

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



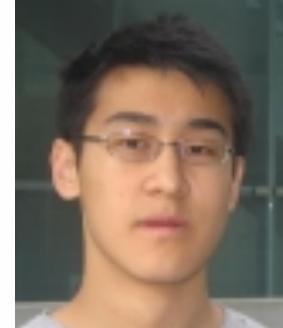
Eun-Gook Moon



S. Nakatsuji



T. Kondo



T. Hsieh



H. Ishizuka

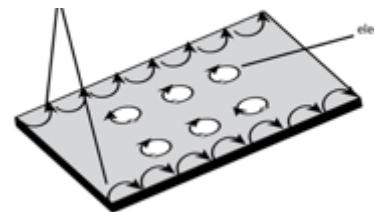
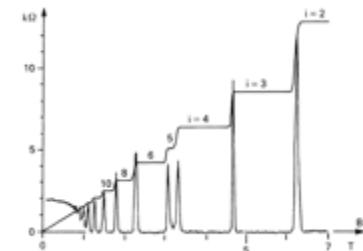
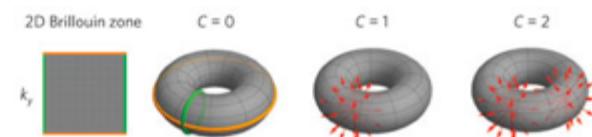
TIs

Broken TRS with TRS

integer Chern number

= Hall conductance

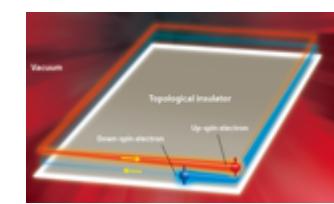
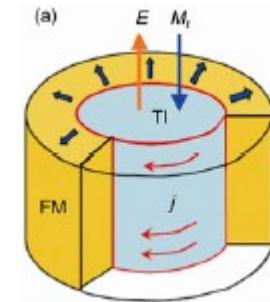
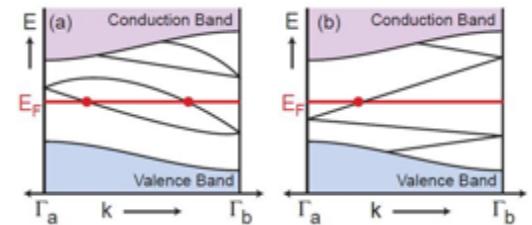
chiral edge states



Z_2 invariant

= M-E polarizability

helical edge/ surface states

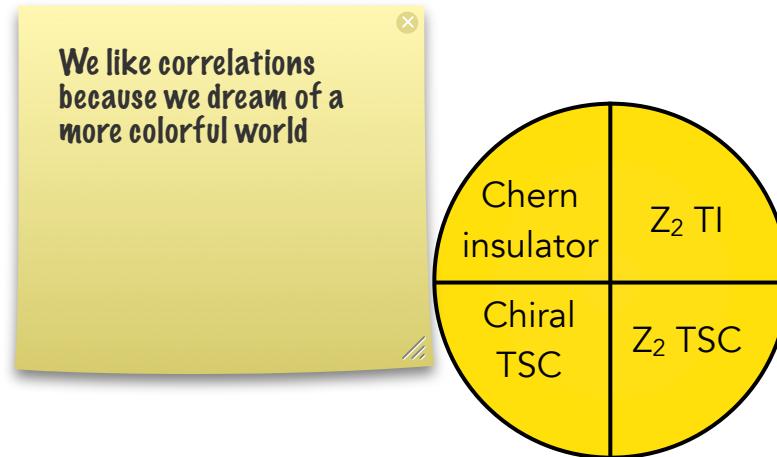


Topological everything

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

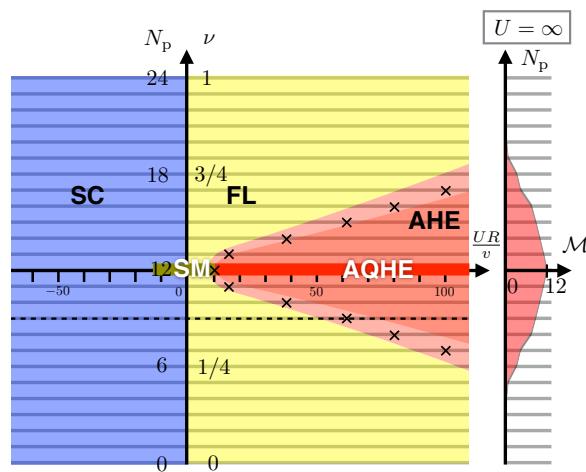
Why correlations?

w/o interactions

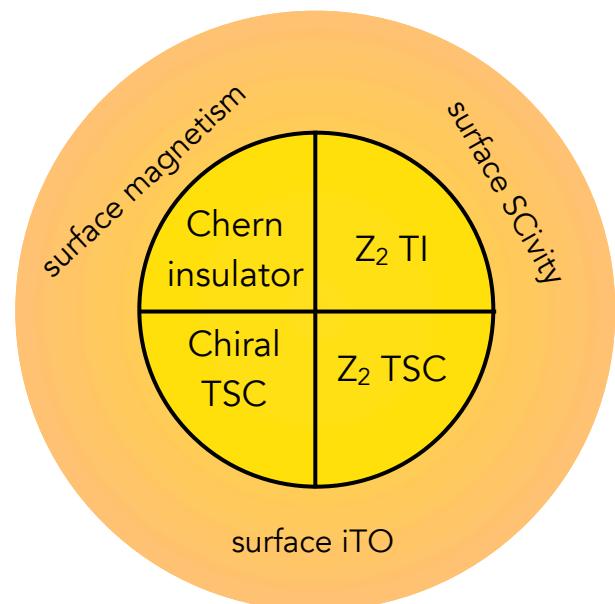


Why correlations?

- Distinct surface states

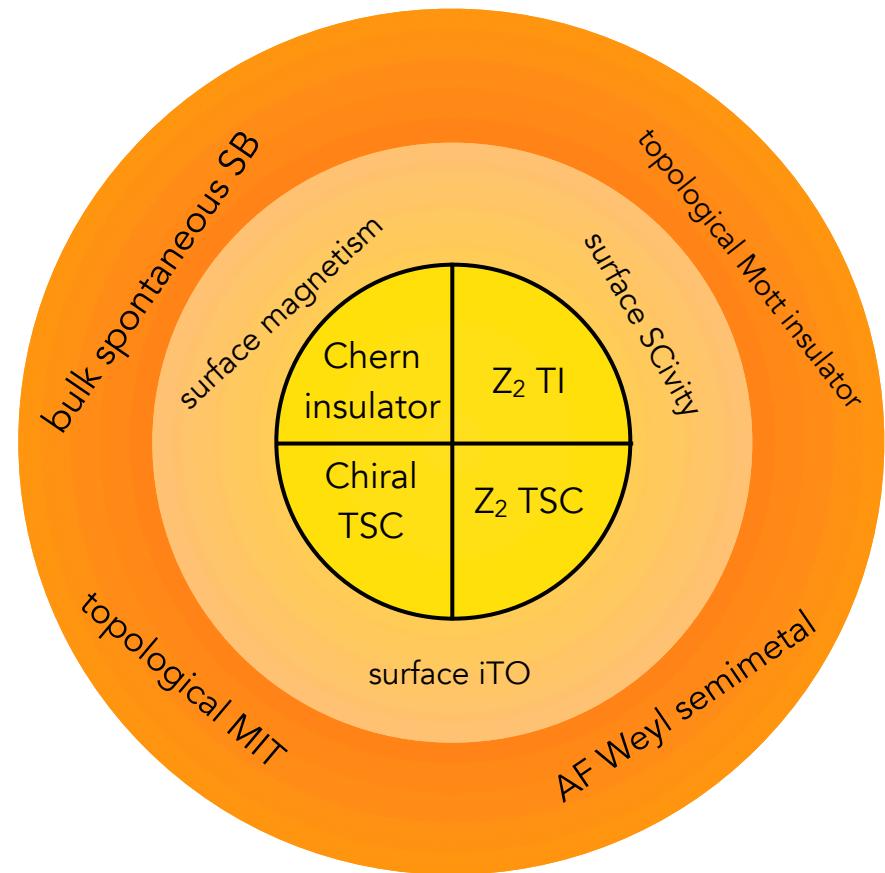


e.g. T. Neupert et al, 2015



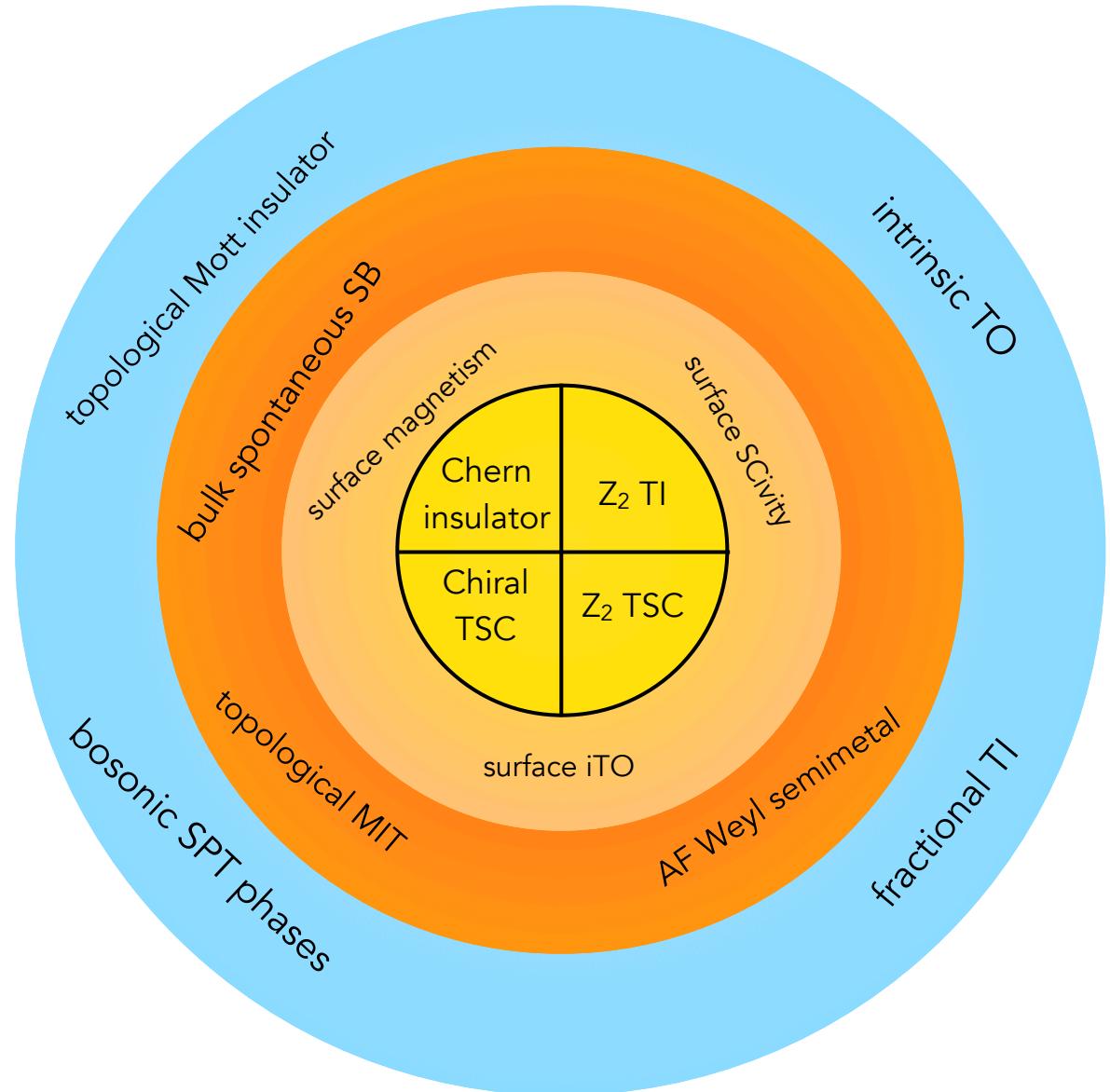
Why correlations?

