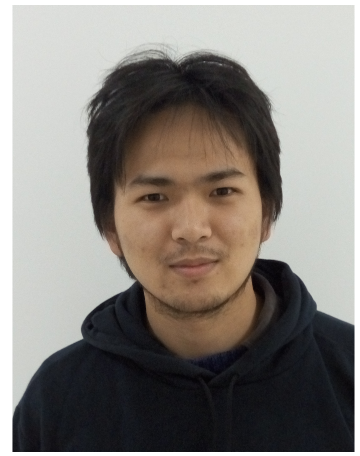
When Luttinger semimetal meets with ordered spin ice state in pyrochlore iridates

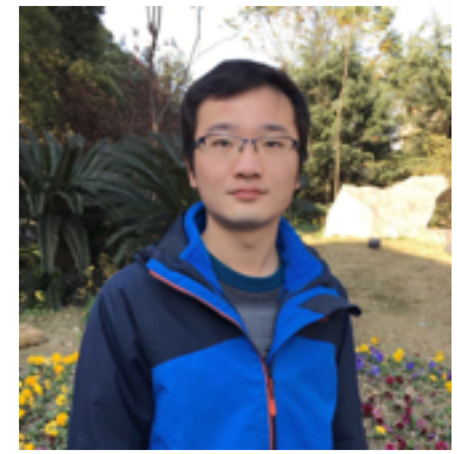
Gang Chen (陈钢)
Fudan University

My theory group on [strongly correlated] quantum matter

Graduate students:



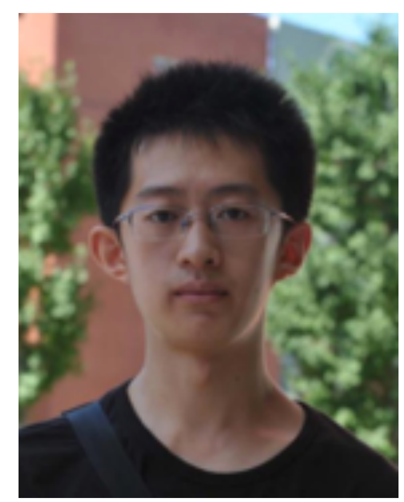
Yao-Dong Li (Fudan -> UCSB) Left 2017



Xu-Ping Yao (Fudan)

Postdocs:

Changle Liu （Fudan） Joined 2017

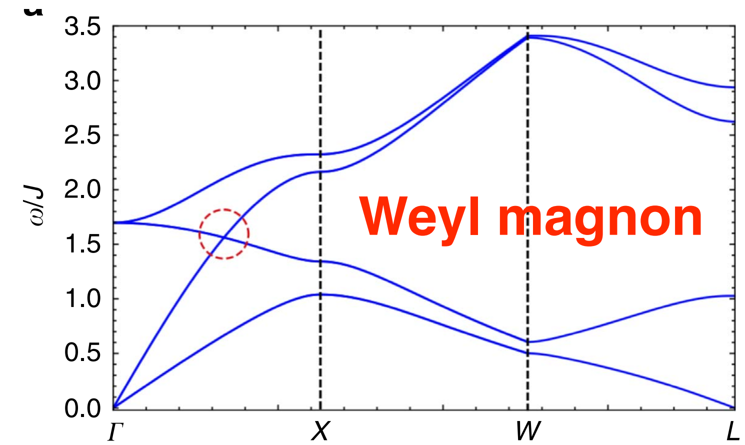


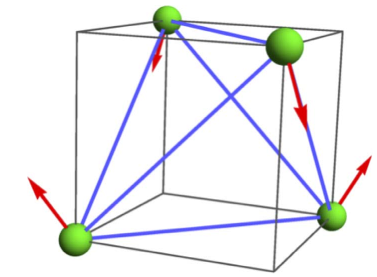
Fei-Ye Li （Fudan）

Some recent topics out of my group (incomplete)

- **Topological Weyl magnons**
  in ordered antiferromagnet

$$H = J\sum_{\langle ij\rangle \in \mathrm{u}} \mathbf{S}_i\cdot\mathbf{S}_j + J'\sum_{\langle ij\rangle\in \mathrm{d}} \mathbf{S}_i\cdot\mathbf{S}_j + D\sum_i (\mathbf{S}_i\cdot\hat{\mathbf{z}}_i)^2$$

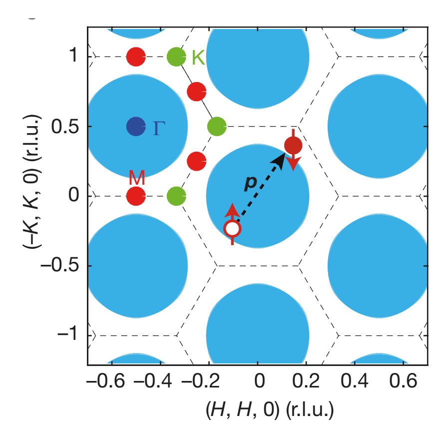


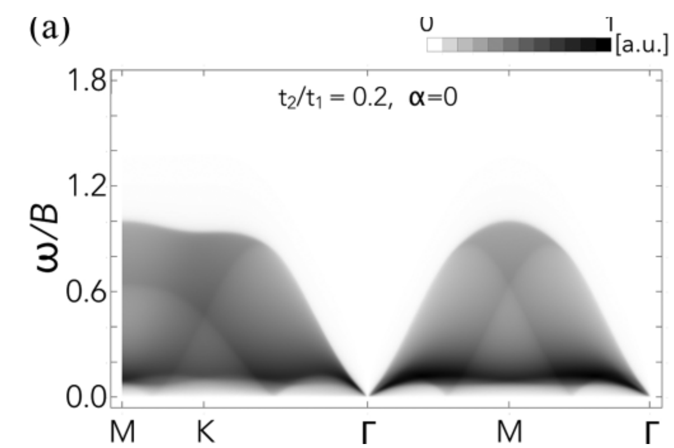


- **Spin liquid & spinon Fermi surface** in YbMgGaO4

$$\boldsymbol{S}_{\boldsymbol{r}} = \frac{1}{2}\sum_{\alpha,\beta} f^{\dagger}_{\boldsymbol{r}\alpha}\boldsymbol{\sigma}_{\alpha\beta} f_{\boldsymbol{r}\beta},$$

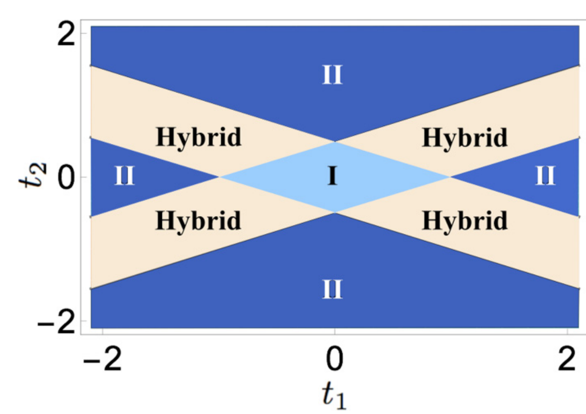
$$H_{\mathrm{MF}} = -\sum_{(\boldsymbol{r}\boldsymbol{r}')}\sum_{\alpha\beta}[\, t_{\boldsymbol{r}\boldsymbol{r}',\alpha\beta} f^{\dagger}_{\boldsymbol{r}\alpha} f_{\boldsymbol{r}'\beta} + \mathrm{H.c.}\,],$$

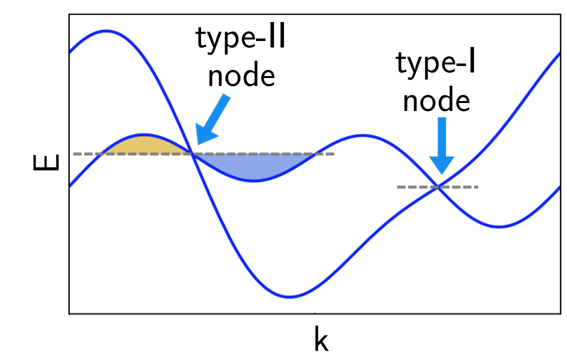




- **Hybrid Weyl semimetal**

$$H = \sum_j [-t_x \boldsymbol{c}^{\dagger}_j \sigma_x \boldsymbol{c}_{j+\hat{x}} - t_y \boldsymbol{c}^{\dagger}_j \sigma_x \boldsymbol{c}_{j+\hat{y}} - t_z \boldsymbol{c}^{\dagger}_j \sigma_x \boldsymbol{c}_{j+\hat{z}}$$
$$- i t'_y \boldsymbol{c}^{\dagger}_j \sigma_y \boldsymbol{c}_{j+\hat{y}} - i t'_z \boldsymbol{c}^{\dagger}_j \sigma_z \boldsymbol{c}_{j+\hat{z}} + \mathrm{H.c.}] + m\boldsymbol{c}^{\dagger}_j \sigma_x \boldsymbol{c}_j .$$

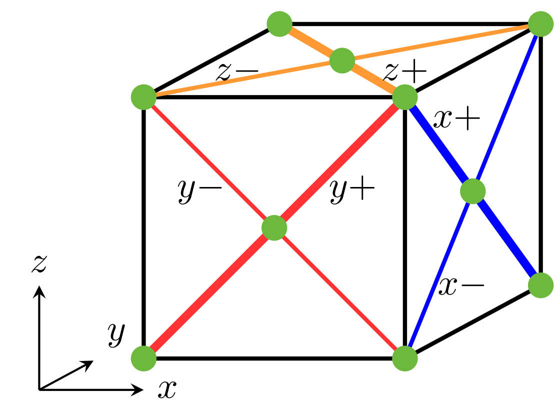




Some recent topics out of my group (incomplete)

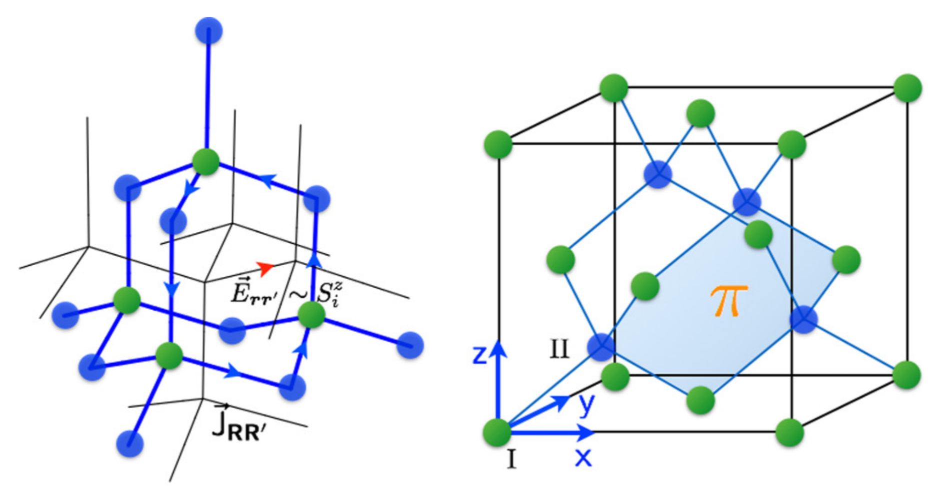
- **Kitaev materials based** on rare-earth magnets

$$H = \sum_{\langle ij\rangle_{\gamma\pm}} \left[J\, \mathbf{S}_i \cdot \mathbf{S}_j + K S_i^{\gamma} S_j^{\gamma} \pm F \left(S_i^{\alpha} S_j^{\beta} + S_i^{\beta} S_j^{\alpha} \right) \right],$$



- **Spinon and magnetic monopoles in pyrochlore quantum spin ice**

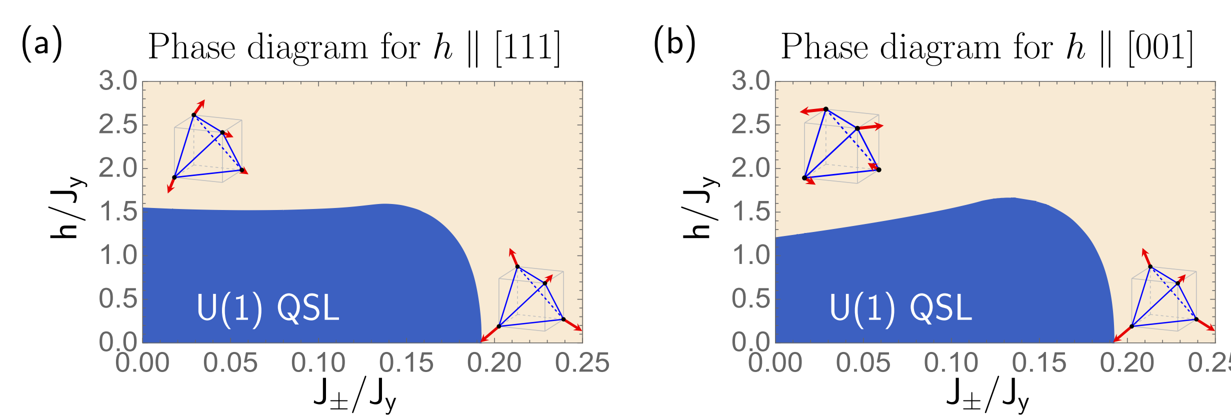
$$T_{\mu}^{m} T_{\nu}^{m} \left(T_{\mu}^{m}\right)^{-1} \left(T_{\nu}^{m}\right)^{-1} = e^{i\pi} = -1.$$



- **Symmetry enriched U(1) topological order** in 3D

$$H = \sum_{\langle ij\rangle} \sum_{\mu=x,y,z} \tilde{J}_{\mu} \tilde{\tau}_i^{\mu} \tilde{\tau}_j^{\mu} - \sum_i h\,(\hat{n}\cdot\hat{z}_i)\,\tau_i^z,$$

