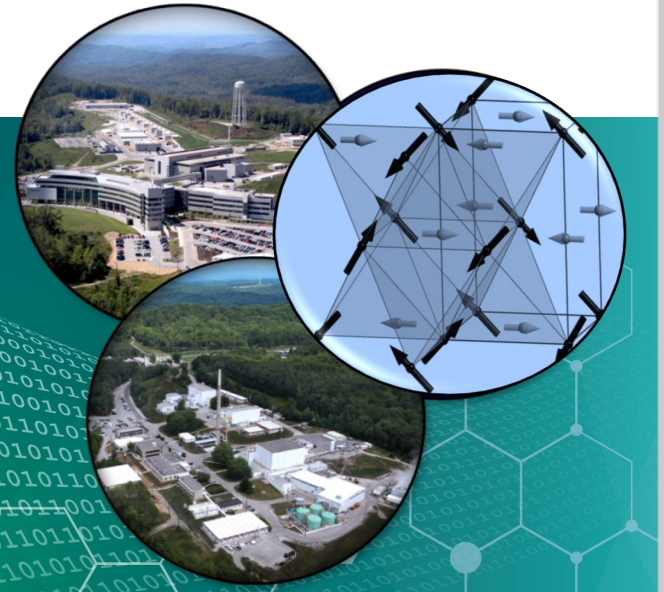
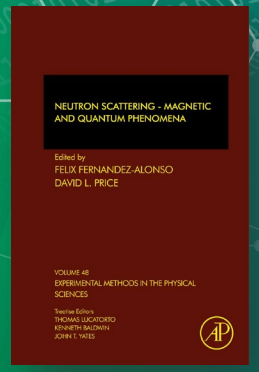
OAK RIDGE National Laboratory

Magnetic Structures in Condensed Matter : A Hierarchy based on Lattice Dimensionality

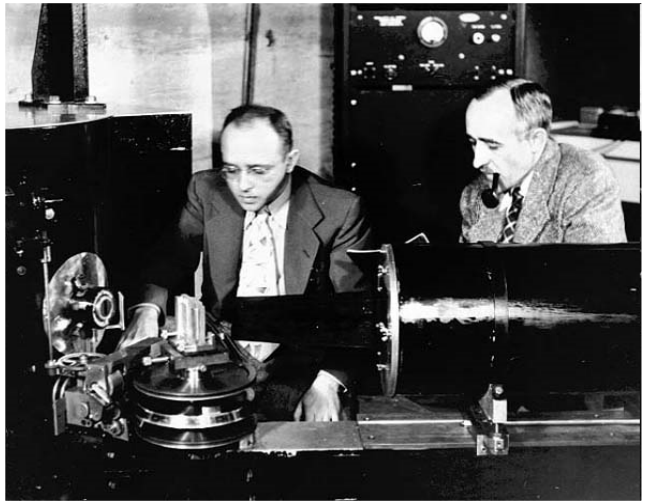


Ovidiu Garlea
Neutron Scattering Division,
Oak Ridge National Laboratory



"Magnetic Structures" chapter in
Experimental Methods in the Physical Sciences
vol. 48, p. 203-290 *Academic Press, 2016*

The beginnings of Magnetic Structure Analysis

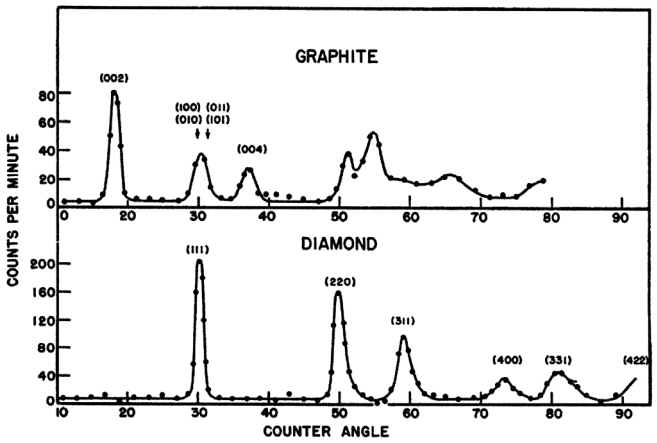


1948: First demonstration of the neutron diffraction

REVIEW VOLUME 73, NUMBER 8

The Diffraction of Neutrons by Crystalline Powders

E. O. WOLLAN AND C. G. SHULL
Oak Ridge National Laboratory, Oak Ridge, Tennessee
(Received January 5, 1948)

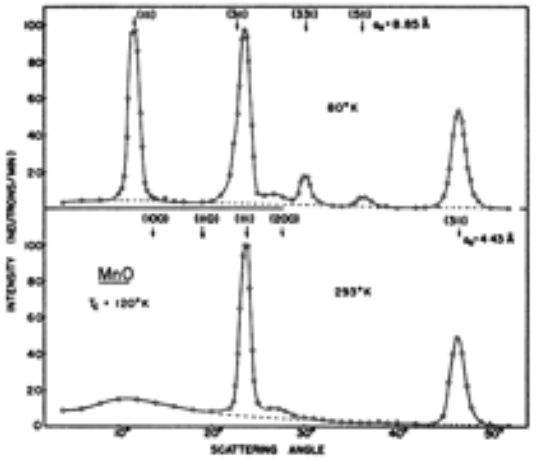


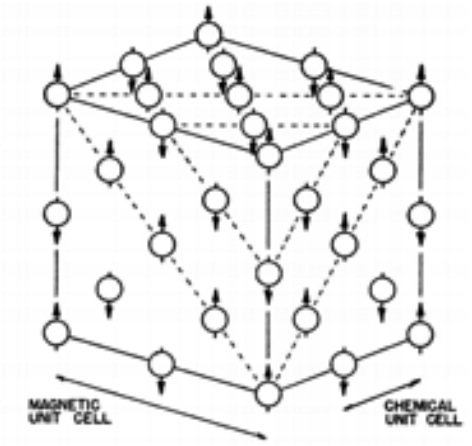
1949: the first direct evidence of Antiferromagnetism (in MnO)

Detection of Antiferromagnetism by Neutron Diffraction*

C. G. SHULL
Oak Ridge National Laboratory, Oak Ridge, Tennessee
AND
J. SAMUEL SMART
Naval Ordnance Laboratory, White Oak, Silver Spring, Maryland
August 29, 1949

AFM: Louis Néel – 1930





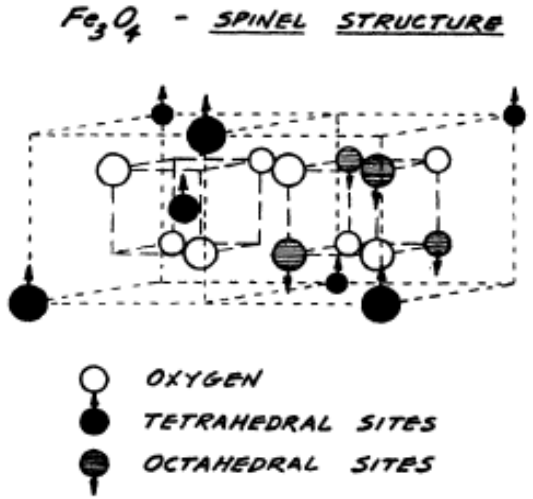
The beginnings of Magnetic Structure Analysis

1951: the Néel model of ferrimagnetism was confirmed

Magnetic Structure of Magnetite and Its Use in Studying the Neutron Magnetic Interaction

C. G. SHULL, E. O. WOLLAN, AND W. A. STRAUSER
Oak Ridge National Laboratory, Oak Ridge, Tennessee
December 8, 1950

Phys. Rev. 81, 483 (1951)



1953: Review articles on magnetic structures began appearing

REVIEWS OF MODERN PHYSICS VOLUME 25, NUMBER 1 JANUARY, 1953

Neutron Diffraction Studies of Various Transition Elements

C. G. SHULL AND M. K. WILKINSON
Oak Ridge National Laboratory, Oak Ridge, Tennessee

Fe_3O_4, MnO, FeO, CoO, NiO, Cr, a-Mn, Ni, Fe (powder and single crystal data & unpolarized and polarized neutrons)

LE JOURNAL DE PHYSIQUE ET LE RADIUM TOME 20, FÉVRIER 1959, PAGE 169

RECENT MAGNETIC STRUCTURE STUDIES BY NEUTRON DIFFRACTION (1)

By C. G. SHULL,
Massachusetts Institute of Technology, Cambridge, Massachusetts, U. S. A.

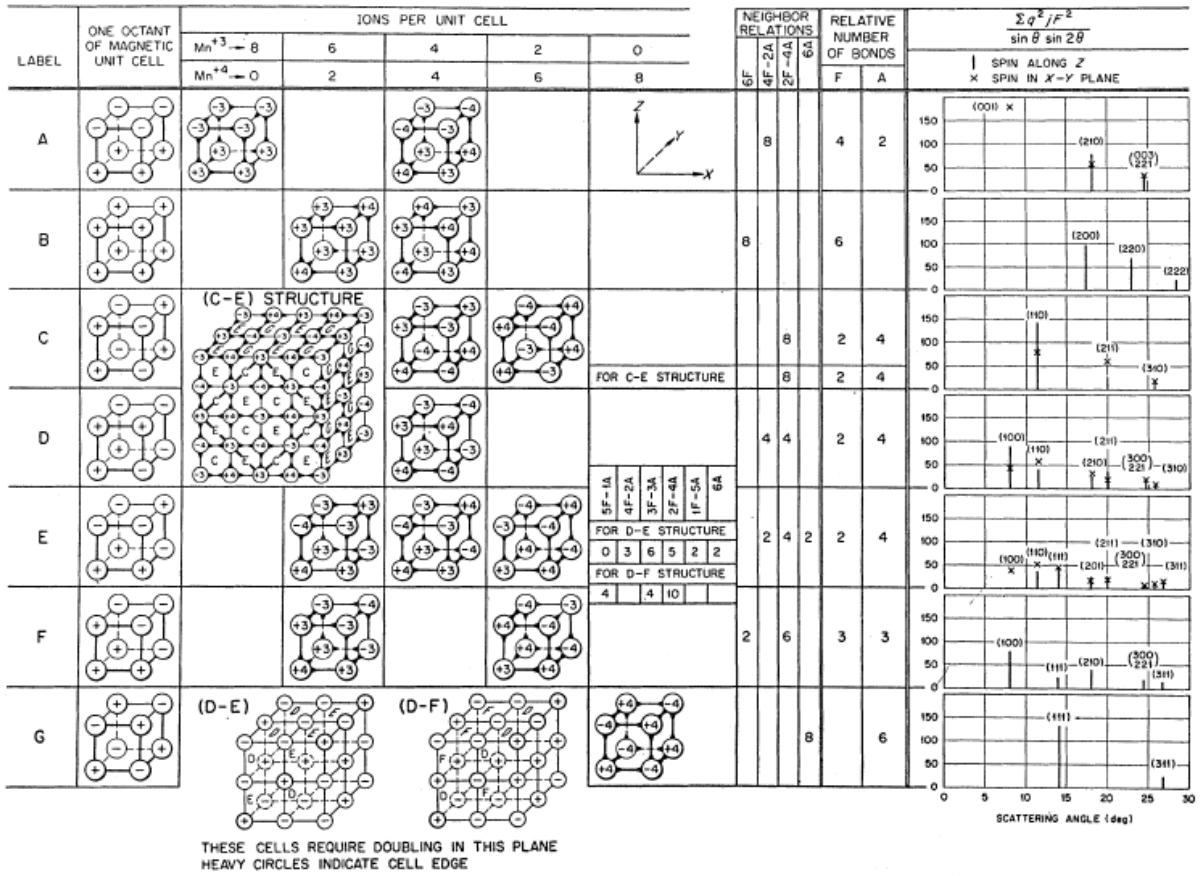
The beginnings of Magnetic Structure Analysis

1955: Scheme of magnetic structures of the perovskite cited over 1900 times

PHYSICAL REVIEW VOLUME 100, NUMBER 2 OCTOBER 15, 1955

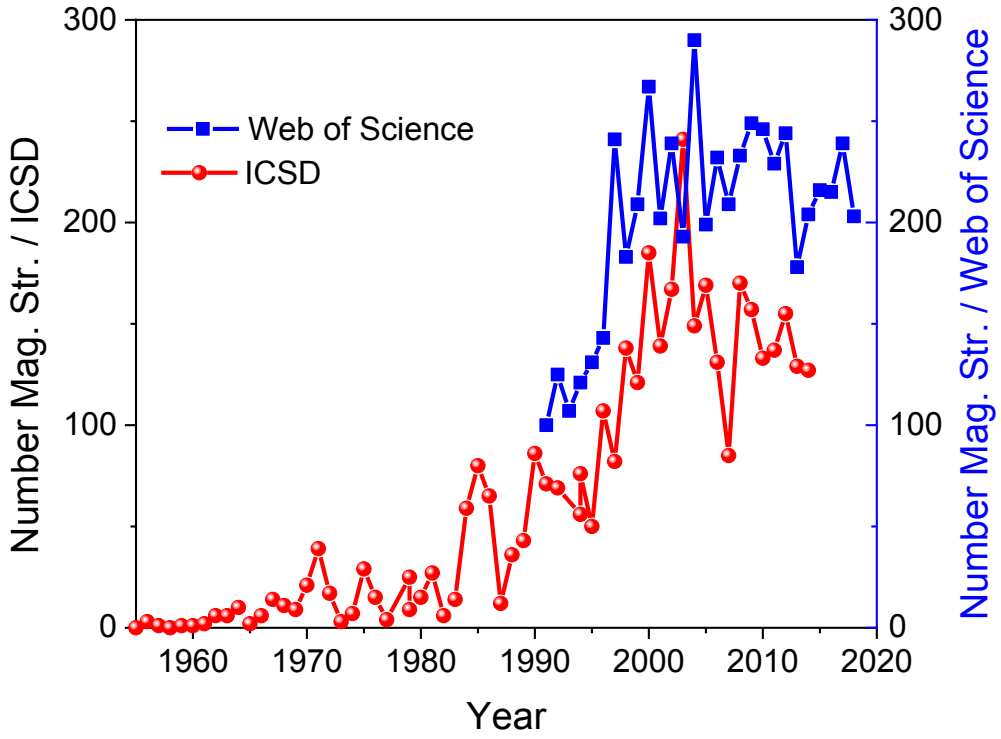
Neutron Diffraction Study of the Magnetic Properties of the Series of Perovskite-Type Compounds $[(1-x)\mathrm{La}, x\mathrm{Ca}]\mathrm{MnO}_3$†