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



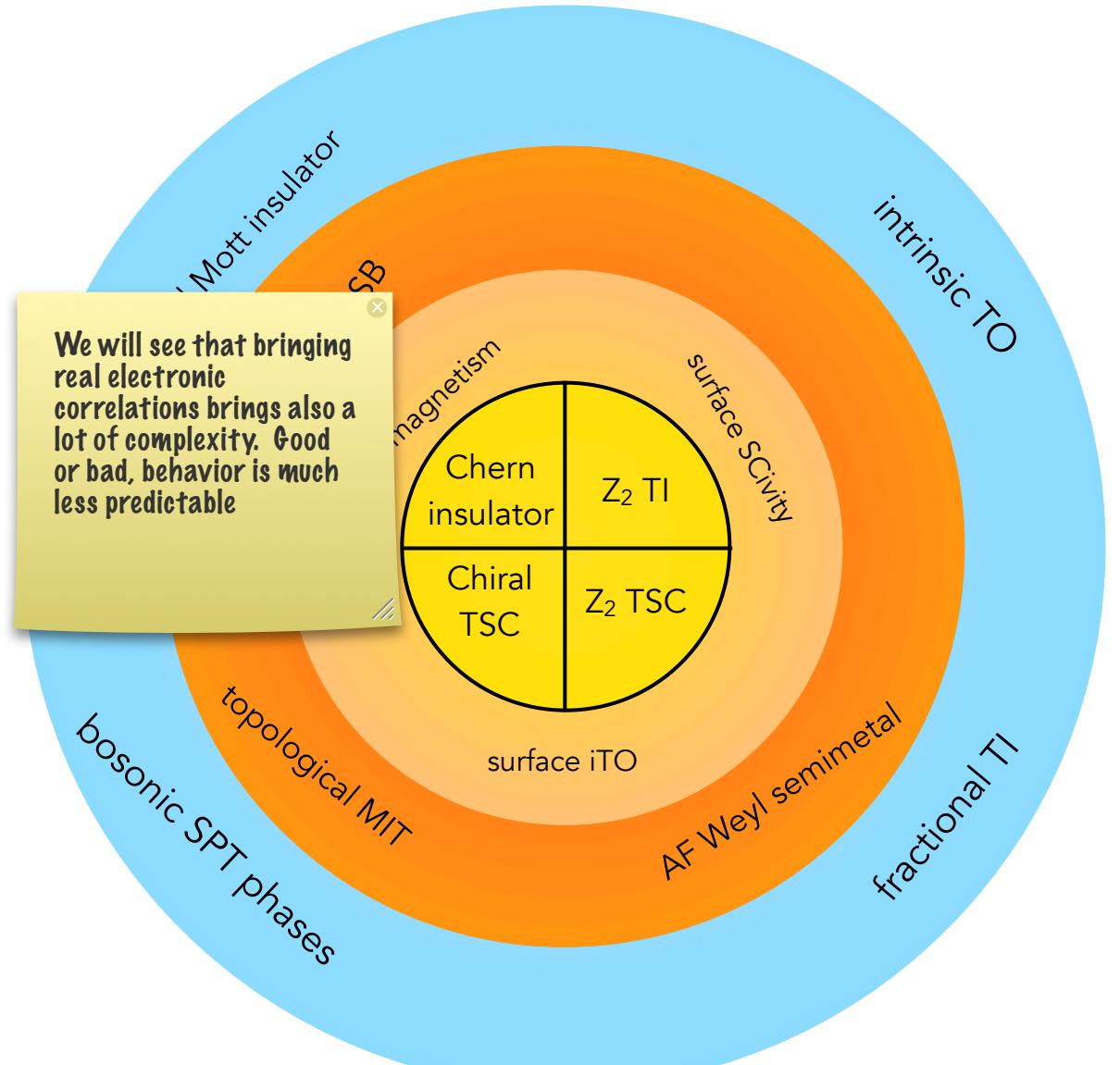
Why correlations?

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



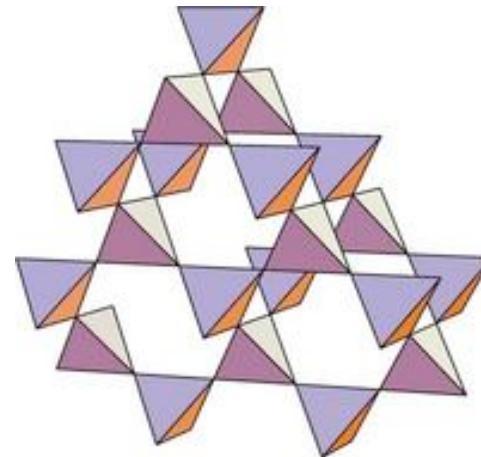
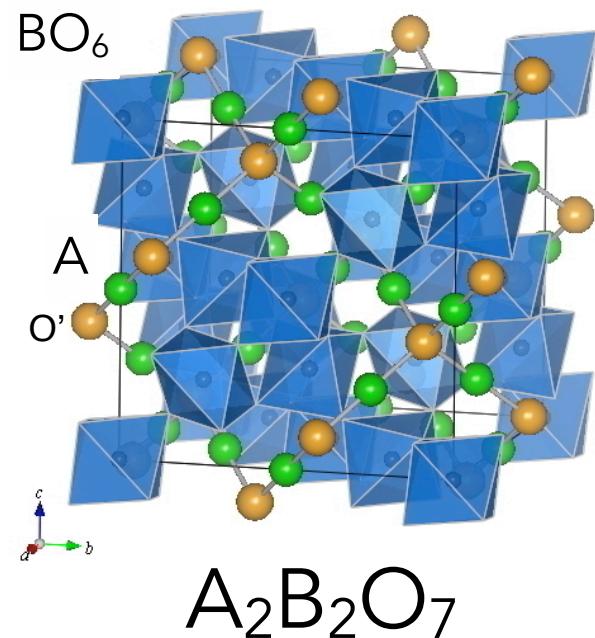
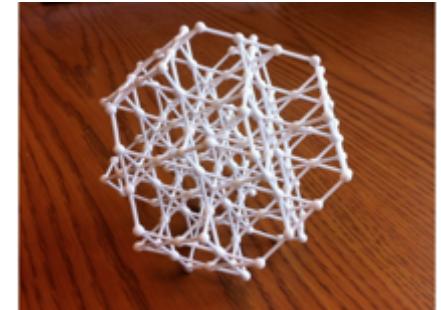
Why correlations?

- Distinct surface states
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This talk: how does this play out in a real example?

Pyrochlores



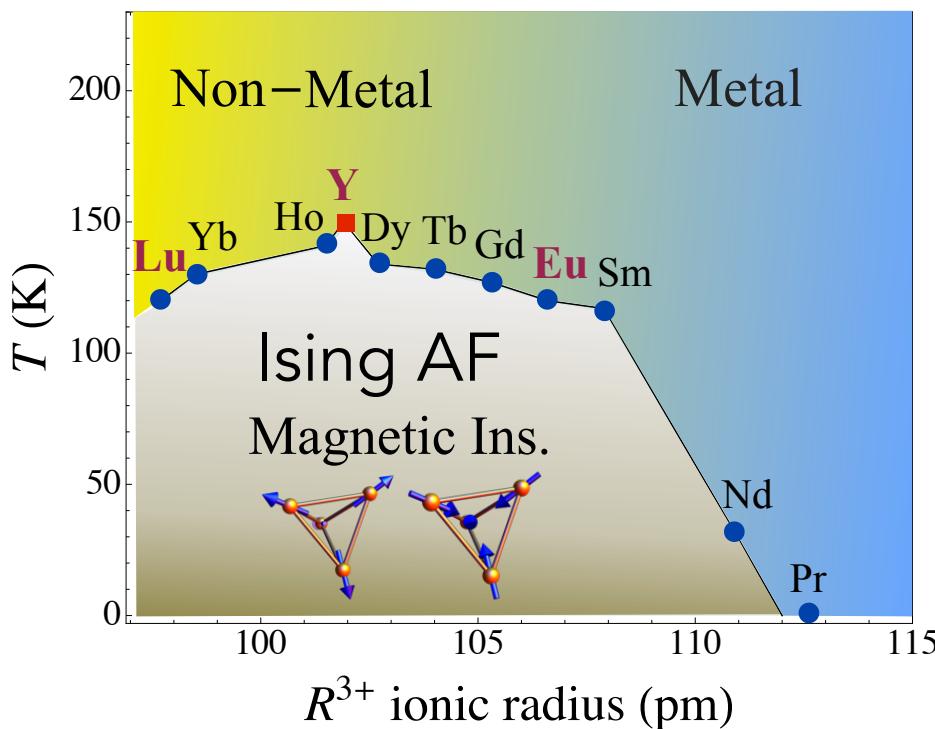
A (B) sublattice

A=Y,Ln ←
B = Ir

f-electron moments, except
when A = Y, Eu

Pyrochlore iridates

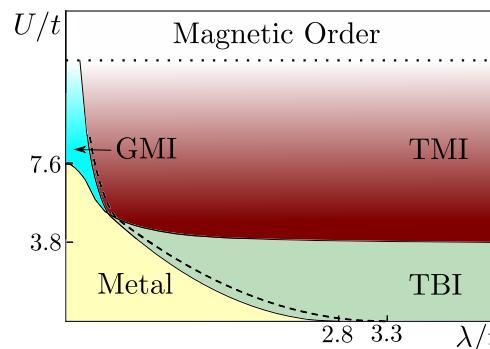
- Continuous magnetic/metal-insulator transitions (compatible with Ising)



