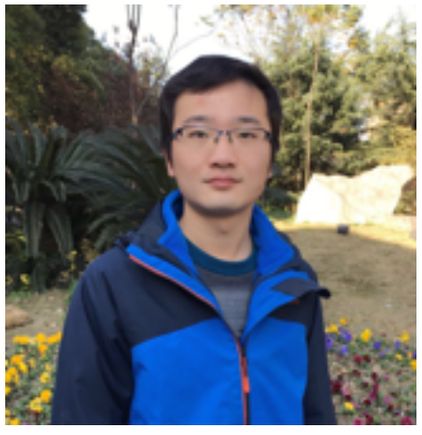
Frustrated metal $Pr_2Ir_2O_7$ and Spin liquid candidate $YbMgGaO_4$

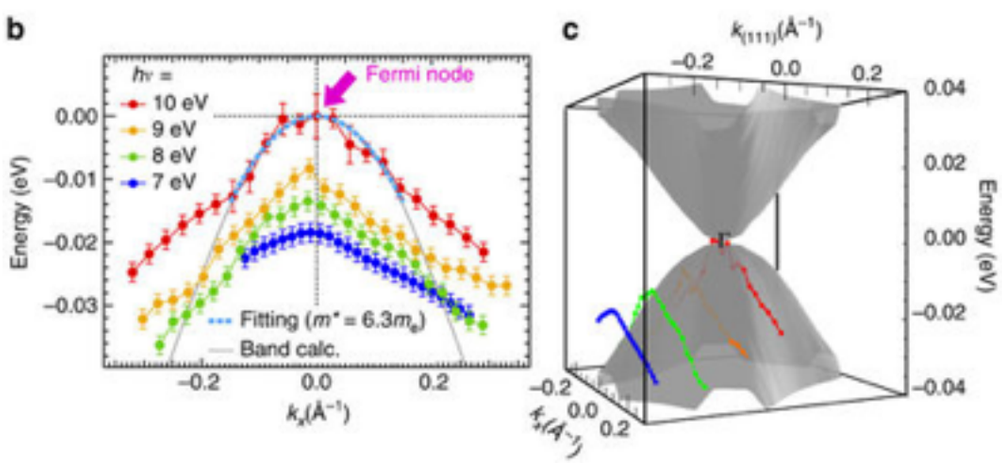
Gang Chen
Fudan University

Part 1



Xu-Ping Yao

When Luttinger semimetal meets Melko-Hertog-Gingras spin ice state in $Pr_2Ir_2O_7$



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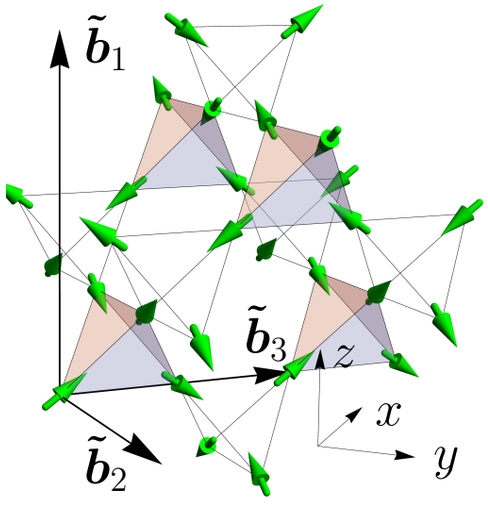

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Ir Luttinger semimetal

MHG spin ice state

Xu-Ping Yao, GC, 1712.06534

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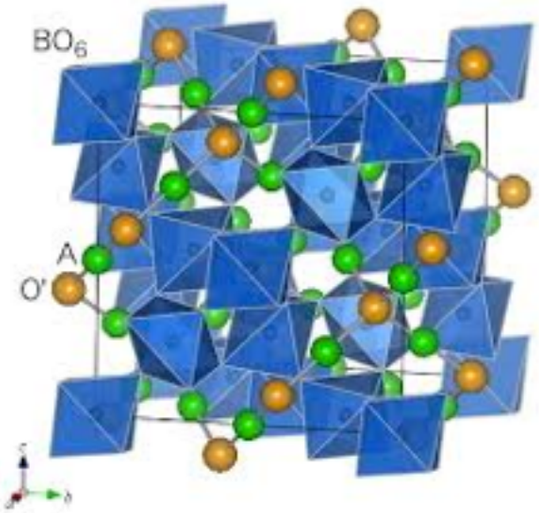
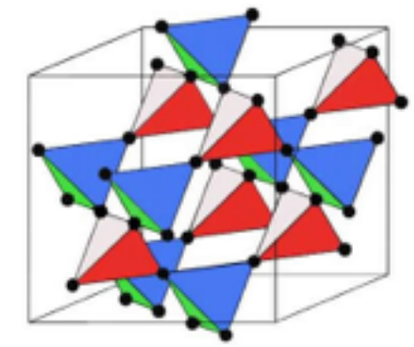
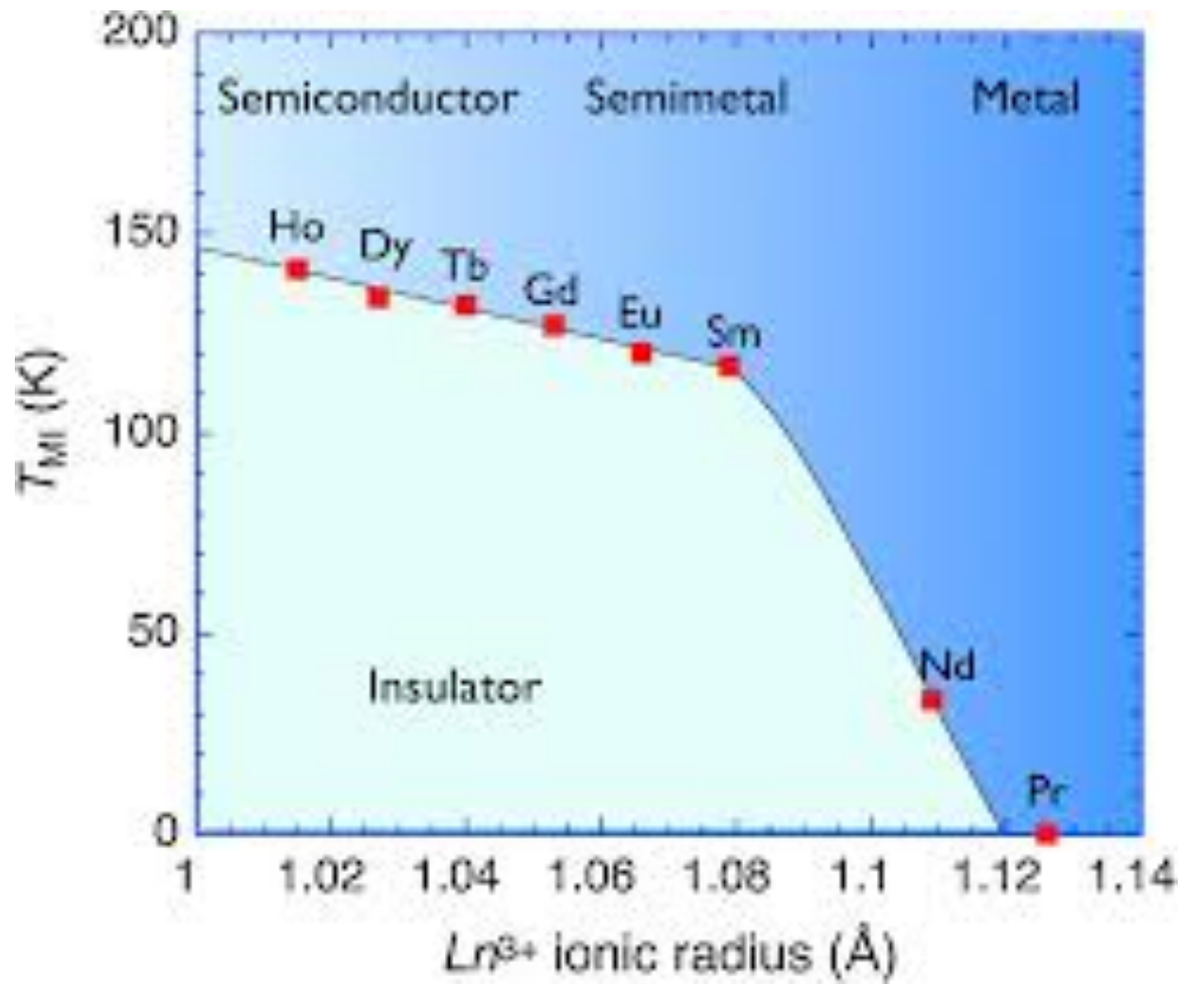
Pyrochlore iridates



$R_2Ir_2O_7$





K Matsuhira, M Wakeshima,
Y Hinatsu, S. Takagi
JPSJ, 2011

$Pr_2Ir_2O_7$ remains metallic and disordered,
all rest have metal-insulator transition with Ir magnetism

Early/pioneering theories: Leon Balents, Dima Pesin, Lucile Savary,
Sungbin Lee, Yong Baek Kim, et al

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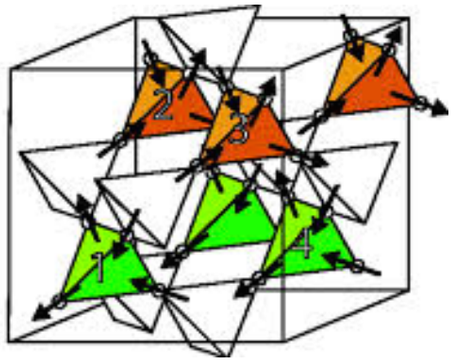
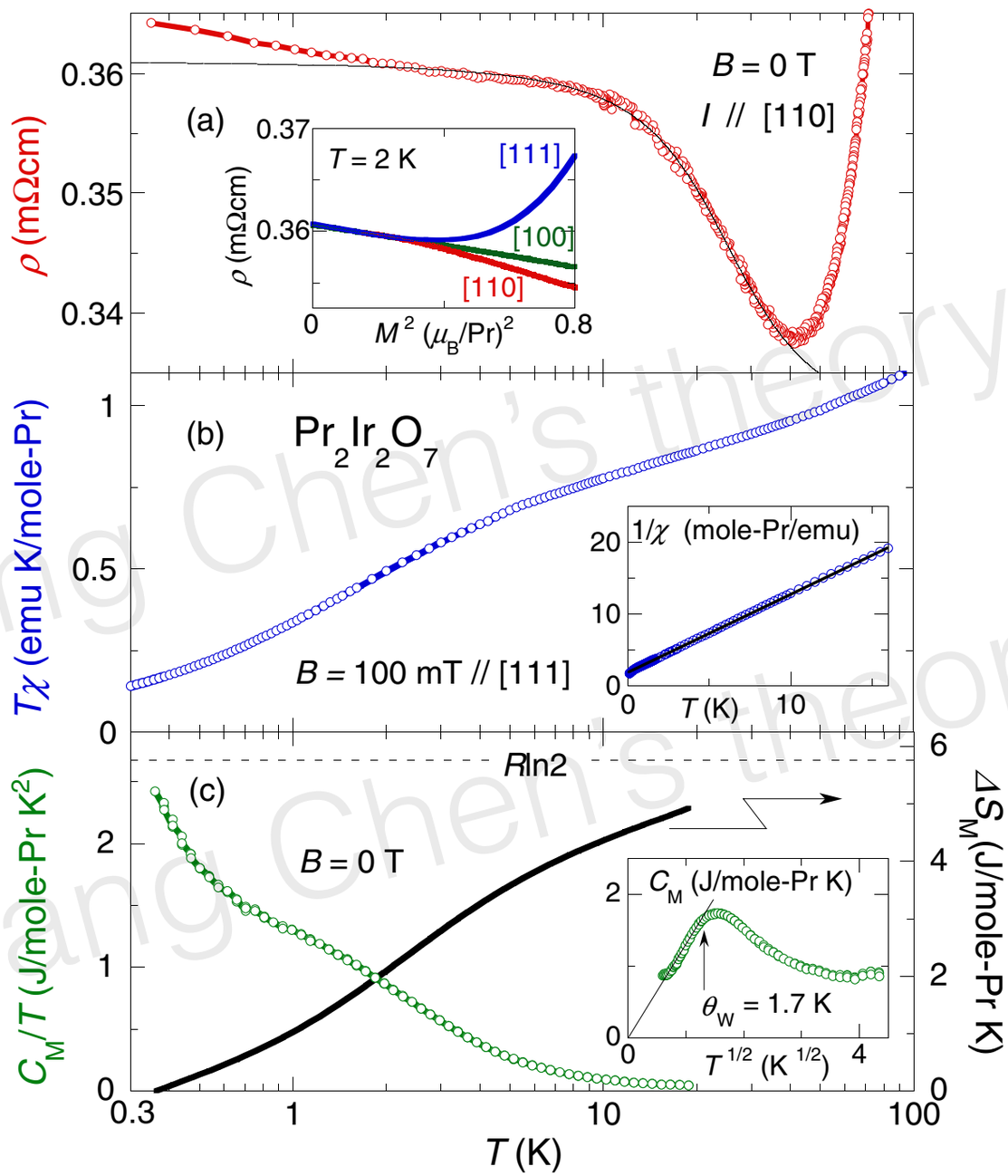
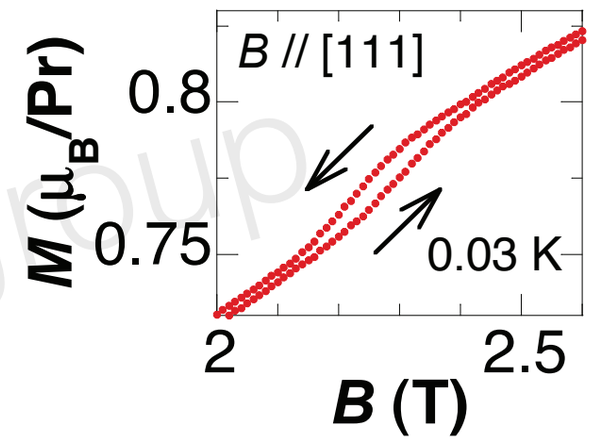


