

Interplay of magnetic and electronic states in the pyrochlore iridates

Leon Balents, KITP, UCSB



- or -
correlations versus
topology

DPG meeting, Regensburg, March 2016

People



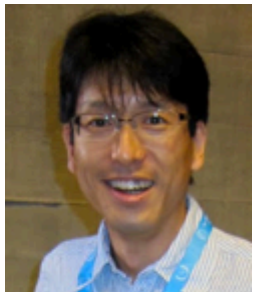
Ru Chen



Lucile Savary



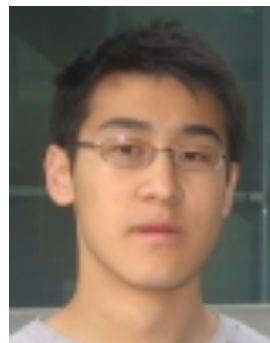
Eun-Gook Moon



S. Nakatsuji



T. Kondo



T. Hsieh



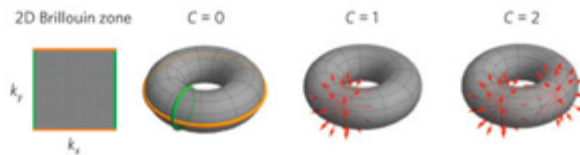
H. Ishizuka

TIs

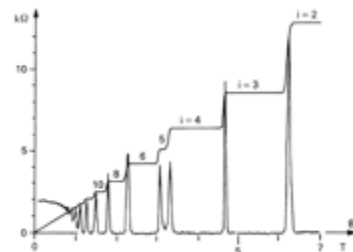
Broken
TRS

with
TRS

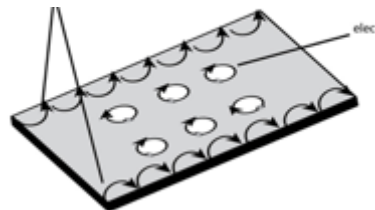
integer Chern
number



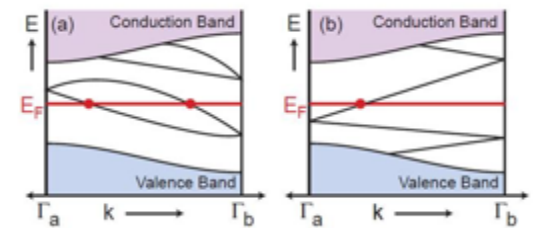
= Hall
conductance



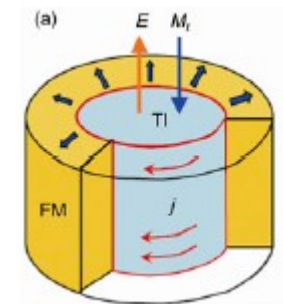
chiral edge
states



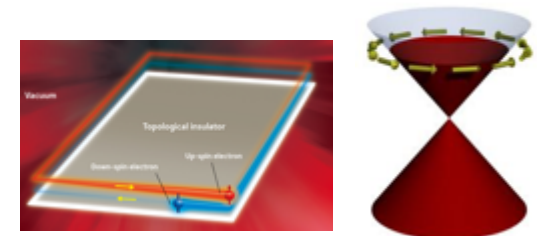
Z_2
invariant



= M-E
polarizability



helical edge/
surface states

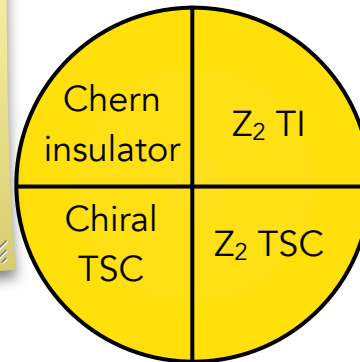
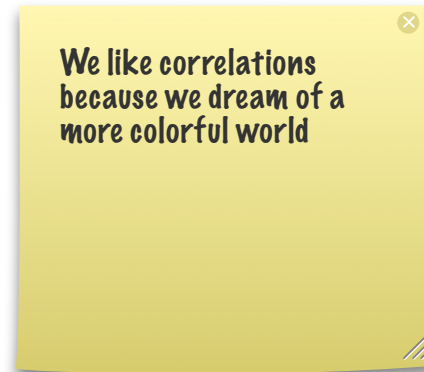


Topological everything

- Chern insulator
- Z_2 topological insulator
- topological crystalline insulators
- topological superconductors
- Dirac semi-metals
- Weyl semi-metals
- Line node semi-metals
- Fermi surface
- ...

Why correlations?

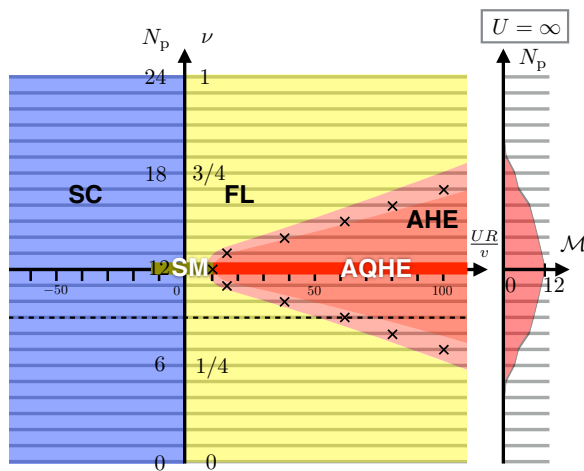
w/o interactions



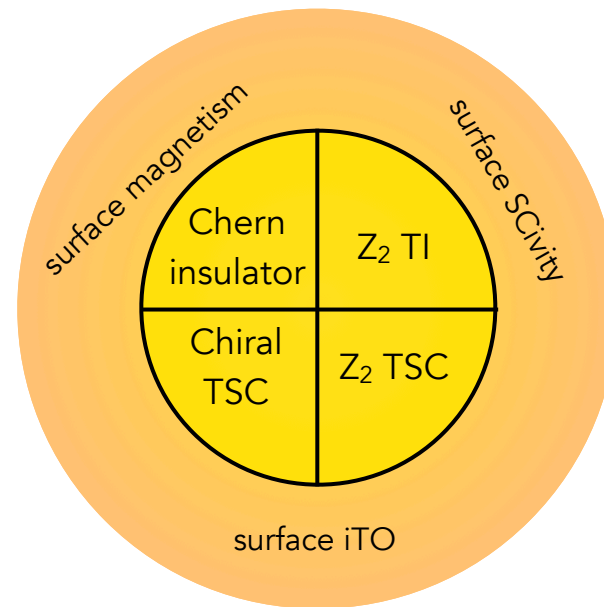
+ Weyl, Dirac...

Why correlations?

- Distinct surface states

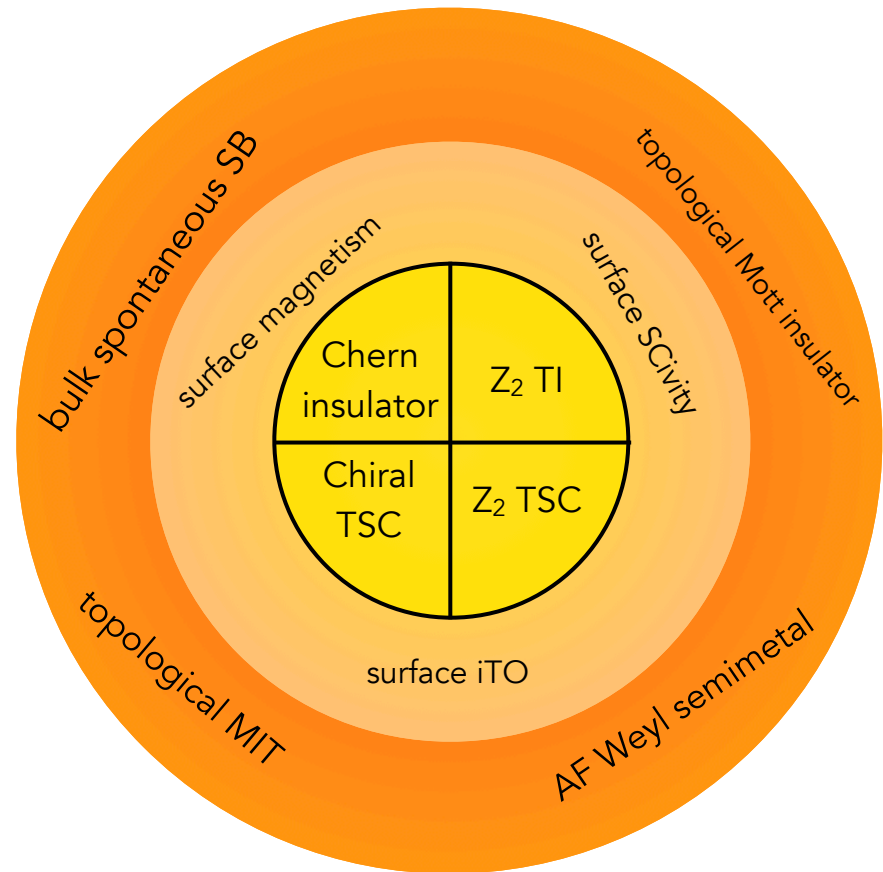


e.g. T. Neupert et al, 2015



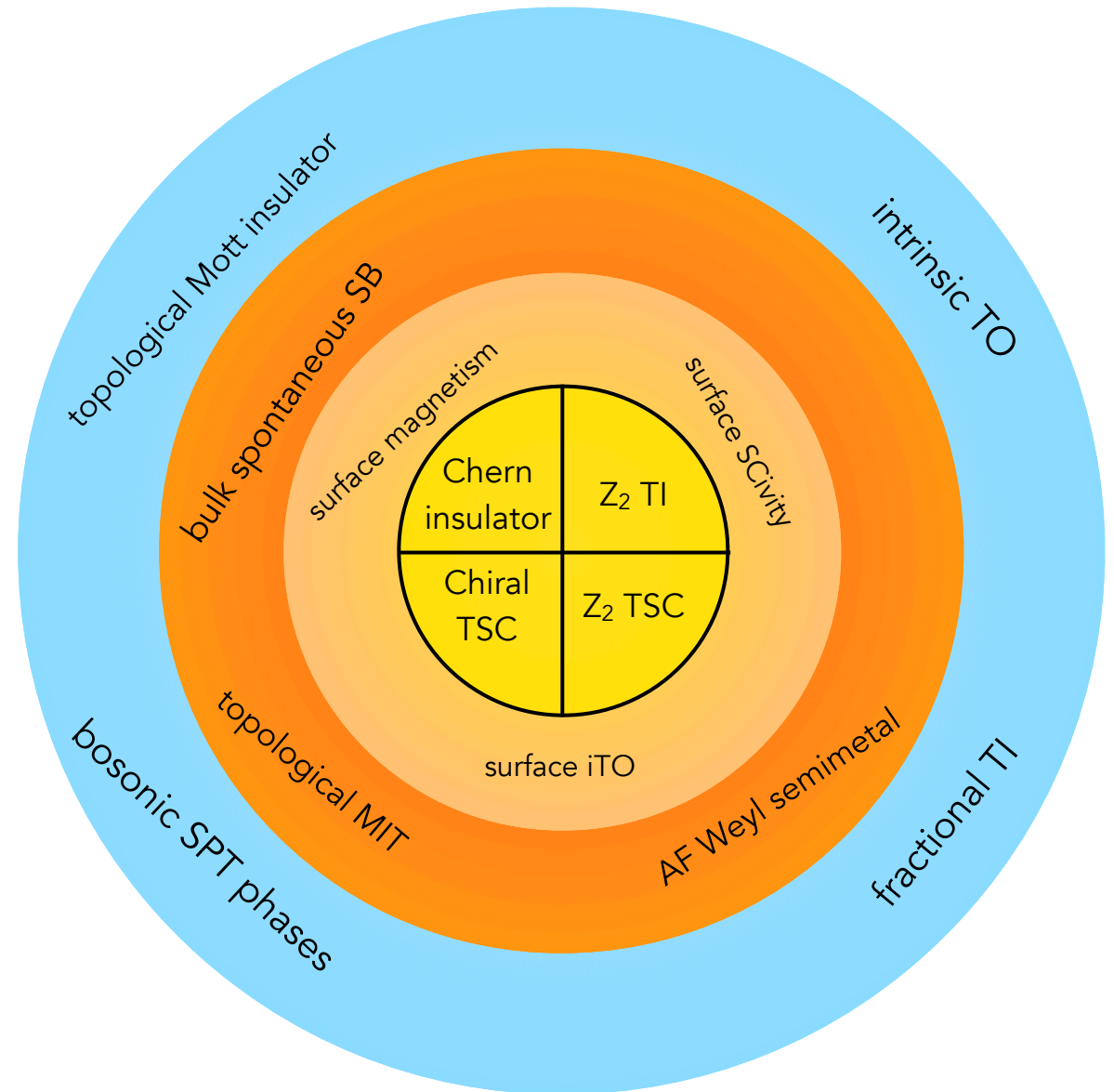
Why correlations?

