

Geometric Magnetic Frustration in the $S=1/2$ Cluster Magnet $\text{LiZn}_2\text{Mo}_3\text{O}_8$

Tyrel M. McQueen

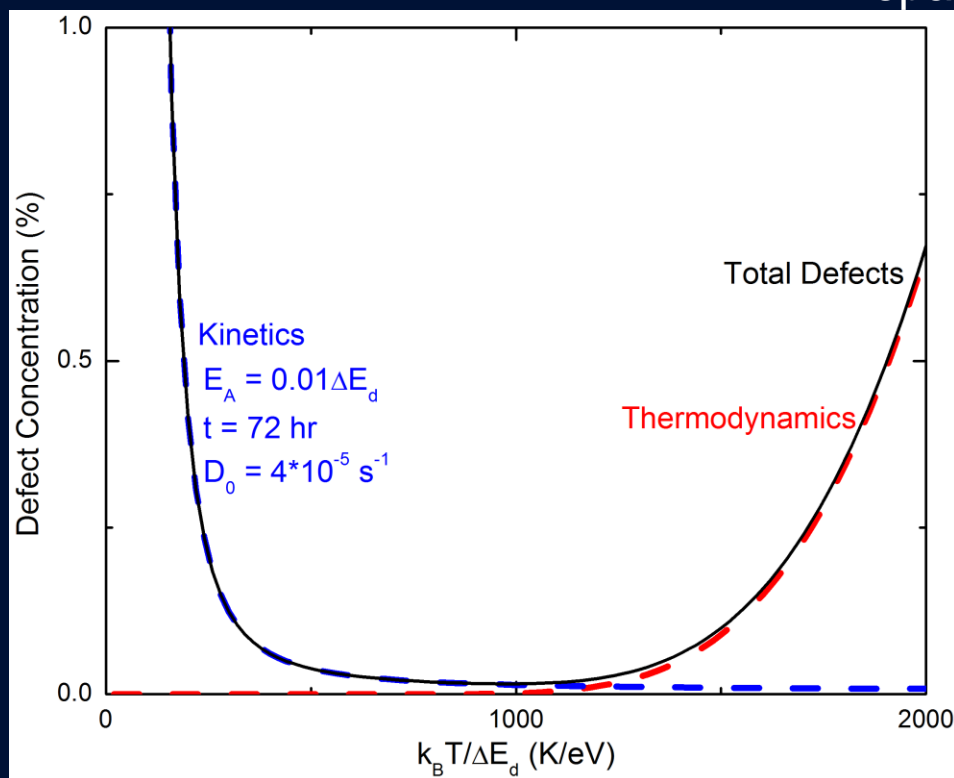
Department of Chemistry

Department of Physics and Astronomy

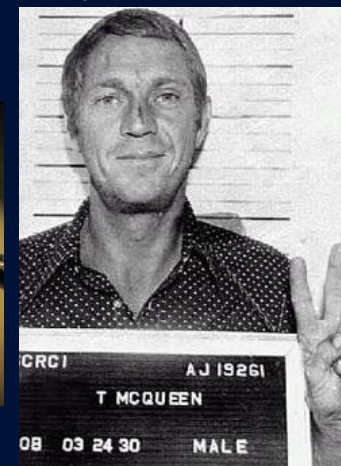
Institute of Quantum Matter

Johns Hopkins University

KITP, October 11, 2012



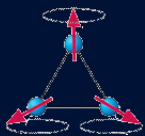
<http://occamy.chemistry.jhu.edu>



“Optimism Does Not Change the Laws of Physics [or Chemistry]”

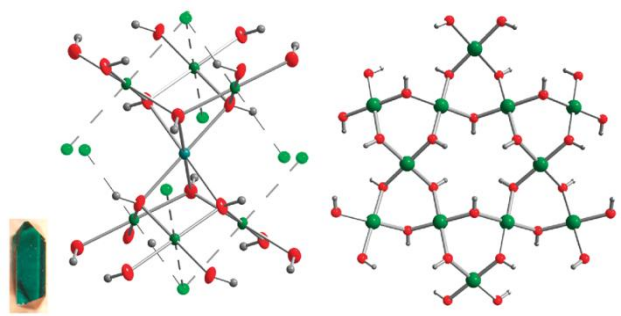
- Science Officer T'Pol, Starship Enterprise





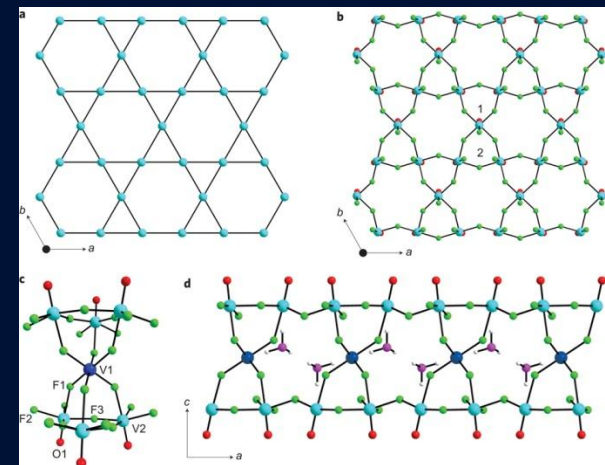
Classes of $S=1/2$ Magnets

Single Ions

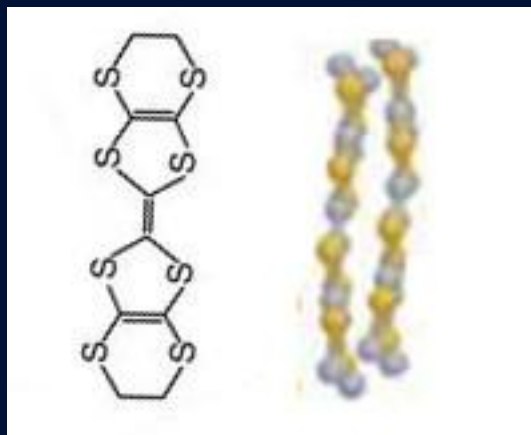


Cu^{2+} (d^9) Minerals

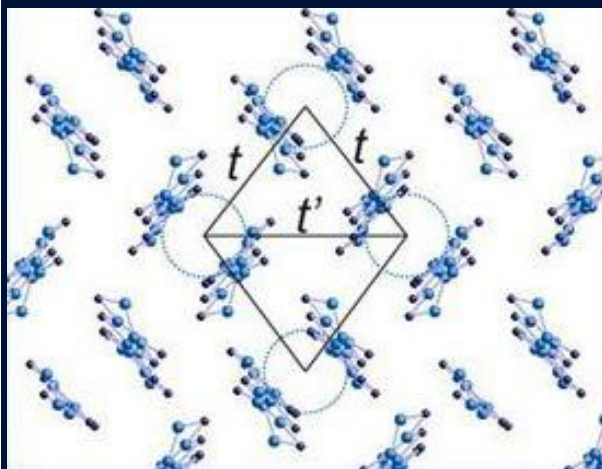
V^{4+} (d^1) Compounds



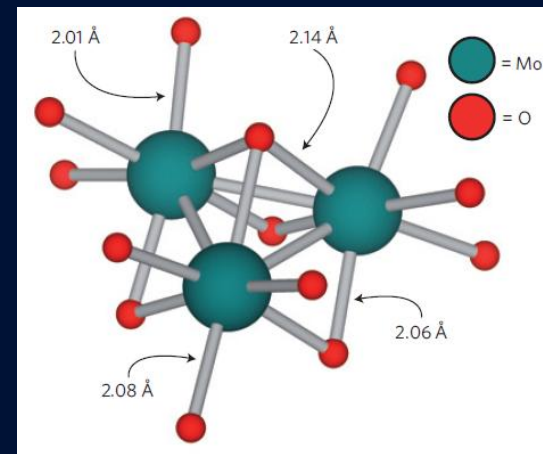
Organic Molecules



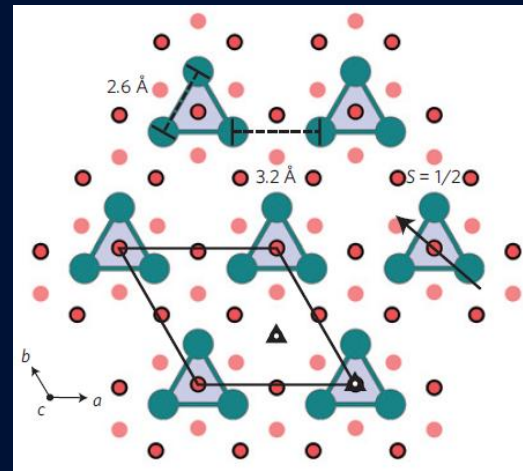
BEDT-TTF Dimers

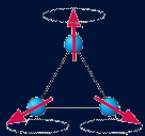


Inorganic "Molecules"