E. O. Wollan and W. C. Koehler
Oak Ridge National Laboratory, Oak Ridge, Tennessee



Evolution in time of the number of magnetic structure entries

marked increases in ~ 80s & 90s likely associated with introduction of computational tools and the discovery of high-Tc superconductors and colossal magnetoresistance (CMR)

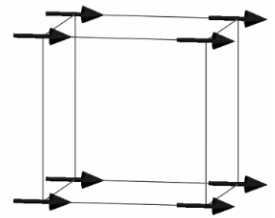


Journals where magnetic structures are reported:

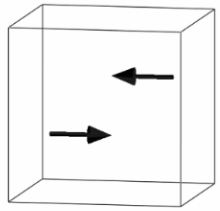
The discovery of novel magnetic structures is unceasing, driven by their relationships to ferroelectricity, thermo-electricity, superconductivity, improved permanent magnets, and spintronic technologies

Classifications of magnetic structures

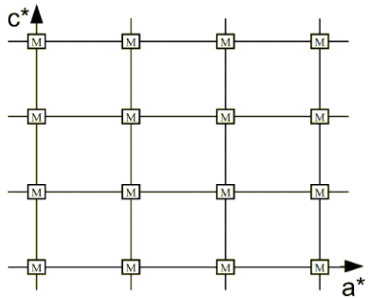
k-vector criteria



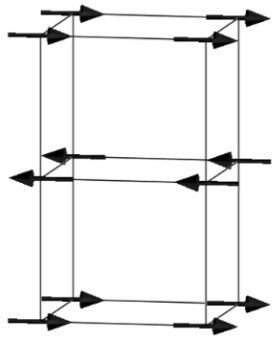
ferromagnet



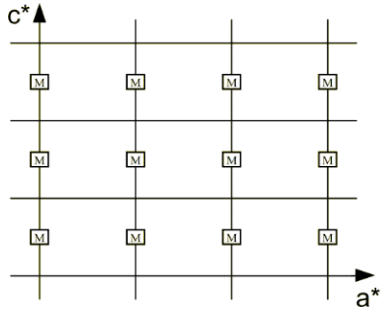
k=0
antiferromagnet



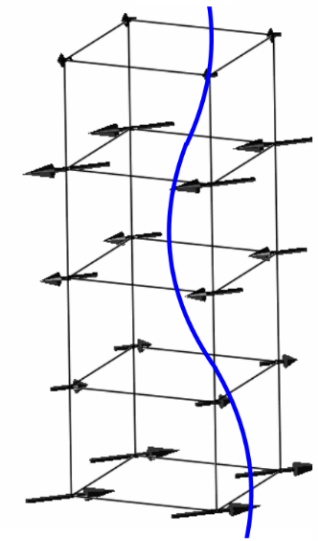
reciprocal space
k=0 magnetic peaks



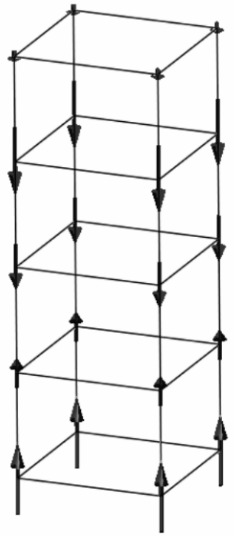
k=(0,0,1/2)
antiferromagnet



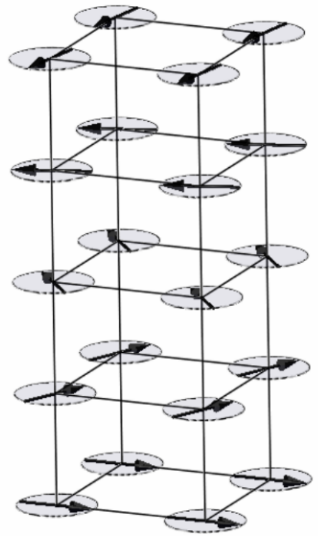
reciprocal space
k=(0,0,1/2)



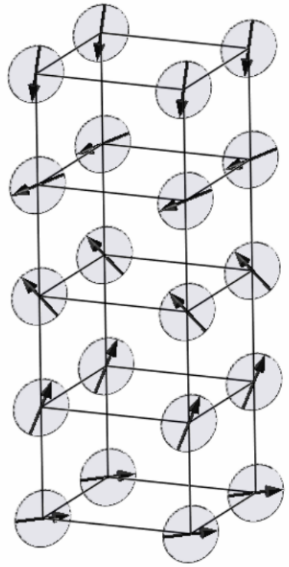
transverse
spin density wave



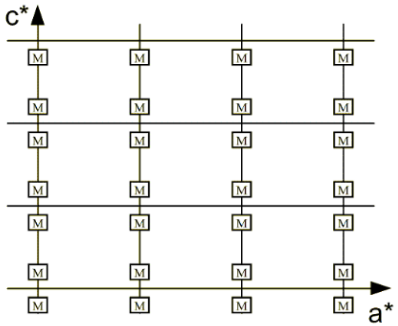
longitudinal
spin density wave



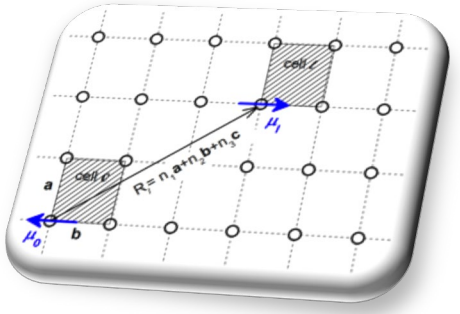
circular helix



circular cycloid



reciprocal space
±k=(0,0,±ξ)



$$\boldsymbol{\mu}_{lj} = \sum_{k} \mathbf{S}_{\mathbf{k}j} e^{i\mathbf{k}\cdot\mathbf{R}_l}$$

Classifications of magnetic structures

"spin-reversal" 1′ operator (aka anti-symmetry or time-inversion) criteria

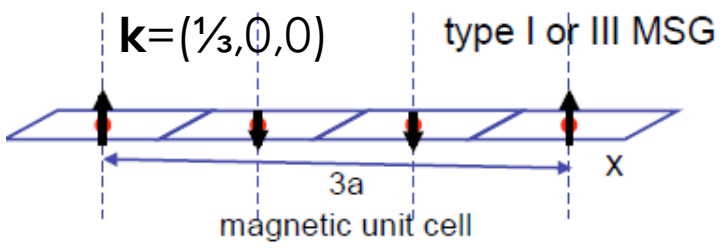
Four types of magnetic space groups (total of 1651):

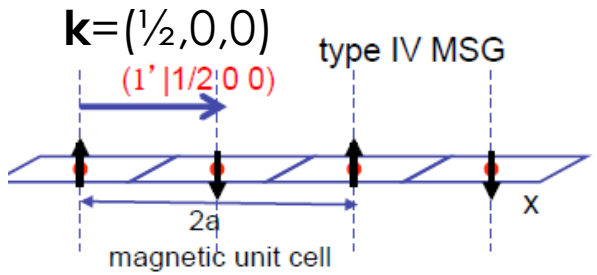
Type I: M = G , made by point groups identical to the 32 crystallographic point groups, not involving the 1' operation. These are termed "single-color" or "**colorless**" (230 groups)

Type II: M = G + G ' , consist of the 32 groups containing symmetry elements in both pure and prime forms. These are named "**grey**" groups, or "**paramagnetic**" groups (230 groups)

Type III : M= D+ (G-D)1', *D = translationgleiche*, involves unprimed elements of the subgroup **D** of index 2 of **G**, and the remaining operators **G** that are being primed. These are called "**black-white**" (674 groups)

Type IV : M= D+ (G-D)1', same as Type III but *D = klassengleiche*, take account of the loss of translations ("anti-translations") (517 groups). Correspond to those defined by the propagation vector **k** = τ/n, n=even → do not allow ferromagnetism





Classifications of magnetic structures

The lack of uniform description has made it impossible to organize the existing magnetic structures into a database.

A *Commission on Magnetic Structures of the International Union of Crystallography* was established in 2011. The commission's mandate covers the following:

- establish standards for the description and dissemination of magnetic structures; (magCIF dictionary proposed by H. Stokes and B. Campbell was formaly approved in Oct 2016; J. M. Perez-Mato and colleagues have started an online database of magnetic structures based on this new magnetic mCIF standard at the Bilbao Crystallographic Server)
- cooperate with other IUCr Commissions in establishing and maintaining standards of common interest, such as magnetic symmetry-group tables, magnetic nomenclature and magnetic form factor data
- Encourage communication and cultivate consensus among research communities that have independently developed diverse approaches to describing magnetic structures.
- Promote the sponsorship and organization of magnetic-structure sessions, symposia, and schools

Current members: B. Campbell (Chair, USA) , M. Avdeev (Australia), M.T. Fernandez-Diaz (France), O. Garlea (USA), M. Henriques (Czech Republic), J.M. Perez-Mato (Spain), J. Rodriguez-Carvajal (France), T. Sato (Japan), A. Wills (UK), O. Zaharko (Switzerland)

A Hierarchy of Magnetic Structures based on Lattice Dimensionality

A magnetic state in a solid is the net result of the competing influences, thermal energy tending to randomize moments versus some quantum mechanical coupling tending to order moments

Spin-Hamiltonian:

isotropic or anisotropic exchange interactions

$$\mathcal{H}_{ex} = -\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j \qquad \mathcal{H}_{an-ex} = -\sum_{ij} J_{ij}^{xy}(\mathbf{S}_{ix} \cdot \mathbf{S}_{jx} + \mathbf{S}_{iy} \cdot \mathbf{S}_{jy}) + J_{ij}^{z}(\mathbf{S}_{iz} \cdot \mathbf{S}_{jz})$$

antisymmetric Dzyaloshinskii-Moriya $\mathcal{H}_{DM} = -\sum_{ij} D_{ij}\mathbf{S}_i \times \mathbf{S}_j$

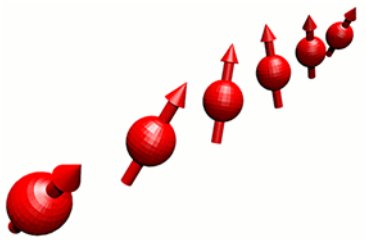
dipolar interactions $\mathcal{H}_{dip} = \sum_{ij} \frac{(g\mu_B)^2}{r_{ij}^3}[3(\mathbf{r}_{ij} \cdot \mathbf{S}_i)(\mathbf{r}_{ij} \cdot \mathbf{S}_j) - \mathbf{S}_i \cdot \mathbf{S}_j]$

single-ion anisotropy $\mathcal{H}_{ani} = -\frac{1}{2}\sum_i D\mathbf{S}_{iz}^2 + \frac{1}{2}\sum_i D'(\mathbf{S}_{ix}^2 - \mathbf{S}_{iy}^2)$

field coupling $\mathcal{H}_H = -\mathbf{H}\sum_i g_i\mu_B\mathbf{S}_i$

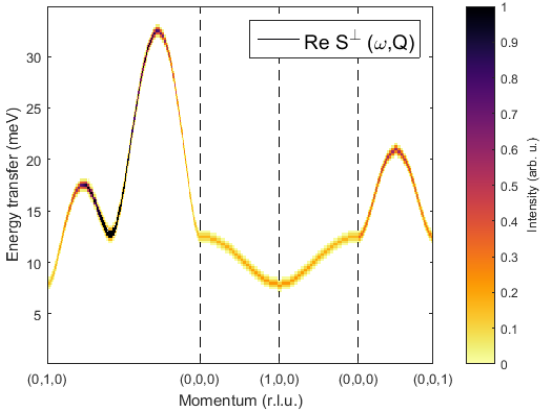
A Hierarchy of Magnetic Structures based on Lattice Dimensionality

- most of the magnetic ground states being realized primarily through the competition between *exchange interactions* ($\sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$)
- all magnetic structures are three-dimensional, but …
- the strength of J_{ij} along different crystal direction, reflected in the velocity of spin-waves propagating in the lattice, can be very different

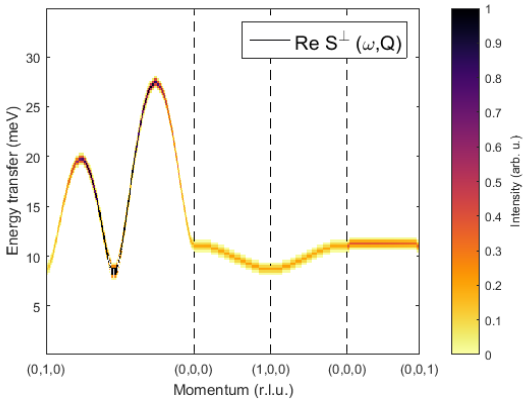


Example:

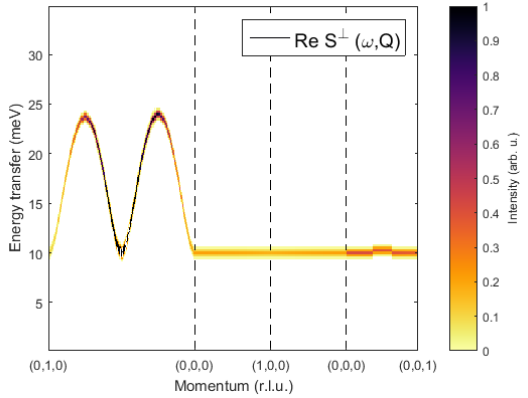
3D: $J_\perp = J_{//}/2$, $J_z = J_{//}/10$

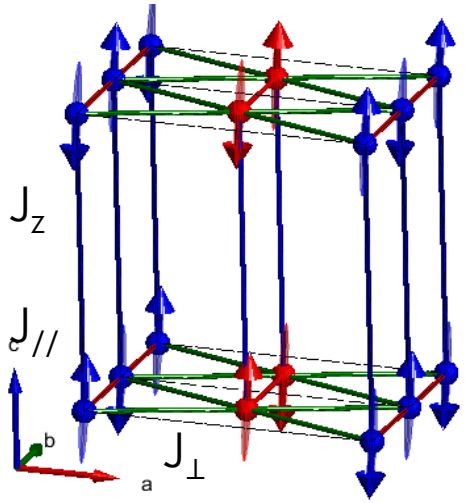


2D: $J_\perp = J_{//}/4$, $J_z = J_{//} \times 10^{-3}$



1D: $J_\perp = J_{//} \times 10^{-2}$, $J_z = J_{//} \times 10^{-3}$





A Hierarchy of Magnetic Structures based on Lattice Dimensionality

→ the effective dimensionality of the lattice plays an important role in the magnetic behavior and selection of magnetic structure

- 3D - networks

  perovskite, pyrochlore - corner-sharing tetrahedral, spinels with pyrochlore and diamond lattices, edge-sharing tetrahedra, …

