

$\text{Pr}_2\text{Ir}_2\text{O}_7$: when Luttinger semimetal meets with Melko-Hertog-Gingras spin ice state

Gang Chen
Fudan University



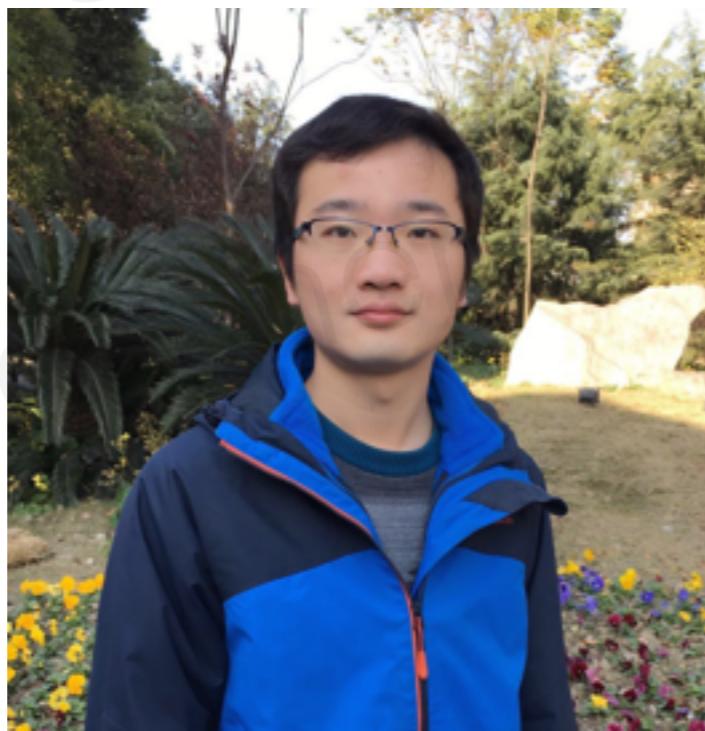
Outline

1. Microscopics of $\text{Pr}_2\text{Ir}_2\text{O}_7$: conduction elections and local moments
2. Pr-magnetism induced Weyl nodes and symmetry protected Dirac band touching

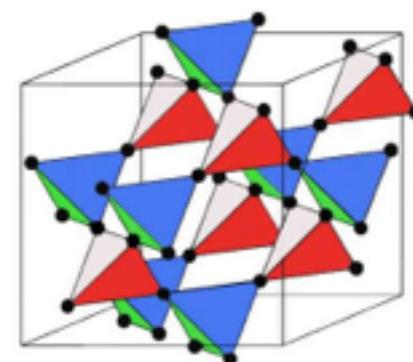
References

Gang Chen, Phys Rev B 94, 205107, (2016)

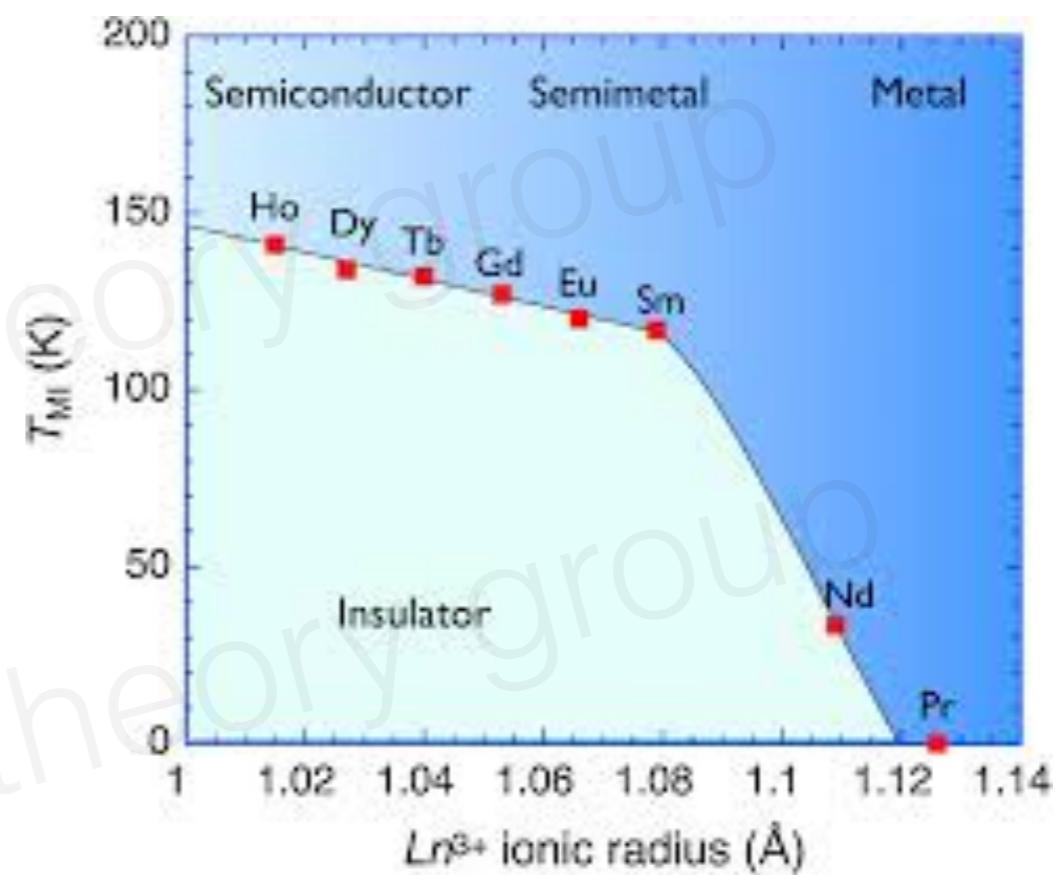
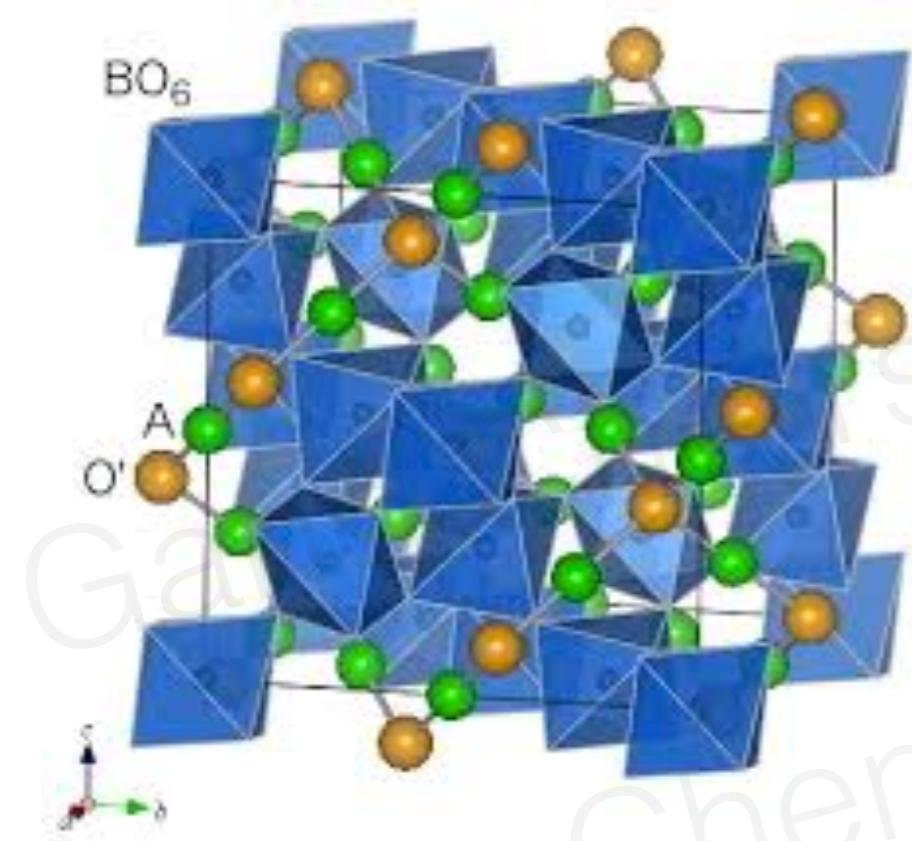
Xu-Ping Yao, Gang Chen, arXiv:1712.06534 PRX



Xu-Ping Yao
(Fudan)



Pyrochlore iridates



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

$Pr_2Ir_2O_7$ remains metallic and disordered !

iridate provides such a setting, has interaction a strong spin-orbit coupling

Leon knows a lot of solid state physics, Mott transition, density of state is suppressed, the longer range part of interaction becomes important and could induce exciton magnetism.