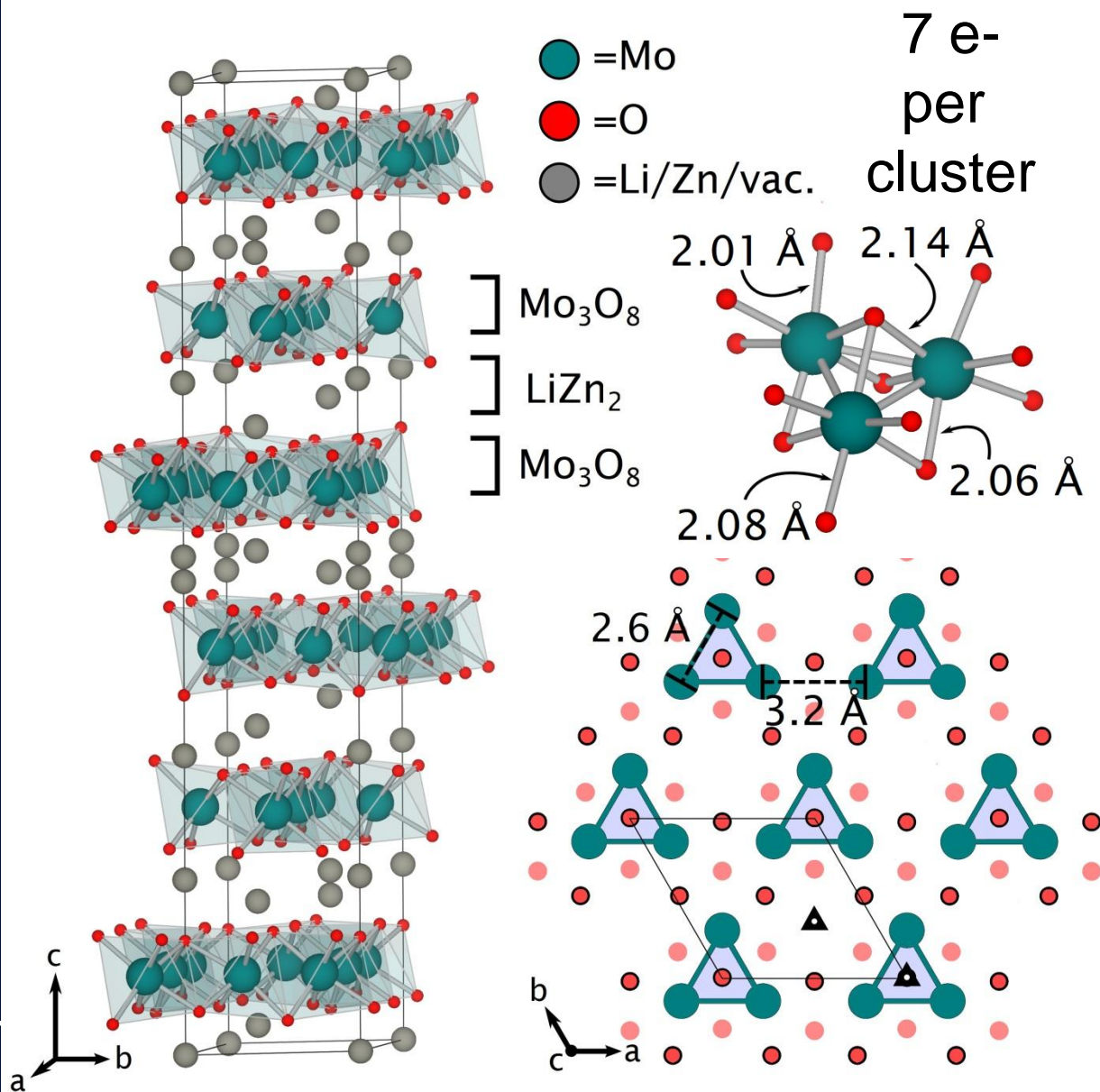


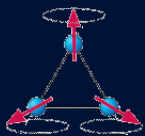
Mo_3O_{13} Cluster



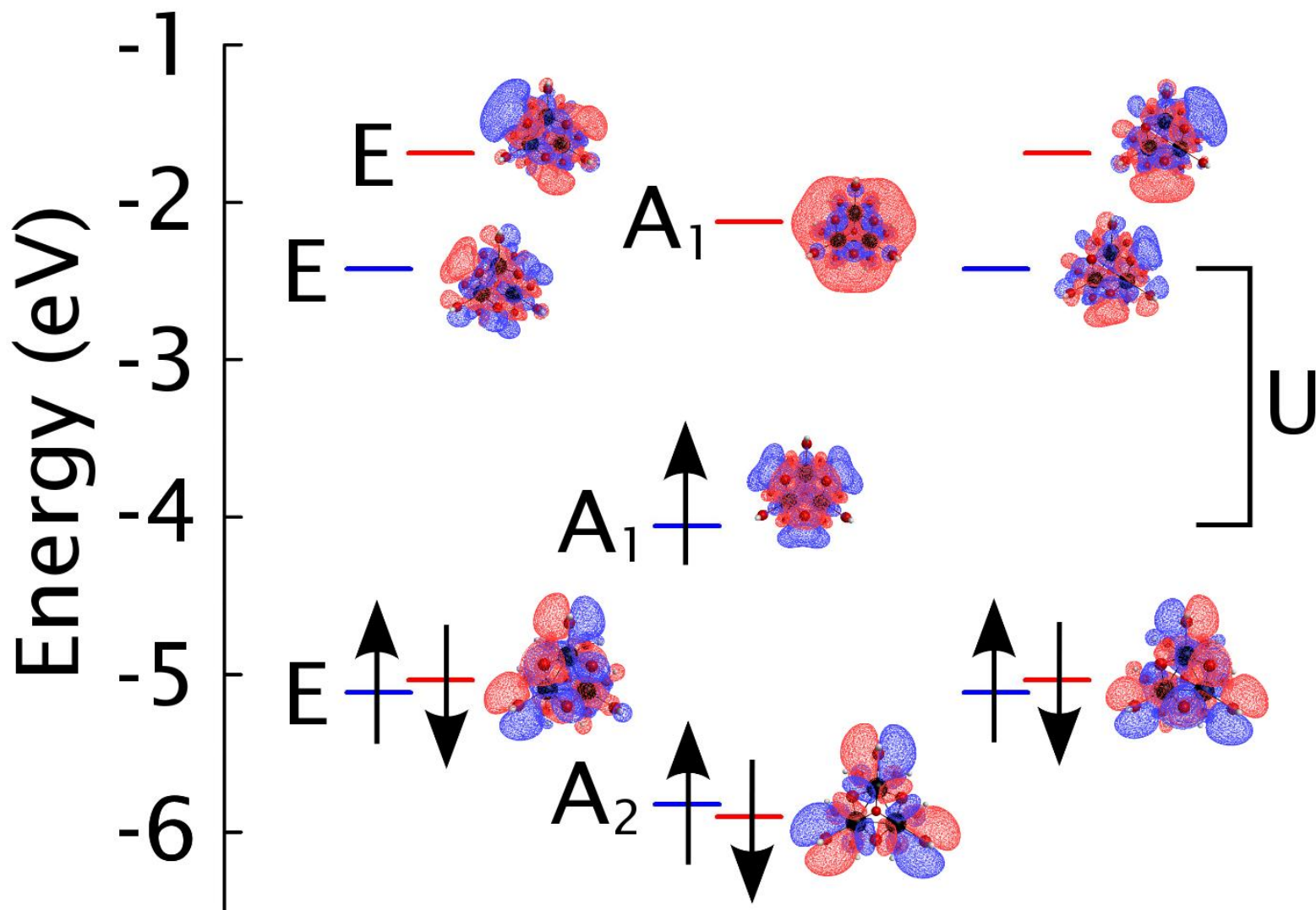


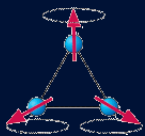
LiZn₂Mo₃O₈ Structure



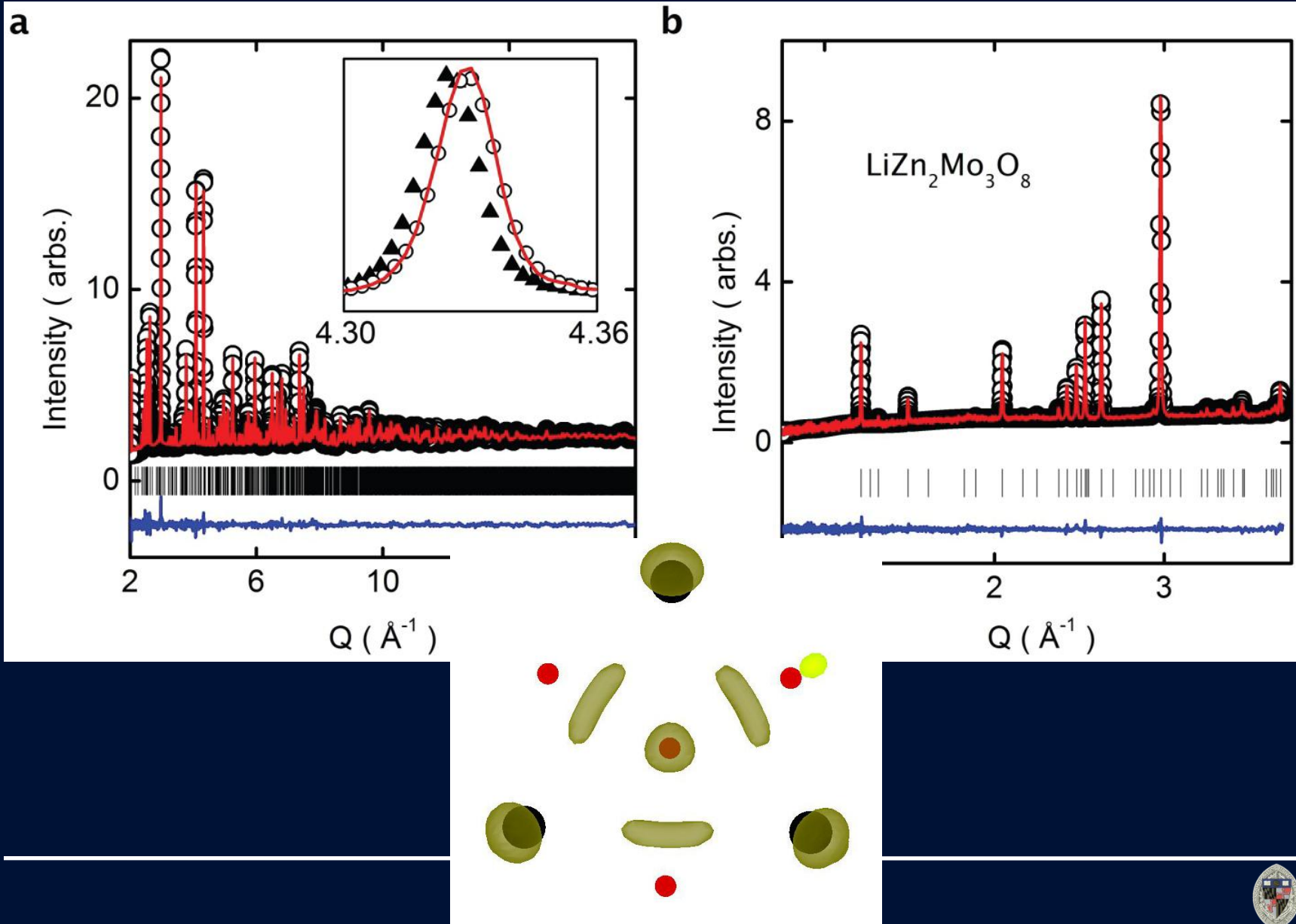


