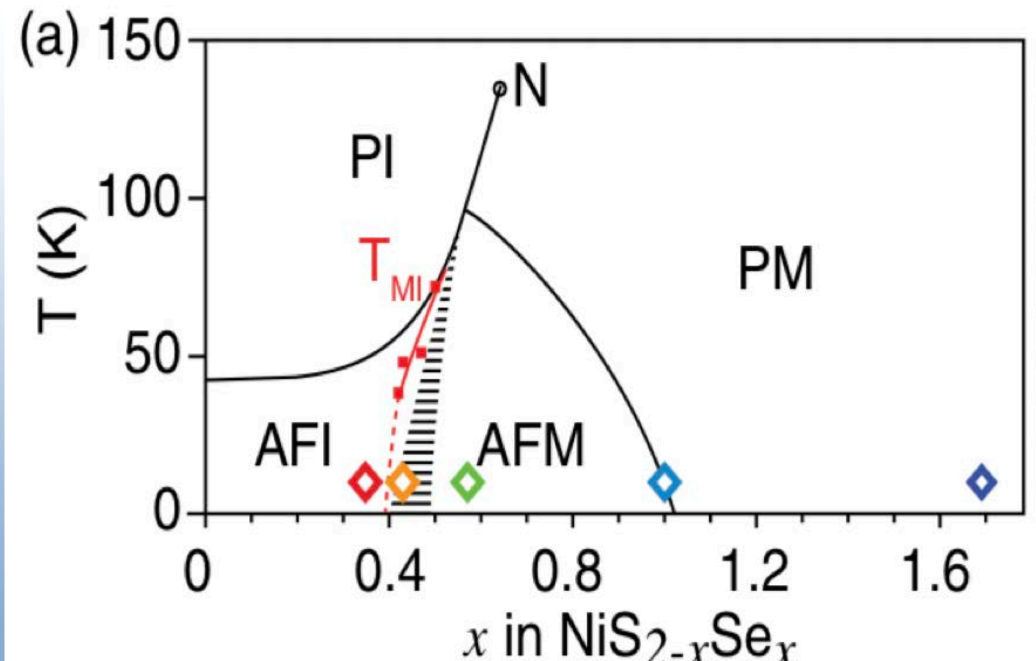


Driven by frustration, the spin-liquid like character of the PI is central to the physics of V2O3

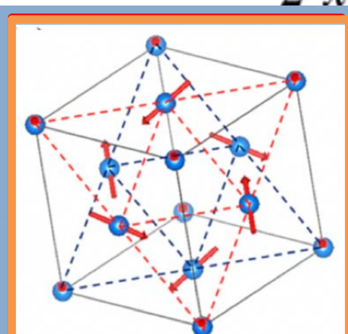
PRL 112, 087603 (2014) PHYSICAL REVIEW LETTERS week ending 28 FEBRUARY 2014

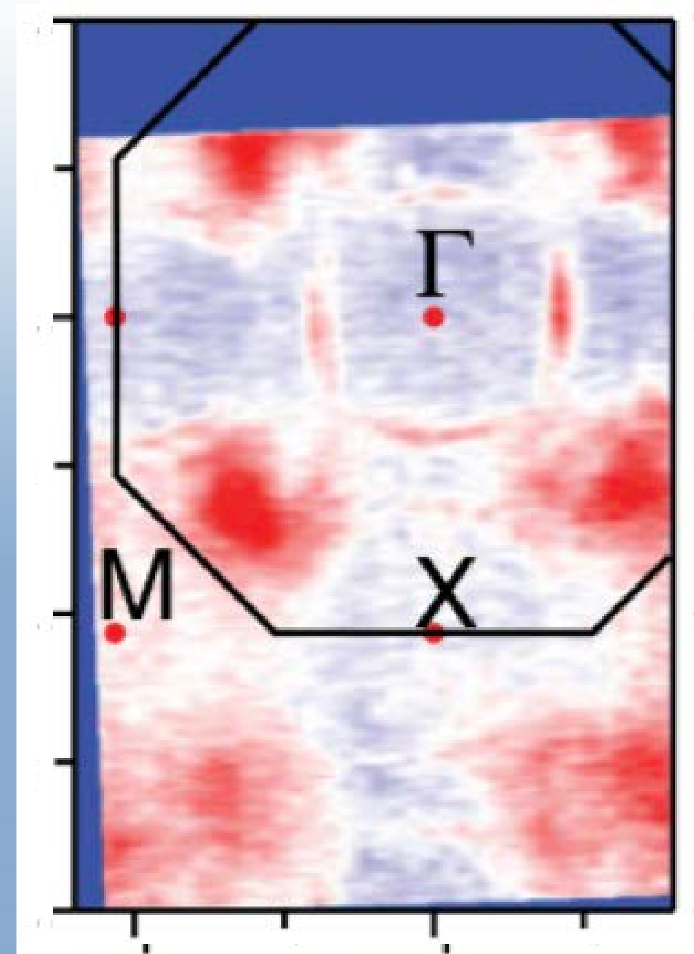
Direct Observation of the Bandwidth Control Mott Transition in the $NiS_{2-x}Se_x$ Multiband System