- Layered structures

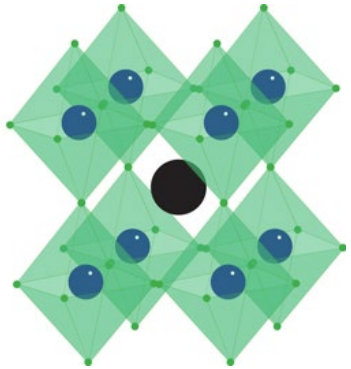
  square-planar, edge-sharing triangles, kagomé, honeycomb lattices, striped-kagomé …

- Quasi-one-dimensional lattices

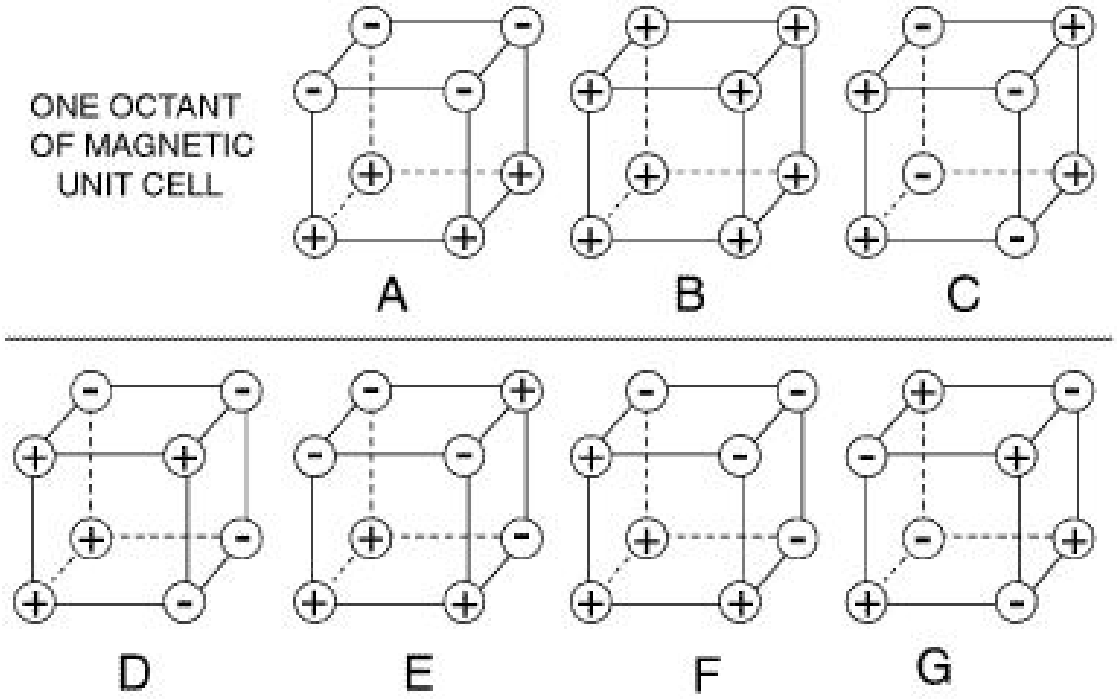
  simple-chain, ladders, sawtooth chains,…

3D - networks : Perovskites

ABO_3



Ordering scheme proposed by:
E. Wollan and W. Koehler, Phys. Rev., 100, 545 (1955)



A-type : antiferro- coupled ferromagnetic planes

B-type: ferromagnetic order (also called F)

C-type: ferromagnetic coupled antiferromagnetic planes

D-type: criss-crossed stripes

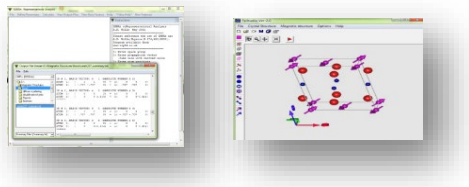
E and F-type: antiferromagnetism with ferrimagnetic planes

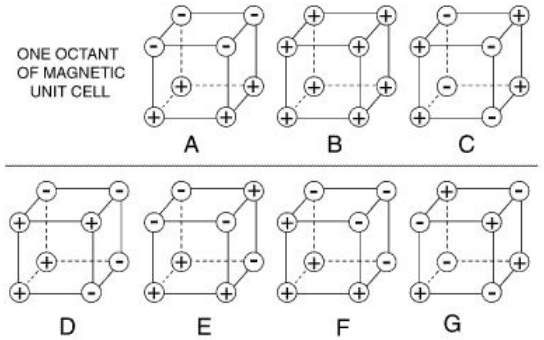
G-type: antiferromagnetically coupled spins in all directions

3D - networks : Perovskites

Symmetry: *Pnma*
k = (0,0,0), M in 4b: (0,0,1/2)

SARAh FPStudio

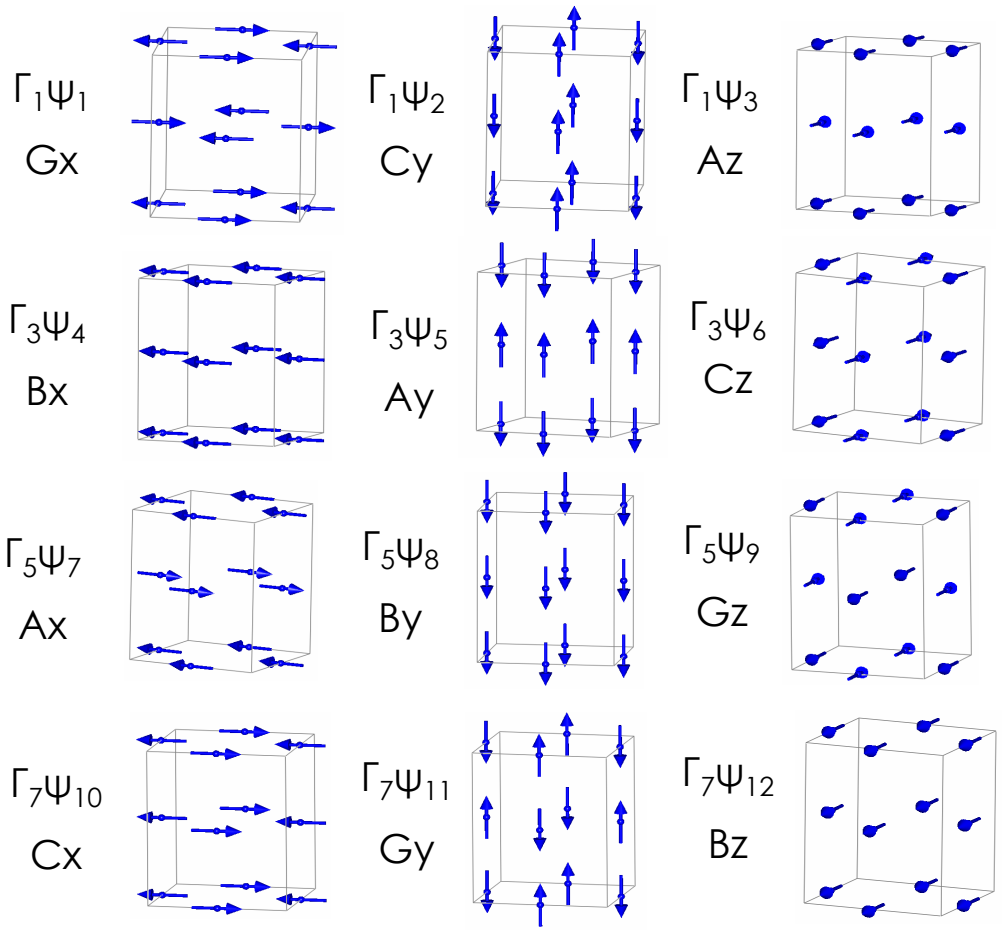




$$\Gamma_{Mag} = 3\Gamma_1^1 + 0\Gamma_2^1 + 3\Gamma_3^1 + 0\Gamma_4^1 + 3\Gamma_5^1 + 0\Gamma_6^1 + 3\Gamma_7^1 + 0\Gamma_8^1$$

in Kovalev notation

IR	BV	Point Group	Shubnikov Group
Γ_1	ψ_1	mmm	$Pnma$, #62.441
	ψ_2	mmm	$Pnma$, #62.441
	ψ_3	mmm	$Pnma$, #62.441
Γ_3	ψ_4	mmm	$Pnm'a'$, #62.447
	ψ_5	mmm	$Pnm'a'$, #62.447
	ψ_6	mmm	$Pnm'a'$, #62.447
Γ_5	ψ_7	mmm	$Pn'ma'$, #62.448
	ψ_8	mmm	$Pn'ma'$, #62.448
	ψ_9	mmm	$Pn'ma'$, #62.448
Γ_7	ψ_{10}	mmm	$Pn'm'a$, #62.446
	ψ_{11}	mmm	$Pn'm'a$, #62.446
	ψ_{12}	mmm	$Pn'm'a$, #62.446



3D - networks : Perovskites

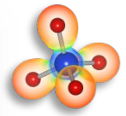
$LaMnO_3$ Moussa et al., *Phys. Rev. B* 54 15149 (1995)

$$\mathcal{H} = -\sum_{i,j} J_{ij}(S_i \cdot S_j) - D\sum_i S_i^{z2}$$

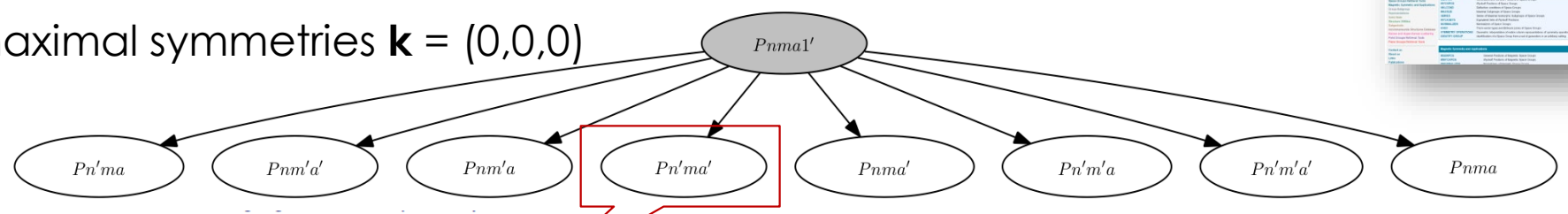
J ~ 9.6 K, J' ~ - 6.7 K, D = 1.92 K

BCS

VESTA



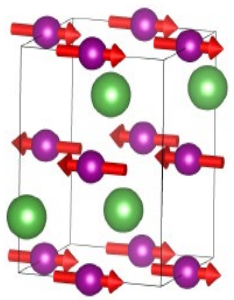
Possible maximal symmetries **k** = (0,0,0)



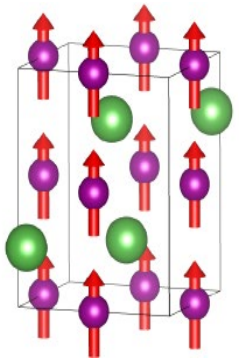
= Γ_5

Multiplicity	Wyckoff letter	Coordinates
8	d	(x,y,z | m_x,m_y,m_z) (x+1/2,-y+1/2,-z+1/2 | -m_x,m_y,m_z) (-x,y+1/2,-z | -m_x,m_y,-m_z) (-x+1/2,-y,z+1/2 | m_x,m_y,-m_z) (-x,-y,-z | m_x,m_y,m_z) (-x+1/2,y+1/2,z+1/2 | -m_x,m_y,m_z) (x,-y+1/2,z | -m_x,m_y,-m_z) (x+1/2,y,-z+1/2 | m_x,m_y,-m_z)
4	c	(x,1/4,z | 0,m_y,0) (x+1/2,1/4,-z+1/2 | 0,m_y,0) (-x,3/4,-z | 0,m_y,0) (-x+1/2,3/4,z+1/2 | 0,m_y,0)
4	b	(0,0,1/2 | m_x,m_y,m_z) (1/2,1/2,0 | -m_x,m_y,m_z) (0,1/2,1/2 | -m_x,m_y,-m_z) (1/2,0,0 | m_x,m_y,-m_z)
4	a	(0,0,0 | m_x,m_y,m_z) (1/2,1/2,1/2 | -m_x,m_y,m_z) (0,1/2,0 | -m_x,m_y,-m_z) (1/2,0,1/2 | m_x,m_y,-m_z)

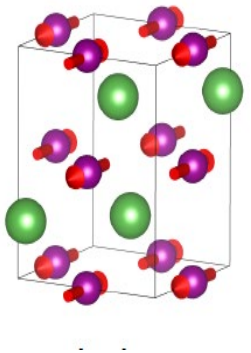
Ax



By



Gz



$LaMnO_3$

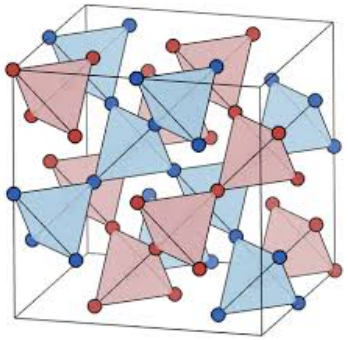
$m(Mn^{3+}) \approx 0\ 3.87\mu_B$

small ferromagnetic component possible due to D-M → AxBy

$YbAlO_3$, Yb ≡ S_{eff} = 1/2 quantum chain material *{Podlesnyak et al. Nature Comm. 10, 698 (2019)}*