Yanagashima+Maeno, JPSJ 2001

K. Matsuhira et al, JPSJ 2011

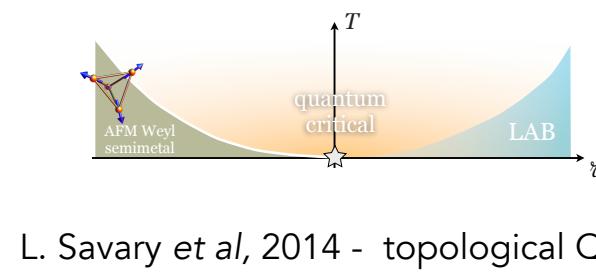
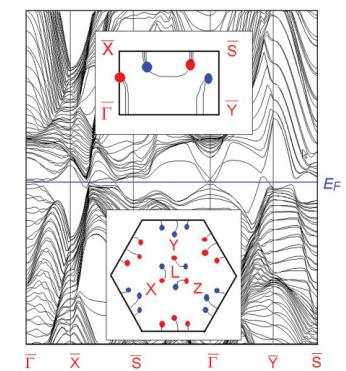
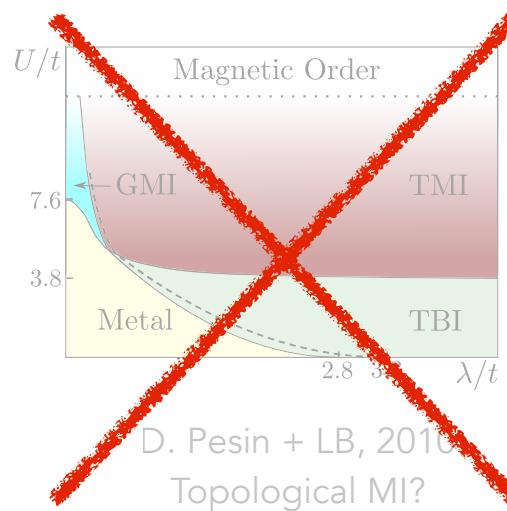
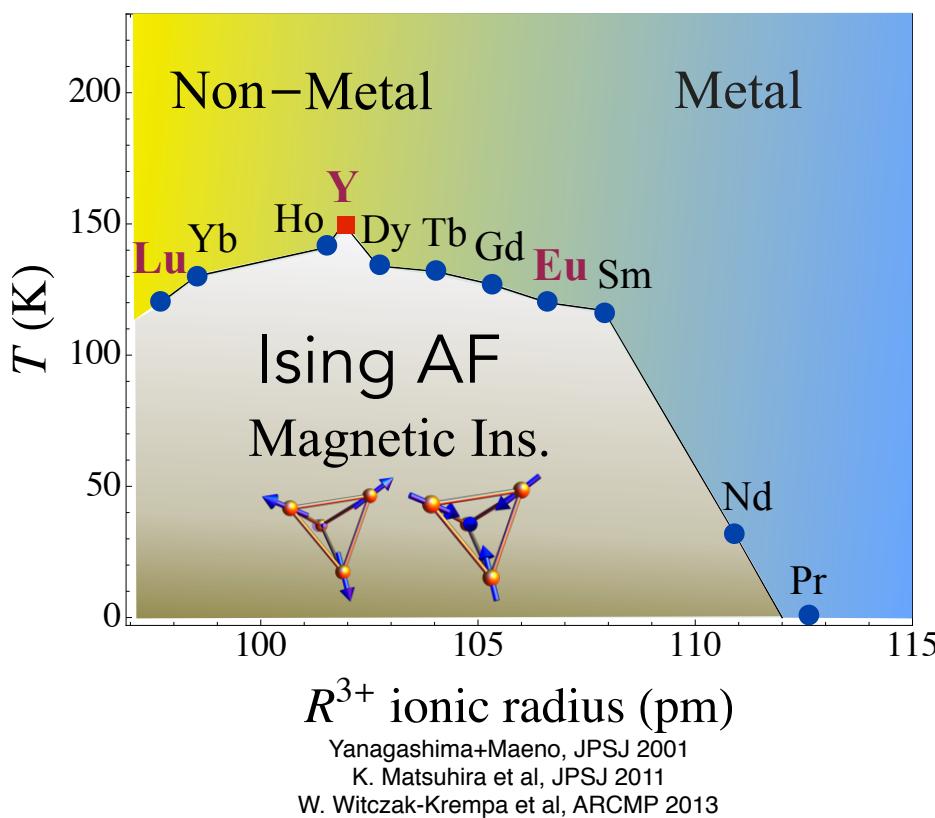
W. Witczak-Krempa et al, ARCMP 2013



D. Pesin + LB, 2010
Topological MI?

Pyrochlore iridates

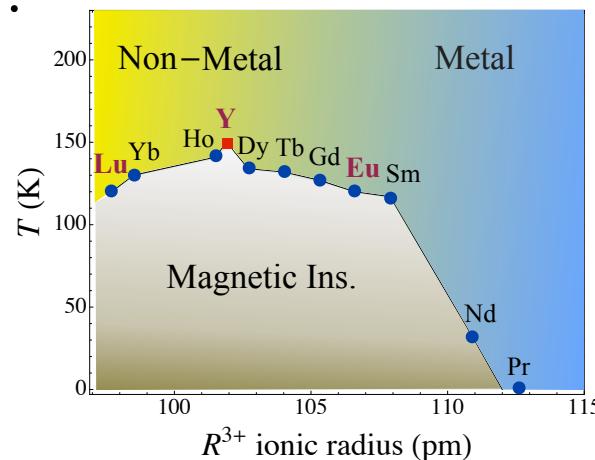
- Continuous magnetic/metal-insulator transitions (compatible with Ising)



Ingredients of a theory

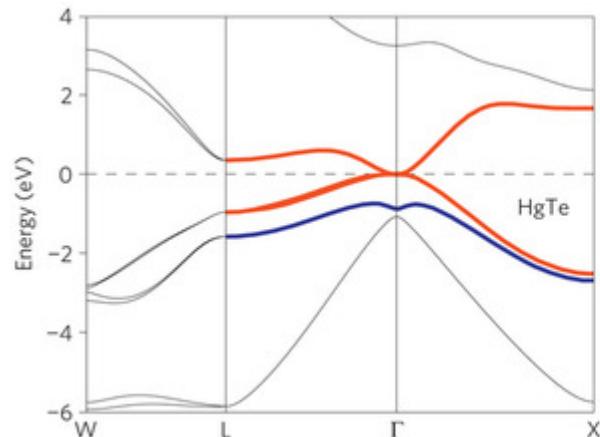
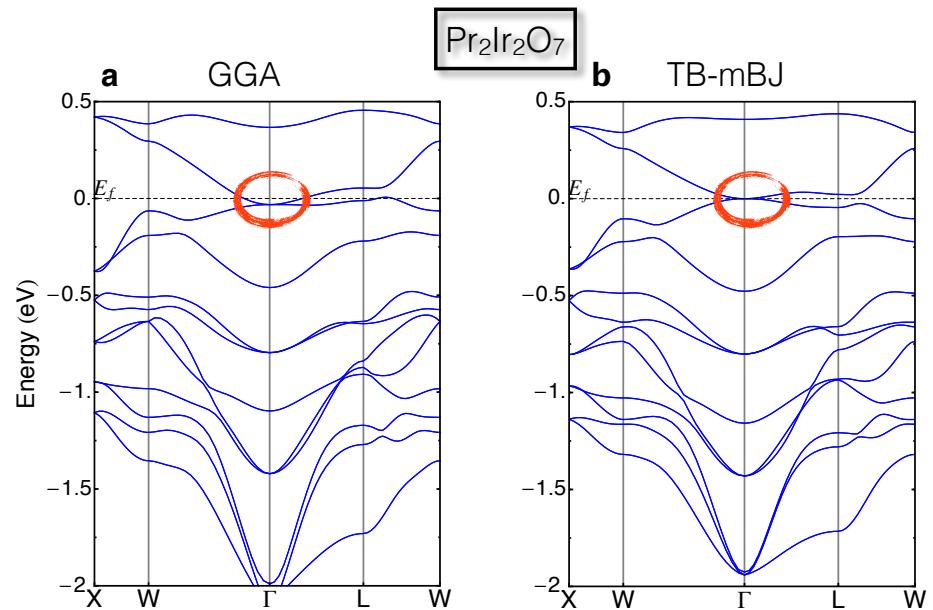
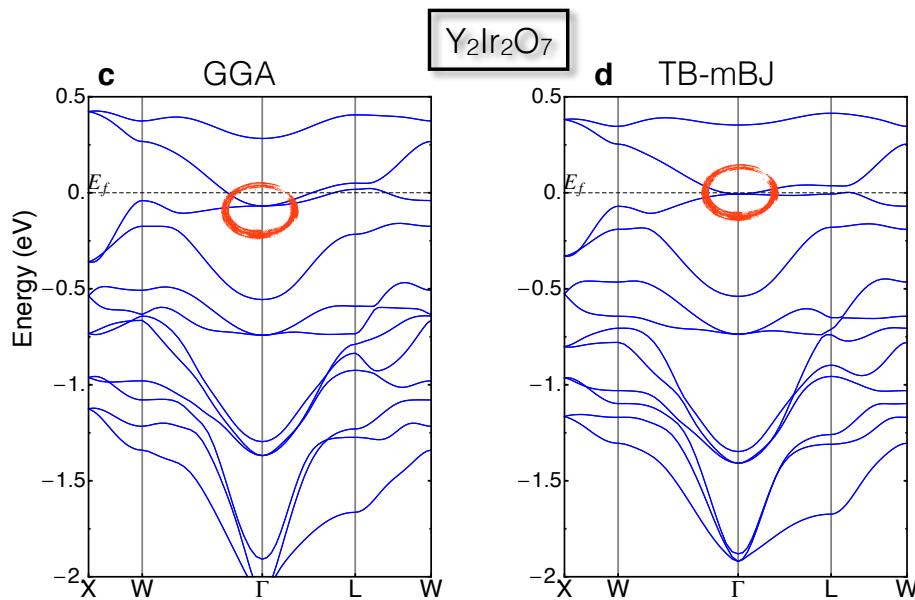
- Unusual electronic structure
- Ir e-e Hubbard interactions
- Rare earth moments?

probably not?