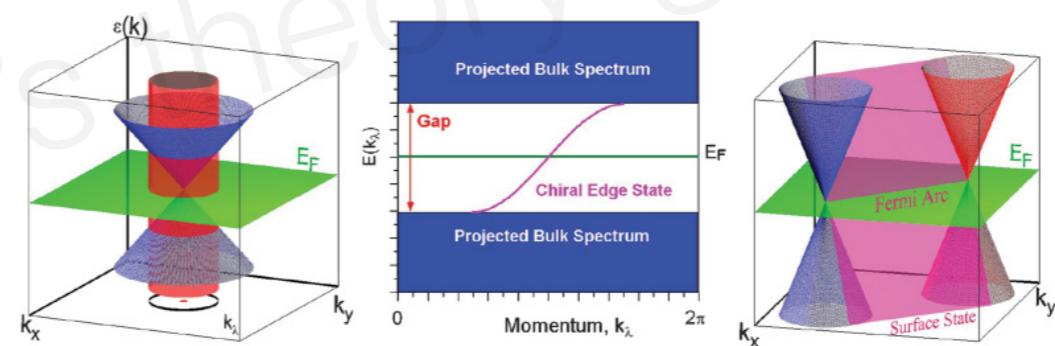
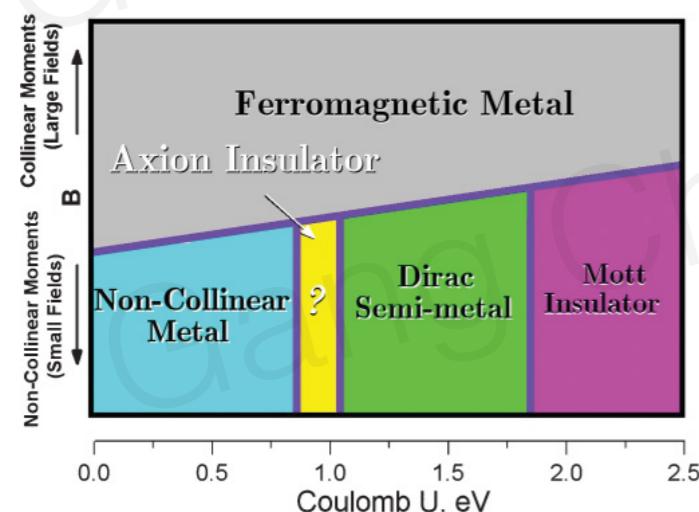
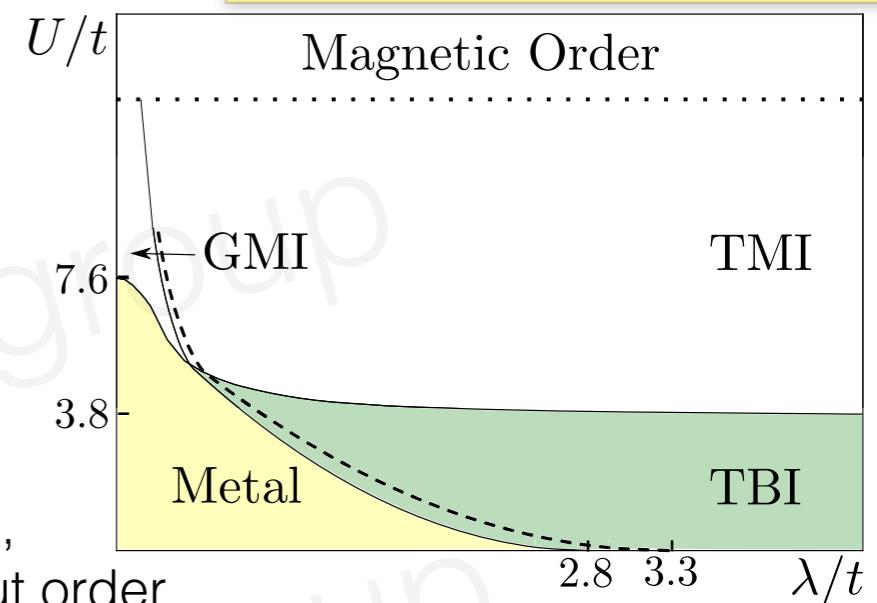
Halperin 1960s.

Early motivation: correlation physics in spin-orbit (to)

D Pesin, L Balents, NatPhys 2010, Topological Mott insulator
(or A 3D U(1) quantum spin liquid)

$$H = \sum_{Ri\alpha} (\varepsilon_\alpha - \mu) d_{Ri\alpha}^\dagger d_{Ri\alpha} + t \sum_{\langle Ri, R'i' \rangle} T_{\alpha\alpha'}^{ii'} d_{Ri\alpha}^\dagger d_{R'i'\alpha'} + \frac{U}{2} \sum_{Ri} \left(\sum_\alpha d_{Ri\alpha}^\dagger d_{Ri\alpha} - n_d \right)^2$$

Xiangang Wan, Turner, Vishwanath, Savrasov, PhysRevB 2011,
Magnetic Weyl semimetal from the Ir correlation driven all-in all-out order.

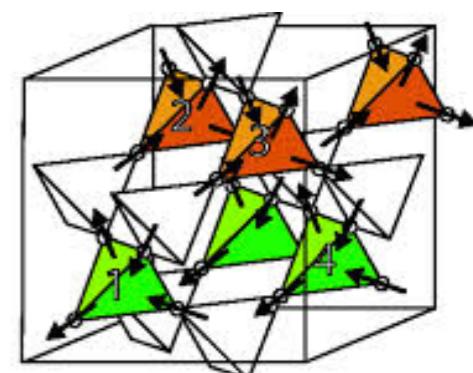


Weyl semimetal and surface Fermi arcs

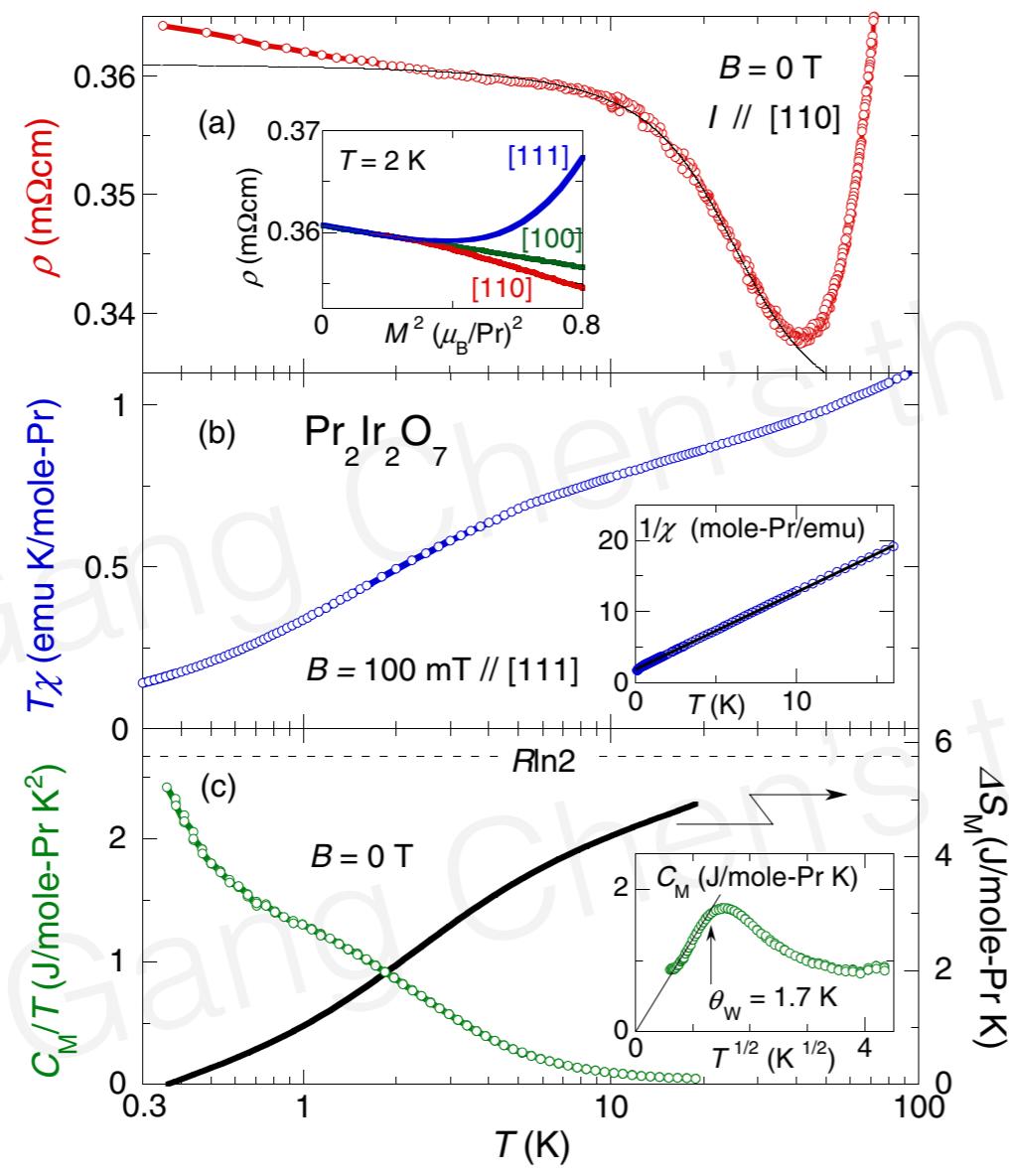
Later on, many interesting works about Iridium physics
(YB Kim, L Savary, L Fu, Xi Dai, Imada, BJ Yang, EG Moon, Nagaosa, etc)