Peculiar one: $Pr_2Ir_2O_7$





metamagnetic transition

Nakatsuji, etc

PRL **96,** 087204 (2006)

Some $Pr_2Ir_2O_7$ sample does order magnetically

Unstable Spin-Ice Order in the Stuffed Metallic Pyrochlore $Pr_{2+x}Ir_{2-x}O_{7-\delta}$

D. E. MacLaughlin,[1,2,*] O. O. Bernal,[3] Lei Shu,[1,4,5] Jun Ishikawa,[2] Yosuke Matsumoto,[2]
J.-J. Wen,[6,†] M. Mourigal,[6,‡] C. Stock,[6,7,§] G. Ehlers,[8] C. L. Broholm,[6,7,8,9] Yo Machida,[2,¶]
Kenta Kimura,[2] Satoru Nakatsuji,[2,10,**] Yasuyuki Shimura,[2] and Toshiro Sakakibara[2]

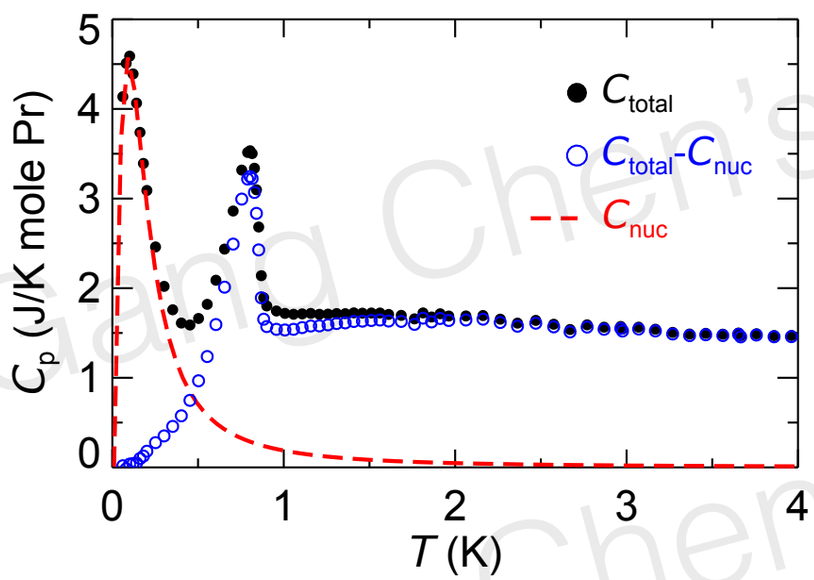


FIG. 1. (color online) Temperature dependence of the specific heat of $Pr_{2+x}Ir_{2-x}O_{7-\delta}$ in zero field. Filled circles: experimental total specific heat. Dashed curve: calculated specific

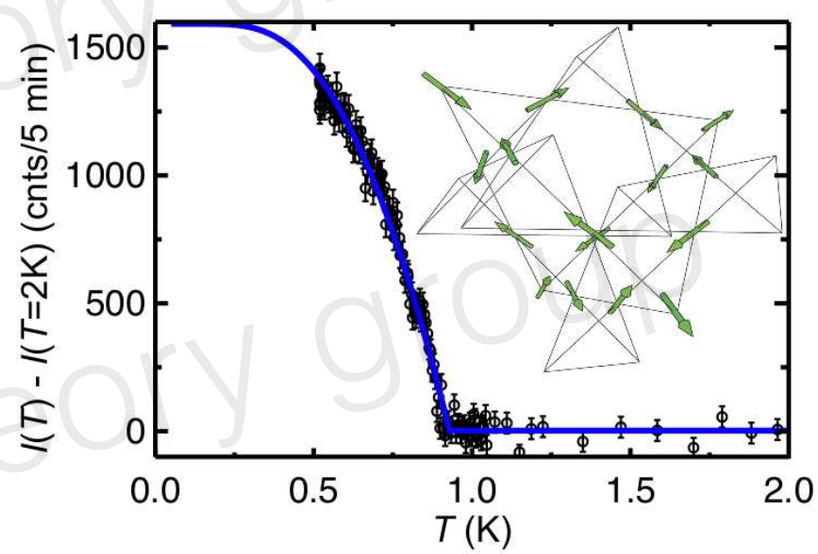
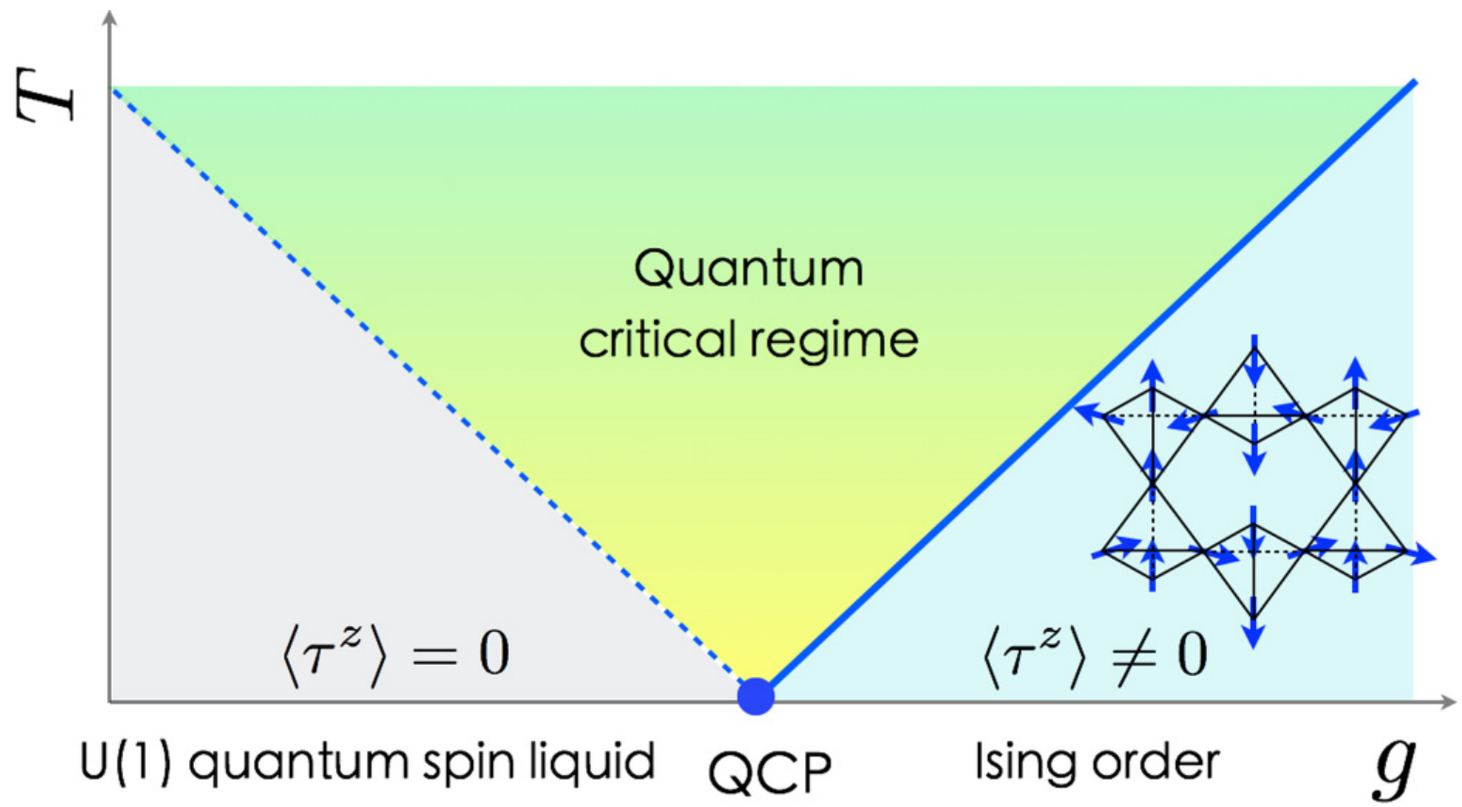


FIG. 2. (color online) Temperature dependence of elastic neutron scattering intensity of $Pr_{2+x}Ir_{2-x}O_{7-\delta}$ at the position of the $\mathbf{q}_m = (100)$ reflection. The intensity measured at $T = 2$ K

actually "Melko-Hertog-Gingras" spin state
(obtained numerically for a **different and classical** system)