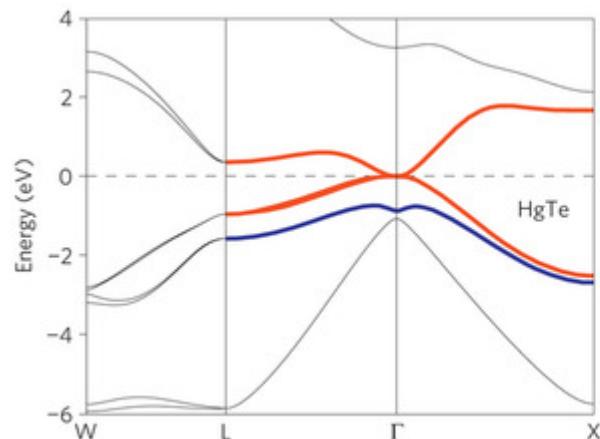
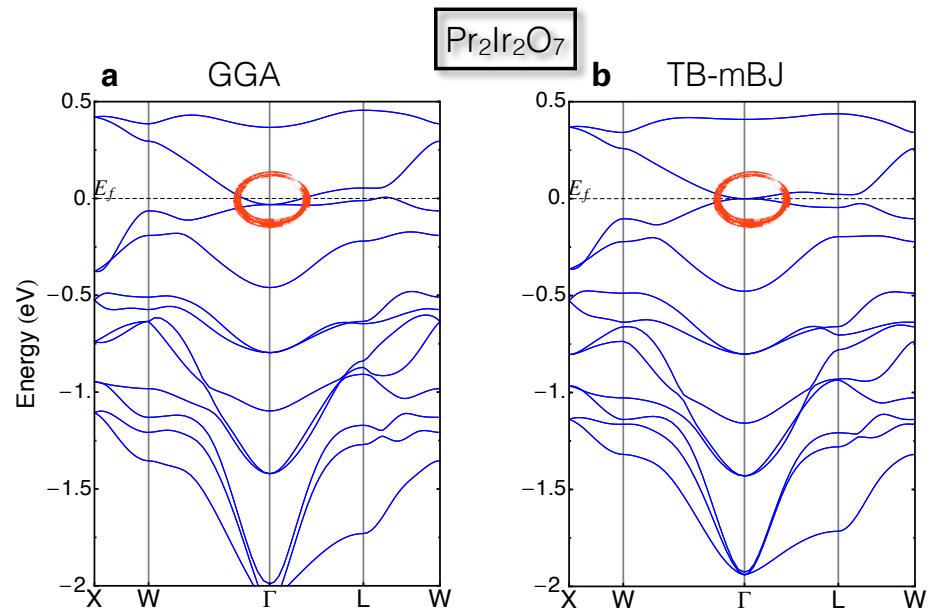
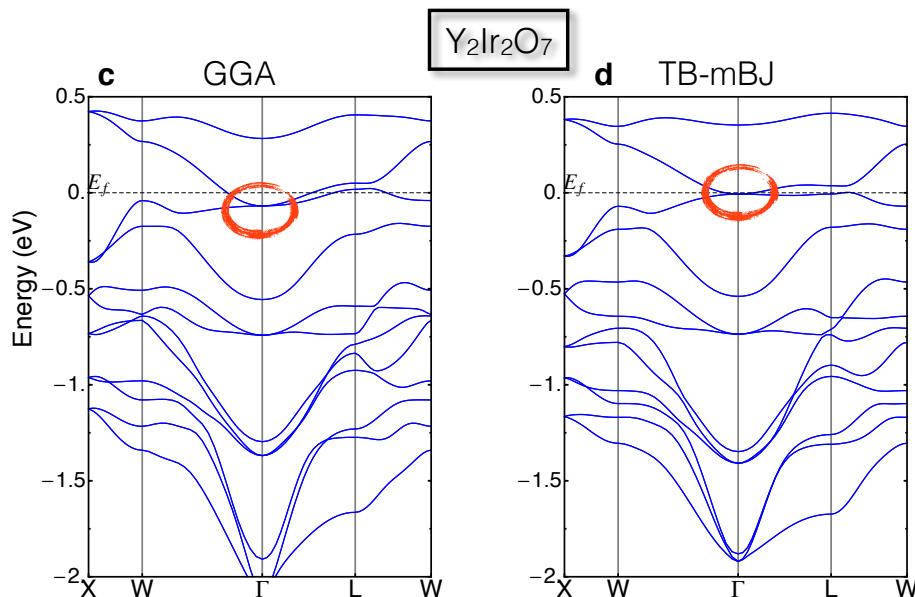
Paramagnetic electronic structure



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

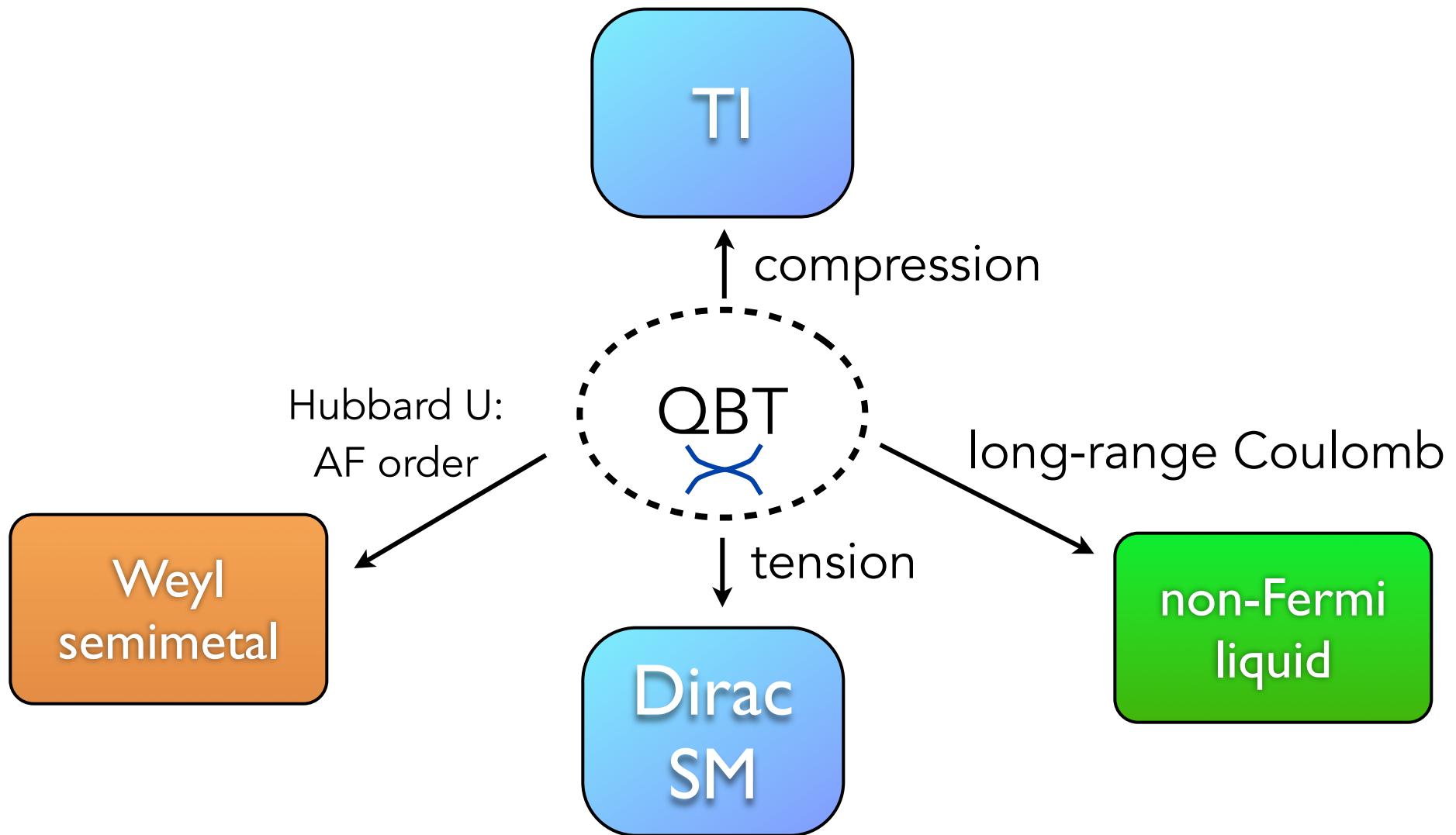


Paramagnetic electronic structure



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

Proximate phases





ARPES

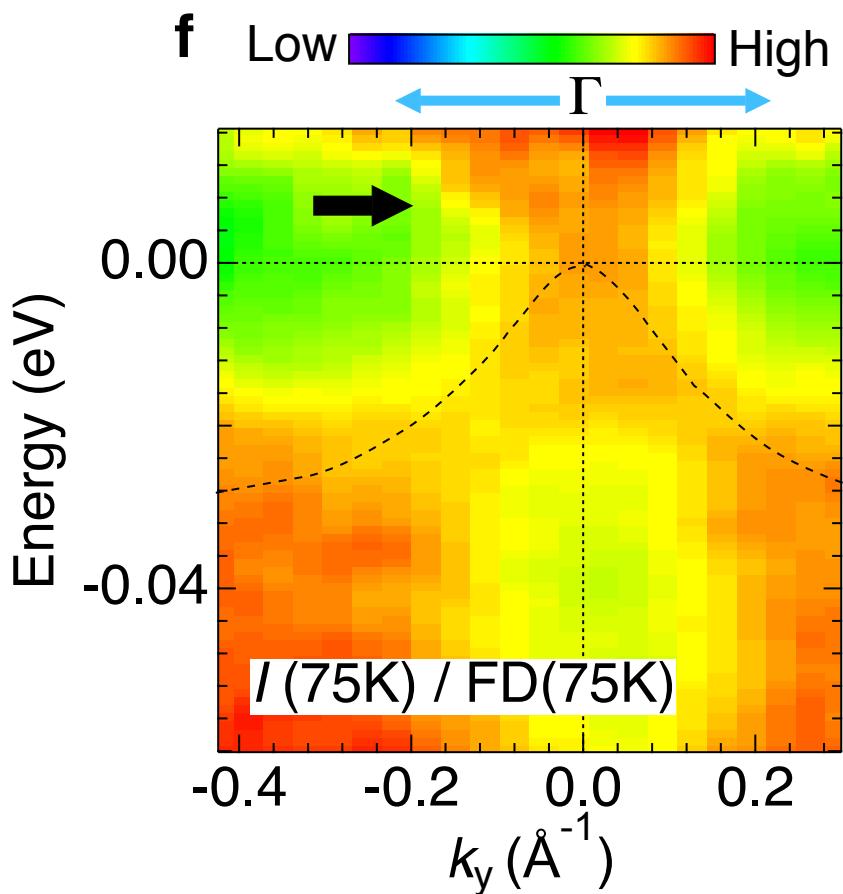
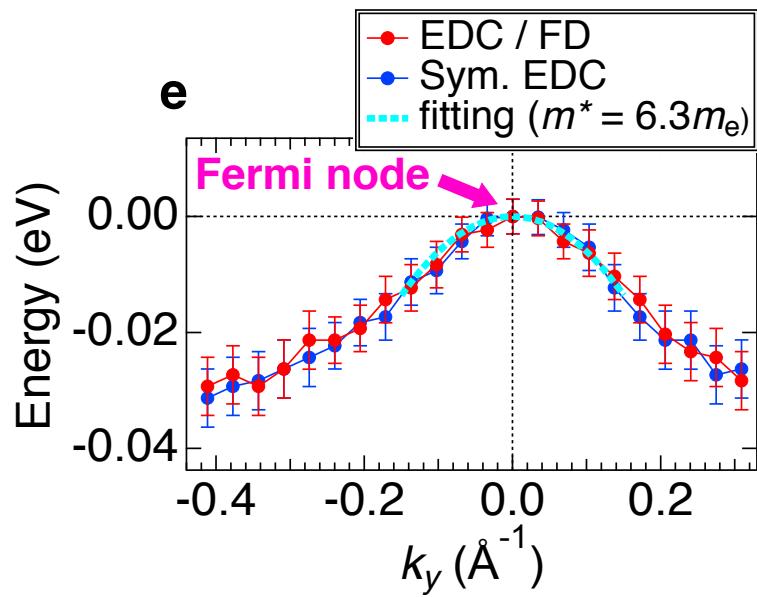
T. Kondo *et al*, Nat. Comm., 2015

