The Abdus Salam
International Centre for Theoretical Physics

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IAEA
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1957-8

Miniworkshop on Strong Correlations in Materials and Atom Traps

4 - 15 August 2008

Physics of 5d Ir oxides.

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Physics of 5d Ir oxides

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東京大学
THE UNIVERSITY OF TOKYO

Outlines

Why Ir oxides??

1. Spin-orbit coupling driven Mott insulating state in Sr_2IrO_4

   ideal playground for “phase sensitive” magnetic x-ray diffraction

   B.J.Kim (UT), S.Fujiyama (RIKEN), K.Ohashi (UT) and T.Takayama (UT)

2. Spin liuquid state in hyper-kagome $Na_4Ir_3O_8$

   _Y.Okamoto (UT), S.Fujiyama (RIKEN), R.Perry (UT) and M.Nohara (UT))

Mott physics in correlated electron system

Hubbard model

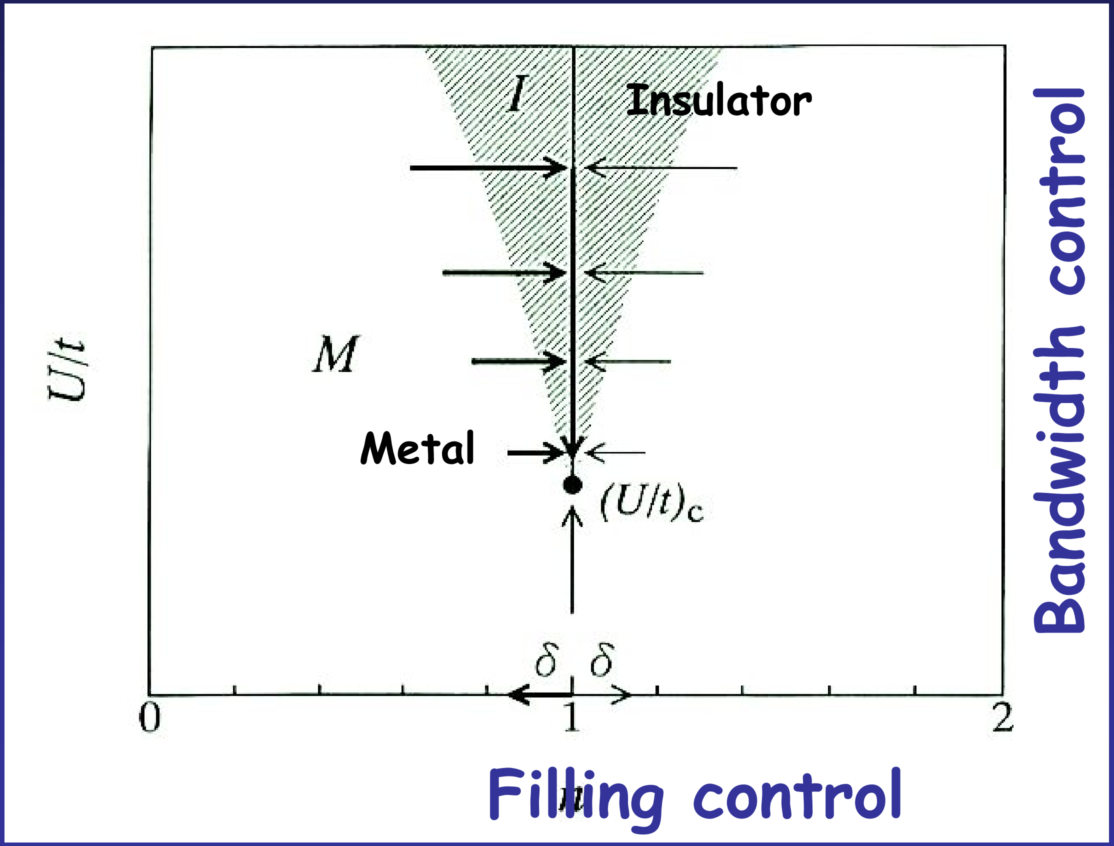
$$H = t\sum a^{+}_{i+1} a_i + U\sum n_{i\uparrow} n_{i\downarrow}$$

Kinetic energy

Coulomb repulsion

U/t, n

Rich variety of exotic electronic phases near Mott insulating state



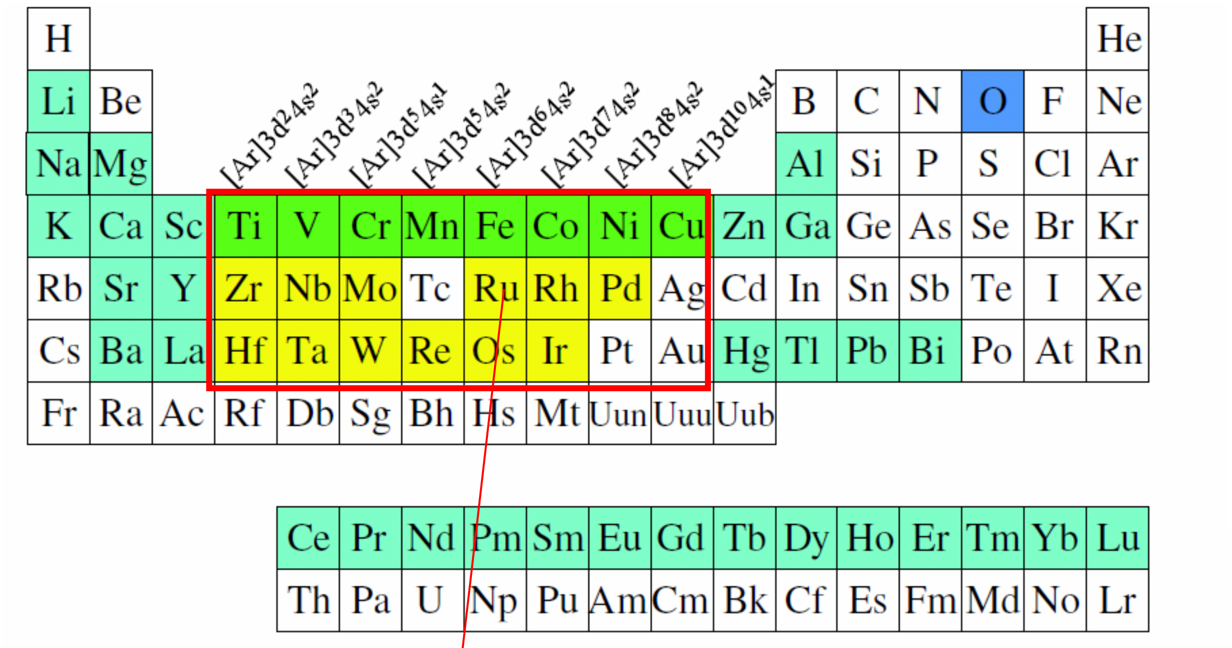
Insulator

Metal

Bandwidth control

Filling control

perovskite (related) oxides as a playground for Mott physics



H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub						
				Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
				Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

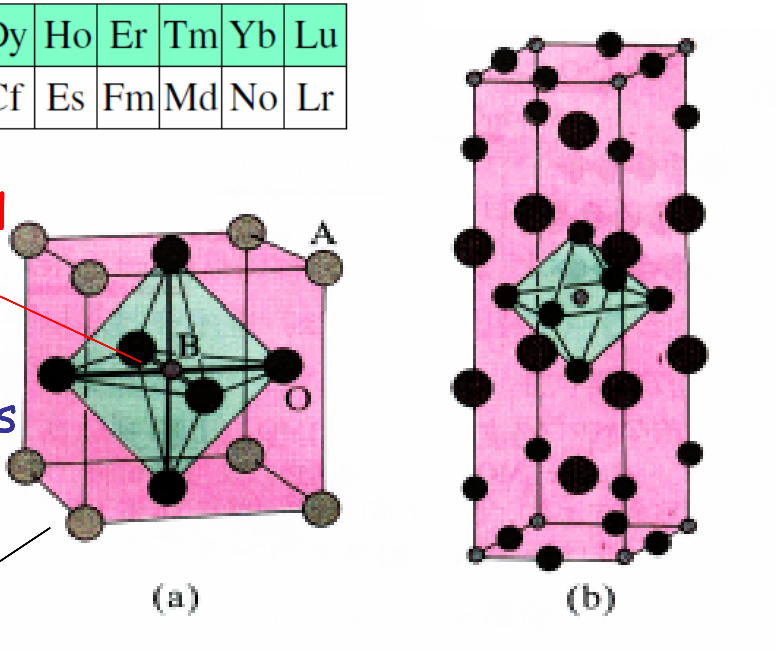
3d transition metal
main playground

Transition Metal

3d: can find Mott Ins.

4d, 5d: hard to find Mott Ins.

Oxygens



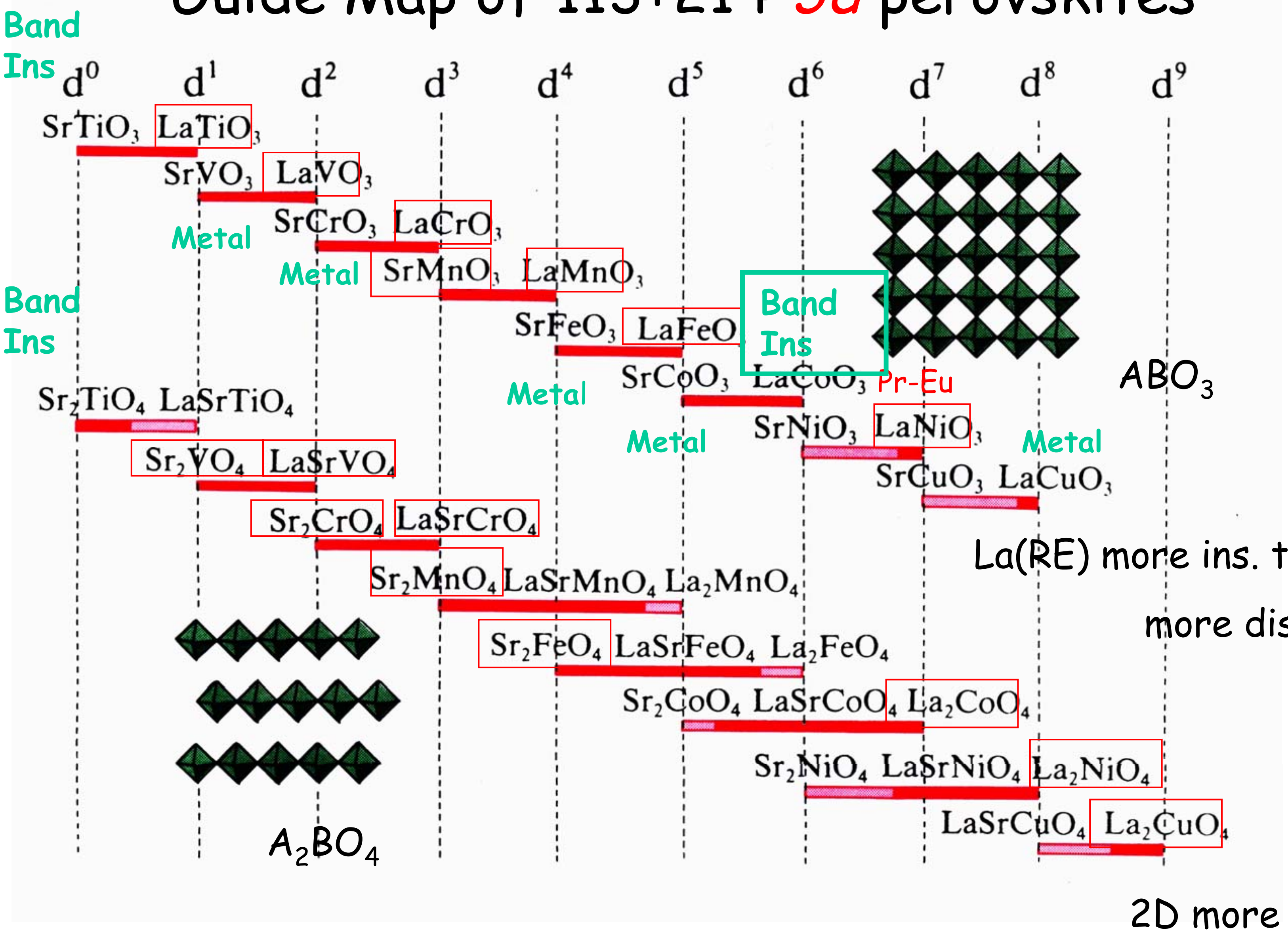
(a) (b)

Rare
earth or
Alkaline
earth
ions

ABO_3

A_2BO_4 (layered)

Guide Map of 113+214 *3d* perovskites



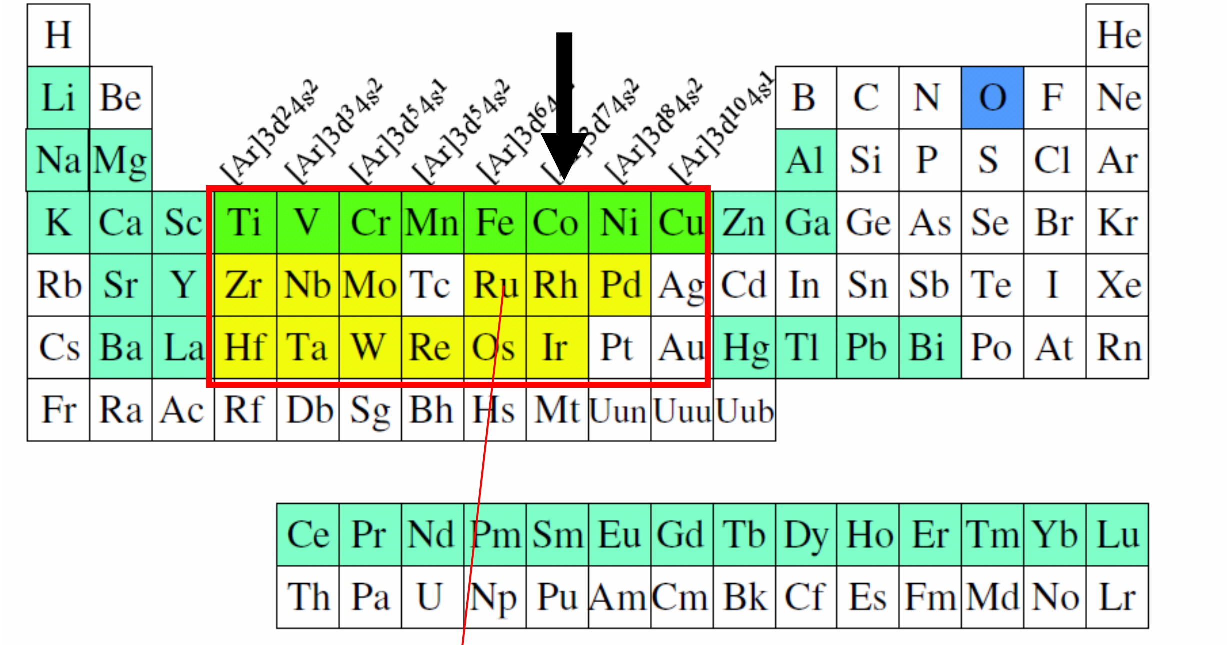
La(RE) more ins. than Sr

more distorted

2D more insulating

🟥 Mott Insulator

3d transition metal perovskite as a playground for Mott physics



			$[Ar]3d^24s^2$	$[Ar]3d^34s^2$	$[Ar]3d^54s^1$	$[Ar]3d^54s^2$	$[Ar]3d^64s^2$	$[Ar]3d^74s^2$	$[Ar]3d^84s^2$	$[Ar]3d^{10}4s^1$							
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub						
				Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
				Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

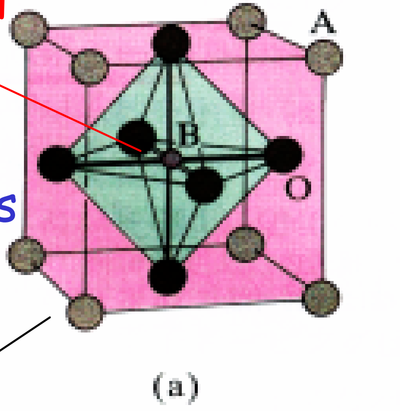
3d transition metal
main playground

Transition Metal

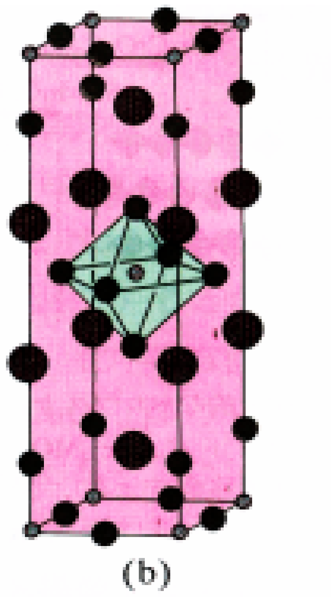
3d: can find Mott Ins.

4d, 5d: hard to find Mott Ins.

Not always the case particulary for 5d because of spin orbit coupling



ABO_3

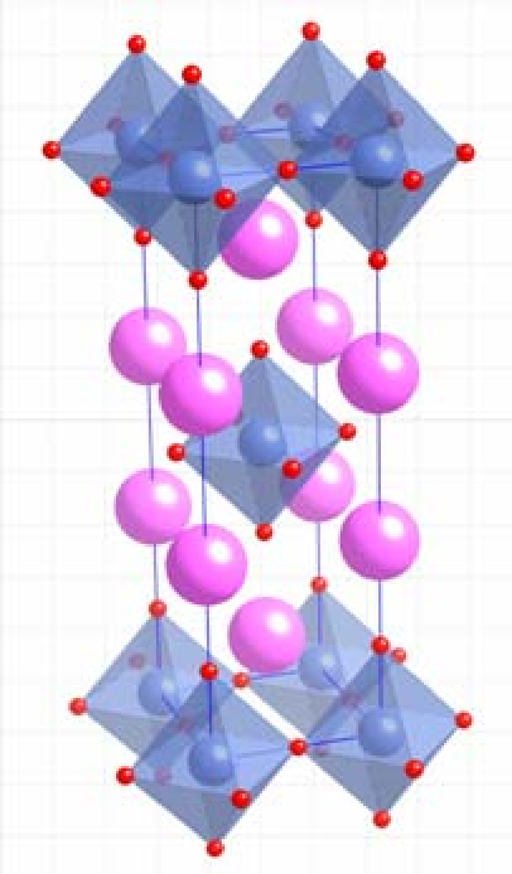


A_2BO_4 (layered)

Group 9 Sr_2MO_4

What is the ground state?

K_2NiF_4 structure



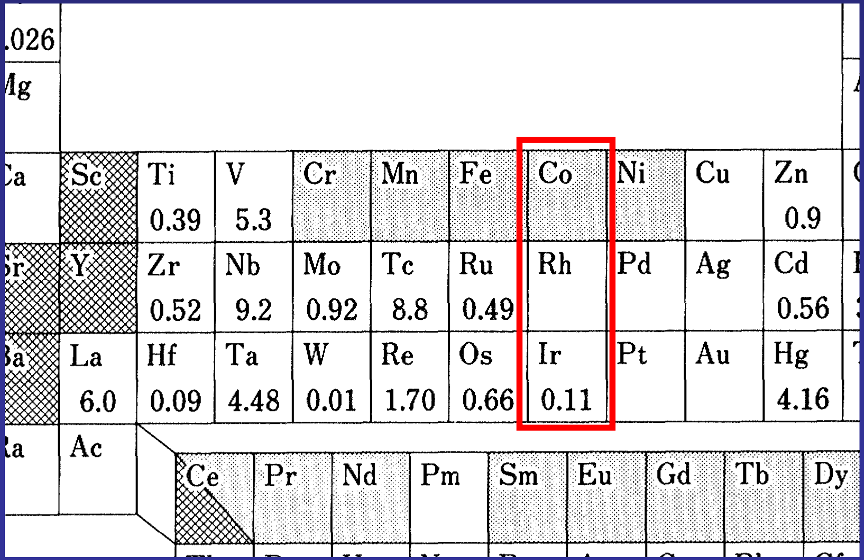
Five d-electrons d^5

3d Sr_2CoO_4

4d Sr_2RhO_4

5d Sr_2IrO_4

Transfer increase



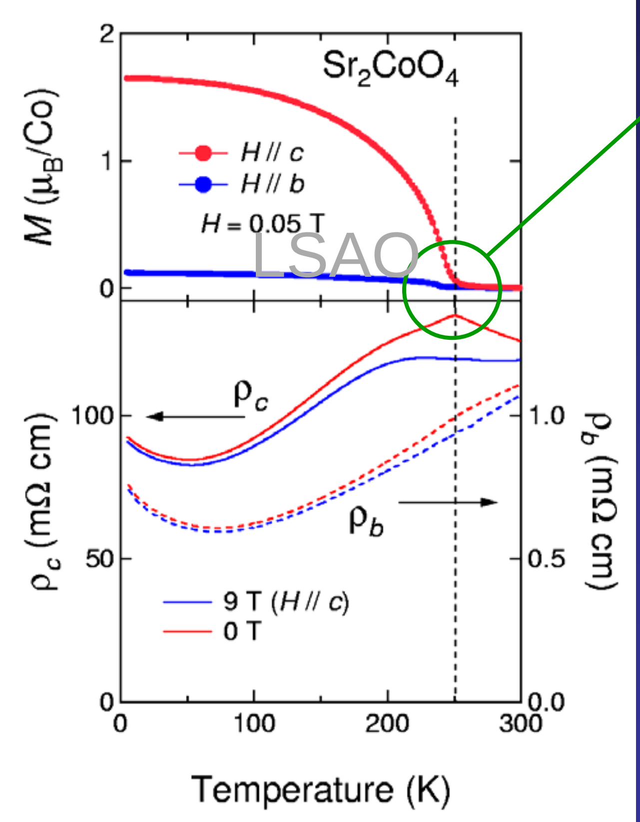
.026										
lg										
a	Sc	Ti 0.39	V 5.3	Cr	Mn	Fe	Co	Ni	Cu	Zn 0.9
r	Y	Zr 0.52	Nb 9.2	Mo 0.92	Tc 8.8	Ru 0.49	Rh	Pd	Ag	Cd 0.56
a	La 6.0	Hf 0.09	Ta 4.48	W 0.01	Re 1.70	Os 0.66	Ir 0.11	Pt	Au	Hg 4.16
a	Ac									