- Distinct surface states
- Control of bulk topology by spontaneous symmetry breaking



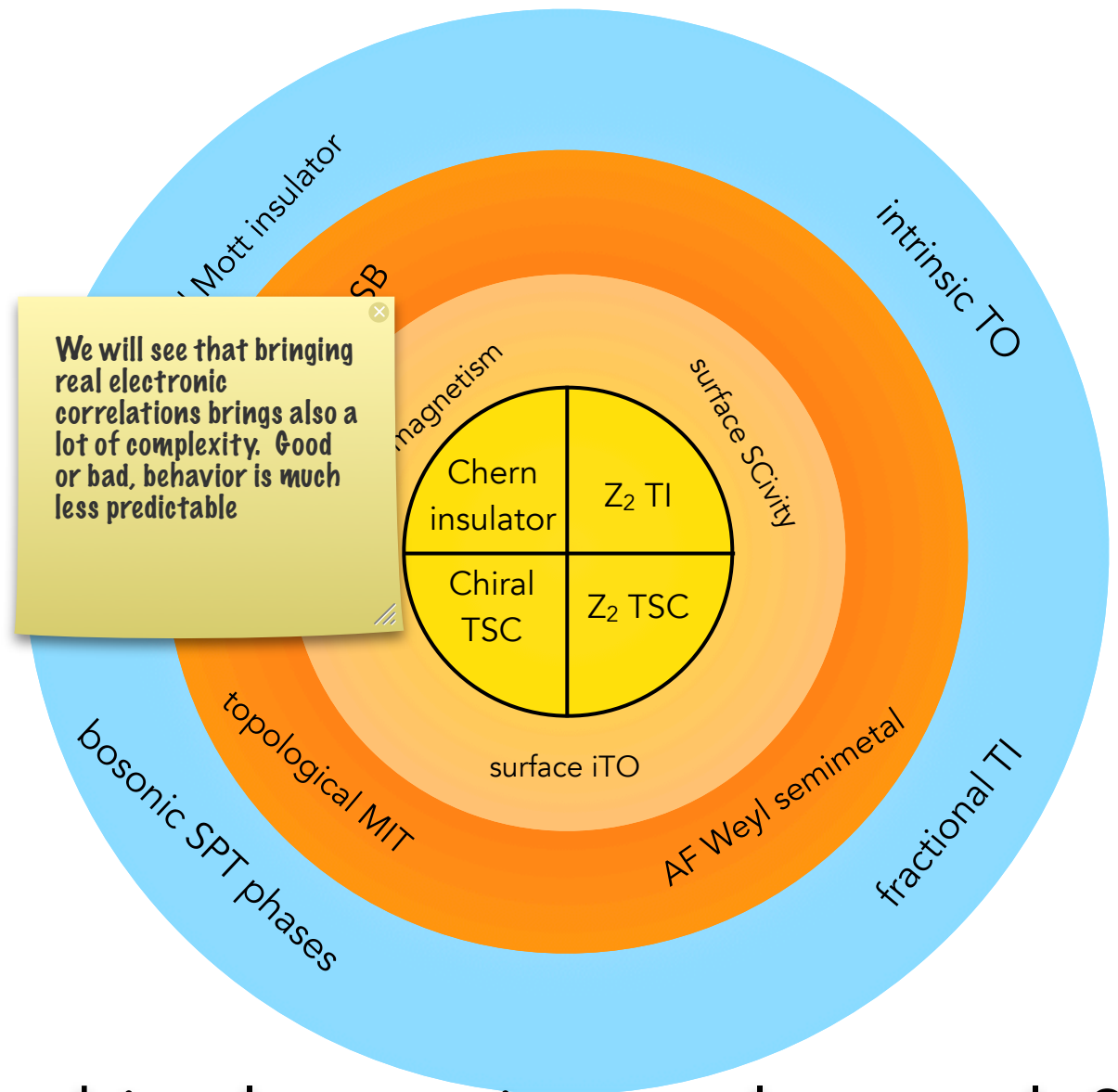
Why correlations?

- Distinct surface states
- Control of bulk topology by spontaneous symmetry breaking
- Entirely new phases requiring strong interactions



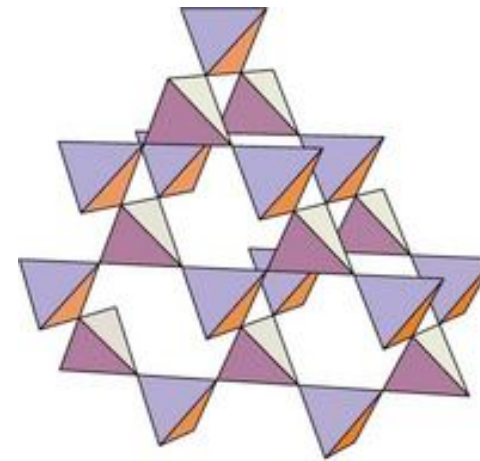
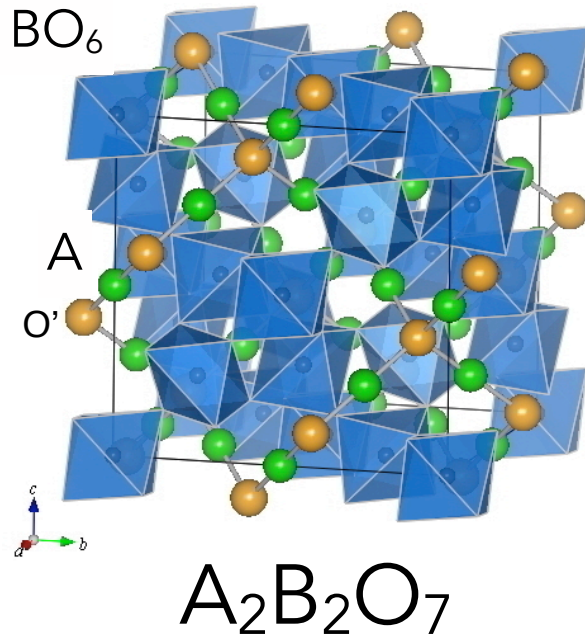
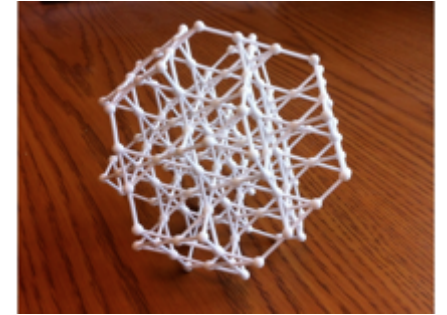
Why correlations?

- Distinct surface states
- Control of bulk topology by spontaneous symmetry breaking
- Entirely new phases requiring strong interactions



This talk: how does this play out in a real example?

Pyrochlores

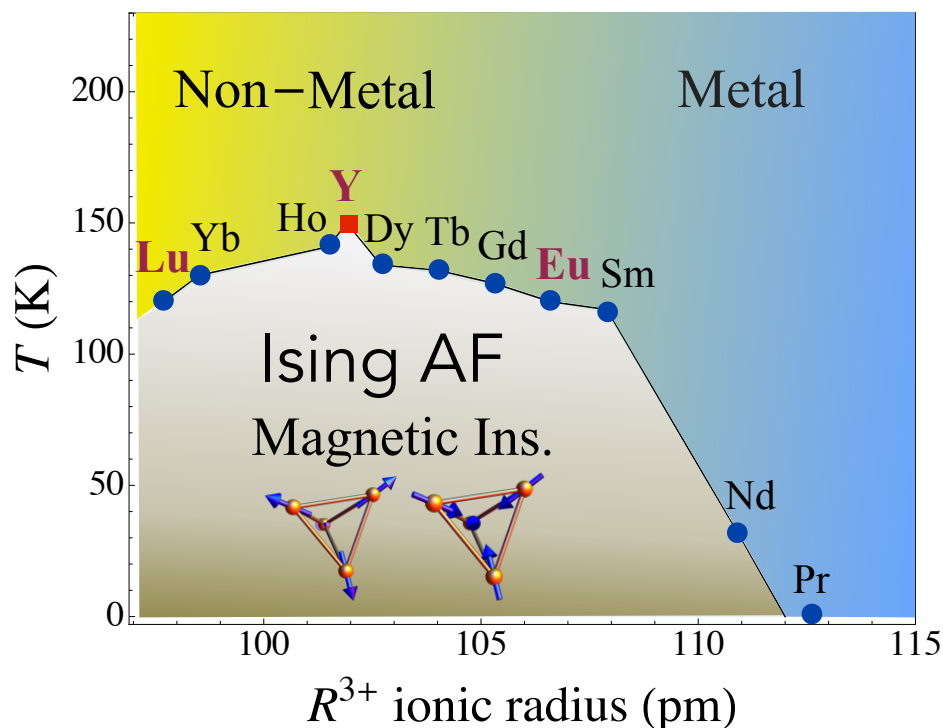


A (B) sublattice

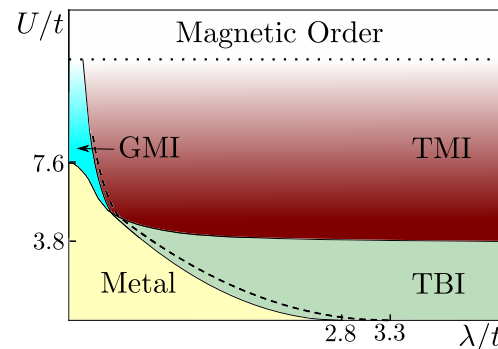
$A = Y, Ln$ ← f-electron moments, except
 $B = Ir$ when $A = Y, Eu$

Pyrochlore iridates

- Continuous magnetic/metal-insulator transitions (compatible with Ising)