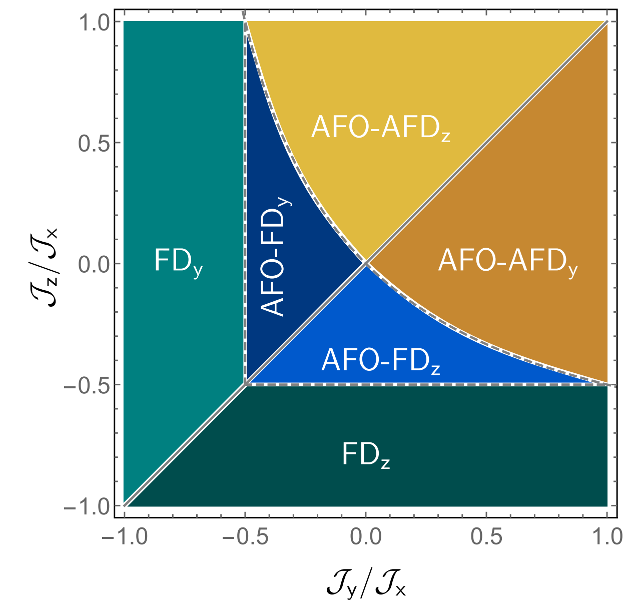
$$H_{\rm sim} = \sum_{\mathbf{r}} \frac{J_y Q_{\mathbf{r}}^2}{2} - \sum_{\mathbf{r}} \sum_{\mu\neq\nu} J_{\pm} \Phi^{\dagger}_{\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_{\mu}} \Phi_{\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_{\nu}} s^{-\eta_{\mathbf{r}}}_{\mathbf{r},\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_{\mu}}$$
$$\times\, s^{+\eta_{\mathbf{r}}}_{\mathbf{r},\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_{\nu}} - \sum_{\langle\mathbf{rr'}\rangle} \frac{h}{2} (\hat{n}\cdot\hat{z}_i)(\Phi^{\dagger}_{\mathbf{r}}\Phi_{\mathbf{r'}} s^{+}_{\mathbf{rr'}} + \text{H.c.}).$$



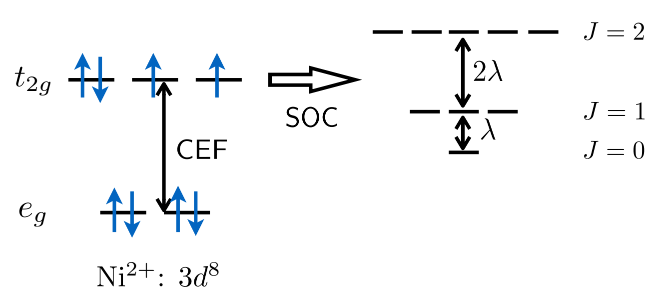
Some recent topics out of my group (incomplete)

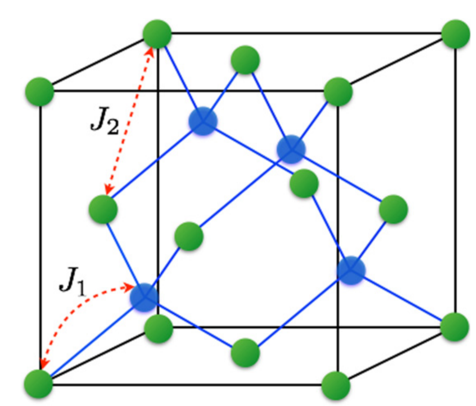
- **Hidden multipolar orders** in quantum magnets

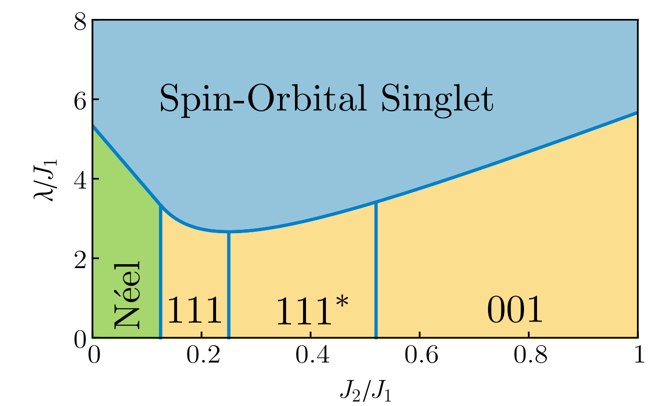
$$H_0 = \sum_{\langle \mathbf{r}\mathbf{r}'\rangle} \left[J_x \tau^x_{\mathbf{r}} \tau^x_{\mathbf{r}'} + J_y \tau^y_{\mathbf{r}} \tau^y_{\mathbf{r}'} + J_z \tau^z_{\mathbf{r}} \tau^z_{\mathbf{r}'} + J_{yz}\left(\tau^y_{\mathbf{r}} \tau^z_{\mathbf{r}'} + \tau^z_{\mathbf{r}} \tau^y_{\mathbf{r}'}\right)\right].$$



- **Quantum criticality** from spin-orbit entanglement for 3d antiferromagnets

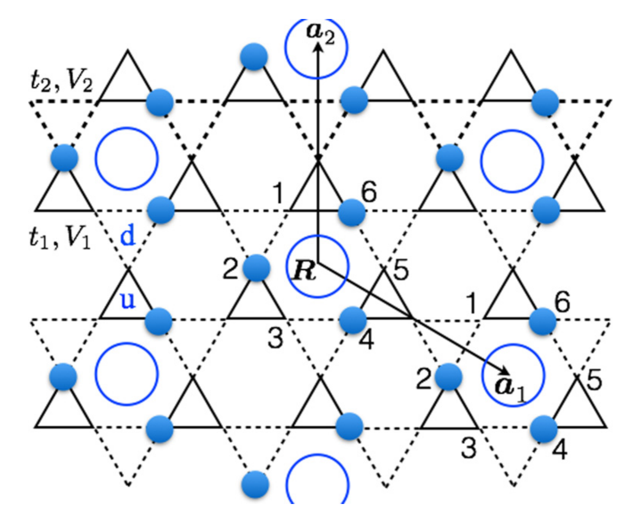






- **Cluster Mott insulators**

$$H = -\sum_{\langle ij\rangle \in \mathrm{u}} (t_1 c^\dagger_{i\sigma} c_{j\sigma} + \mathrm{H.c.}) - \sum_{\langle ij\rangle \in \mathrm{d}} (t_2 c^\dagger_{i\sigma} c_{j\sigma} + \mathrm{H.c.}) + \sum_{\langle ij\rangle \in \mathrm{u}} V_1 n_i n_j + \sum_{\langle ij\rangle \in \mathrm{d}} V_2 n_i n_j + \sum_i U n_{i\uparrow} n_{i\downarrow},$$

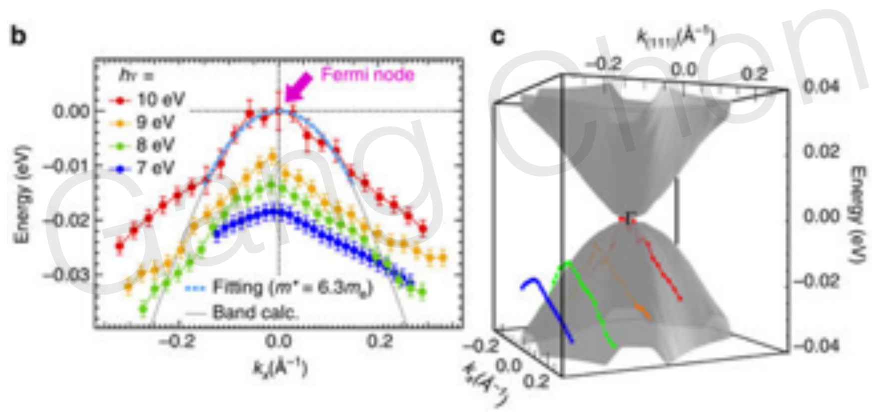


Outline

1. Introduction to pyrochlore iridates:
   spin-orbit coupling + electron correlation

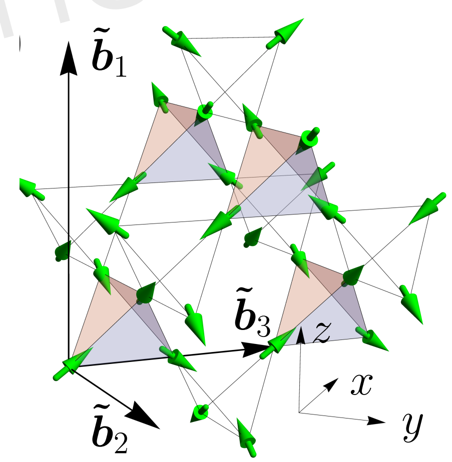
2. Microscopics of $Pr_2Ir_2O_7$:
   conduction elections and local moments

3. Magnetism induced Weyl nodes and
   symmetry protected Dirac nodes, magnetic controls.



Luttinger semimetal

+



Ordered spin ice

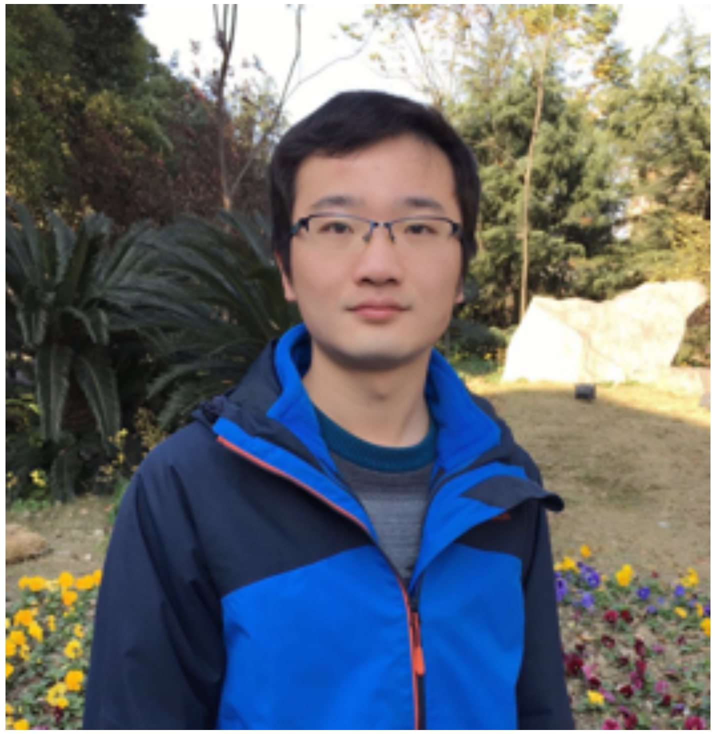
= ???

References

Gang Chen, Michael Hermele, Phys Rev B, 86, 235129 (2012)

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

Xu-Ping Yao, Gang Chen, arXiv:1712.06534, Phys Rev X in press

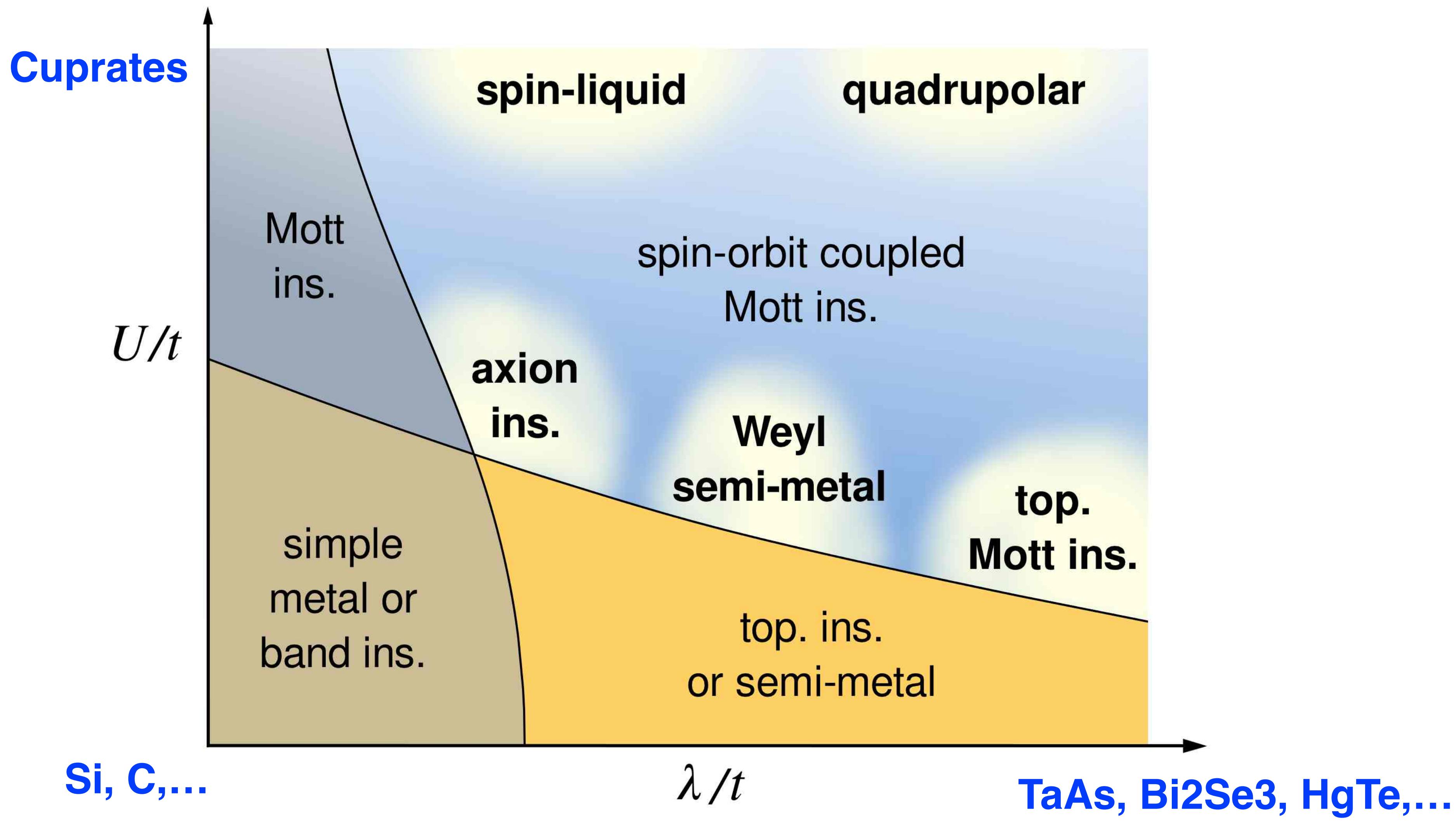


Xu-Ping Yao

(Fudan)

