Interplay of magnetic and electronic states in the pyrochlore iridates

Leon Balents, KITP, UCSB

- or -

correlations versus topology

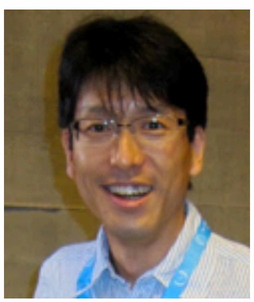
APS meeting, Baltimore, March 2016

People

Ru Chen

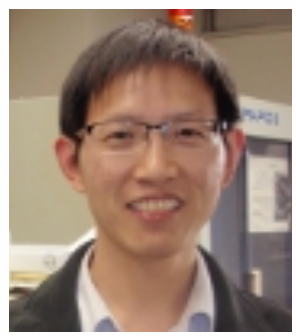
Lucile Savary

Eun-Gook Moon

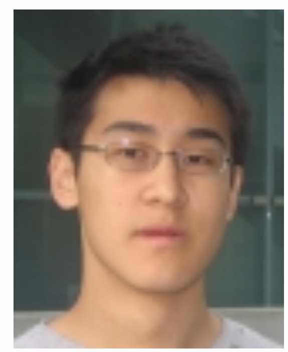


S. Nakatsuji

T. Kondo



Z. Tian



T. Hsieh

H. Ishizuka

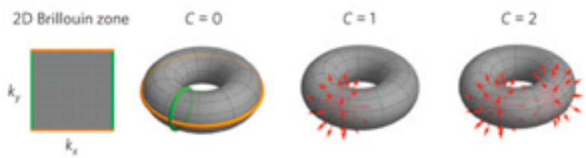
General questions about pyrochlore iridates

- How correlated are these materials?
  - Lots of theory uses mean-field. Does this work? If so why?
- What is the role of interactions beyond mean-field? Slater versus Mott.
- What is the nature of the MIT?
- Any real signatures of topology?

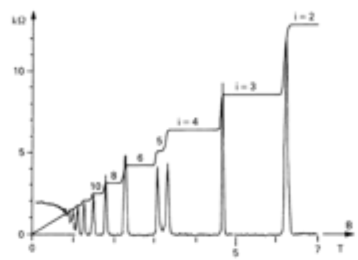
TIs

Broken TRS	with TRS
integer Chern number	Z_2 invariant
= Hall conductance	= M-E polarizability
chiral edge states	helical edge/ surface states

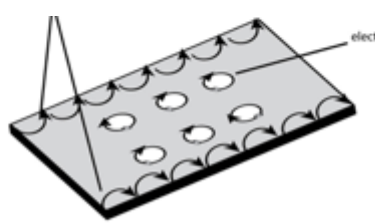
integer Chern number



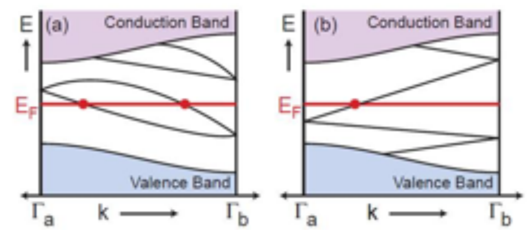
= Hall conductance



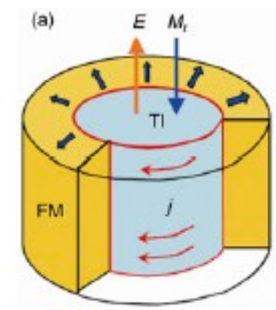
chiral edge states



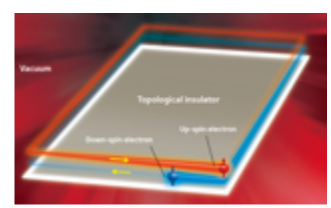
Z_2 invariant



= M-E polarizability



helical edge/ surface states

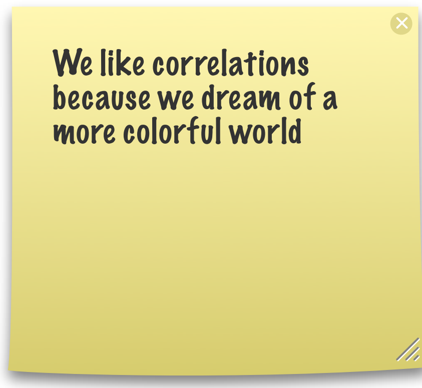


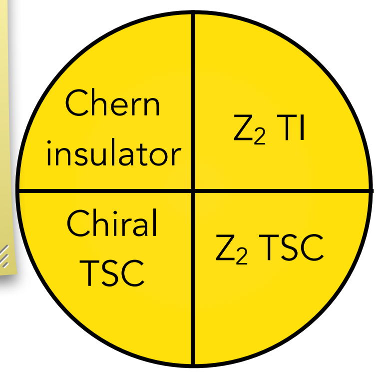
Topological everything

- 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

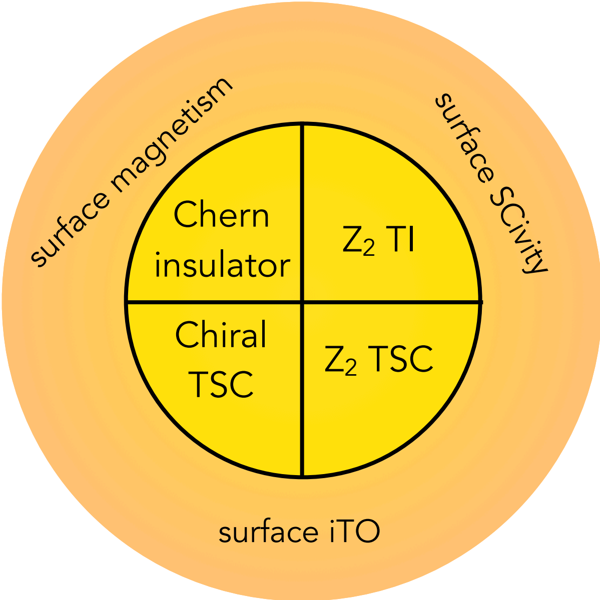




+ Weyl, Dirac...

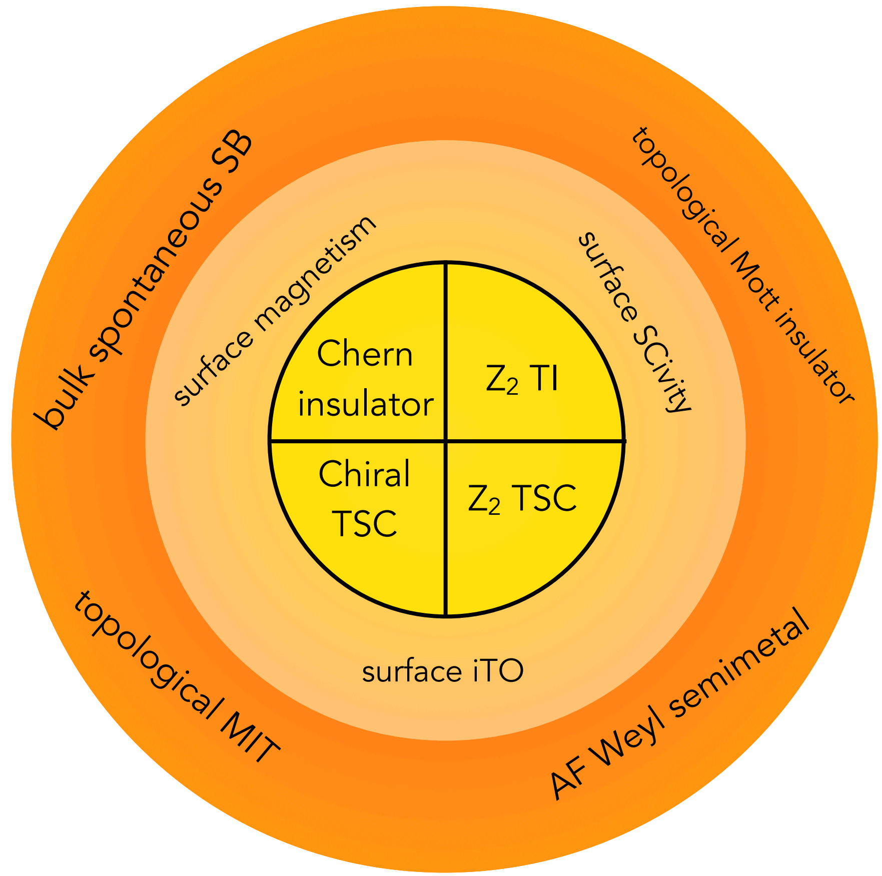
Why correlations?