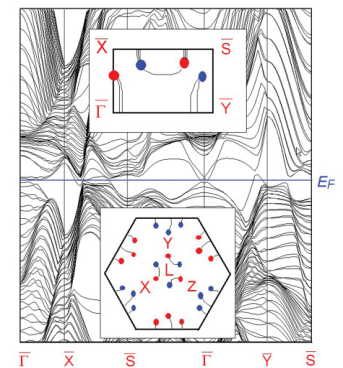
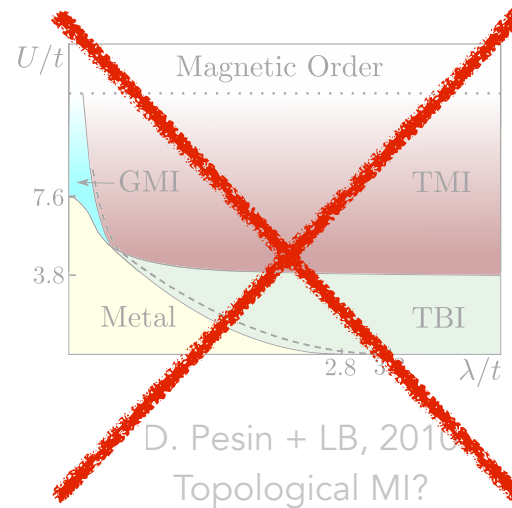
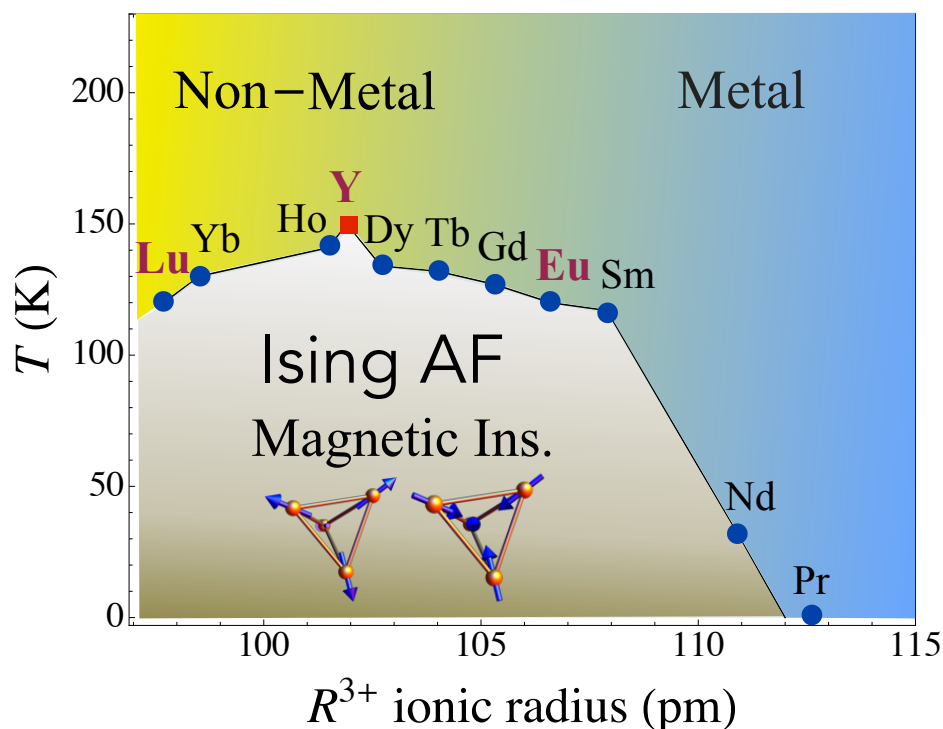
Yanagashima+Maeno, JPSJ 2001
 K. Matsuhira et al, JPSJ 2011
 W. Witczak-Krempa et al, ARCOMP 2013



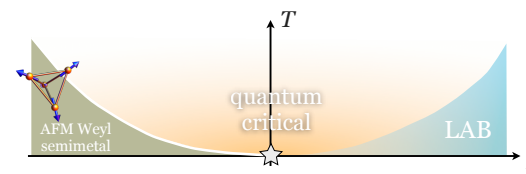
D. Pesin + LB, 2010
 Topological MI?

Pyrochlore iridates

- Continuous magnetic/metal-insulator transitions (compatible with Ising)



X. Wan et al, 2011
AF Weyl semimetal?

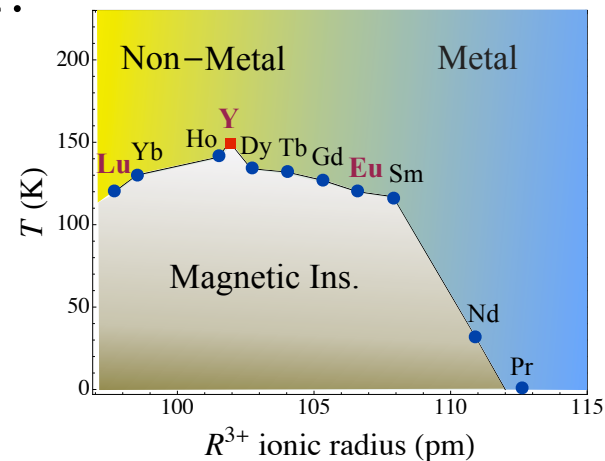


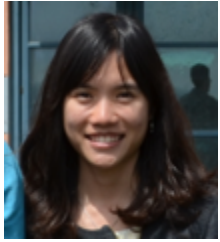
L. Savary et al, 2014 - topological QCP?

Ingredients of a theory

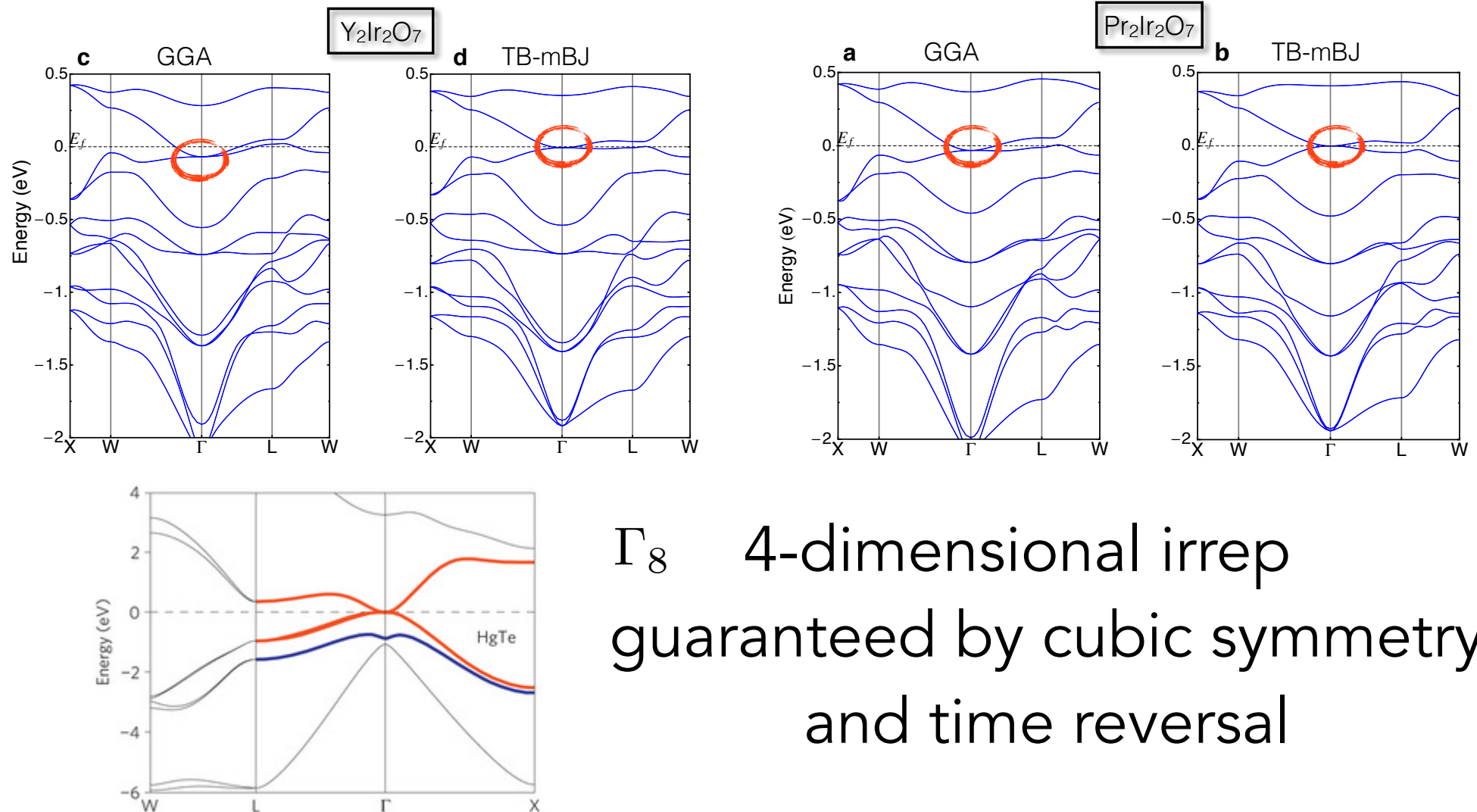
- Unusual electronic structure
- Ir e-e Hubbard interactions
- Rare earth moments?

probably not?