Our proposal for Pr subsystem

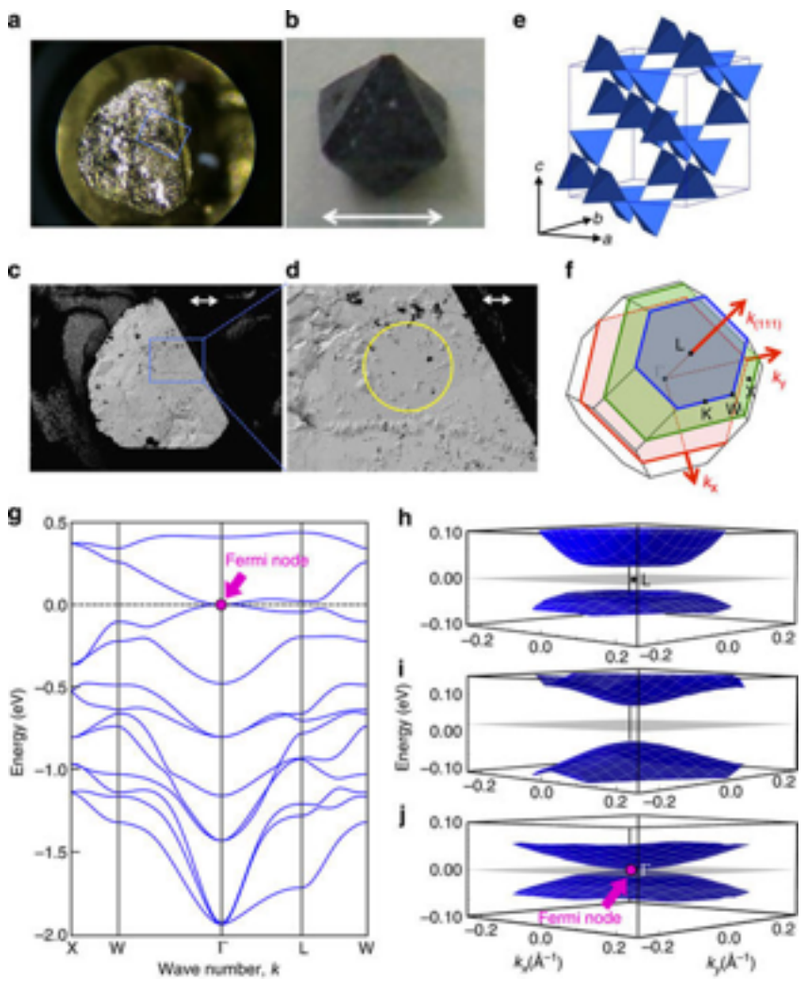


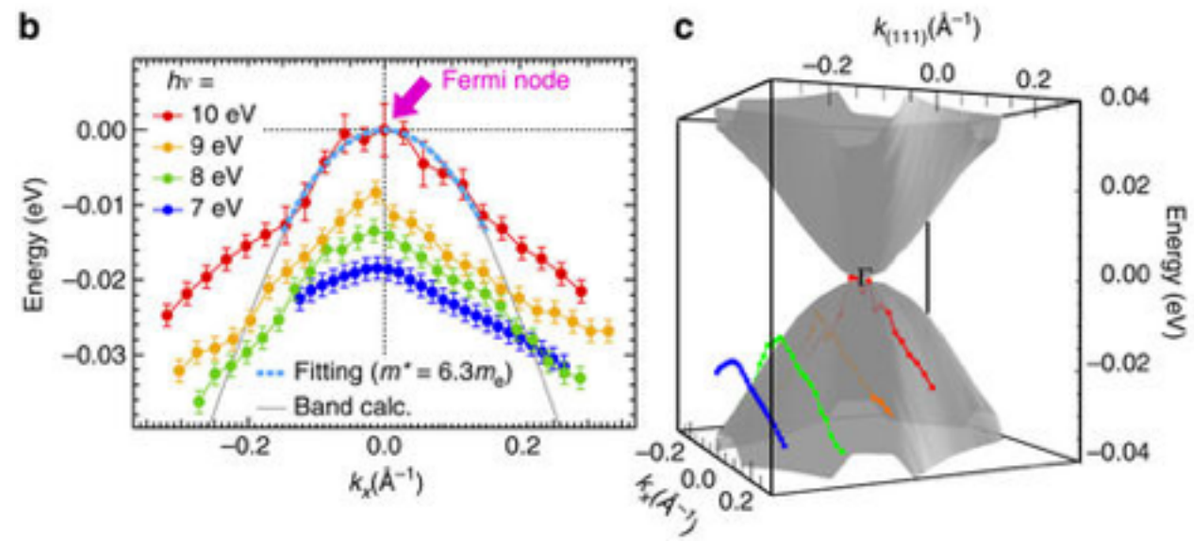
The Pr subsystem is proximate to a quantum phase transition from pyrochlore ice U(1) QSL to Ising magnetic order.

Microscopics: different samples have different Fermi energy, induces different RKKY interaction between Pr local moments.

Gang Chen, PRB 94, 205107 (2016)

Ir conduction electron: Luttinger semimetal



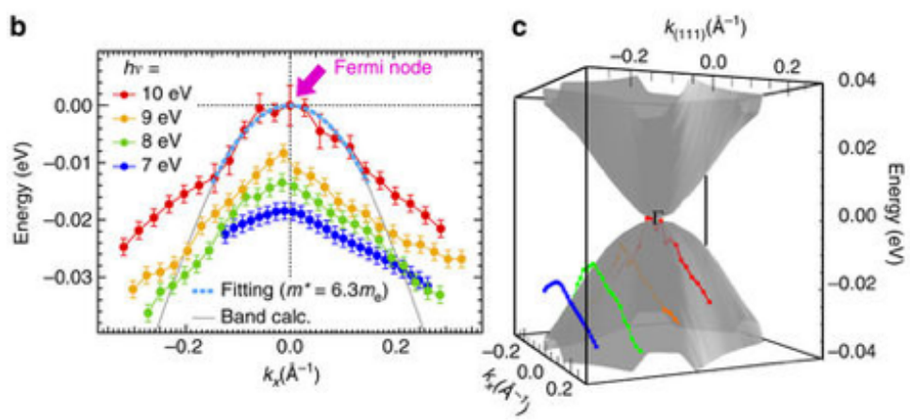


ARPES: Quadratic band touching

T Kondo, …Ru Chen, …, Nakatsuji, Balents, Shin
Nature Comm, 2015
P Amitage's optical measurement 2017
Correlation effect: EG Moon, L Savary, YB Kim, Cenke Xu, L Balents

Partial screening of long range Coulomb interaction

What is the impact of Pr magnetism
on Ir conduction electrons in the **ordered** regime?



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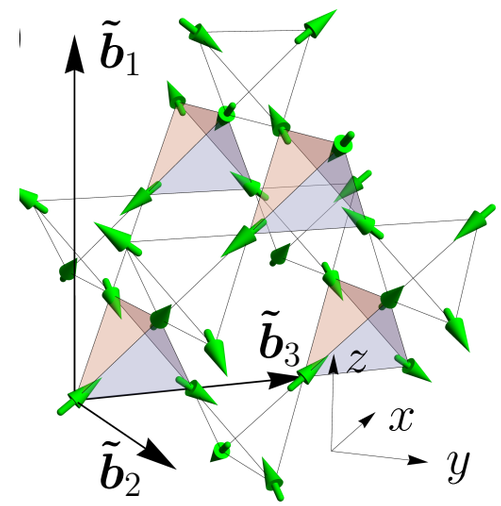

= ????

Ir Luttinger semimetal

MHG spin ice state

T Kondo, etc, 2015

C Broholm, etc, 2015

When electron behaves as electron,
when spin behaves as spin !

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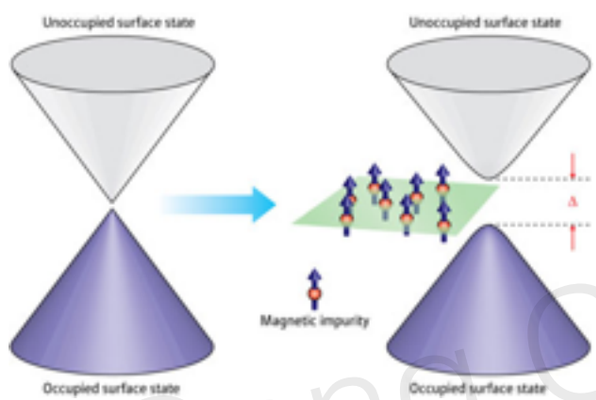
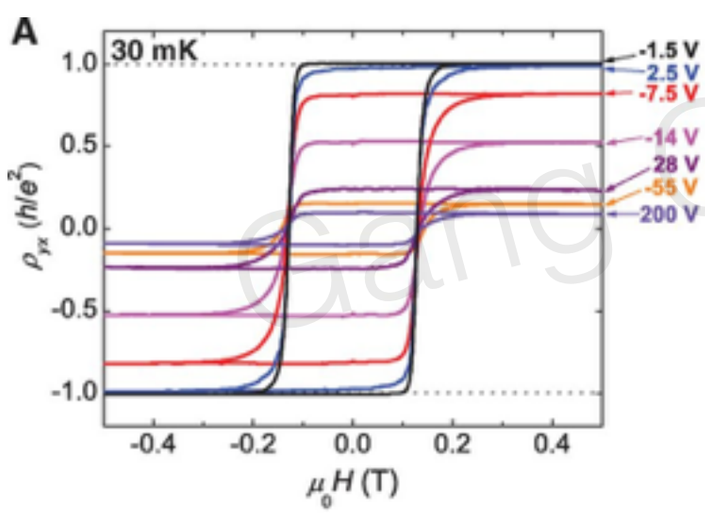
Digression: Quantum Anomalous Hall Effect

Qikun Xue's group



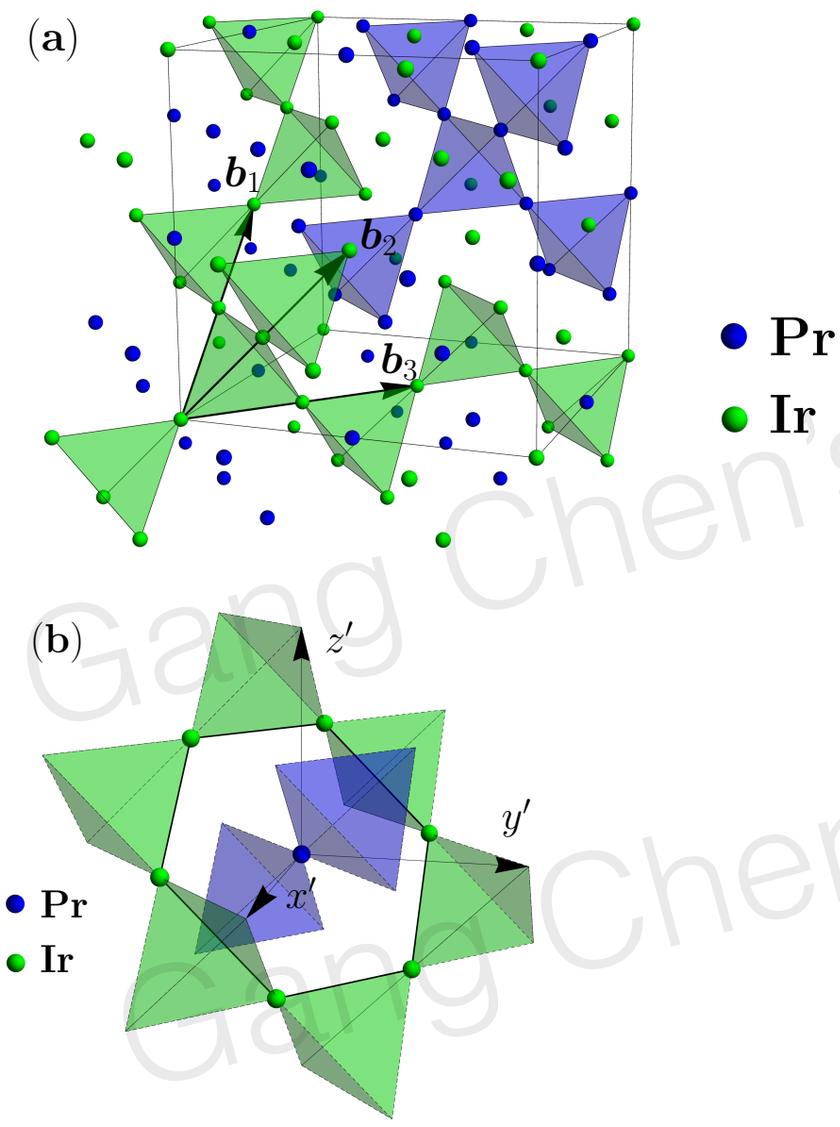


1. One understanding: TI -> Dirac cone ferromagnetism -> gapped Dirac fermion -> QAHE

2. Our understand: QAHE is an example of interplay between conduction electron and local moments. Here in QAHE, itinerant electron band topology is modulated by magnetism, and magnetism is rather simple.