- Distinct surface states



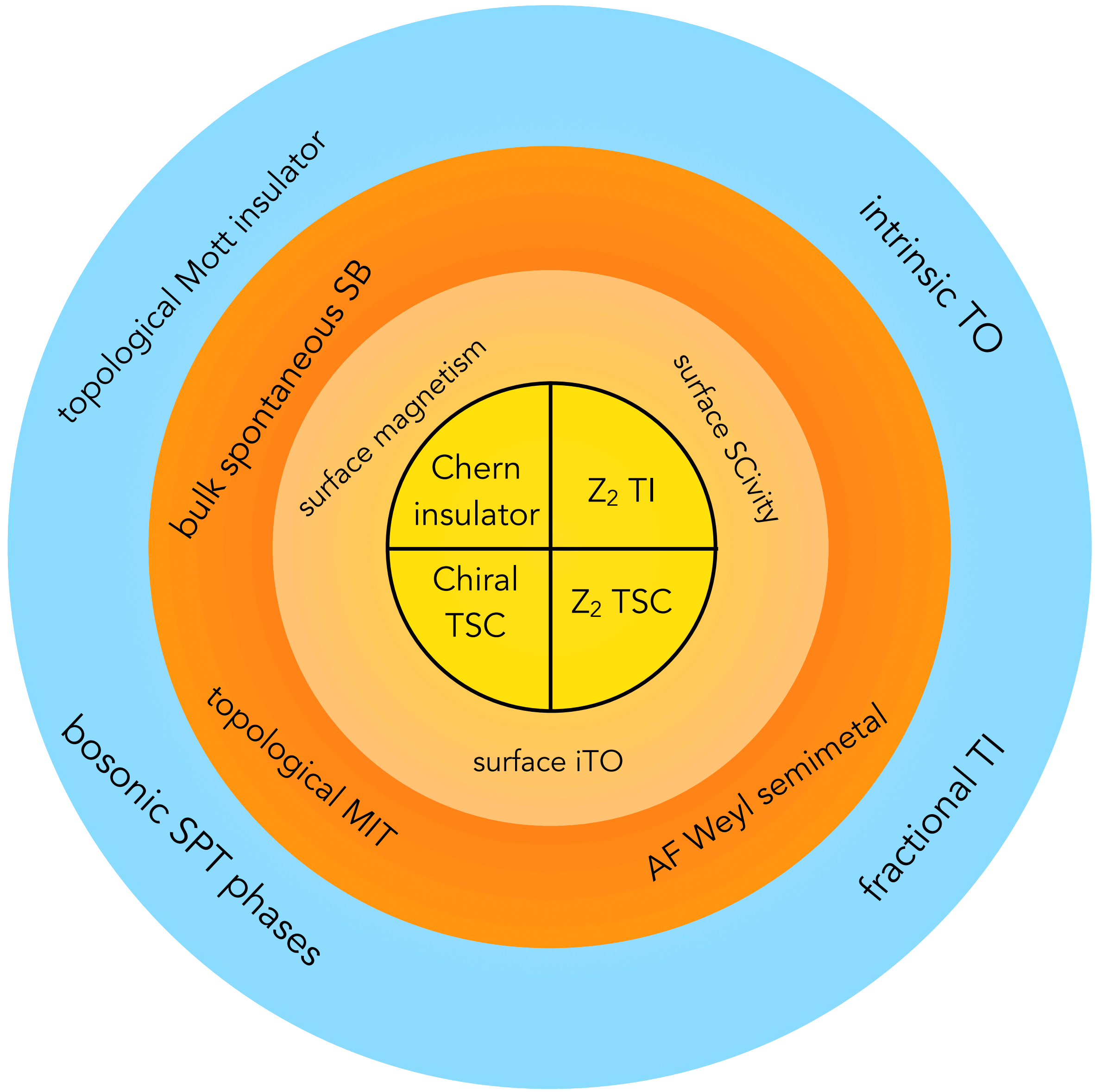
Why correlations?

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



Why correlations?

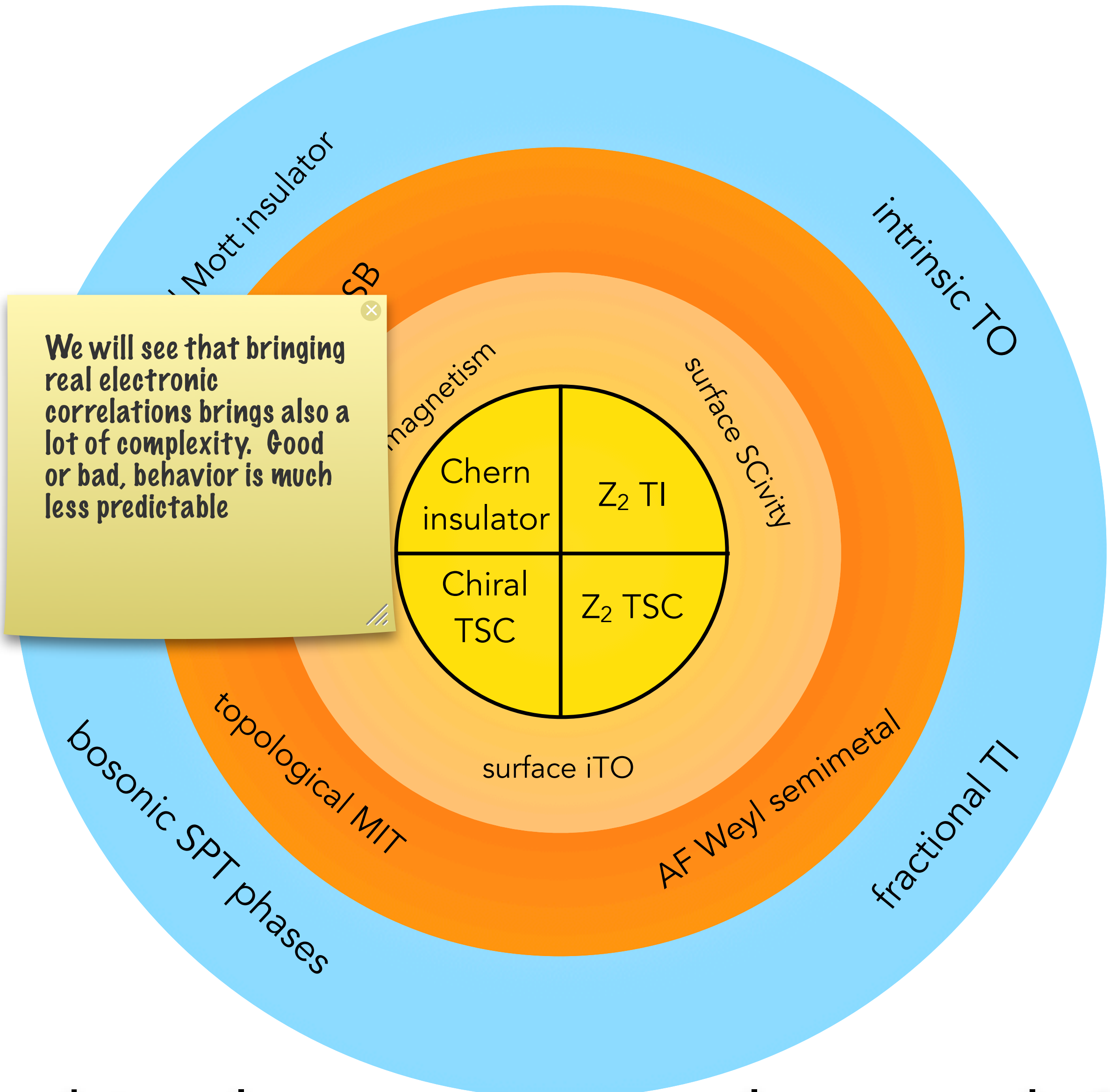
- Distinct surface states
- Control of bulk topology by spontaneous symmetry breaking
- Entirely new phases requiring strong interactions



Why correlations?