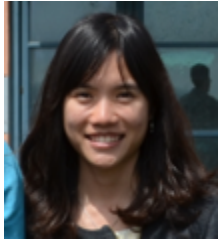




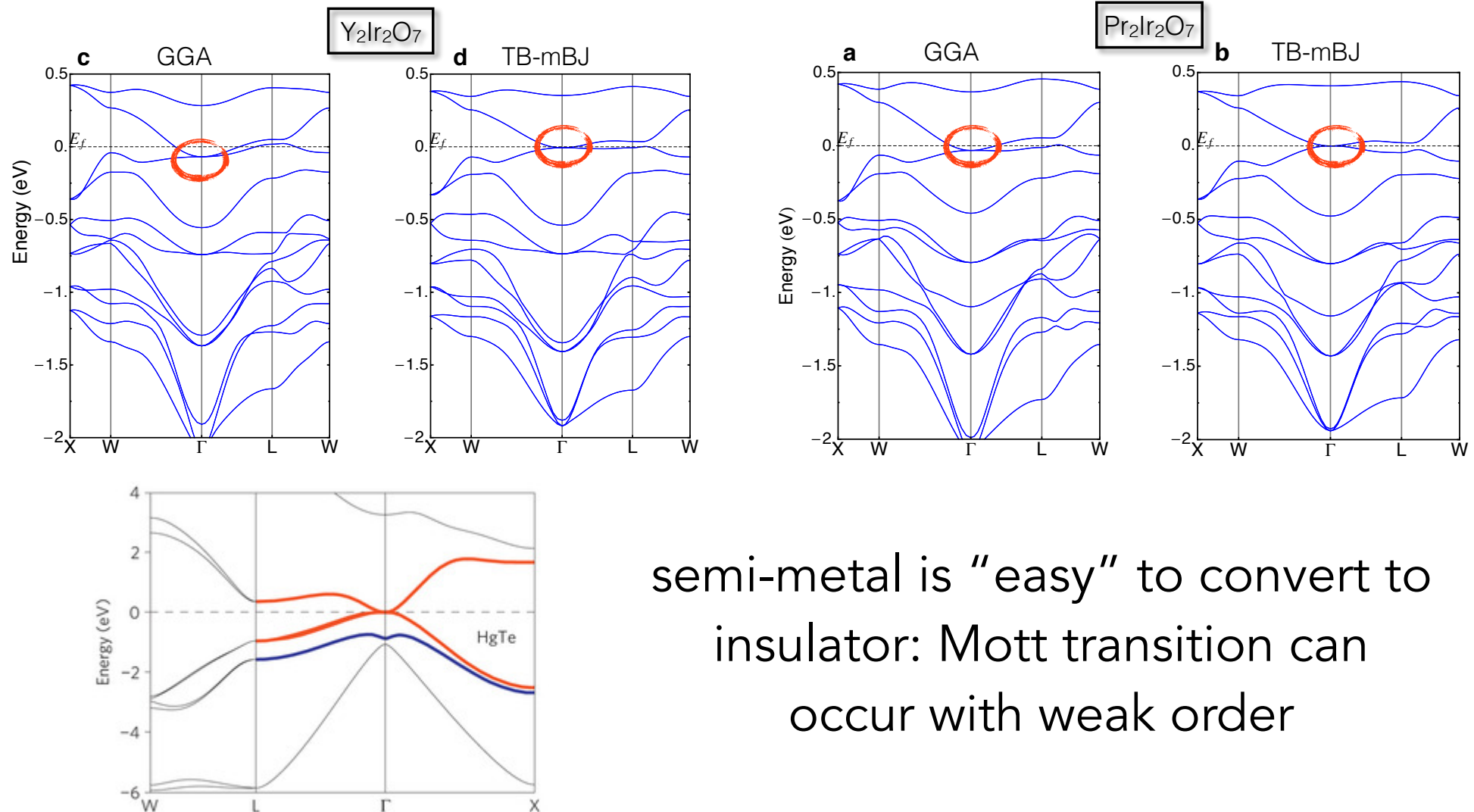
Paramagnetic electronic structure



Γ_8 4-dimensional irrep
guaranteed by cubic symmetry
and time reversal

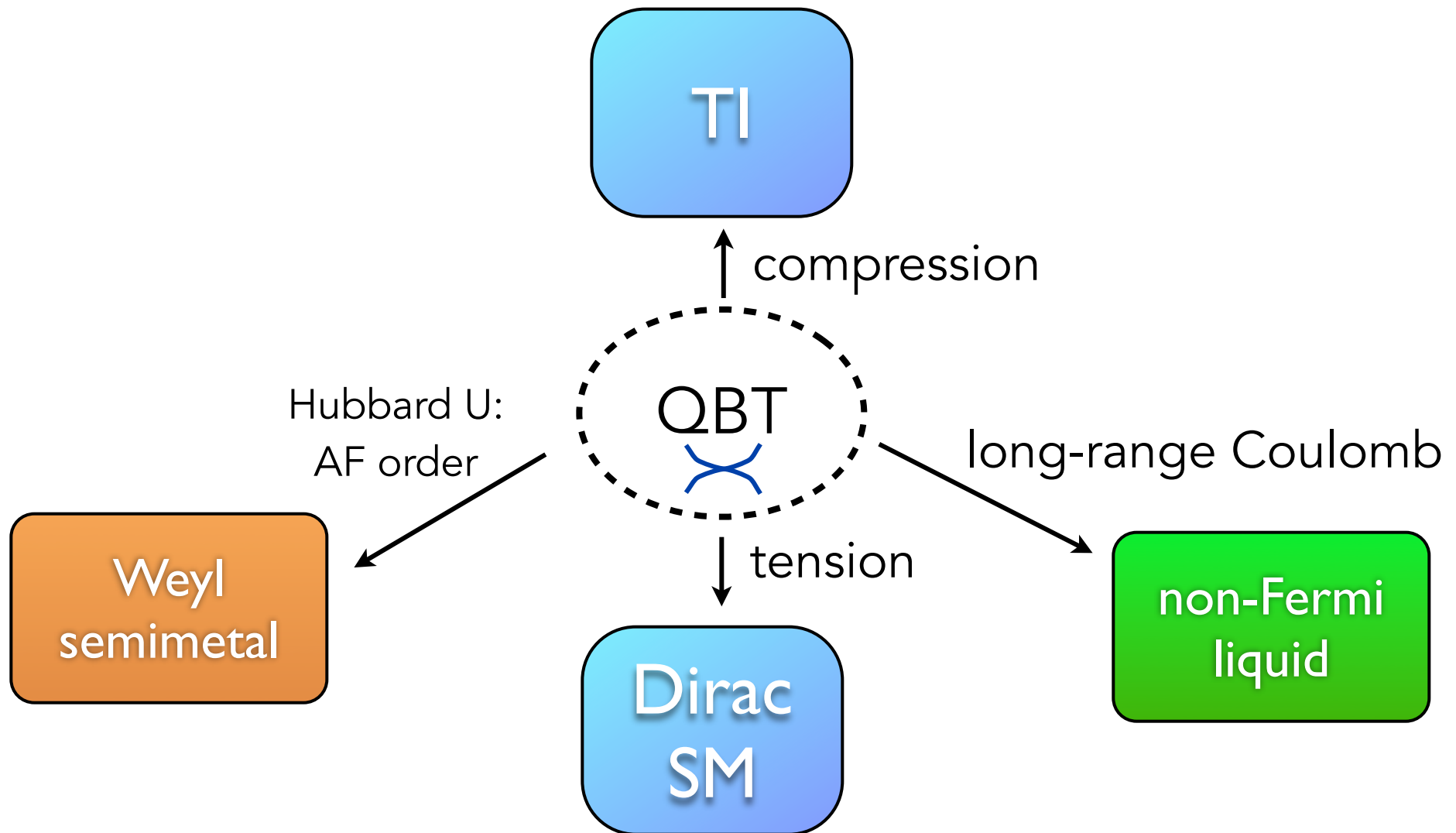


Paramagnetic electronic structure



semi-metal is "easy" to convert to insulator: Mott transition can occur with weak order

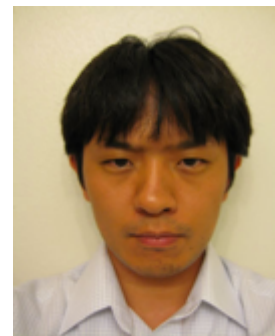
Proximate phases





ARPES

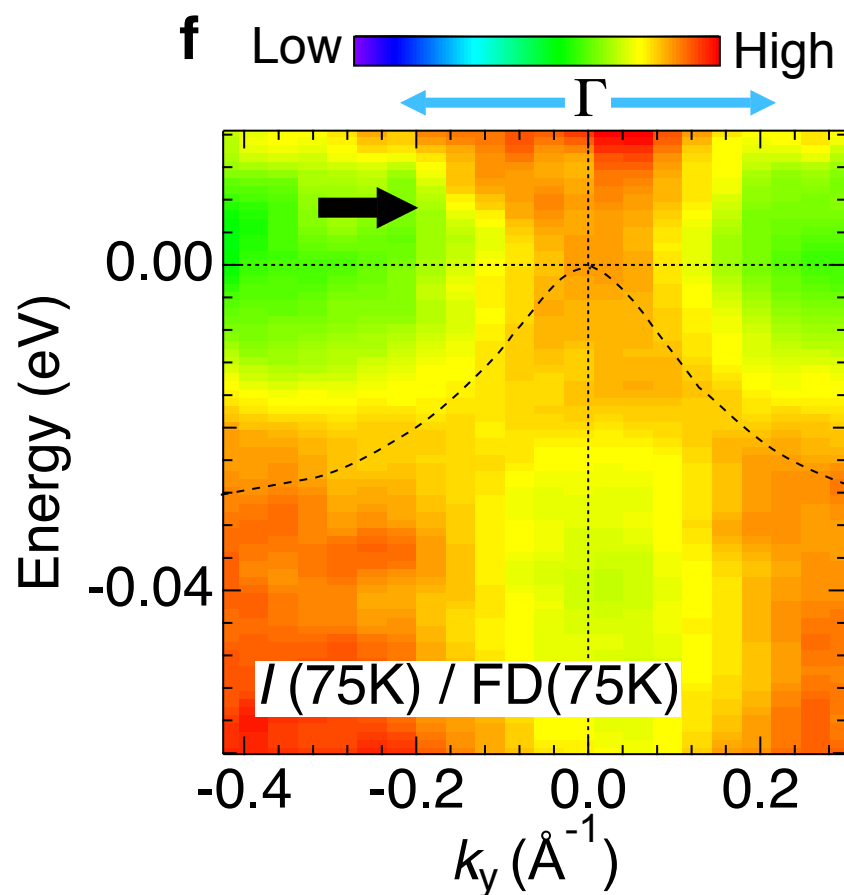
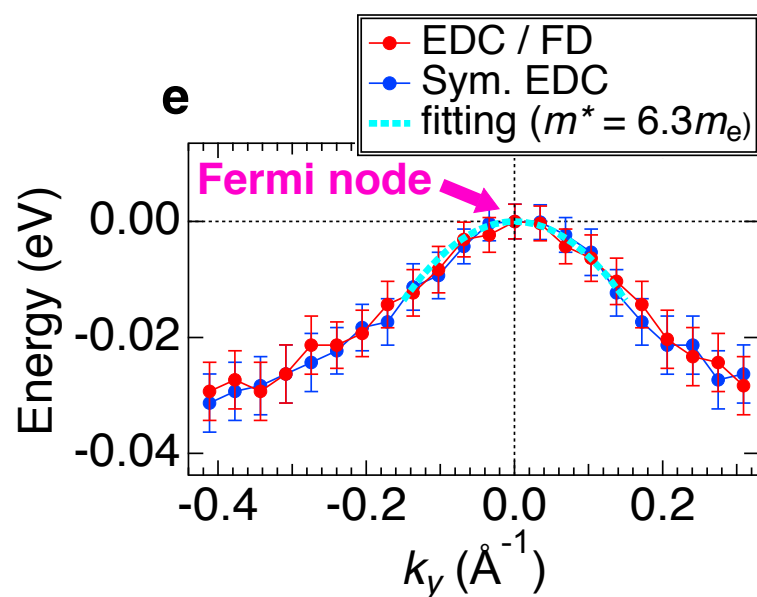
T. Kondo et al, Nat. Comm., 2015