Here, we study the system with both local moments and itinerant electrons, trying to understand their interplay and interactions. How local moments influence conduction electrons, and ice versa.

Microscopics: Ir conduction electron + Pr local moments

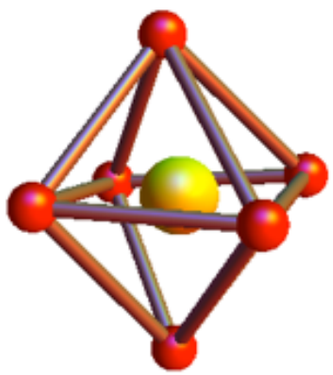


GC, Hermele, PRB 2012
X-P Yao, GC, 1712.06534

Energy Scale	
~<1eV	Ir 5d electron: hopping, SOC, interaction
~	**Pr-Ir interaction: f-d exchange**
~10K	Pr 4f electron: exchange interaction

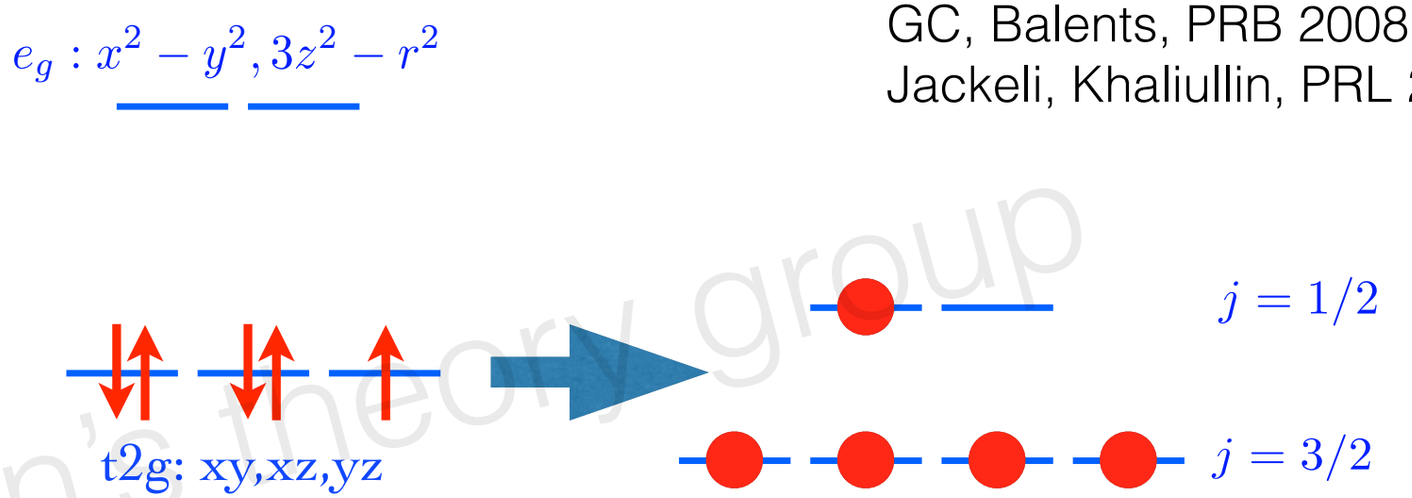
Ir 5d electron: SOC, hopping and correlation

BJ Kim, etc 2008,
GC, Balents, PRB 2008
Jackeli, Khaliullin, PRL 2009



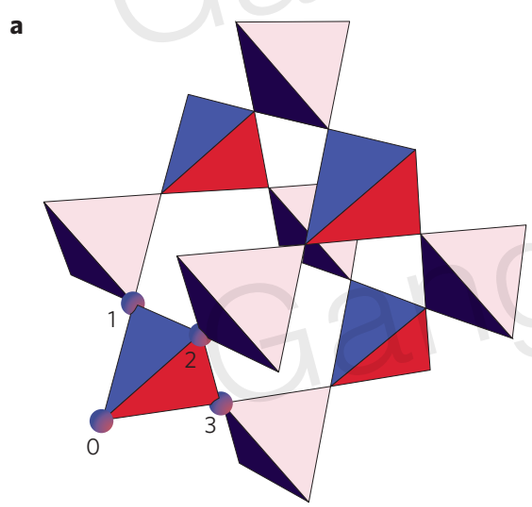
IrO6 octahedron

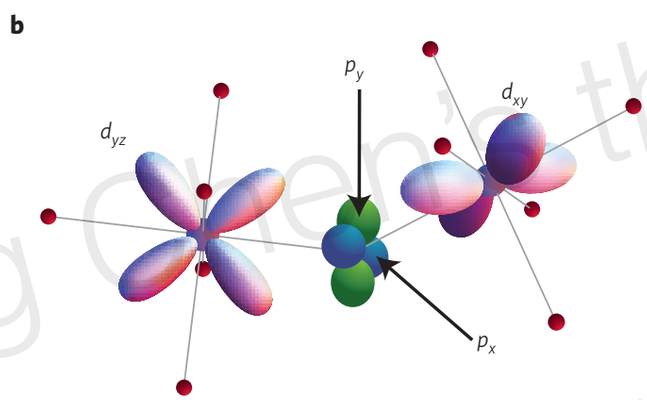
$\mathrm{Ir}^{4+} : 5d^5$



Crystal electric field

Spin-orbit coupling



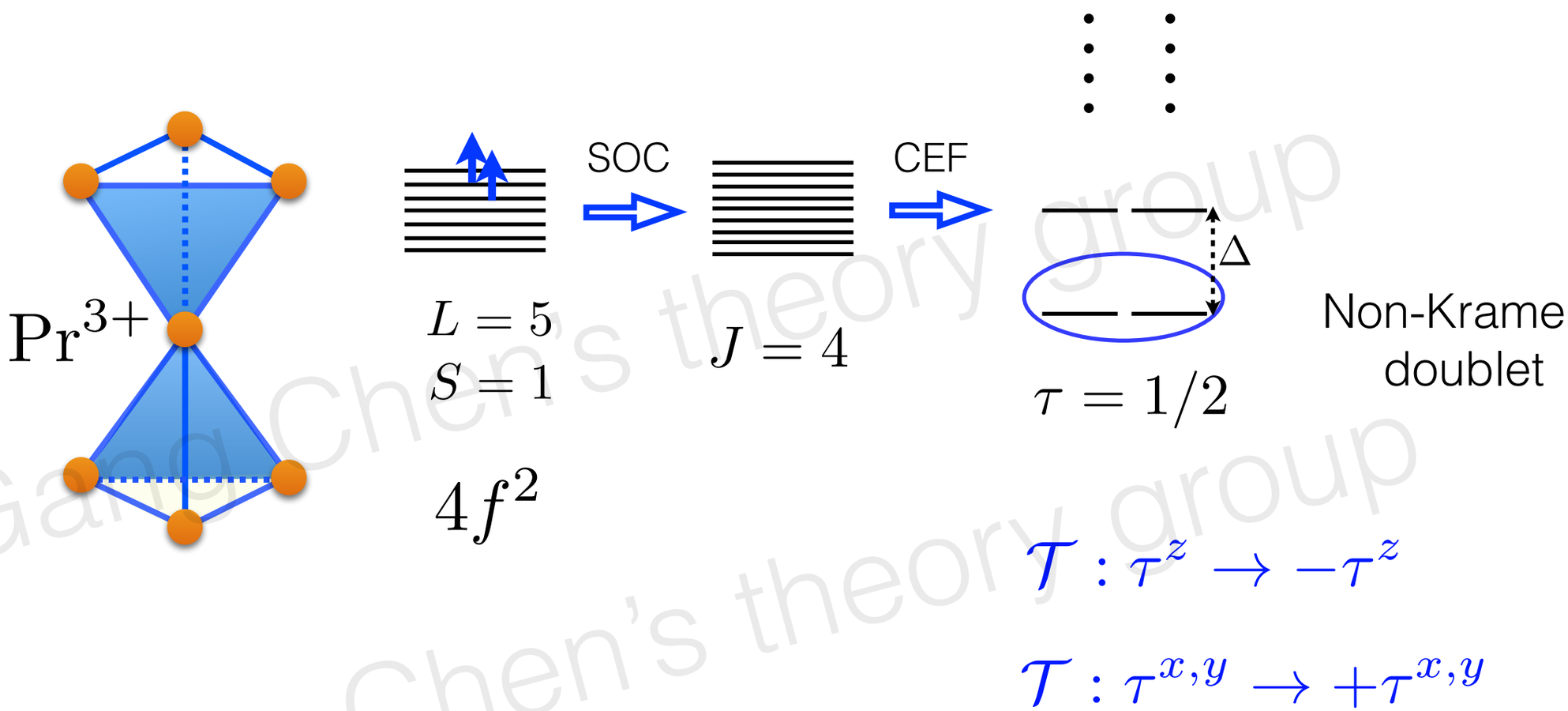


Besides Ir electron hopping via intermediate oxygens, there is direct electron hopping (Yong Baek Kim)

For $Pr_2Ir_2O_7$, correlation renormalizes the overall band width.

quickly skip

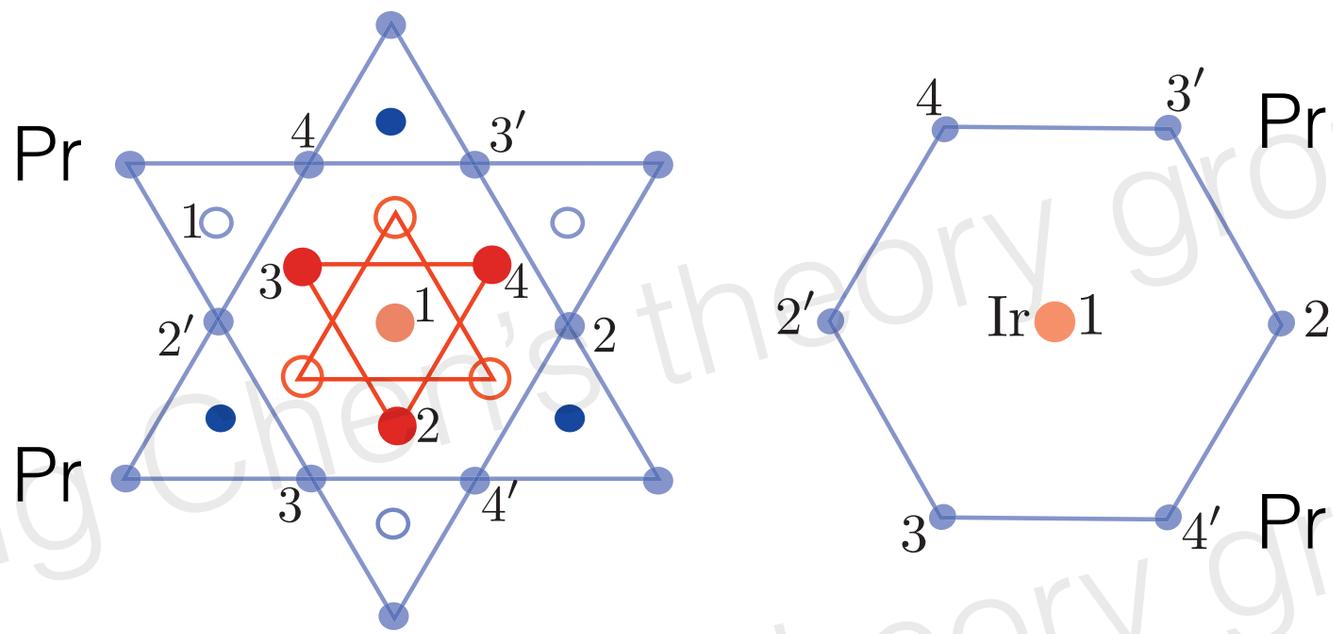
Pr local moments: non-Kramers dou



Indication:
1. Only z (or Ising) component couples to external magnetic field.
2. Magnetic order necessarily implies z (or Ising) component ordering.
3. Only z (or Ising) component couples to the Ir electron spin density.