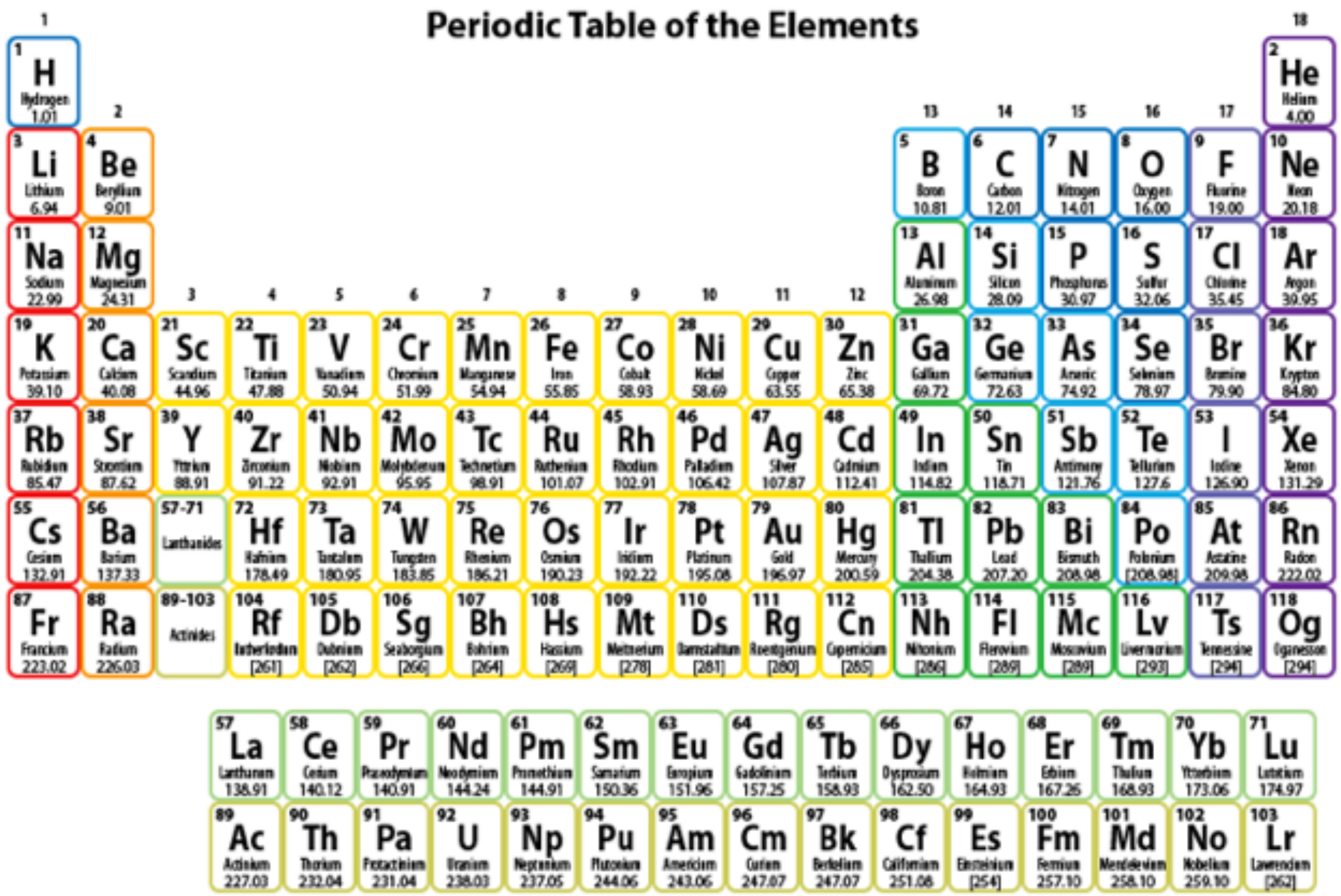
复旦大学 FUDAN UNIVERSITY

Spin-orbit-coupled correlated matter



W Witczak, **Gang Chen**, YB Kim, L Balents,
Annual Review of Condensed Matter Physics, 2014

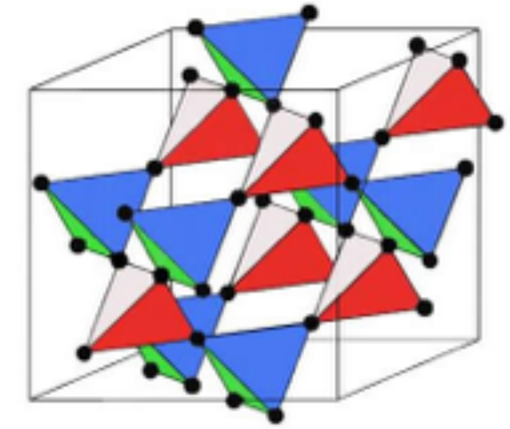
Ir, Os, Ta, …,4d/5d,… ,4f electrons,…

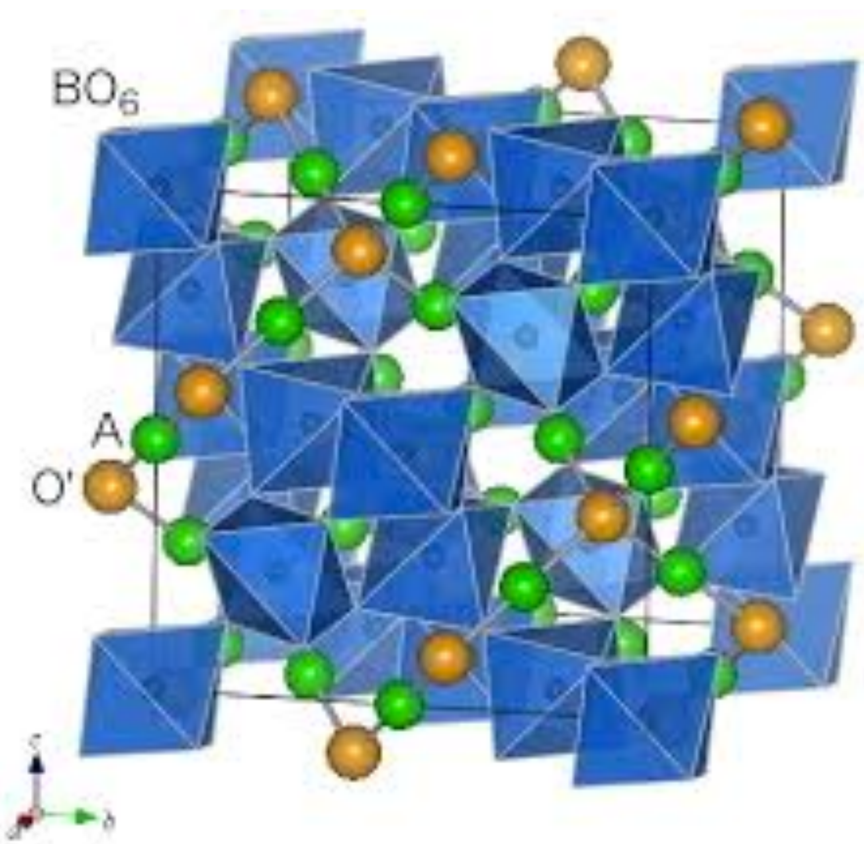


Iridates, osmates, rheniumates…, 4d/5d materials

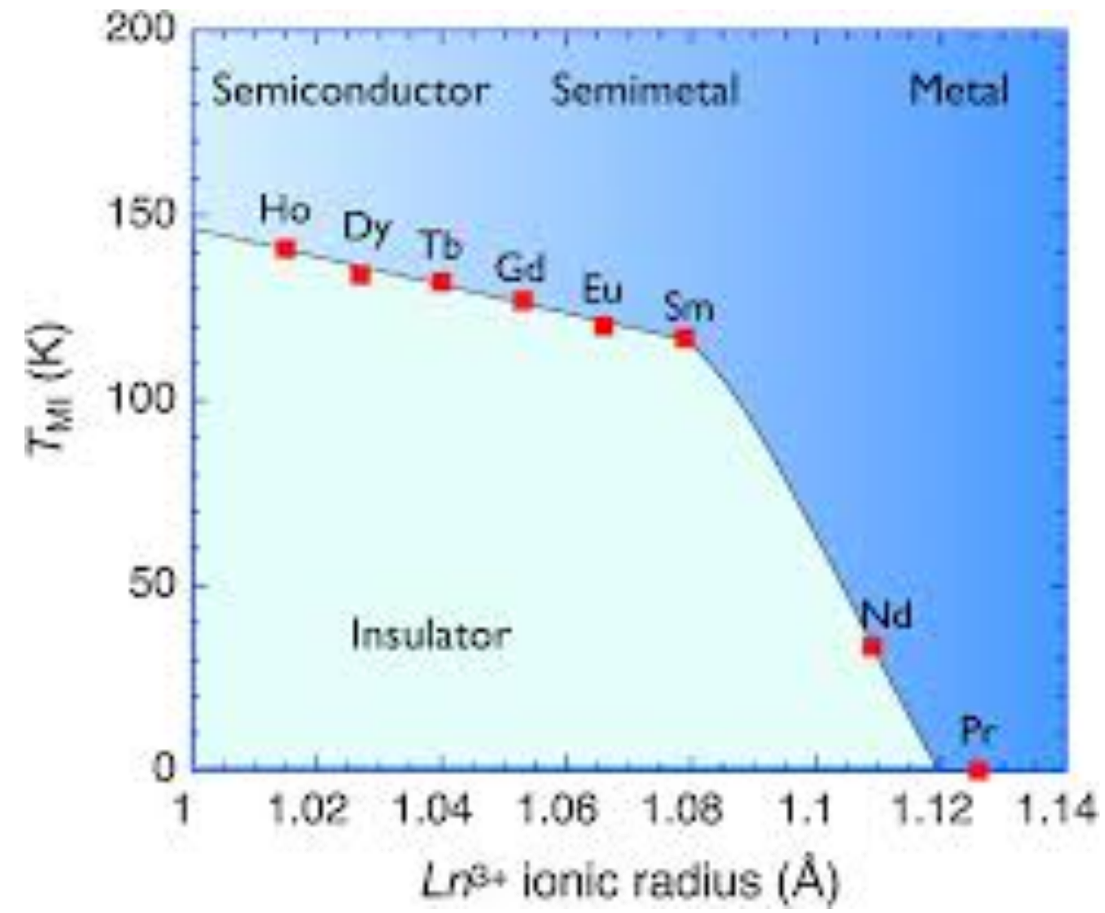
Pr, Yb, Er, Nd… , rare-earth materials

Pyrochlore iridates





$R_2Ir_2O_7$



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

$Pr_2Ir_2O_7$ remains metallic and disordered.

Correlation physics in spin-orbit (topological) matter

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

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

at that time, p
effect on topo

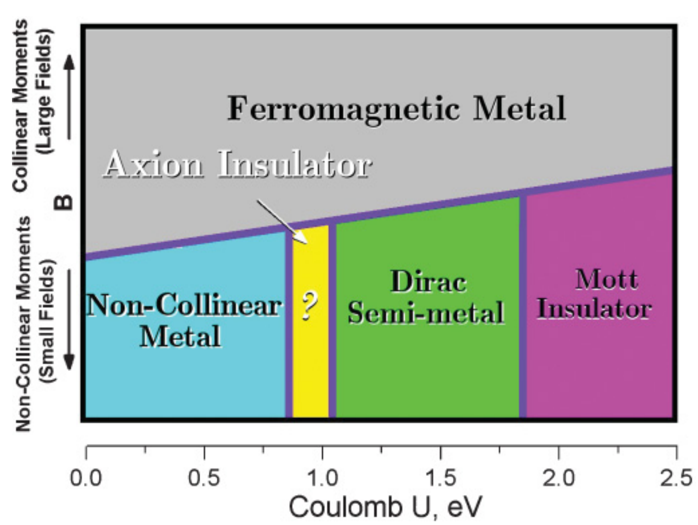
iridate provide
strong spin-o

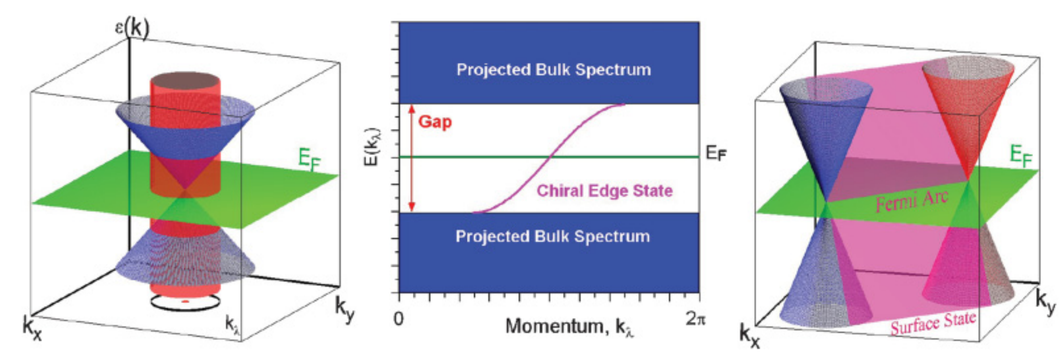
Leon knows a
transition, der
longer range p
and could ind

Halperin 1960

Xiangang Wan

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

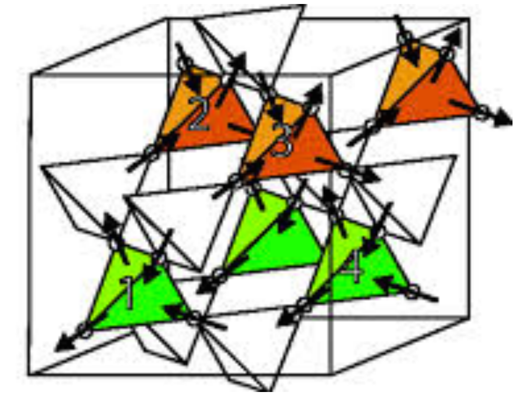
Later on, many interesting works about Iridium physics
(YB Kim, L Savary, L Fu, Xi Dai, Imada, BJ Yang, EG Moon, Nagaosa, ZX Shen, etc)