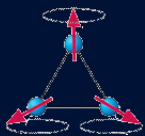
LiZn₂Mo₃O₈ MO Calculation



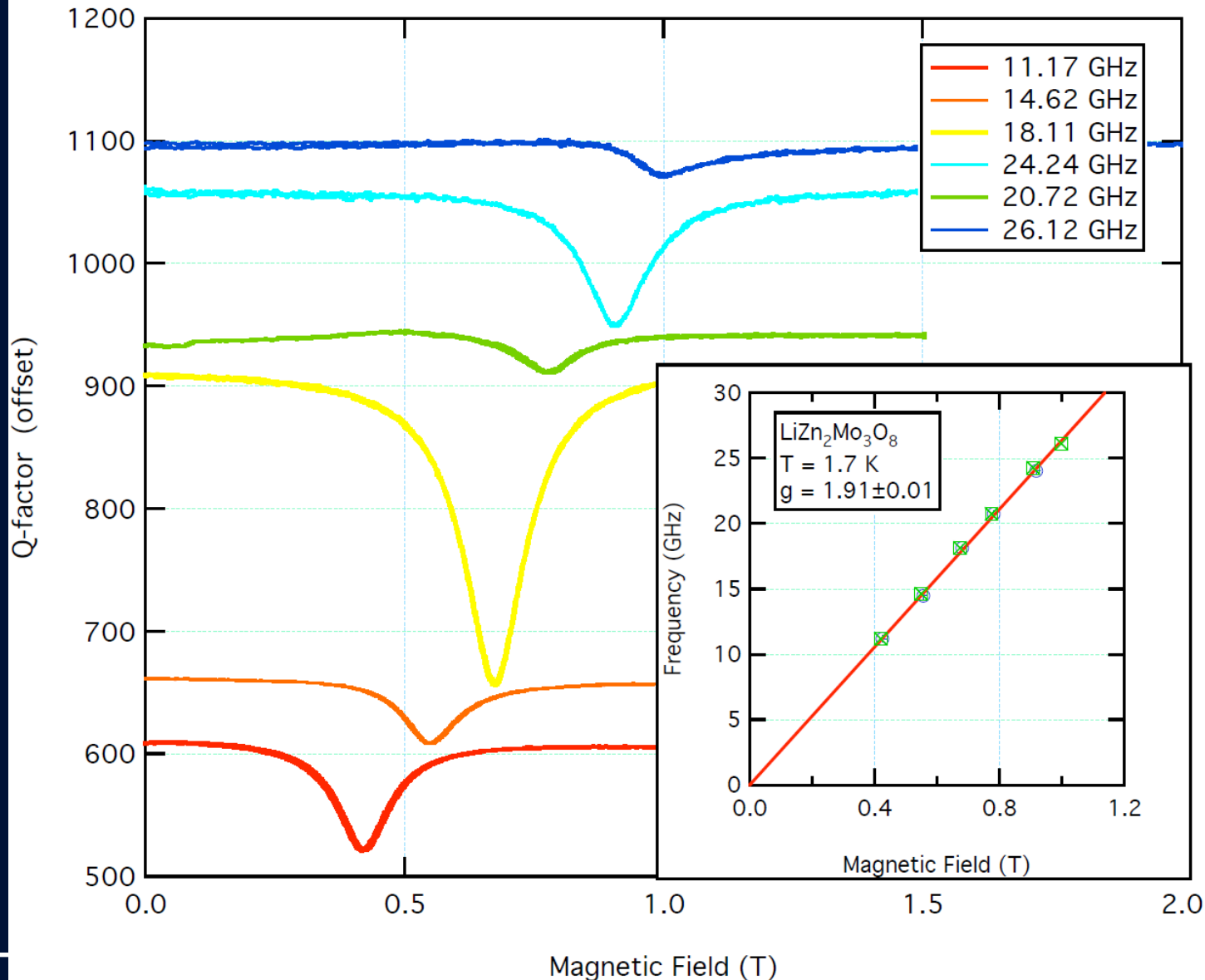


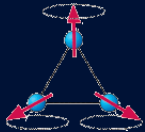
Trigonal Structure



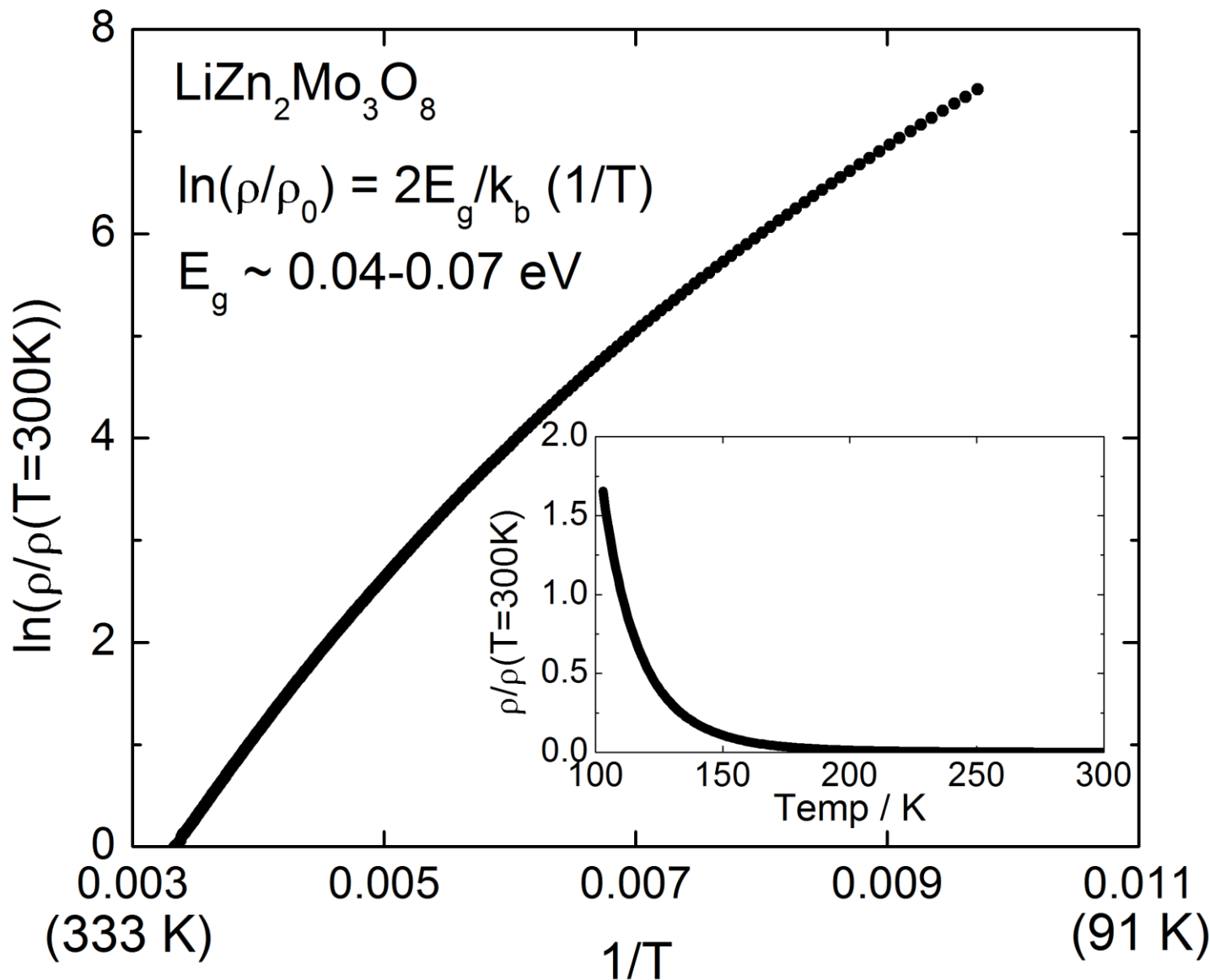


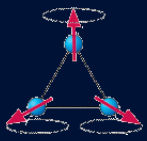