quickly skip

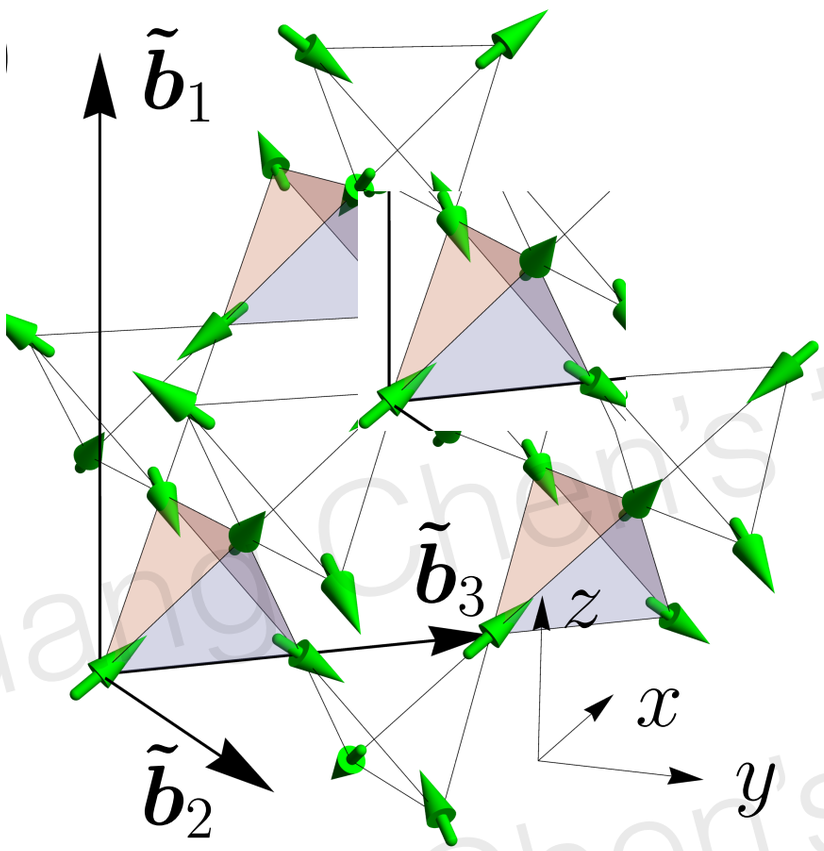
Pr-Ir interaction: 4f-5d exchan

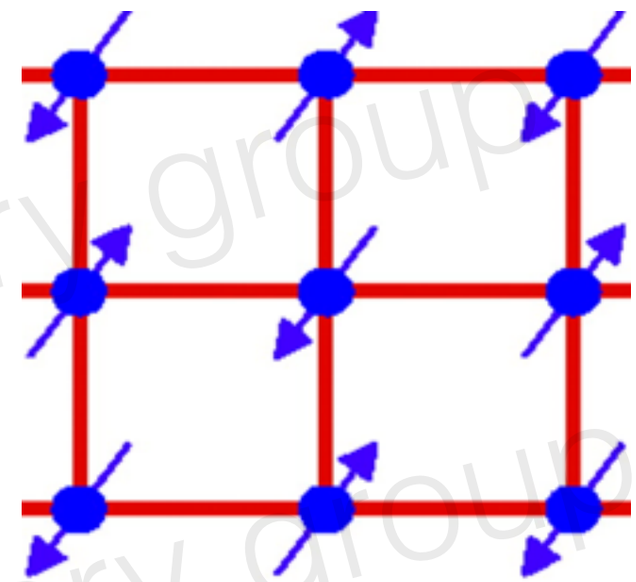


$$\mathcal{H}_{\rm fd} = \left[c_1\tau_4^z - c_2\left(\tau_2^z + \tau_3^z\right)\right] j_1^x + \left[c_1\tau_3^z - c_2\left(\tau_2^z + \tau_4^z\right)\right] j_1^y$$
$$+ \left[c_1\tau_2^z - c_2\left(\tau_3^z + \tau_4^z\right)\right] j_1^z + [2 \leftrightarrow 2', 3 \leftrightarrow 3', 4 \leftrightarrow 4'],$$

GC, Hermele, PRB 2012

Magnetic translation of MHG spin ice state

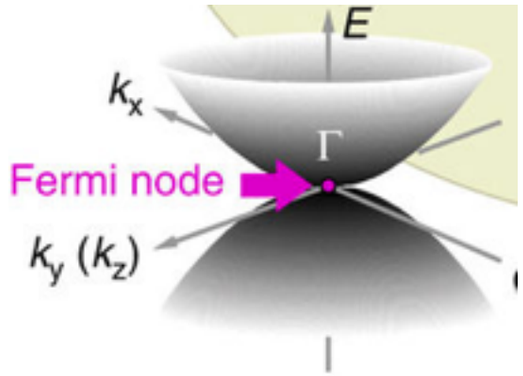




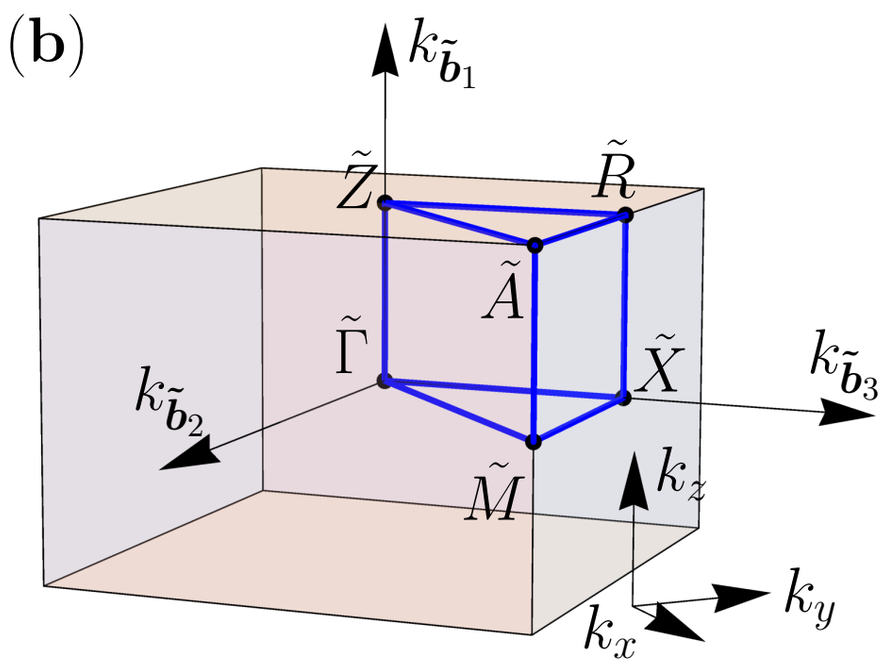
Neel state on square lattice

$$\tilde{\mathcal{T}} \equiv \mathcal{T} \circ t$$

3D analogue of the magnetic translation for Neel state

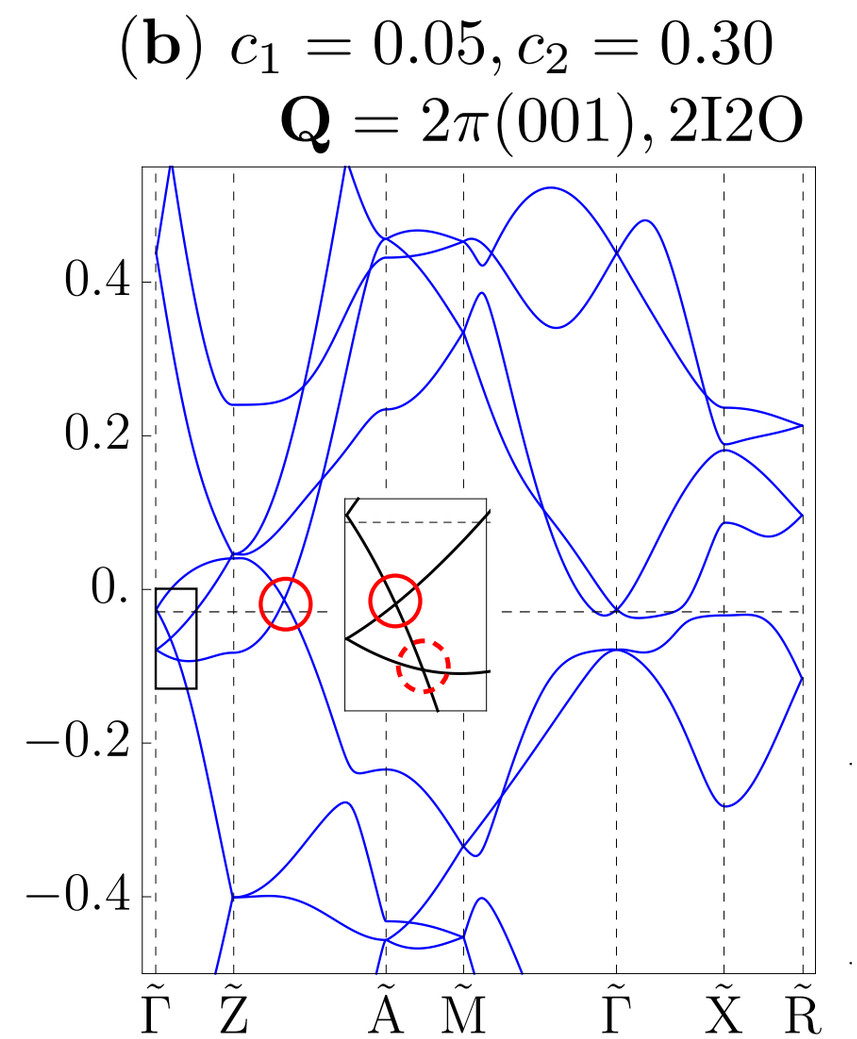


Symmetry protected Dirac band touching



magnetic Brillouin zone

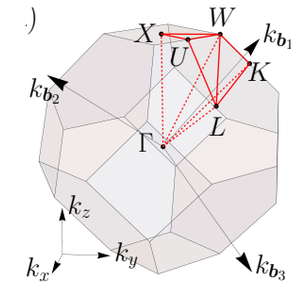
$\tilde{\mathcal{T}}^2 = -1$ at $\tilde{\Gamma}$ point