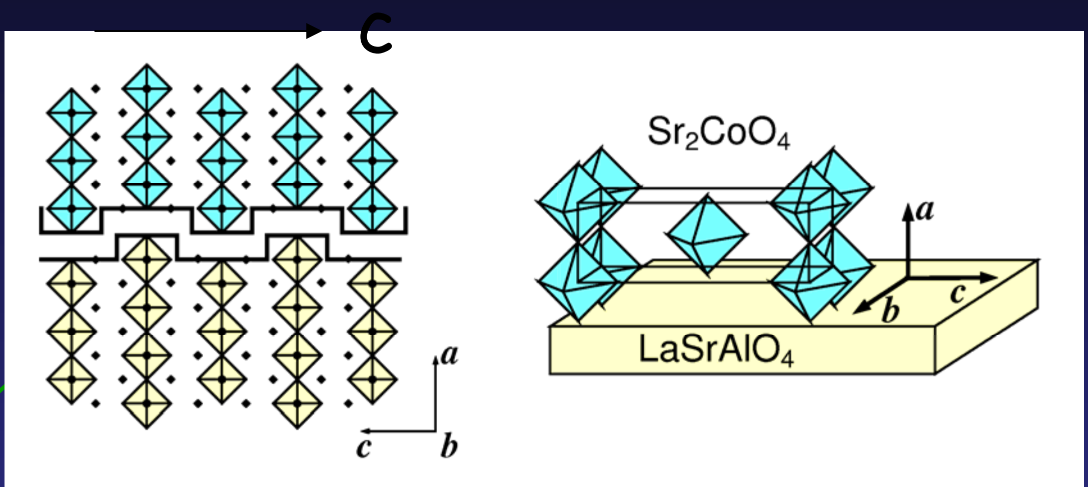
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy

New itinerant ferro-magnet Sr_2CoO_4 developed by "atomic graphoepitaxy"

Matsuno PRL (2004)

SCO

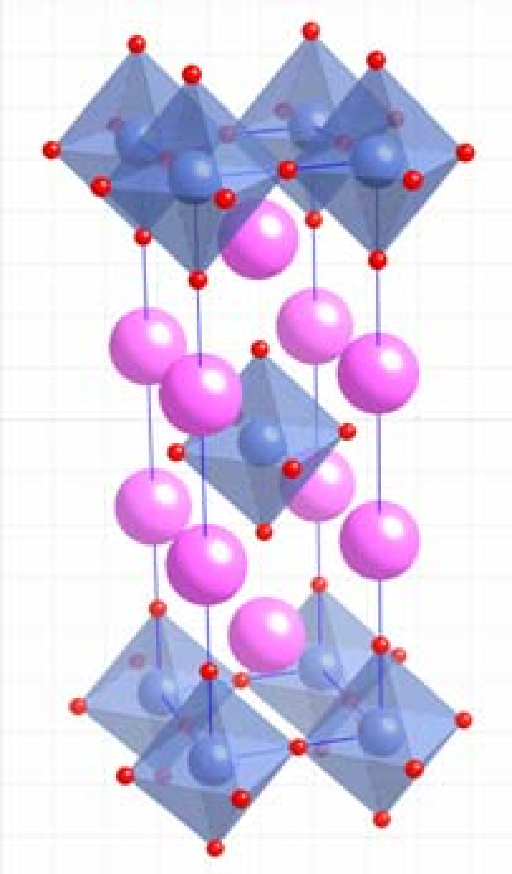




- Ferromagnet: $T_C \sim 250$ K
  cf. $SrCoO_3$ ($T_C \sim 280$ K)
- Metallic conduction below T_C
- Anisotropy $\rho_c/\rho_b \sim 10^2$
  quasi-two-dimensionality

Group 9 Sr_2MO_4

K_2NiF_4 structure



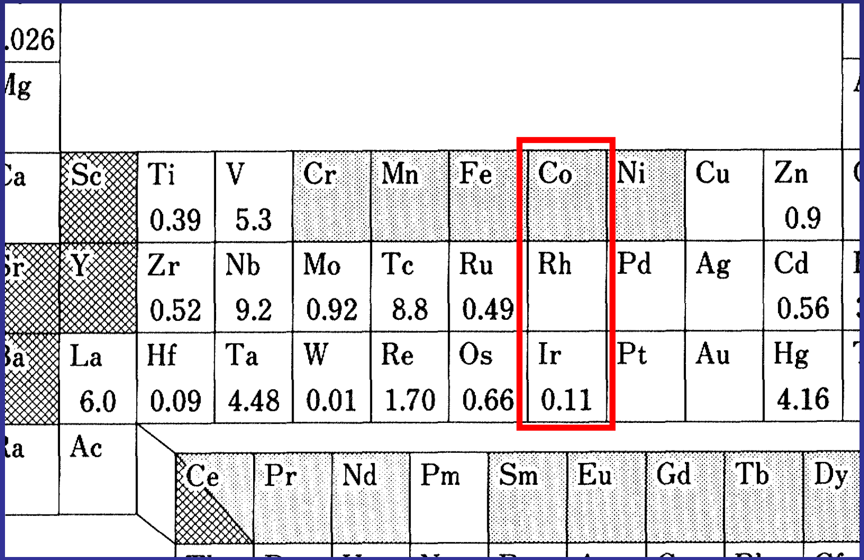
Five d-electrons d^5

3d Sr_2CoO_4 Ferromagnetic metal

4d Sr_2RhO_4

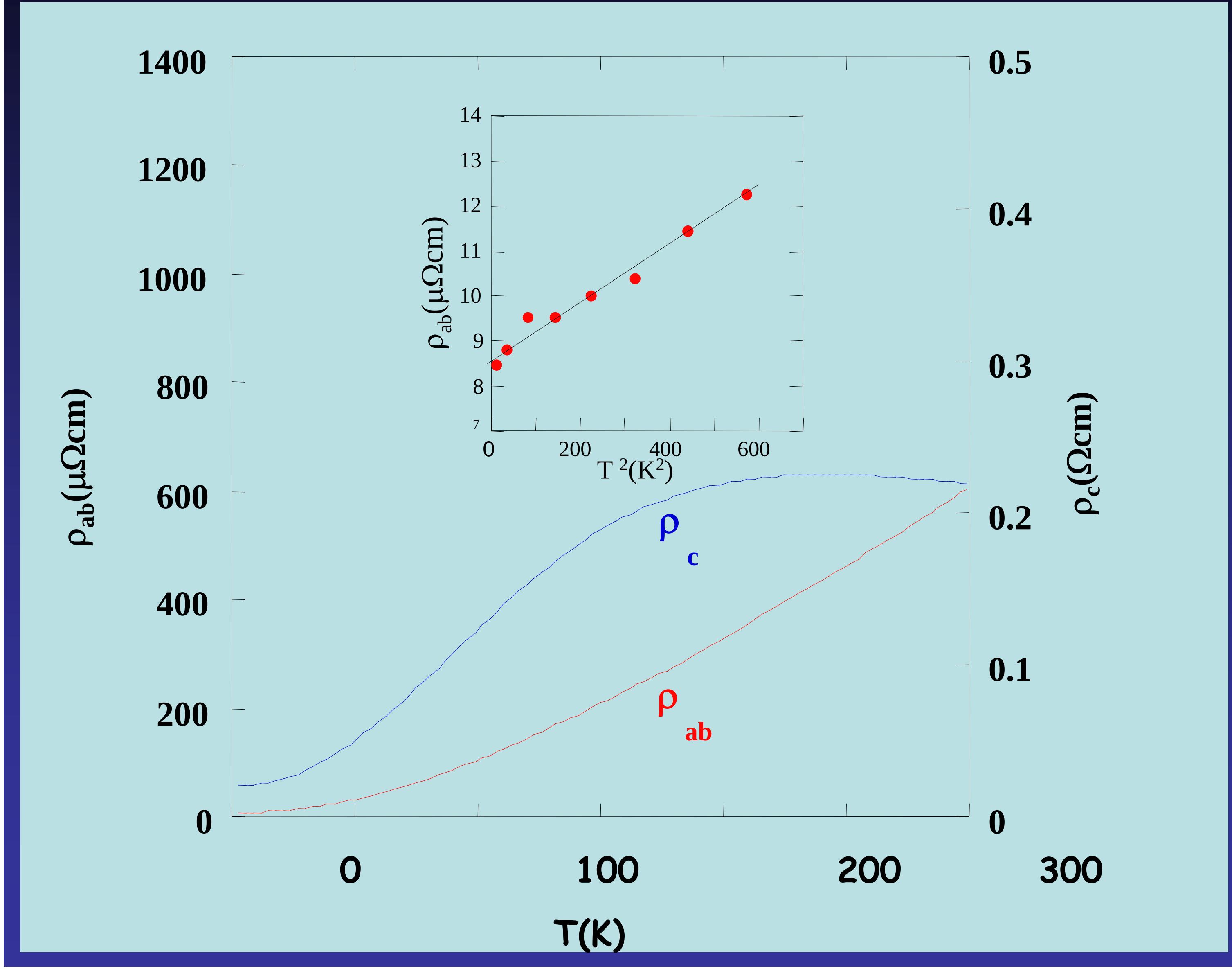
5d Sr_2IrO_4

Transfer increase



.026										
lg										
a	Sc	Ti 0.39	V 5.3	Cr	Mn	Fe	Co	Ni	Cu	Zn 0.9
Sr	Y	Zr 0.52	Nb 9.2	Mo 0.92	Tc 8.8	Ru 0.49	Rh	Pd	Ag	Cd 0.56
a	La 6.0	Hf 0.09	Ta 4.48	W 0.01	Re 1.70	Os 0.66	Ir 0.11	Pt	Au	Hg 4.16
a	Ac									
		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy

Sr_2RhO_4, a paramagnetic metal



low spin
$t2g^5$ metal

Quasi 2D
Fermi liquid

No magnetism

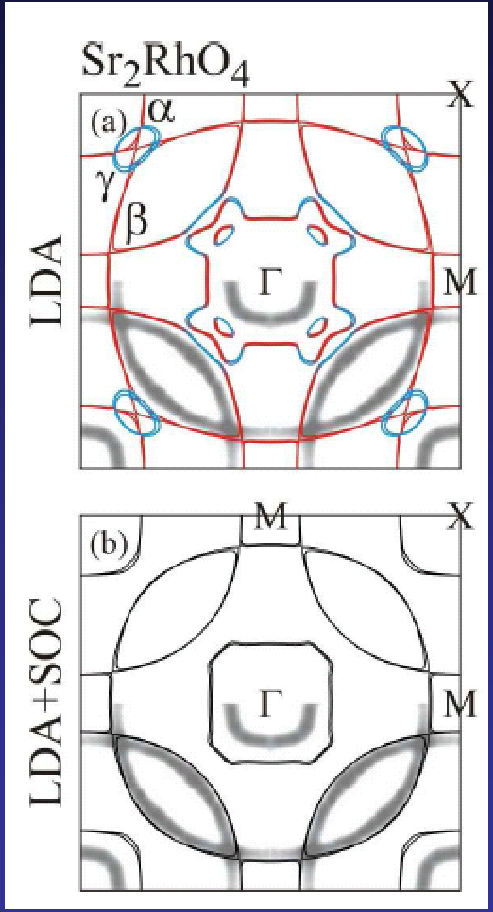
I. Nagai et al.
unpublished

Importance of SOC in Sr_2RhO_4

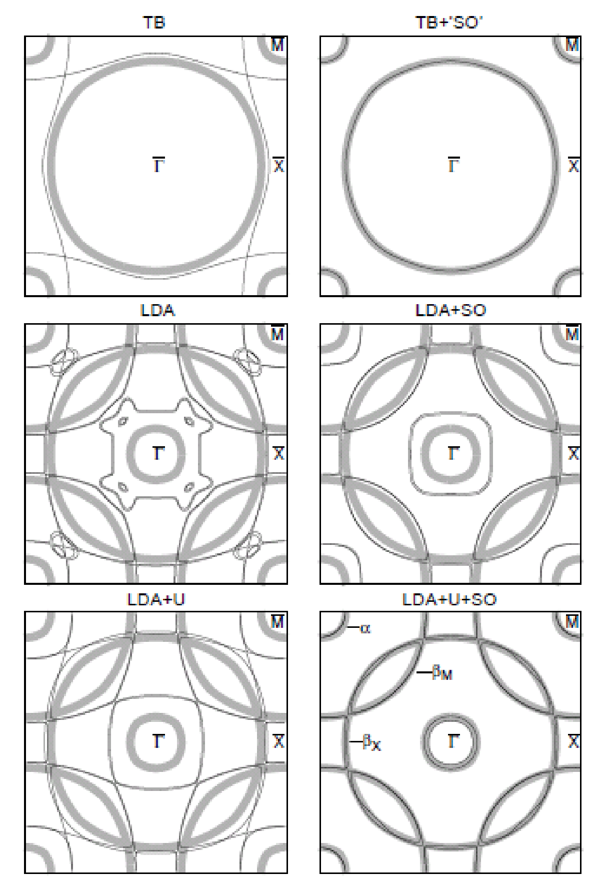
ARPES FS
not 100% consistent with LDA FS

SOC
100-200meV

Tend to make FS isotropic



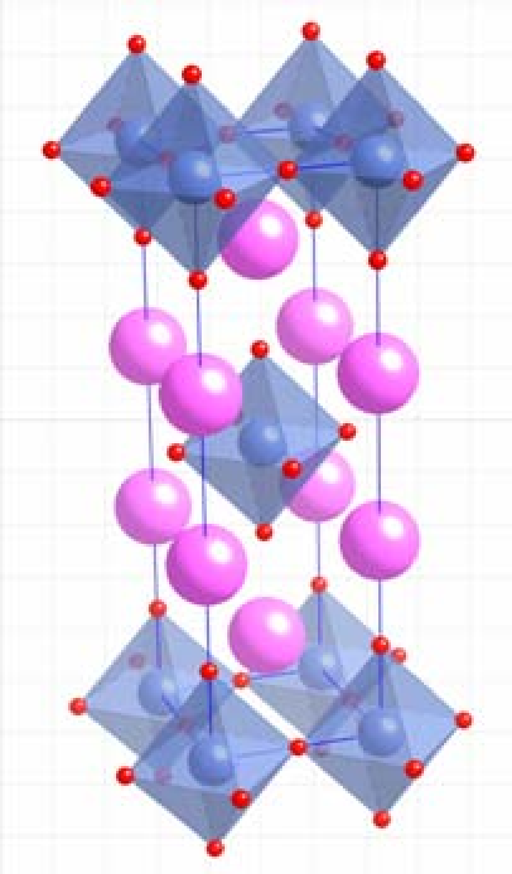
Haverkort et al. PRL(2008)



Liu et al. PRL(2008)

Group 9 Sr_2MO_4

K_2NiF_4 structure



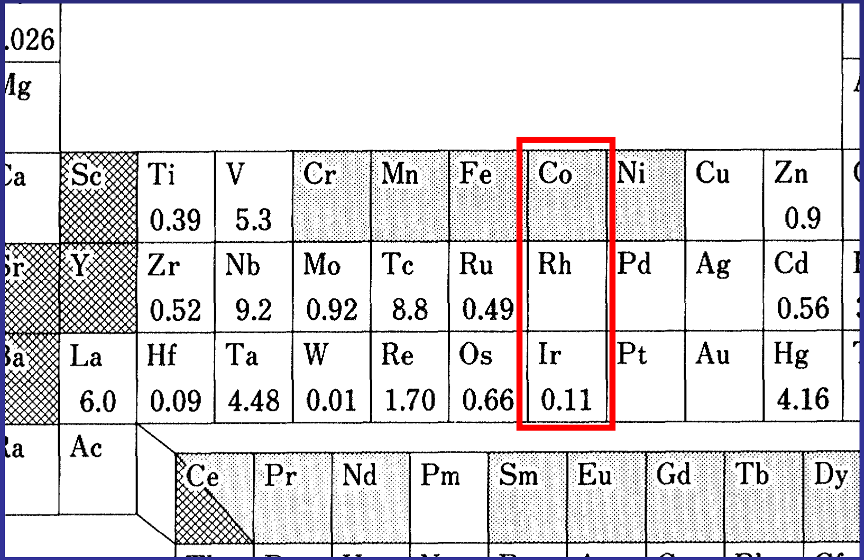
Five d-electrons d^5

3d Sr_2CoO_4 Ferromagnetic metal

4d Sr_2RhO_4 paramagnetic metal

5d Sr_2IrO_4

Transfer increase



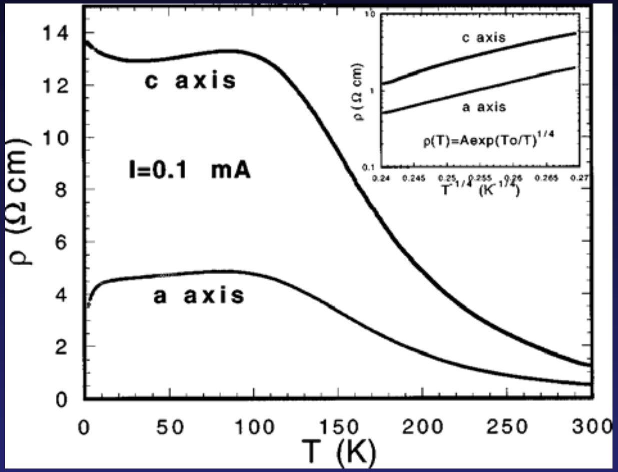
.026										
Mg										
Ca	Sc	Ti 0.39	V 5.3	Cr	Mn	Fe	Co	Ni	Cu	Zn 0.9
Sr	Y	Zr 0.52	Nb 9.2	Mo 0.92	Tc 8.8	Ru 0.49	Rh	Pd	Ag	Cd 0.56
Ba	La 6.0	Hf 0.09	Ta 4.48	W 0.01	Re 1.70	Os 0.66	Ir 0.11	Pt	Au	Hg 4.16
Ra	Ac									

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy

Sr_2IrO_4, a magnetic insulator

G.Cao et al. PRB 1998

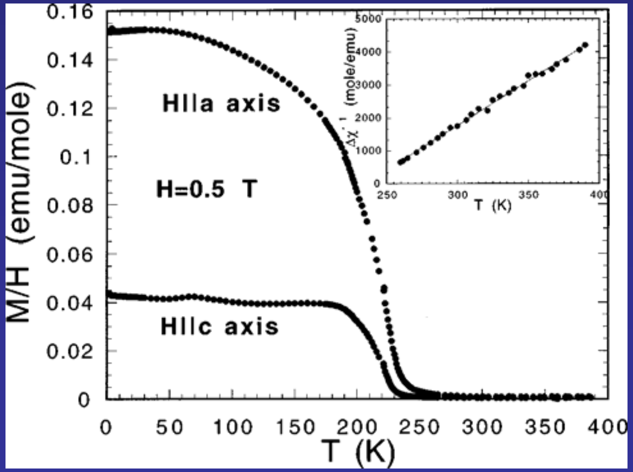
Electric



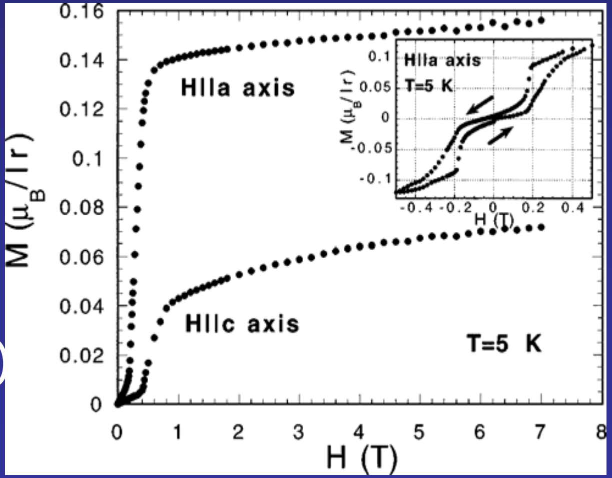
Mott insulator?

Metamagnetic transition
Weakly ferromagnetic
at least H>Hc

Magnetic

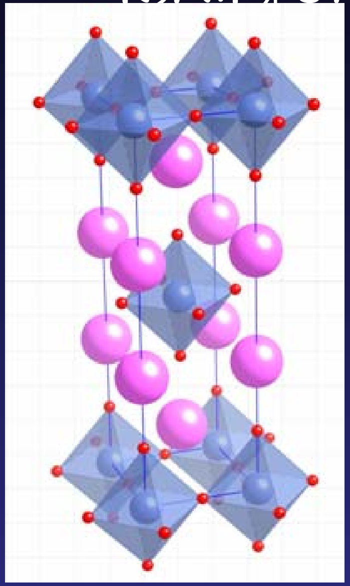


- Tc~240K
- μ_s~0.1 μ_B/Ir
- μ_{eff}=0.5 μ_B/Ir
- Magnetic anisotropy (easy axis along a axis)



Why Sr_2IrO_4 insulating?