ESR Confirms $S=1/2$ Nature



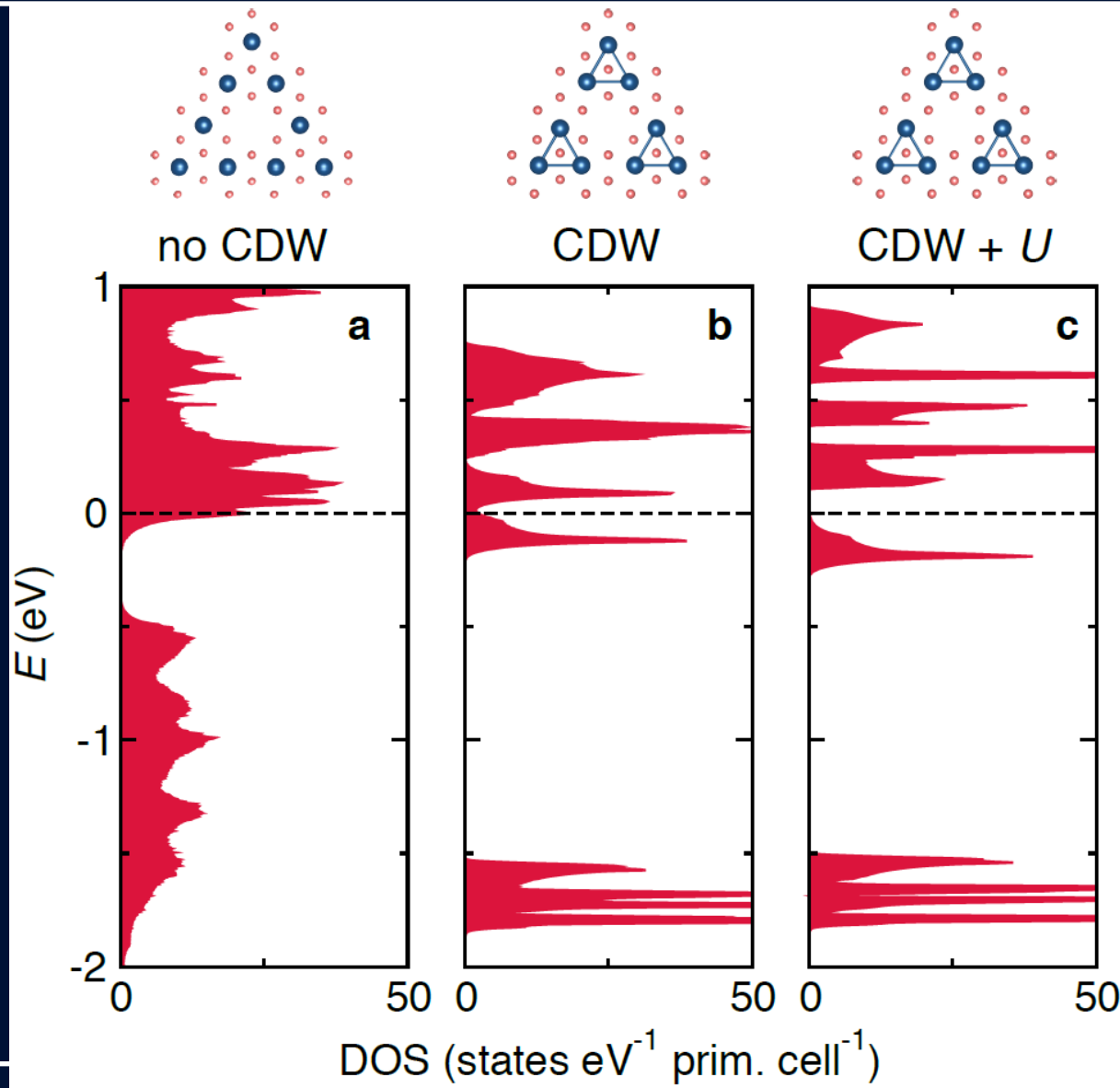


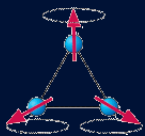
LiZn₂Mo₃O₈ resistivity



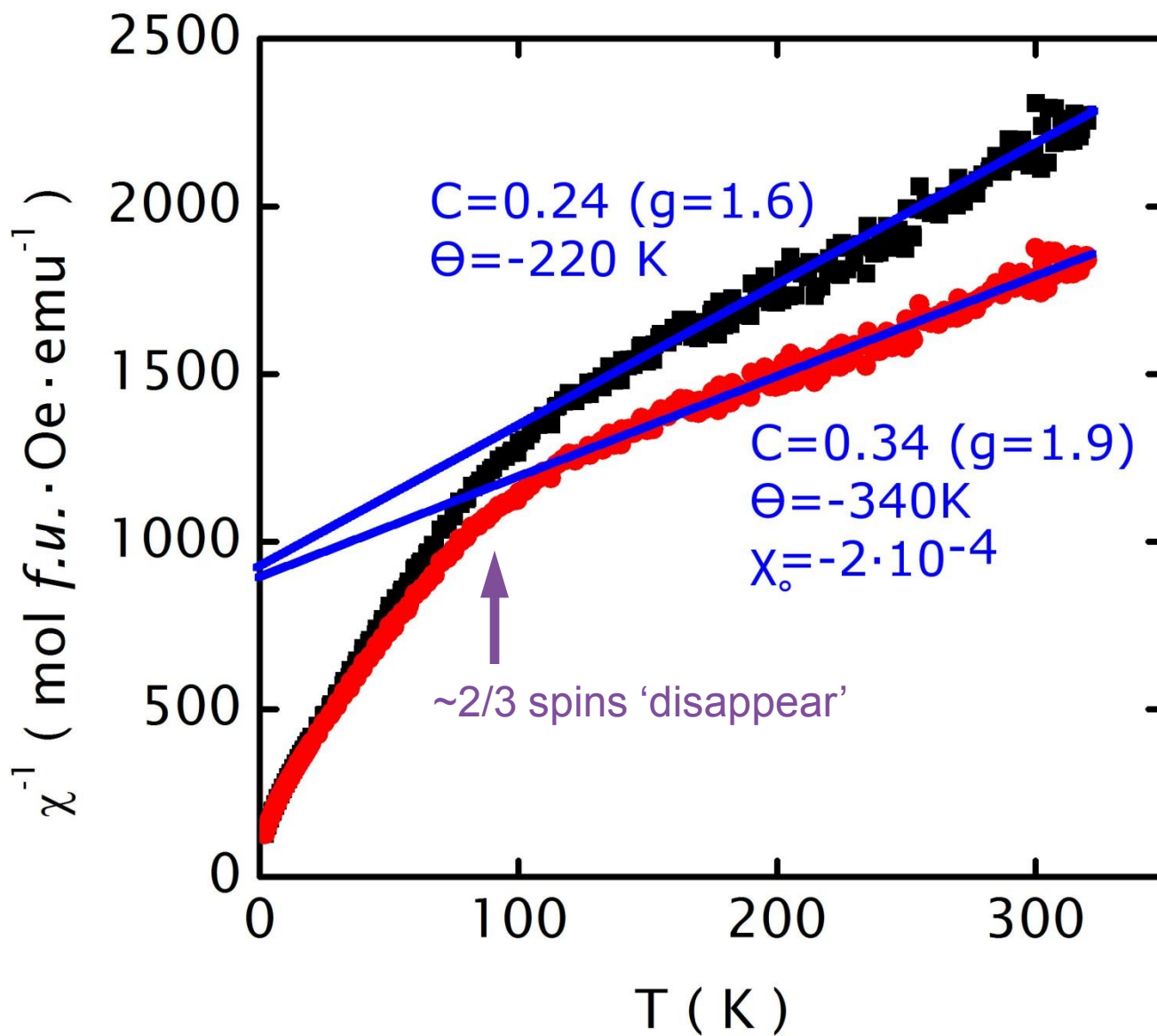


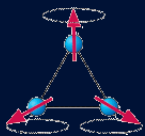