Peculiar one: Pr₂Ir₂O₇

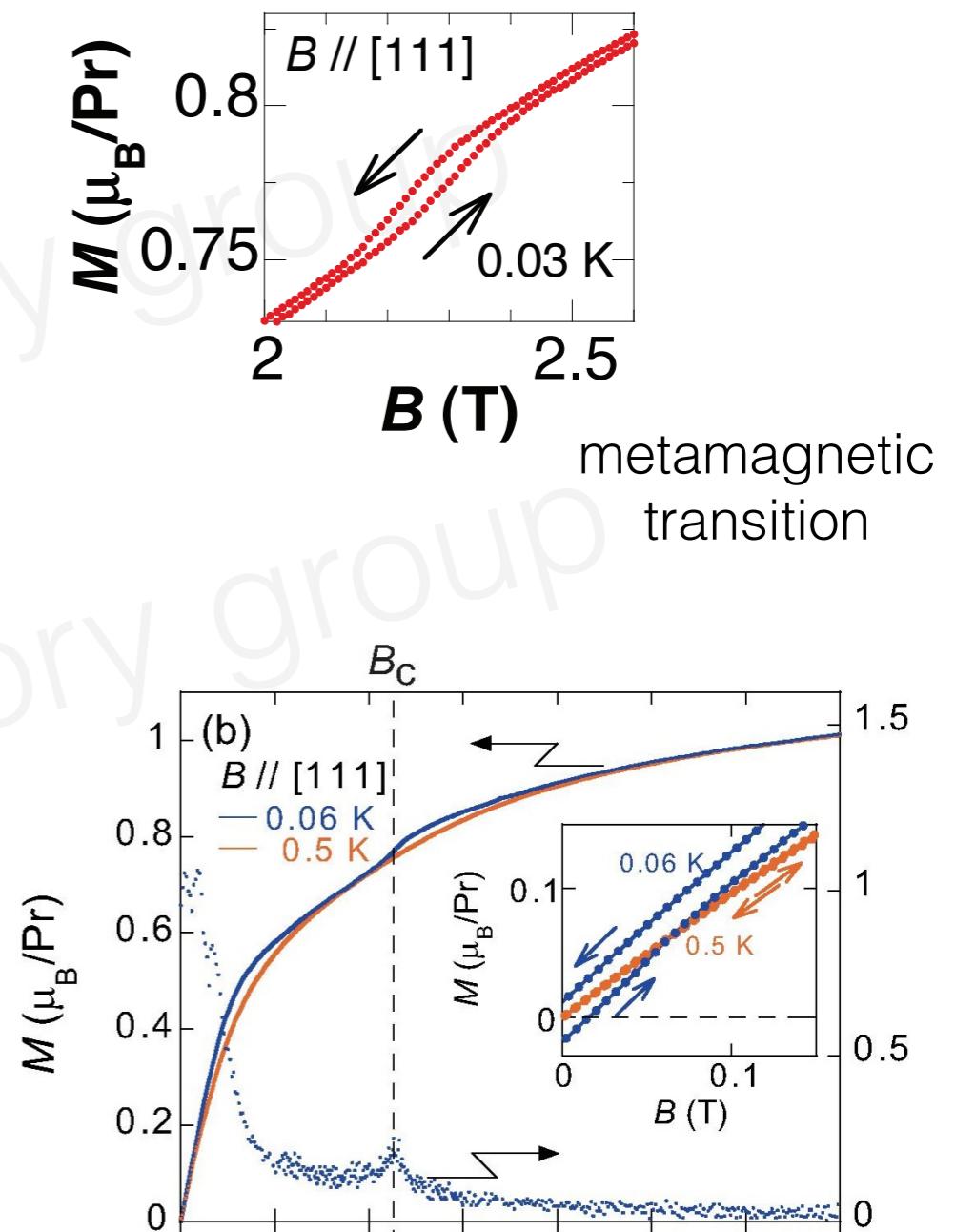


Satoru Nakatsuji



Nakatsuji, etc

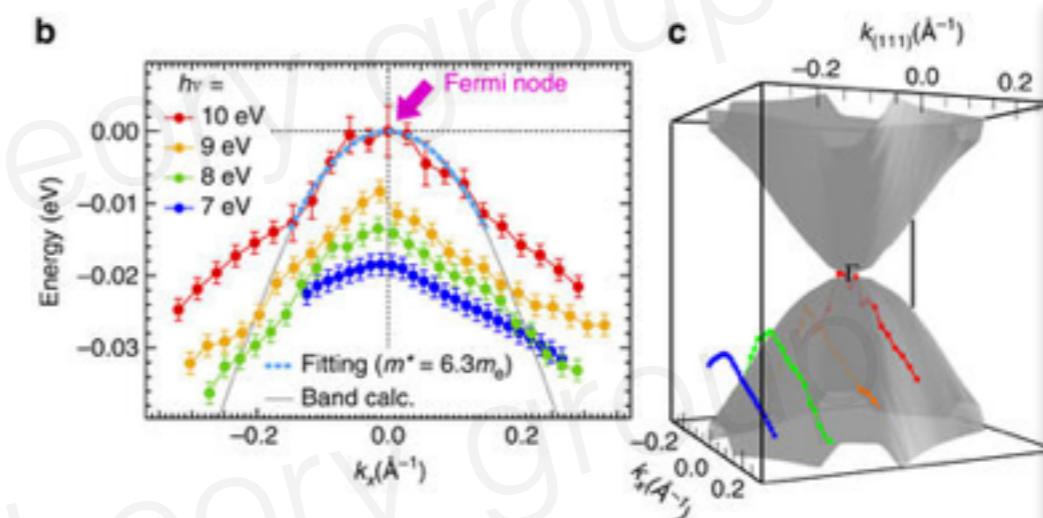
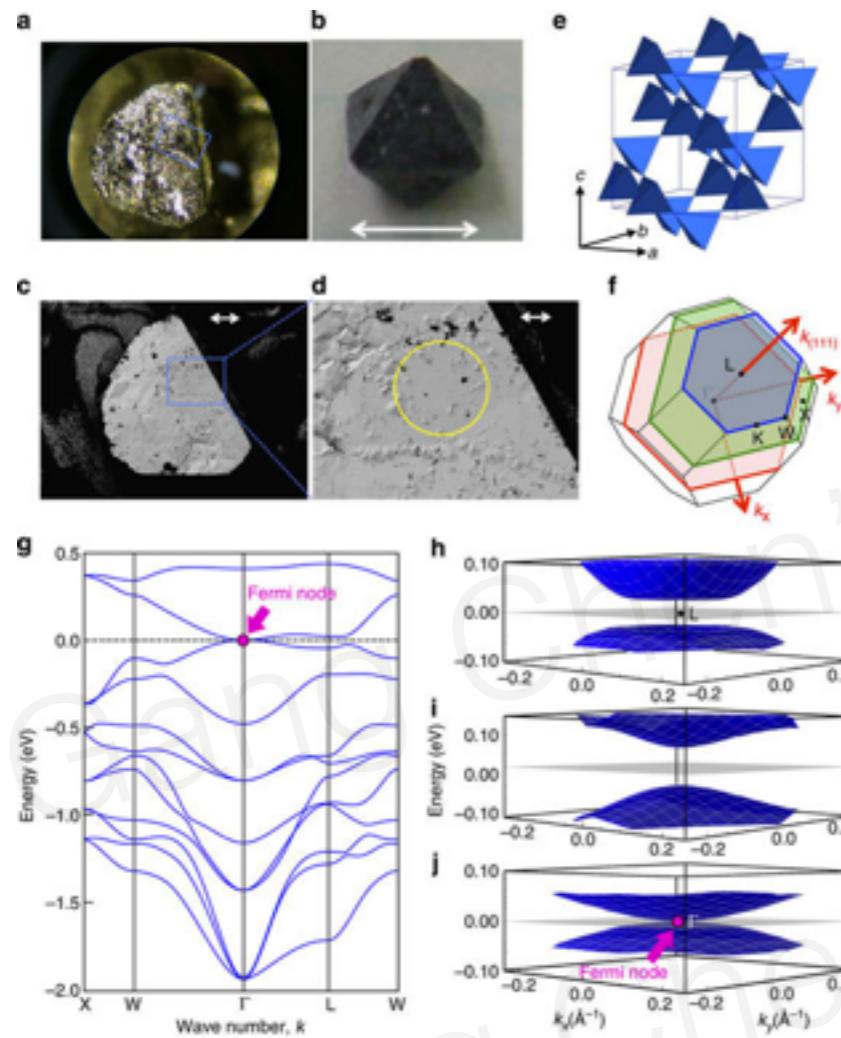
PRL 96, 087204 (2006)



Ir conduction electron: Luttinger semimetal



T Kondo



ARPES: Quadratic band

vanishing DOS, p
the coulomb interac

T Kondo, ... **Ru Chen**, ..., Nakatsuji, Balents, Shin

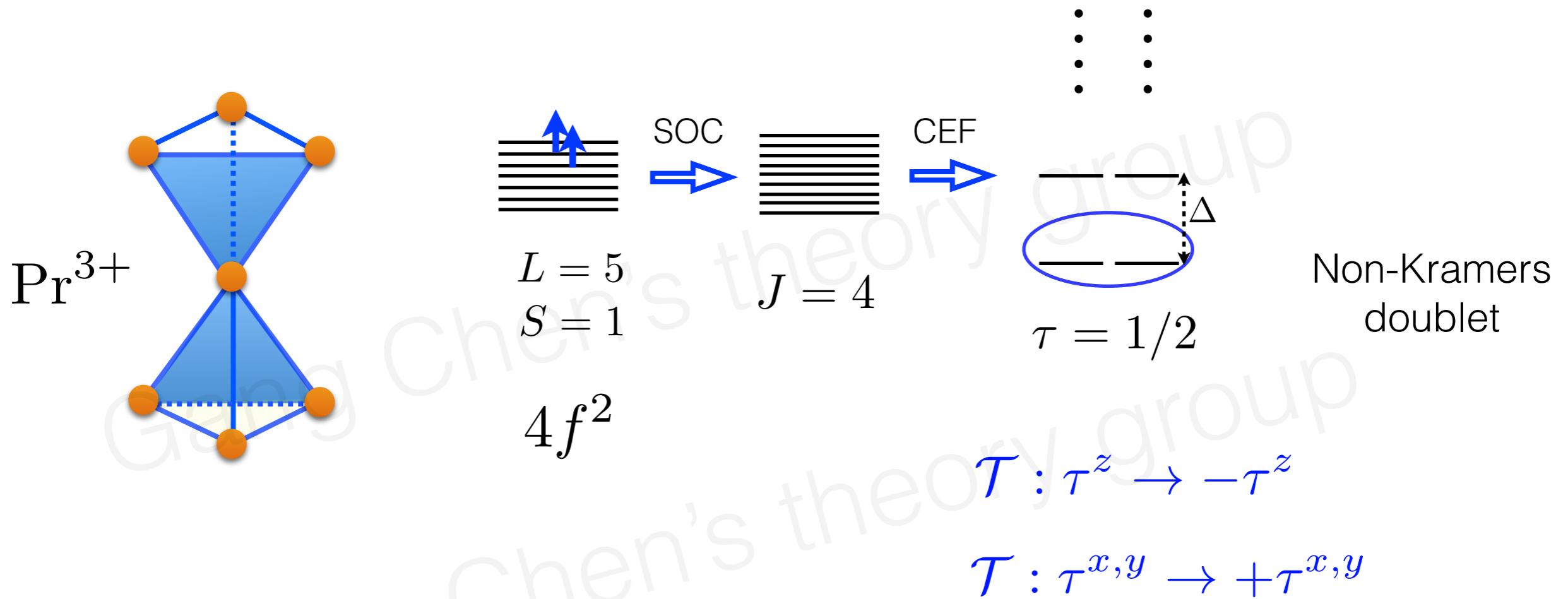
Nature Comm, 2015

P Amitage's optical measurement 2017

Correlation effect: EG Moon, L Savary, YB Kim,
C Xu, L Balents

Partial screening of long
range Coulomb interaction

Pr local moments: non-Kramers doublets



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.