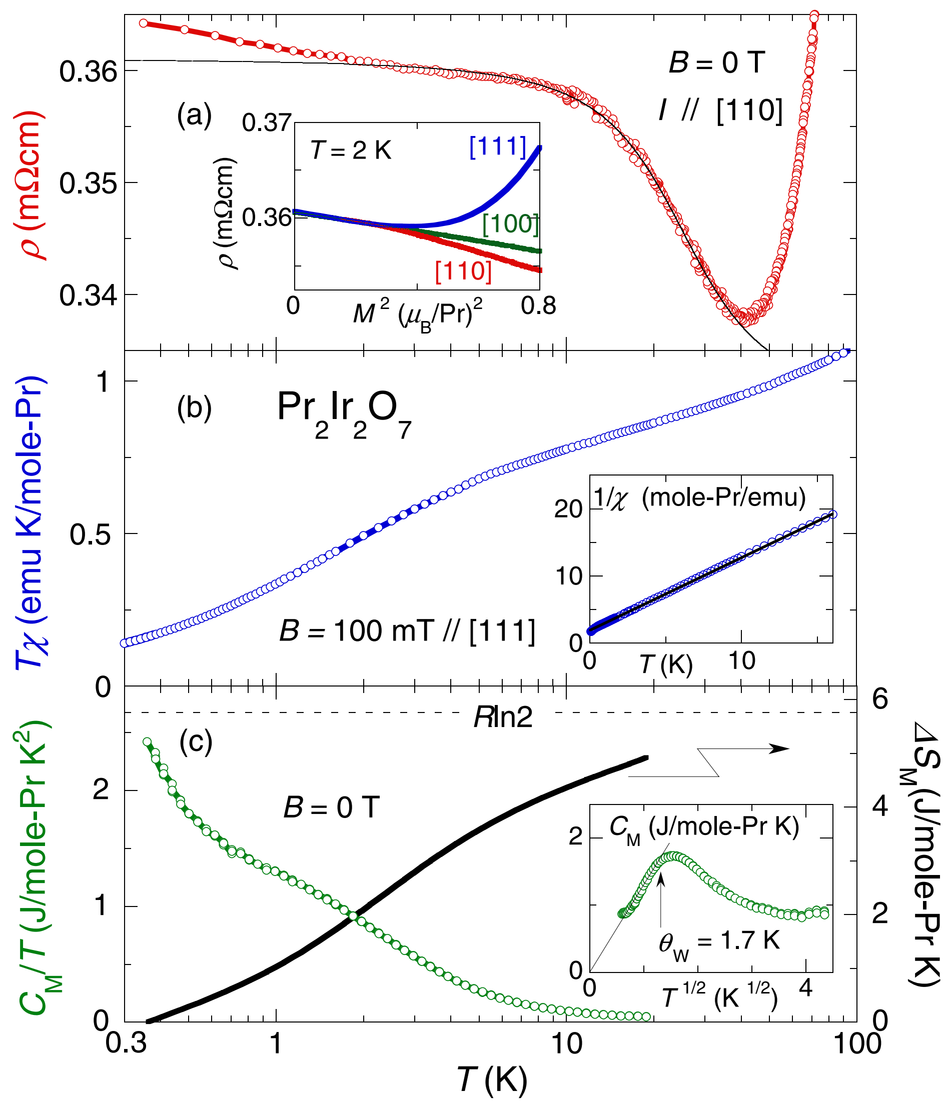
lex

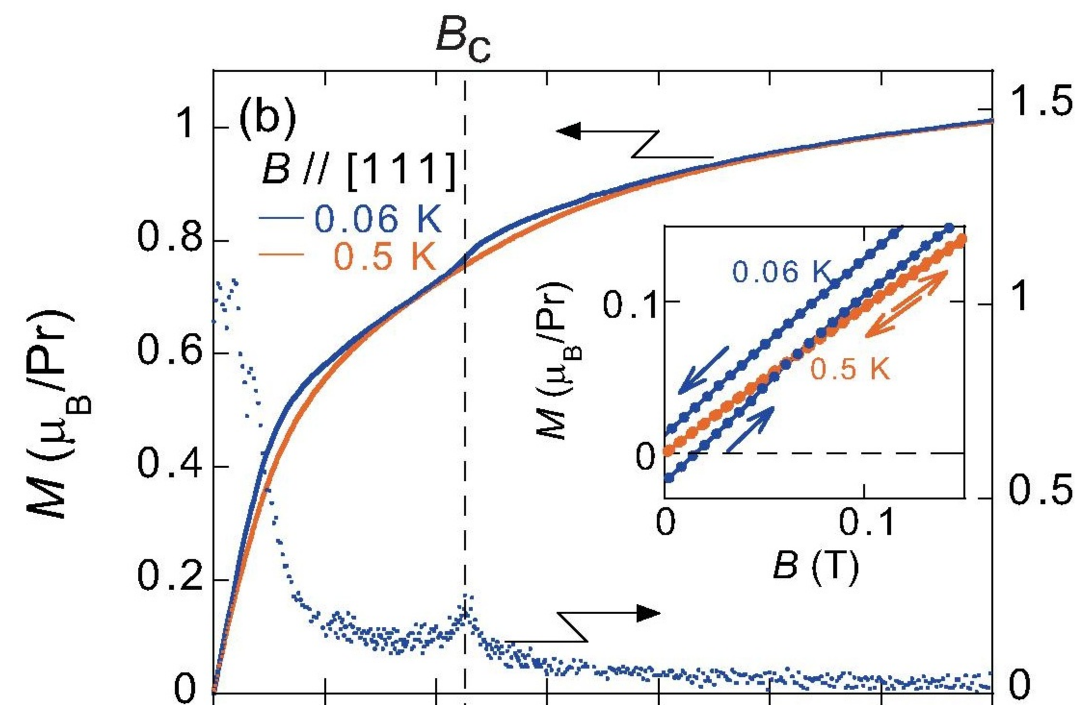
Satoru Nakatsuji

Peculiar one: $Pr_2Ir_2O_7$

contains extremely rich and complex physics







metamagnetic transition
for field along 111,
indicating strong anisotropy.

Nakatsuji, etc PRL **96,** 087204 (2006)

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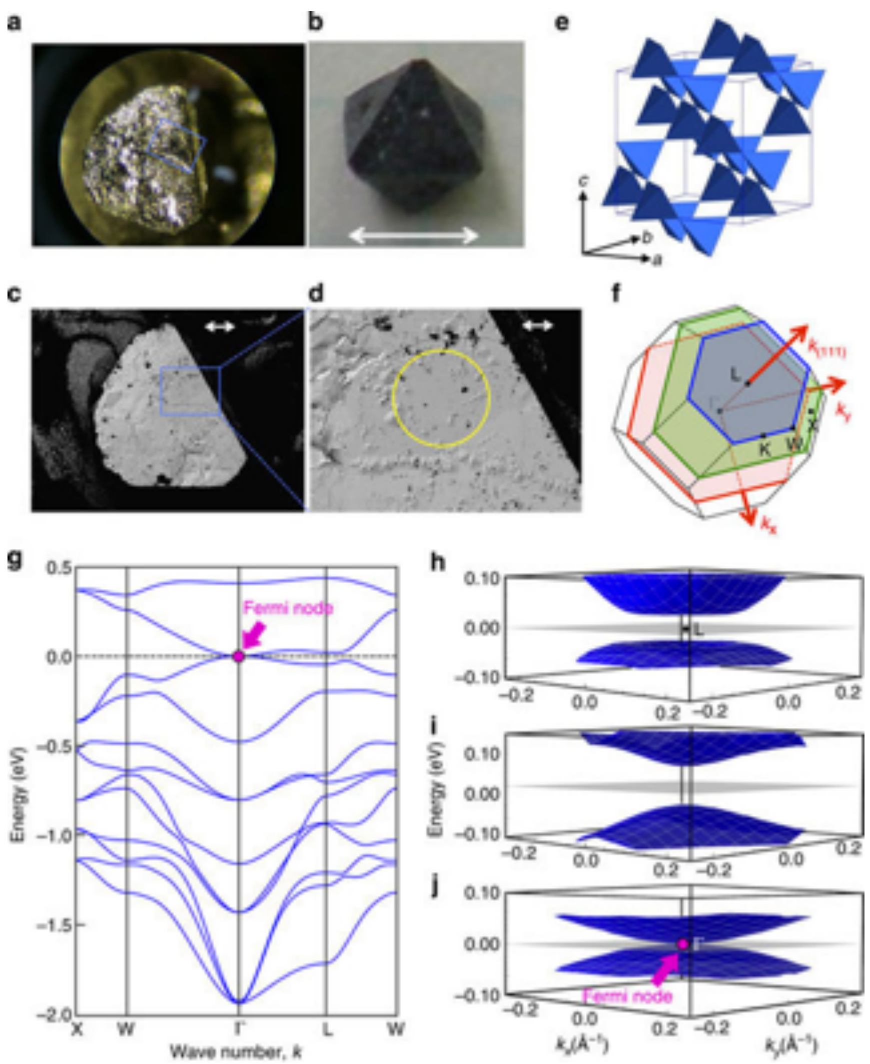
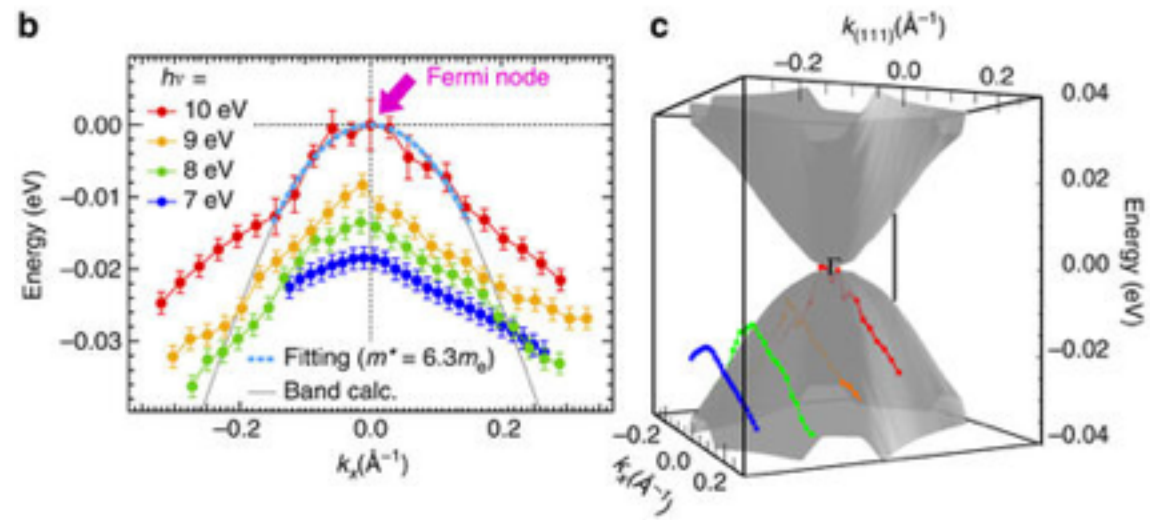
Ir conduction electron: Luttinger semimetal

T Kondo





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, C Xu, L Balents

Partial screening of long range Coulomb interaction

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]

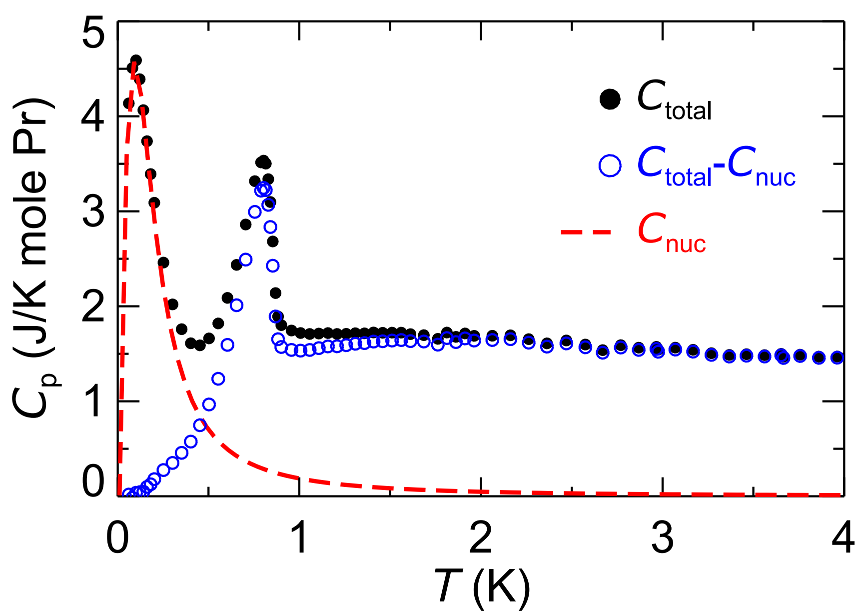


FIG. 1. (color online) Temperature dependence of the specific heat of $Pr_{2+x}Ir_{2-x}O_{7-\delta}$ in zero field. Filled circles: experimental total specific heat. Dashed curve: calculated specific