3D - networks : Pyrochlore: Corner-sharing tetrahedral lattices

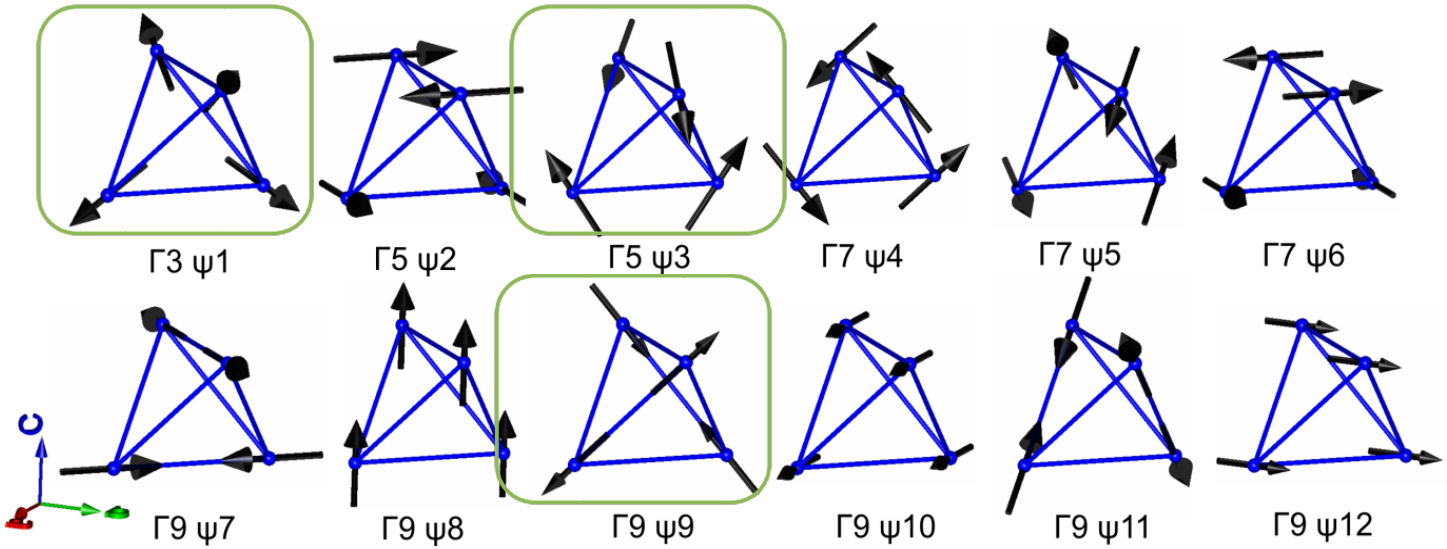
$A^{3+}_2B^{4+}_2O_7$

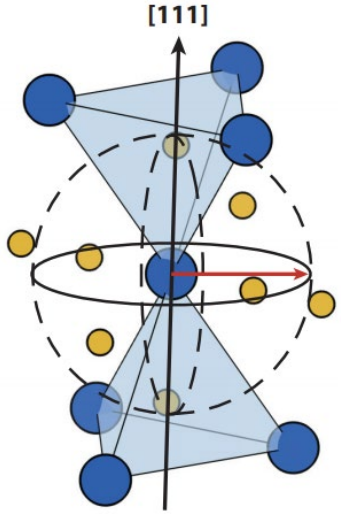


- two interpenetrating lattices (A, B) of corner-sharing tetrahedra (*Fd*$\bar{3}$*m*, sites 16c and 16d)
- strong geometrically frustrated NN AFM interactions → single-ion anisotropy, dipolar interactions, antisymmetric D-M are relevant

Fd$\bar{3}$*m*, **k** = (0, 0, 0)

$$\Gamma_{mag}(A) = 1\,\Gamma_3^{(1)} + 2\,\Gamma_5^{(1)} + 3\,\Gamma_7^{(1)} + 3\,\Gamma_9^{(2)}$$

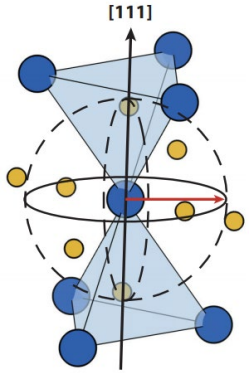




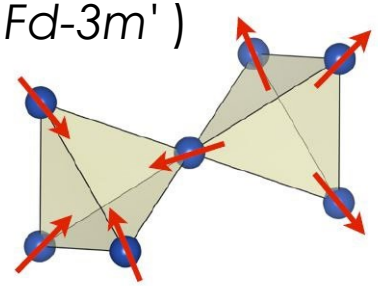
3D - networks : Pyrochlore lattices

	Anisotropy	Free moment	θ_{CW}	T_N, T_C, or T_f	Ground State
$Sm_2Ti_2O_7$ [35]	Ising	1.5 μ_B	−0.3 K	0.3 K	All-in/All-out
$Gd_2Ti_2O_7$ [53]	Heisenberg	7.9 μ_B	−9 K	1 K	Partial order
$Tb_2Ti_2O_7$ [54]	Ising	9.7 μ_B	−19 K	–	Spin liquid?
$Dy_2Ti_2O_7$ [39]	Ising	10.6 μ_B	+0.5 K	∼1 K	Spin Ice
$Ho_2Ti_2O_7$ [38]	Ising	10.4 μ_B	+1.9 K	∼1 K	Spin Ice
$Er_2Ti_2O_7$ [46]	XY	9.5 μ_B	−22 K	1.2 K	XY AFM
$Yb_2Ti_2O_7$ [55]	XY	4.5 μ_B	+0.6 K	0.25 K	Canted FM

A. Hallas et al. Annu. Rev. Cond. Matter Phys. 9,105, 2018

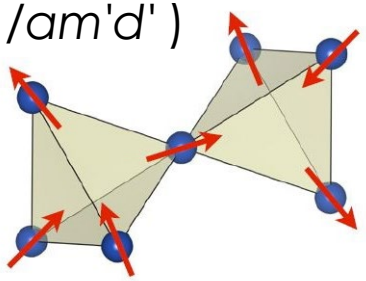


$\Gamma_3\psi_1$ (*Fd-3m'*)



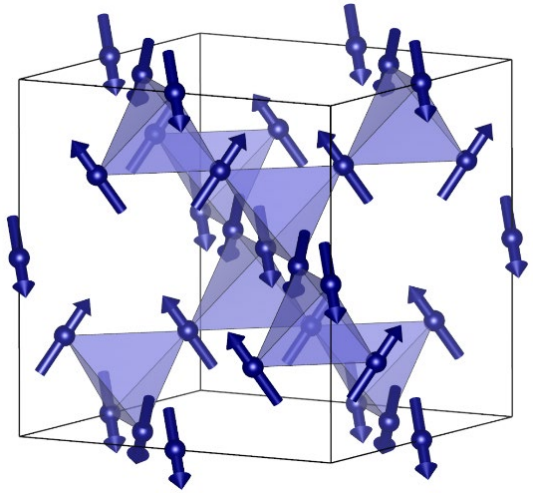
$Sm_2Ti_2O_7$: Ising all-in/all-out

$\Gamma_9\psi_9$ (*I4$_1$/am'd'*)



$Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$:
Ising two-in/two-out, spin ice

$\Gamma_5\psi_3$ (*I4$_1$'/am'd*)

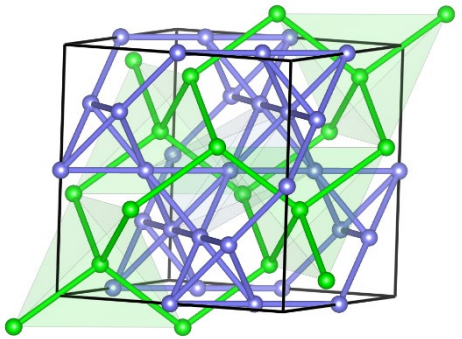


$Er_2Ti_2O_7$: AFM- XY pyrochlore

$Pr_2Hf_2O_7$ – Quantum Spin Ice (Sibille et al, Nat. Physics 14, 2018)
$NaCaNi_2F_7$ – S=1 Heisenberg model- spin liquid (Plumb et al, Nat. Physics 15, 2019)

3D - networks : Spinel

AB_2X_4 : corner-sharing tetrahedra (B) and diamond lattice (A)

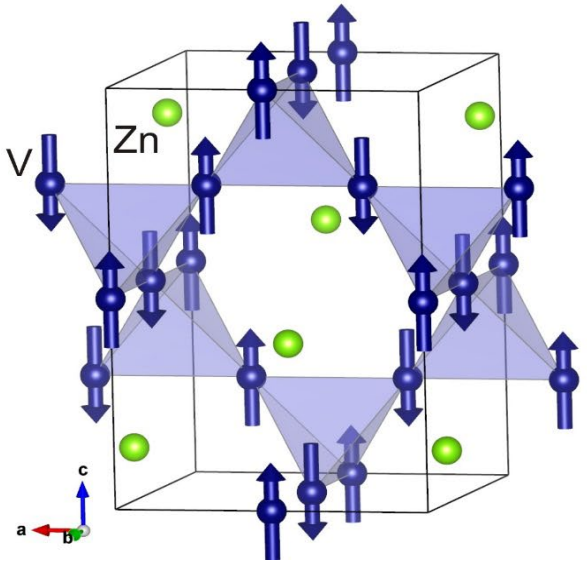


chemically versatile: transition metal Oxides, Sulfides and Selenides

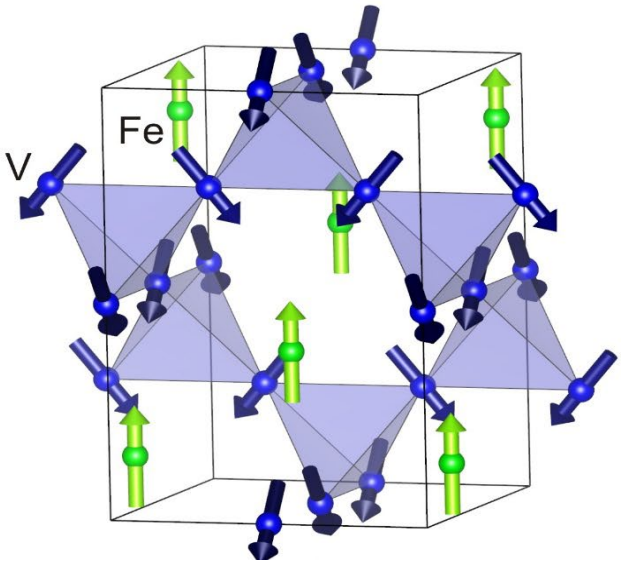
- ACr_2O_4 with non-magnetically A-site exhibit simultaneous lattice distortion and magnetic order due to the spin–lattice coupling

- AV_2O_4, with V^{3+} ($3d^2$) - model systems for studying orbital order in frustrated lattice. Sequence of phase transitions: structural distortion followed by a magnetic transition.

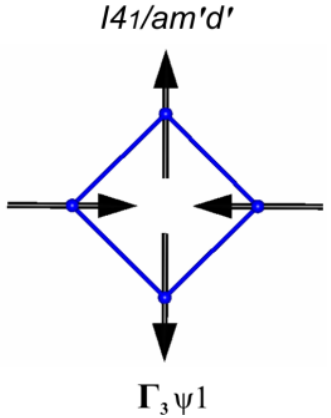
ZnV_2O_4 $Fd\bar{3}m \rightarrow I4_1/amd$ (T_S=50K)
k = (0, 0, 1), *AFM* (T_N=40K)



FeV_2O_4 (A = Fe^{2+} ($3d^6$) S=2)
$Fd\bar{3}m \rightarrow I4_1/amd \rightarrow Fddd \rightarrow I4_1/amd$.
collinear FerriM (T_{N1}= 110K) → canted FerriM (60K)



"two-in/two-out"



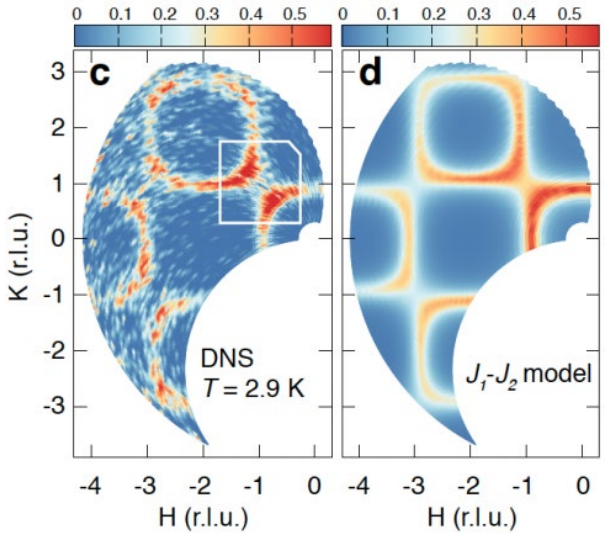
3D - networks : Diamond-lattice in Spinel systems

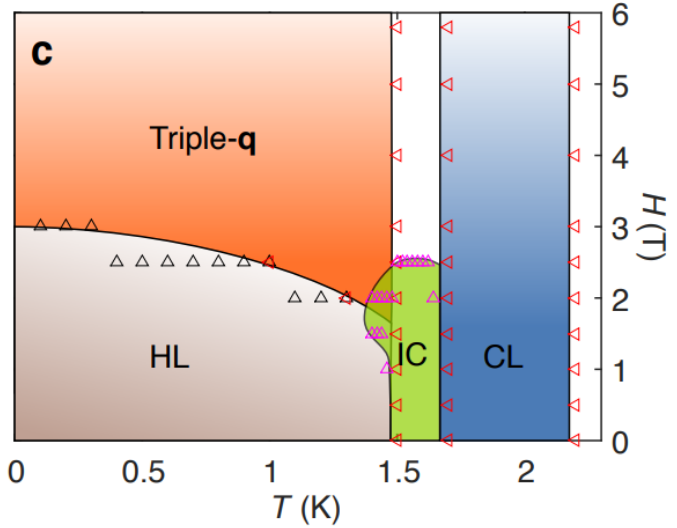
Only the A-site of the spinel lattice is occupied by magnetic atoms

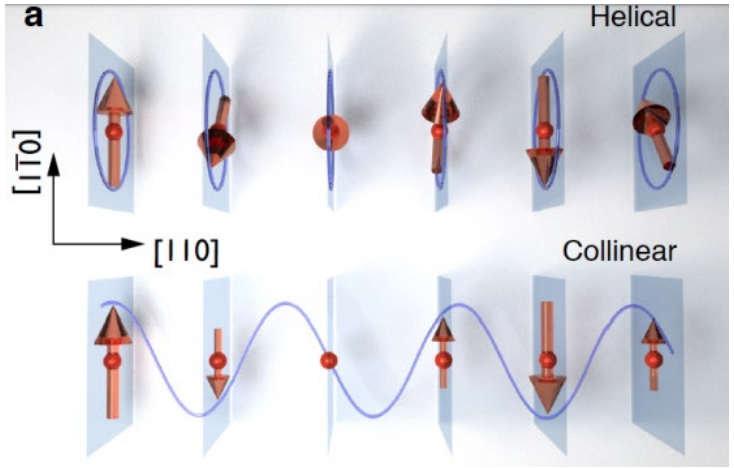
- two interpenetrating FCC sublattices : four NN (J_1) and twelve NNN (J_2) competing exchange interactions
- for $J_2/J_1 > 1/8$ → large ground-state degeneracy and the possibility of spin-liquid behavior. The degeneracy could be lifted by thermal or quantum effects to enable a magnetic ordering via the "order-by-disorder" mechanism ($CoAl_2O_4$, $MnSc_2S_4$, $FeSc_2S_4$ …)

$MnSc_2S_4$: Commensurate (C) → IC below T_{N2} = 1.9 K, **k** = (3/4 ± 0.02, 3/4 ± 0.02, 0)