Some $\text{Pr}_2\text{Ir}_2\text{O}_7$ sample does order magnetically

Unstable Spin-Ice Order in the Stuffed Metallic Pyrochlore $\text{Pr}_{2+x}\text{Ir}_{2-x}\text{O}_{7-\delta}$

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 Sakakibara²

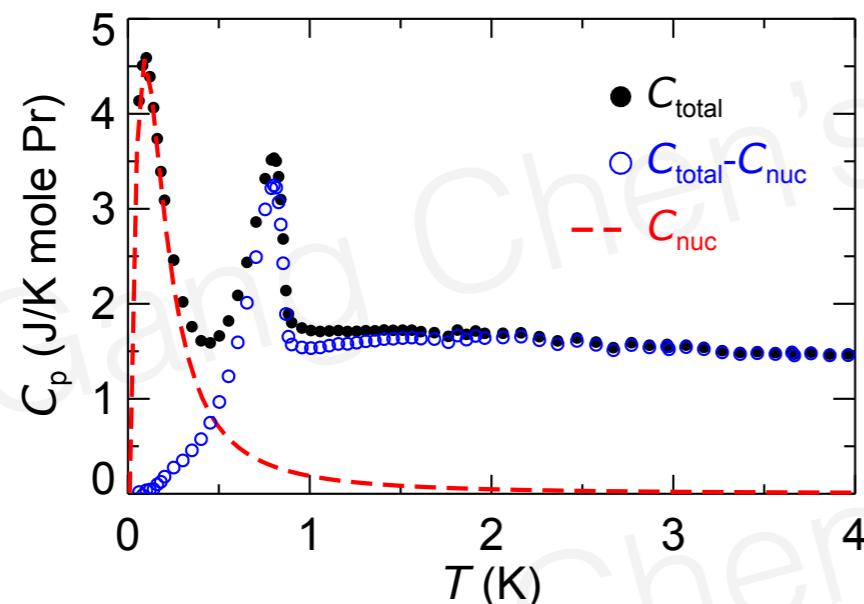


FIG. 1. (color online) Temperature dependence of the specific heat of $\text{Pr}_{2+x}\text{Ir}_{2-x}\text{O}_{7-\delta}$ in zero field. Filled circles: experimental total specific heat. Dashed curve: calculated specific

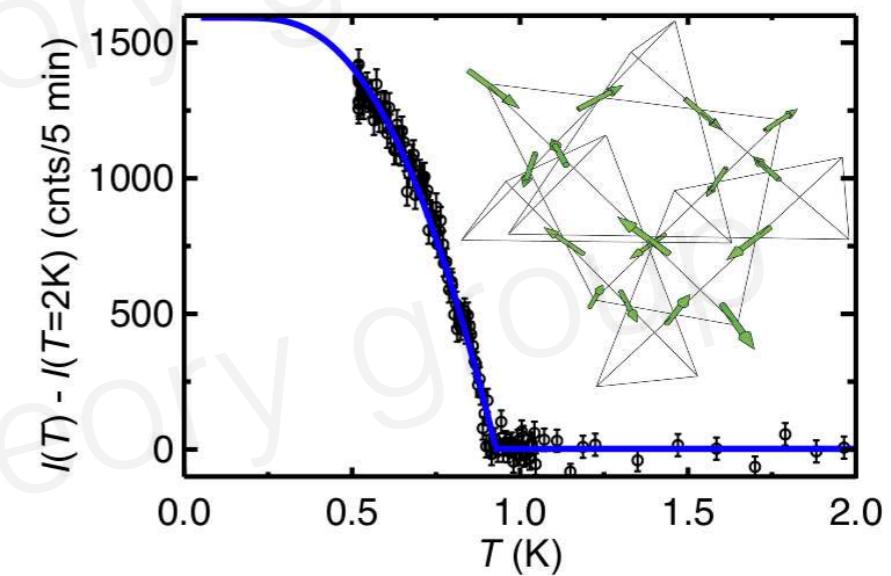
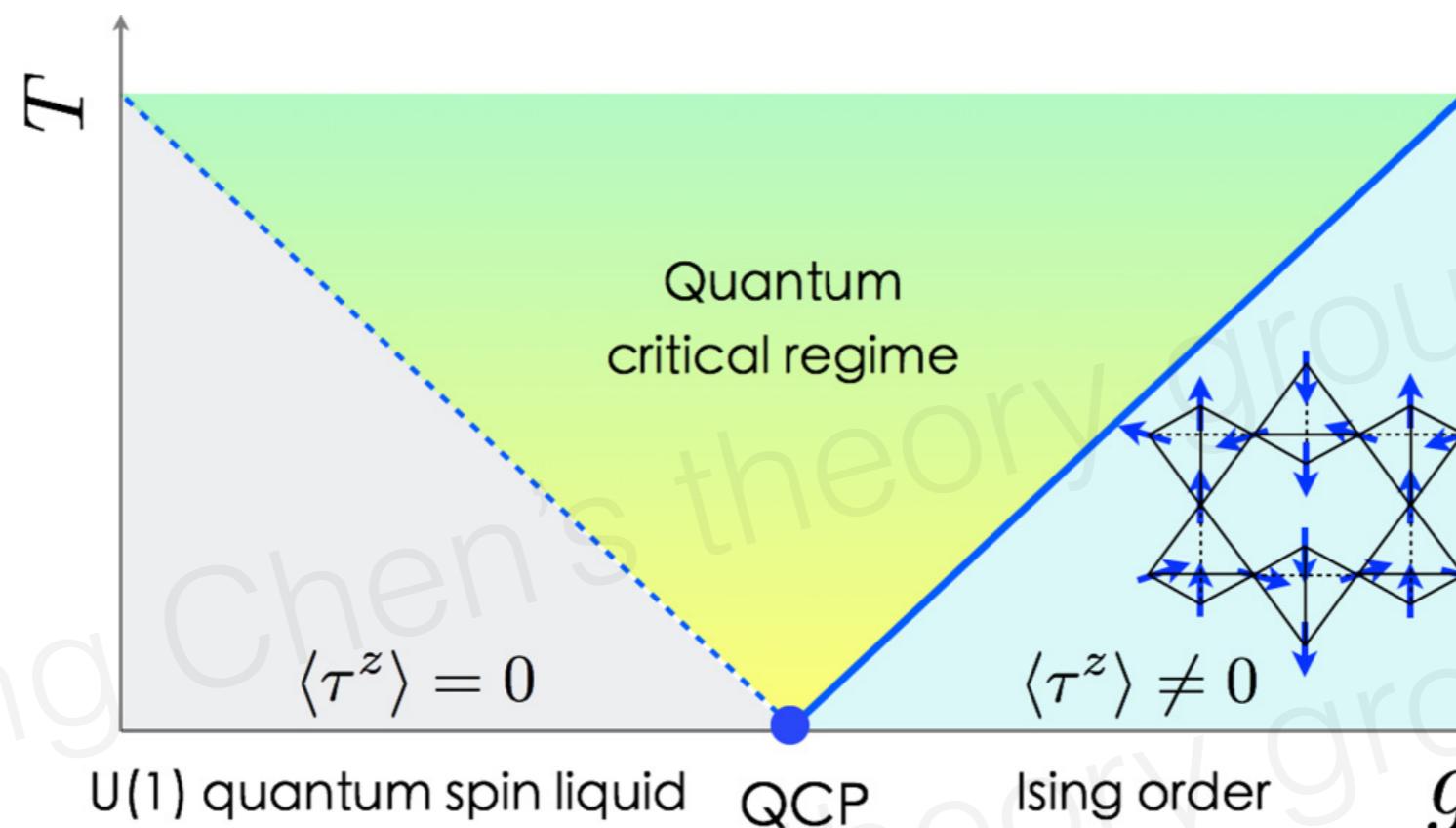


FIG. 2. (color online) Temperature dependence of elastic neutron scattering intensity of $\text{Pr}_{2+x}\text{Ir}_{2-x}\text{O}_{7-\delta}$ at the position of the $\mathbf{q}_m = (100)$ reflection. The intensity measured at $T = 2\text{ K}$

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

Our suggestion



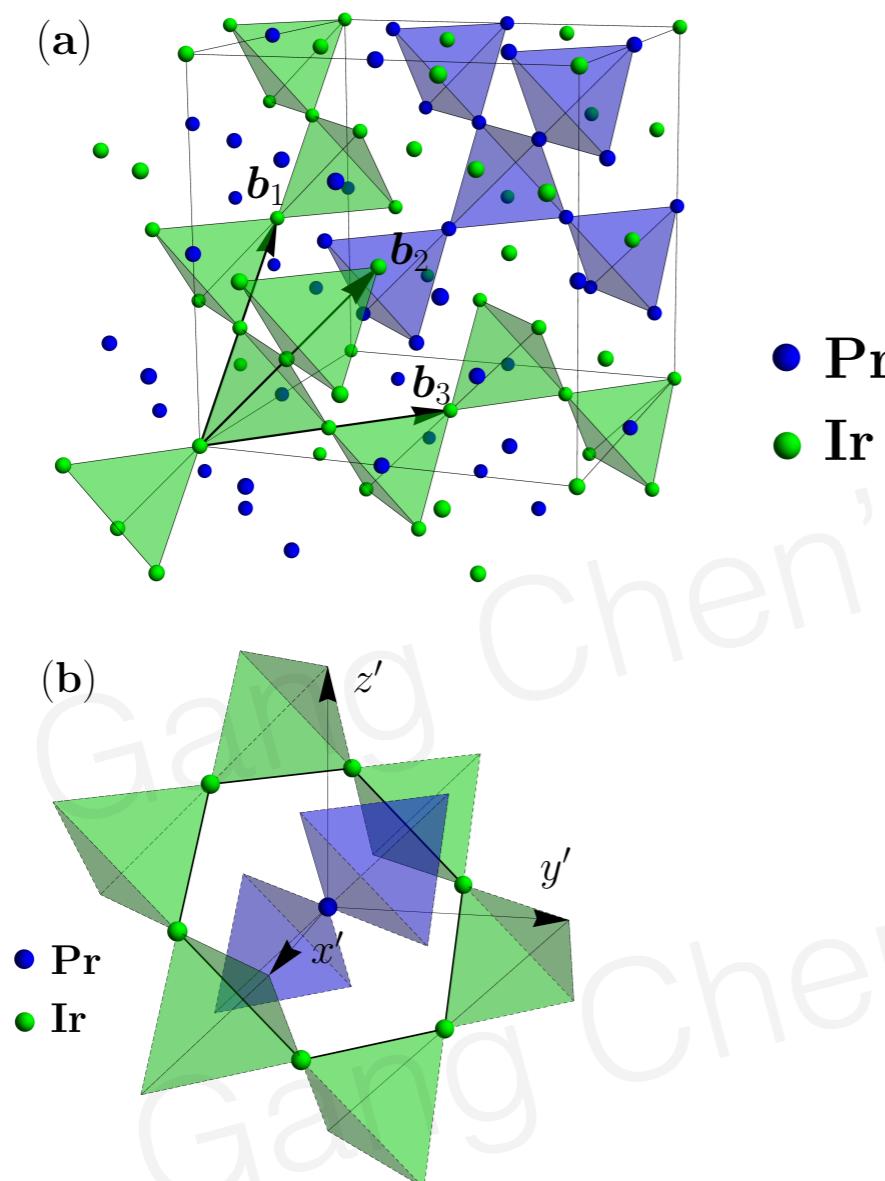
The Pr subsystem is proximate to a quantum phase transition from pyrochlore ice $U(1)$ QSL to Ising magnetic order.