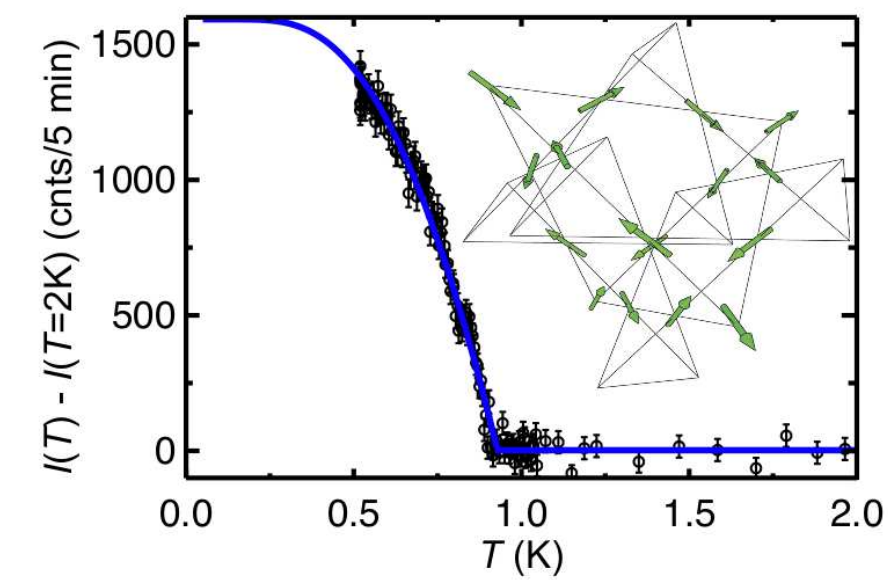
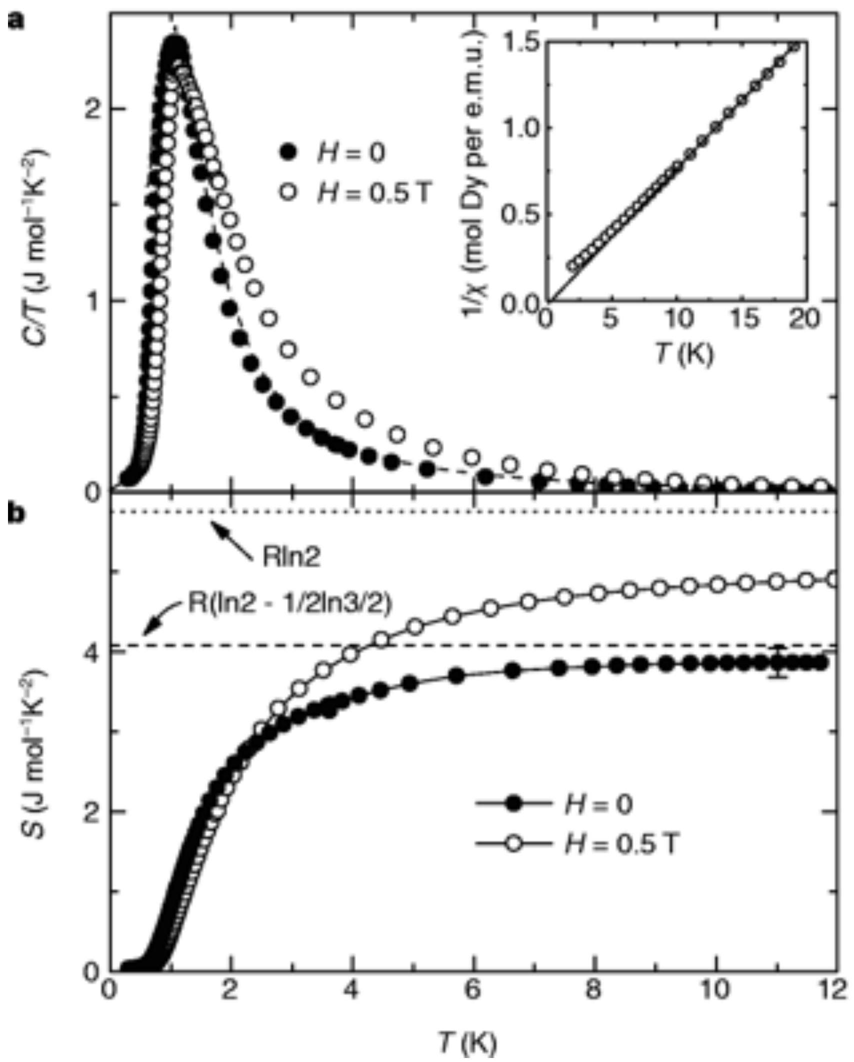


FIG. 2. (color online) Temperature dependence of elastic neutron scattering intensity of $Pr_{2+x}Ir_{2-x}O_{7-\delta}$ at the position of the $\mathbf{q}_m = (100)$ reflection. The intensity measured at $T = 2$ K

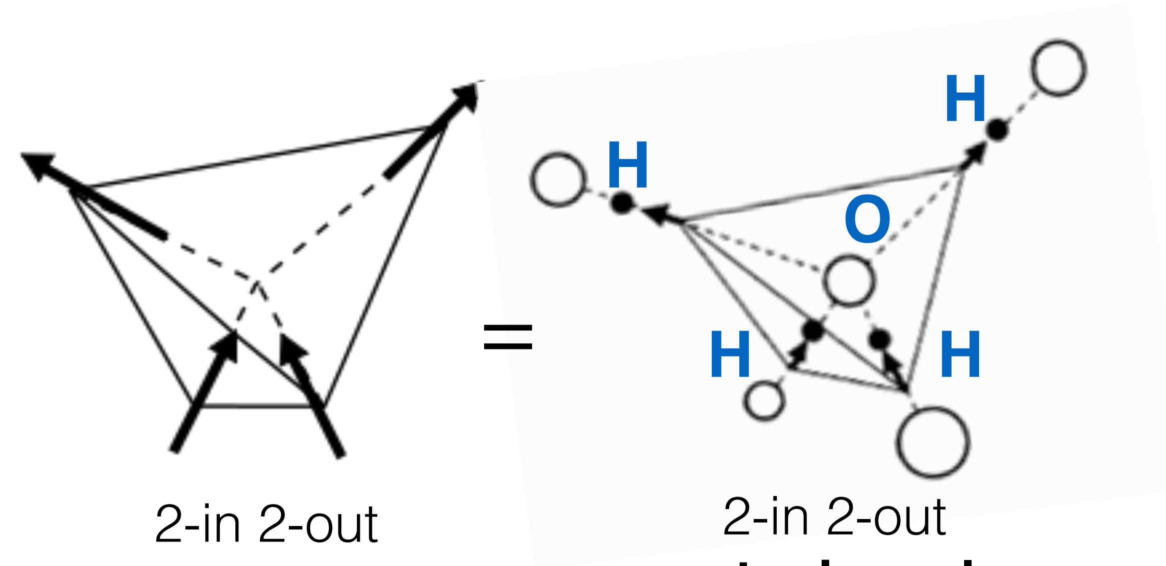
actually “Melko-Hertog-Gingras" spin state
(obtained numerically for a **different and classical** system)

Spin ice

$Dy_2Ti_2O_7$

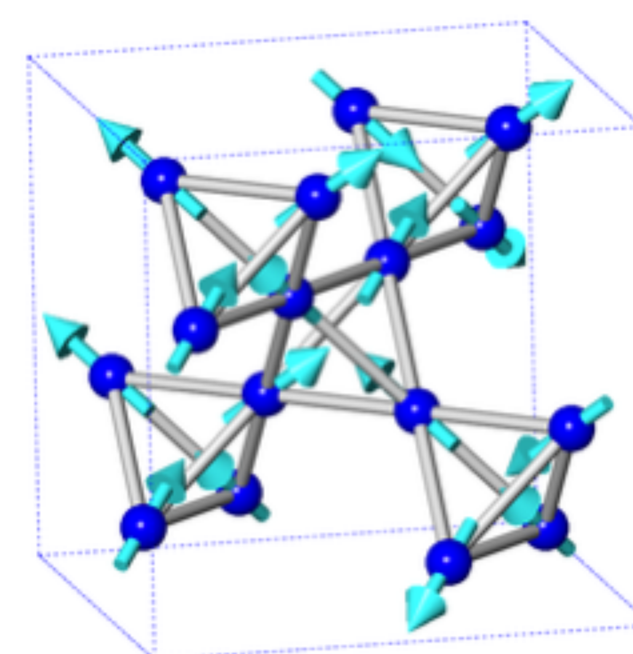


Pauling entropy in spin ice,
Ramirez, etc, Science 1999



2-in 2-out
spin ice rule

2-in 2-out
water ice rule



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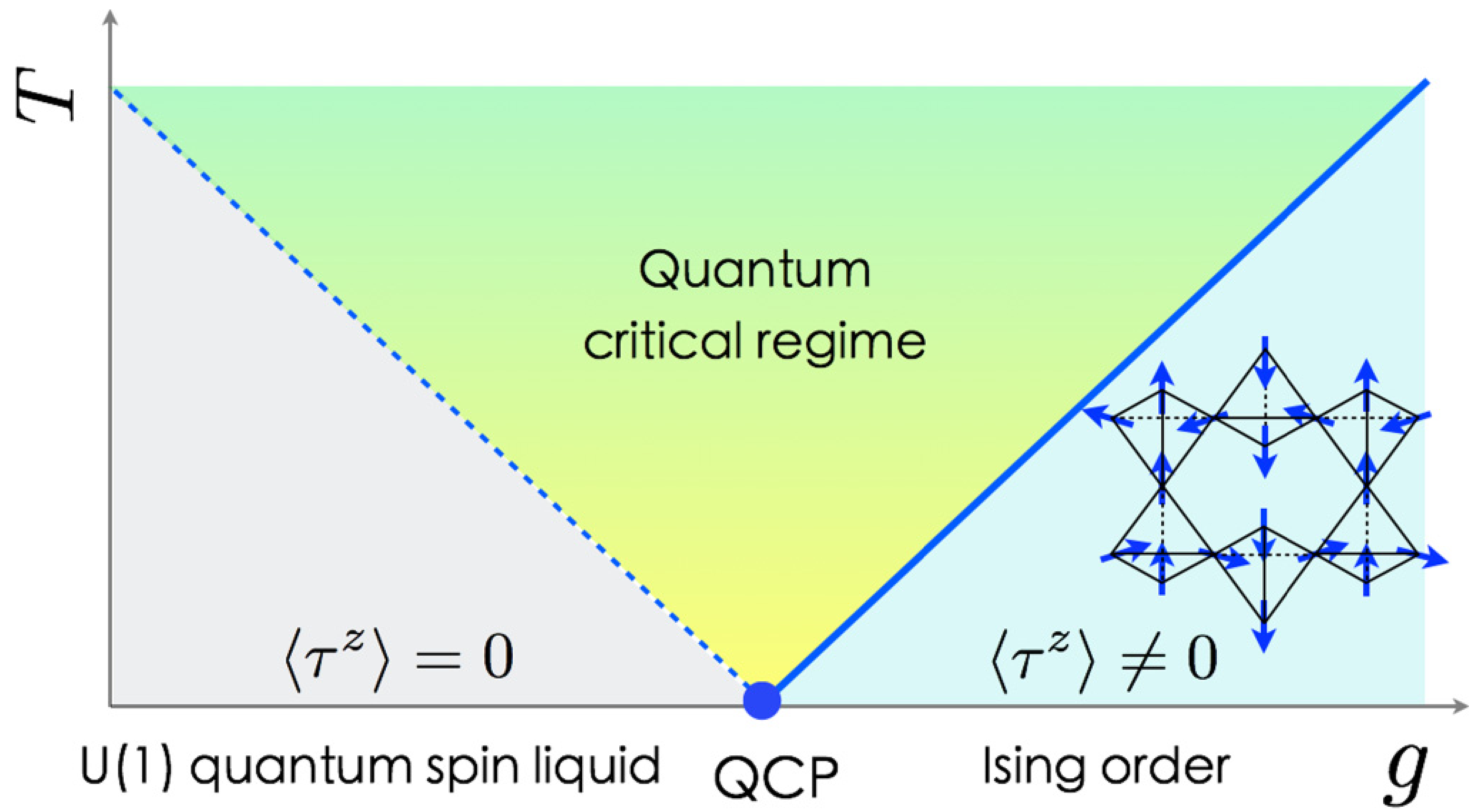
My suggestion: proximity to quantum criticality



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

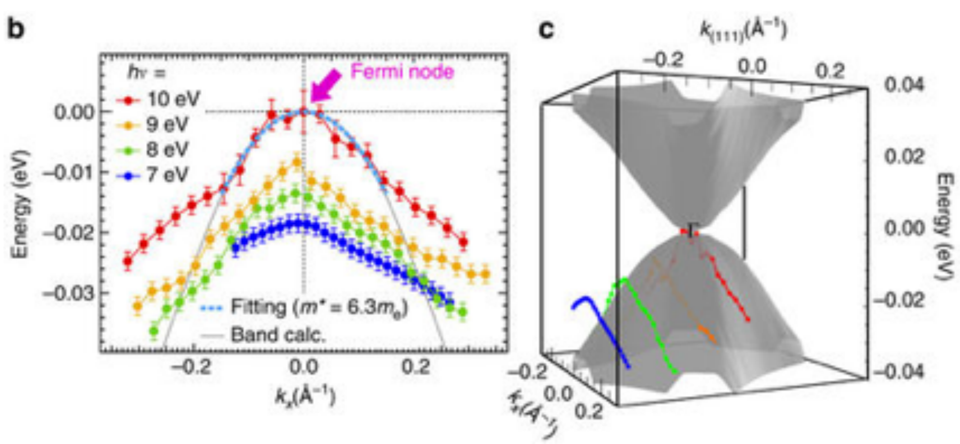
Microscopics: different samples have different Fermi energy, induces different RKKY interaction between Pr local moments.

Gang Chen, PRB 94, 205107 (2016)

2. Microscopics of $Pr_2Ir_2O_7$:
conduction elections and local moments

Let's focus on the ordered side/sample.

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



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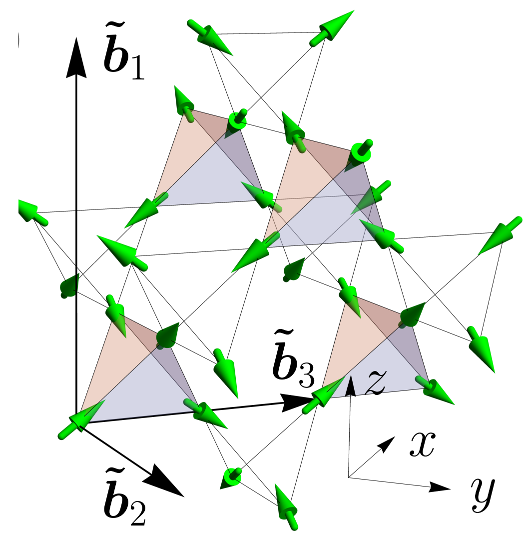


= ????