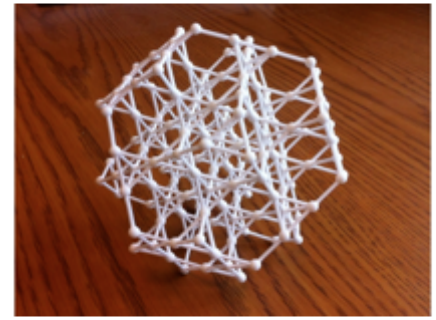
- Distinct surface states
- Control of bulk topology by spontaneous symmetry breaking
- Entirely new phases requiring strong interactions

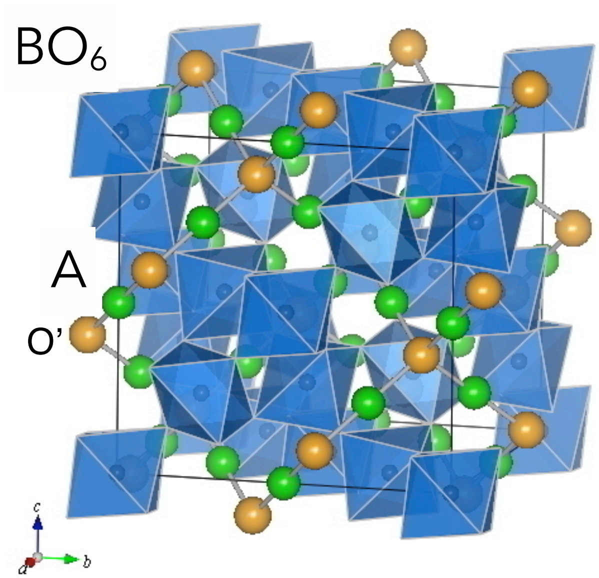
We will see that bringing real electronic correlations brings also a lot of complexity. Good or bad, behavior is much less predictable



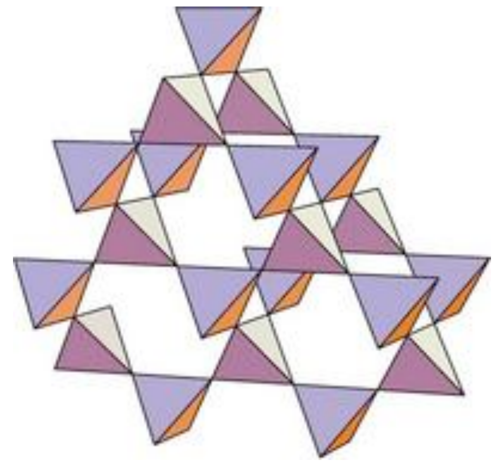
This talk: how does this play out in a real example?

Pyrochlores





$A_2B_2O_7$



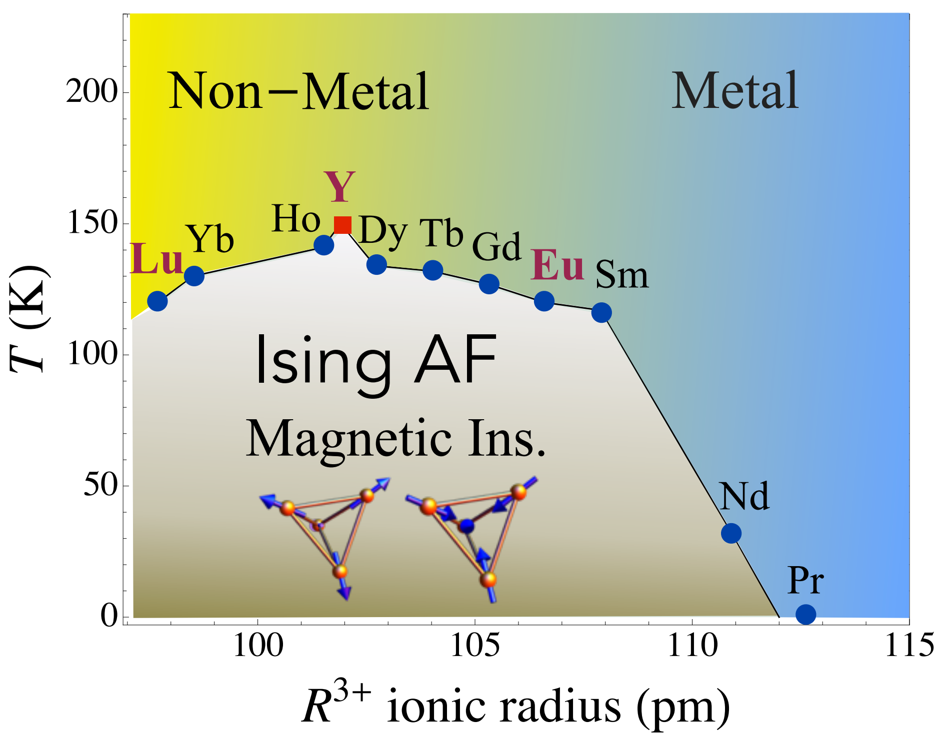
A (B) sublattice

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

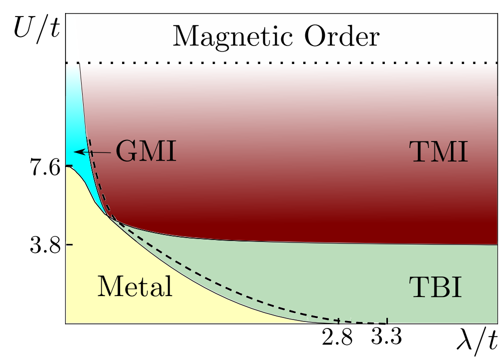
B = Ir

Pyrochlore iridates

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



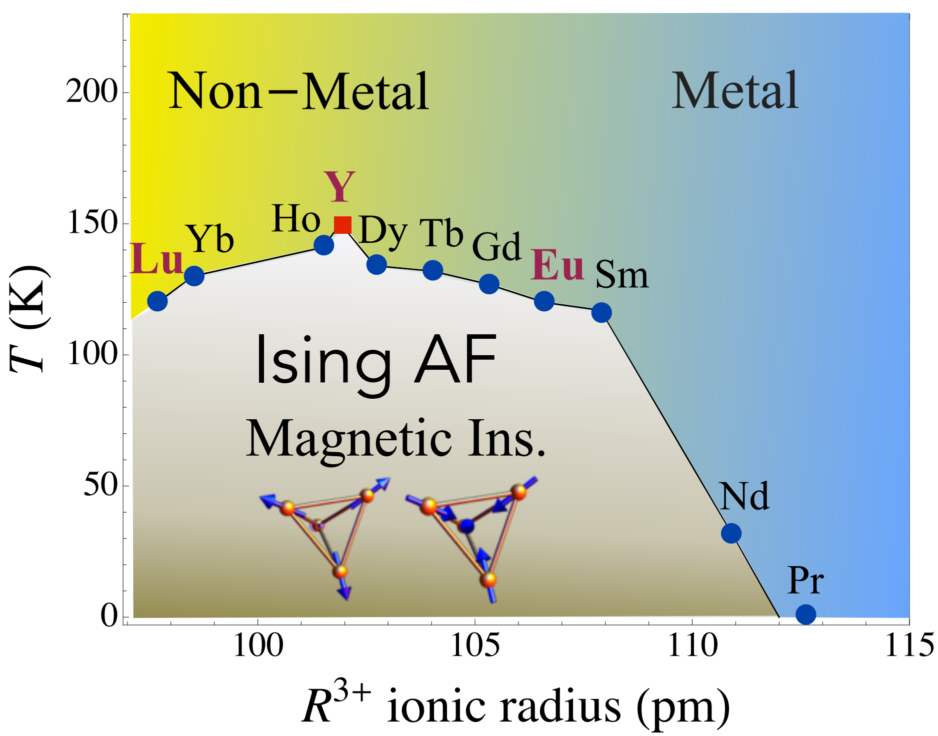
Yanagashima+Maeno, JPSJ 2001
K. Matsuhira et al, JPSJ 2011
W. Witczak-Krempa et al, ARCMP 2013