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

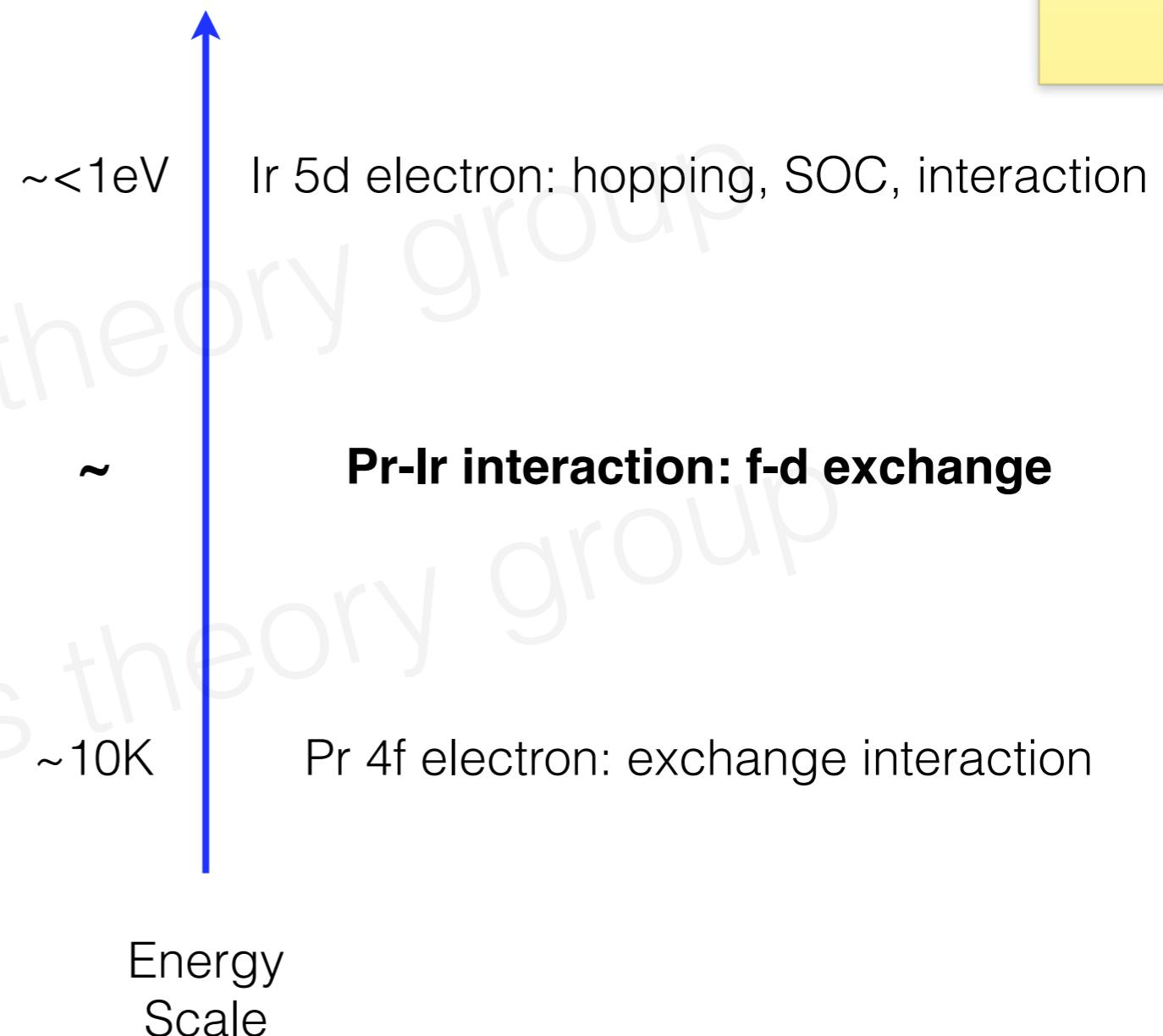
GC, PRB 94, 205107 (2016)

interact with
interact with
very complex
system

Microscopics: Ir conduction electron + Pr local moment

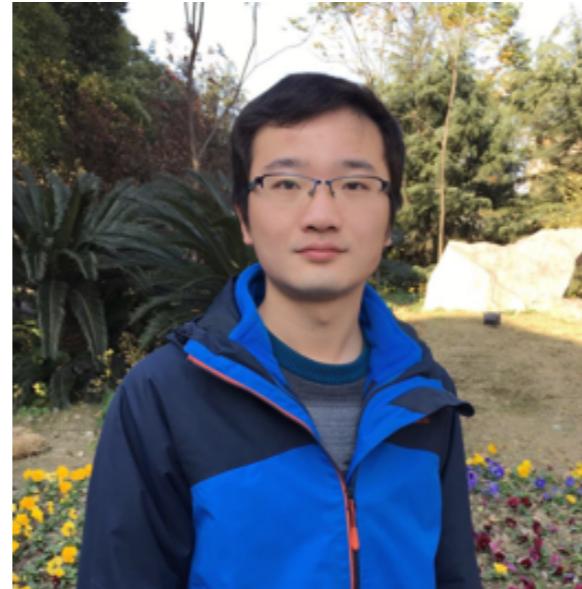


GC, Hermelé, PRB 2012
X-P Yao, GC, 1712.06534



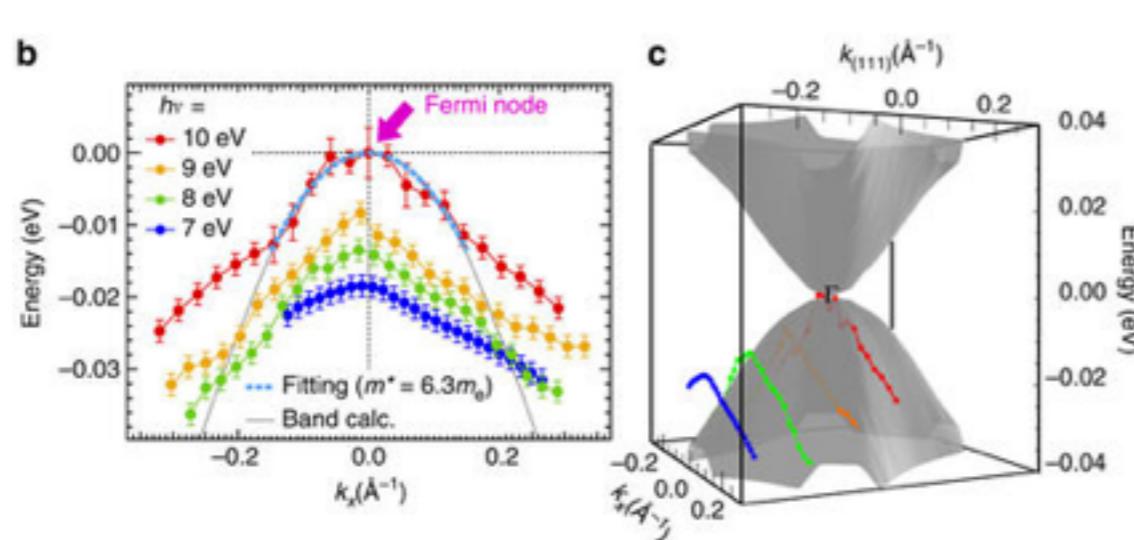
2. Pr-magnetism induced Weyl nodes and symmetry protected Dirac band touching

Here we focus on the ordered side/sample.

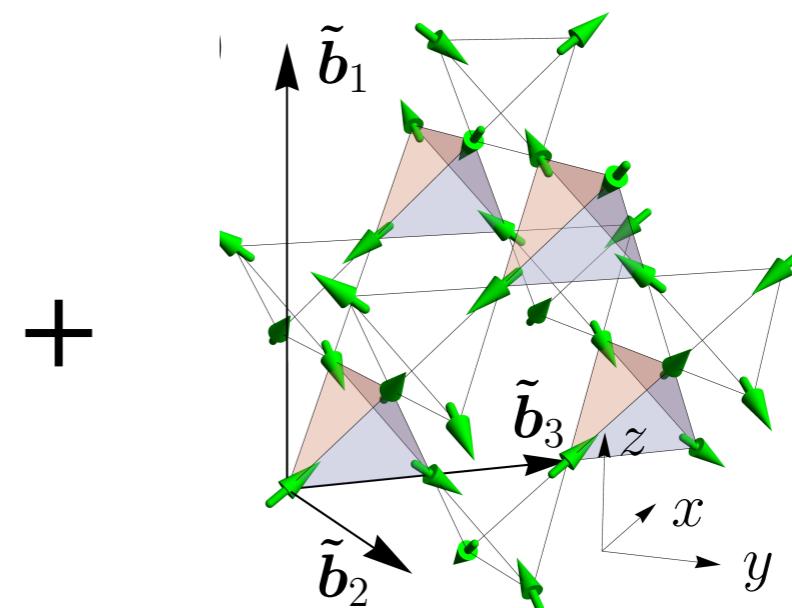


Xu-Ping Yao, GC, 1712.06534

What is the impact of the Pr magnetism
on Ir conduction electrons?