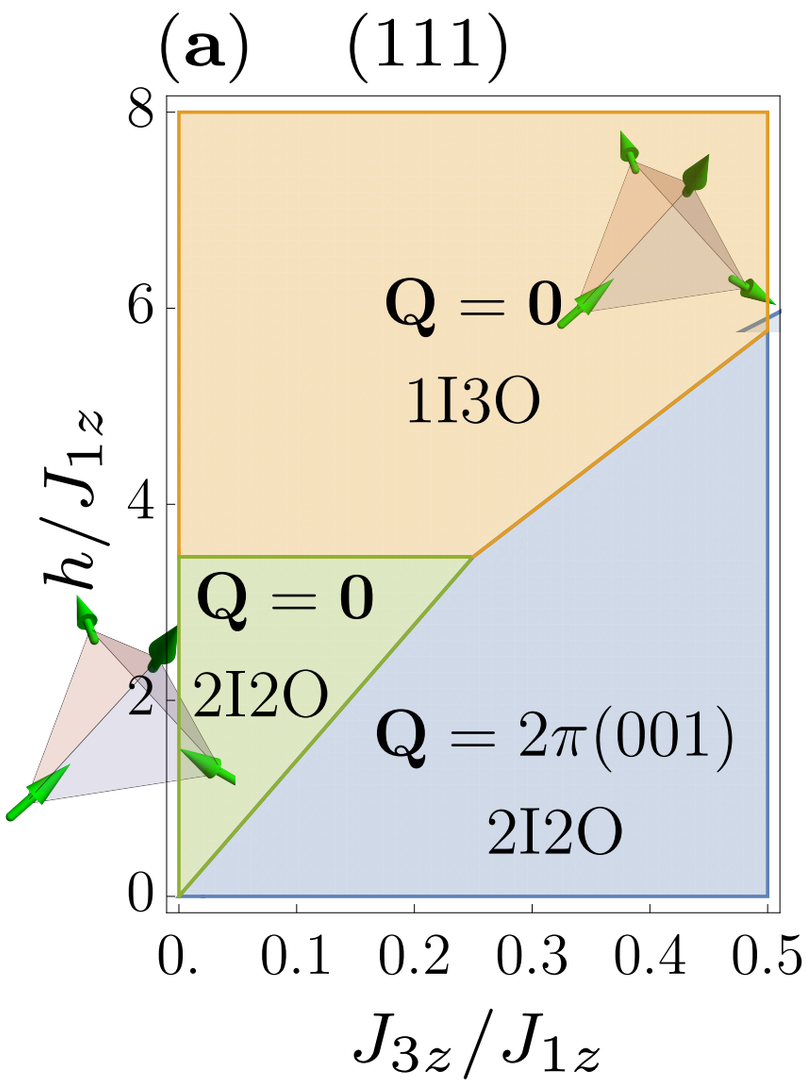


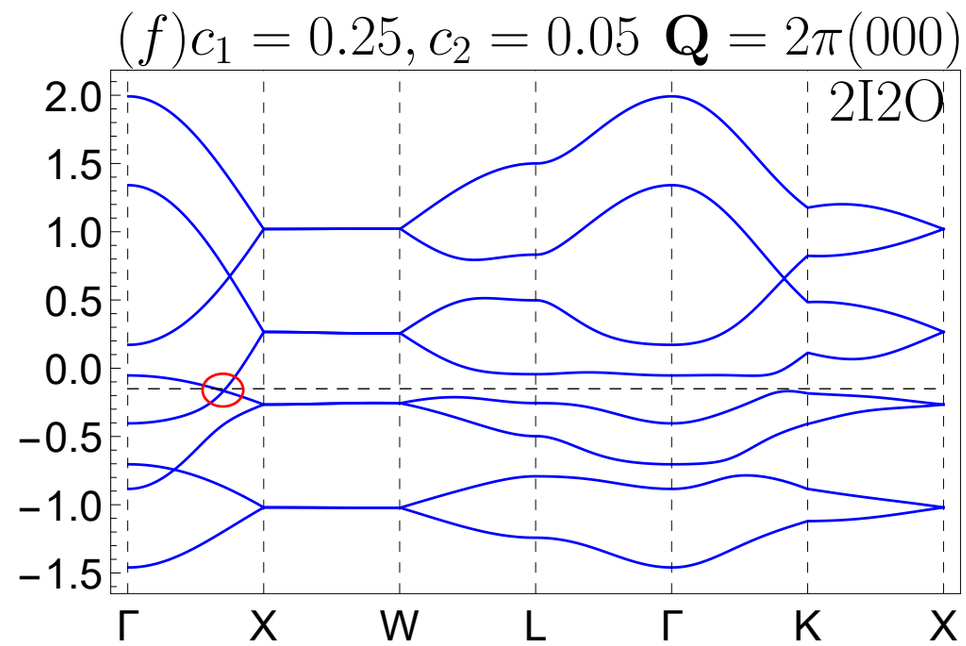
in addition, there are Weyl nodes
whose existence does not require symmetry

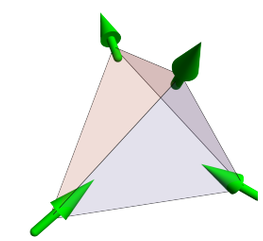
Pr magnetic order transfers its time reversal
symmetry breaking to Ir Luttinger semimetal.

Band engineering by external magnetic field





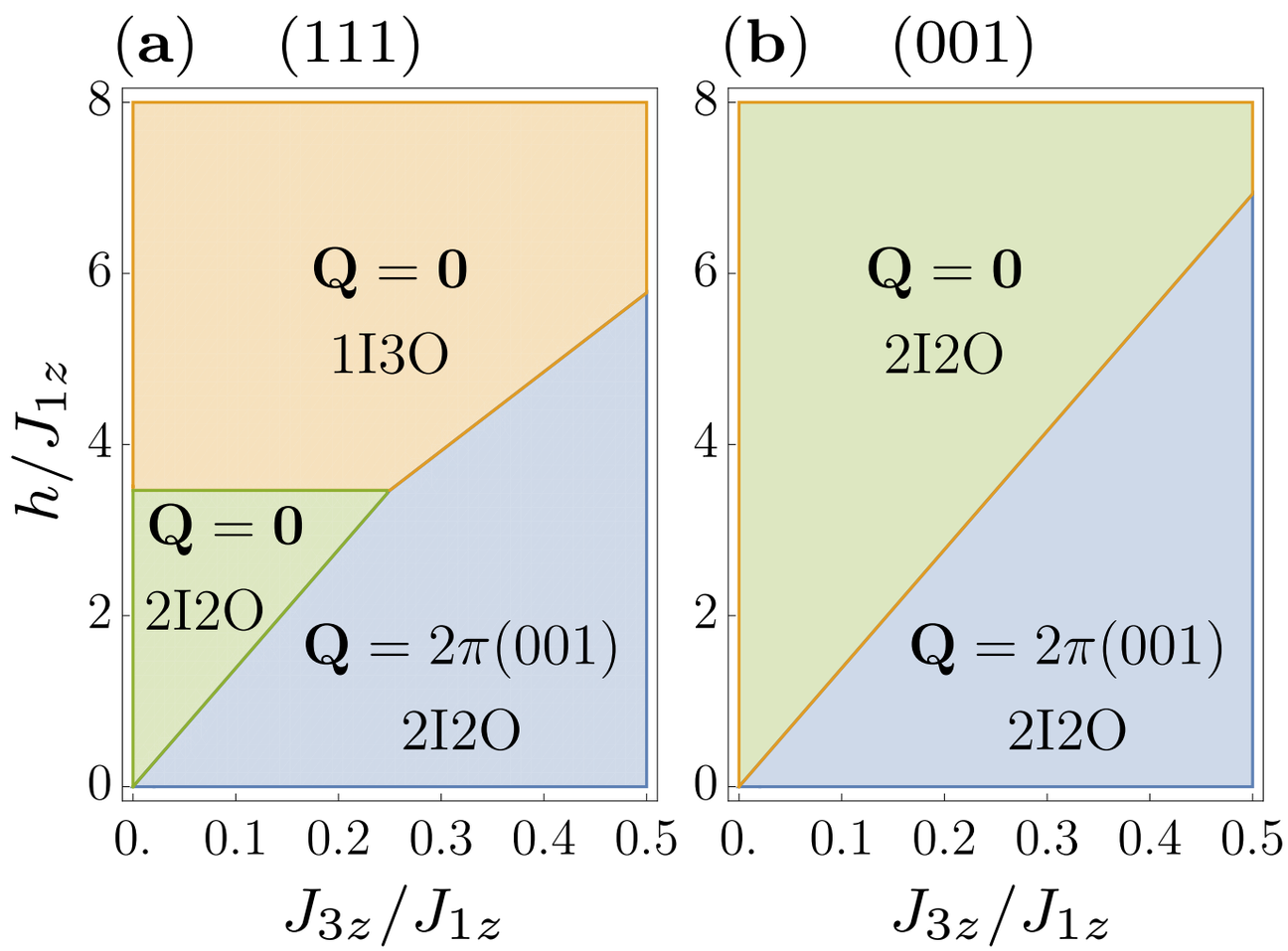




example: double Weyl nodes

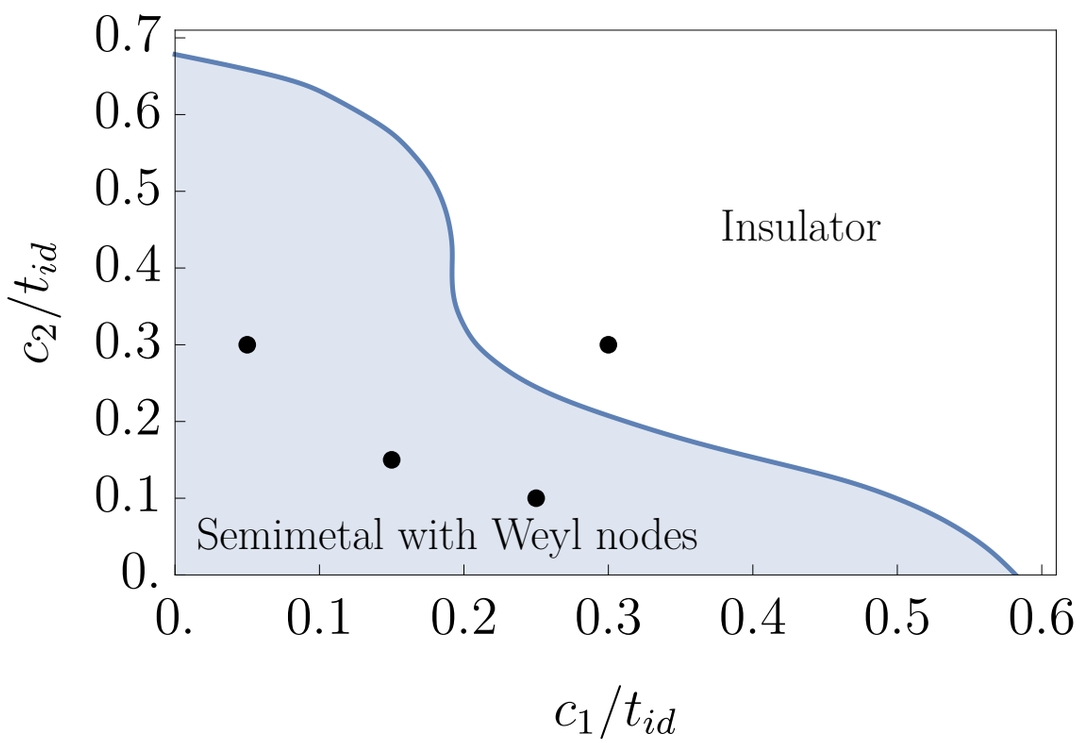
1. Magnetic field primarily couples to Pr moments, modifies Pr spin state, thereby indirectly influence the Ir band structure,
2. Field immediately removes the Dirac band touching,
3. Field induces Weyl nodes on the Ir band structure as well, anomalous Hall effect