D. Pesin + LB, 2010
Topological MI?

Pyrochlore iridates

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



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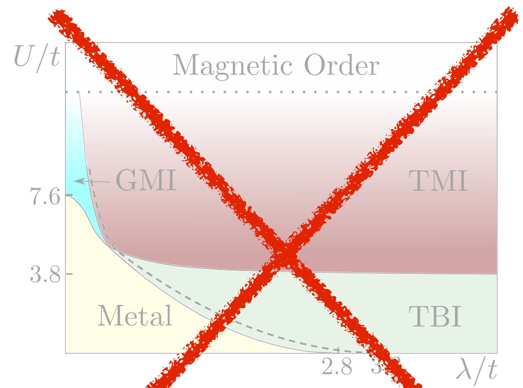

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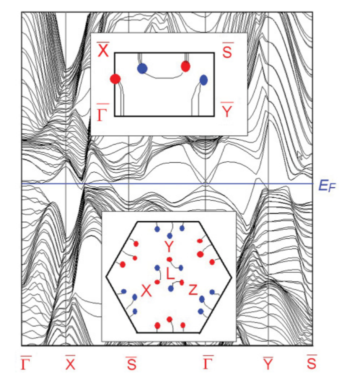
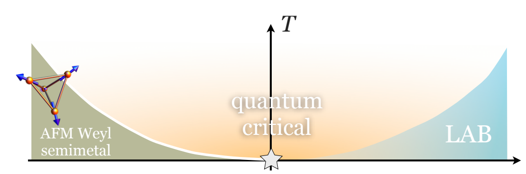


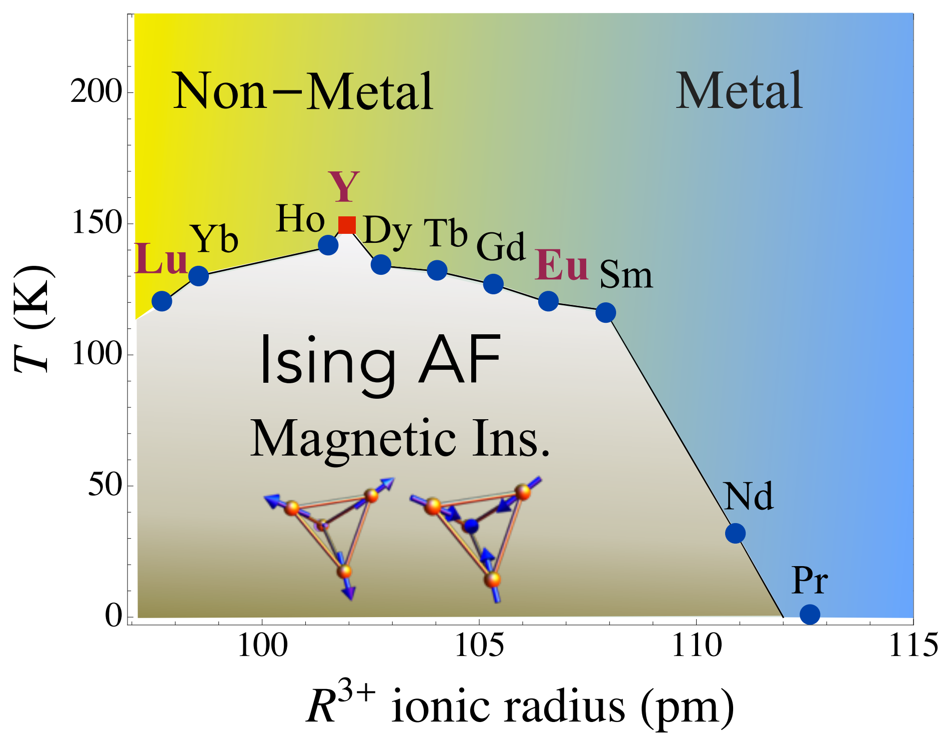
X. Wan *et al*, 2011
AF Weyl semimetal?



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

Pyrochlore iridates

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



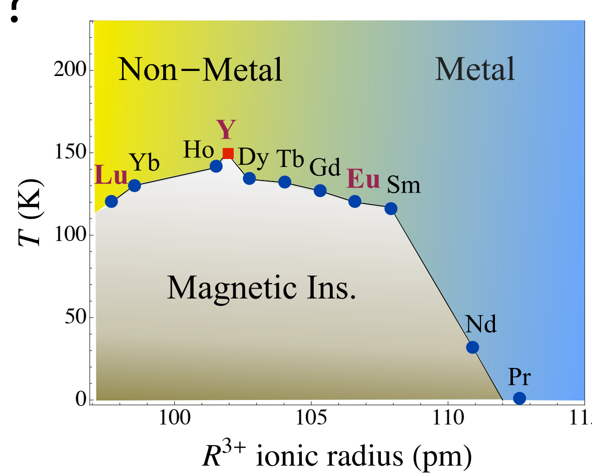
Yanagashima+Maeno, JPSJ 2001
K. Matsuhira et al, JPSJ 2011
W. Witczak-Krempa et al, ARCMP 2013

How correlated are these materials? Is there physics beyond mean-field? If yes, what is its role?

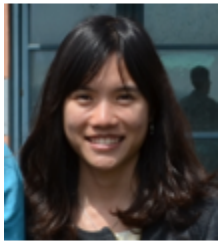
Ingredients of a theory

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

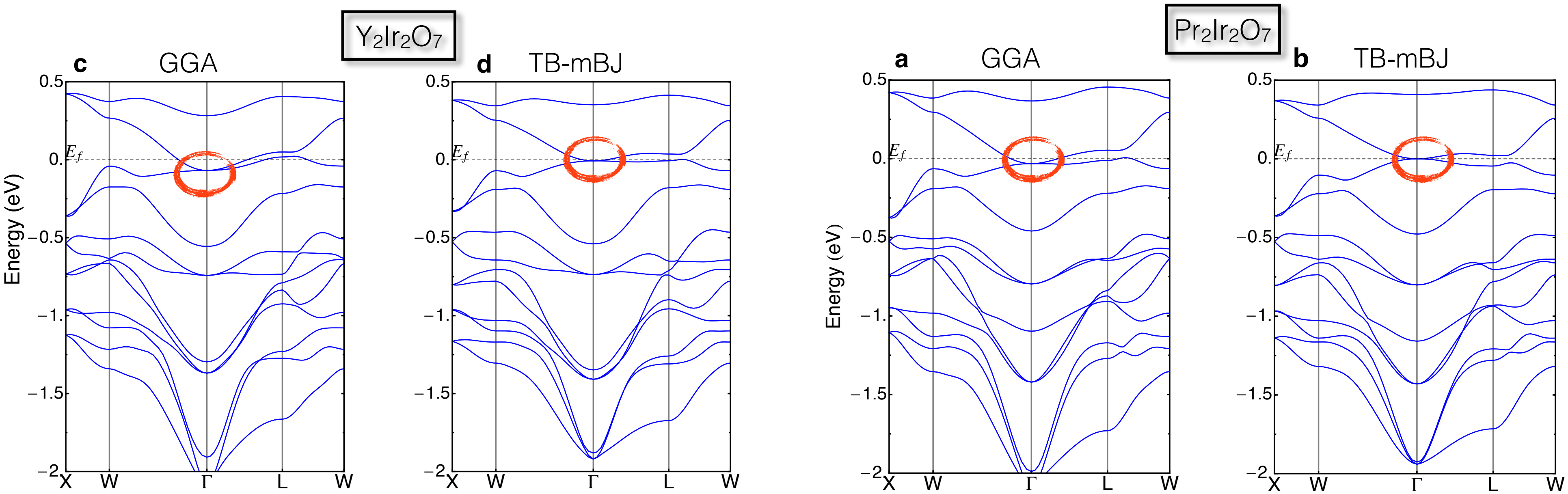
probably not?