$\text{Pr}_2\text{Ir}_2\text{O}_7$ S. Nakatsuji

T. Kondo

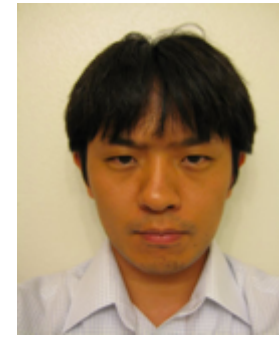
S. Shin





ARPES

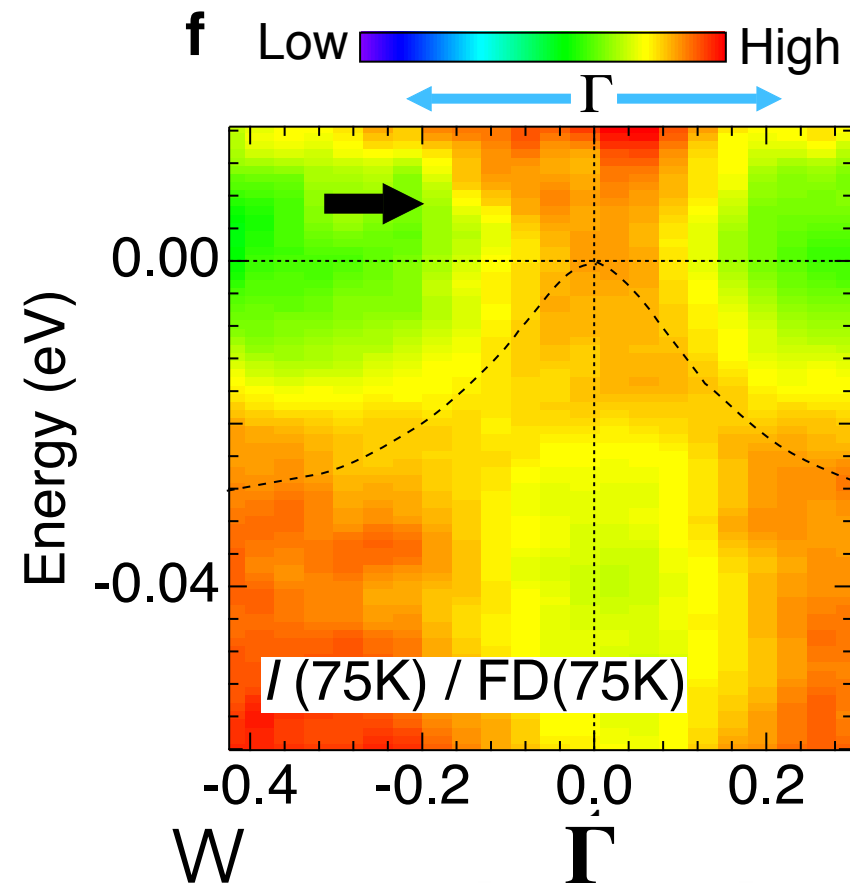
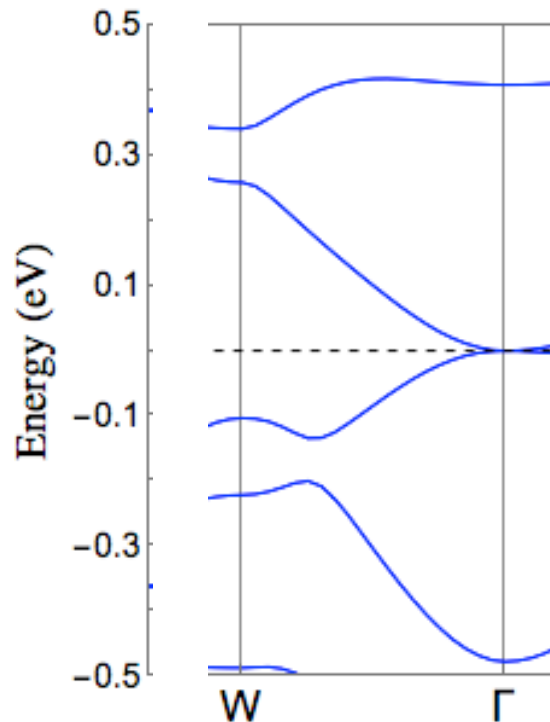
T. Kondo et al, Nat. Comm., 2015



$\text{Pr}_2\text{Ir}_2\text{O}_7$ S. Nakatsuji

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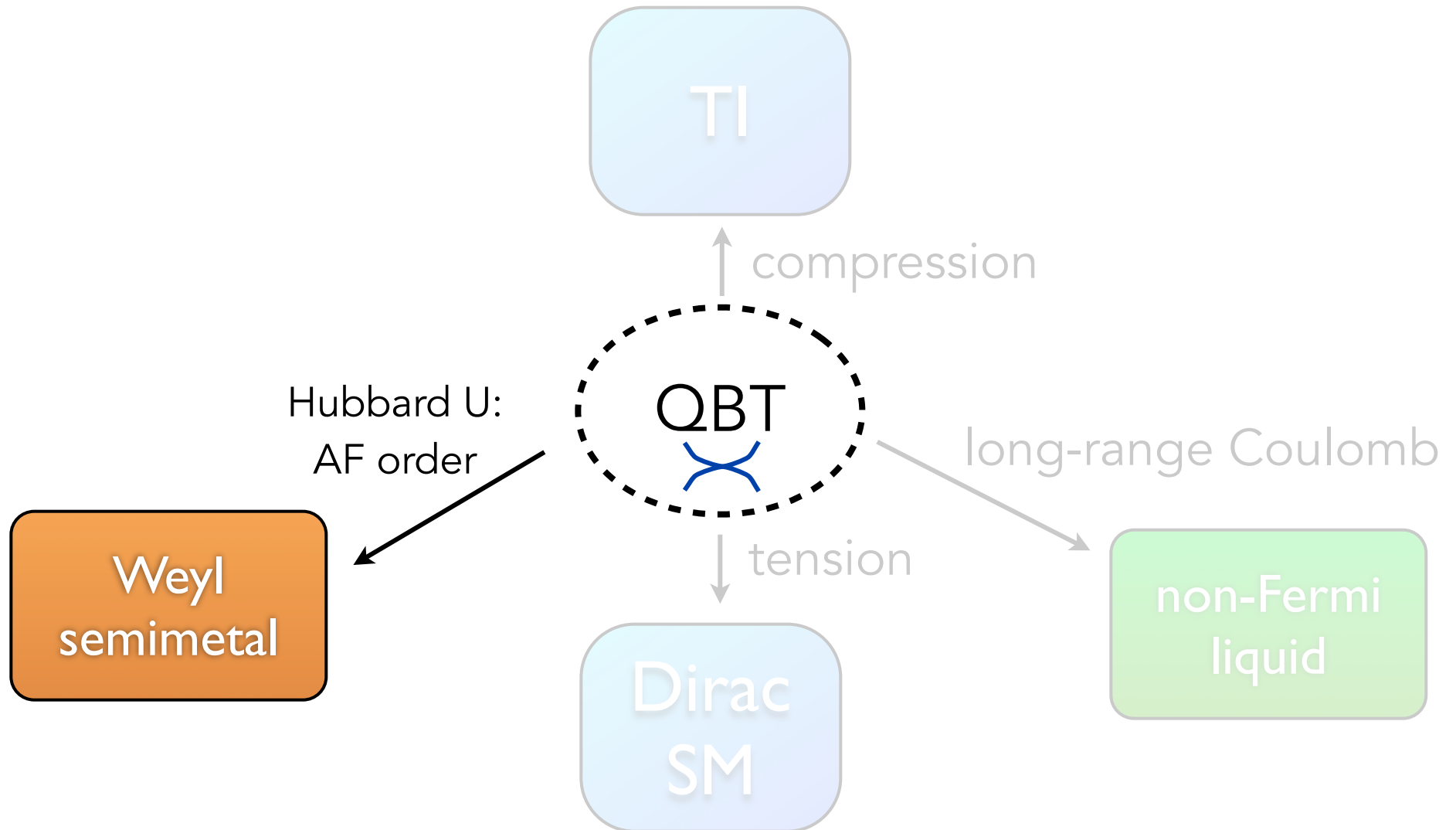
S. Shin



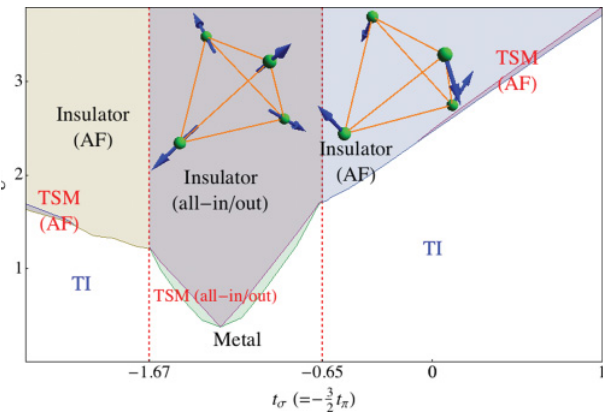
overall bandwidth \sim 3-5 times reduced!!

substantial U

Proximate phases

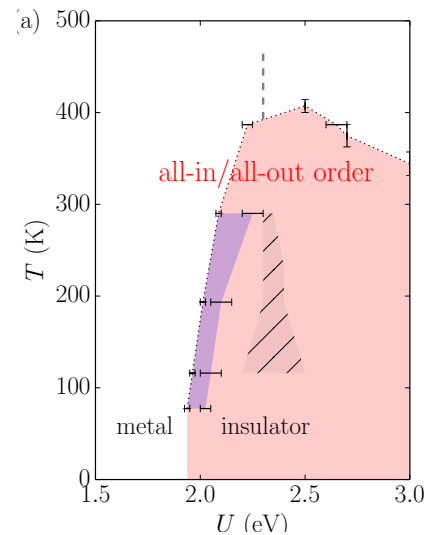


Ordering: theory



W. Witzak-Krempa + YB Kim, 2012

Hartree-Fock

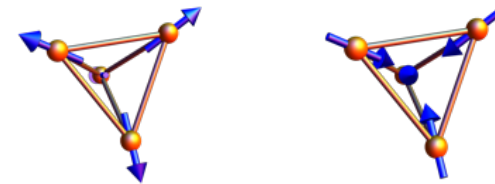


H. Shinaoka et al, 2015

DMFT

Jay-Z model

$$H = J_z \sum_{\langle i,j \rangle} S_i^z S_j^z$$



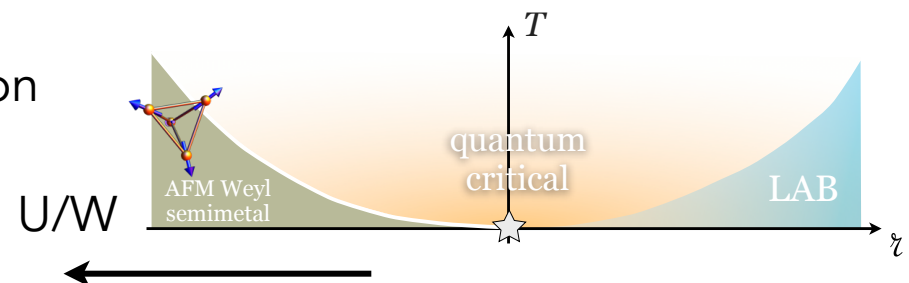
$J_z < 0$: all-in/all-out order

superexchange

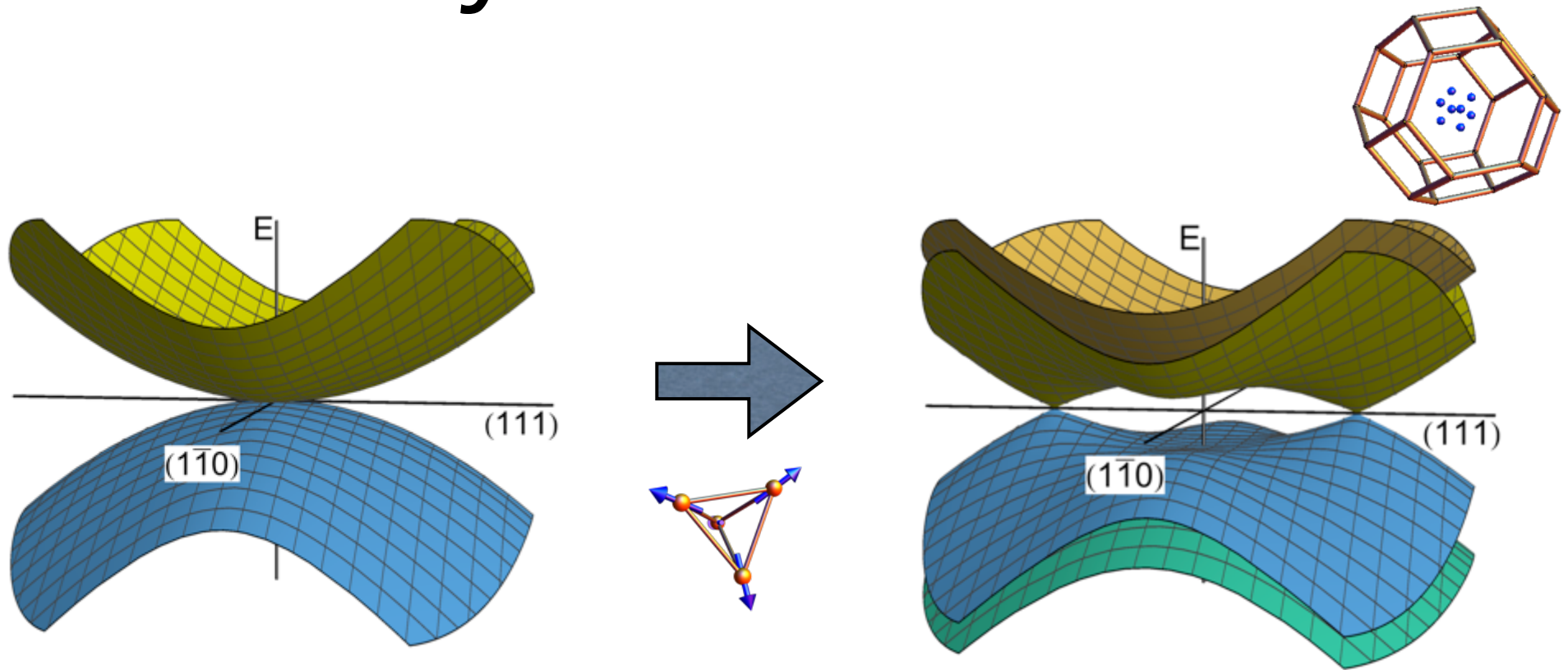
- General agreement: transition to AlAO Ising AF order