LiZn₂Mo₃O₈ Calculation



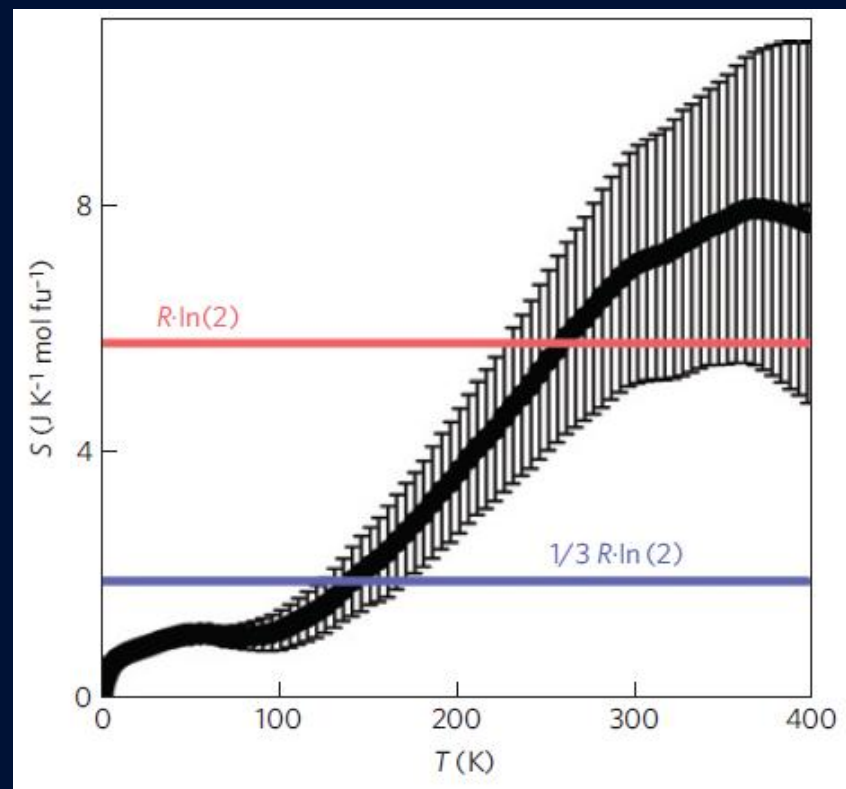
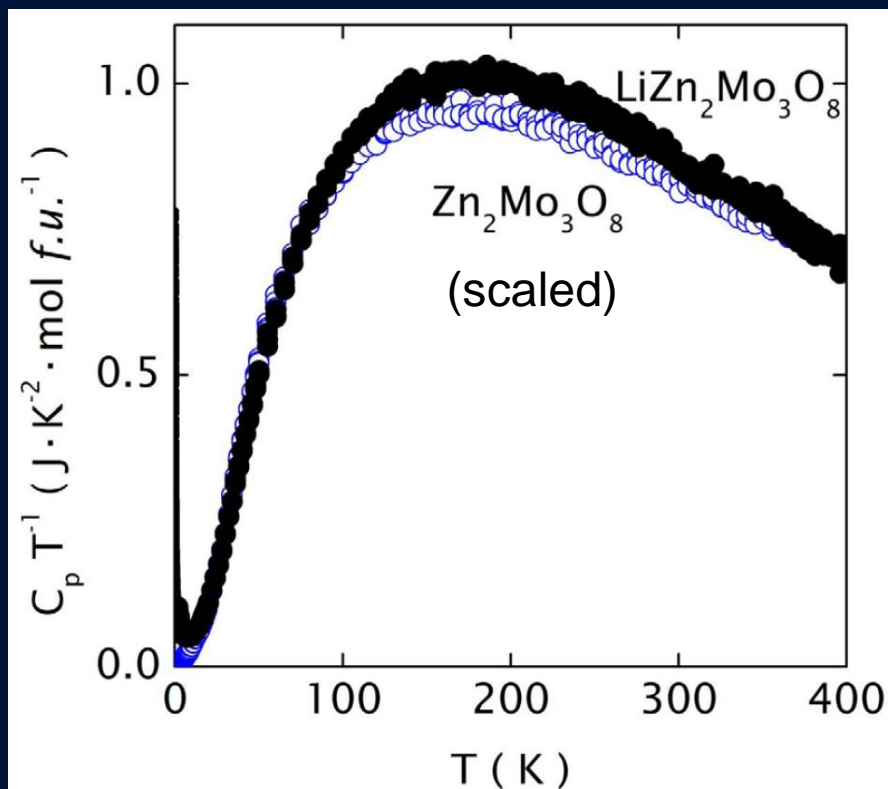


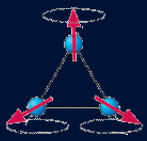
LiZn₂Mo₃O₈ Susceptibility



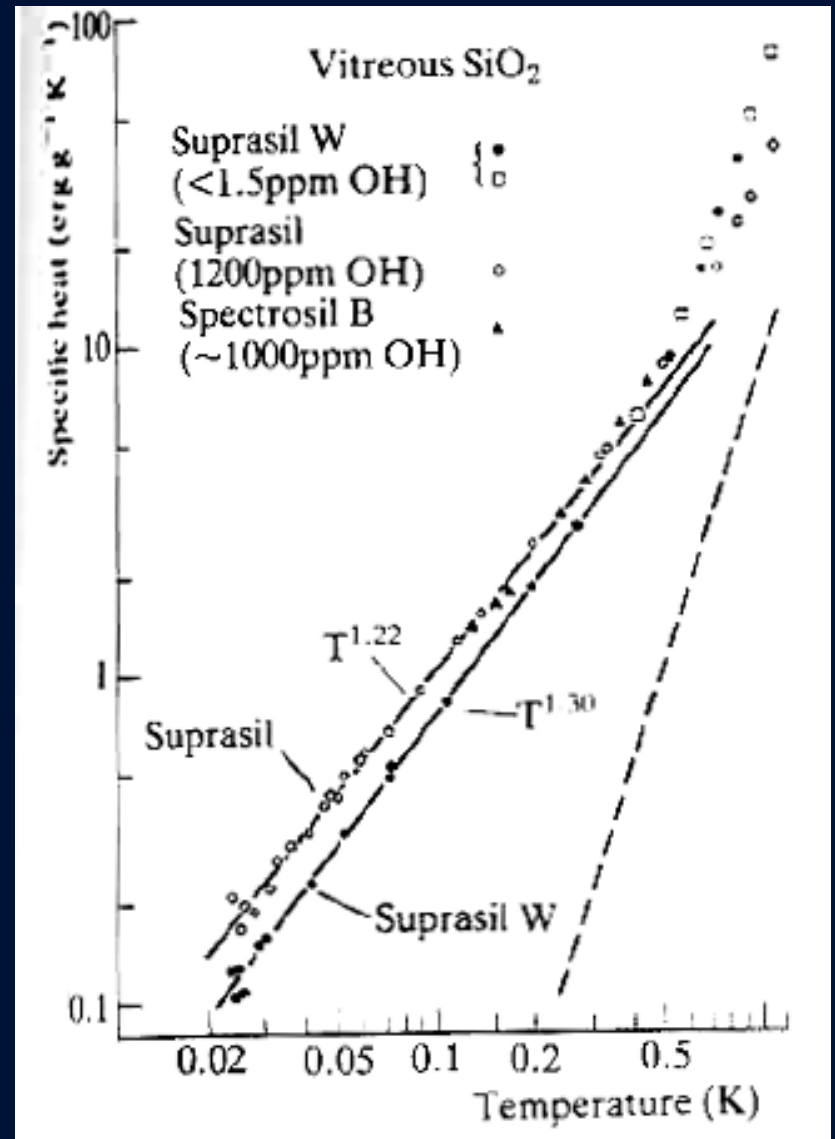
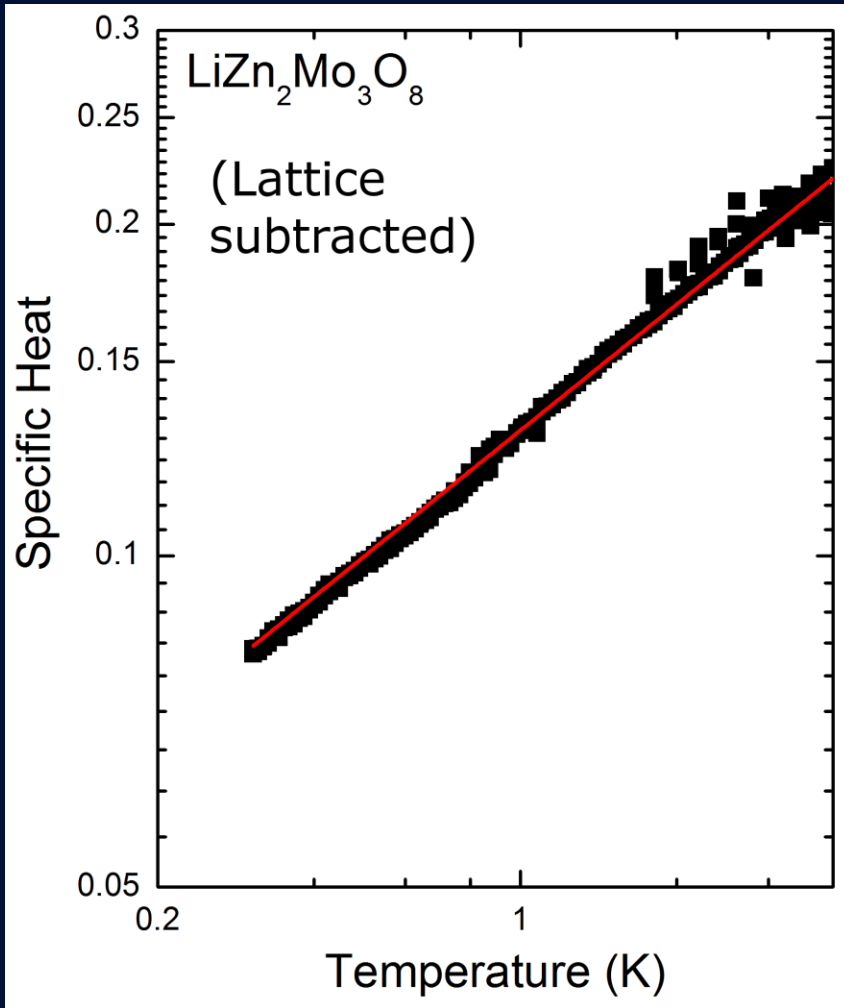