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,†]



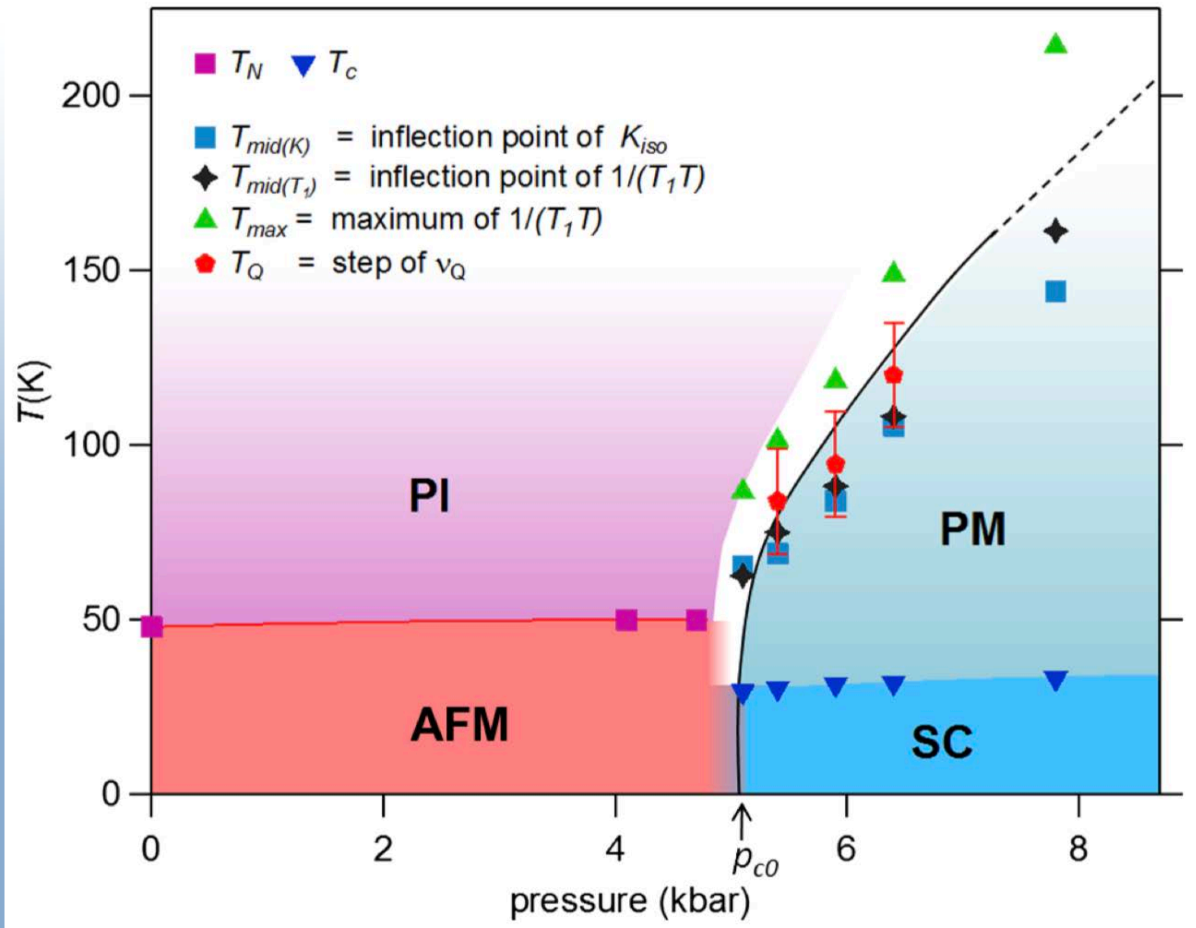
Magnetic Structures by D. Louca et al.