K_2NiF_4 structure



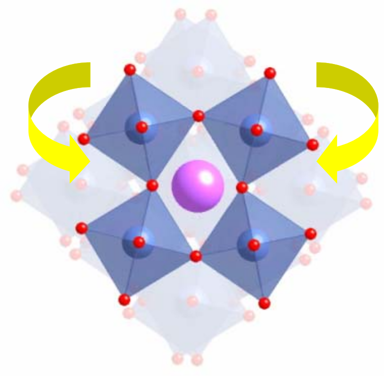
Five d-electrons d^5

3d Sr_2CoO_4 ferromagnetic metal

4d Sr_2RhO_4 paramagnetic metal

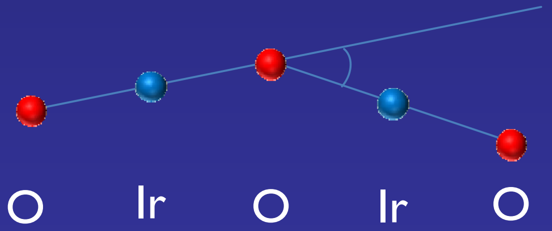
5d Sr_2IrO_4 magnetic insulator

Transfer increase

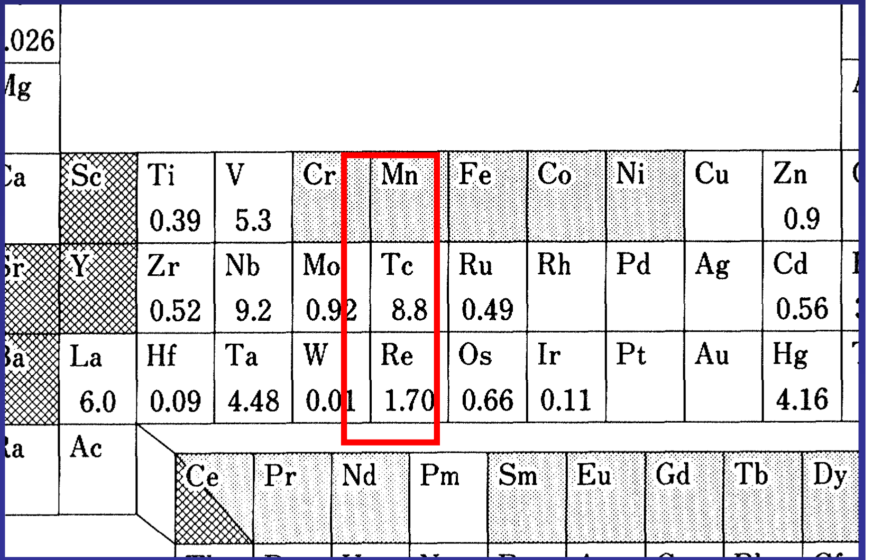


Octahedron rotates 11°

M-O-M bond angle ~ 22°



Sr_2RhO_4 20° !



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g										
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r	Y	Zr 0.52	Nb 9.2	Mo 0.92	Tc 8.8	Ru 0.49	Rh	Pd	Ag	Cd 0.56
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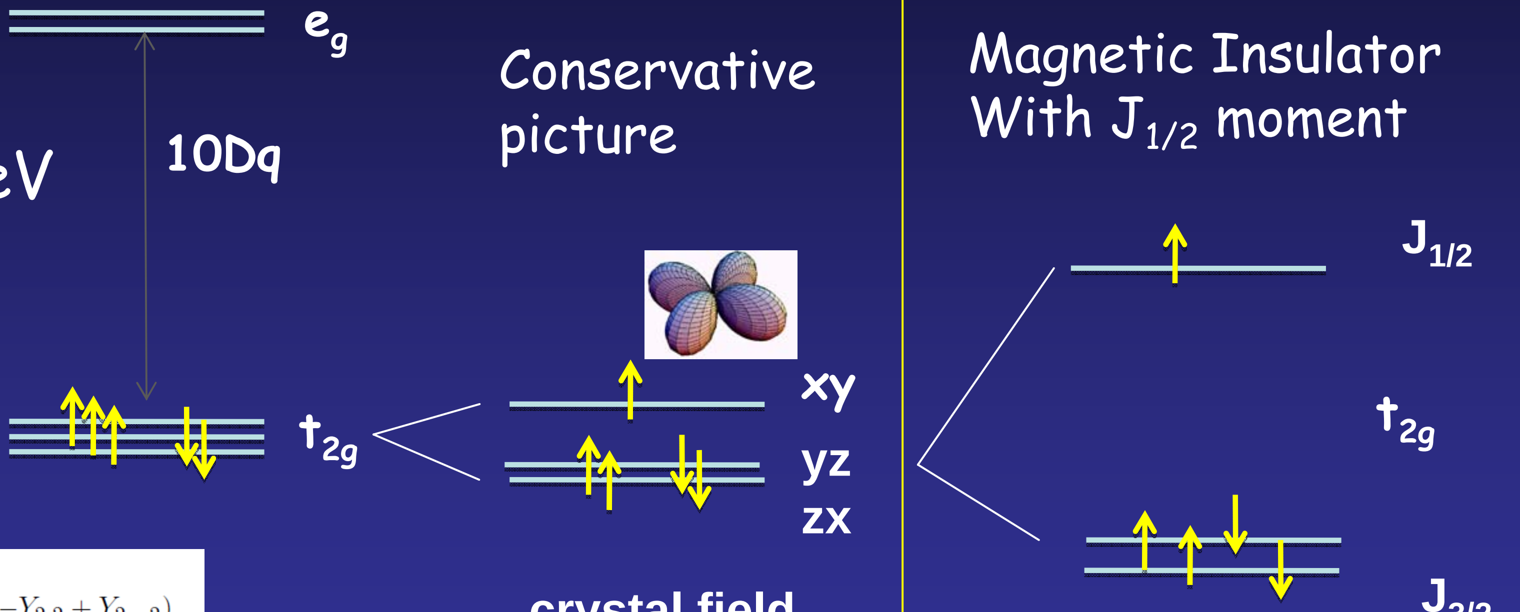
Sr_2IrO_4 Spin-orbit driven Mott insulator?

B.J.KIM

Ir 4+ ($5d^5$), low spin config.



e_g

3-4 eV

10Dq

|0> eff

|1>+|-1>

|1>-|-1>

t_{2g}

Conservative picture

xy

yz

zx

crystal field

S=1/2?

Magnetic Insulator
With $J_{1/2}$ moment

$J_{1/2}$

t_{2g}

$J_{3/2}$

spin-orbit coupling ~0.5 eV
(> crystal field)

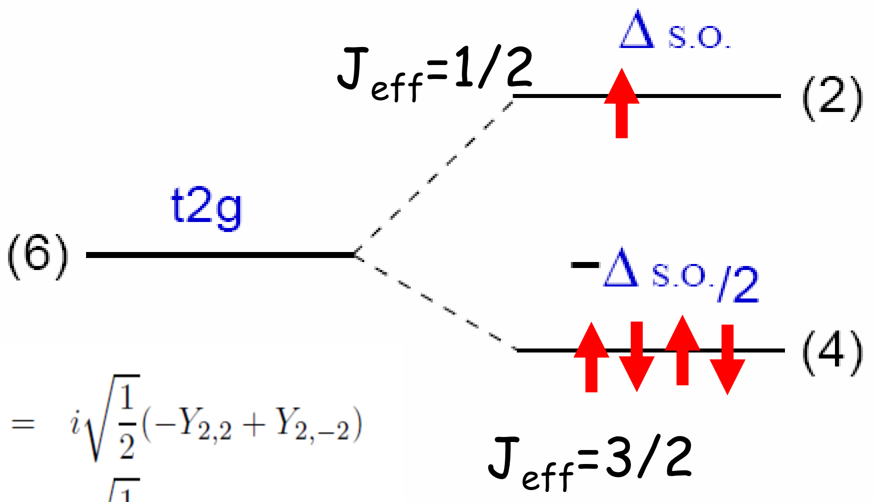
$$
\begin{aligned}
|xy\rangle &= i\sqrt{\frac{1}{2}}(-Y_{2,2}+Y_{2,-2}) \\
|yz\rangle &= i\sqrt{\frac{1}{2}}(Y_{2,1}+Y_{2,-1}) \\
|zx\rangle &= \sqrt{\frac{1}{2}}(-Y_{2,1}+Y_{2,-1})
\end{aligned}
$$

Octrahedron elongated along c
A few to several 100 meV

J_{eff}=1/2 states

$L_{t_{2g}} \rightarrow -L_{2p}$ inverts the energy order of J_{eff} multiplets

$$H_{SO} = \Delta \boldsymbol{L}\cdot\boldsymbol{S} = \left(\begin{array}{ccc|ccc} 0 & \Delta/2 & -i\Delta/2 & & & \\ \Delta/2 & 0 & -i\Delta/2 & & & \\ i\Delta/2 & i\Delta/2 & 0 & & & \\ \hline & & & 0 & -\Delta/2 & i\Delta/2 \\ & & & -\Delta/2 & 0 & i\Delta/2 \\ & & & -i\Delta/2 & -i\Delta/2 & 0 \end{array}\right), basis = \left(\begin{array}{c} xy\uparrow \\ yz\downarrow \\ zx\downarrow \\ \hline xy\downarrow \\ yz\uparrow \\ zx\uparrow \end{array}\right)$$



|xy,↑> + |yz,↓> + i |zx,↓>,
|xy,↓> − |yz,↑> + i|zx,↑>

|yz,↓> + i|zx,↓>
|yz,↑> − i|zx,↑>
|xy,↑> − (|yz,↓> + i|zx,↓>)/2
|xy,↓> + (|yz,↑> − i|zx,↑>)/2

$$|xy\rangle = i\sqrt{\frac{1}{2}}(-Y_{2,2}+Y_{2,-2})$$

$$|yz\rangle = i\sqrt{\frac{1}{2}}(Y_{2,1}+Y_{2,-1})$$

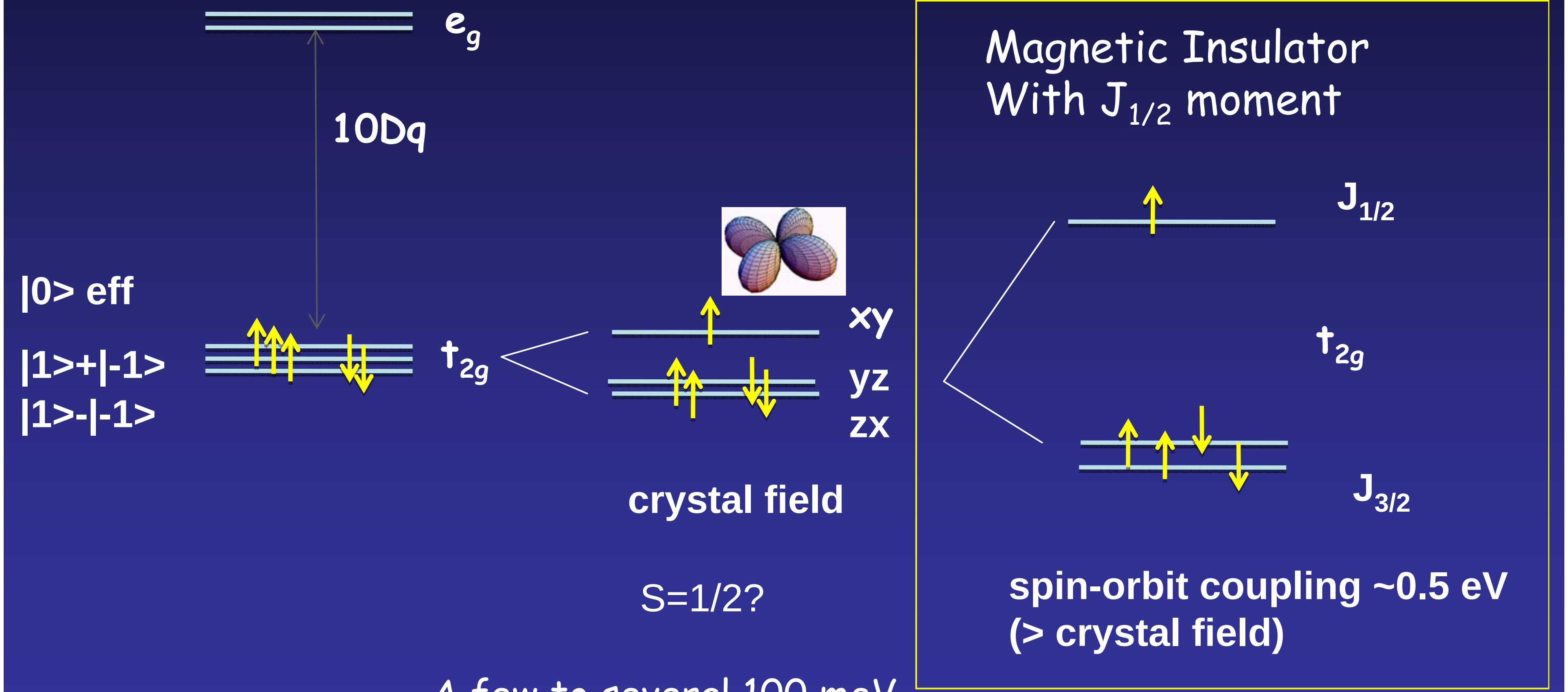
$$|zx\rangle = \sqrt{\frac{1}{2}}(-Y_{2,1}+Y_{2,-1})$$

in strong SO limit

Sr_2IrO_4 Spin-orbit driven Mott insulator?

B.J.KIM

Ir 4+ ($5d^5$), low spin config.



e_g

10Dq

|0> eff

|1>+|-1>

|1>-|-1>

t_{2g}

xy

yz

zx

crystal field

S=1/2?

A few to several 100 meV

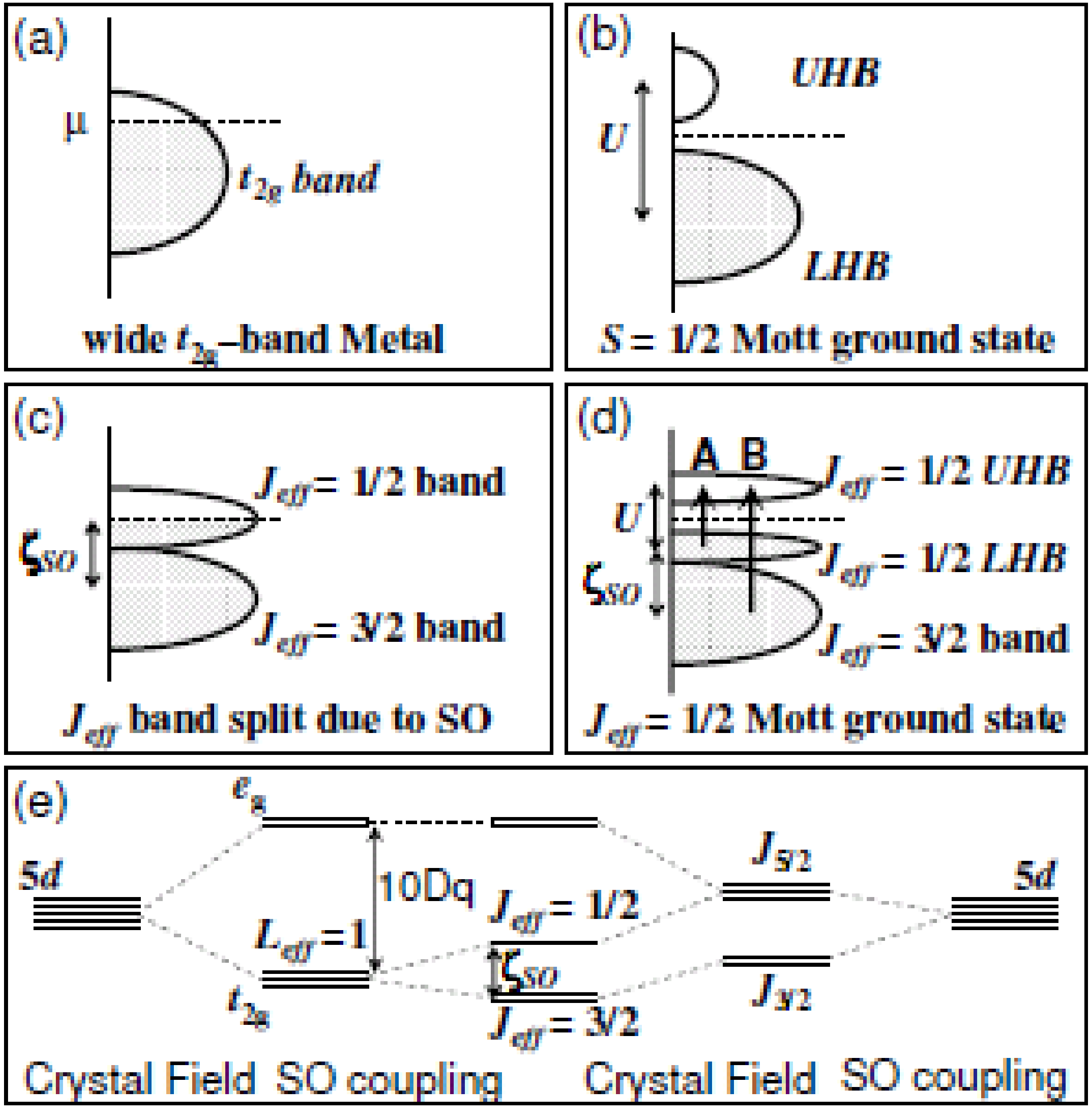
Magnetic Insulator
With $J_{1/2}$ moment

$J_{1/2}$

t_{2g}

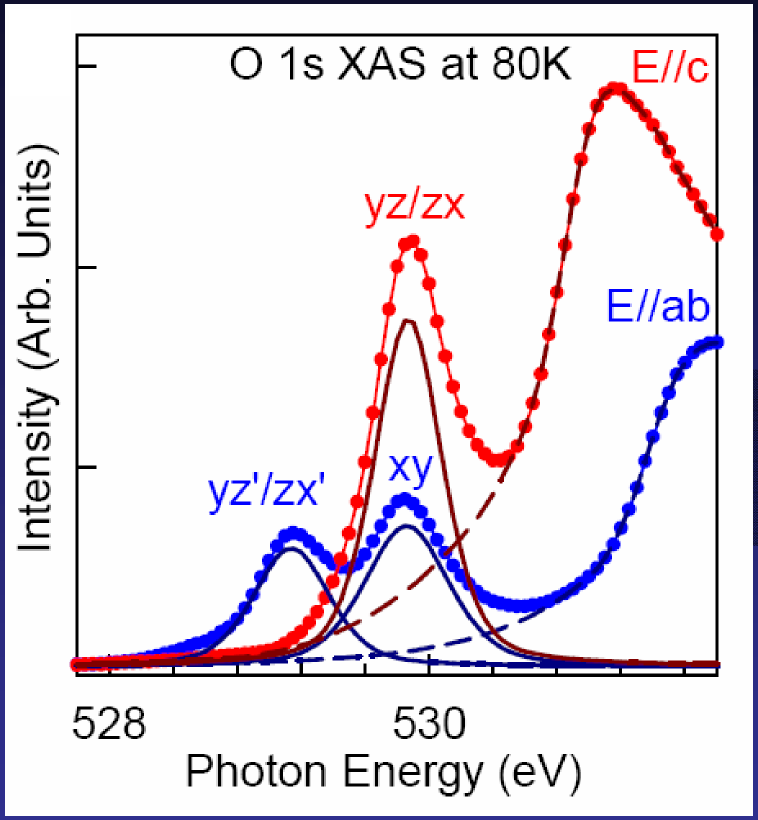
$J_{3/2}$

spin-orbit coupling ~0.5 eV
(> crystal field)


(a)
μ
t_{2g} band
wide t_{2g}–band Metal
(b)
UHB
U
LHB
$S = 1/2$ Mott ground state
(c)
$J_{eff} = 1/2$ band
ζ_{SO}
$J_{eff} = 3/2$ band
J_{eff} band split due to SO
(d)
A
B
$J_{eff} = 1/2$ UHB
U
$J_{eff} = 1/2$ LHB
ζ_{SO}
$J_{eff} = 3/2$ band
$J_{eff} = 1/2$ Mott ground state
(e)
e_g
5d
10Dq
$J_{eff} = 1/2$
$L_{eff} = 1$
ζ_{SO}
t_{2g}
$J_{eff} = 3/2$
$J_{5/2}$
$J_{3/2}$
5d
Crystal Field
SO coupling
Crystal Field
SO coupling

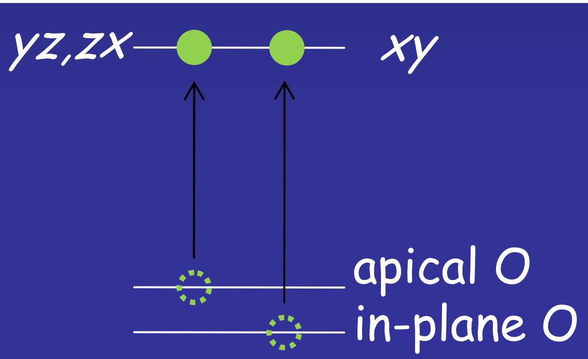
B.J.KIM

X-ray Absorption Spectroscopy cosistent with 1:1:1 xy yz zx



$$J_{eff1/2} = \frac{1}{\sqrt{3}}\left(|xy,\pm 1/2\rangle \pm |yz,\mp 1/2\rangle + i|zx,\mp 1/2\rangle \right)$$

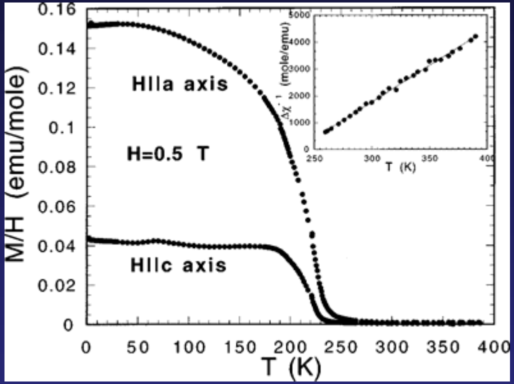
Characteristic orbital state with xy:yz:zx=1:1:1 ratio of $J_{eff}=1/2$ is confirmed by O K-edge XAS



B.J.KIM

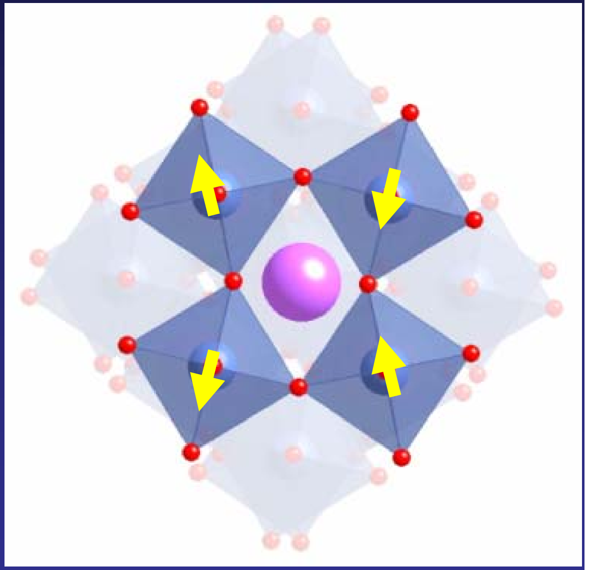
Points to be clarified

$$J_{eff1/2}=\frac{1}{\sqrt{3}}\left(|xy,\pm 1/2\rangle \pm |yz,\mp 1/2\rangle + i|zx,\mp 1/2\rangle\right) \qquad \langle L_z\rangle=\frac{2}{3},\langle S_z\rangle=\frac{1}{6},\langle L_z+2S_z\rangle=1$$



1. Magnetism??

J_{eff}=1/2 canted
AF magnet because of rotation of octahedra?