Spiral spin-liquid state → helical long-range ordered state due to dipolar and J_3 perturbations



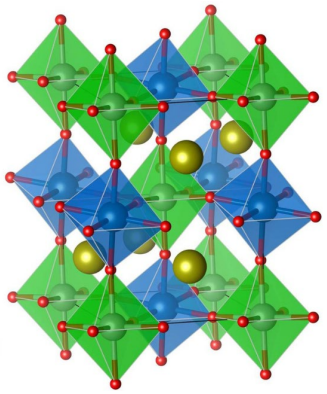




Gao *et al.* Nature Physics 13, 157 (2017)

3D - networks : Double Perovskites with edge-sharing tetrahedra

$A_2BB'O_6$

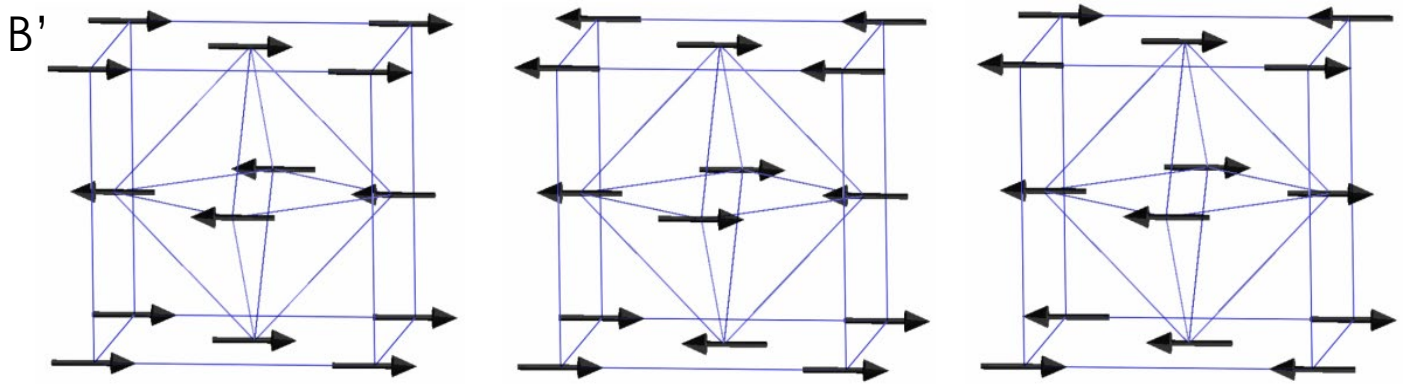


B' magnetic site = frustrated FCC lattice.
A = diamagnetic alkaline earth or lanthanide cation

spin-orbit coupling → monoclinic distortion (*I4/m* or $P2_1/n$, $\sqrt{a_p} \times \sqrt{a_p} \times 2\,a_p$)

C. Jones and P. D. Battle, J. Solid State Chem. 78, 108, 1989

- Type I: dominant (B'-O-O-B') NN interactions → AFM order between successive (001) ferro planes ; **k** = (0, 0, 1)
- Type II: dominant (B'-O-A-O-B') NNN exchange interactions → spins alternate along two directions
- Type III: comparable NN and NNN ; **k** = (½, ½, ½)



Sr_2LuRu0_6
Ba_2YRu0_6

Ca_2WMnO_6
Sr_2MoMnO_6

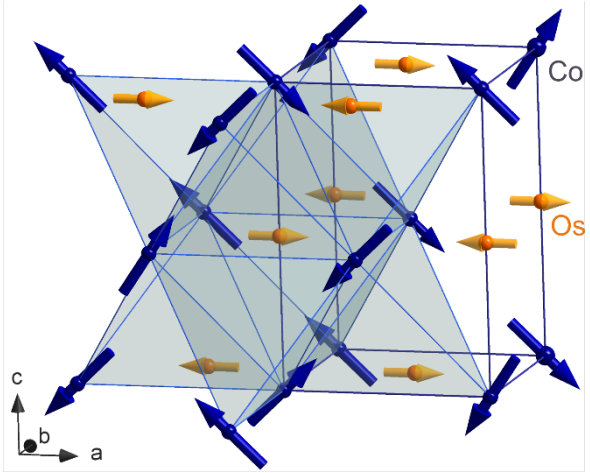
Ba_2LaRuO_6

3D - networks : Double Perovskites

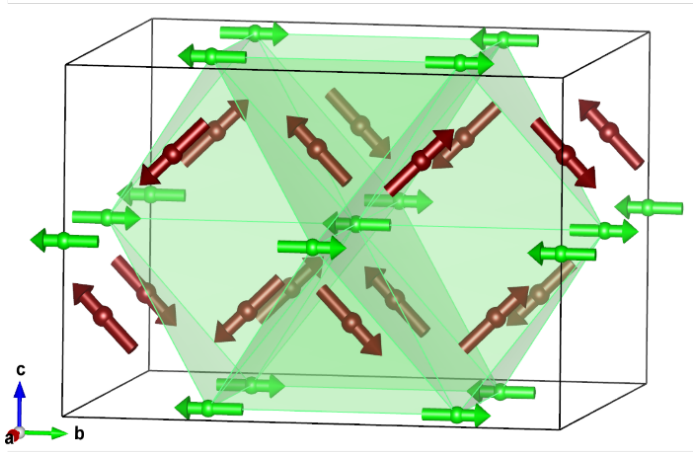
$A_2BB'O_6$ - when B, B' or A, B' are magnetic: the interplay between intra-lattice frustration and the inter-lattice interaction can lead to a wide variety magnetic states

FM metals (B–O–B'–O–B coupling mediated by itinerant electrons) :
Sr_2FeMoO_6 (T_C= 420 K), Sr_2CrReO_6 (T_C = 625 K)
Ferri insulators : Sr_2CrOsO_6 (T_C =725 K), Ca_2FeReO_6 (520 K), Sr_2MnReO_6, …
AFM insulators : Sr_2FeOsO_6, Sr_2CoOsO_6 , Nd_2NaOsO_6 , …

Sr_2CoOsO_6 , *I*4/*m* → *I*2/*m*
Os: T_{N1}= 108 K, $\mathbf{k}_1$ = (½, ½, 0)
Co: T_{N2}= 67 K, $\mathbf{k}_2$ = (½, 0, ½)

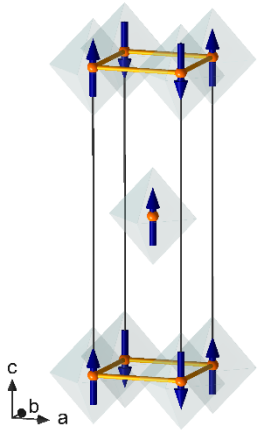


Nd_2NaOsO_6, $P2_1/n$
T_N = 16 K, $\mathbf{k}$= (½, ½, 0)



2D structures: Square-planar metal-oxygen/halogen

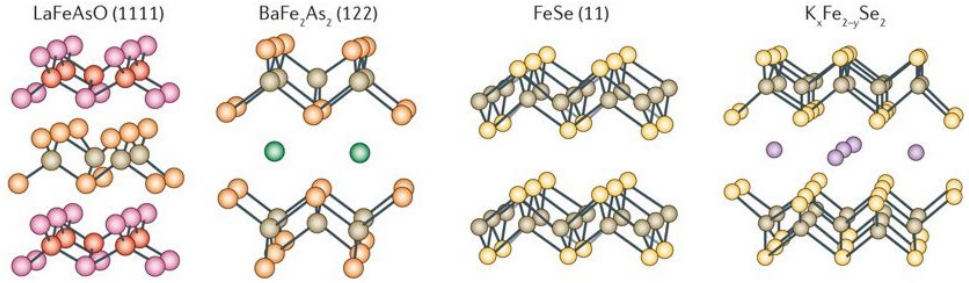
K_2NiF_4,



R. Plumier and E. Legrand, *J. Phys. Radium,* 24, 741 (1963)
R. J. Birgeneau, H. J. Guggenheim, and G. Shirane, *PRL* 22, 720 (1969)

Inter-layer exchange smaller than the intra-plane exchange by at least three orders of magnitude → 2D Heisenberg antiferromagnet. ("Bragg ridges" rather than Bragg peaks)

Layered perovskite - high-Tc Cuprates
Fe - pnictides: ZrCuSiAs–type (1111)
or $ThCr_2Si_2$-type (122), Fe(Se,Te) (11)



structure distorts at T_N

D. J. Singh, *Sci. Technol. Adv. Mater.,* 13, 054304 (2012)

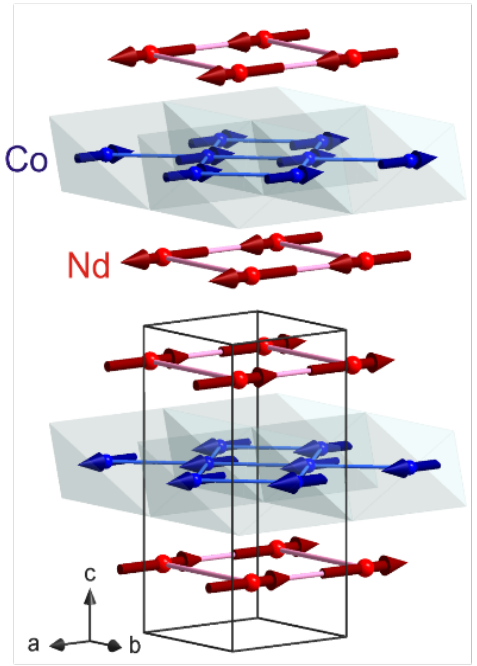
2D structures: Square-planar metal-pnictogen lattices

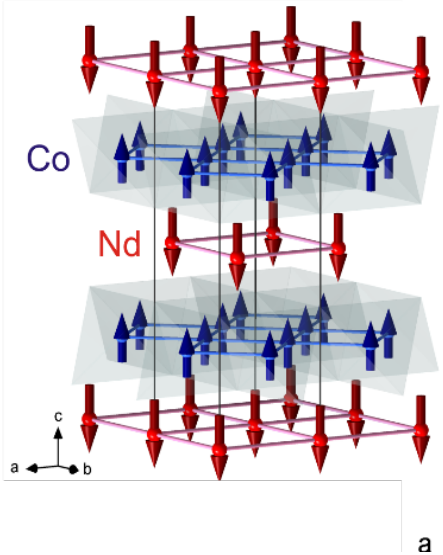
Co – pnictides containing two magnetic sublattices (Co, RE)

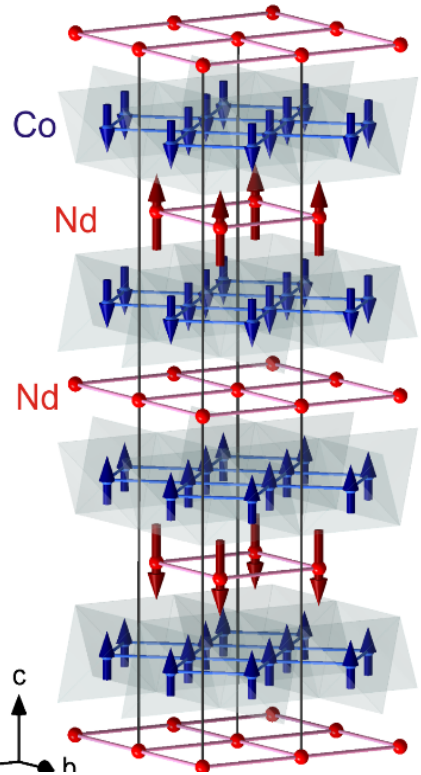
NdCoAsO
Tc = 69 K, FM-Co
T_{N1} = 14 K, AFM-Co
T_{N2} = 3.5 K, AFM-Nd/Co
k = (0, 0, ½)

$NdCo_{1.7}As_2$
Tc = 69 K, FM-Co
T_N = 6 K, FiM-Nd/Co
k = (0, 0, 0)

$NdCo_2P_2$
T_{N1} = 309 K, AFM-Co
T_{N2} ~ 100 K, AFM-Nd/Co
k = (0, 0, ½)



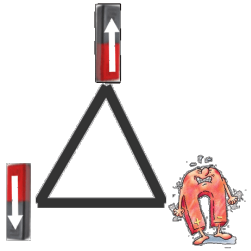




m(Nd) ≠ 0

m(Nd) =0

2D structure: edge-sharing equilateral triangles



- simplest geometrical frustrated lattice
- planar 120° spin structure or "three-sublattice $\sqrt{3} \times \sqrt{3}$ state"
- other ordered states can be stabilized by NNN interactions, anisotropy of the orbital configuration, or magnetoelastic coupling.