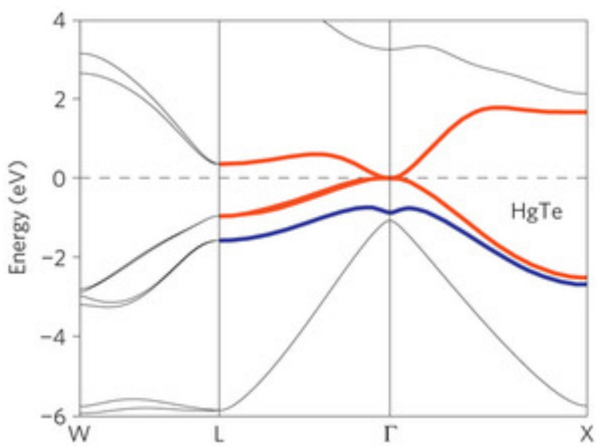


T. Kondo *et al*, Nat. Comm., 2015



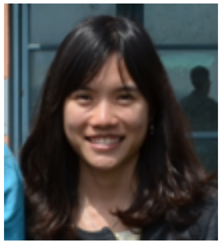
Paramagnetic electronic structure



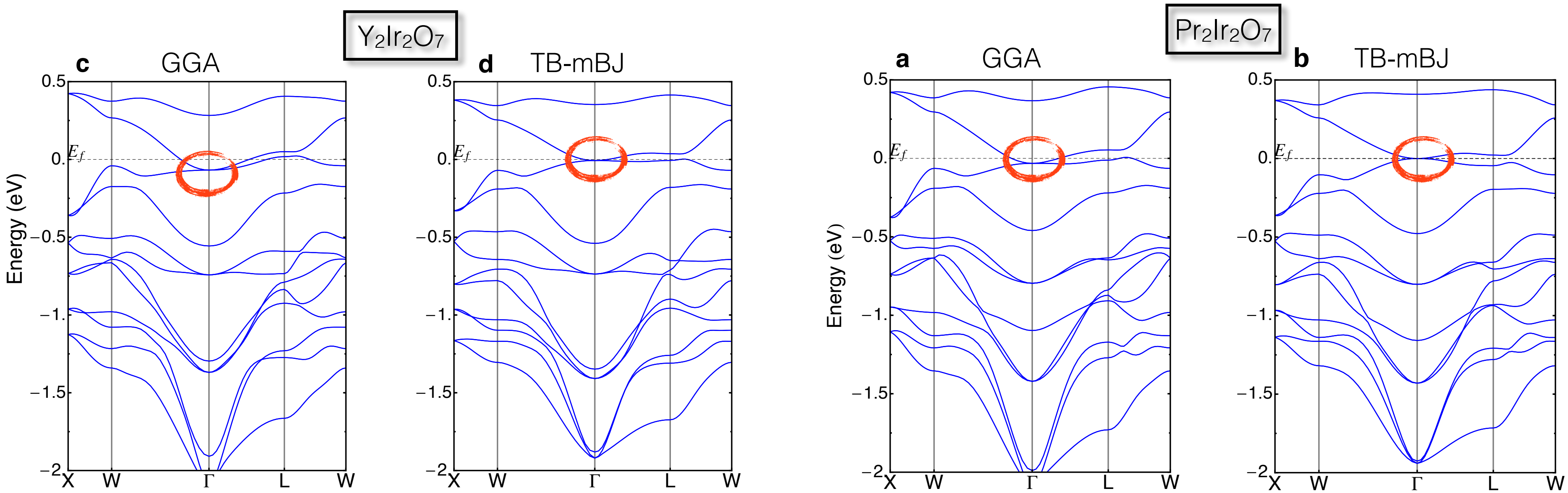


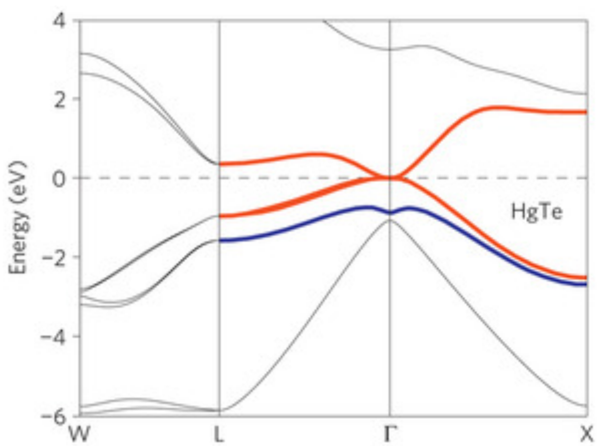
Γ_8 4-dimensional irrep guaranteed by cubic symmetry and time reversal