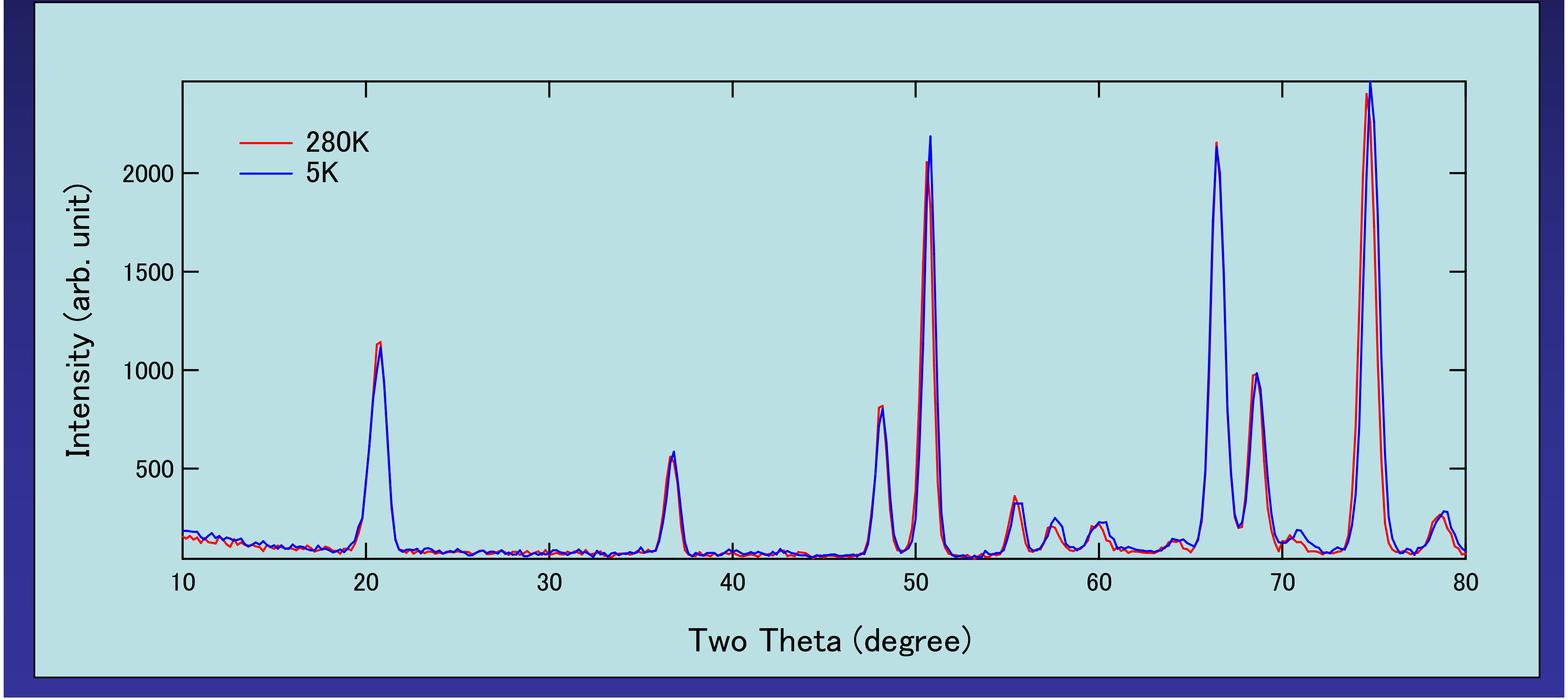
2. Determination of wave function?

complex phase
L S separation

Neutron could not detect magnetic signal

Ir is strong neutron absorber
Moment small (1/2?)
Large single crystal not available

Neutron does not distinguish L and S



Points to be clarified

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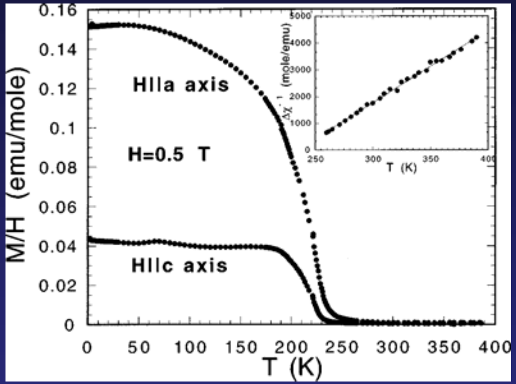

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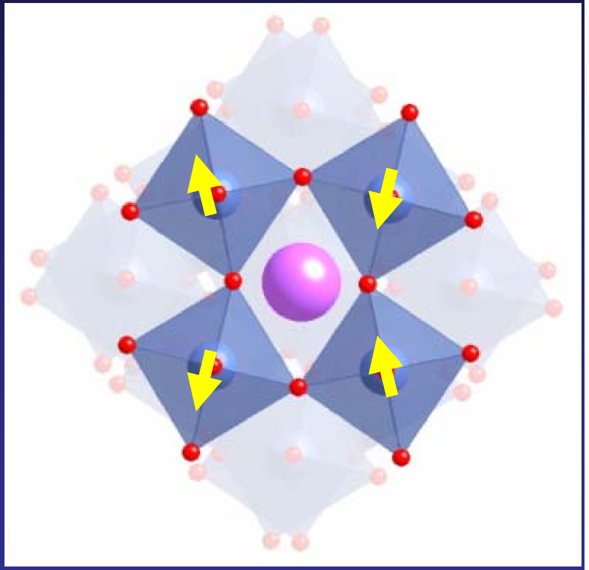
J_{eff}=1/2 canted
AF magnet because of rotation of octahedra?

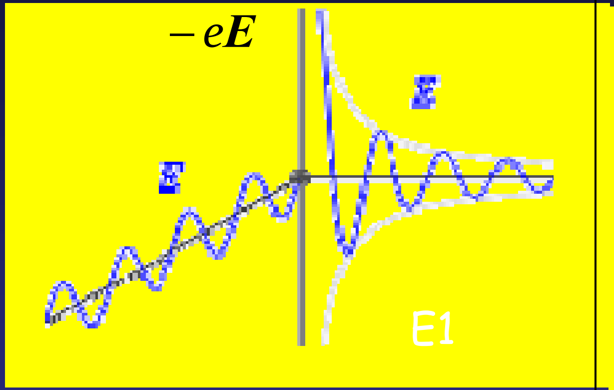


2. Determination of wave function?

complex phase
L S separation

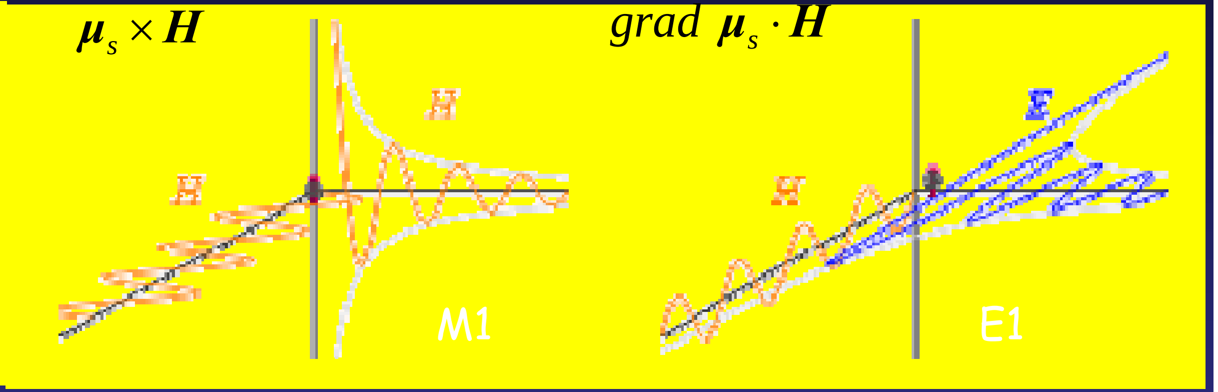
X-ray scattering by electrons

Charge scattering
(Thomson scattering)



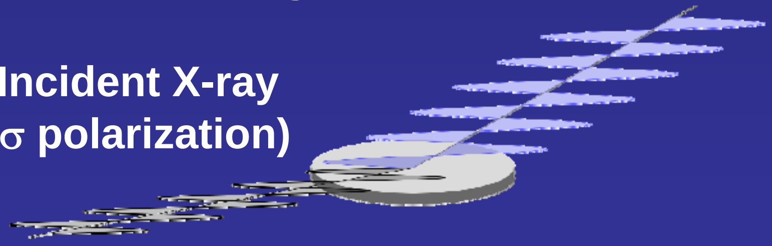
Charge amplitude $\sim N_{total}$

Magnetic scattering



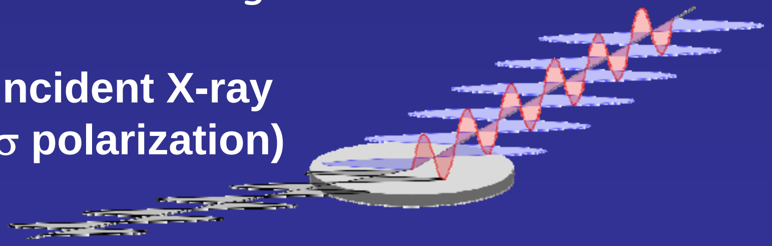
$$\text{Magnetic amplitude} \sim N_{mag} \cdot \frac{\hbar\omega}{mc^2} \sim \frac{\text{Charge amplitude}}{1000}$$

Not induce orthogonal waves



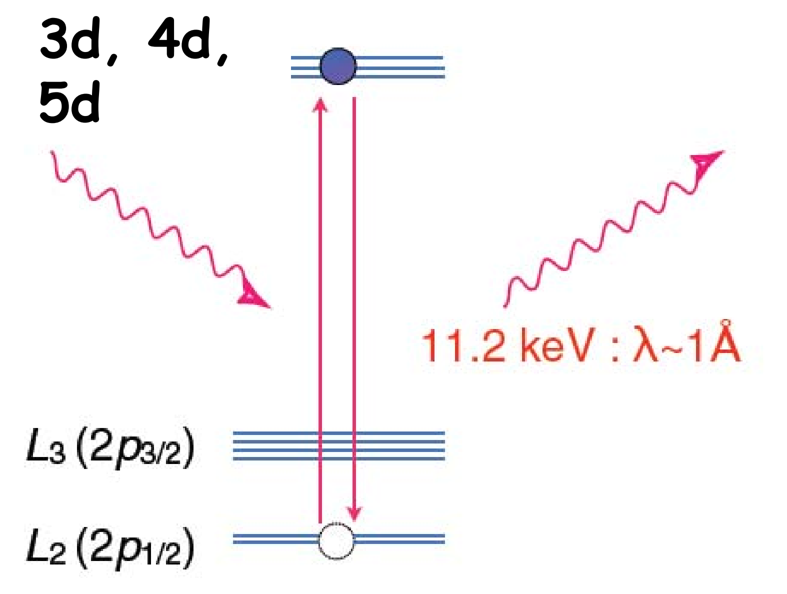
Incident X-ray
(σ polarization)

Induce orthogonal waves



Incident X-ray
(σ polarization)

Resonant magnetic x-ray



$$f_{\alpha\beta} = \sum_m \frac{m_e \omega_{im}^3}{\omega} \frac{\langle i | R_\beta | m \rangle \langle m | R_\alpha | i \rangle}{\hbar\omega - \hbar\omega_{im} + i\Gamma/2} .$$

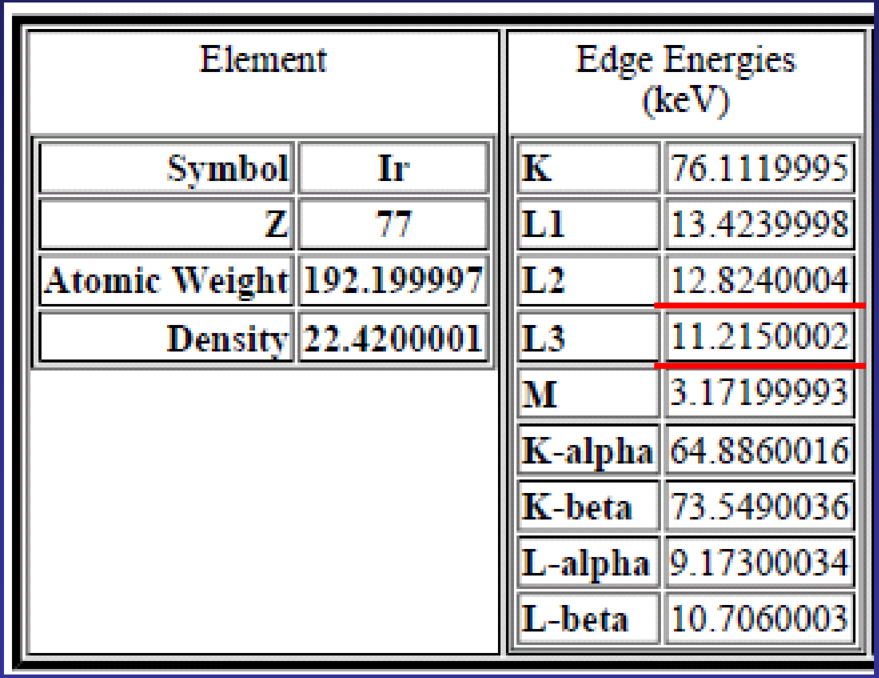
Enhance signal from t_{2g} in charge of magnetism
can gain more magnetic scattering

Can expect quantum interference through intermediate state
detection of phase

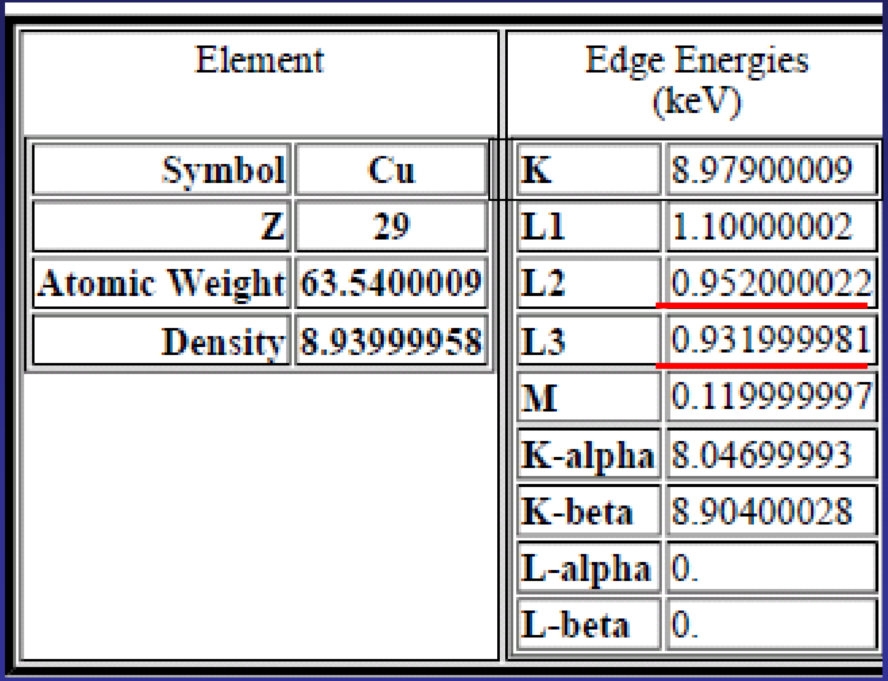
Ir compounds as an ideal playground for magnetic x-ray diffraction using L-edge (2p→d)

Ir wave length 0.1 nm because of high energy!!

3d Cu as long as 1nm!! Only long wave length modulation
the same is true for 4f

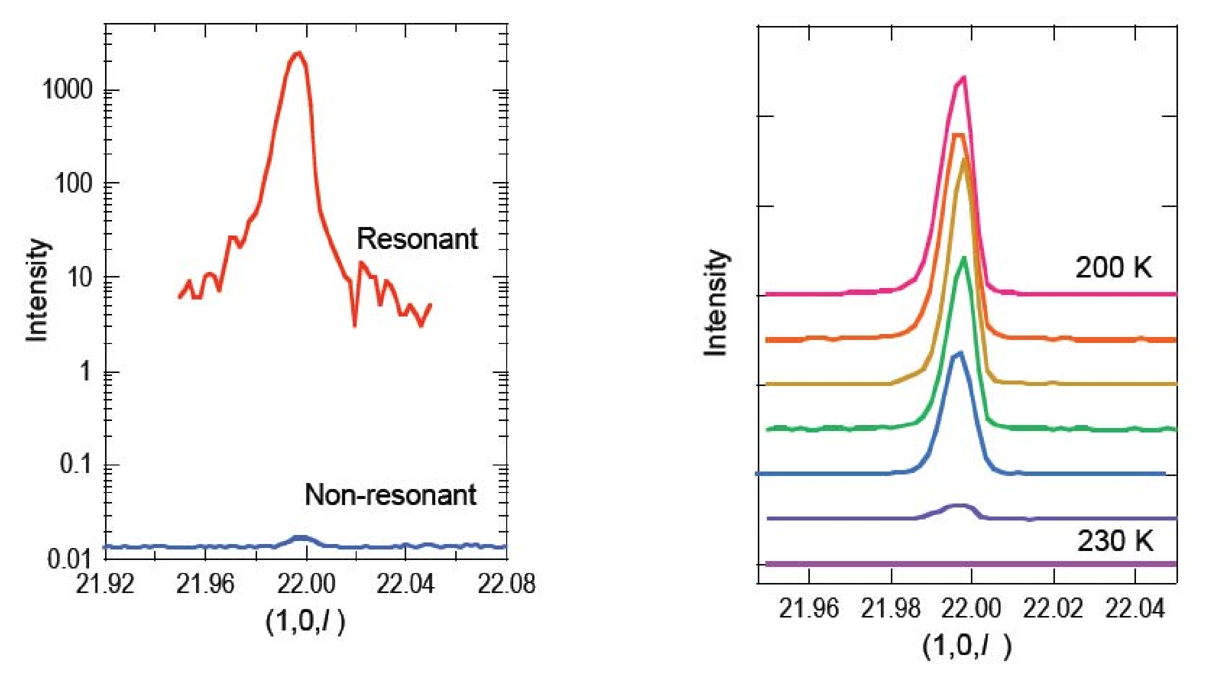


Element		Edge Energies (keV)	
Symbol	Ir	K	76.1119995
Z	77	L1	13.4239998
Atomic Weight	192.199997	L2	12.8240004
Density	22.4200001	L3	11.2150002
		M	3.17199993
		K-alpha	64.8860016
		K-beta	73.5490036
		L-alpha	9.17300034
		L-beta	10.7060003

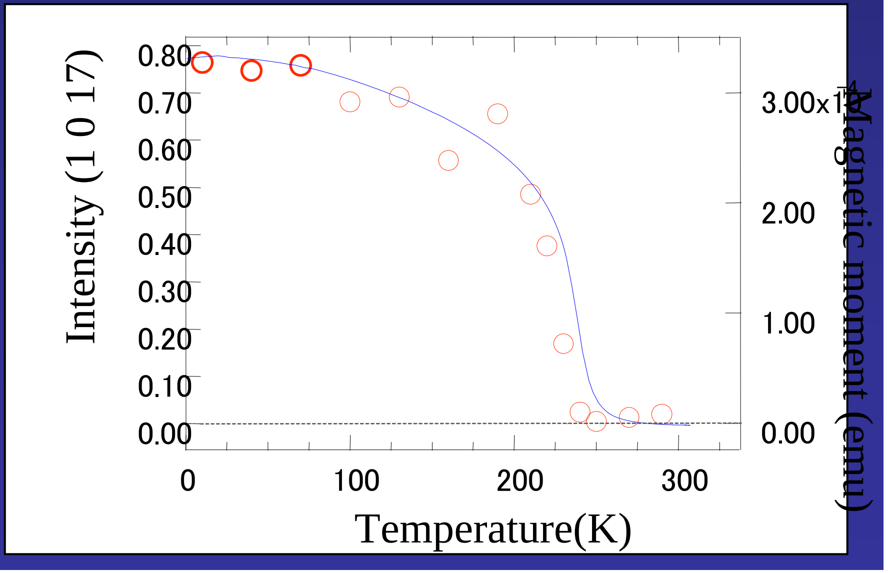


Element		Edge Energies (keV)	
Symbol	Cu	K	8.97900009
Z	29	L1	1.10000002
Atomic Weight	63.5400009	L2	0.952000022
Density	8.93999958	L3	0.931999981
		M	0.119999997
		K-alpha	8.04699993
		K-beta	8.90400028
		L-alpha	0.
		L-beta	0.