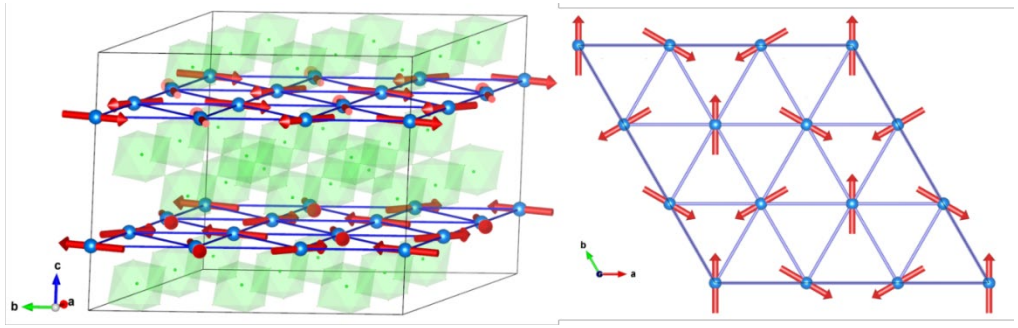
✓ VX_2 and AMX_3, where A = Cs, Rb, X = Cl, Br, I

✓ $A^+M^{3+}O_2$ series with delafossite or a-$NaFeO_2$ structures

✓ 6H-perovskites $Ba_3M'M''_2O_9$ with M' = Ni, Co, Mn, and M''= Nb or Sb

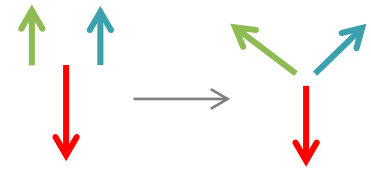
✓ $RbFe(MoO_4)_2$, $Rb_4Mn(MoO_4)_3$, $K_2M^{2+}{}_3(VO_4)_2CO_3$, $Na_2BaM^{2+}(VO_4)_2$, $K_3RE^{3+}(VO_4)_2$

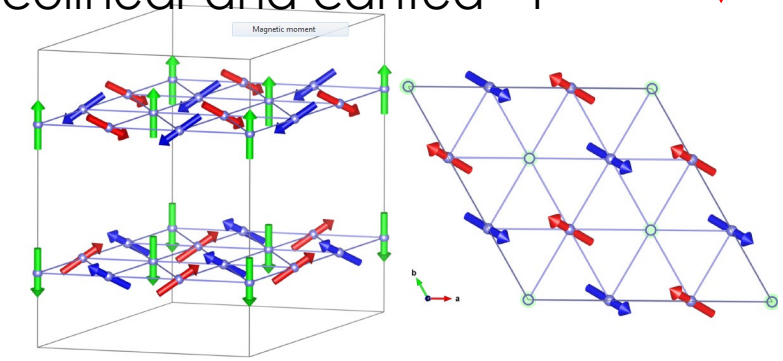
XY -type anisotropy (D ≤ 0)
120° spin structure in *ab plane*



$Ba_3NiNb_2O_9$, k = (⅓, ⅓, ½)

easy-axis anisotropy (D>0)
successive transitions:
colinear and canted "Y"





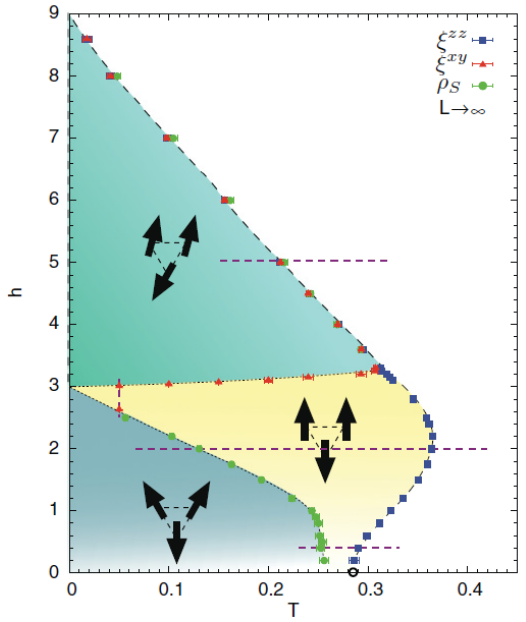
$2.2\ \mathrm{K} \leq T \leq 3\ \mathrm{K}$
$P6'_3/m$

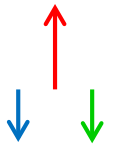
$T < 2.2\ \mathrm{K}$
$P2'_1$

$K_2Mn_3(VO_4)_2CO_3$, k = (⅓, ⅓, 0)

2D structure: edge-sharing equilateral triangles

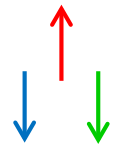
triangular Heisenberg antiferromagnet: rich range of phases in applied field





k =(1/3,1/3,0),

vs.



$\mathbf{k_1}$ =(1/3,1/3,0)

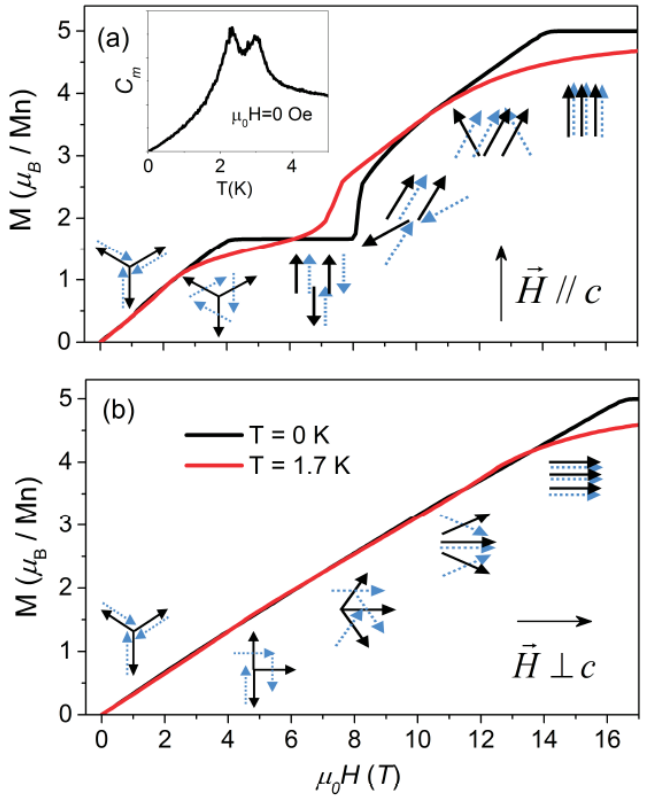
$\mathbf{k_2}$ =(0,0,0)

thermal and quantum fluctuations stabilize:

- coplanar, three-sublattice "*Y* state,"
- "uud" state - one-third magnetization plateau
- a coplanar 2:1 canted phase

← *Seabra et al, PRB, 84, 214418 (2011)*

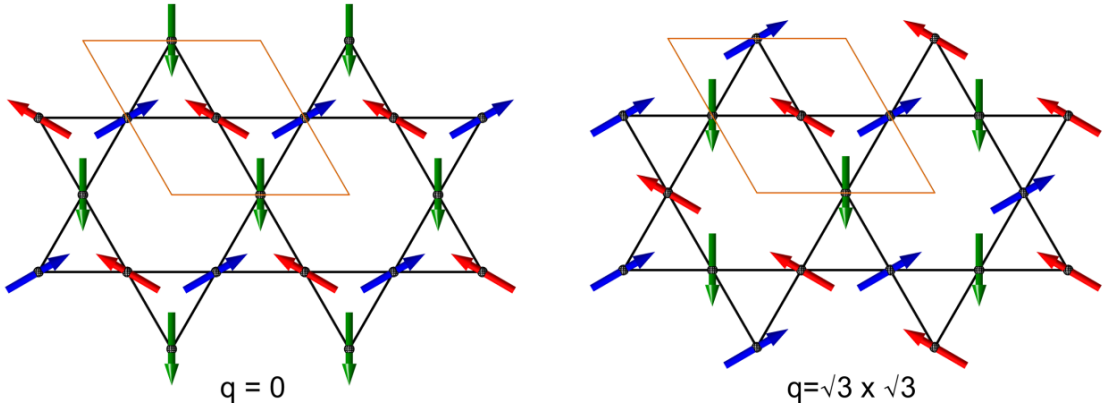
$K_2Mn_3(VO_4)_2CO_3$ – AFM with easy- axis anisotropy



Garlea et al, PRX, 9, 011038 (2019)

2D structure: Kagomé (corner-shared triangular) lattice

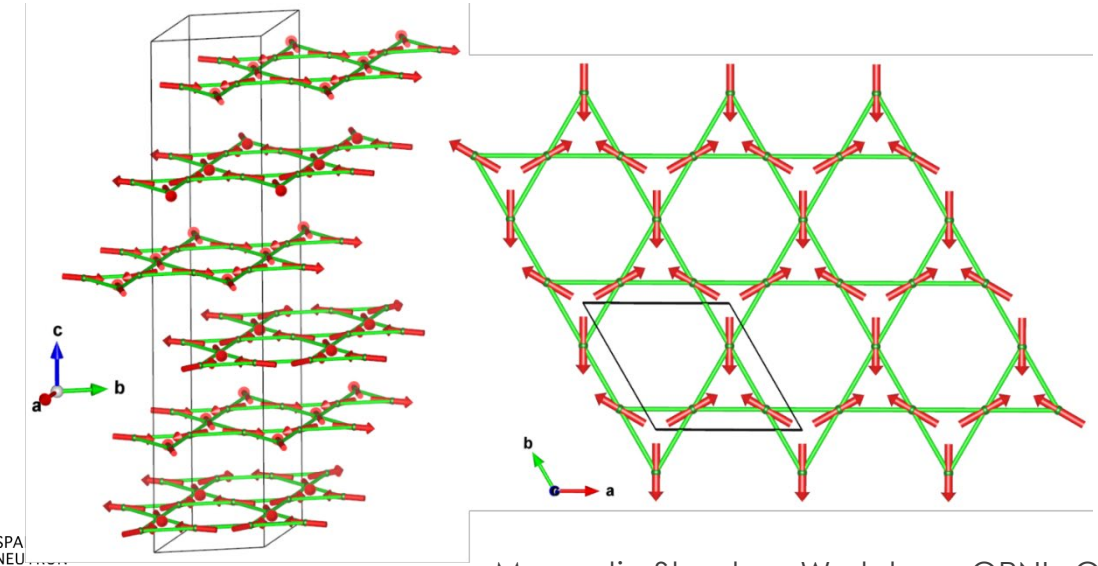
- variety of ground states: spin liquid, short-range order, or long-range order that can be stabilized by further-neighbor and D-M interactions
  - classical kagomé lattice orders with planar *120°* between *NN* spins



***q* = 0** : spin arrangement with uniform vector chirality

***q* = √3 x √3** : alternative spin arrangement with staggered vector chirality

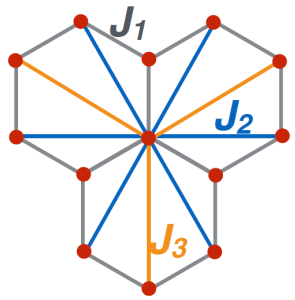
  - volborthite, herbertsmithite, kapellasite and jarosite series

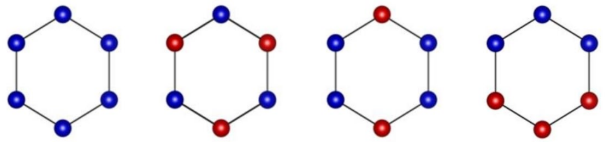


Fe-based jarosites $AFe_3(SO_4)_2(OH)_6$, with A = K, Na, Ag, (*R-3m* symmetry)
k = (0, 0, 3/2) order into planar "**q = 0**" type with AFM stacking of the layers)

A. Wills, PRB , 63, 064430 (2001)

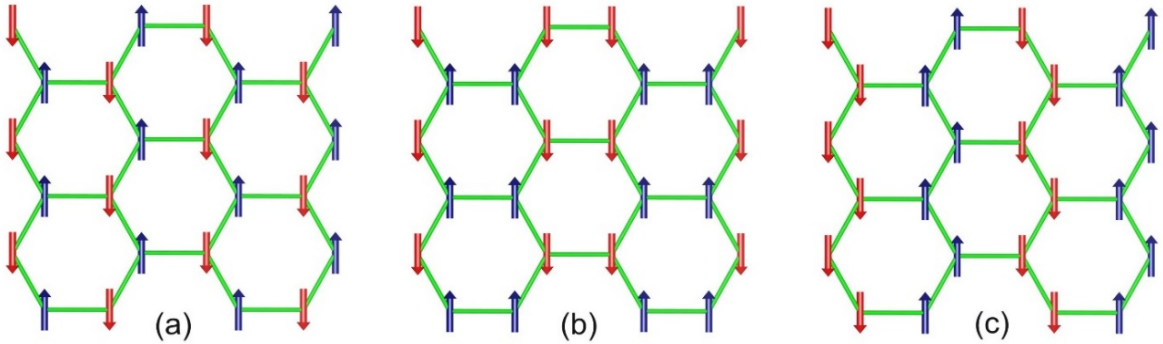
2D structure: honeycomb lattices





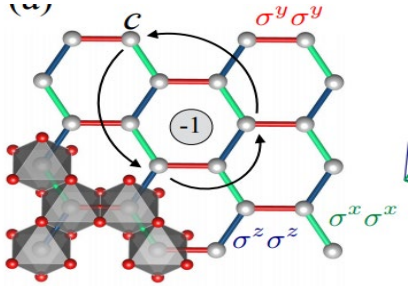
$$H = J_1 \sum_{n} S_i \cdot S_j + J_2 \sum_{nn} S_i \cdot S_j + J_3 \sum_{nnn} S_i \cdot S_j + Jz \sum_{nn} S_i \cdot S_j$$

Néel Stripe Zigzag



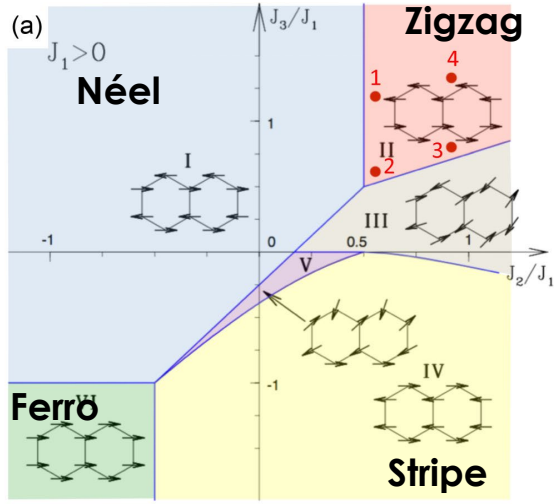
the Kitaev model (S=1/2 interacting via anisotropic bond-dependent coupling → Majorana-like excitations, or Zigzag ordered state (a-$RuCl_3$, Na_2IrO_3, …)

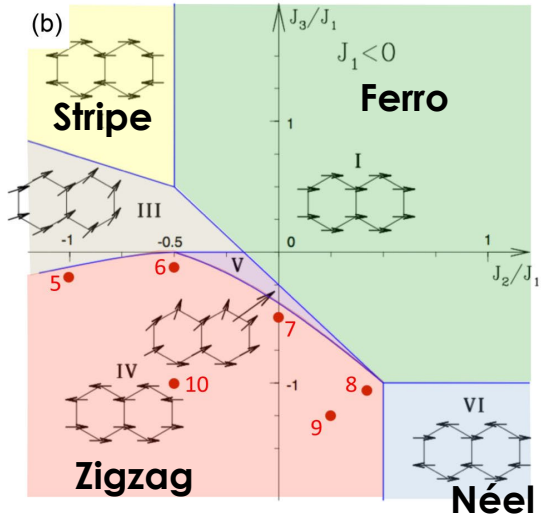
Hermanns, et al., Annu. Rev. Cond. Matter 9, 17 (2018)



J_2/J_1 – J_3/J_1 phase diagrams for AF $J_1 > 0$ and for FM $J_1 < 0$

Lefrancois, PRB B 94, 214416 (2016)
Fouet, Eur. Phys.J. B 20, 241 (2001)