Quantum control under magnetic field

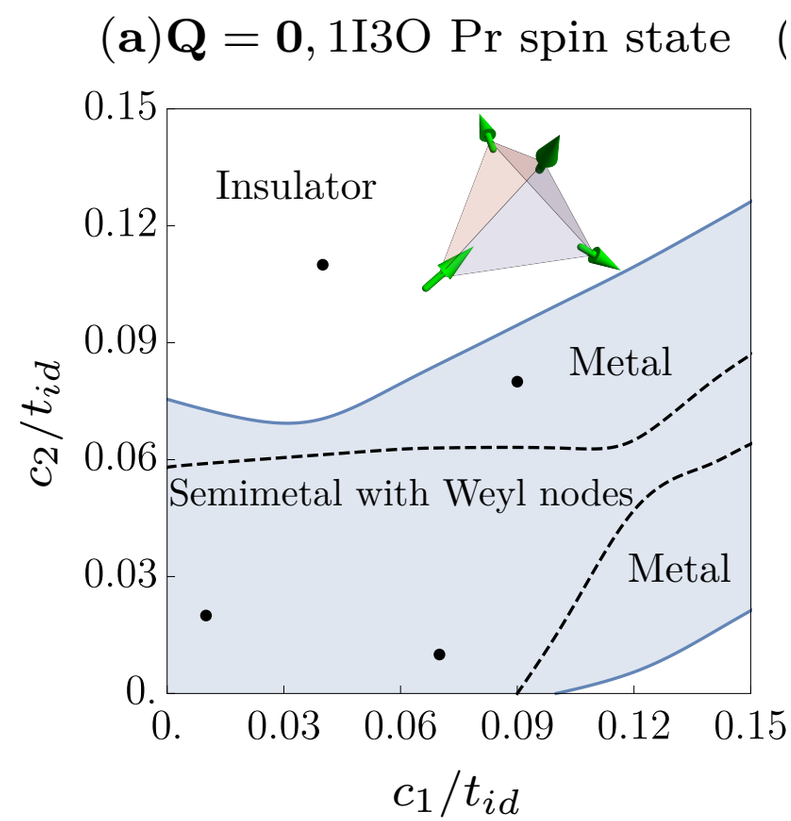


The Pr magnetic state under
different direction magnetic field

Ir band property under 111 field



zero field



finite field

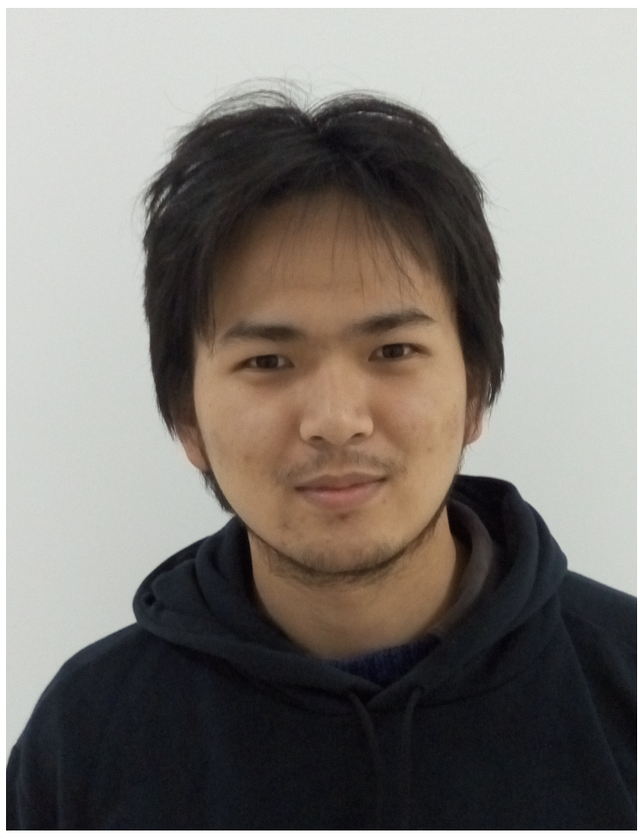
Magnetic field modifies the Pr magnetic structure, thereby modifies the Ir band structure.

We predict that external magnetic field destroy the symmetry protected Dirac band touching, and Weyl nodes still persist and give to anomalous Hall effect.

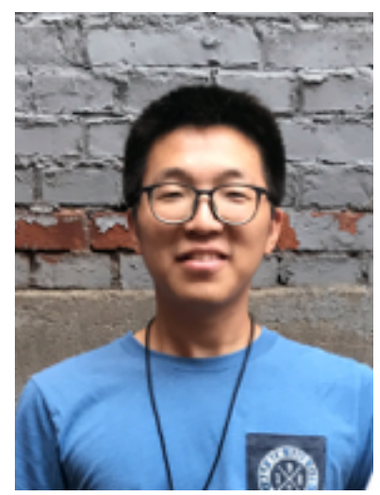
Xu-Ping Yao, Gang Chen, arXiv 1712.06534

Part 2

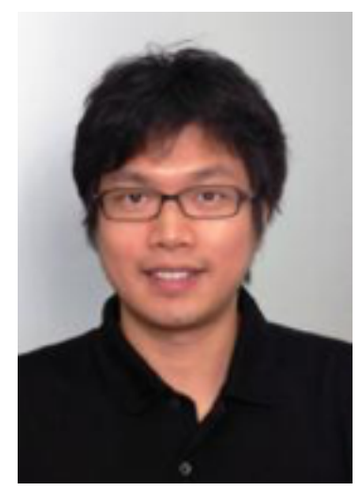
Fractionalization in a spin liquid candidate $YbMgGaO_4$: a **weak-field** regime



Yaodong Li
(now at UCSB)



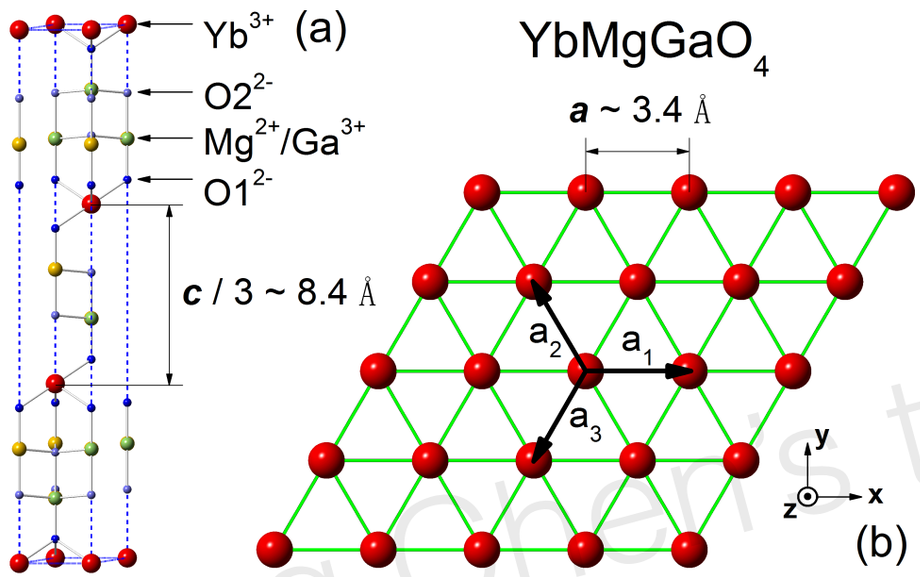
Yao Shen
(Fudan)

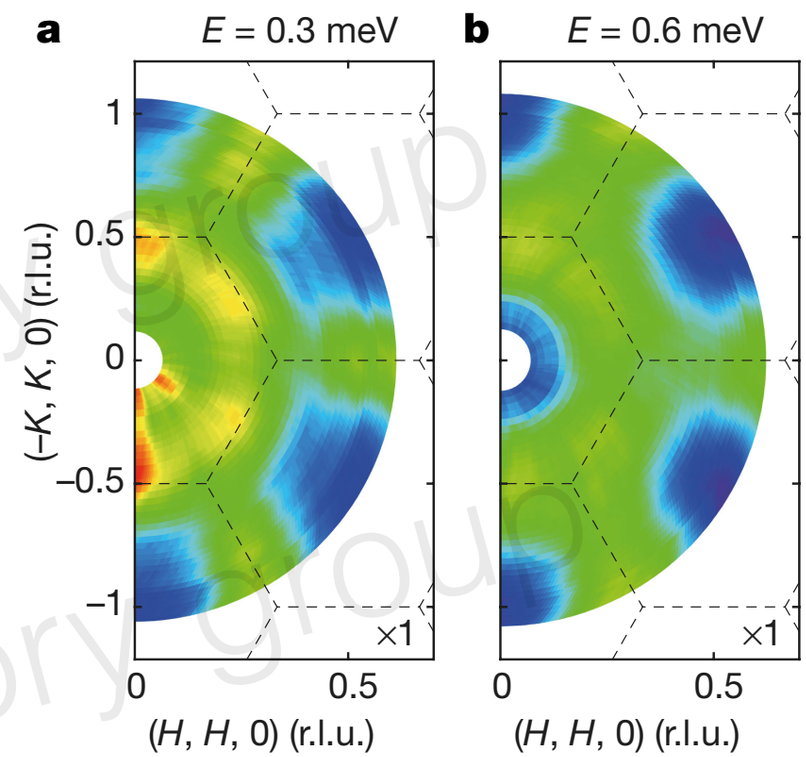


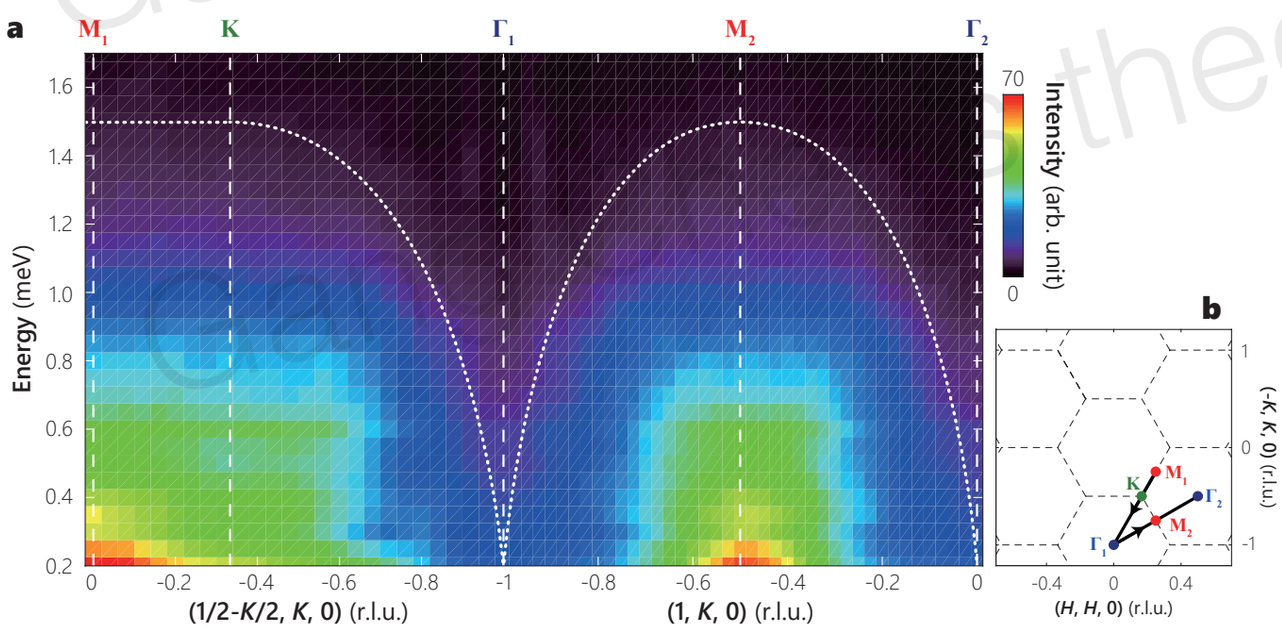
Jun Zhao
(Fudan)

復旦大學
FUDAN UNIVERSITY

Rare-earth triangular lattice magnets: spin liquid







with Yuesheng Li, Qingming Zhang, Jun Zhao, Yao Shen, Yaodong Li

Proposal of spinon Fermi surface U(1) QSL

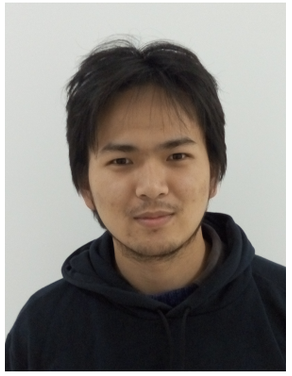
The proposed spinon particle-hole continuum of a spinon Fermi surface is consistent with the experimental results.

Refs:

YD Li, XQ Wang, GC*,	PRB 94, 035107 (2016)
YD Li, XQ Wang, GC*,	PRB 94, 201114 (2016)
YD Li, Y Shen, YS Li, J Zhao, GC*,	PRB 97, 125105 (2018)
YD Li, YM Lu, GC*,	PRB 96, 054445 (2017)
YD Li, GC*,	PRB 96, 075105 (2017)
YS Li, GC*, .., QM Zhang*,	PRL 115, 167203 (2015)
Y Shen, YD Li, .., GC*, J Zhao*,	Nature, 540, 559 (2016)
Y Shen, YD Li, .., GC*, J Zhao*,	arXiv 1708.06655

Probably most important question is whether the continuum represents the fractionalized spinon excitation.