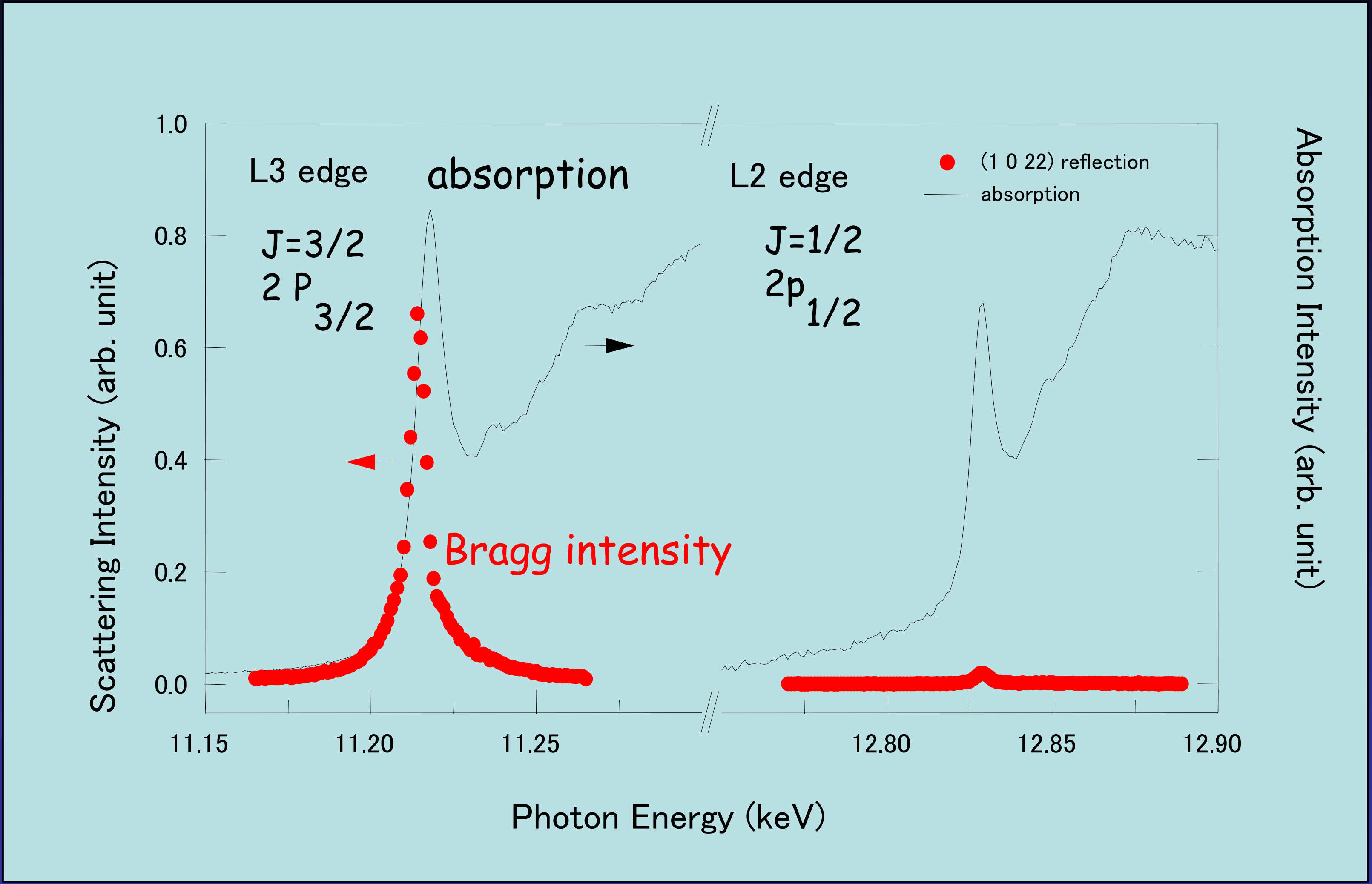
Gigantic enhancement of magnetic x-ray diffraction peak



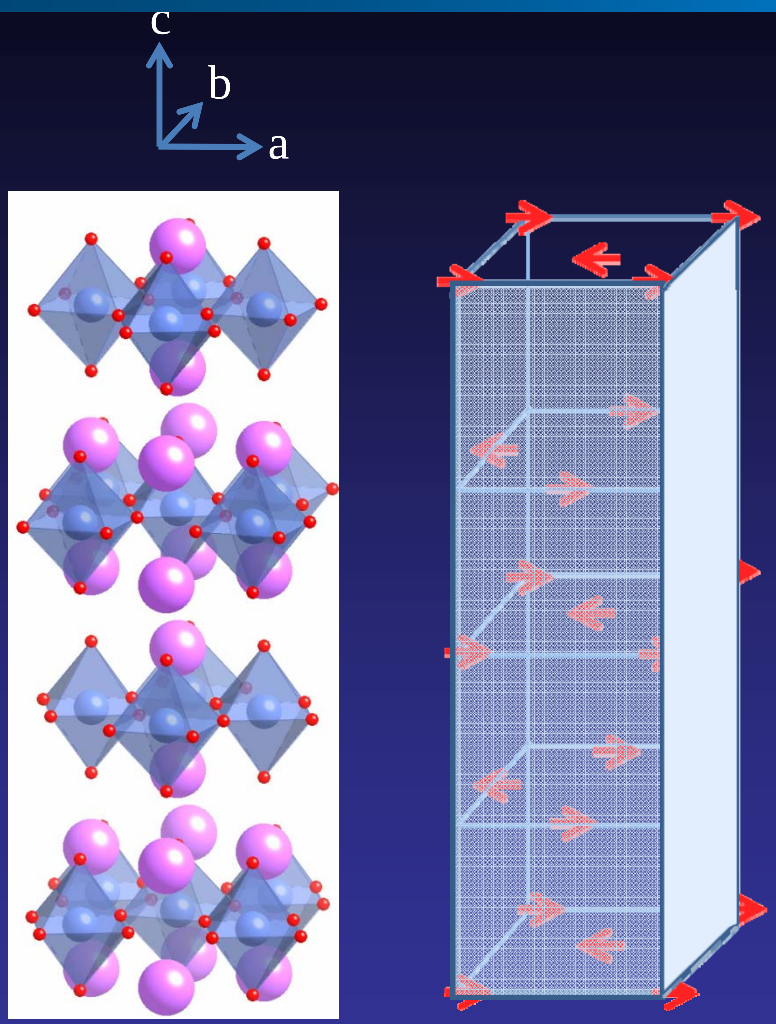
10^6 enhancement
due to resonance

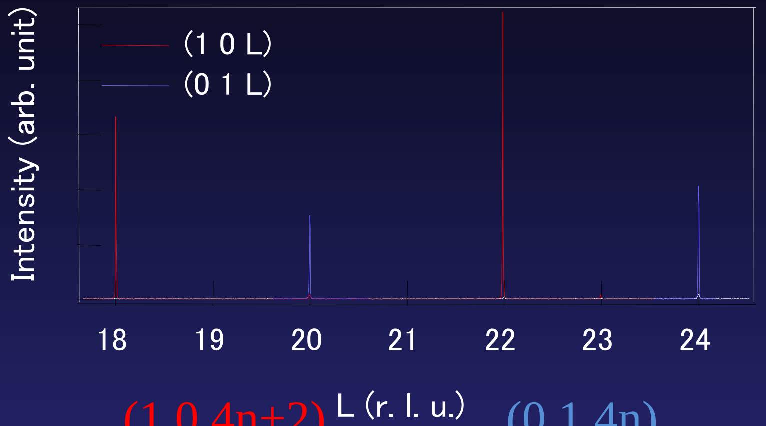


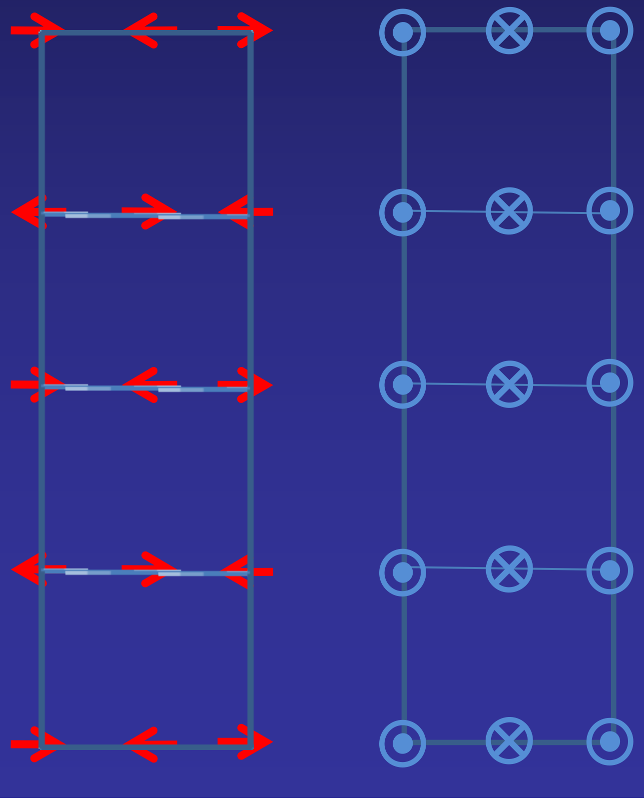
Gigantic enhancement of magnetic x-ray diffraction



Magnetic Bragg peak consistent with canted AF

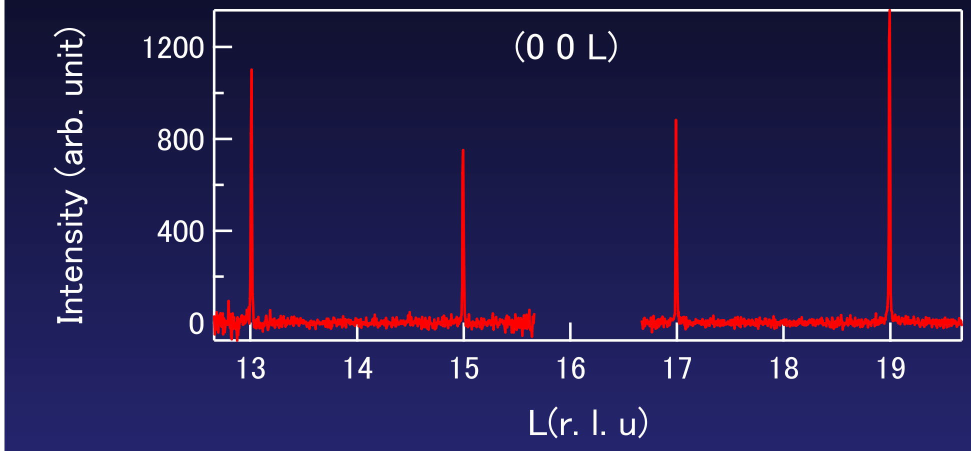


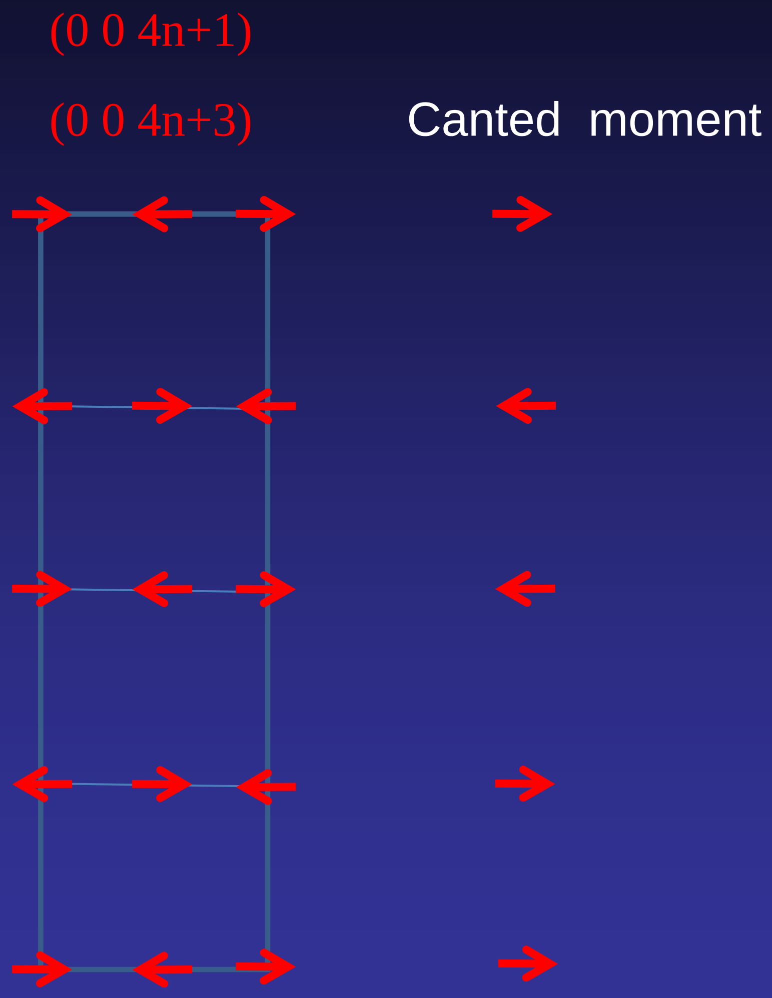




Stacking of 2D AF layers
Along c-axis

Magnetic Bragg peak consistent with canted AF




(0 0 4n+1)

(0 0 4n+3)