Ir Luttinger semimetal

MHG spin ice state

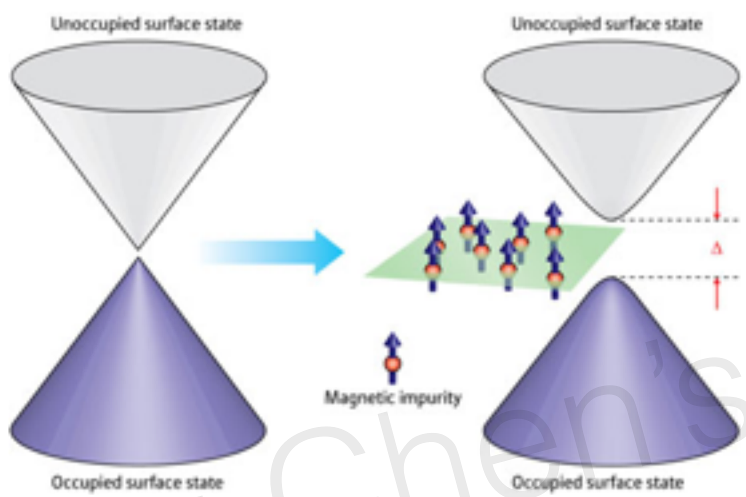
T Kondo, etc, 2015

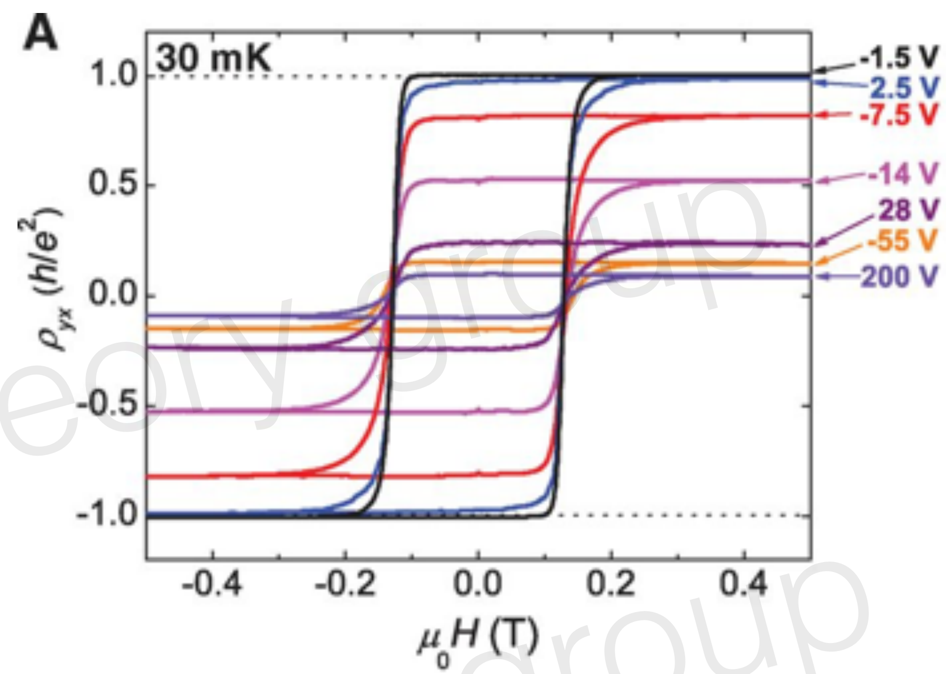
C Broholm, etc, 2015

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

Qikun Xue's group

Quantum Anomalous Hall Effect





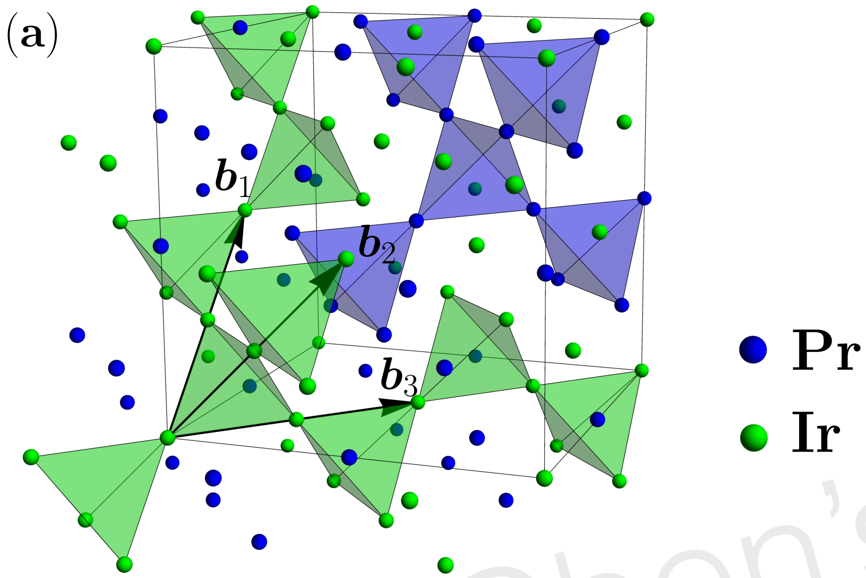
Our understand: QAHE is an example of interplay between conduction electron and local moments. Here in QAHE, itinerant electron band topology is modulated by magnetism, and magnetism is rather simple.

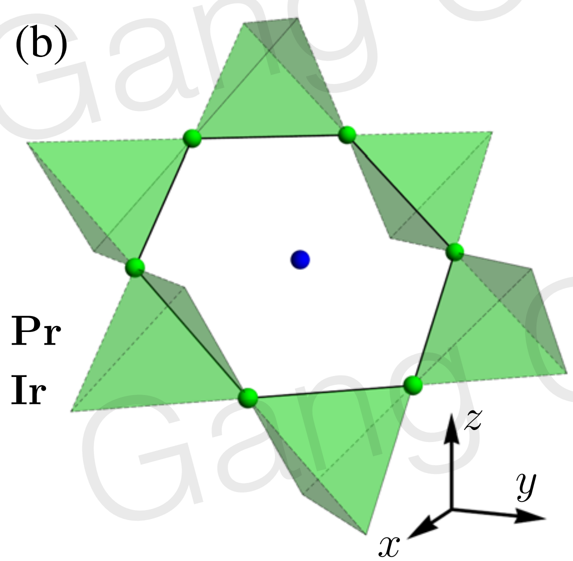
Here, we study the system with both local moments and itinerant electrons, trying to understand their interplay and interactions. How local moments influence conduction electrons, and ice versa.

J Checkelsky's kagome metal, Claudia's magnetic Weyl metal,
Rongying Jin's Berry phsae in magnetic materials, Tokura's skyrmion lattice metal,
all belong to this category's problems.

Microscopics: Ir conduction electron + Pr local moment

interact with
interact with
very comple
system





~<1eV Ir 5d electron: hopping, SOC, interaction

~ **Pr-Ir interaction: f-d exchange**

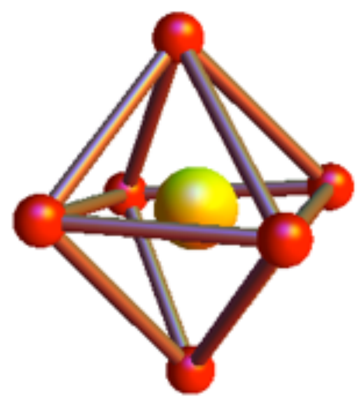
~10K Pr 4f electron: exchange interaction

Energy Scale

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

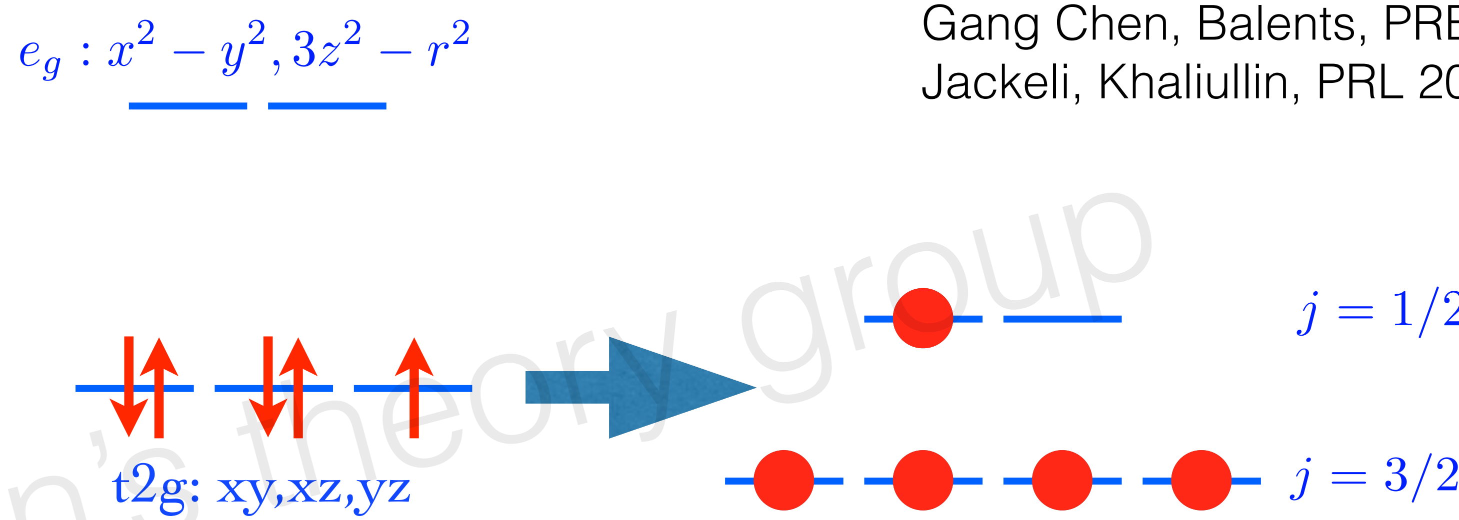
Ir 5d electron: SOC, hopping and correlation

BJ Kim, etc 2008,
Gang Chen, Balents, PRB 2008
Jackeli, Khaliullin, PRL 2009



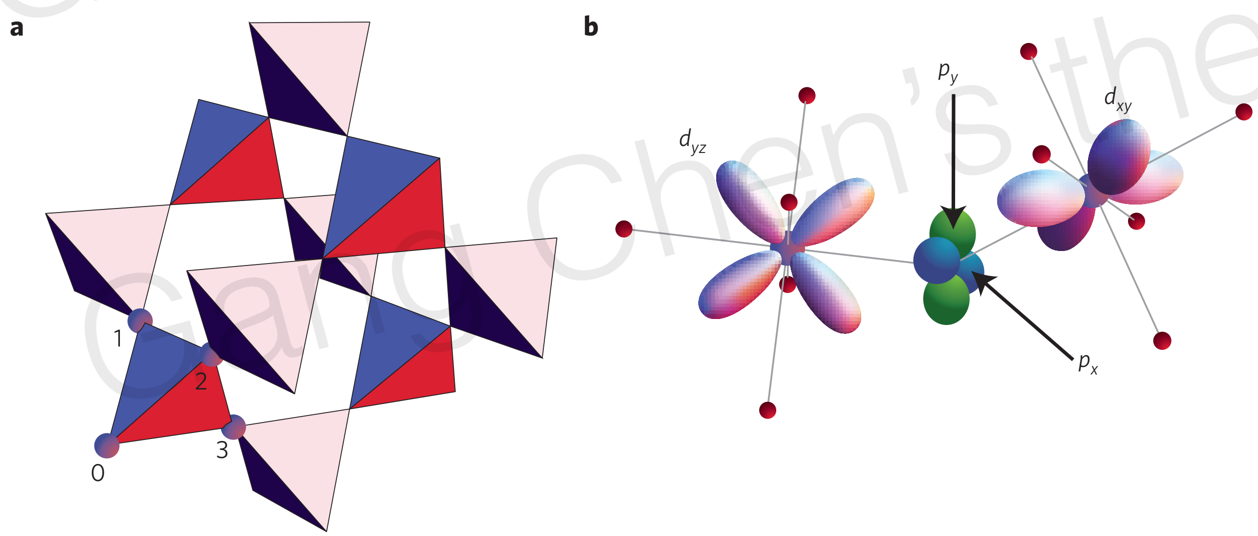
IrO6 octahedron

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



Crystal electric field

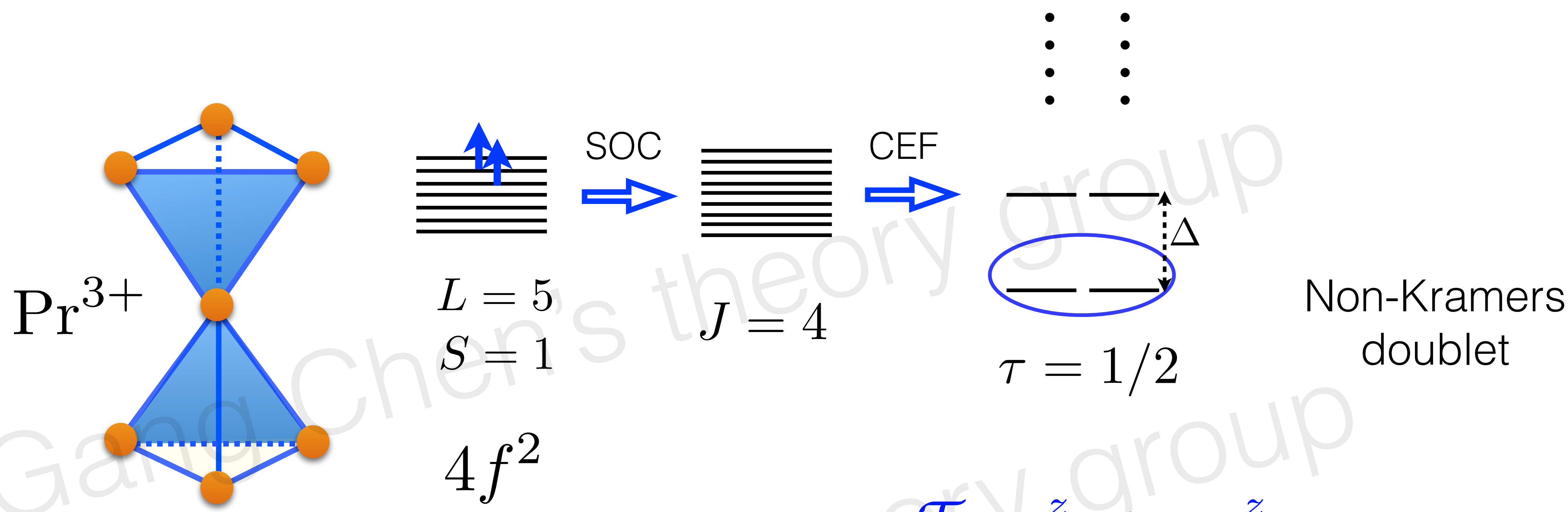
Spin-orbit coupling



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

For $Pr_2Ir_2O_7$, correlation renormalizes the band width.