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



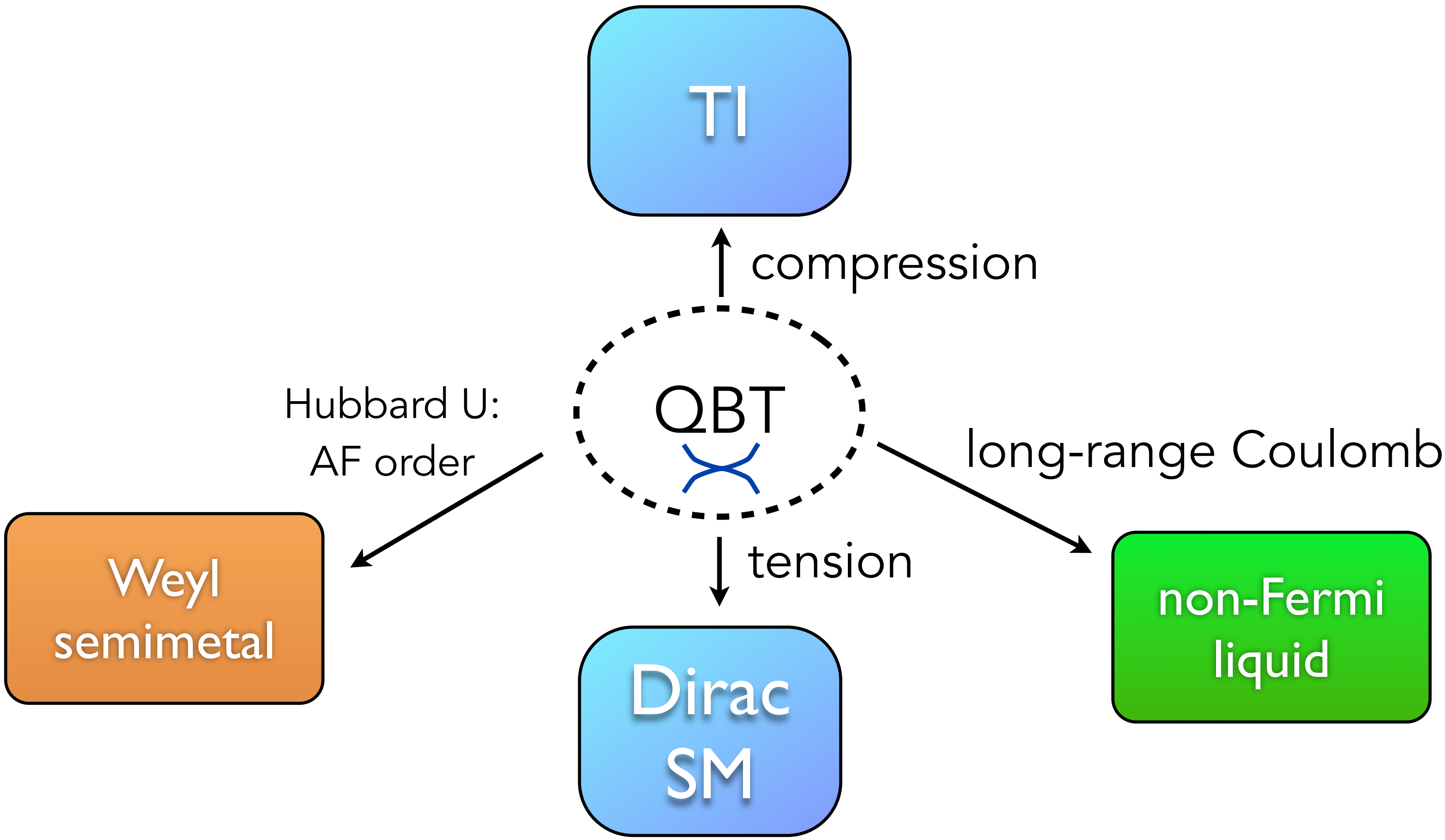
Paramagnetic electronic structure





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

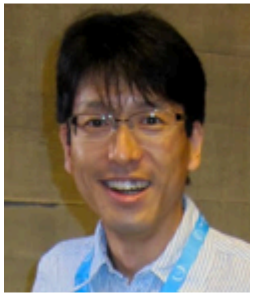
Proximate phases



ARPES

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

$Pr_2Ir_2O_7$



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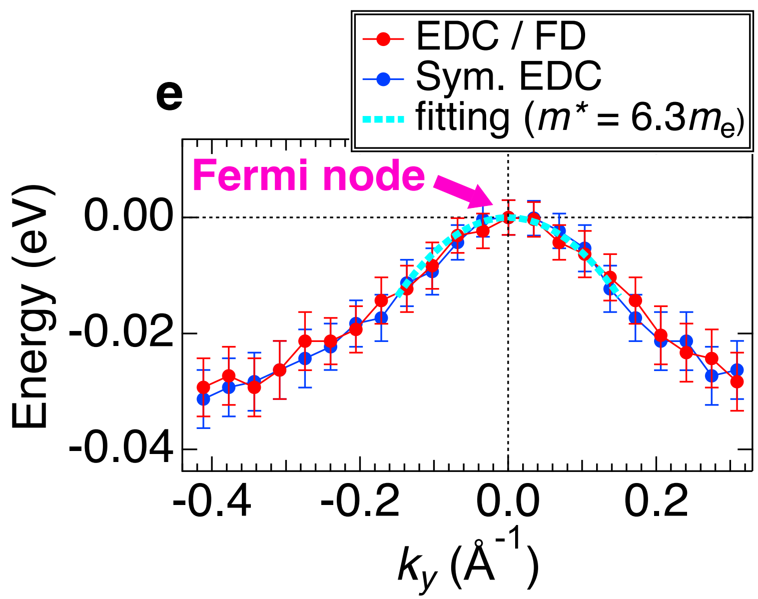
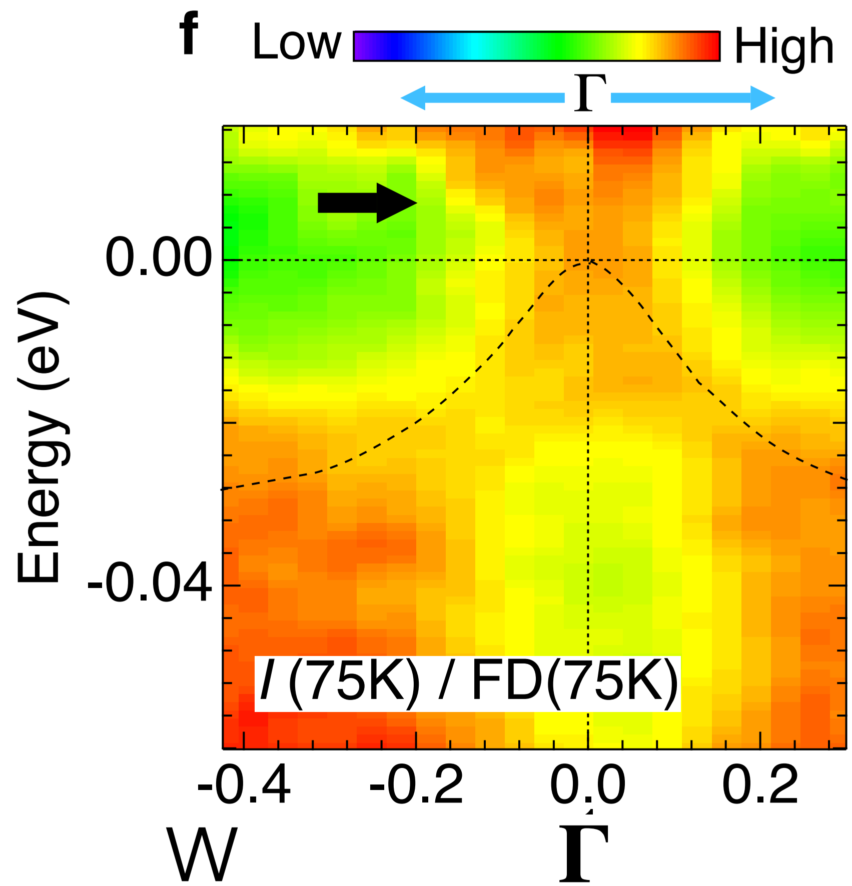
S. Shin