Canted moment

up up down down
stacking of canted moments
along c-axis

Magnetic structure

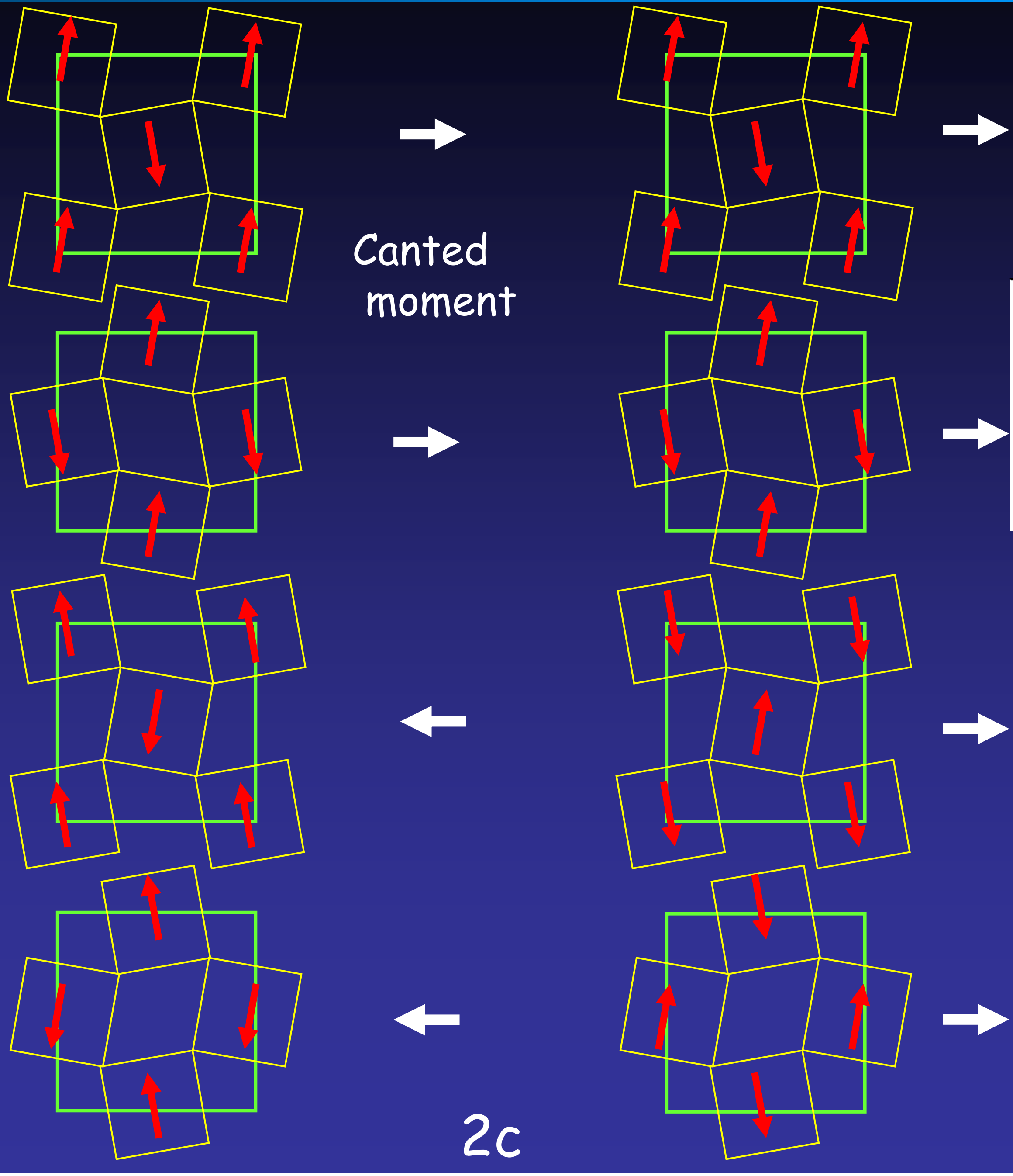
H=0

1st IrO$_2$layer

2nd IrO$_2$layer

3rd IrO$_2$layer

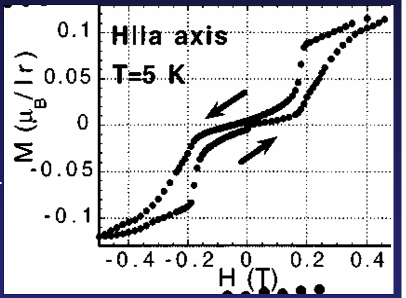
4th IrO$_2$layer



Canted moment

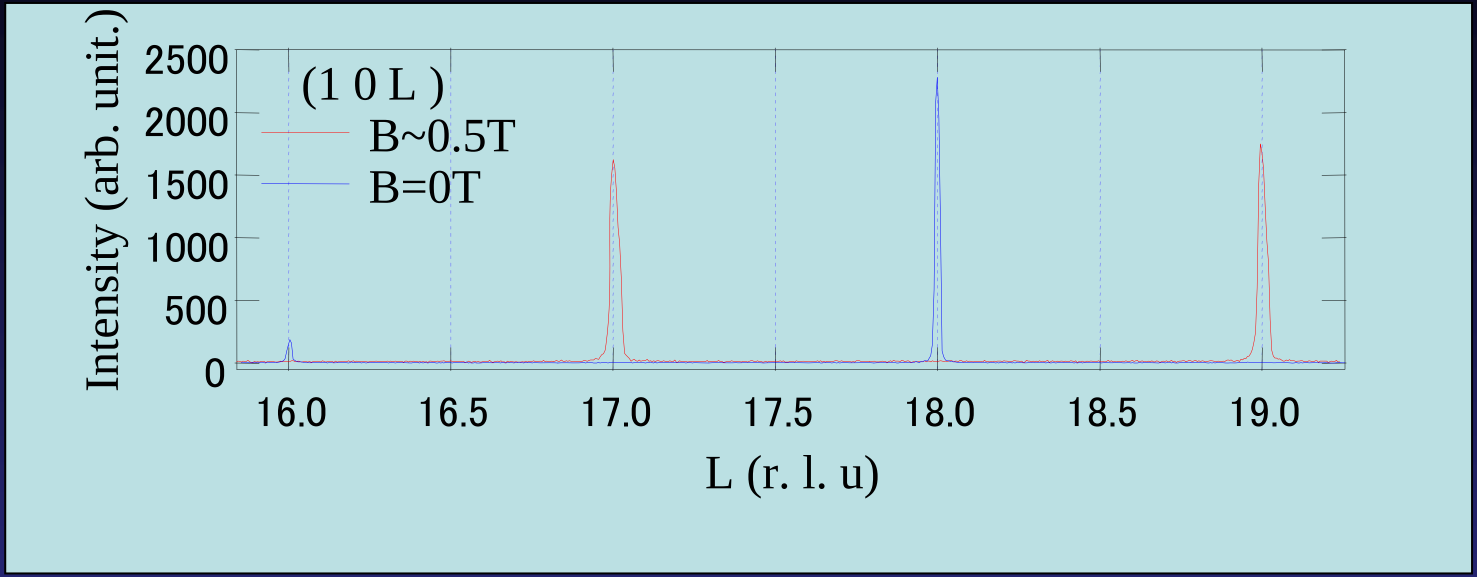
2c

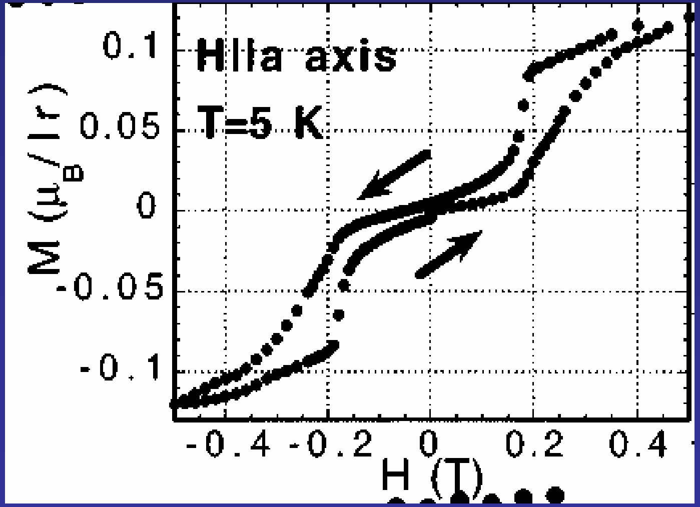
H>Hc
Meta
-magnetic



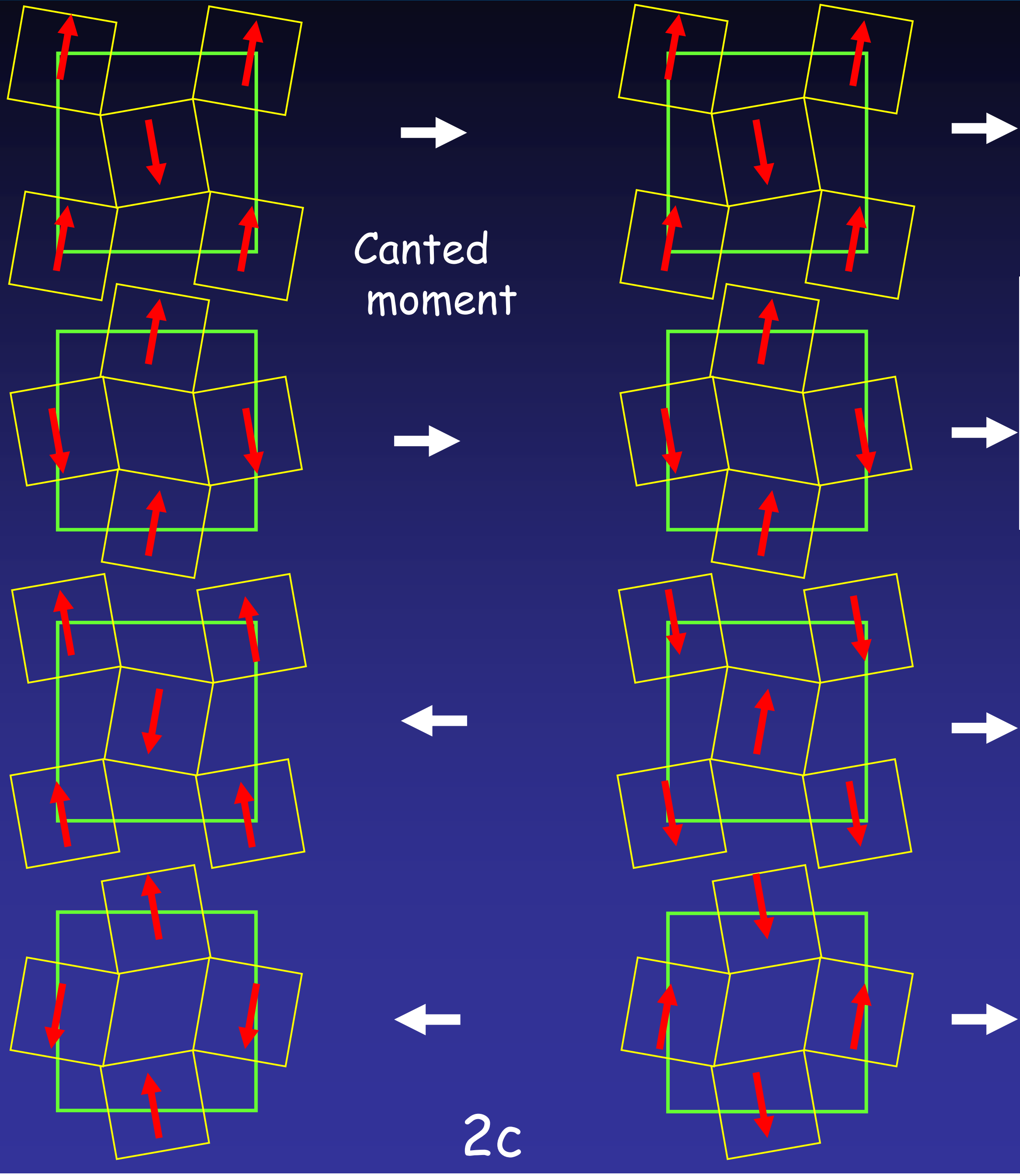
c

Metamagnetism seen in magnetic x-ray diffraction





Magnetic structure



H=0

1st IrO_2layer

2nd IrO_2layer

3rd IrO_2layer

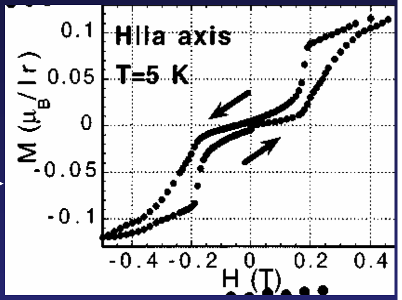
4th IrO_2layer

Canted moment

2c

H>Hc
Meta
-magnetic

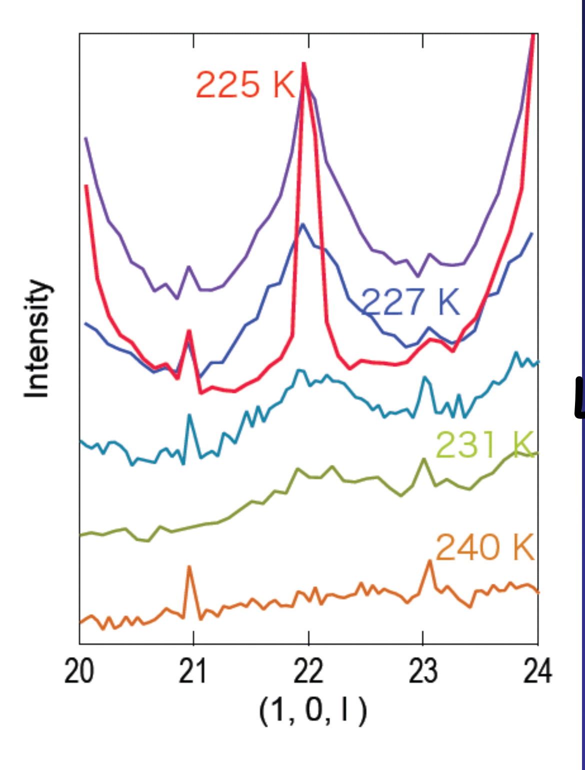
c

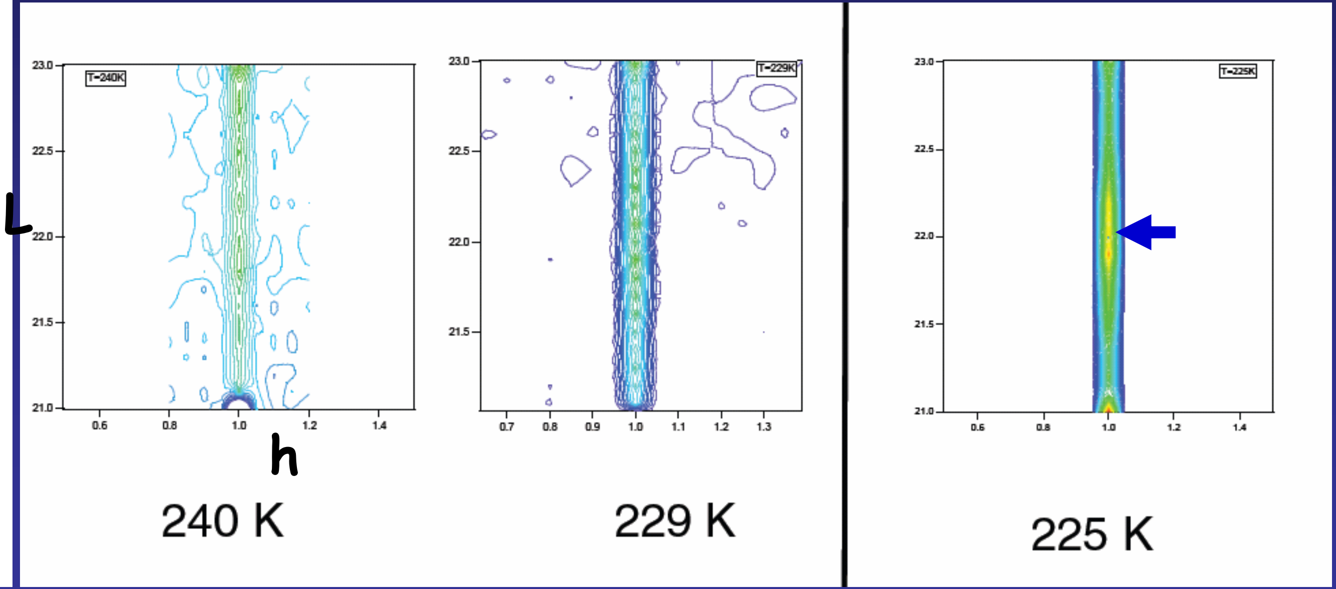


2D spin correlations observed by magnetic diffuse x-ray scattering

with 100 μm size crystals!!!

Contour plot in (h,0, l) plane



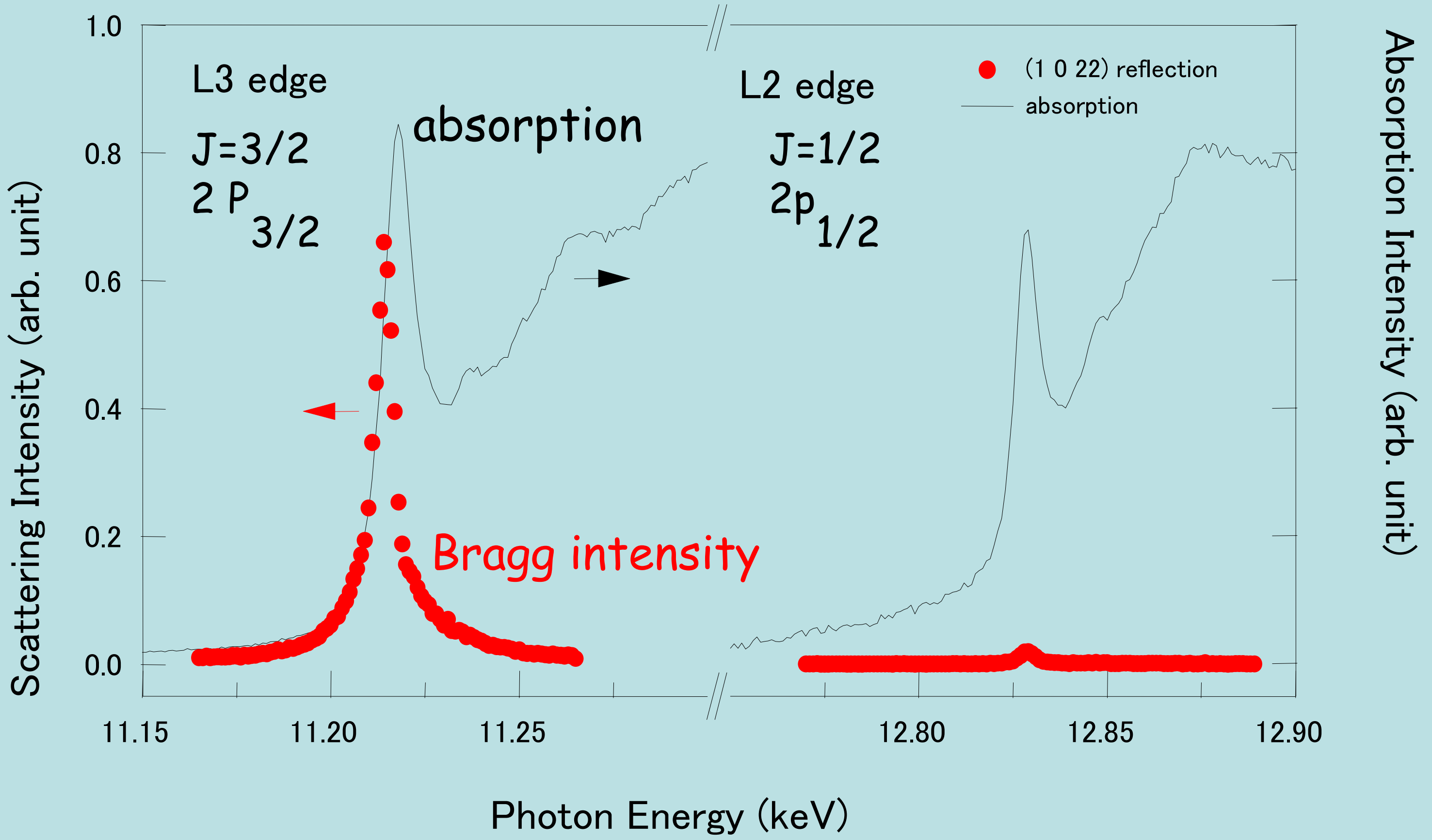


Diffuse scattering
Dynamic magnetic correlation

$T>T_N$
2D rod

$T<T_N$
Bragg point

Selection rule for magnetic x-ray diffraction



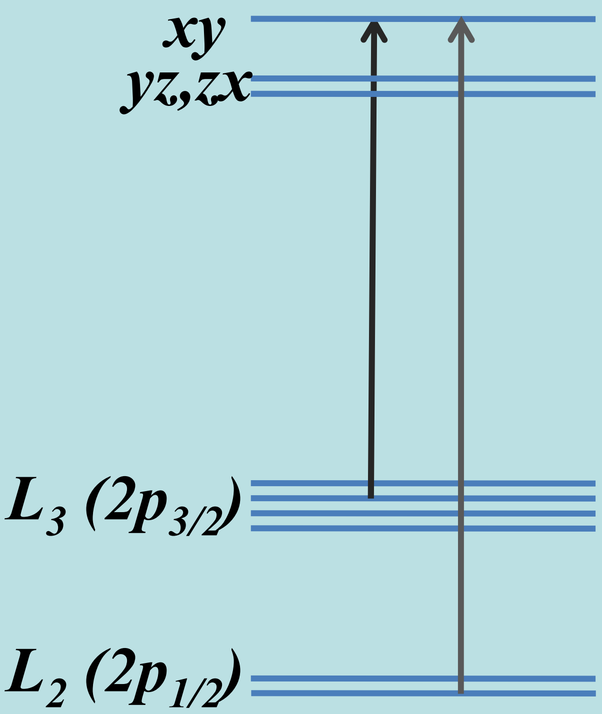
Beyond neutron!

Almost no resonance at L_2:

L_2 scattering intensity is only about 1% of that of the L_3.

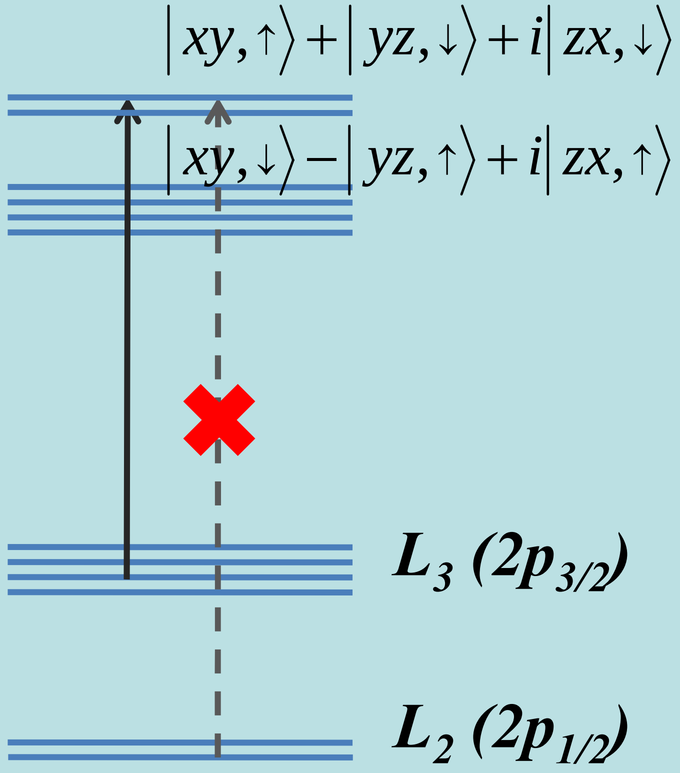
Selection rule in magnetic x-ray scattering

$S=1/2$



1:1 intensity ratio between L3 and L2 is expected

$J_{eff}=1/2$



Zero intensity at L2 is expected

Extinction rule for L2 and L3 edges

$$f_{\alpha\beta} = \sum_m \frac{m_e \omega_{im}^3}{\omega} \frac{\langle i|R_\beta|m\rangle\langle m|R_\alpha|i\rangle}{\hbar\omega - \hbar\omega_{im} + i\Gamma/2}.$$

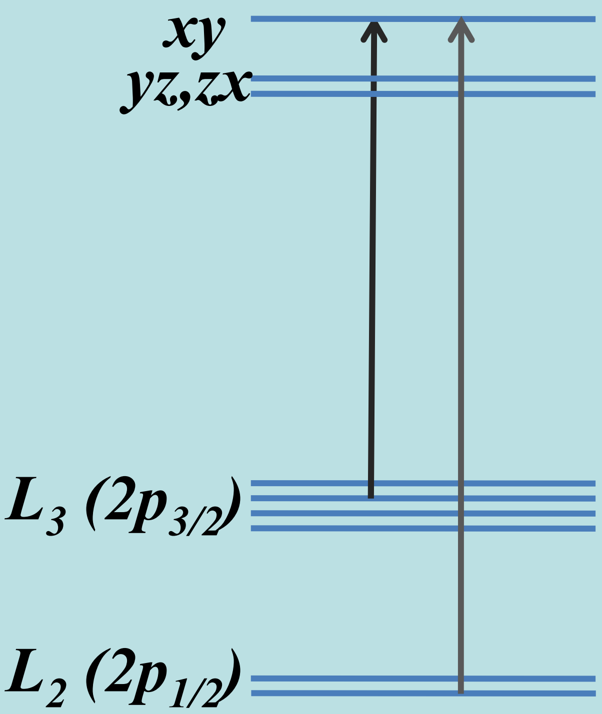
$$c_1|xy,\uparrow\rangle + c_2|yz,\downarrow\rangle + c_3|zx,\downarrow\rangle.$$

$$f^{L2}_{\alpha\beta} = \frac{1}{6}\begin{pmatrix} (c_1 + ic_3)(c_1^* - ic_3^*) & (ic_1^* + c_3^*)(c_1 - c_2) & 0 \\ (-ic_1 + c_3)(c_1^* - c_2^*) & (c_1 - c_2)(c_1^* - c_2^*) & 0 \\ 0 & 0 & (c_2 + ic_3)(c_2^* - ic_3^*) \end{pmatrix}.$$

S=1/2 model(xy orbital)	J_{eff}=1/2 model
L3 $f^{\alpha\beta}_{(L_3)} = \begin{pmatrix} 1/3 & i/6 & 0 \\ -i/6 & 1/3 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$f^{\alpha\beta}_{(L_3)} = \begin{pmatrix} 1/3 & i/6 & 0 \\ -i/6 & 1/3 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
L2 $f^{\alpha\beta}_{(L_2)} = \begin{pmatrix} 1/6 & i/6 & 0 \\ -i/6 & 1/6 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$f^{\alpha\beta}_{(L_2)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

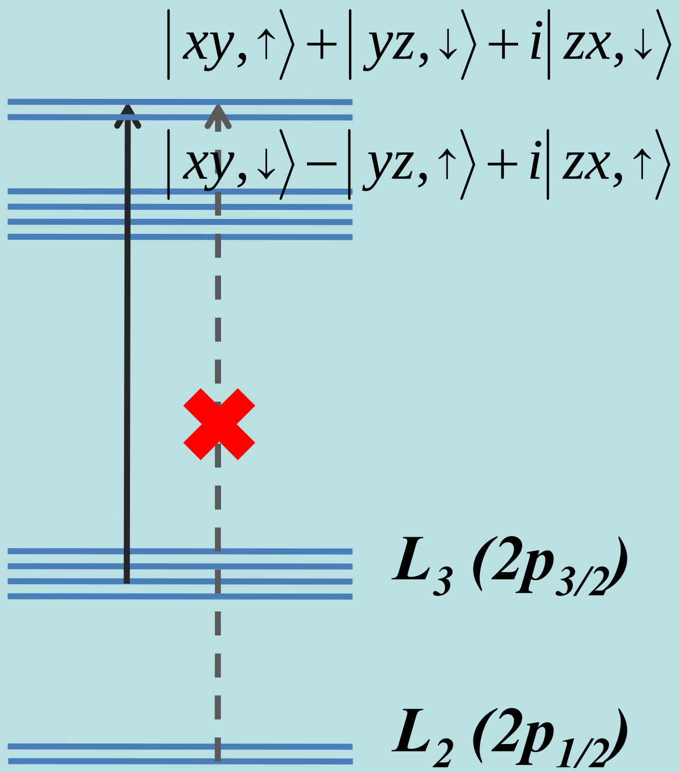
Selection rule consistent with $J_{eff}=1/2$

$S=1/2$



1:1 intensity ratio between L3 and L2 is expected

$J_{eff}=1/2$



Zero intensity at L2 is expected

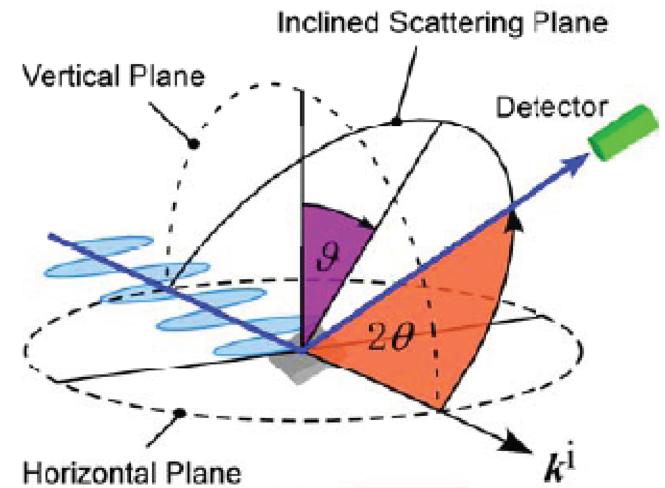
LS decoupling by “non-resonant” scattering