- ◆ Quantum critical theory of this transition

L. Savary et al, 2014 - topological QCP



Weyl semimetal

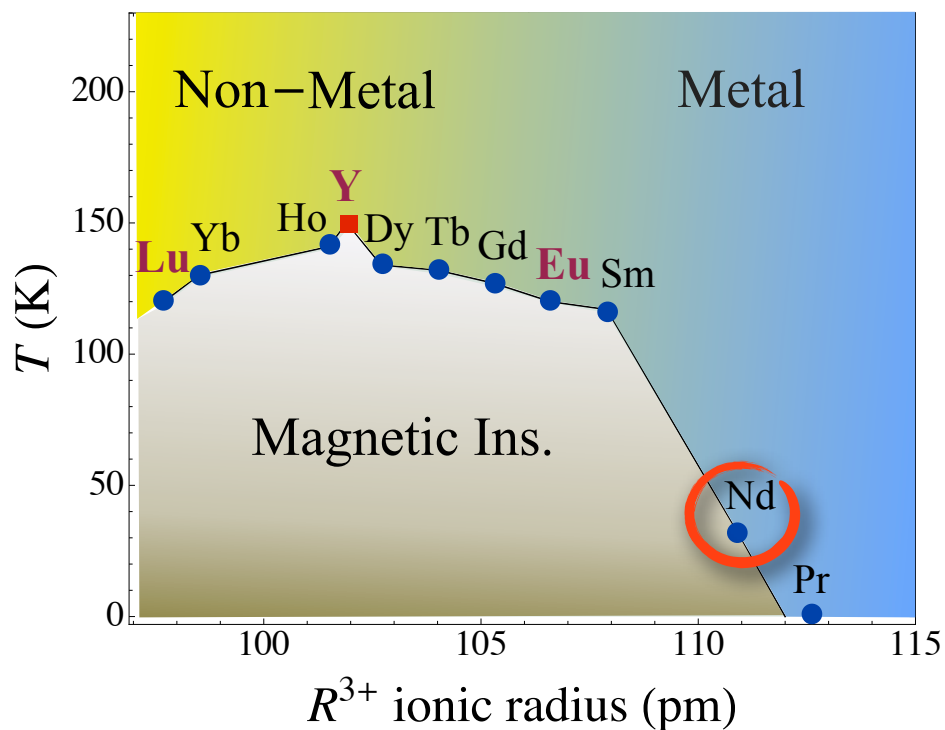


If quasiparticle picture applies at low energy, a *weakly* ordered AIAO state *must* be a Weyl semimetal

Weyl?

- Weyl semimetal?

Best candidate
should be
 $\text{Nd}_2\text{Ir}_2\text{O}_7$

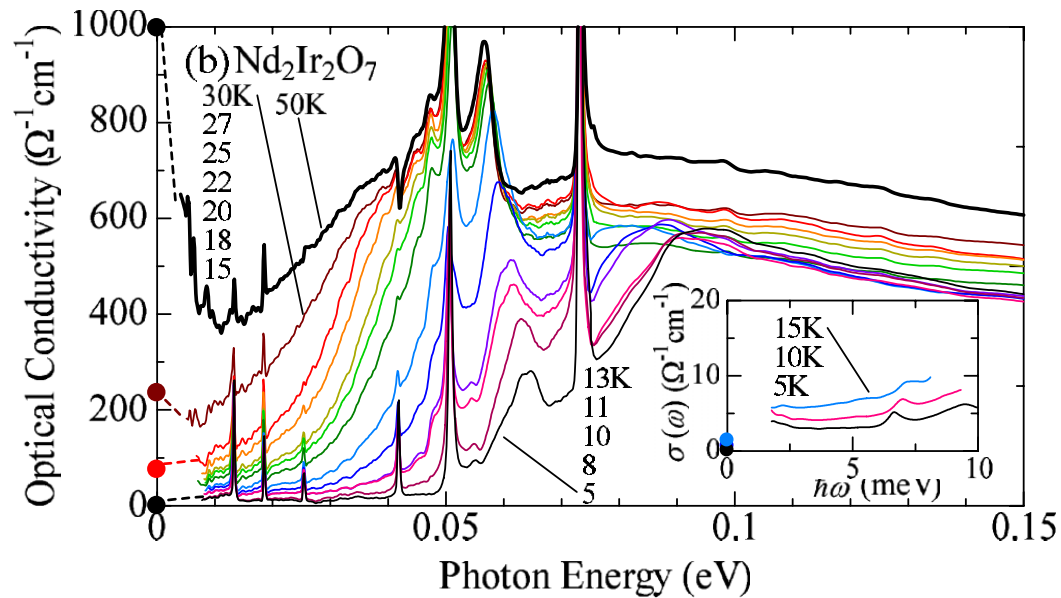


R^{3+} ionic radius (pm)
Yanagashima+Maeno, JPSJ 2001
K. Matsuhira et al, JPSJ 2011
W. Witczak-Krempa et al, ARCOMP 2013



Weyl not?

K. Ueda *et al*, 2012



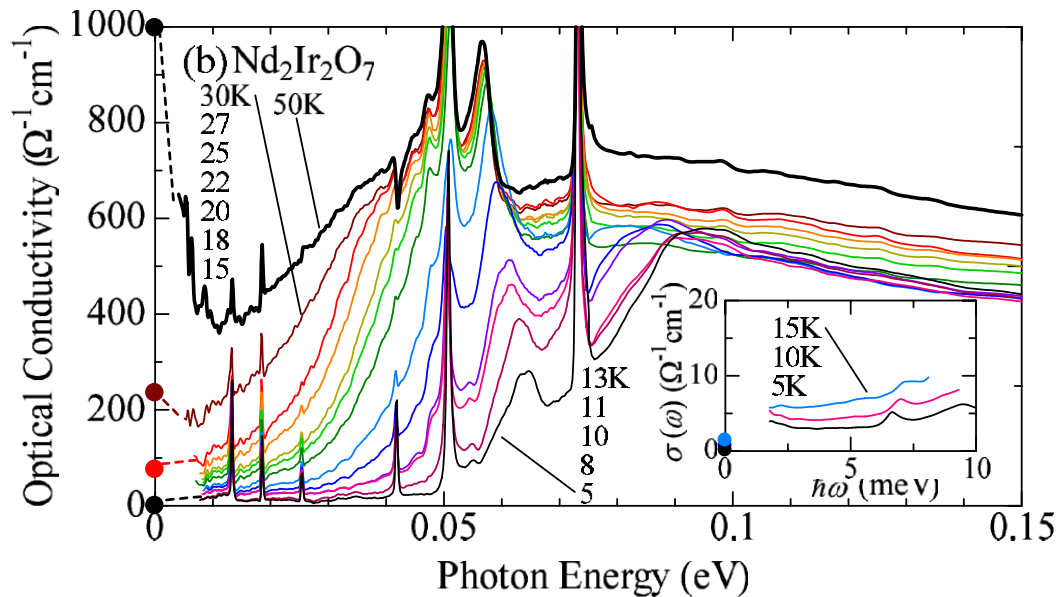
charge gap \sim
45meV

n.b. Gap $\sim 18T_c$



Weyl not?

K. Ueda *et al*, 2012

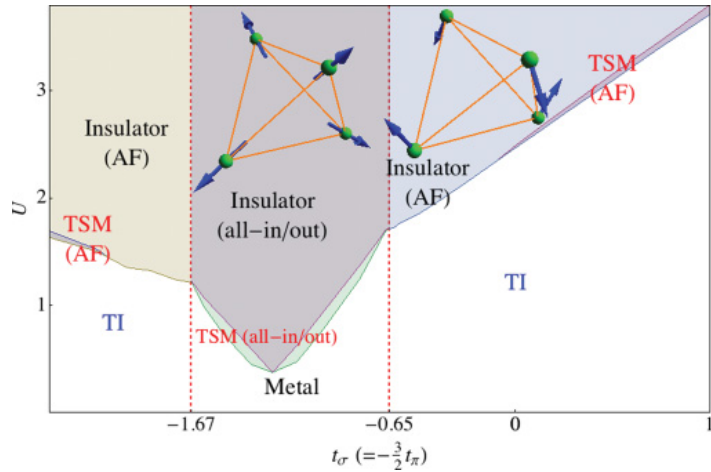


charge gap \sim
45meV

If quasiparticle picture applies at low energy, a *weakly* ordered AIAO state *must* be a Weyl semimetal

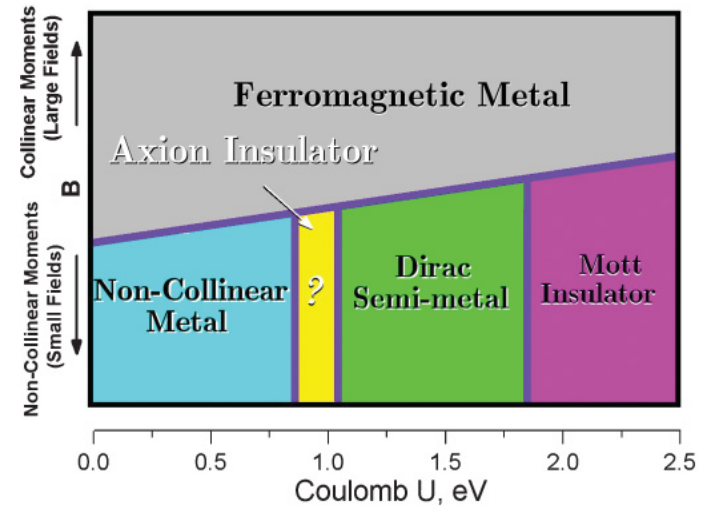
- ◆ Not weakly ordered?
- ◆ No quasiparticles?
- ◆ Weyl with very small DOS?

Weak or not?



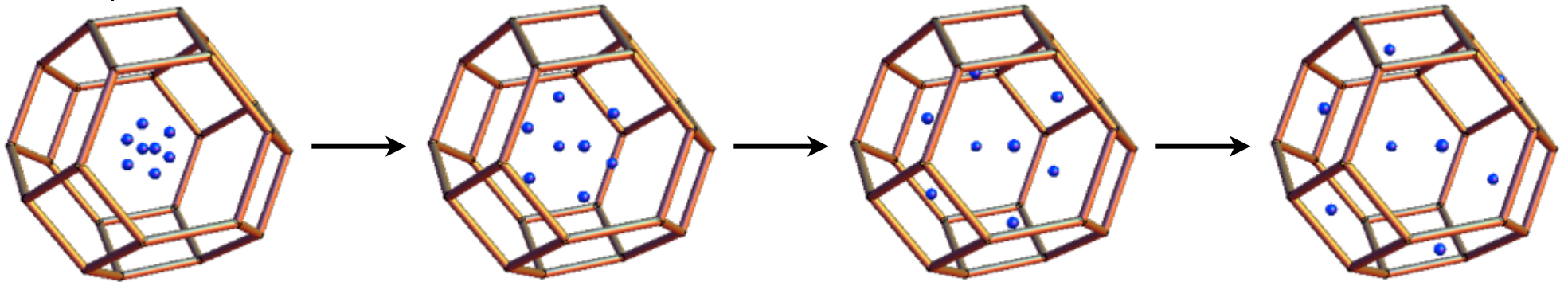
W. Witzak-Krempa + YB Kim, 2012

VS



X. Wan et al, 2011

Weyl points move to zone boundary and annihilate with increasing order?