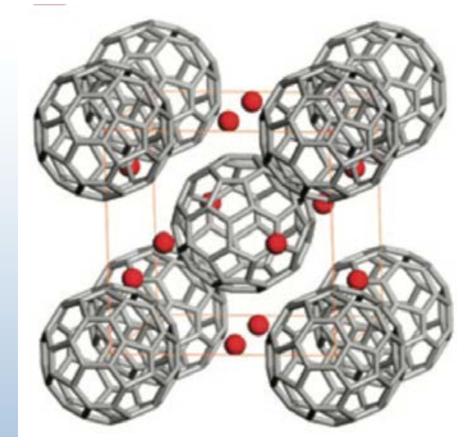


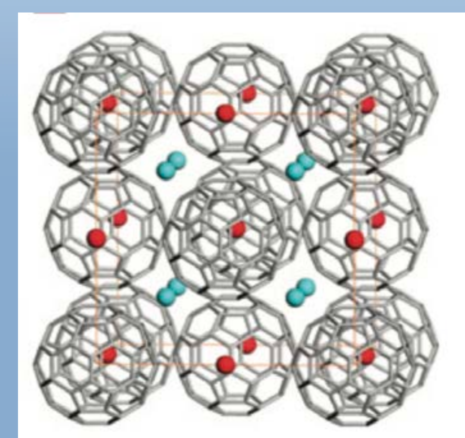


Mott Transition in the *A*15 Phase of Cs_3C_{60}: Absence of a Pseudogap and Charge Order

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]