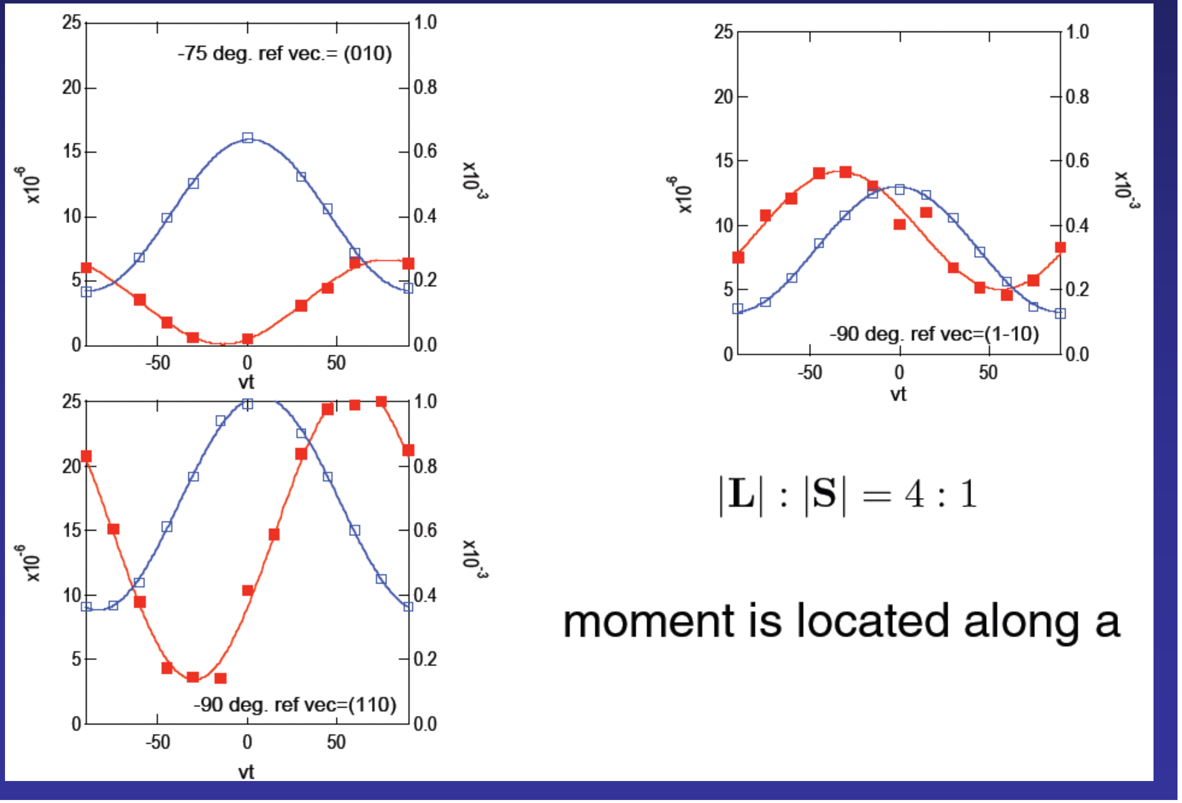
$$\begin{pmatrix} E'_\sigma \\ E'_\pi \end{pmatrix} = \begin{pmatrix} S_2 \sin 2\theta & -2\sin^2\theta\left[(S_1+L_1)\cos\theta - S_3\sin\theta\right] \\ 2\sin^2\theta\left[(S_1+L_1)\cos\theta + S_3\sin\theta\right] & \left[2L_2\sin^2\theta\cos\theta + S_2\right]\sin 2\theta \end{pmatrix}\begin{pmatrix} E_\sigma \\ E_\pi \end{pmatrix}$$

M. Blume and Doon Gibbs, Phys. Rev. B **37**, 1779 (1988).

$$J_{eff1/2} = \frac{1}{\sqrt{3}}\left(|xy,\pm1/2\rangle \pm |yz,\mp1/2\rangle + i|zx,\mp1/2\rangle\right)$$

$$\langle L_z\rangle = \frac{2}{3}, \langle S_z\rangle = \frac{1}{6}, \langle L_z + 2S_z\rangle = 1$$





$$|\mathbf{L}| : |\mathbf{S}| = 4:1$$

moment is located along a

Summary of Sr_2IrO_4

"J_{eff}=1/2" Mott insulator not S=1/2 Mott insulator

Wave function
$$J_{eff1/2} = \frac{1}{\sqrt{3}}\left(\left| xy, \pm 1/2 \right\rangle \pm \left| yz, \mp 1/2 \right\rangle + i \left| zx, \mp 1/2 \right\rangle \right)$$

in strong SOC limit

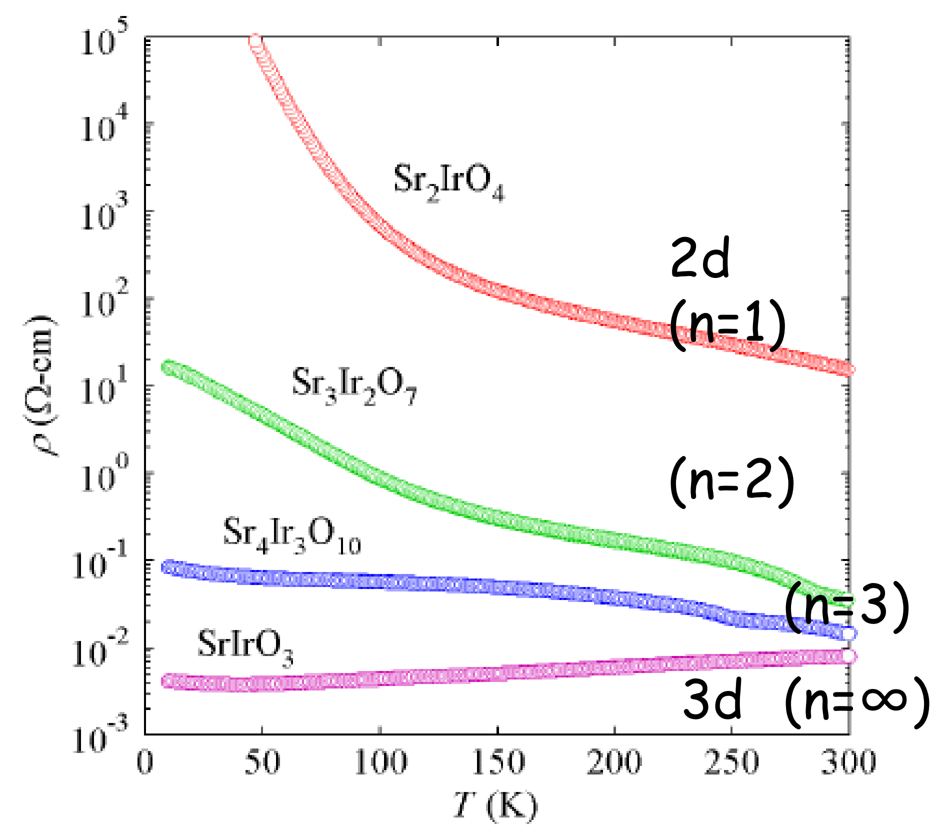
- interplay between coulomb U and a large SOC

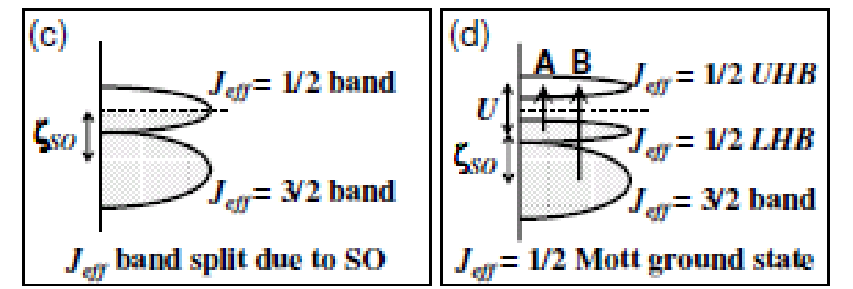
-Why crystal field splitting ~ a few 100 meV, comparable to SOC, behave as if the were absent??

J_{eff} =1/2 Canted antiferromagnet

Perfect playground for magnetic x-ray because of L-edge being hard x-ray region

Mott transition within J_{eff}=1/2 band - increase dimensionality

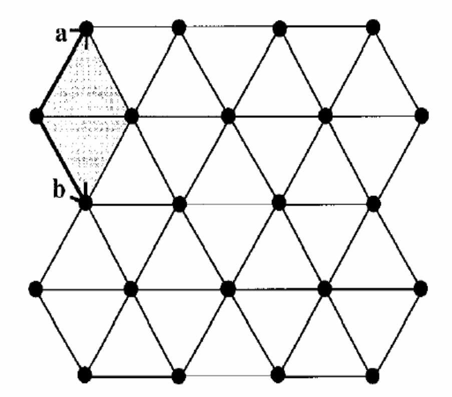




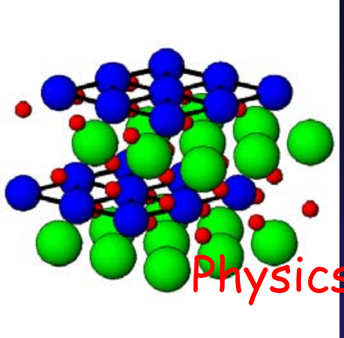
Metallic state can be described as a half filled J_{eff}=1/2 band?
If so, any exotic transport due to strong SOC??
Thin film without inversion symmetry??

Develop compounds with more exotic structure?

Geometrically Frustrated Lattices

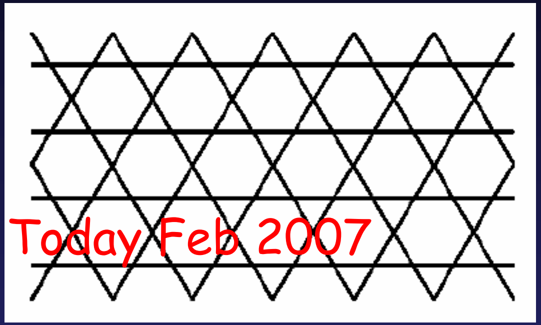


2D Triangular lattice

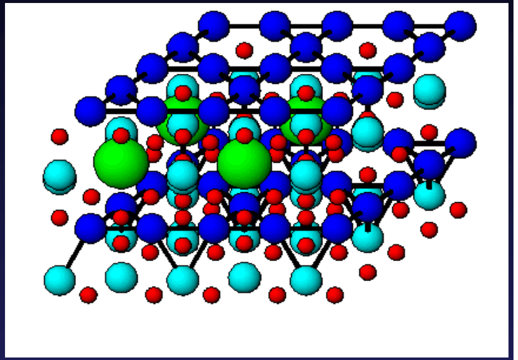


$NiGa_2S_4$, BEDT-TTFCu(NCS) $NaTiO_2$

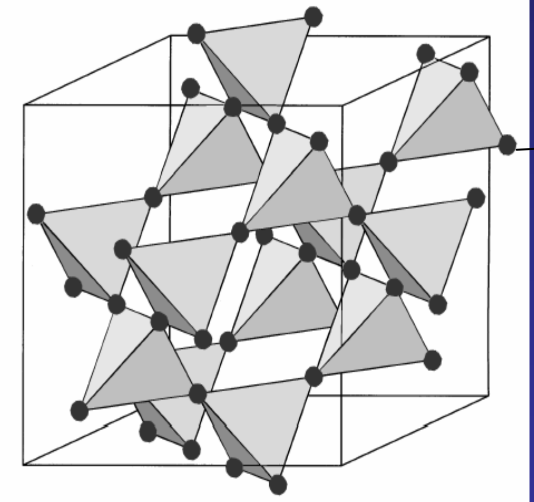
Physics Today Feb 2007



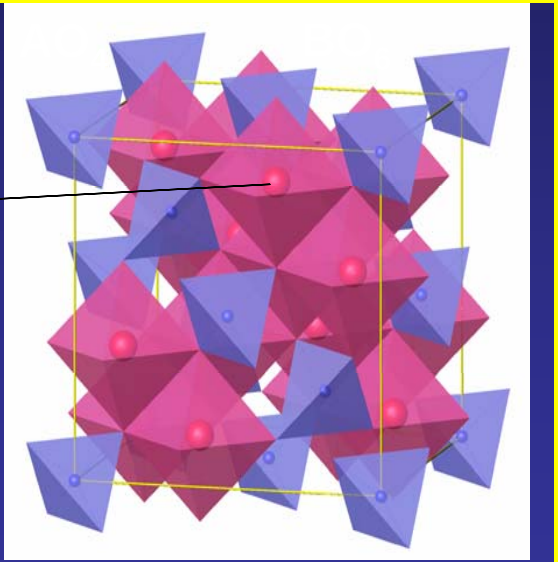
2D Kagome lattice



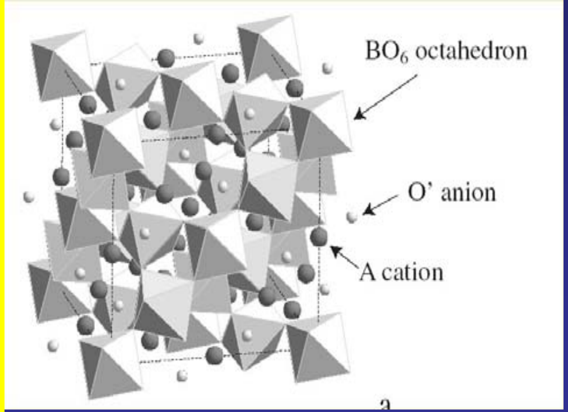
$ZnCu_3(OH)_6Cl_2$
$SrCr_9Ga_3O_{19}$,



3D Pyrochlore lattice



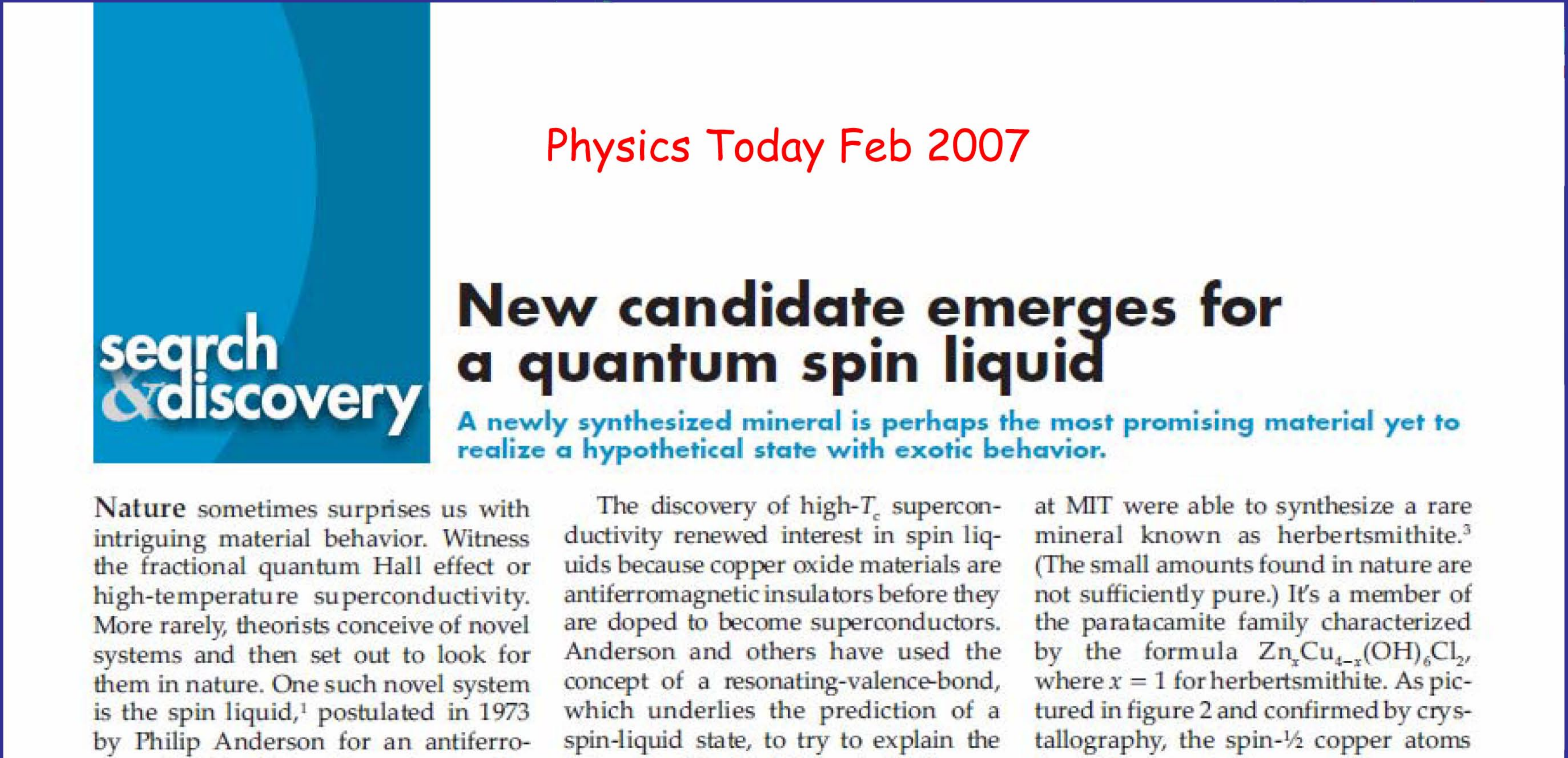
Spinel (AB_2O_4)
Fe_3O_4=$FeFe_2O_4$



Pyrochlore($A_2B_2O_7$)
$Y_2Mo_2O_7$

a wide variety of materials, most popular oxide structure

Geometrically Frustrated Lattices



Physics Today Feb 2007

search & discovery

New candidate emerges for a quantum spin liquid

A newly synthesized mineral is perhaps the most promising material yet to realize a hypothetical state with exotic behavior.

Nature sometimes surprises us with intriguing material behavior. Witness the fractional quantum Hall effect or high-temperature superconductivity. More rarely, theorists conceive of novel systems and then set out to look for them in nature. One such novel system is the spin liquid,[1] postulated in 1973 by Philip Anderson for an antiferro-

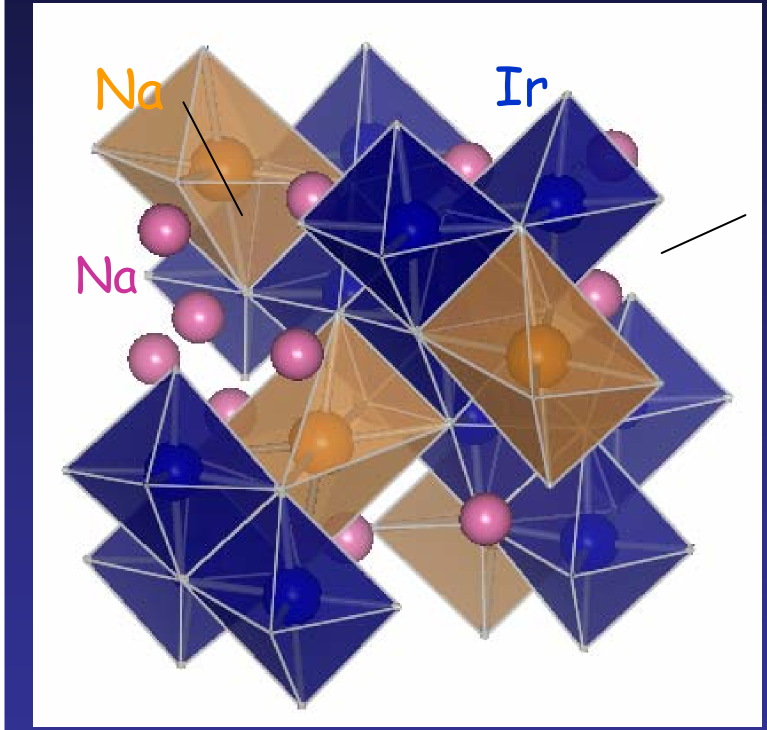
The discovery of high-T_c superconductivity renewed interest in spin liquids because copper oxide materials are antiferromagnetic insulators before they are doped to become superconductors. Anderson and others have used the concept of a resonating-valence-bond, which underlies the prediction of a spin-liquid state, to try to explain the

at MIT were able to synthesize a rare mineral known as herbertsmithite.[3] (The small amounts found in nature are not sufficiently pure.) It's a member of the paratacamite family characterized by the formula $Zn_xCu_{4-x}(OH)_6Cl_2$, where $x = 1$ for herbertsmithite. As pictured in figure 2 and confirmed by crystallography, the spin-½ copper atoms

$Na_4Ir_3O_8$: Ir^{4+} oxide with hyper-kagome structure

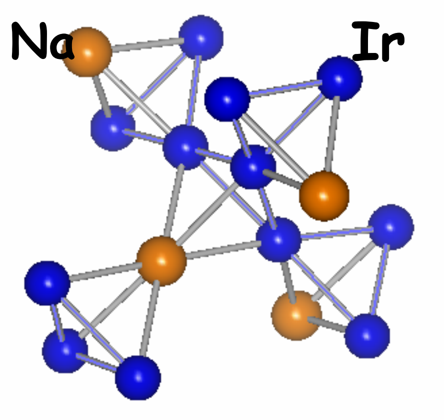
B-cation ordered spinel

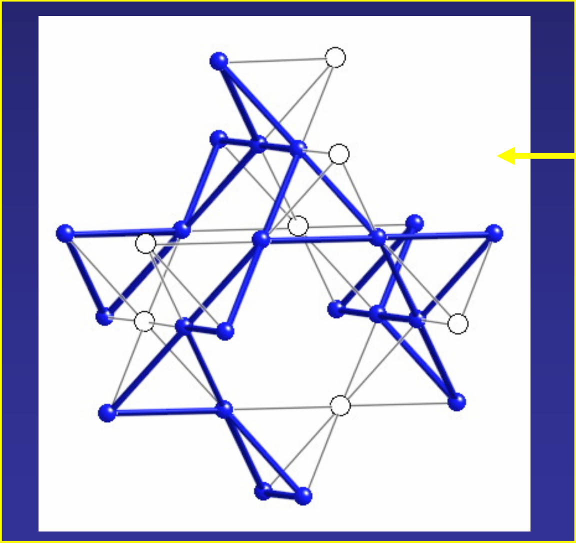
$2\ (Na_{3/2})_1\ (Ir_{3/4}, Na_{1/4})_2 O_4$



$Na_4Ir_3O_8$: cubic $P4_132$, $a = 8.985$ Å

Isostructural to $Na_4Sn_3O_8$



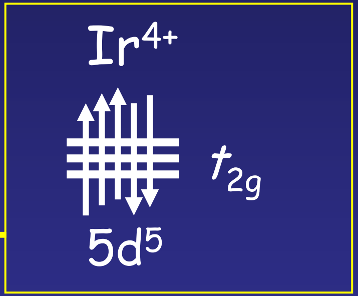


"hyper-Kagome"
frustration

B-site

$\frac{3}{4}$: Ir, $\frac{1}{4}$: Na

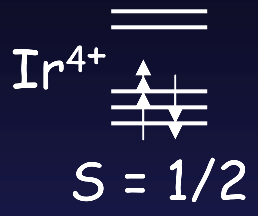
Cation ordering



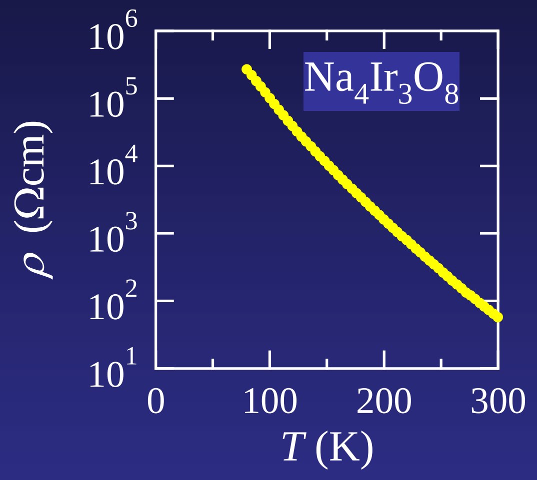
S=1/2
or
J=1/2 ??