ARPES

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

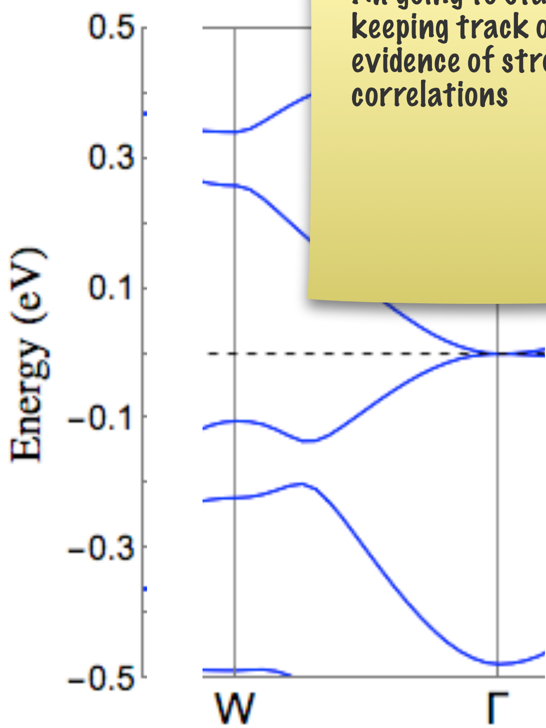
$Pr_2Ir_2O_7$

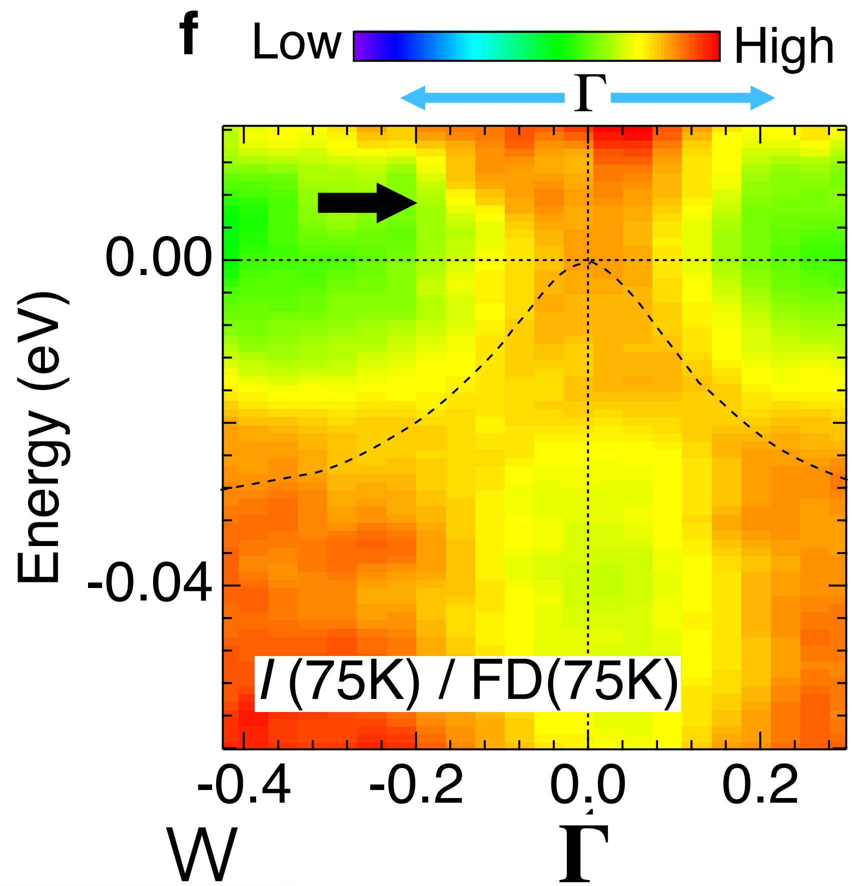
S. Nakatsuji

T. Kondo

S. Shin

I'm going to start keeping track of evidence of strong correlations



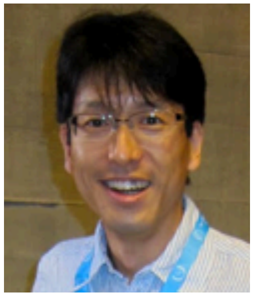


✓Bandwidth reduced by 3-5 from DFT

ARPES

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

$Pr_2Ir_2O_7$



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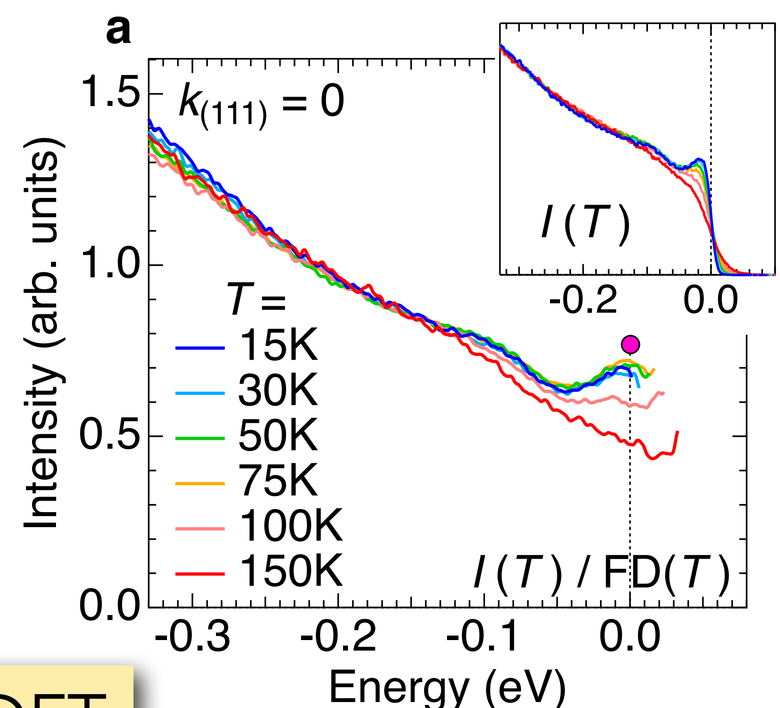
T. Kondo