A new idea: explore the weak field regime



Yao-Dong Li
(UCSB)

Continuing the recent proposal of the spinon Fermi surface U(1) spin liquid state for $YbMgGaO_4$ in Yao-Dong Li, *et al*, arXiv:1612.03447 and Yao Shen, *et al*, Nature 2016, we explore the experimental consequences of the external magnetic fields on this exotic state. Specifically, we focus on the *weak field regime* where the spin liquid state is preserved and the fractionalized spinon excitations remain to be a good description of the magnetic excitations. From the spin-1/2 nature of the spinon excitation, we predict the unique features of spinon continuum when the magnetic field is applied to the system. Due to the small energy scale of the rare-earth magnets, our proposal for the spectral weight shifts in the magnetic fields can be immediately tested by inelastic neutron scattering experiments. Several other experimental aspects about the spinon Fermi surface and spinon excitations are discussed and proposed. Our work provides a new way to examine the fractionalized spinon excitation and the candidate spin liquid states in the rare-earth magnets like $YbMgGaO_4$.

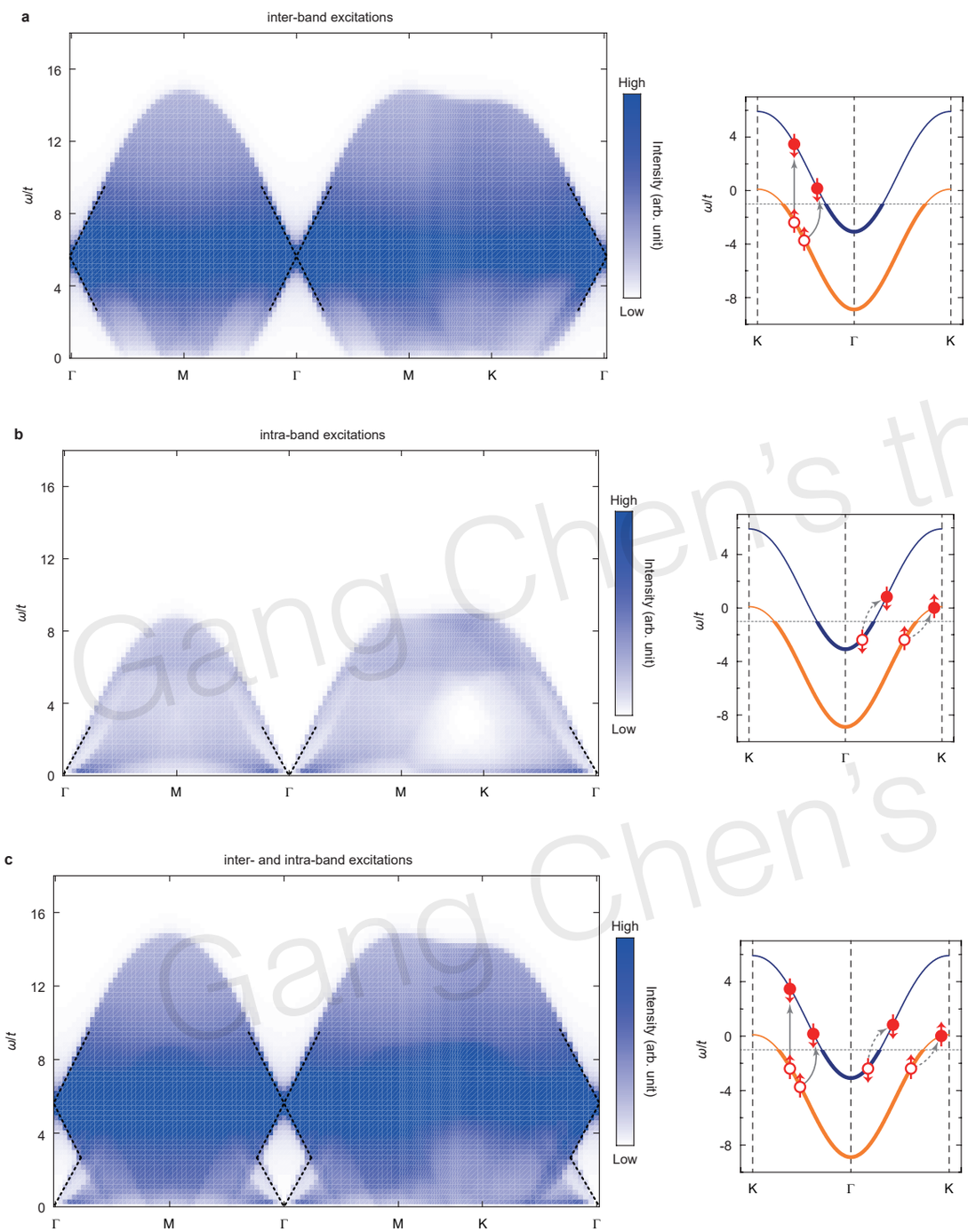
Realizable and Predictable.

Yao-Dong Li, **GC**, PRB 96, 075105 (2017)

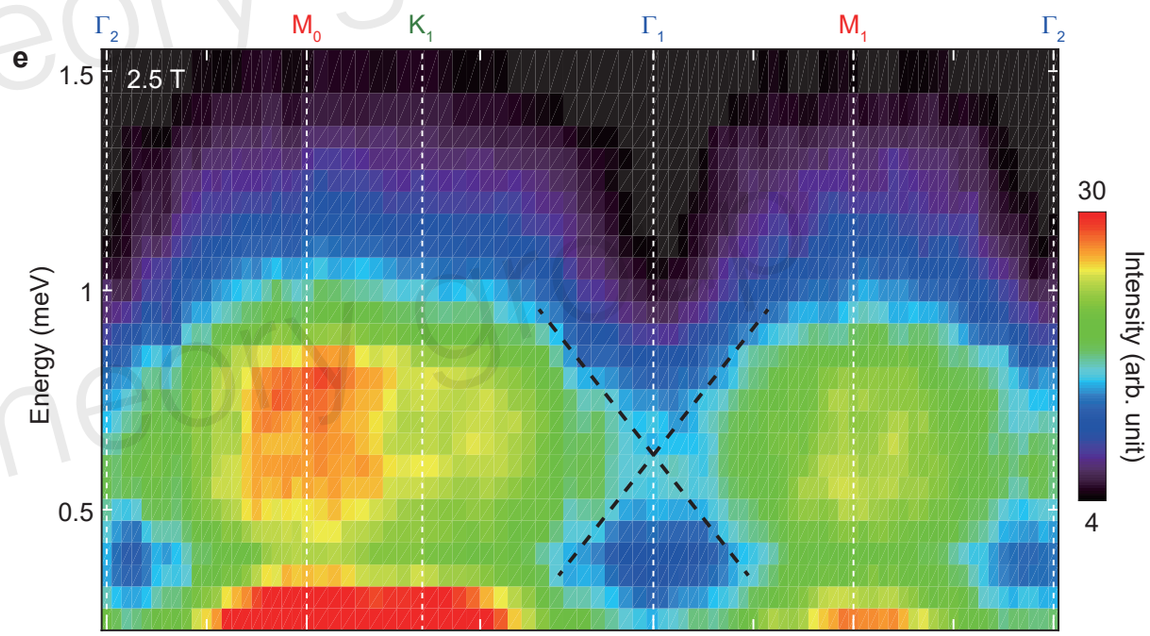
isotope effect in BCS superconductor

復旦大學 FUDAN UNIVERSITY

Strong Mott regime: only Zeeman coupling



$$\mathcal{H}_{\mathrm{MFT}} = -t \sum_{\langle ij \rangle, \alpha} f_{i\alpha}^{\dagger} f_{j\alpha} - \mu \sum_{i} f_{i\alpha}^{\dagger} f_{i\alpha} - g_z \mu_{\mathrm{B}} H \sum_{i} f_{i\alpha}^{\dagger} \frac{\sigma_{\alpha\beta}^{z}}{2} f_{i\beta}$$



experiment at 2.5T

Use new materials to support materials

Compound	Magnetic ion	Space group	Local moment	Θ_{CW} (K)	Magnetic transition	Frustration para. f	Refs.
$YbMgGaO_4$	$Yb^{3+}(4f^{13})$	$R\bar{3}m$	Kramers doublet	-4	PM down to 60 mK	$f > 66$	[4]
$CeCd_3P_3$	$Ce^{3+}(4f^1)$	$P6_3/mmc$	Kramers doublet	-60	PM down to 0.48 K	$f > 200$	[5]
$CeZn_3P_3$	$Ce^{3+}(4f^1)$	$P6_3/mmc$	Kramers doublet	-6.6	AFM order at 0.8 K	$f = 8.2$	[7]
$CeZn_3As_3$	$Ce^{3+}(4f^1)$	$P6_3/mmc$	Kramers doublet	-62	Unknown	Unknown	[8]
$PrZn_3As_3$	$Pr^{3+}(4f^2)$	$P6_3/mmc$	Non-Kramers doublet	-18	Unknown	Unknown	[8]
$NdZn_3As_3$	$Nd^{3+}(4f^3)$	$P6_3/mmc$	Kramers doublet	-11	Unknown	Unknown	[8]

YD Li, XQ Wang, GC*, PRB 94, 035107 (2016)

Magnetism in the $KBaRE(BO_3)_2$ (RE=Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) series: materials with a triangular rare earth lattice

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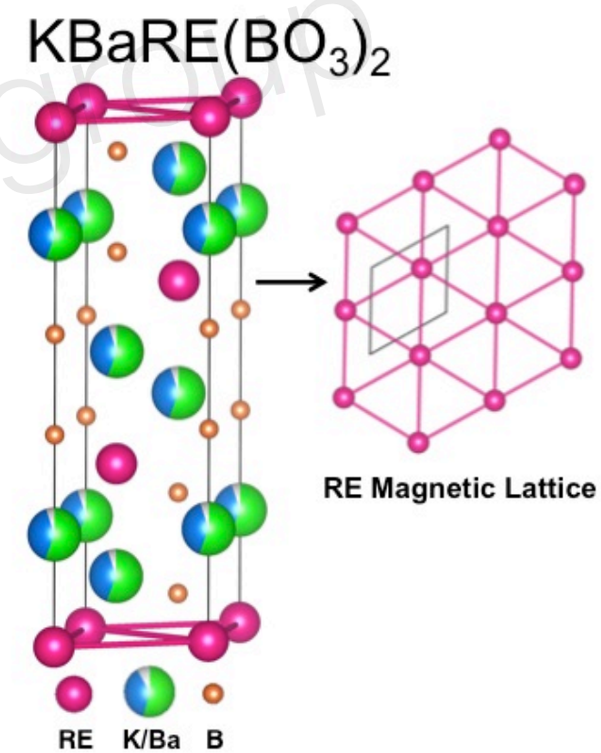

many ternary chalcogenides NaRES2 , NaRESe2 , KRES2 , KRESe2 , KRETe2 , RbRES2 , RbRESe2 , RbRETe2 , CsRES2 , CsRESe2, etc.)

Lots of isostructural materials

Summary

1. We predict the band structure reconstruction of the Ir conduction electrons by the Pr magnetic order. We predict symmetry protected Dirac band touching and topologically protected Weyl nodes. We point out the interesting interplay of conduction electron and local moments in **hybrid quantum materials**.

2. We propose the weak field regime to detect the signatures of fractionalization. Such a regime can be realized in current laboratory settings. It has already been performed and observed by Jun Zhao's group.

   further directions: how to detect spinon-gauge coupling? how to detect gauge field? any other material with similar properties?