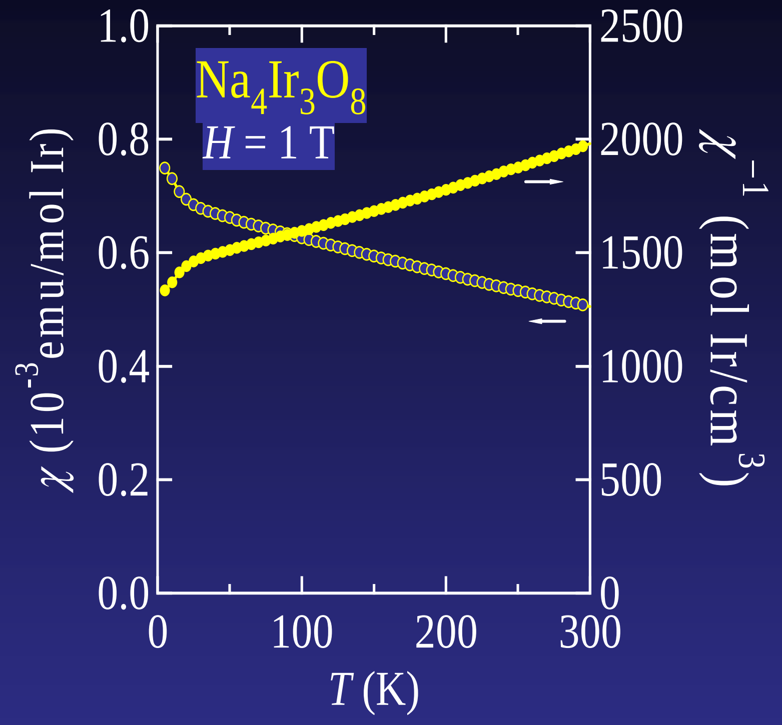
Locally more distorted

$Na_4Ir_3O_8$ J or S=1/2 Mott Ins. with AF interaction



$5d^5$





Mott insulator

J=1/2 or S=1/2

θ_W = -650 K

strong AF int.

J=650 K estimated

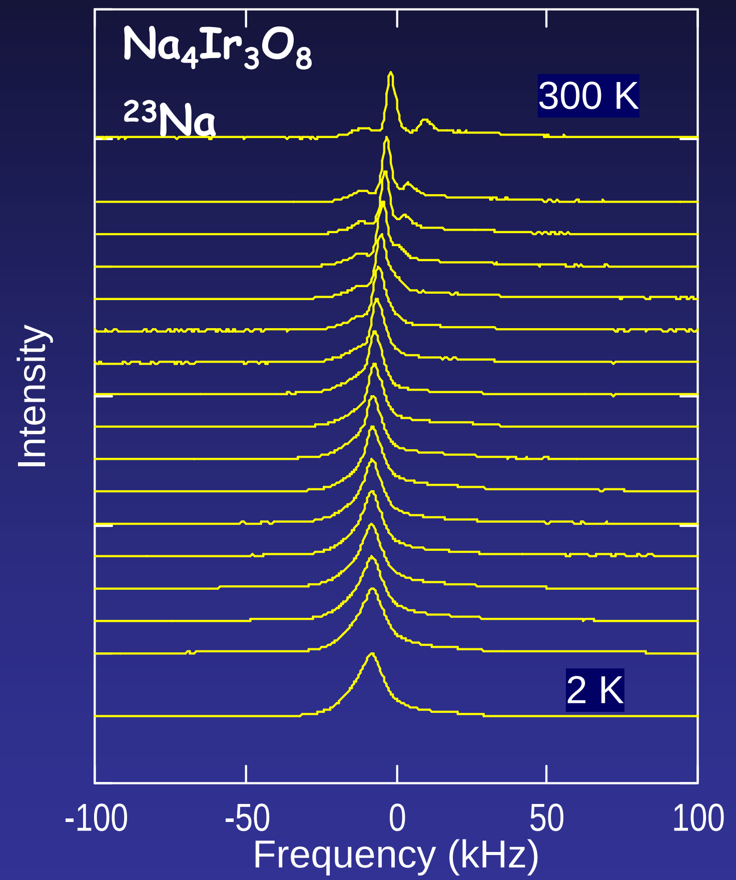
μ_{eff} = 1.96 μ_B / Ir

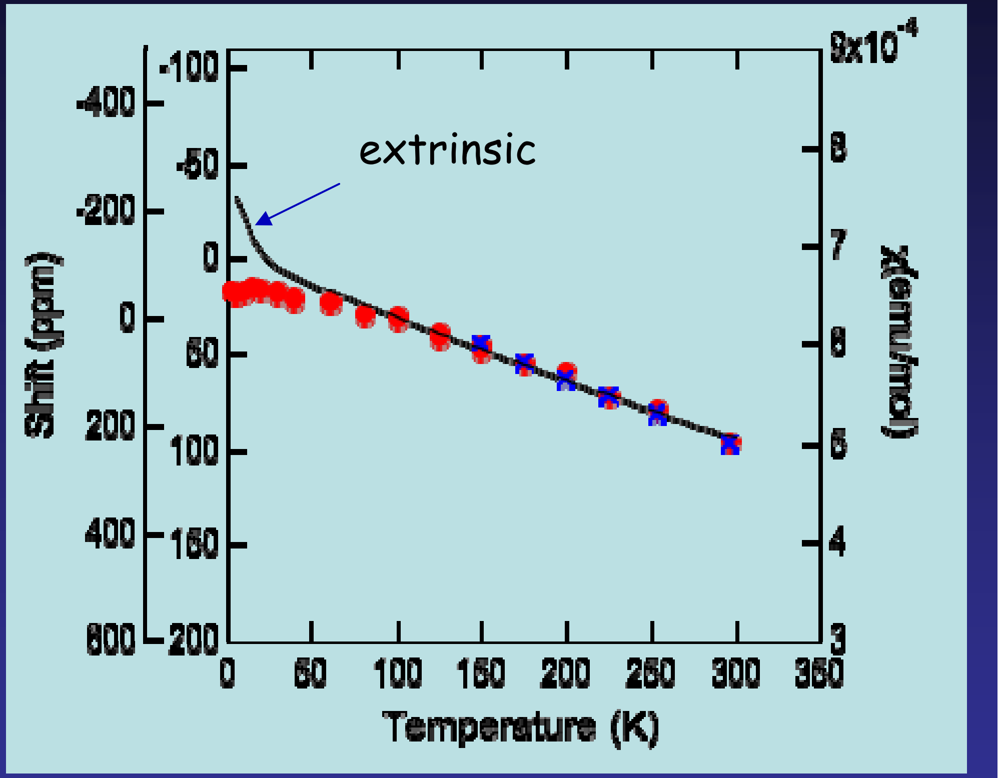
(S = 1/2 → 1.73 μ_B)

No ordering in χ down to 1.8 K << θ_{cw}= 650K   Strong frustration

No long range ordering detected by neutron down to 4K

^{23}Na NMR indicates absence of magnetic ordering down to 2 K (J=650 K) - evidence for spin liquid





χ(T) → constant at T=0 limit

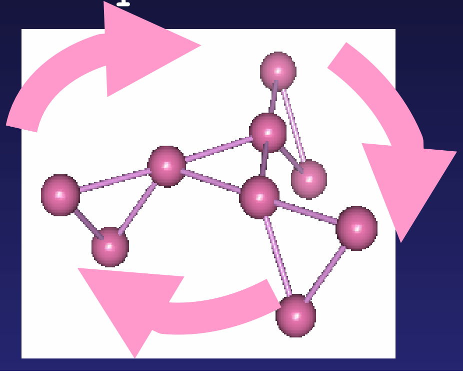
gapless

Spin correlation
should be checked by x-ray!

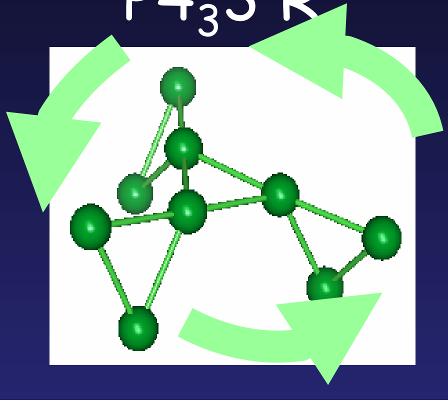
Fujiyama, Kanoda

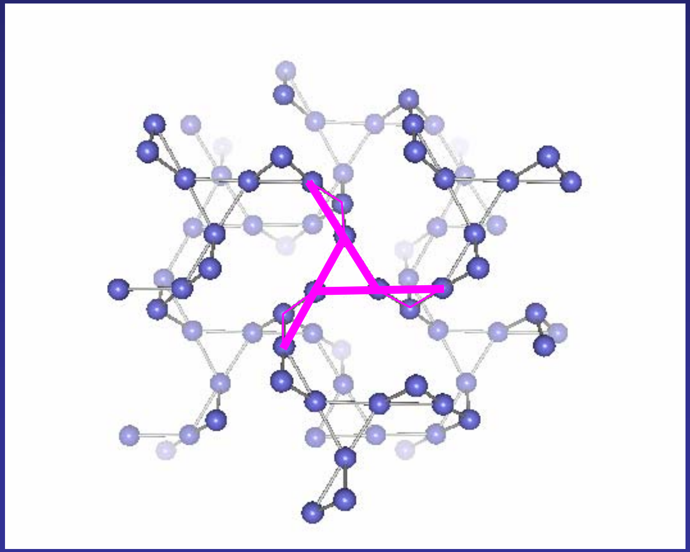
Hyperkagome (ordered spinel) lattice has “chirality“

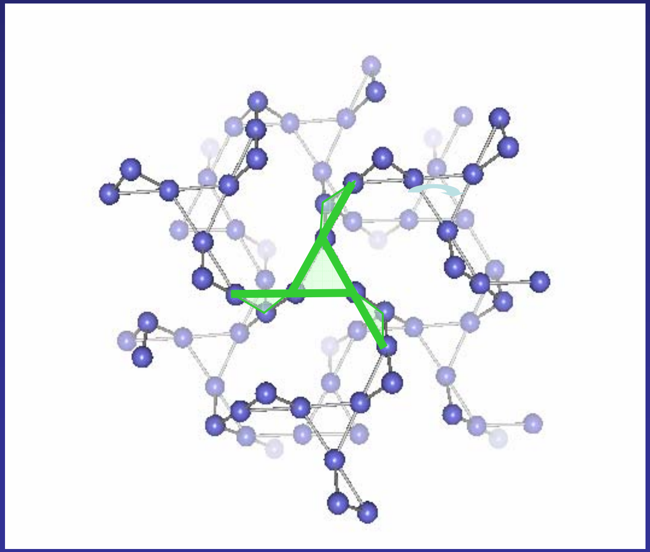
$P4_132$ L



$P4_33$ R



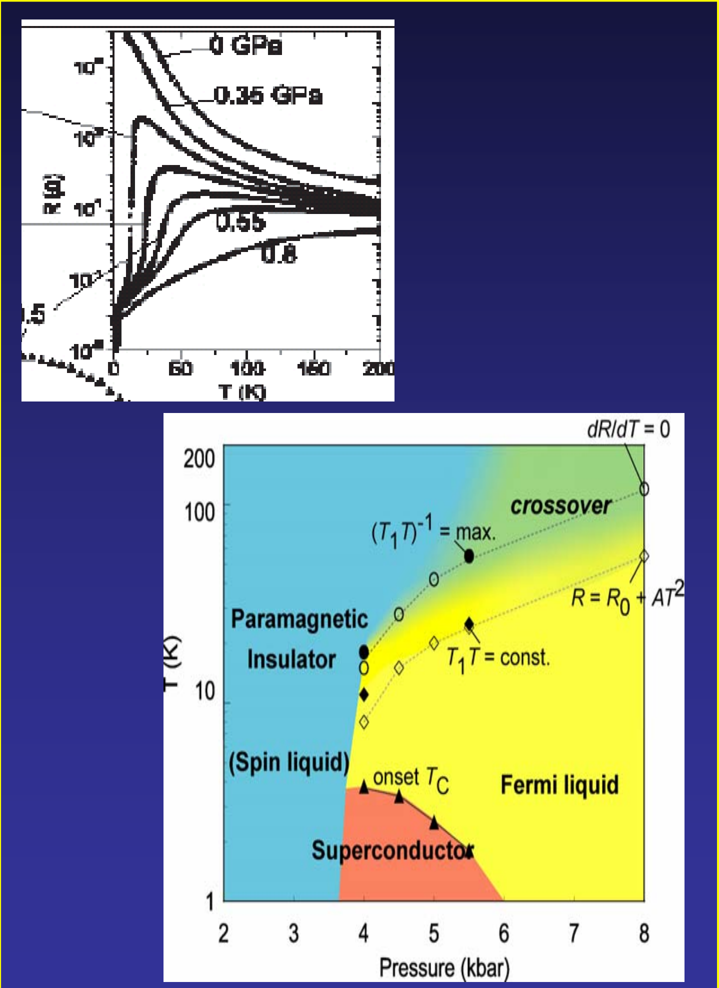




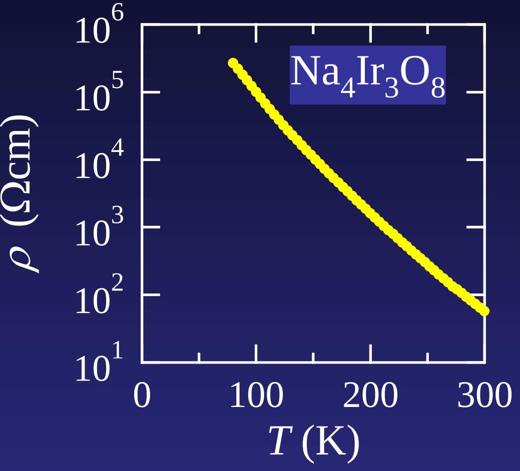
Spin liquid formed on chiral lattice!
(+ strong spin orbit coupling)

Itinerancy and stabilization of spin liquid

common physics with BEDT salt (Kanoda) S=1/2 triangular?



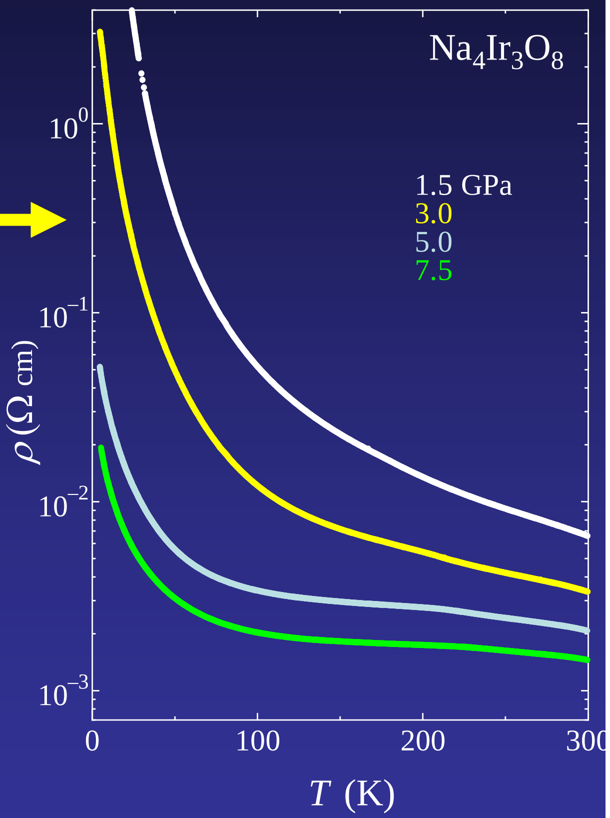
Kanoda



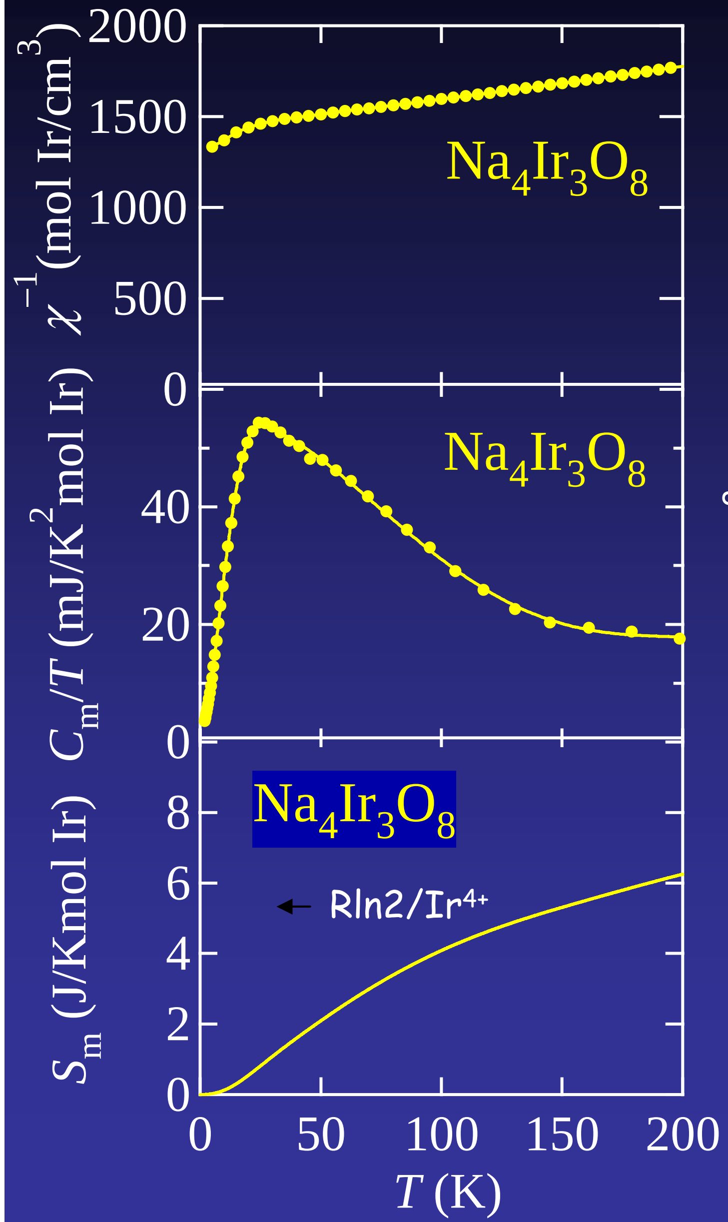
Close proximity to M-I

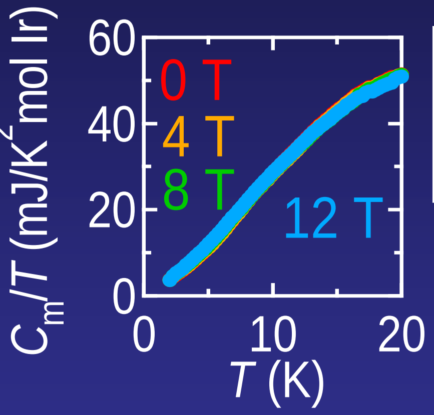
Large band width of Ir5d

transport in the presence of strong SOC!!
Inversion symmetry absent



Spin excitation puzzle by comparing C(T) and χ(T)





$C_m(T) \propto T^2$ down to 2K
E linear DOS (gap node)

But

$\chi(T \to 0)$ = finite
Not zero

←

<< θ_{cw} = 650K

Spin orbit coupling??
Leo Balents