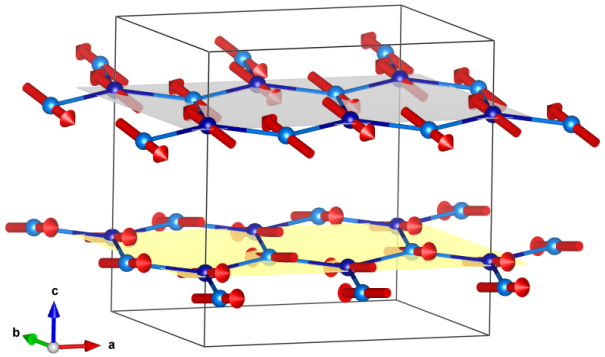


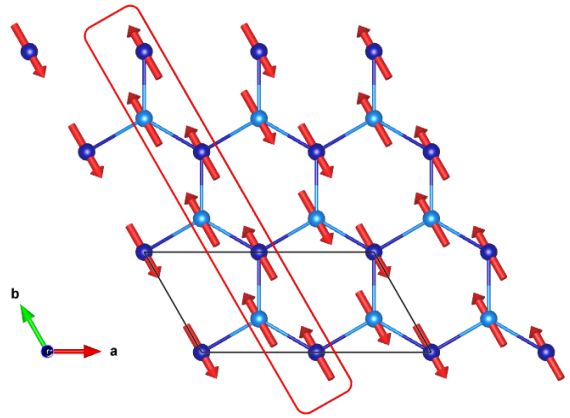
2D structure: honeycomb lattices

Examples of honeycomb lattice compounds:

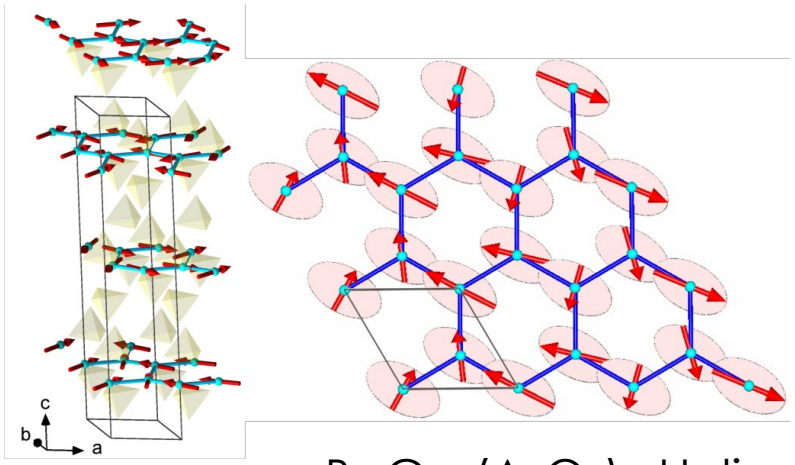
- MnTiO3, - Néel order,
- $Cu_3M_2SbO_6$, $Na_3M_2SbO_6$ (M=Cu, Mn, Co, Ni) - zigzag order

- $Na_2Co_2TeO_6$, Zigzag
  k = (1/2, 0, 0), $P_C2_12_12_1$

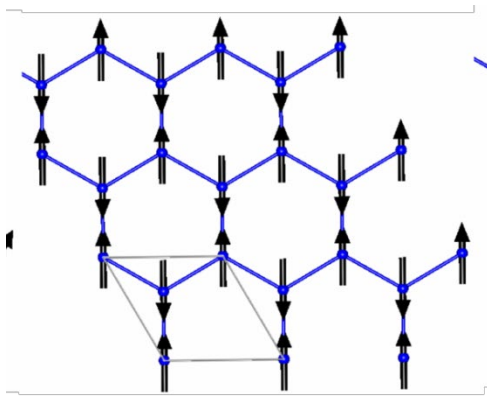




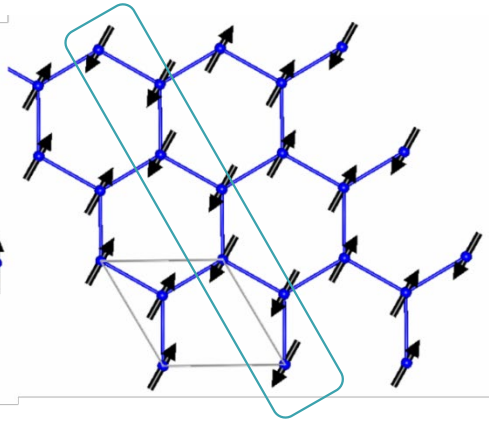
- $BaM_2(XO_4)_2$
  (M = Co, Ni, and X = P, As, V),



$BaCo_2(AsO_4)_2$, Helical
k = (0.261, 0, -4/3)



$BaNi_2(PO_4)_2$, Néel
k = (0, 0, 0)

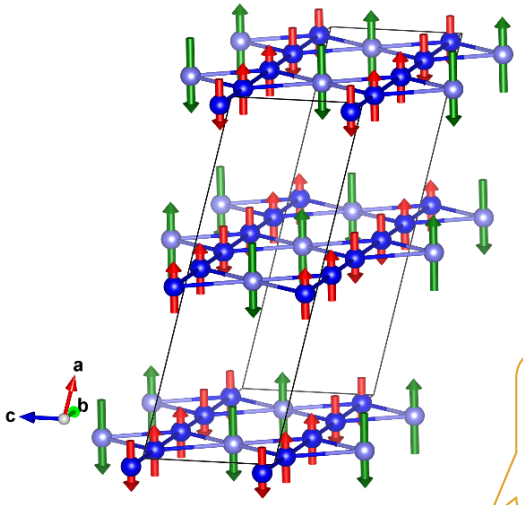


$BaNi_2(AsO_4)_2$, Zigzag
k = (½, 0, ½)

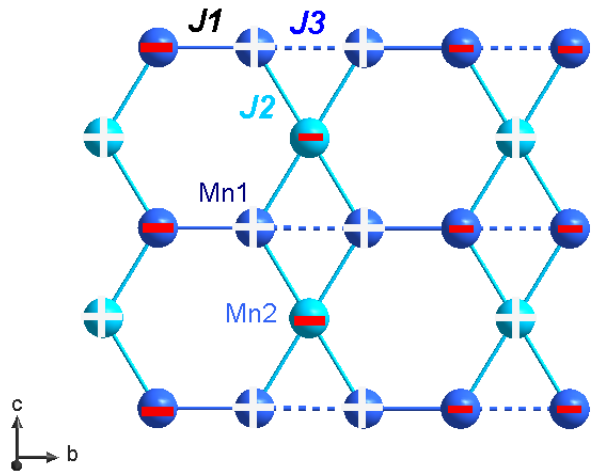
2D structure: frustrated "bow-tie" lattices

"bow-tie" or striped kagomé

$Ca_2Mn^{4+}{}_3O_8$, $K_2Mn^{2+}{}_3(VO_4)_2(OH)_2$



k = (0, ½ , 0)
m(Mn1) ≈ 1.7 μ_B
m(Mn2) ≈ 2.5 μ_B



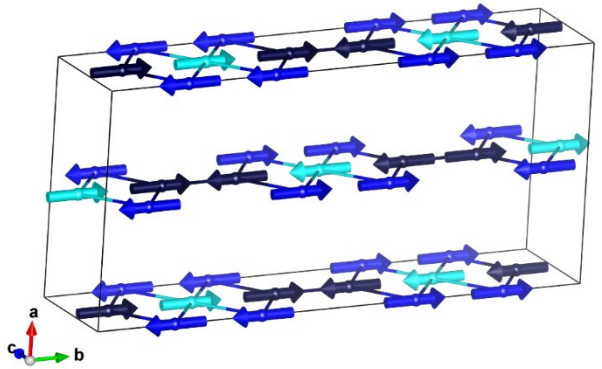
AFM - NN

Mn1, 3 NN

Mn2, 4 NN

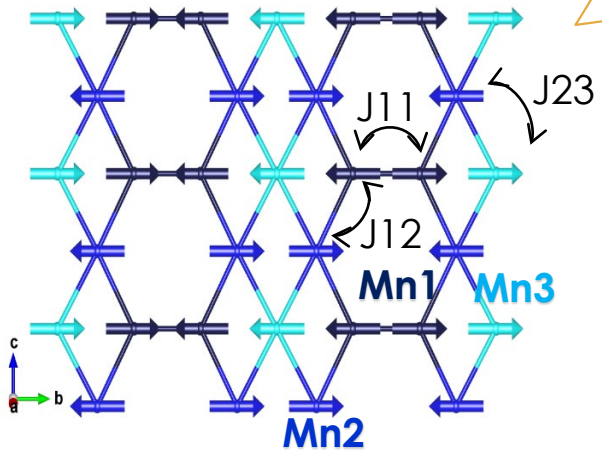
striped triangular lattice

$Mn^{2+}{}_5(VO_4)_2(OH)_4$



P_b2/c

k = (0, ½ , 0)
m(Mn1) ≈ 1.98 μ_B
m(Mn2) ≈ 2.43 μ_B
m(Mn3) ≈ 2.48 μ_B



AFM - NN

Mn1 , 3 NN

Mn2 , 4 NN

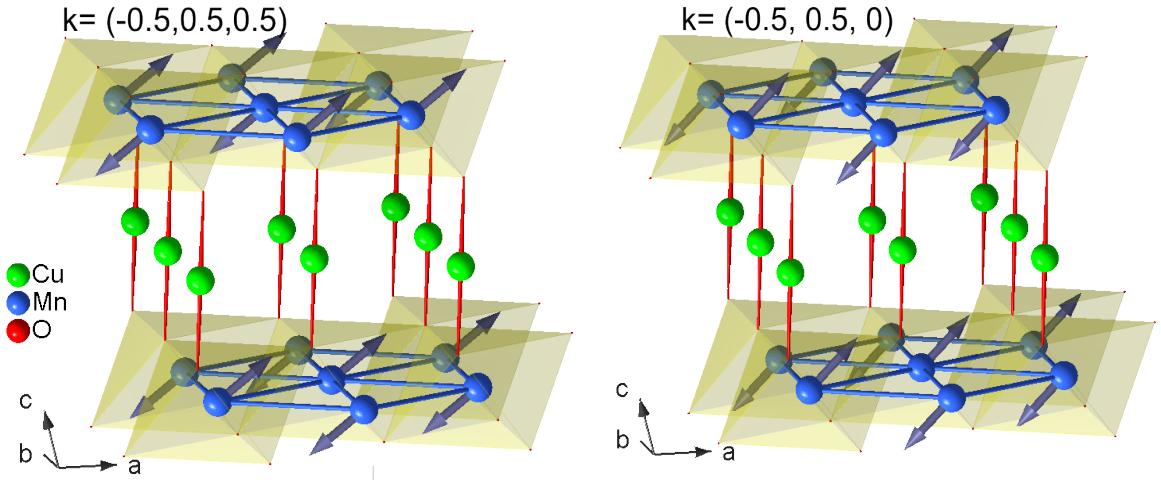
Mn1 , 4 NN

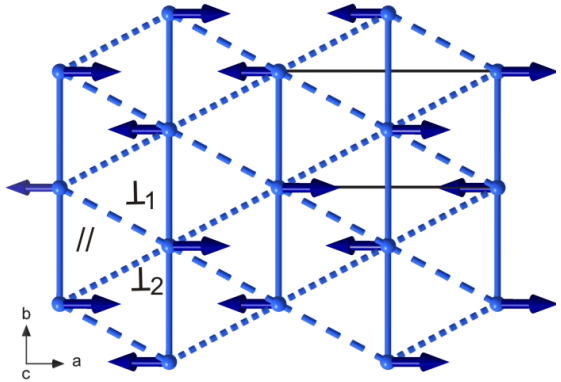
2D structure: Isosceles triangle lattice → possible Quasi-1D

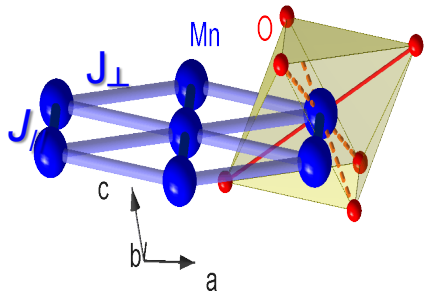
$NaMnO_2$ $Cu_{1+x}Mn_xO_2$, $Mn^{3+}(t_{2g}^3 e_g^1)$

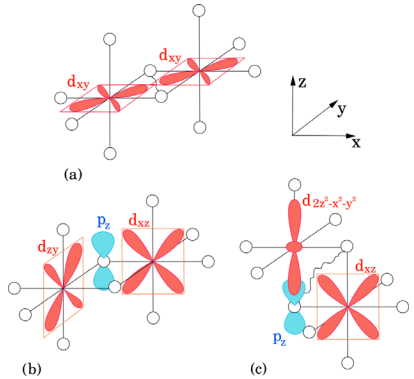
k = (½, ½, 0) or (½, ½, ½)

C2/m → *P-1* , $T_S \approx 65$ K (Cu) and $T_S \approx 45$ K (Na)



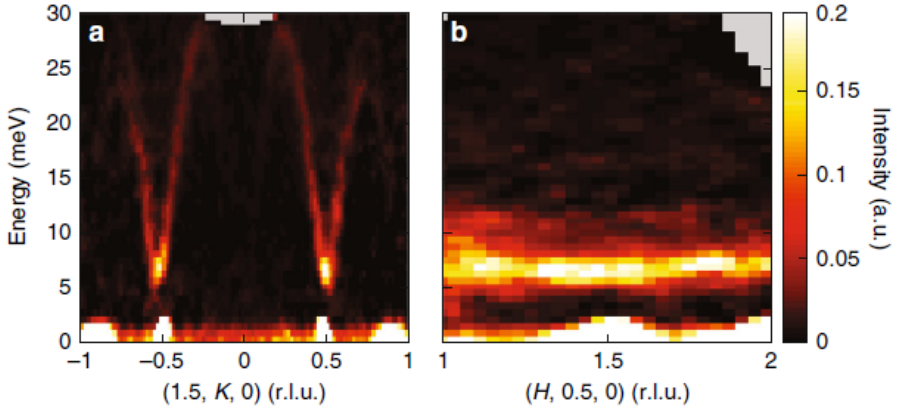






$$H = J_{\parallel} \sum_{nn} S_i \cdot S_j + J_{\perp} \sum_{nnn} S_i \cdot S_j + Jz \sum_{nnn} S_i \cdot S_j \quad -D \sum_n (S_n^z)^2$$

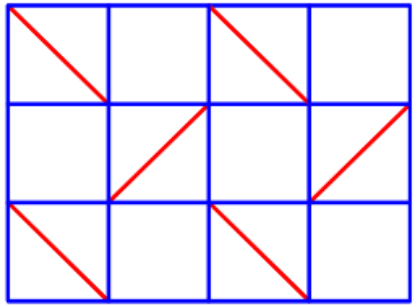
1D character of spin dynamics

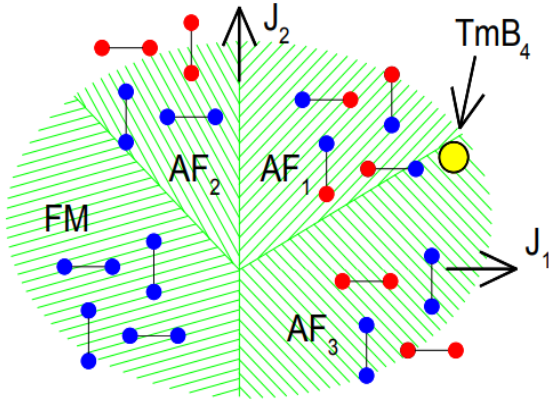


Dally et al. Nature Comm. **9**, *2188 (2018)*

2D structure: Shastry-Sutherland lattice → possible 0 D

Interpenetrating planar sublattices of orthogonal dimers

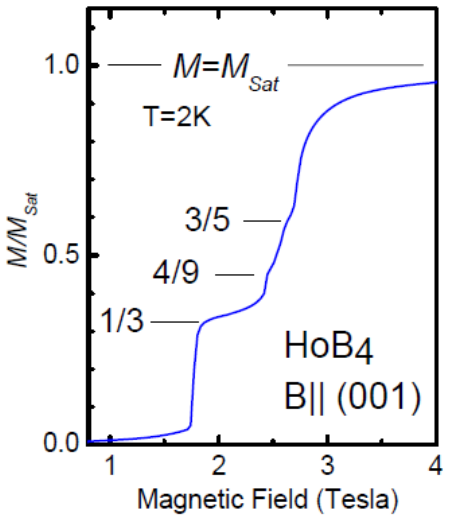




REB_4 : RE = Er, Tm - strong Ising
RE = Ho - XY anisotropy.