Ir Luttinger semimetal



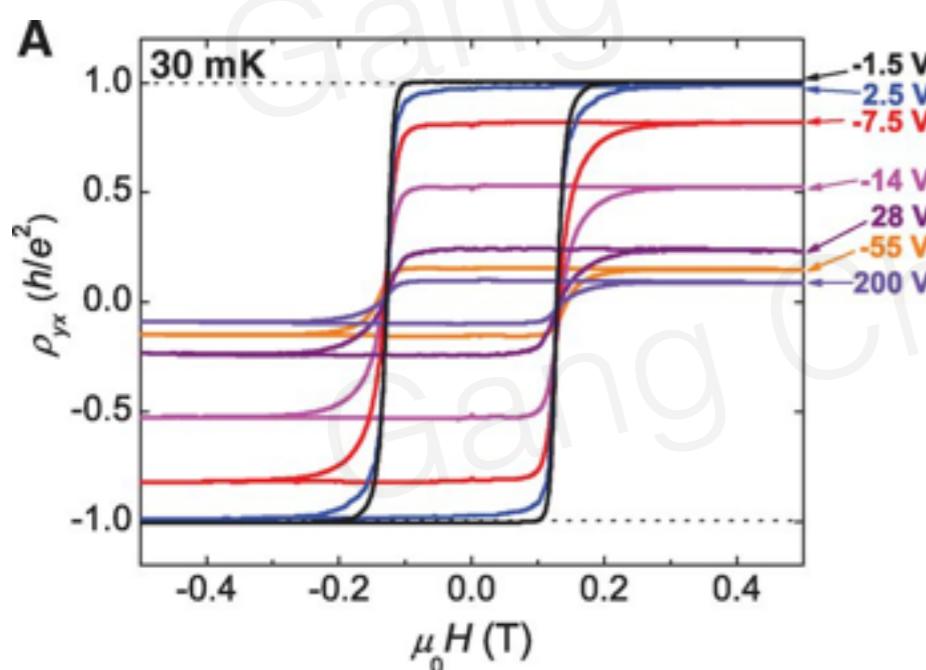
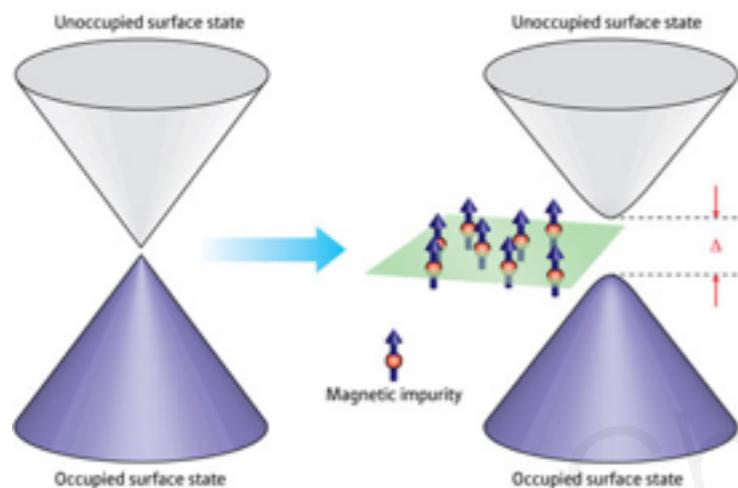
Pr magnetism

= ???

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

Quantum Anomalous Hall Effect

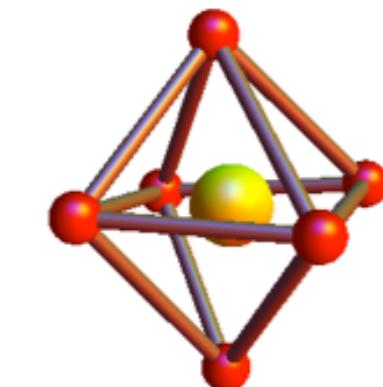
Experiments of Prof Xue's group



1. One understanding: TI \rightarrow Dirac cone ferromagnetism \rightarrow gapped Dirac fermion \rightarrow 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 vice versa.

Ir 5d electron: SOC, hopping and correlation



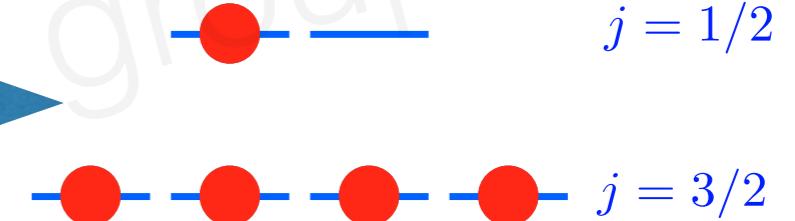
IrO₆ octahedron

Ir⁴⁺ : 5d⁵

$e_g : x^2 - y^2, 3z^2 - r^2$

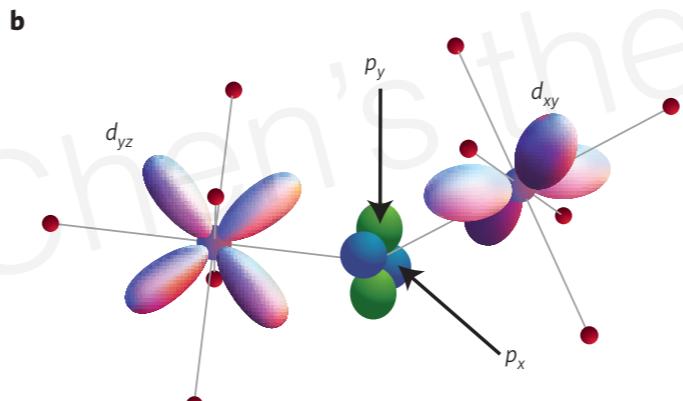
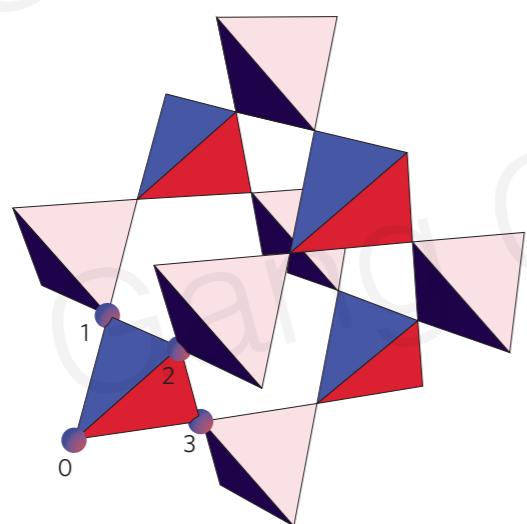
$\downarrow \uparrow$
t_{2g}: xy,xz,yz

Crystal electric field



Spin-orbit coupling

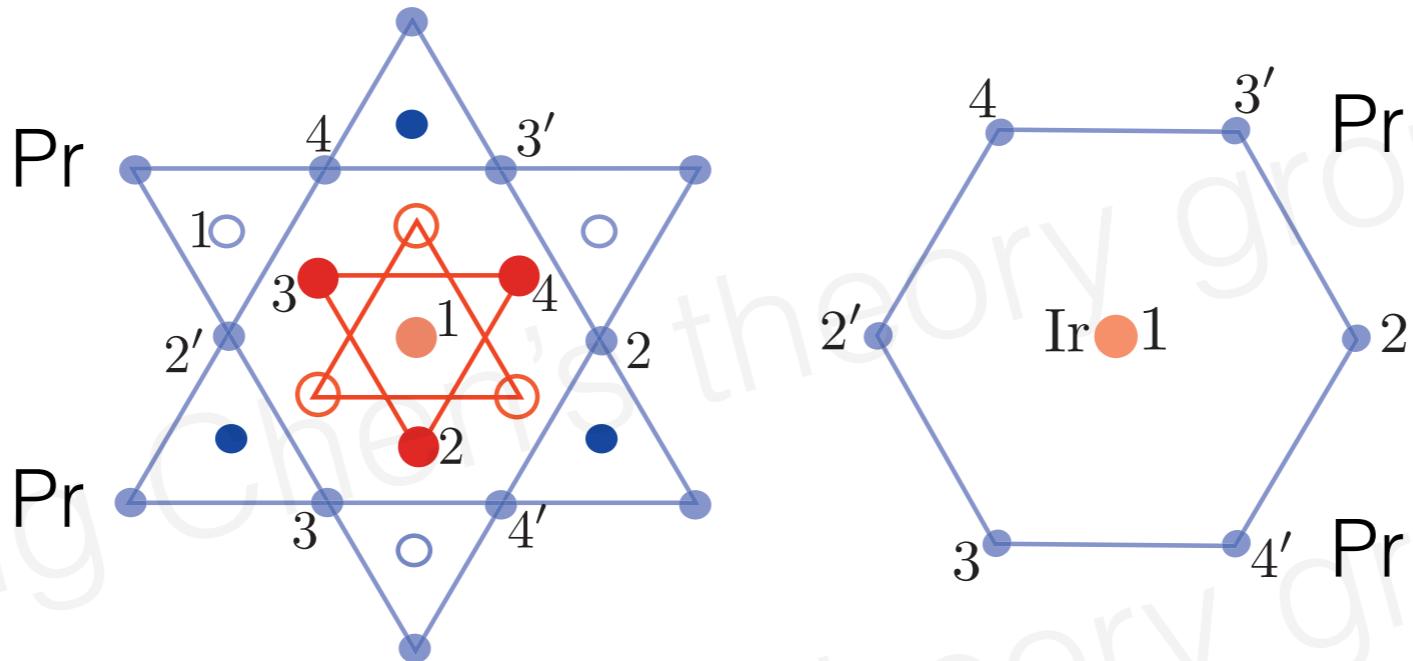
BJ Kim, etc 2008,
GC, Balents, PRB 2008
Jackeli, Khaliullin, PRL 2009



Besides Ir electron hopping via intermediate oxygens, there is also direct electron hopping