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



T. Kondo

S. Shin





ARPES

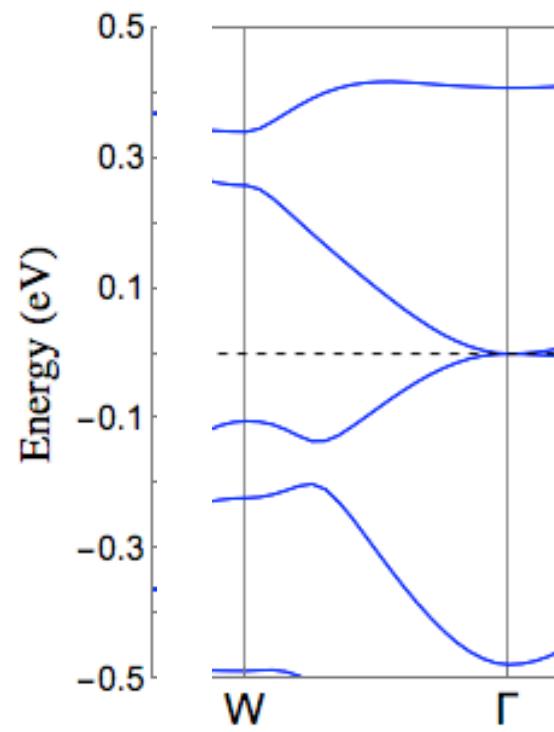
T. Kondo *et al*, Nat. Comm., 2015

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

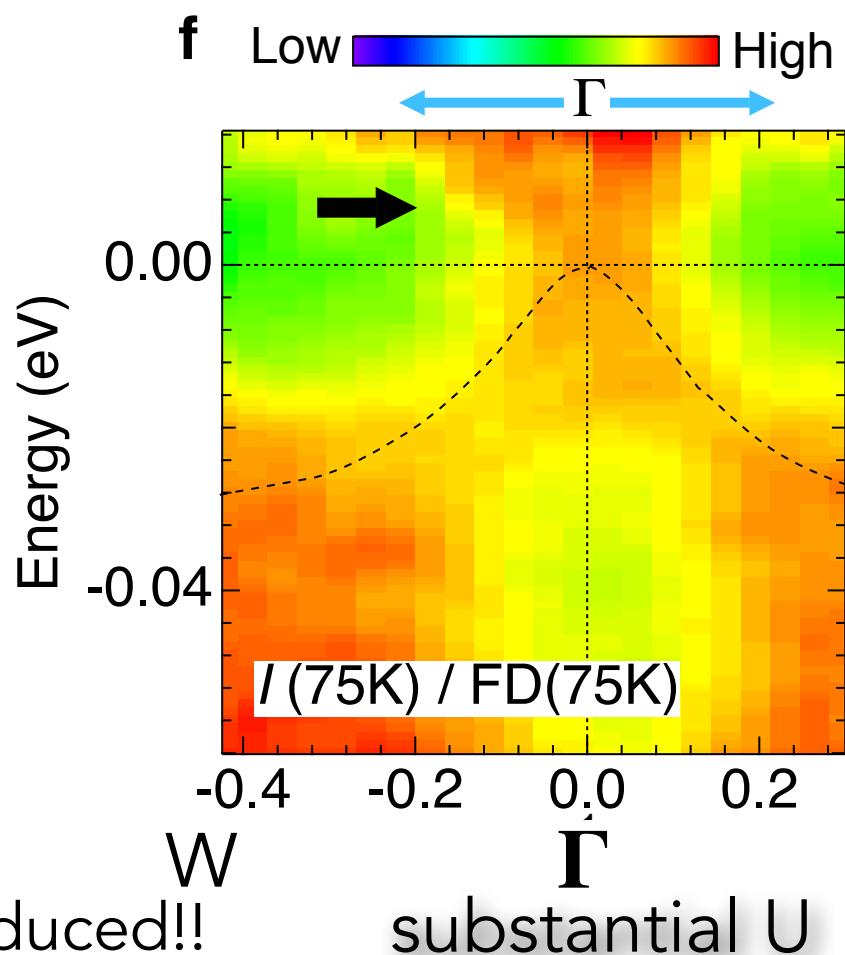


T. Kondo

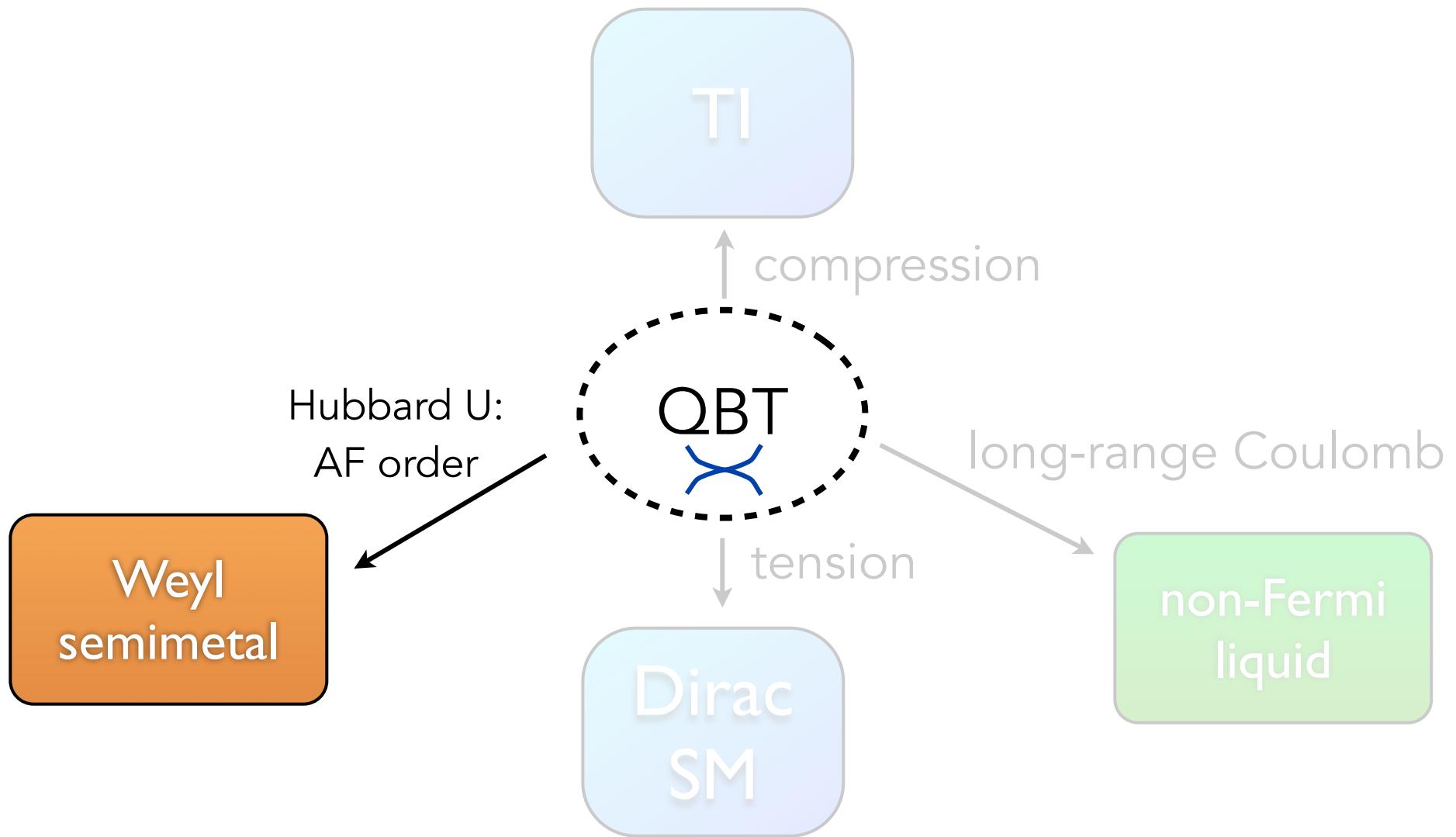
S. Shin



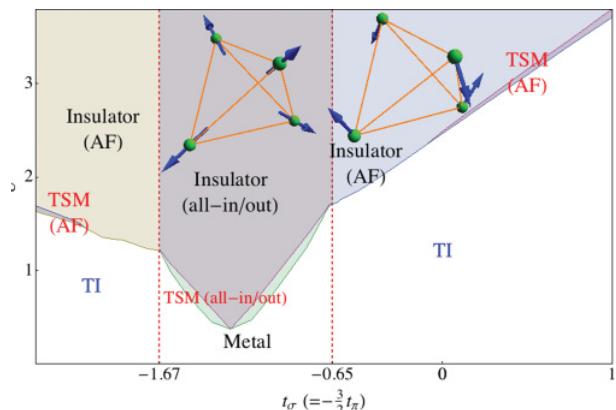
overall bandwidth \sim 3-5 times reduced!!