Spin-orbit for Pr ion: non-Kramers doublets



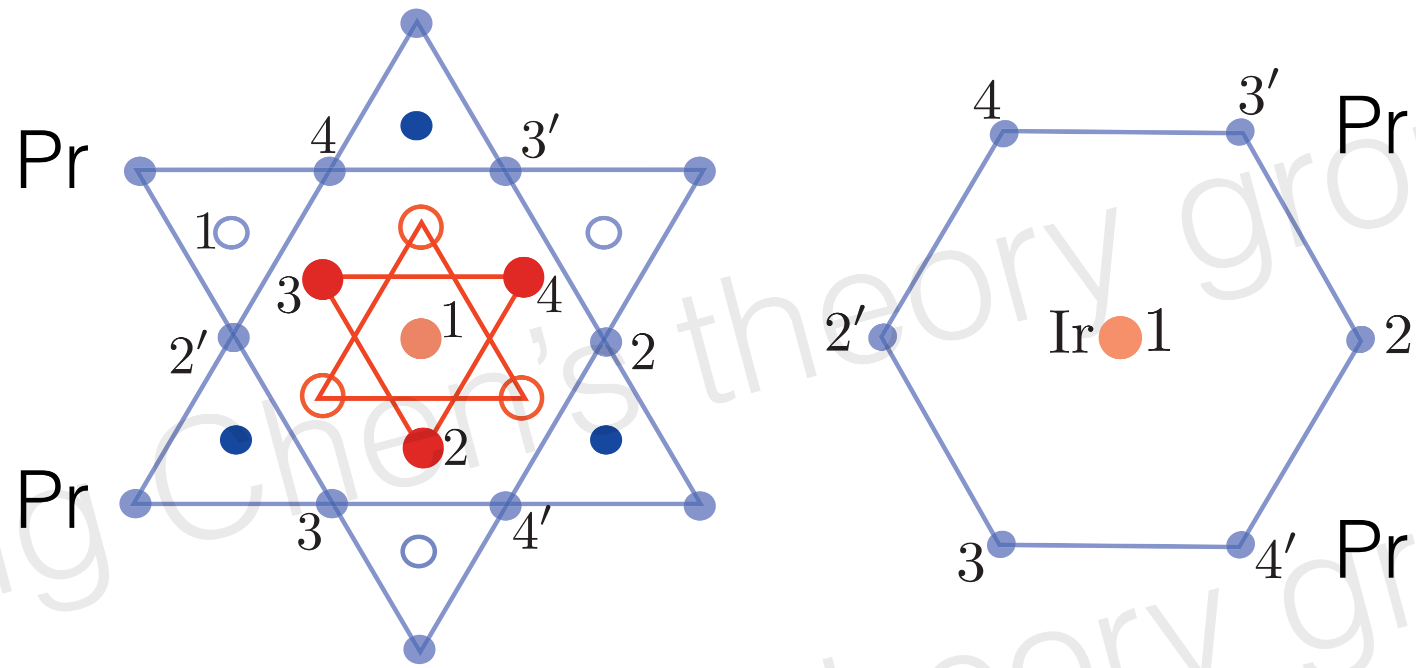
$$\mathcal{T} : \tau^z \rightarrow -\tau^z$$

$$\mathcal{T} : \tau^{x,y} \rightarrow +\tau^{x,y}$$

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.

Pr-Ir interaction: f-d exchange

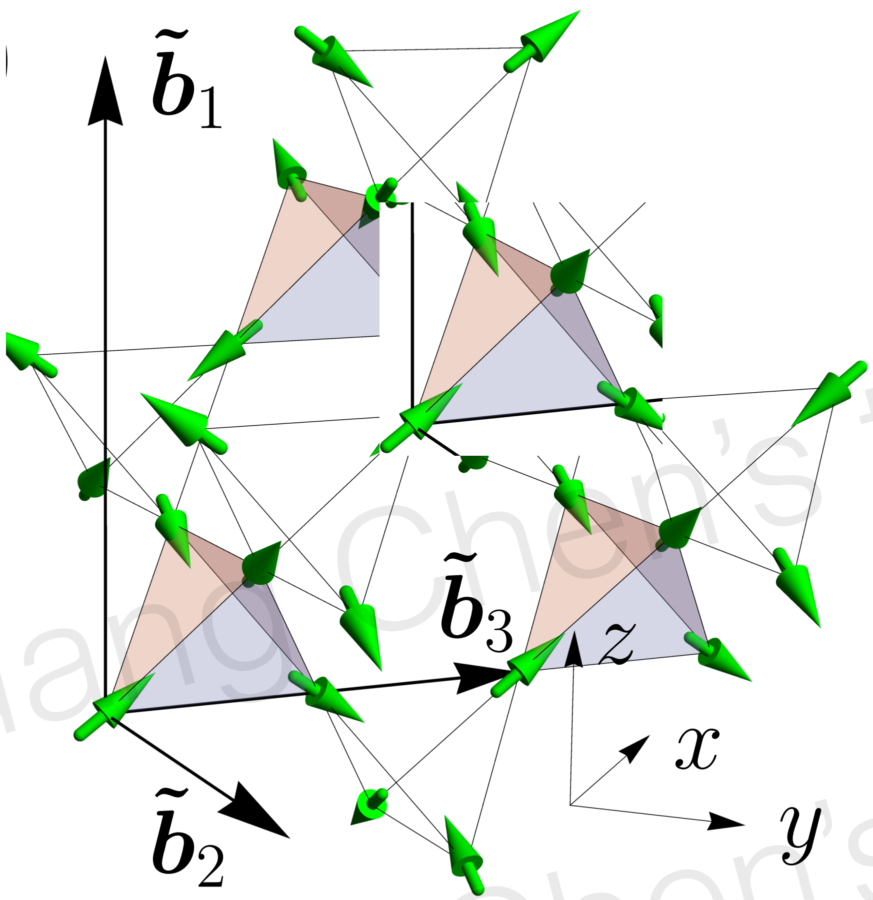


$$
\mathcal{H}_{\text{fd}} = \big[c_1 \tau_4^z - c_2(\tau_2^z + \tau_3^z)\big] j_1^x + \big[c_1 \tau_3^z - c_2(\tau_2^z + \tau_4^z)\big] j_1^y + \big[c_1 \tau_2^z - c_2(\tau_3^z + \tau_4^z)\big] j_1^z + [2 \leftrightarrow 2', 3 \leftrightarrow 3', 4 \leftrightarrow 4'],
$$

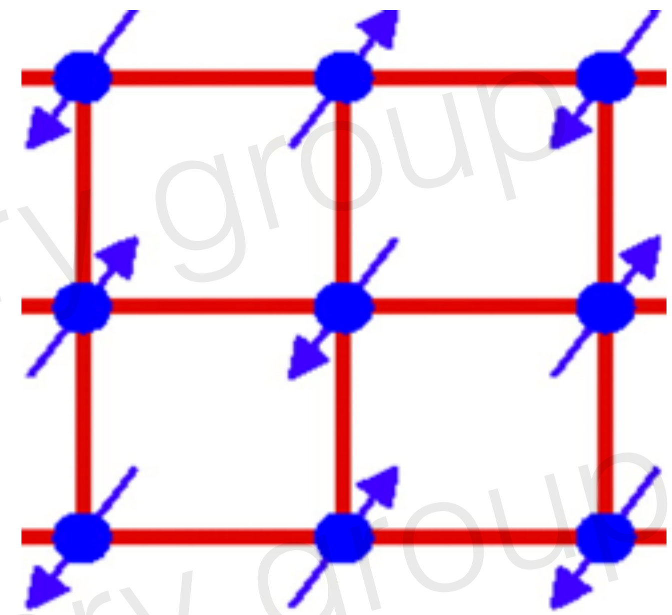
3. Magnetism induced Weyl nodes and
symmetry protected Dirac nodes, magnetic controls.

Here we focus on the ordered side/sample.

Magnetic translation of MHG spin ice state

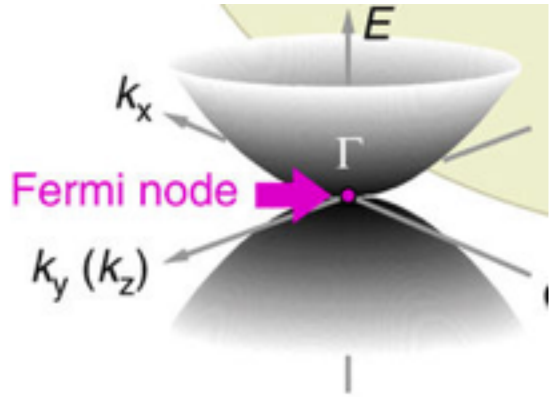


$$\tilde{\mathcal{T}} \equiv \mathcal{T} \circ t$$

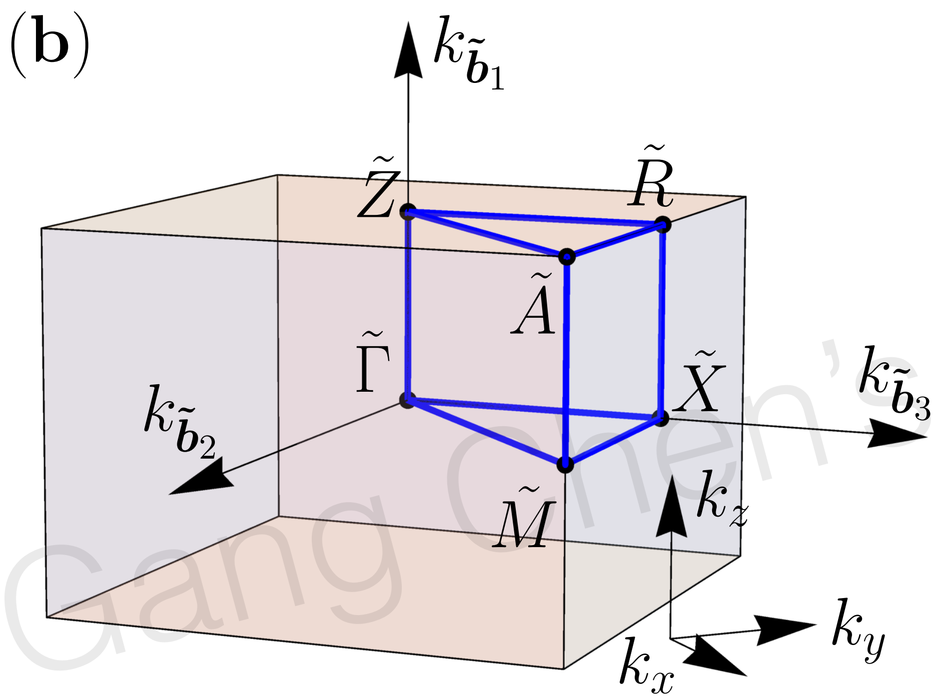


Neel state on square lattice for cuprate AFM.

3D analogue of the magnetic translation for Neel state

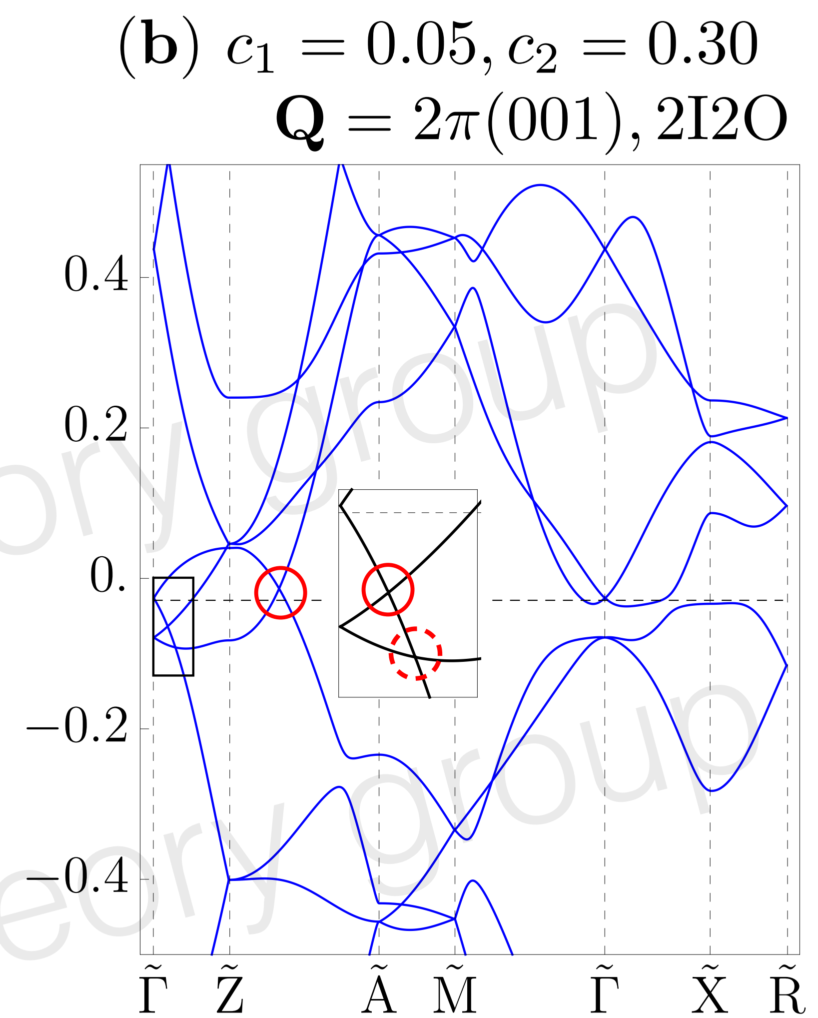


Symmetry protected Dirac band touching



magnetic Brillouin zone

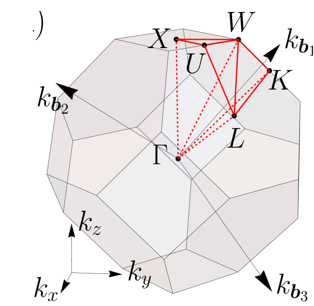
$\tilde{\mathcal{T}}^2 = -1$ at $\tilde{\Gamma}$ point