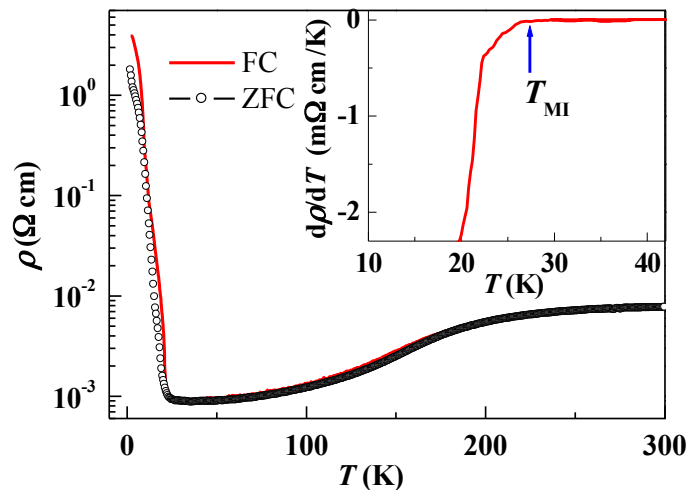


Could this have happened already for Nd?

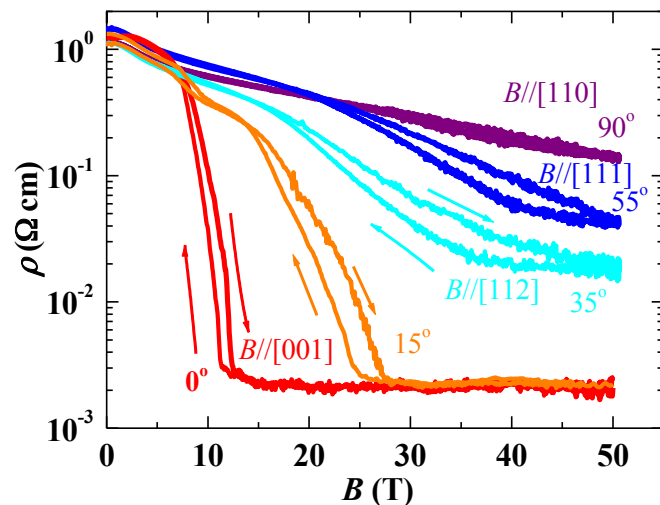


Transport

To explore this in more detail, let's look at transport

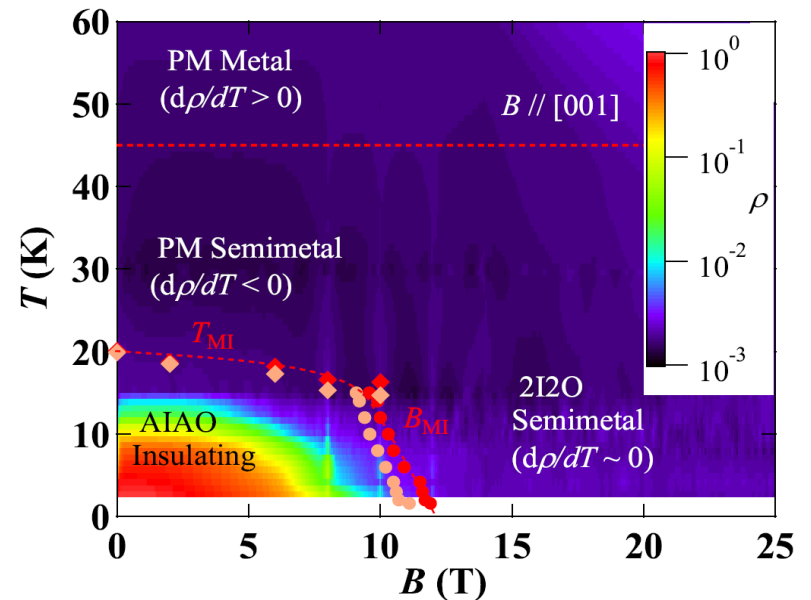
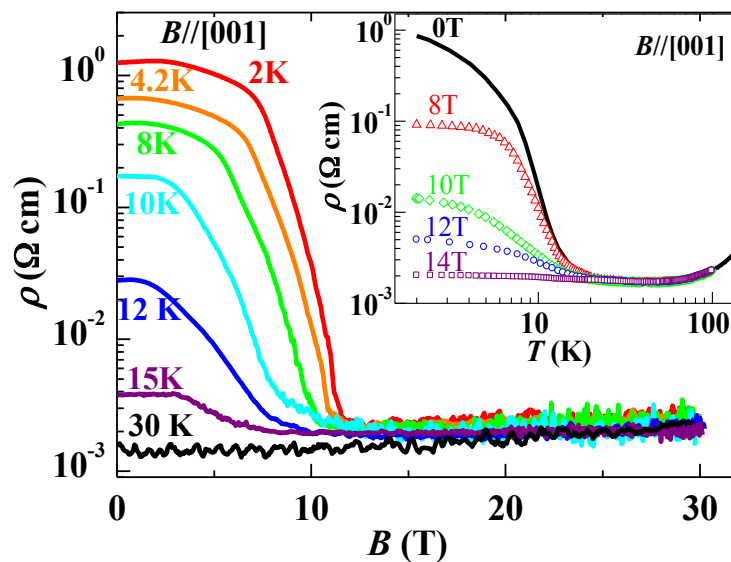


- Seems to be a transition with hard gap
- thermal transition is continuous



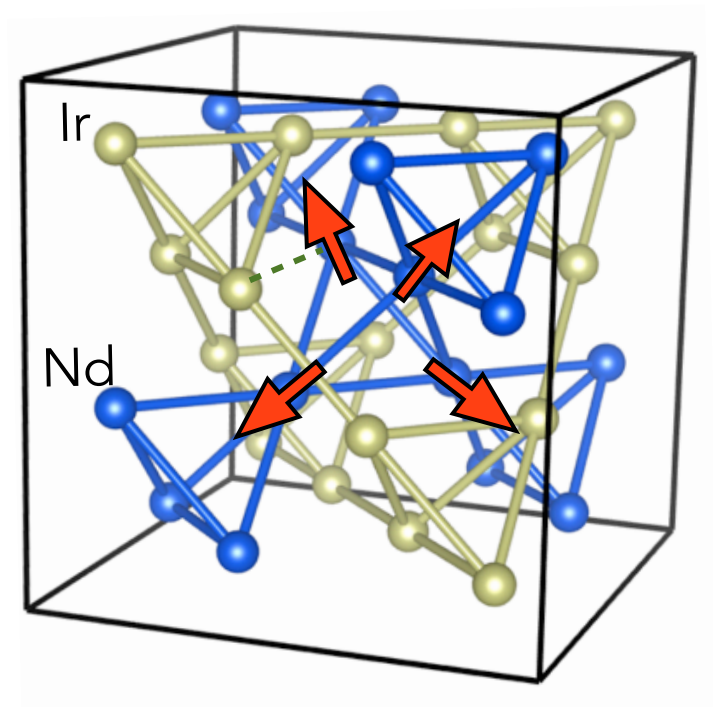
- However, abrupt first order transition appears at low T in a field
- Insulator-metal transition *only* occurs for fields along (100)

Metal-Insulator Transition



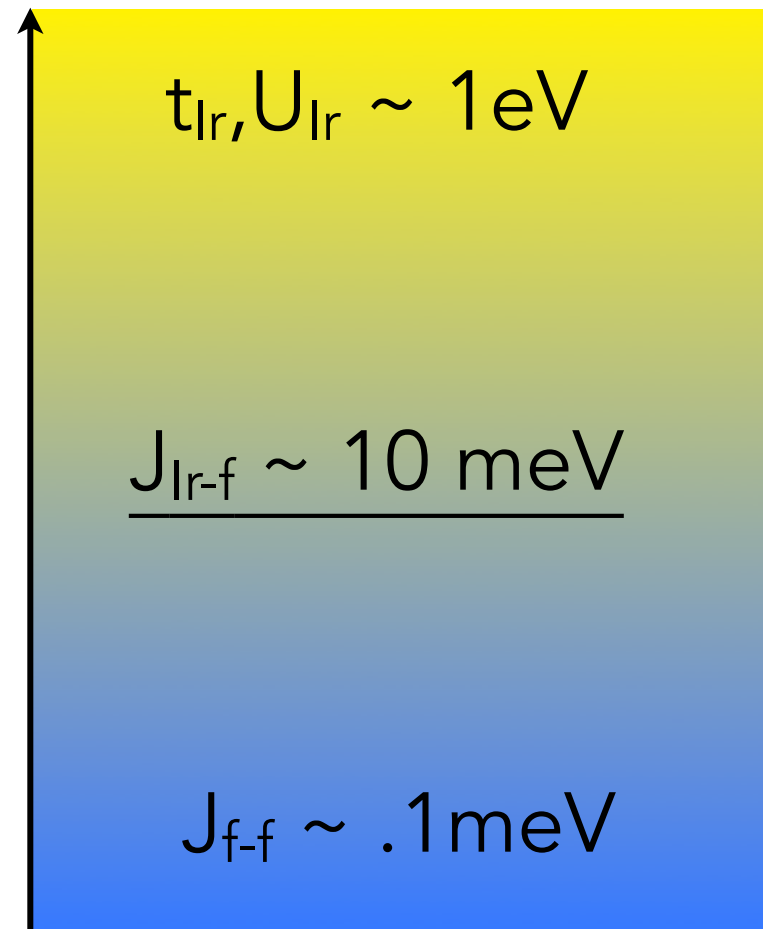
- First order transition at low temperature: mechanism of MIT is vanishing of condensation energy, not gap closing.
- Anisotropy: clear indication that Nd plays a direct role in the MIT - probably this is a unique feature for R=Nd

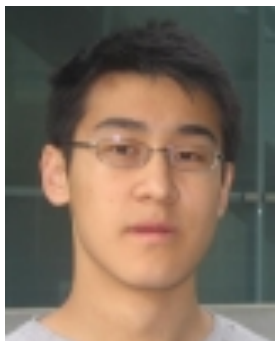
Nd physics



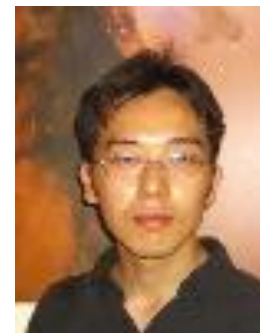
- Much of gap (45meV) is *due* to Nd-Ir exchange
- Intrinsic g-tensor anisotropy of Nd explains anisotropy of MIT

(100) field achieves maximum Nd polarization of 2in-2out type, "opposite" to AIAO Ising order