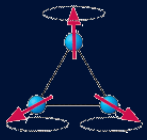
LiZn₂Mo₃O₈ Specific Heat



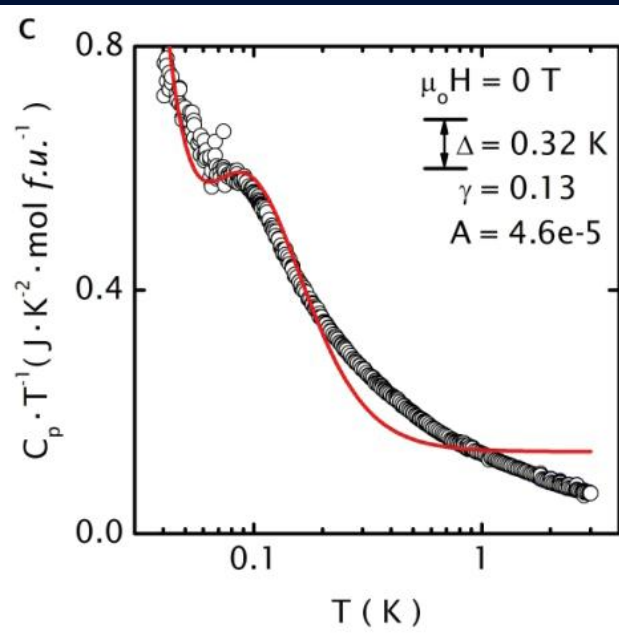
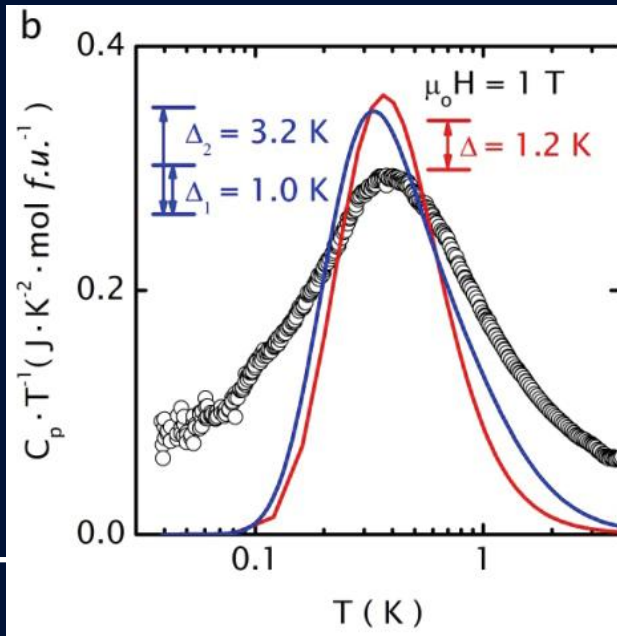
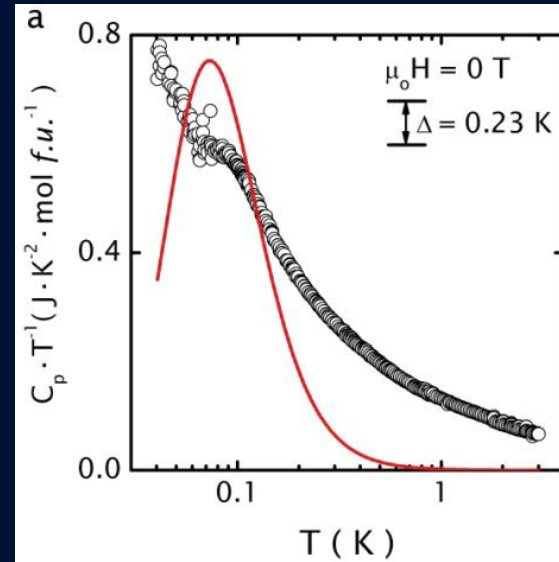
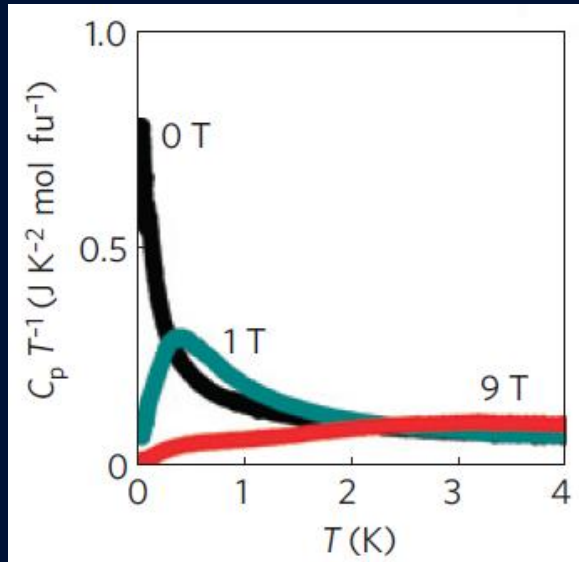