Proximate phases

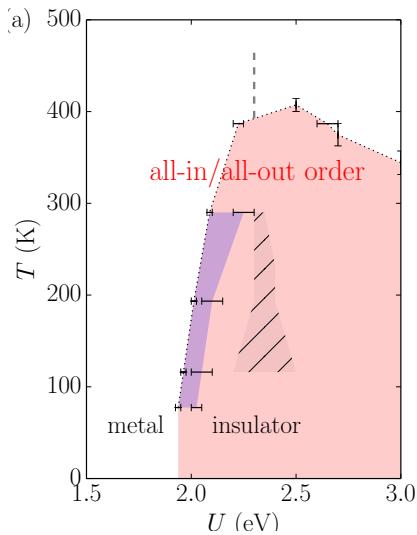


Ordering: theory



W. Witzak-Krempa + YB Kim, 2012

Hartree-Fock

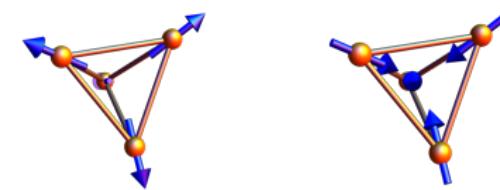


H. Shinaoka *et al*, 2015

DMFT

Jay-Z model

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

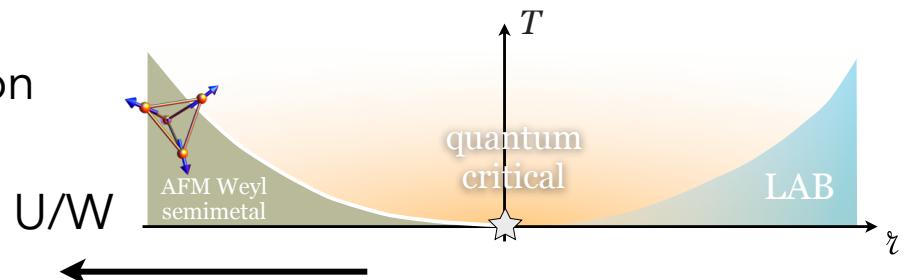


$J_z < 0$: all-in/all-out order
superexchange

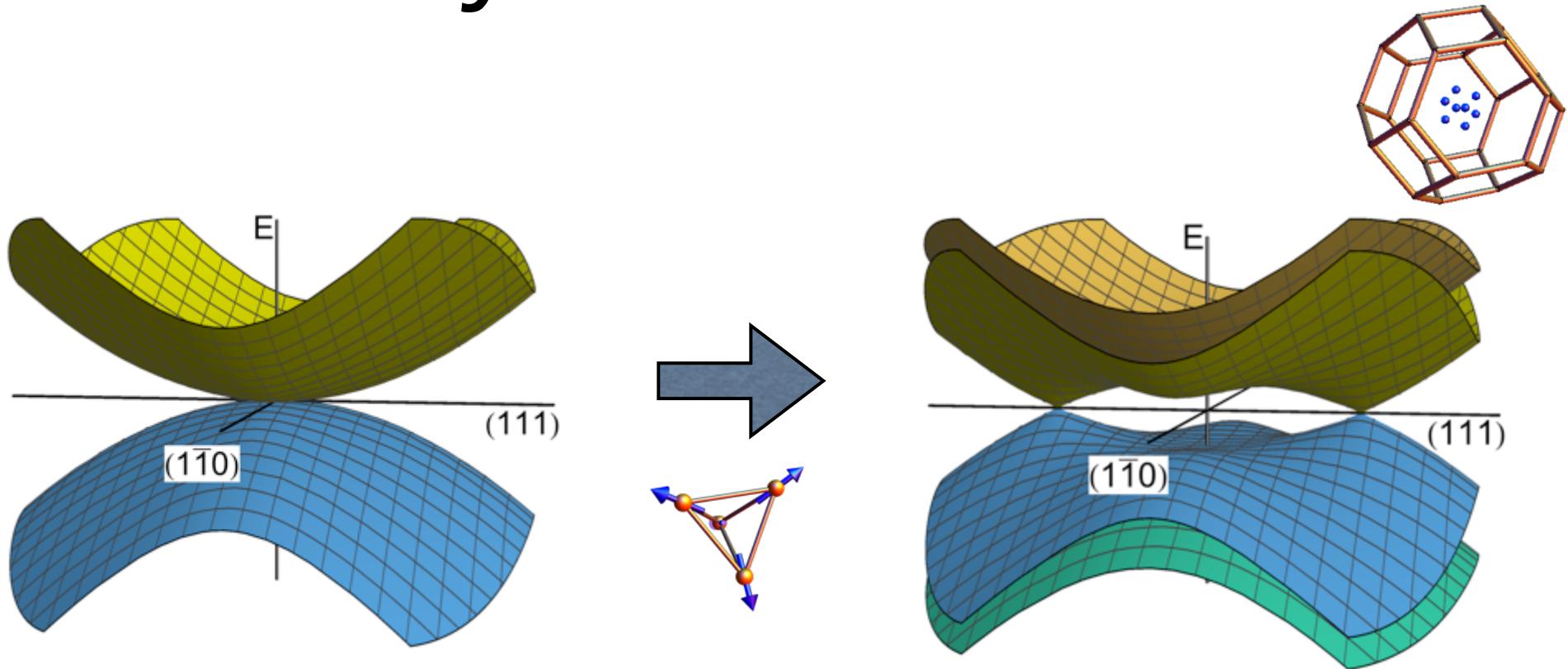
- General agreement: transition to AlAO Ising AF order

- ♦ Quantum critical theory of this transition

L. Savary *et al*, 2014 - topological QCP



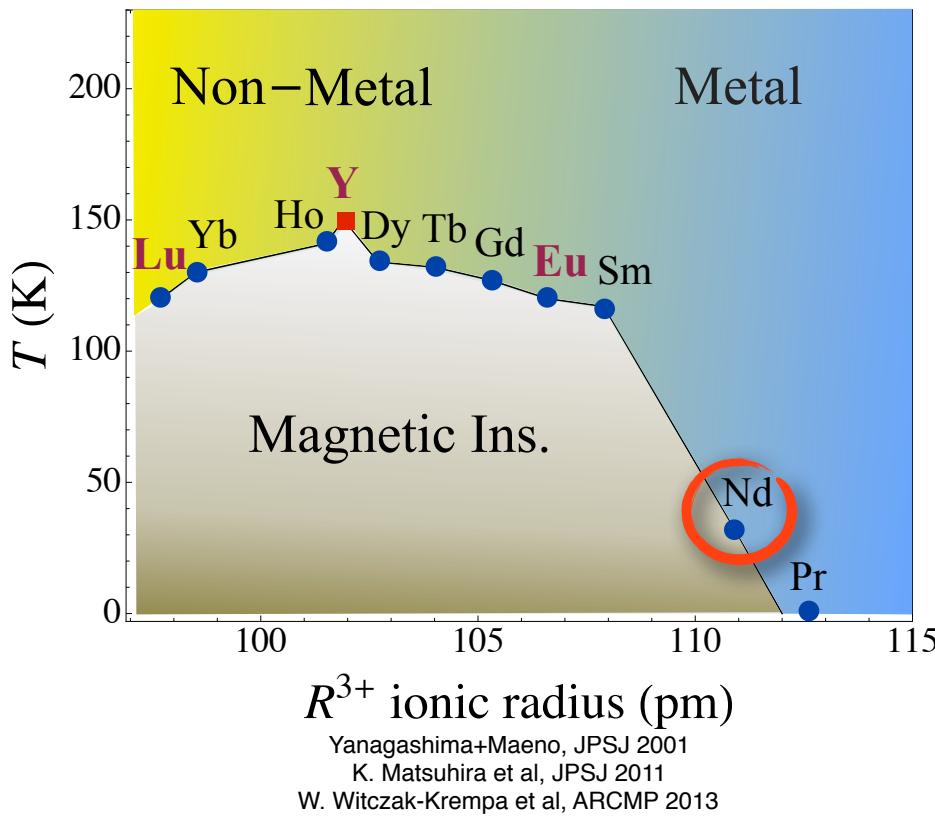
Weyl semimetal



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

Weyl?

- Weyl semimetal?

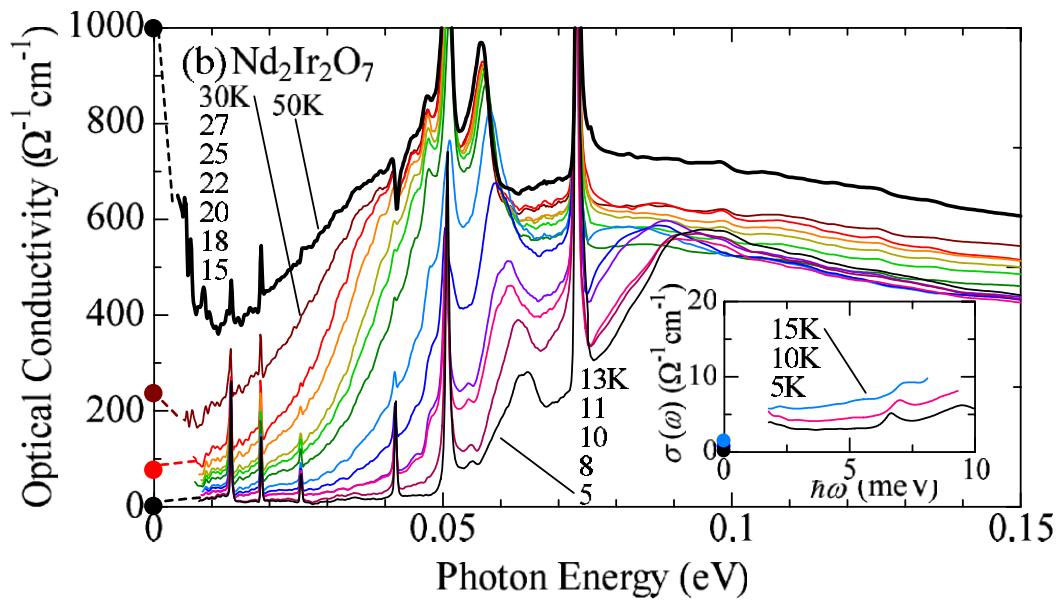


Best candidate
should be
 $\text{Nd}_2\text{Ir}_2\text{O}_7$



Weyl not?