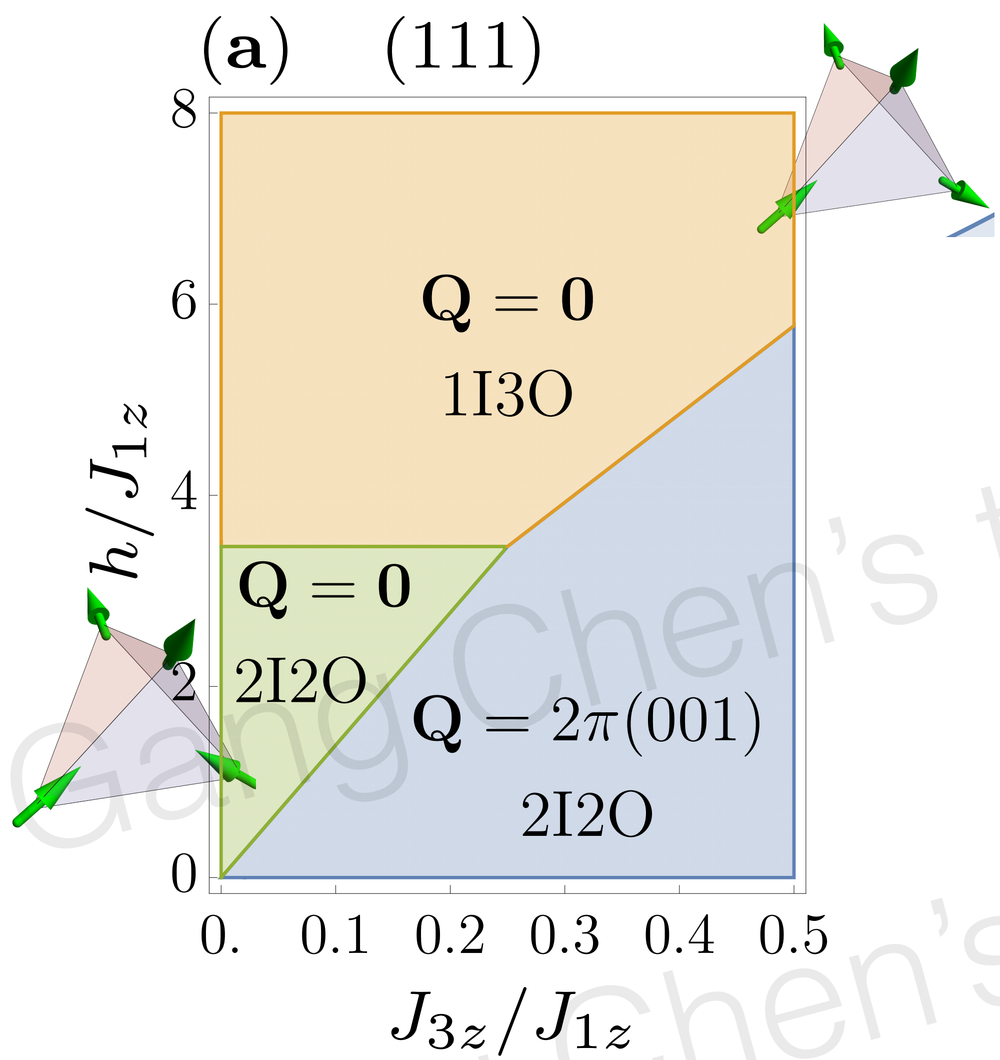


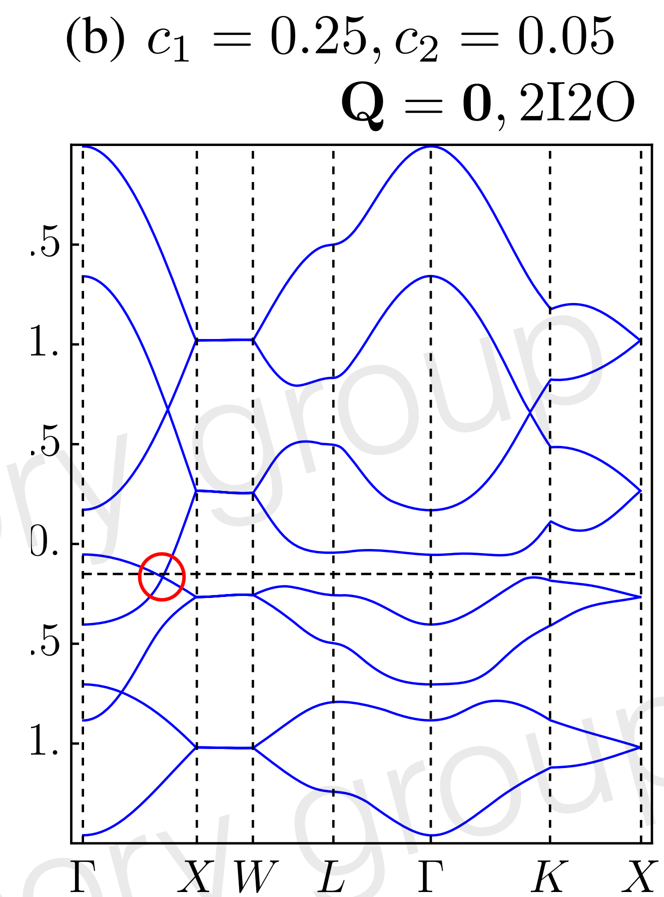
in addition, there are Weyl nodes
whose existence does not require symmetry

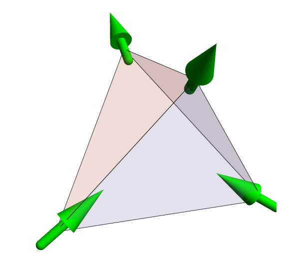
Pr magnetic order transfers its time reversal
symmetry breaking to Ir Luttinger semimetal.

Band topology control: external field amplified internally









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

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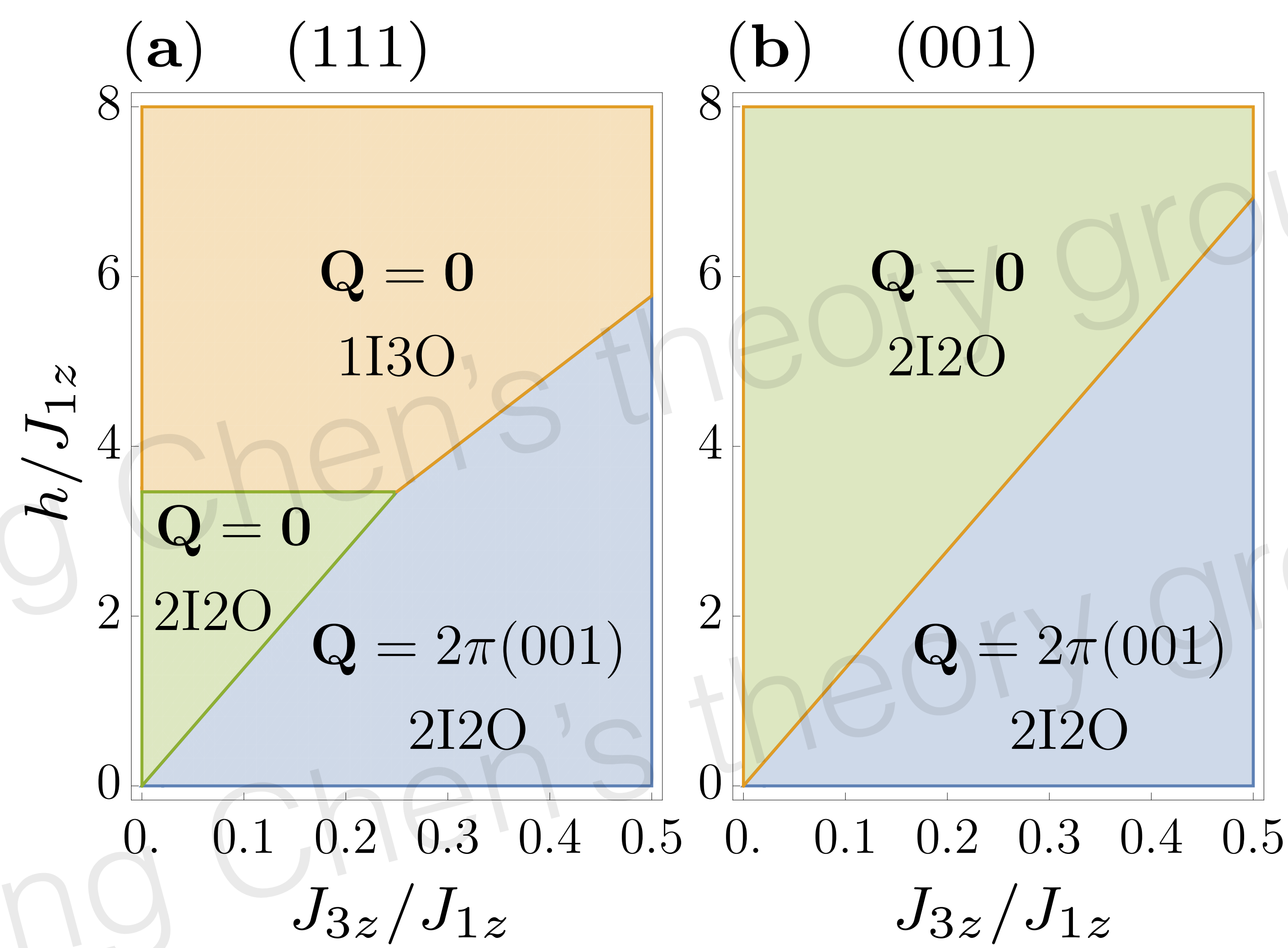
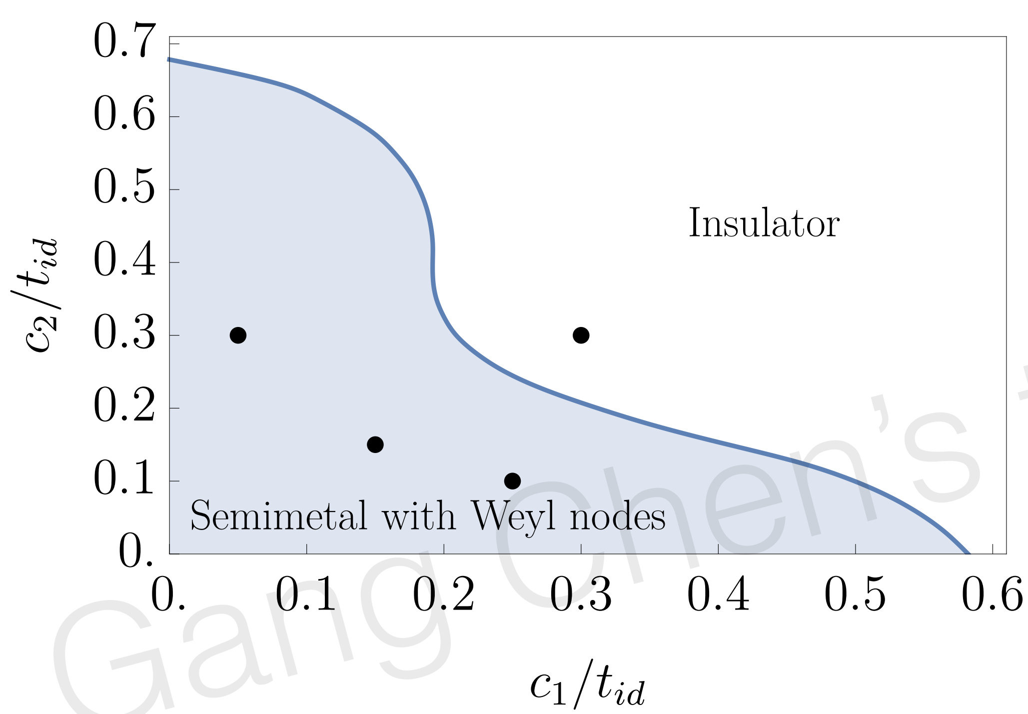
Quantum control under magnetic field

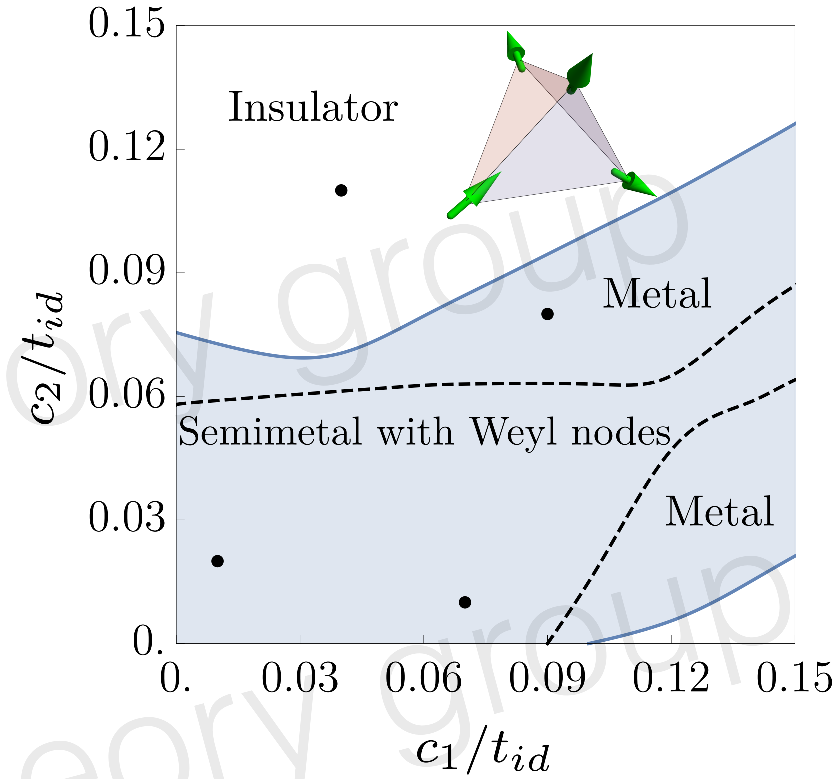


The Pr magnetic state under
different direction magnetic field

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, PRX in press

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.
- **Hybrid quantum materials with both itinerant electrons and local moments** can be a quite interesting direction of research for topological phenomena, correlation physics, band structure engineering, et al.