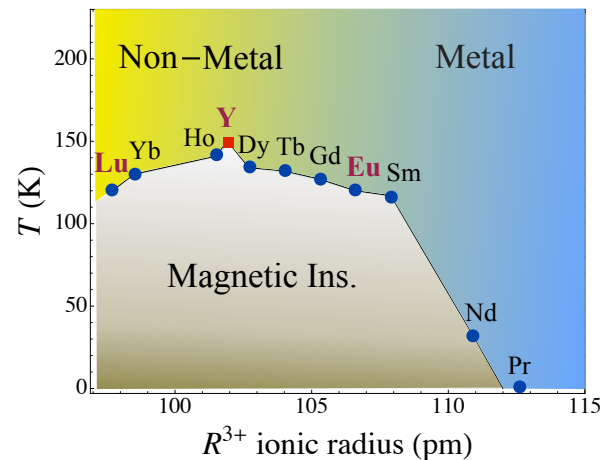
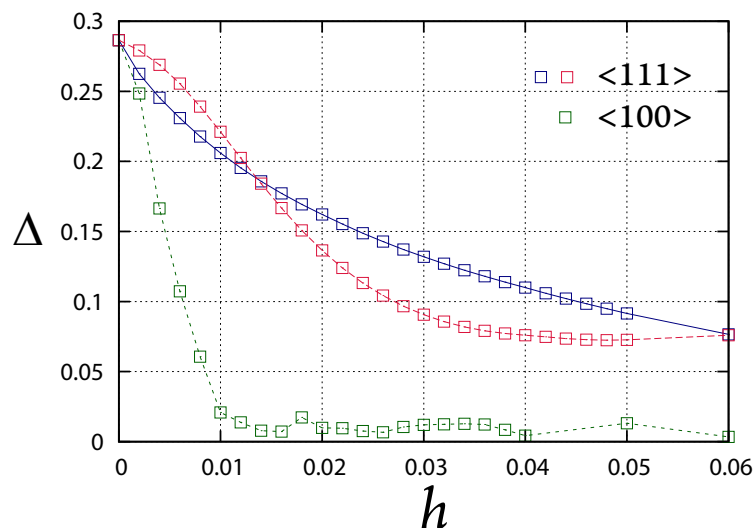


Anisotropy



- Nd sensitivity to direction is transferred to Ir

$$H_K = \sum_{ia} \vec{S}_i \cdot \mathbf{J}_{ia} \cdot \vec{\tau}_a \quad \text{acts like } h_{\text{eff}} \sim 10 \text{ meV local field on Ir}$$

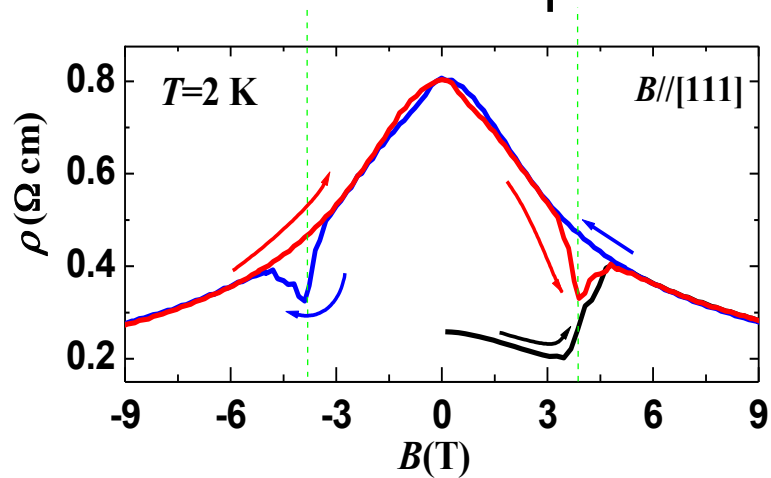


Hartree-Fock on Hubbard
+Kondo lattice model

- h_{eff} is significant for Nd case
- can explain the anisotropy

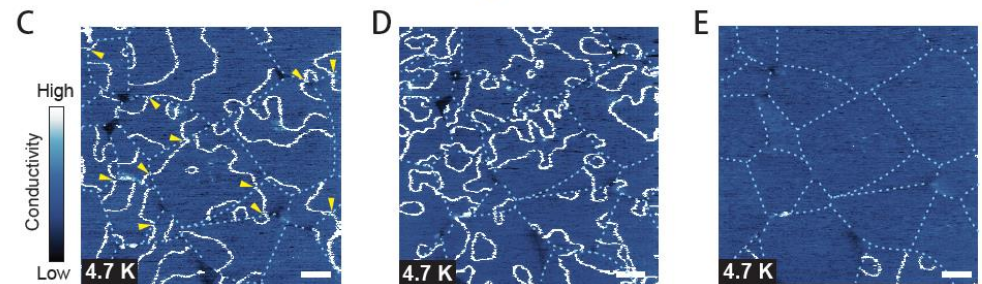
Domains

- Large magnetic moment of Nd allows manipulation of domains



Z. Tian *et al*, 2015

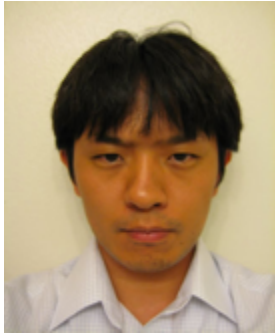
c.f. K. Ueda *et al* (2014)



local conductivity

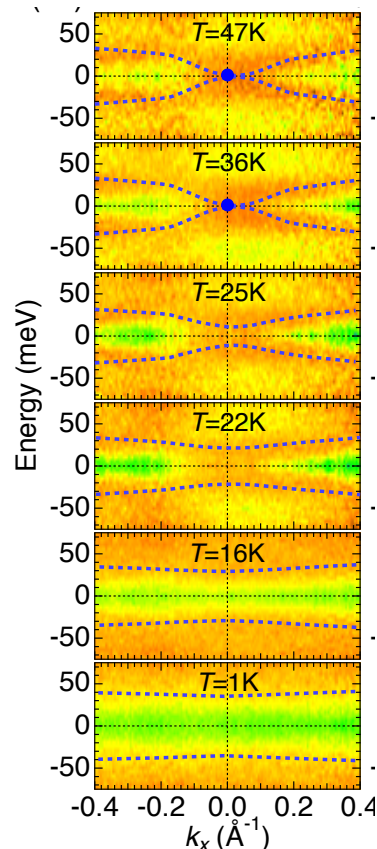
E. Y. Ma *et al*, 2015

conducting domain walls!



Quasiparticles?

- Already observed bandwidth reduction in $\text{Pr}_2\text{Ir}_2\text{O}_7$ - what happens for Nd?



$T > T_c$: like Pr

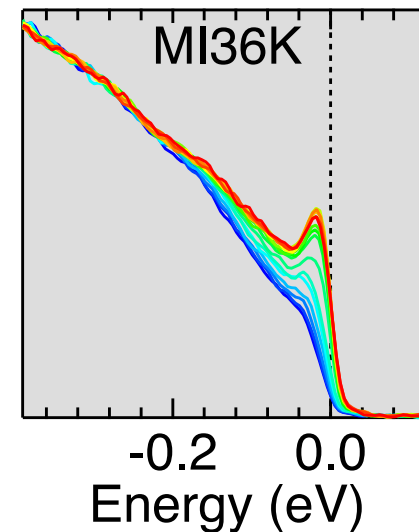
$T = T_c$: no precursor - Slater

$T < T_c$: gap developing

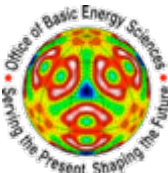
Slater to Mott
crossover?

$T \ll T_c$: remarkably flat

In strong Mott localized regime non-trivial band topology is unlikely



loss of quasiparticle peak

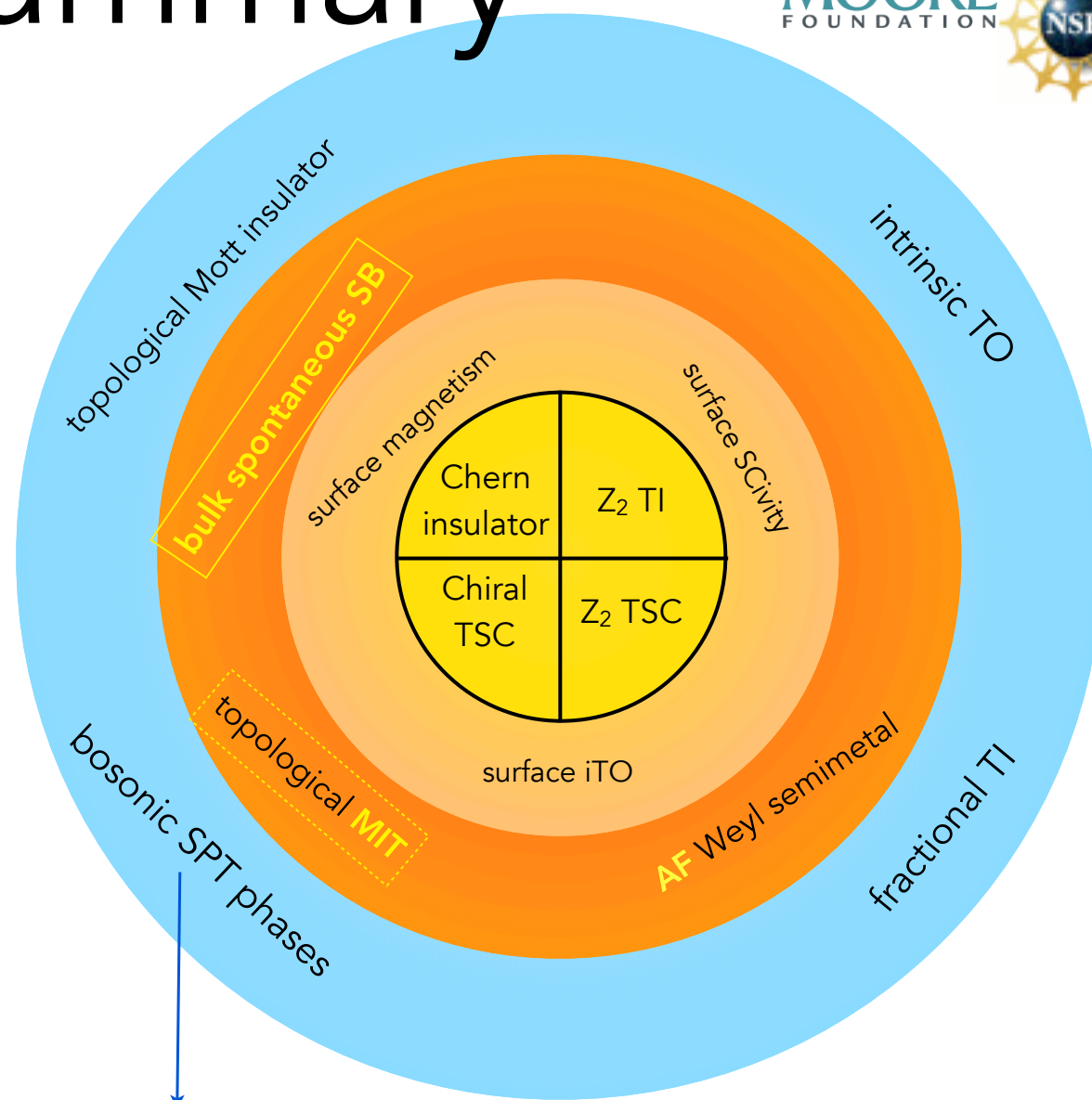


GORDON AND BETTY
MOORE
FOUNDATION



Summary

- Pyrochlore iridates show a rich phenomenology with nodal and gapped states, metal-insulator transitions, and strong anisotropic response
- Correlations induce antiferromagnetism but also Mott localization, which, helped by Nd f-moments, seems to subdue the Weyl fermions expected from the former alone
- Quite a bit still to explore! Correlated materials prove surprising and challenging



Advertisement: Zhen Bi et al, arXiv:1602.03190