K. Ueda *et al*, 2012



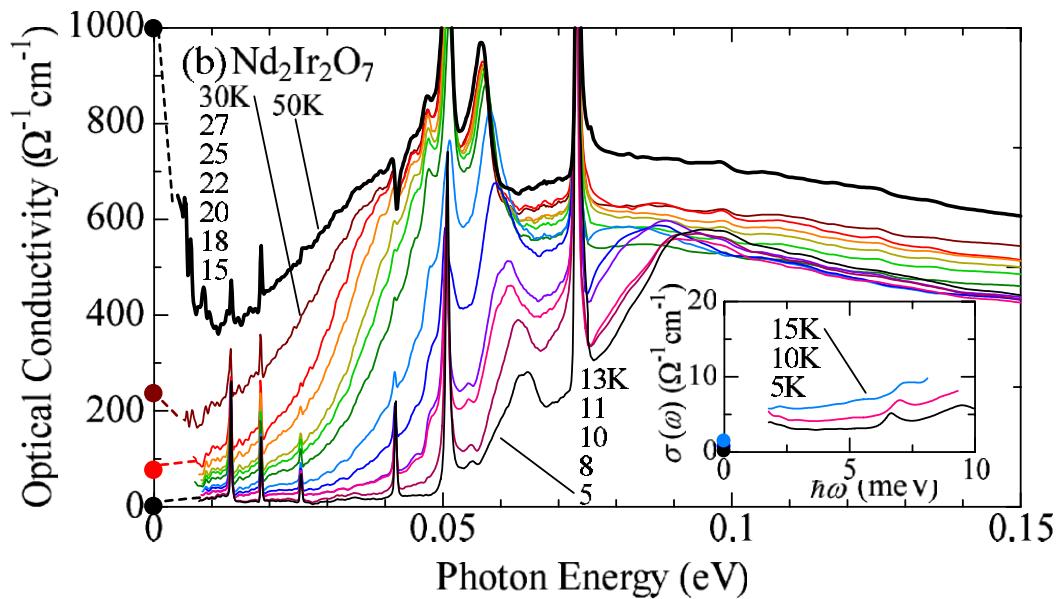
charge gap ~
45meV



n.b. Gap ~ $18T_c$

Weyl not?

K. Ueda *et al*, 2012

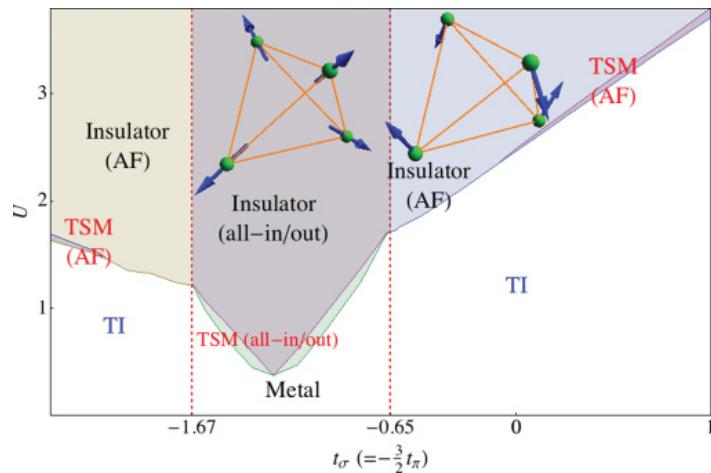


charge gap ~
45meV

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

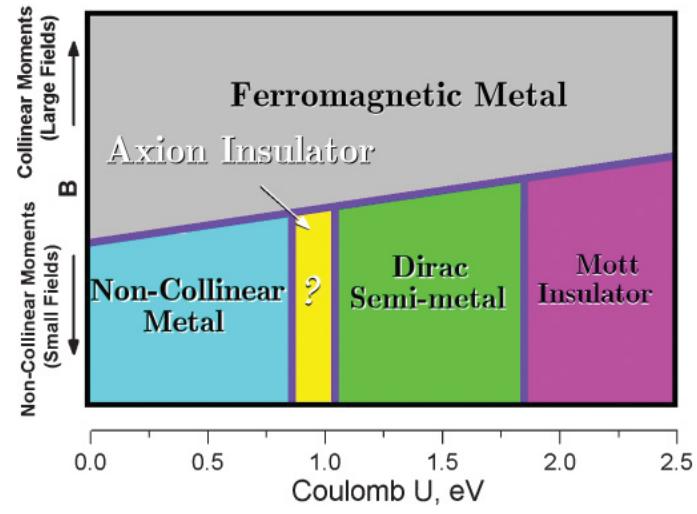
- ◆ Not weakly ordered?
- ◆ No quasiparticles?
- ◆ Weyl with very small DOS?

Weak or not?



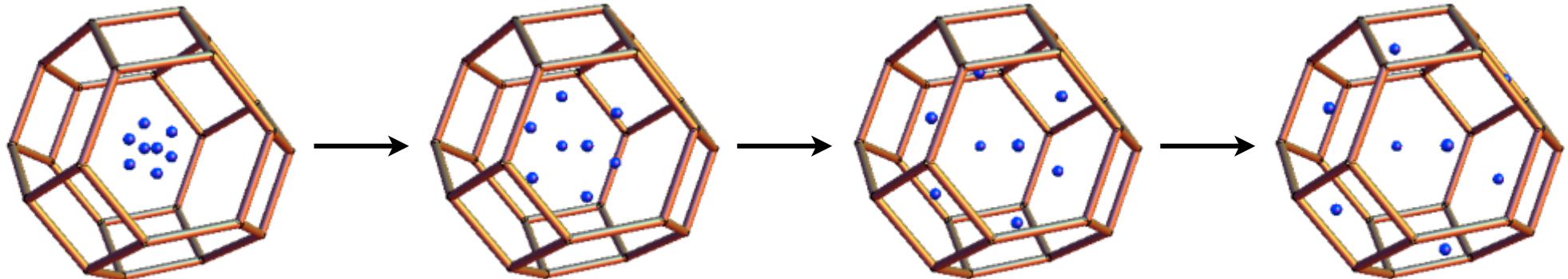
W. Witzak-Krempa + YB Kim, 2012

VS



X. Wan et al, 2011

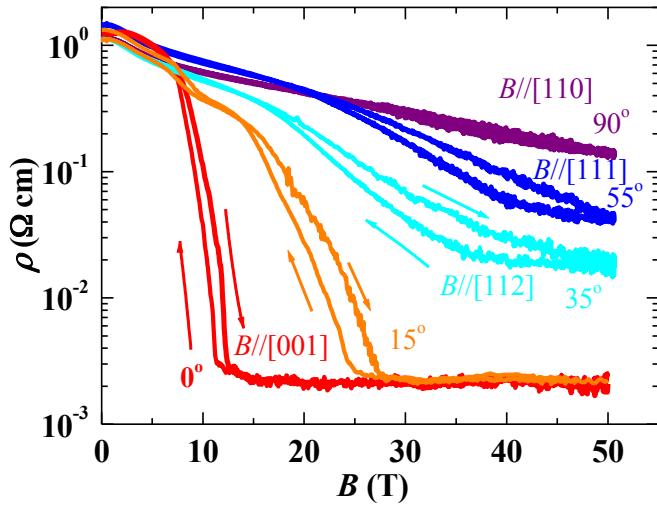
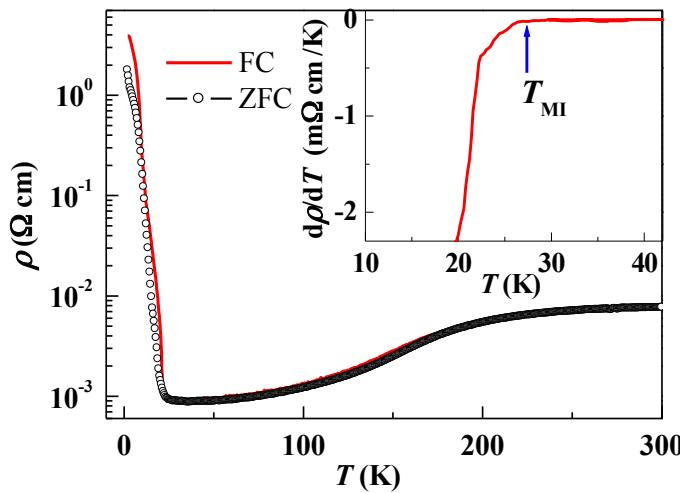
Weyl points move to zone boundary and annihilate with increasing order?



Could this have happened already for Nd?



Transport



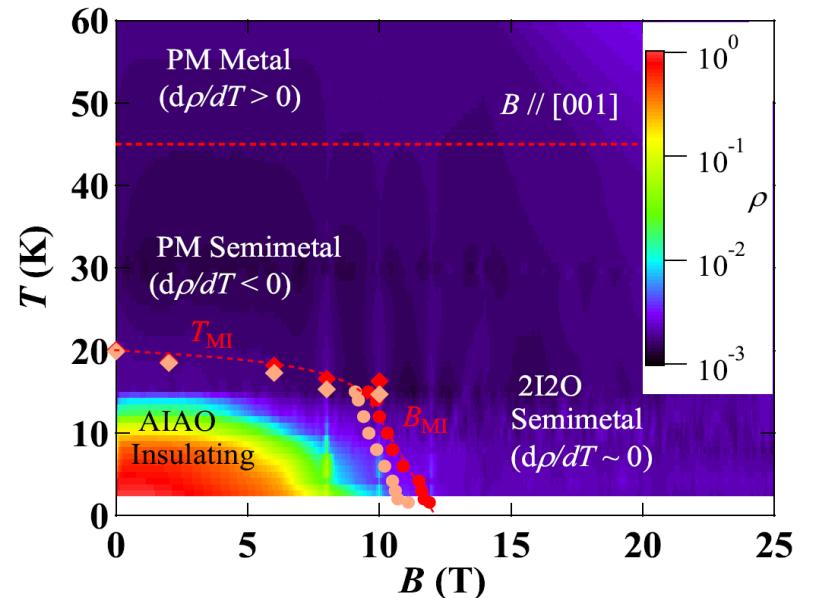
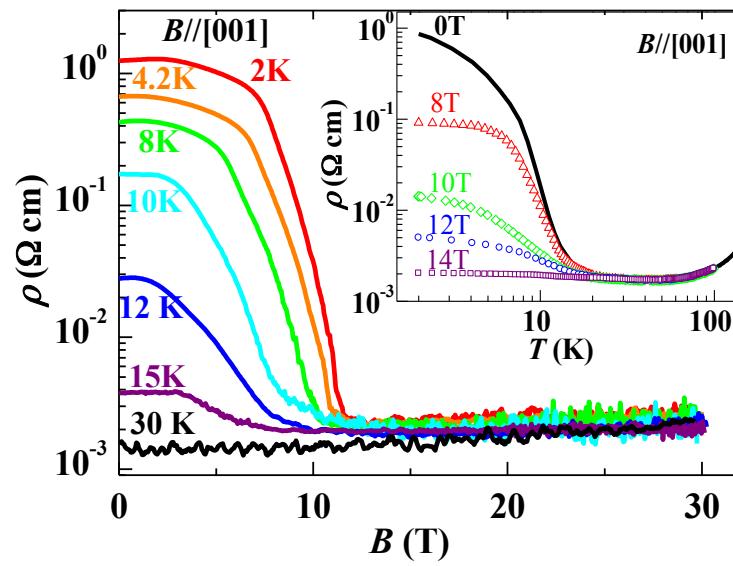
To explore this in more detail, let's look at transport