HoB_4:

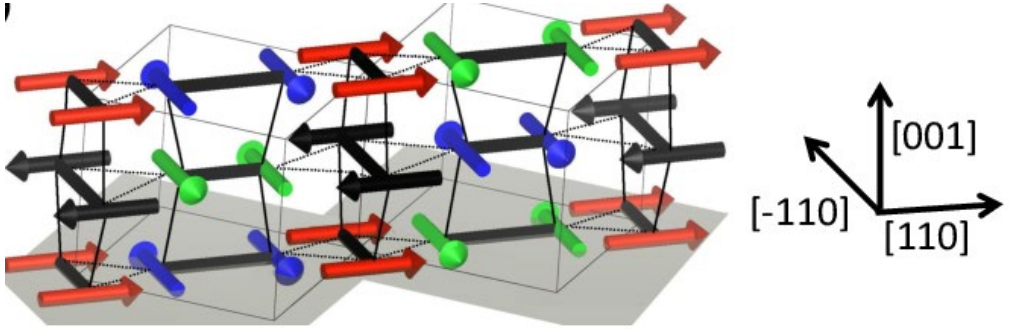
- T_{N1} = 7K, k_1 = (0.02, 0.02, 0.4) and T_{N2} = 5K , k_2 = (1 0 0)
- Fractional magnetization plateaus in applied field



Mat'aš et al J. Phys. 200, 032041 (2010)

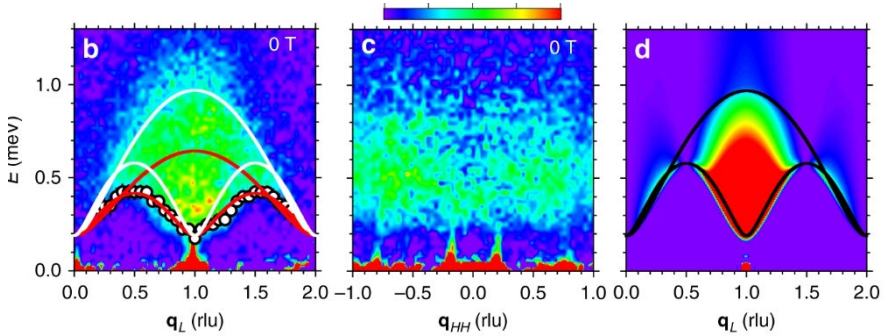
Yb_2Pt_2Pb, Yb -strong Ising anisotropy

$\mathbf{k_1}$ = (1/5,1/5, 0) & $\mathbf{k_2}$ = (-1/5,1/5, 0)



Miiler et al., PRB 93, 104419 (2016)

spinon dispersion along the c axis typical of the S=1/2 Heisenberg-Ising XXZ spin Hamiltonian



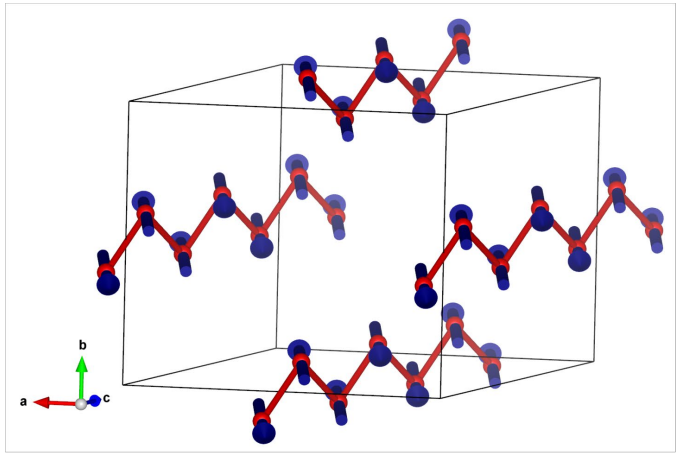
L. Wu Science 352, 1206 (2016)
Gannon et al. , Nature Comm., 10, 1123 (2019)

Quasi-1D structures

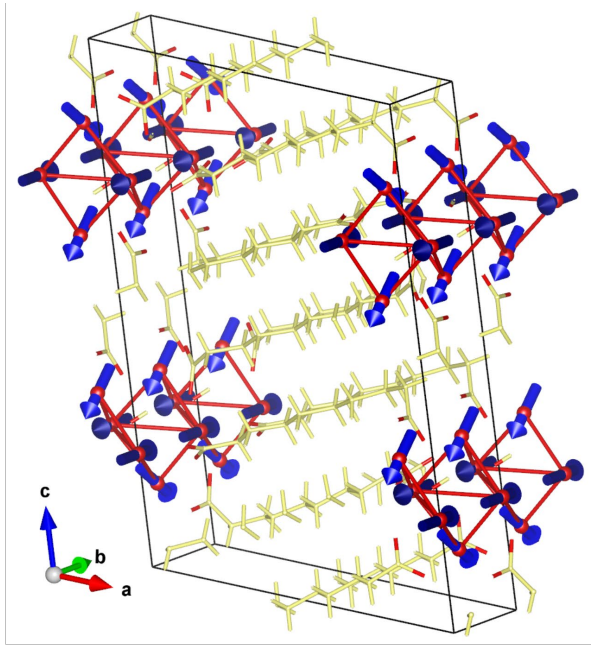
strong exchange coupling between magnetic ions only along one direction

- metal-organic frameworks (MOFs): connected low-dimensional inorganic subnetworks through non-magnetic molecules
- alkali-metal pyroxenes AMX_2O_6 , A = Li^+, Na^+; M = Ti^{3+}, V^{3+}, Cr^{3+}, Mn^{3+}, and Fe^{3+}; X = Si^{4+}, Ge^{4+}
- brackebuschite $Ba_2M^{3+}(VO_4)_2(OH)$ and descloizite $SrM^{2+}(VO_4)(OH)$ transition metal vanadate

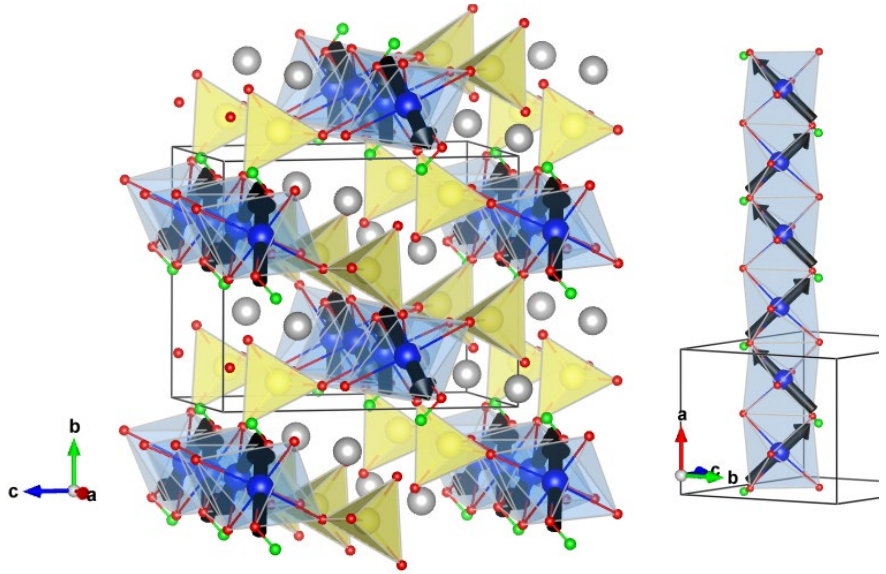
$NaMnGe_2O_6$ pyroxene
k = (0, 0, ½)



$Co_4(OH)_2(C_{10}H_{16}O_4)_3$
k = (0, 0, 0), $d_{interchain}$ ~ 12A

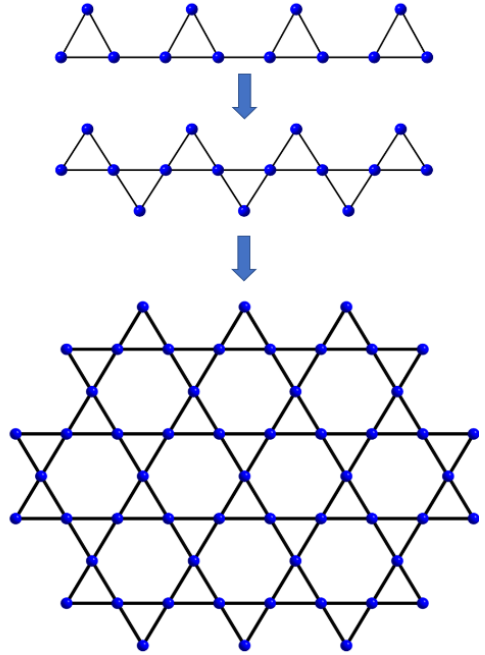


$SrCo^{2+}(VO_4)(OH)$
k = (0, 0, 0)



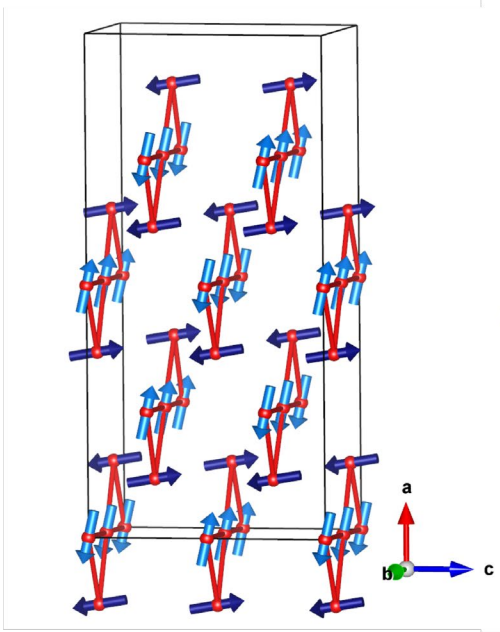
Quasi-1D structures : delta or "sawtooth" chains

prototype example of highly frustrated lattices; can be seen as derived from a kagomé lattice by removing magnetic sites in periodic lines perpendicular to the kagomé spine direction

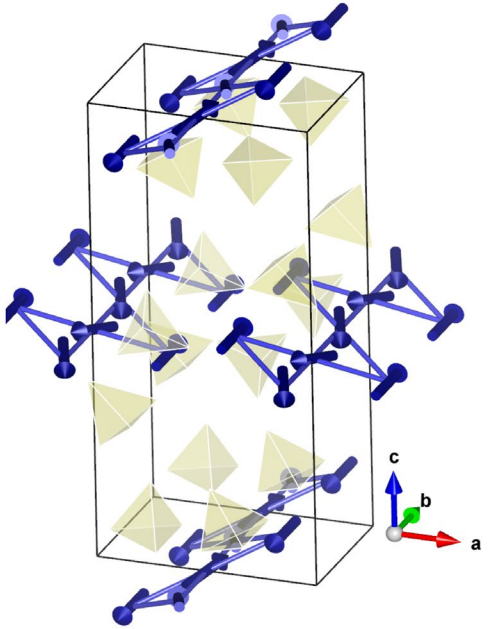


- olivines (M_2XO_4, X = Si , Ge) , oxy-arsenates $A_2Fe_2O(AsO_4)_2$, and alkali Transition Metal Molybdates $CsM_2(MoO_4)_2(OH)$ (M = Mn, Fe, Co, Zn), $Rb_2M_3(MoO_4)_3(OH)_2$ (A = K, Rb; M = Mn, Co),

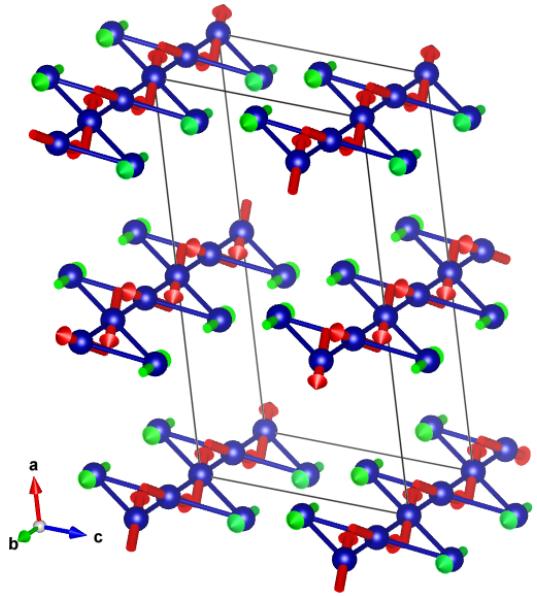
Ni_2SiO_4
k = (½, 0, ½);



$Rb_2Fe_2O(AsO_4)_2$
k = (0, 0, 0)



$CsM_2(MoO_4)_2(OH)$
k = (½, 0, 0)



Summary

The effective dimensionality & topology of the crystal lattice plays an important role in defining the magnetic ordered state

A hierarchy of magnetic structures based on lattice dimensionality can be established. Exceptions to this classification can lead to discovery of new physics

Magnetic structure determination is an important step in understanding materials, as it places your system inside a magnetic phase diagram.

Think of the mechanisms that are responsible for the static order. Consider complementing your findings with spin dynamics studies to answer the “So What?“ question.

Thank you !