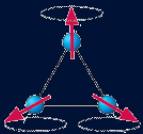
LiZn₂Mo₃O₈ Specific Heat Continued



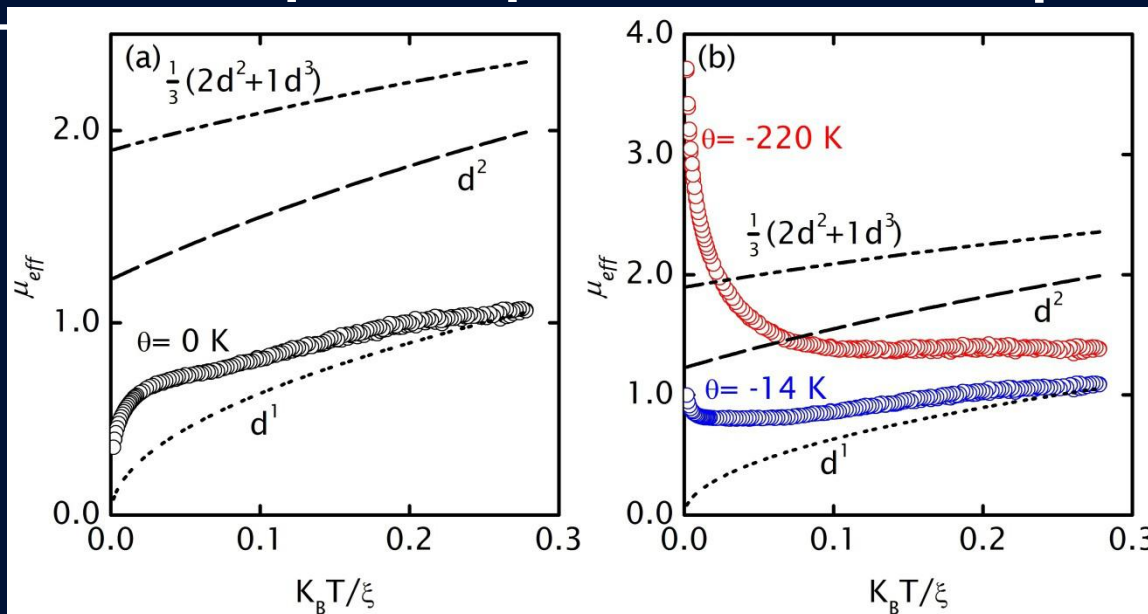


LiZn₂Mo₃O₈ Specific Heat Continued





Not 'simple' spin-orbit coupling



$$g_m = g_e \left(1 - A \frac{\xi}{\Delta E}\right)$$

Mo-d

$$\xi = 0.068 \text{ eV}$$

$$\Delta E \approx 1.5 \text{ eV}$$

$$g_m \approx 1.6-1.9$$

$$g_{\text{obs}} = 1.9$$

Cu-d

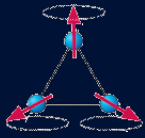
$$\xi = 0.100 \text{ eV}$$

$$\Delta E \approx 2.4 \text{ eV}$$

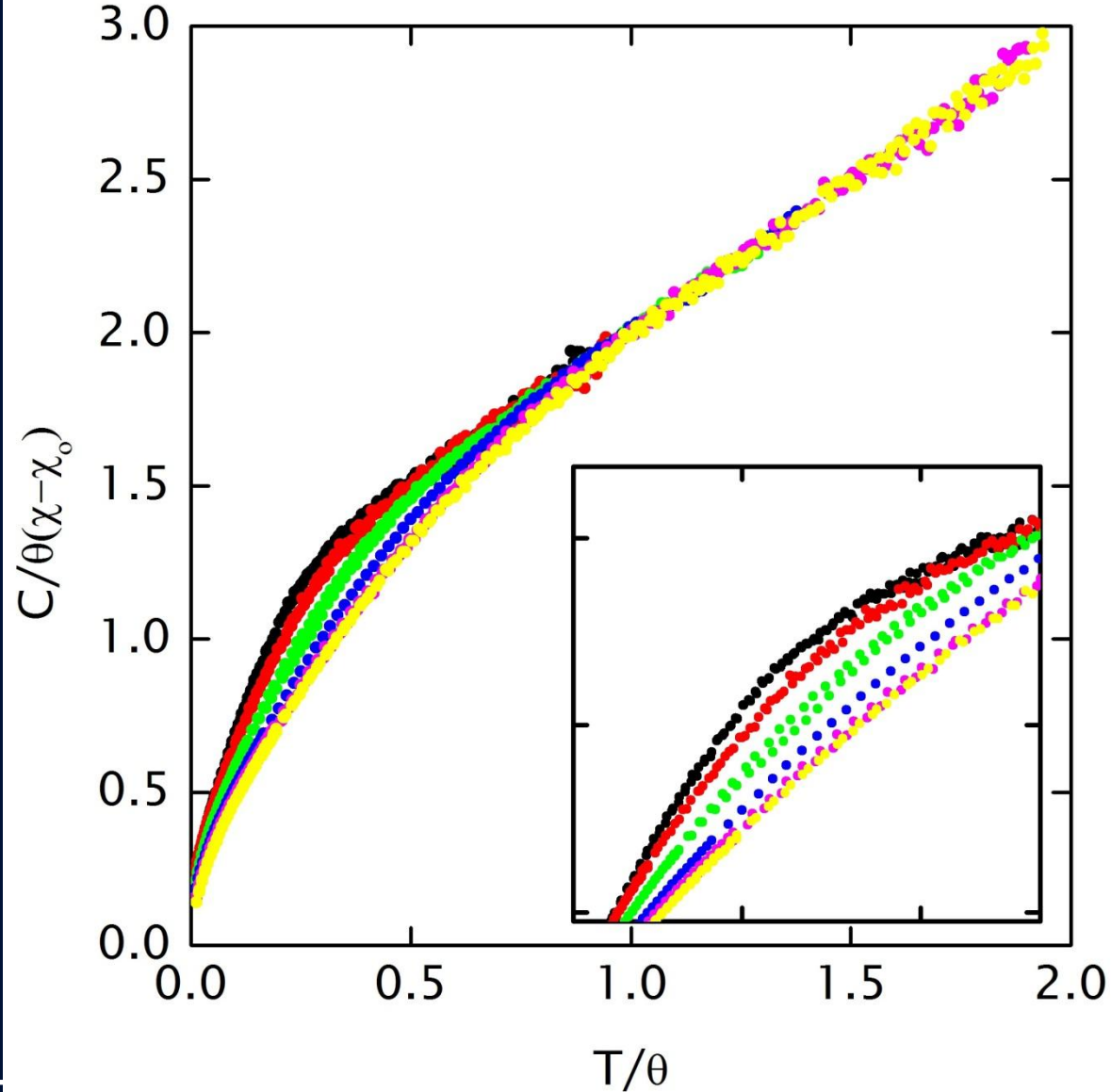
$$g_m \approx 2.1-2.4$$

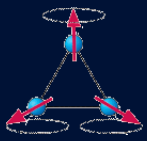
$$g_{\text{obs}} = 2.2$$



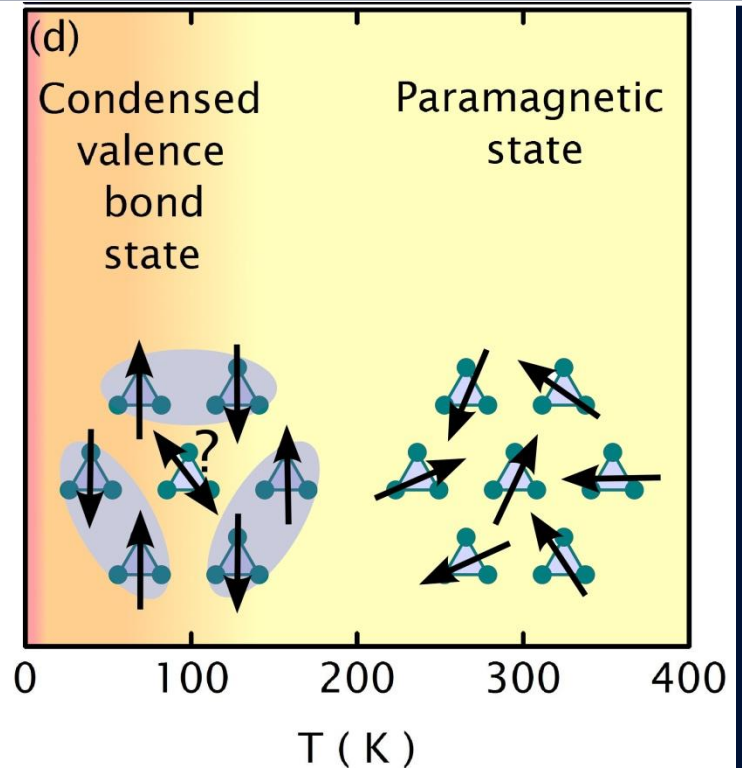
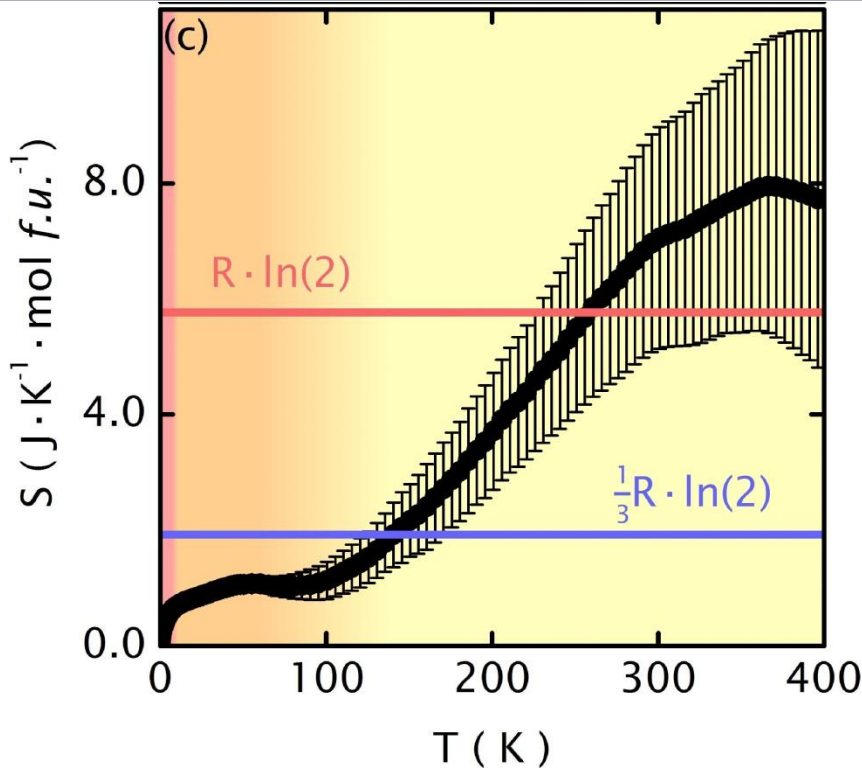


Not single ion physics



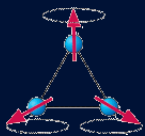


Geometric Frustration in $\text{LiZn}_2\text{Mo}_3\text{O}_8$

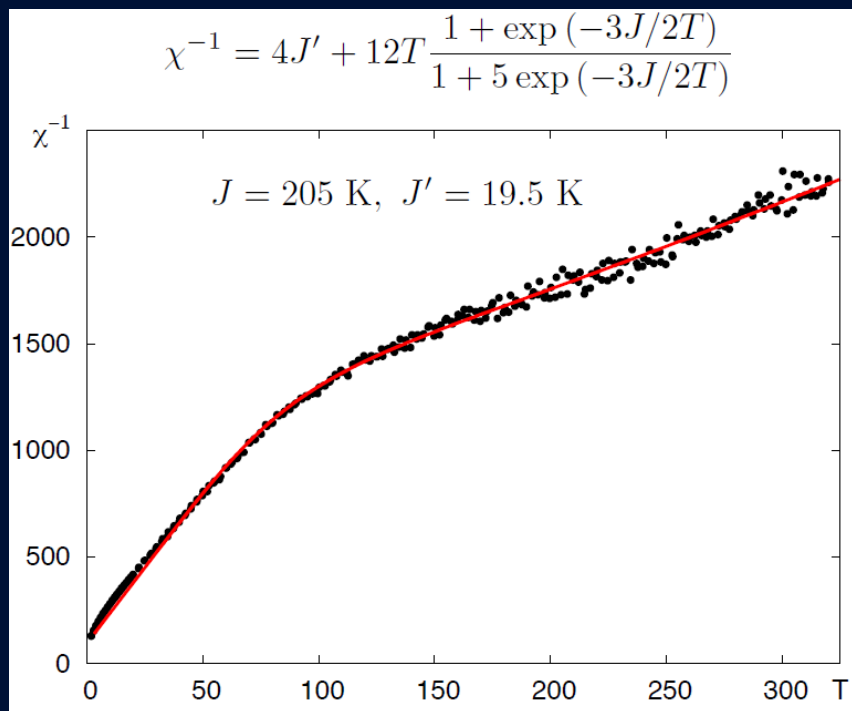


- Loss of $\sim 2/3$ of spin susceptibility at $T = 96$ K
- No observed structural transition down to $T = 7$ K
- No observed magnetic order greater than $0.2(2) \mu_B/\text{Mo}$
- Calculations and data support $S = 1/2$ model with SOC as a perturbation (a la Cu)
- Electrically insulating, likely a Mott insulator, $U \sim 1.5$ eV
- Dynamic or static singlets?