- Seems to be
- thermal tra

with hard gap
continuous

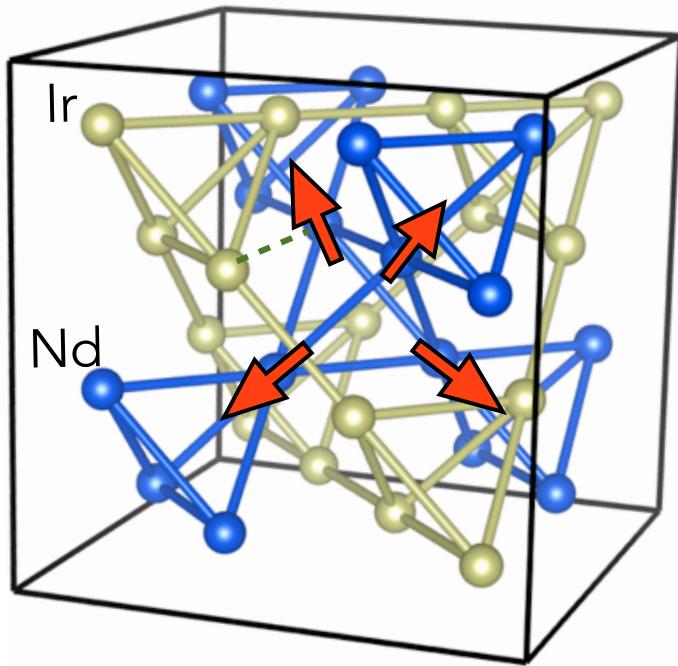
- However, abrupt first order transition appears at low T in a field
- Insulator-metal transition only occurs for fields along (100)

Metal-Insulator Transition



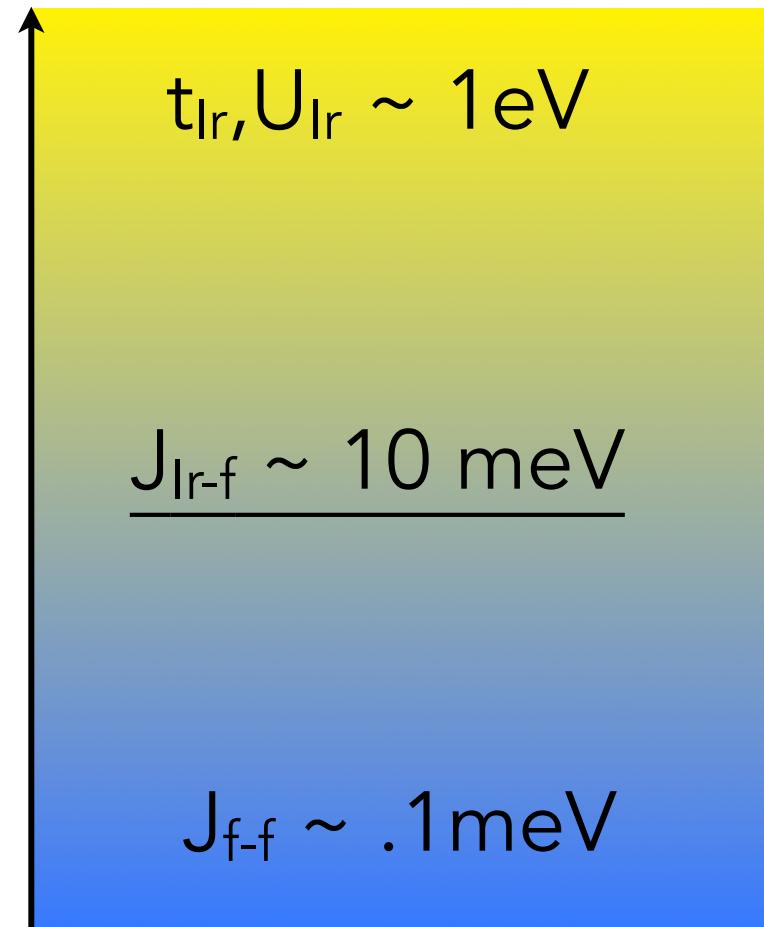
- First order transition at low temperature: mechanism of MIT is vanishing of condensation energy, not gap closing.
- Anisotropy: clear indication that Nd plays a direct role in the MIT - probably this is a unique feature for R=Nd

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 AlAO Ising order

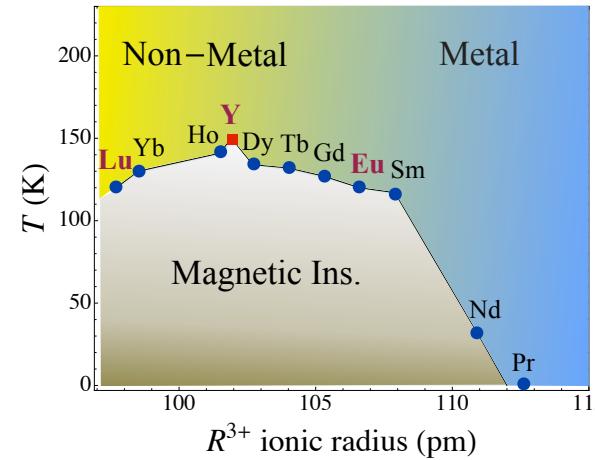
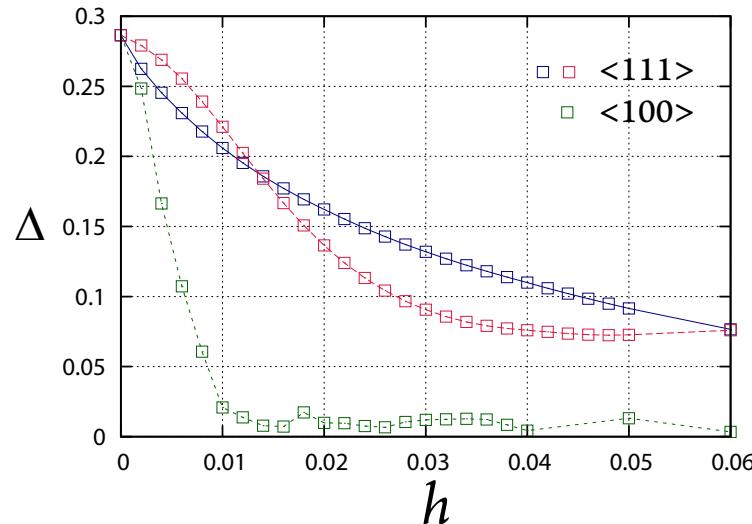




Anisotropy

- Nd sensitivity to direction is transferred to Ir

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

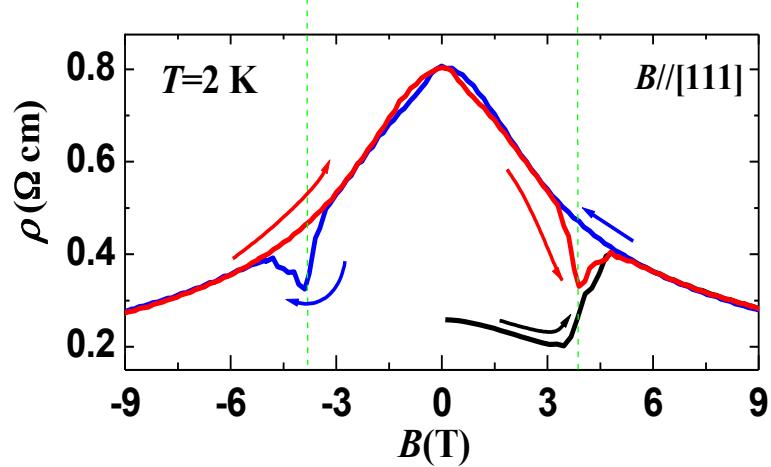


Hartree-Fock on Hubbard
+Kondo lattice model

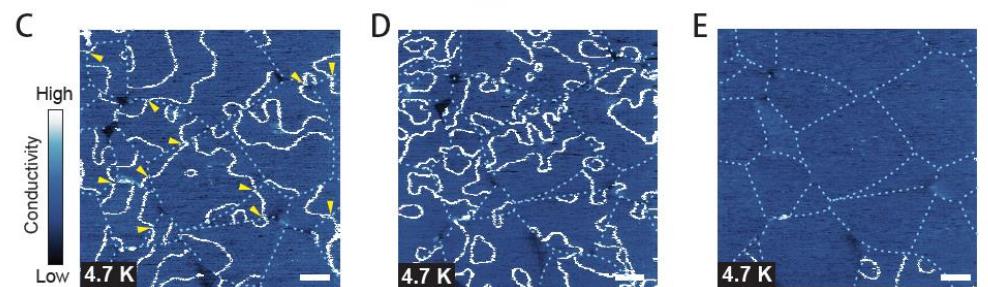
- h_{eff} is significant for Nd case
- can explain the anisotropy

Domains

- Large magnetic moment of Nd allows manipulation of domains



Z. Tian *et al*, 2015
c.f. K. Ueda *et al* (2014)



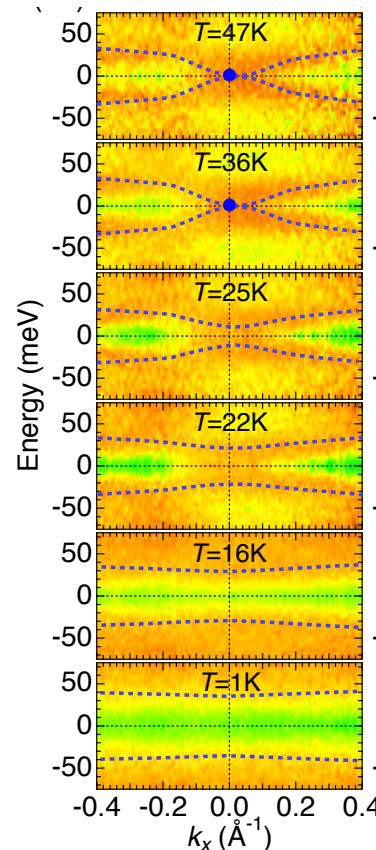
local conductivity
E. Y. Ma *et al*, 2015

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

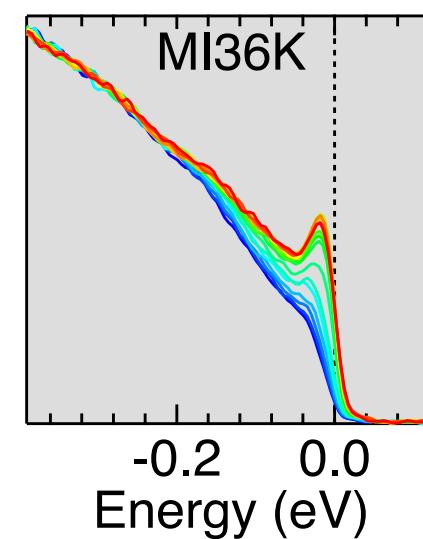
$T = T_c$: no precursor - Slater

$T < T_c$: 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

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