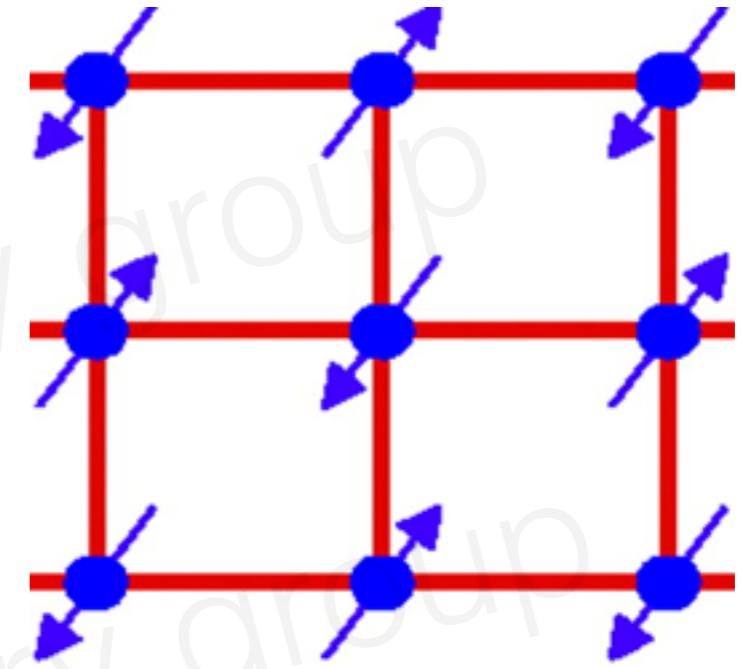
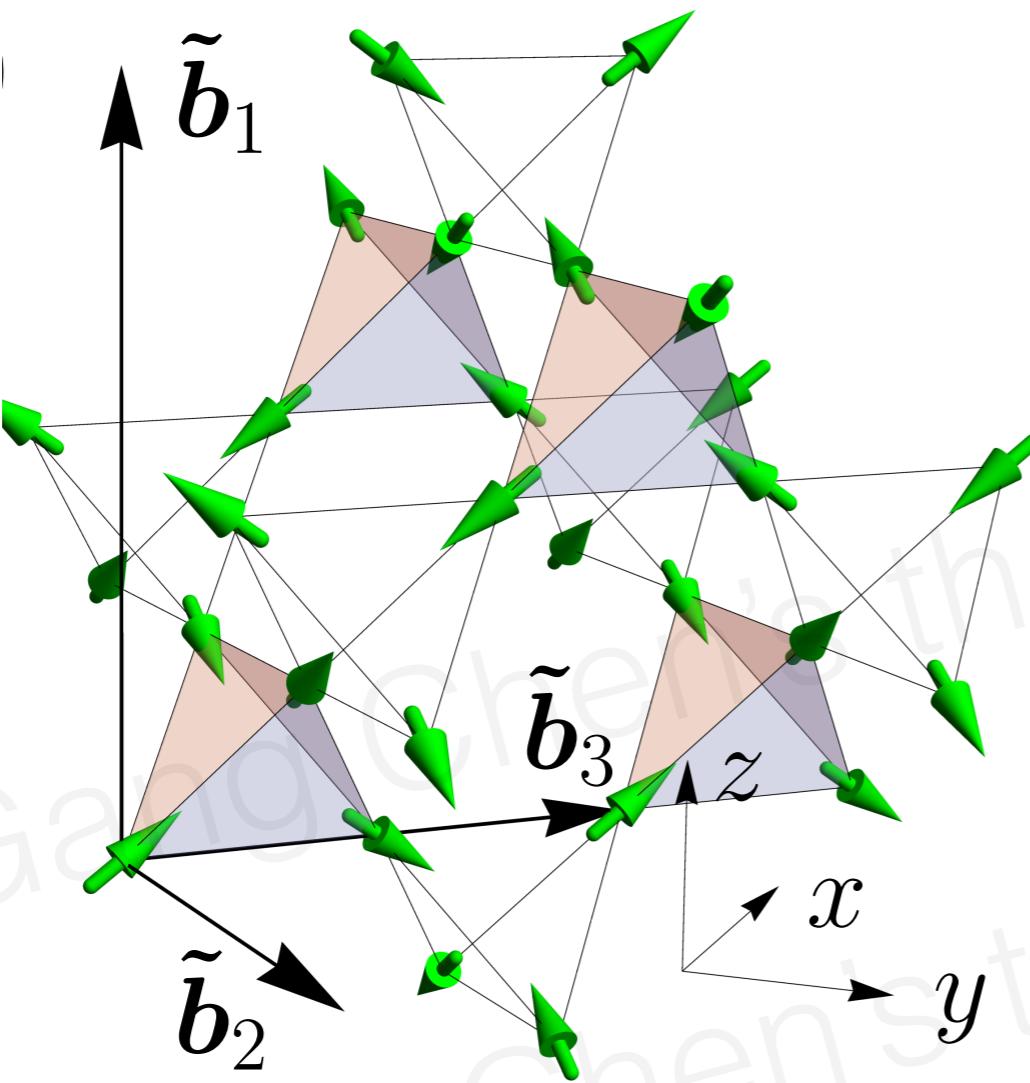
For Pr₂Ir₂O₇, correlation renormalizes the band width.

Pr-Ir interaction: 4f-5d exchange



$$\begin{aligned}\mathcal{H}_{\text{fd}} = & [c_1 \tau_4^z - c_2 (\tau_2^z + \tau_3^z)] j_1^x + [c_1 \tau_3^z - c_2 (\tau_2^z + \tau_4^z)] j_1^y \\ & + [c_1 \tau_2^z - c_2 (\tau_3^z + \tau_4^z)] j_1^z + [2 \leftrightarrow 2', 3 \leftrightarrow 3', 4 \leftrightarrow 4'],\end{aligned}$$

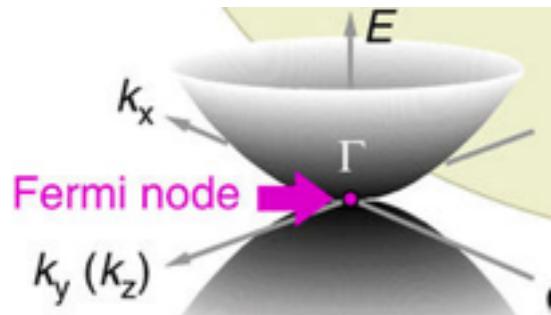
Magnetic translation of Pr magnetic state



Neel state on square lattice

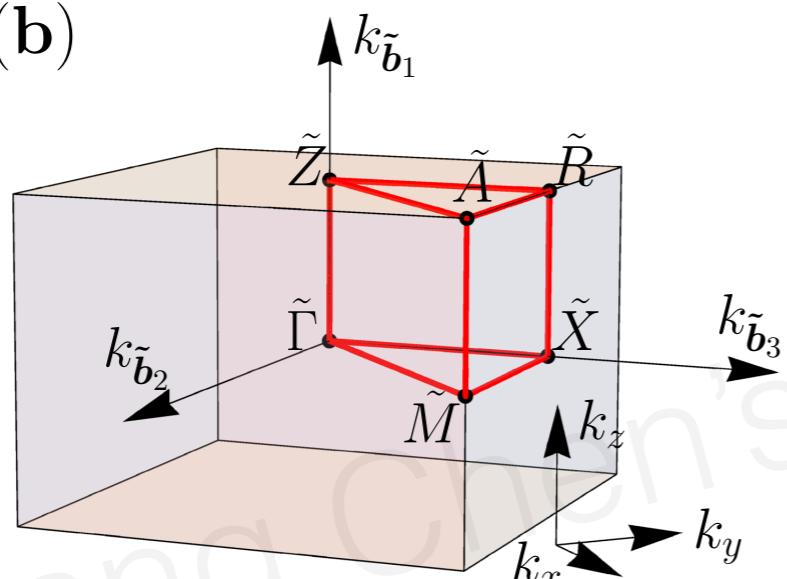
$$\tilde{\mathcal{T}} \equiv \mathcal{T} \circ t$$

3D analogue of the magnetic translation for Neel state



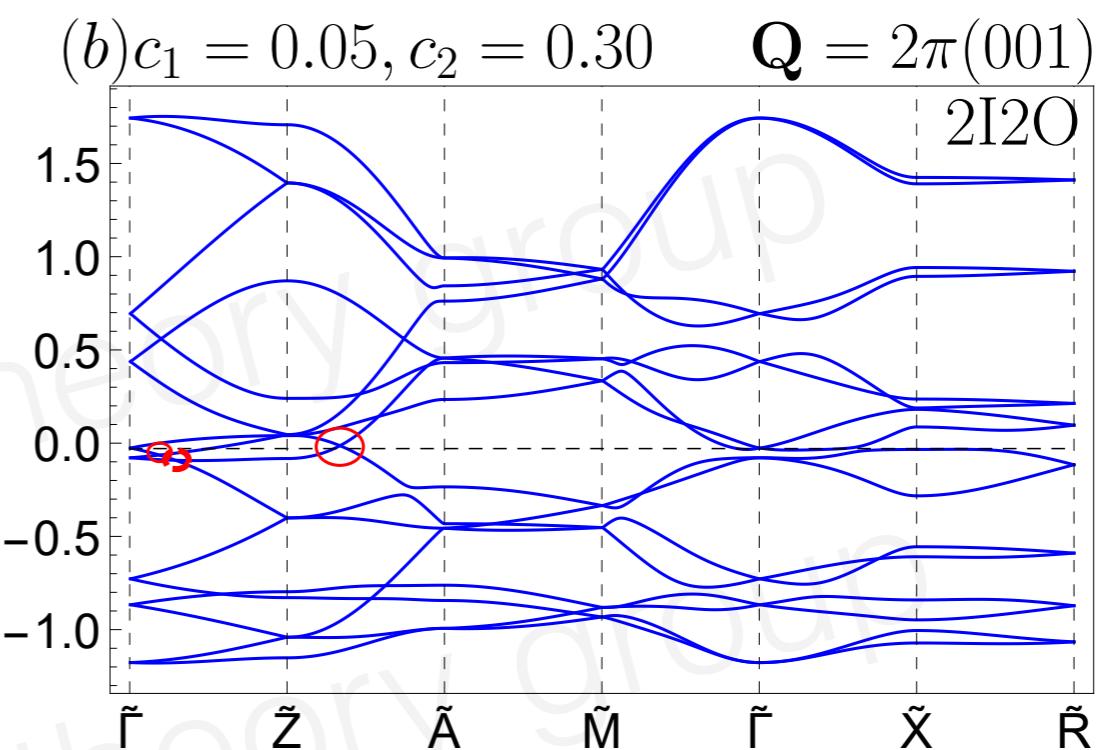
Symmetry protected Dirac band touching

(b)