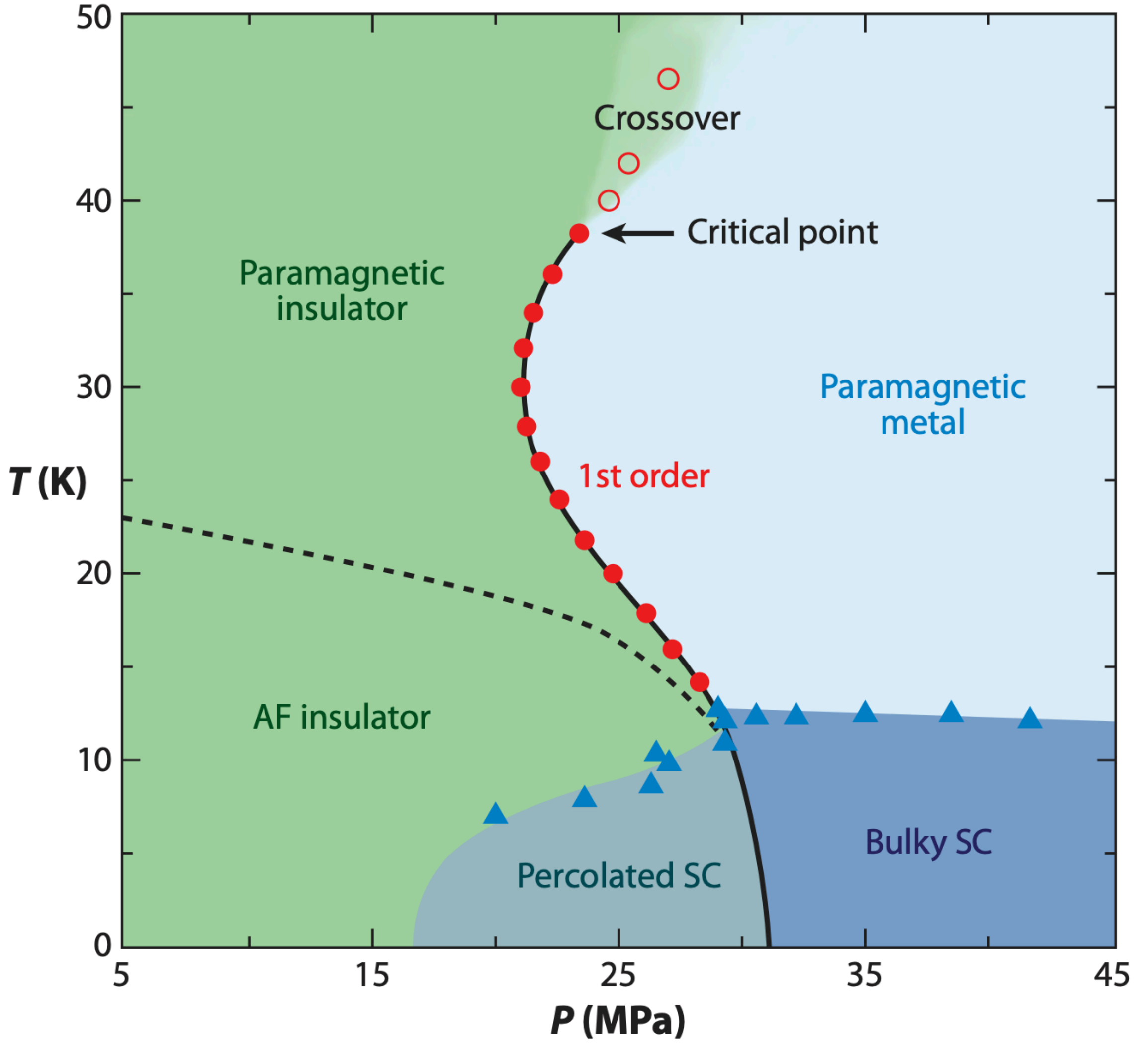


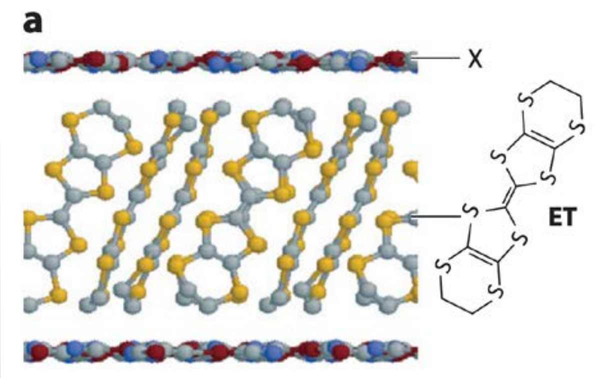


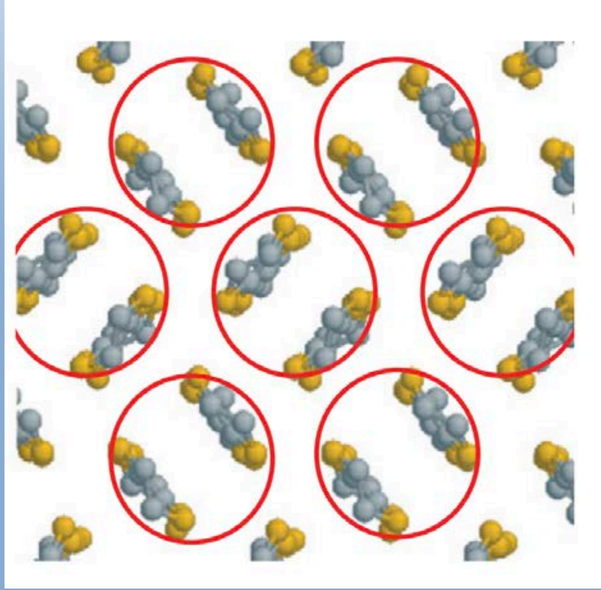


Mott Physics in triangular organic lattices

Kazushi Kanoda et al.







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