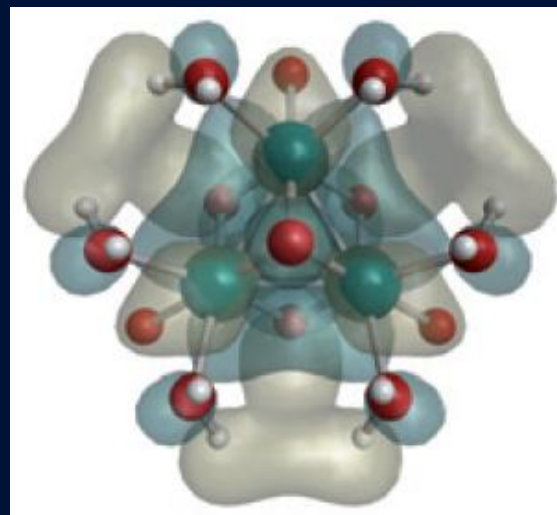




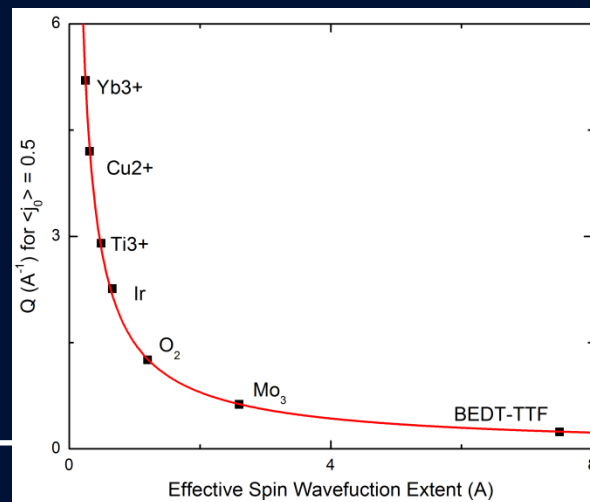
Theories?



- “Triangles of triangles” model
- O. Tchernyshyov & Y. Wan (private communication)

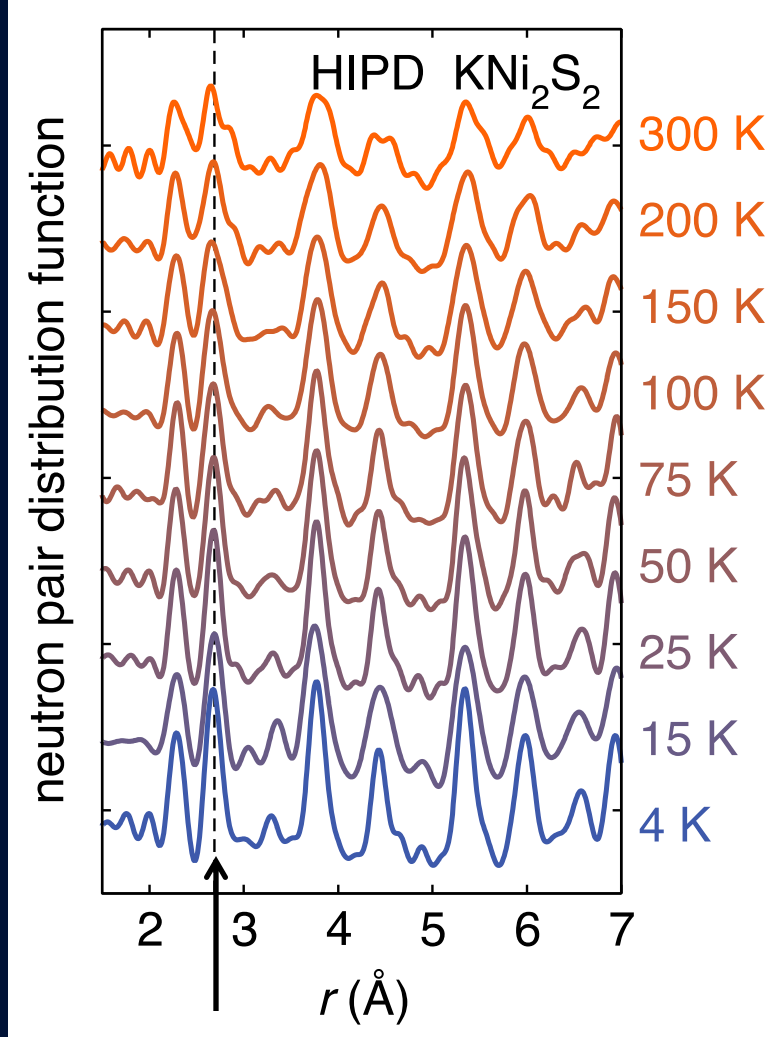
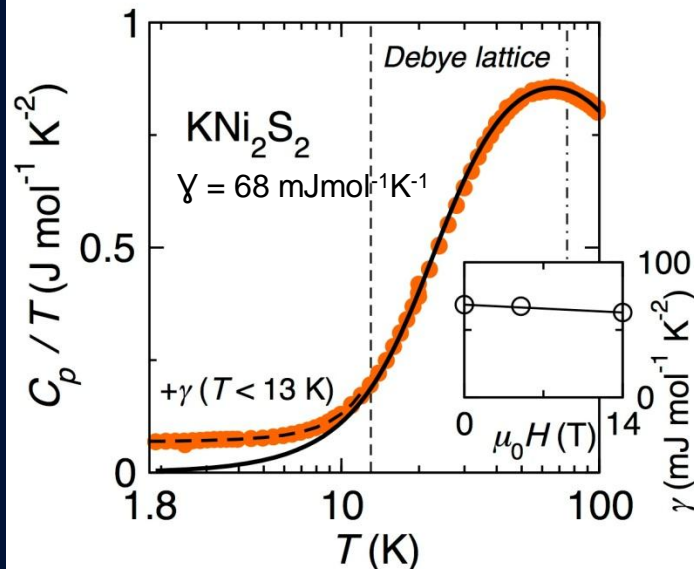
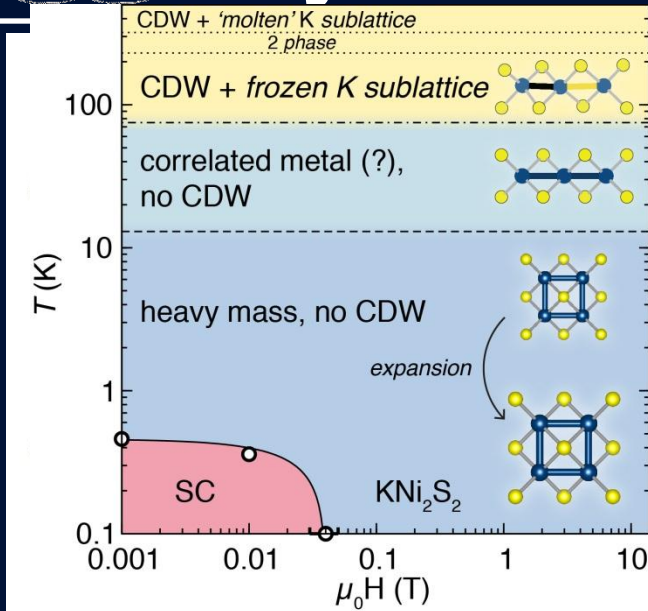


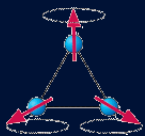
- Isotropic exchange from a_1 totally symmetric HOMO



Only a small part of my group...

Charge driven Heavy fermion behavior?



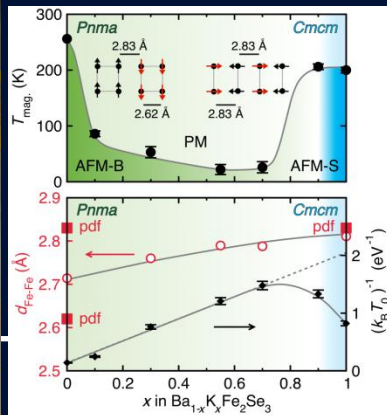
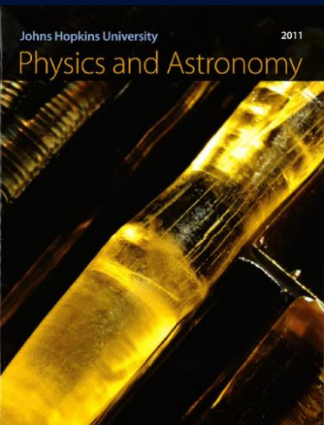


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- Dr. Minyea Lee (CSU)
- Dr. Takashi Imai (McMaster)
- JHU Collaborators
- All collaborators on other projects



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Office of Science, Basic Energy Sciences
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ANL/APS: Beamline 11-BM



NPDF upgrade
Dilution Refrigerator

Johns Hopkins University
Start-up funds to Prof. T. M. McQueen
<http://occamy.chemistry.jhu.edu/>