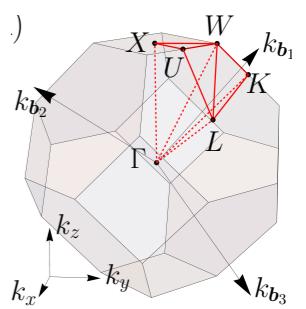
magnetic Brillouin zone

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

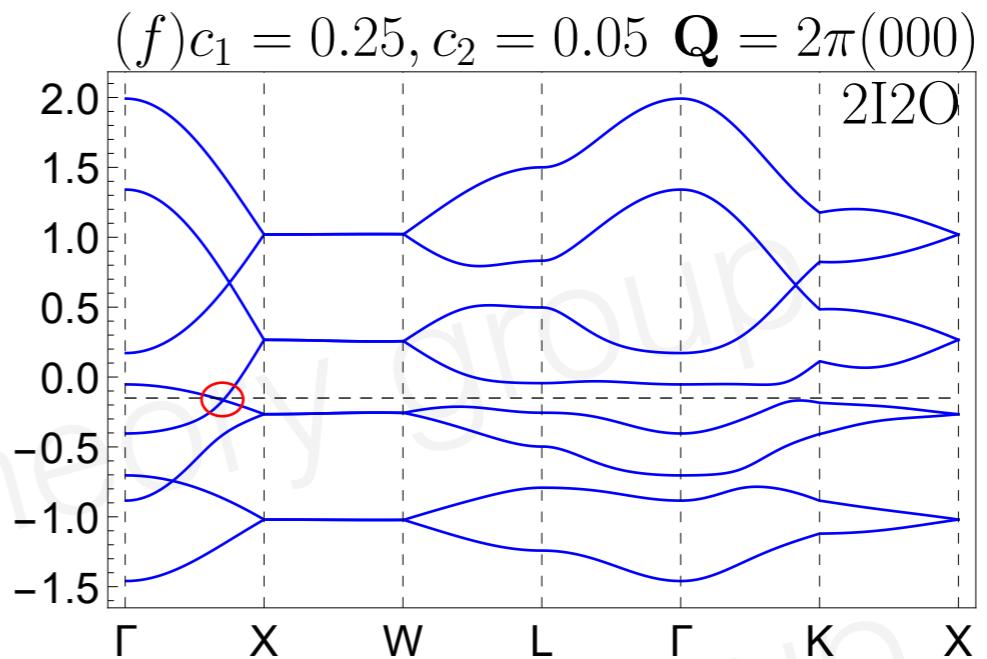
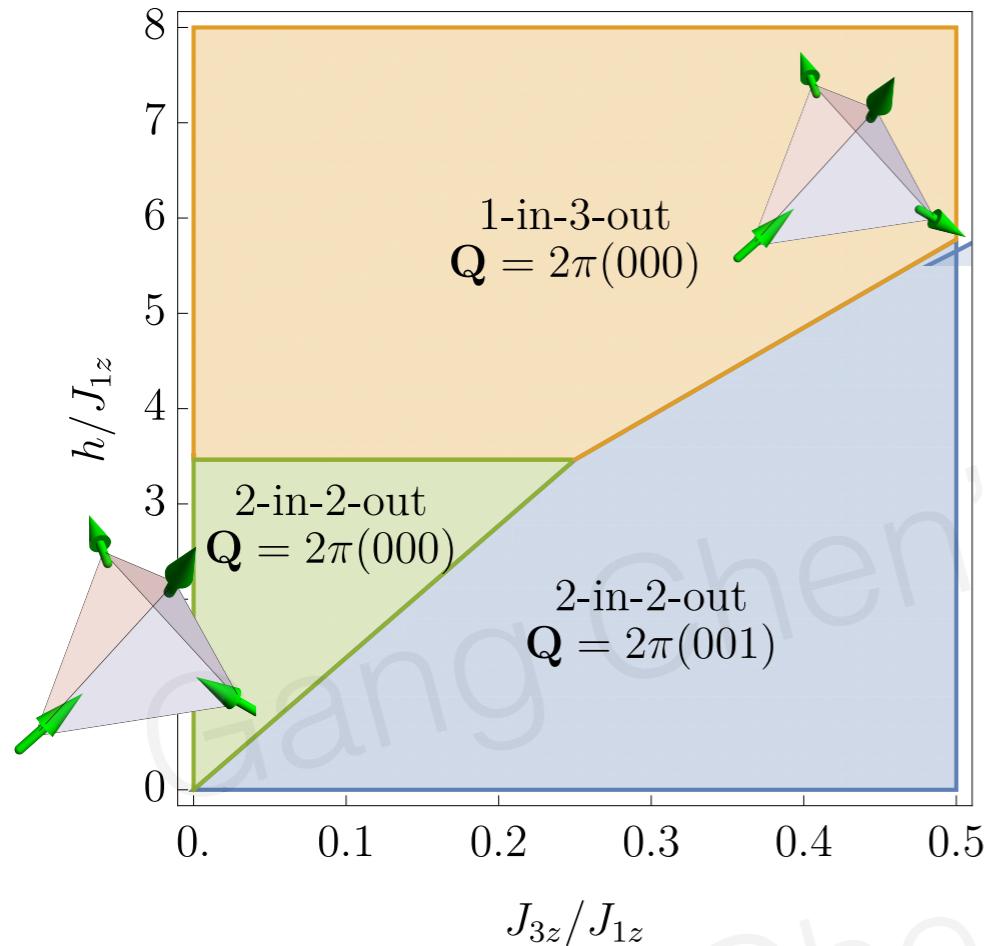


in addition, there are Weyl nodes
whose existence does not require symmetry

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



Band engineering by external magnetic field

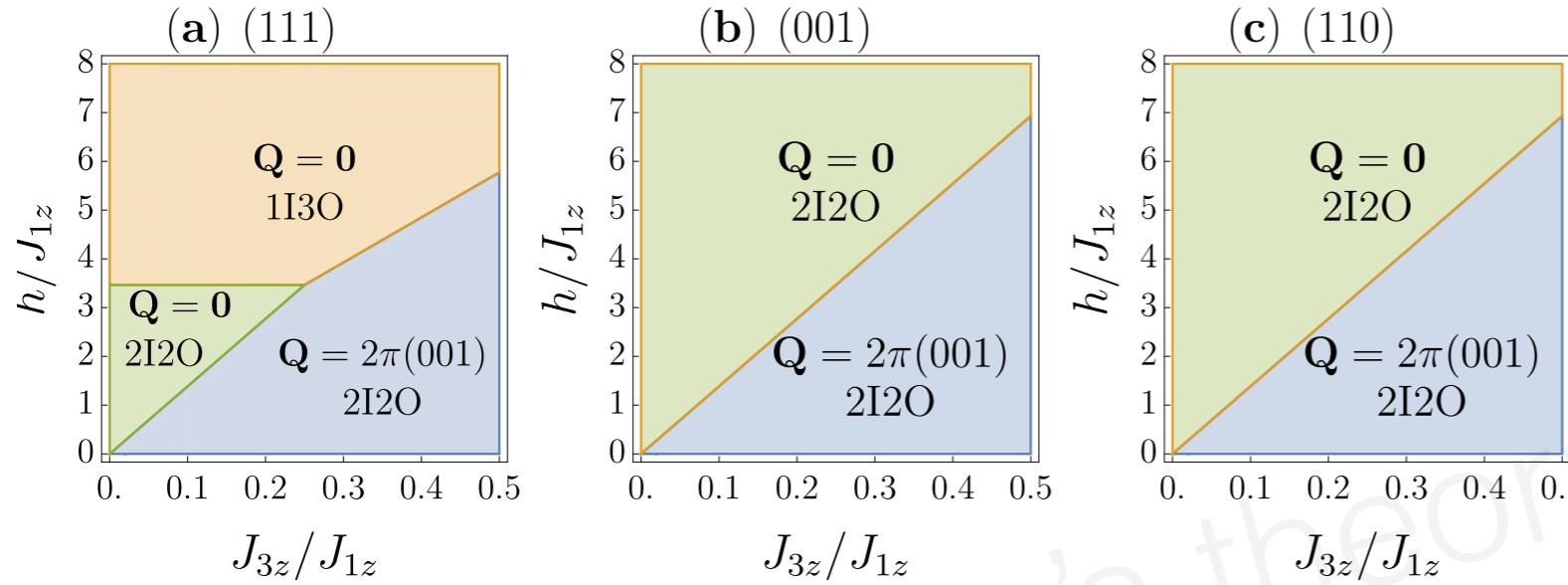


example: double Weyl nodes

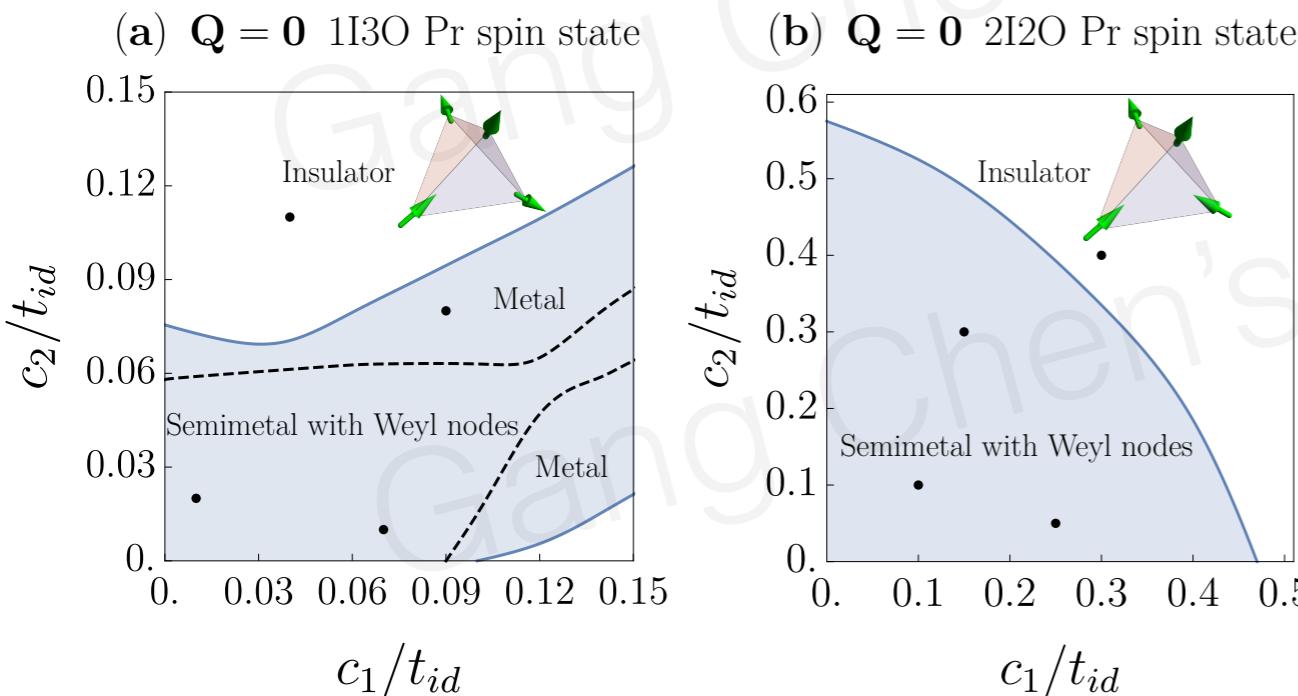
e.g. **HgCr₂Se₄**, HM Weng, X Dai, Z Fang

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



111 magnetic field, Ir band structure

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

Conclusion

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.

Some prediction has been confirmed by Nakatsuji's experiments.