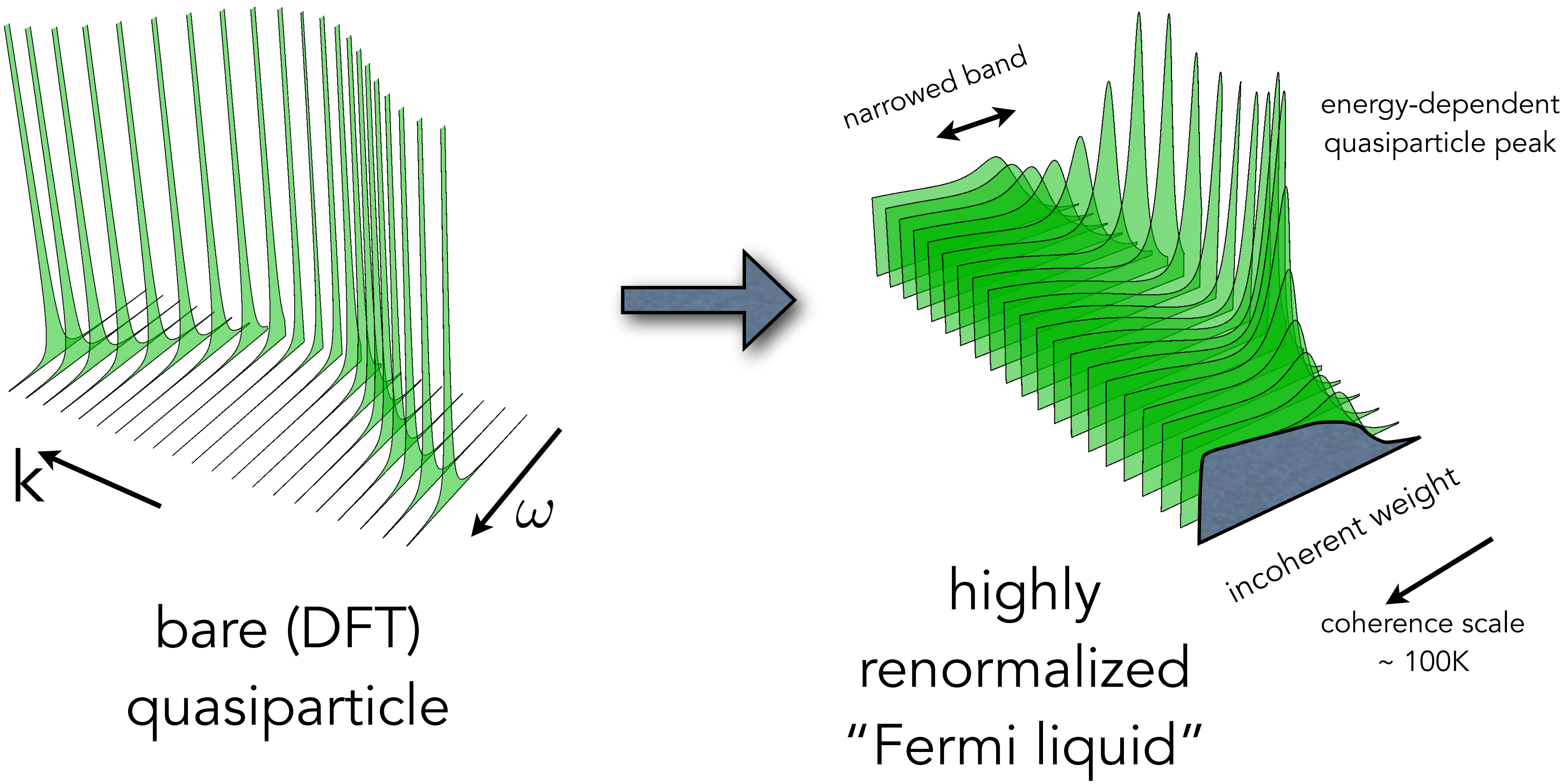
S. Shin



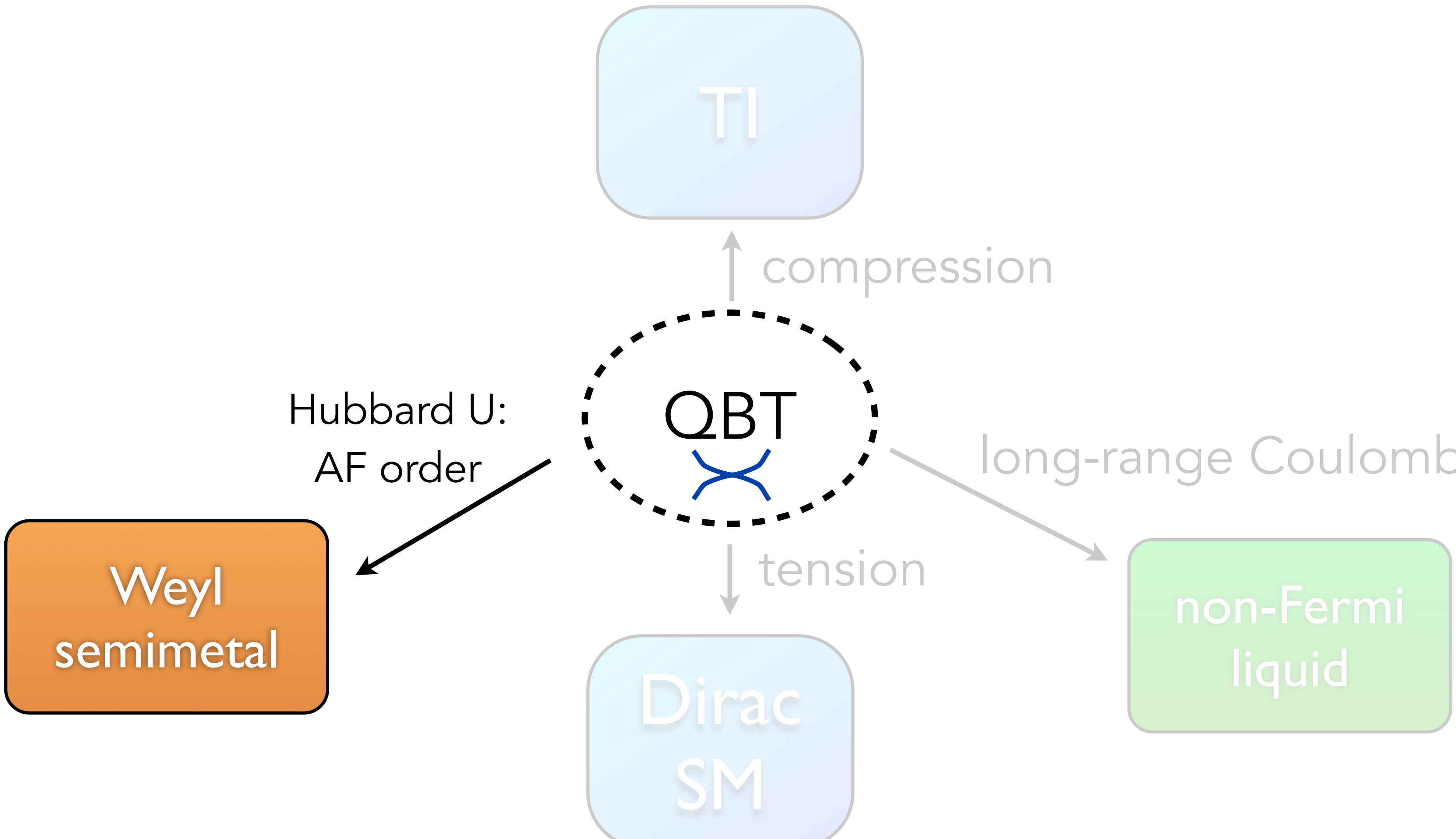
✓Bandwidth reduced by 3-5 from DFT

✓Quasiparticle weight strongly suppressed with temperature

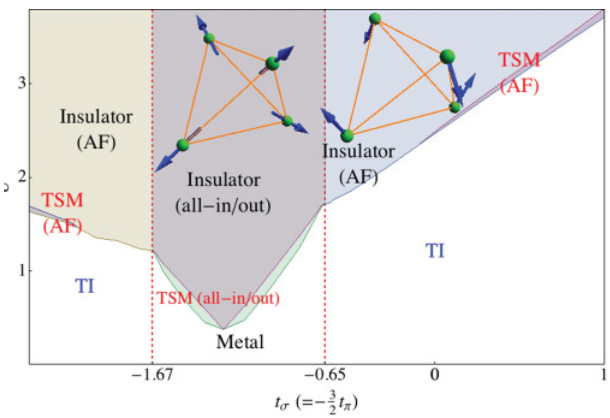
Correlated quasiparticles



Proximate phases

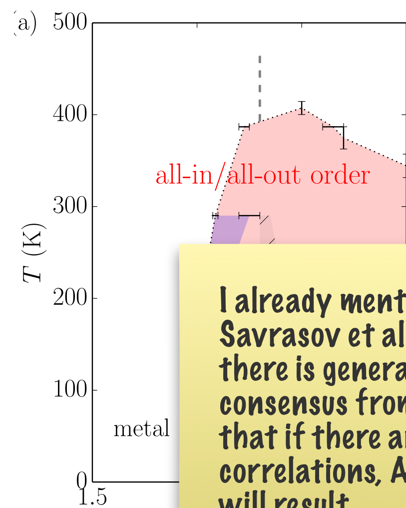


Ordering: theory



W. Witzak-Krempa + YB Kim, 2012

Hartree-Fock



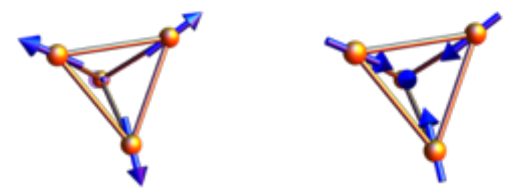
I already mentioned Savrasov et al. But there is general consensus from theory that if there are enough correlations, AIAO order will result.

H. Sh

DMFT

Jay-Z model

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



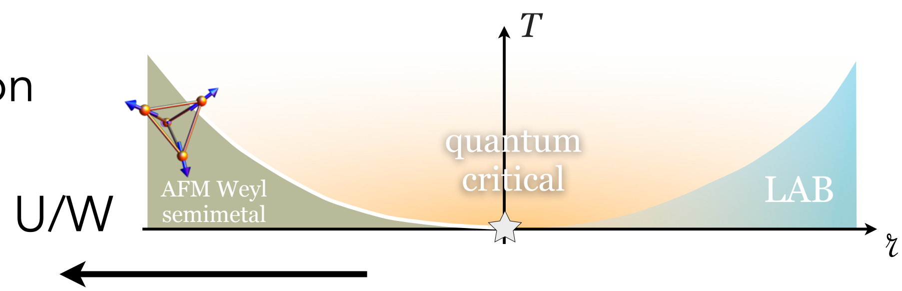
$J_z < 0$: all-in/all-out order

superexchange

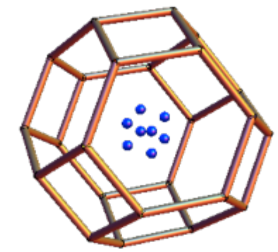
- General agreement: transition to AIAO Ising AF order

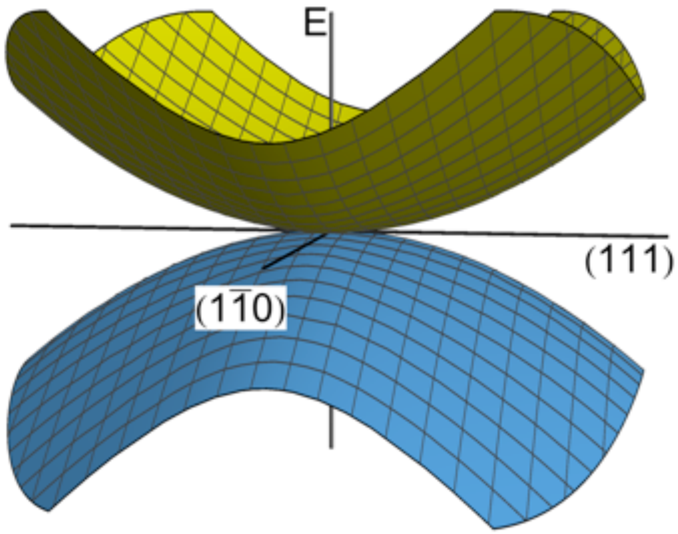
✦Quantum critical theory of this transition

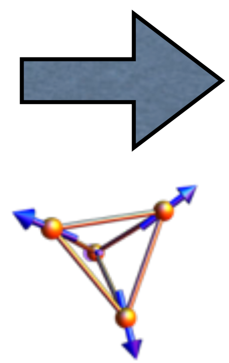
L. Savary *et al*, 2014 - topological QCP

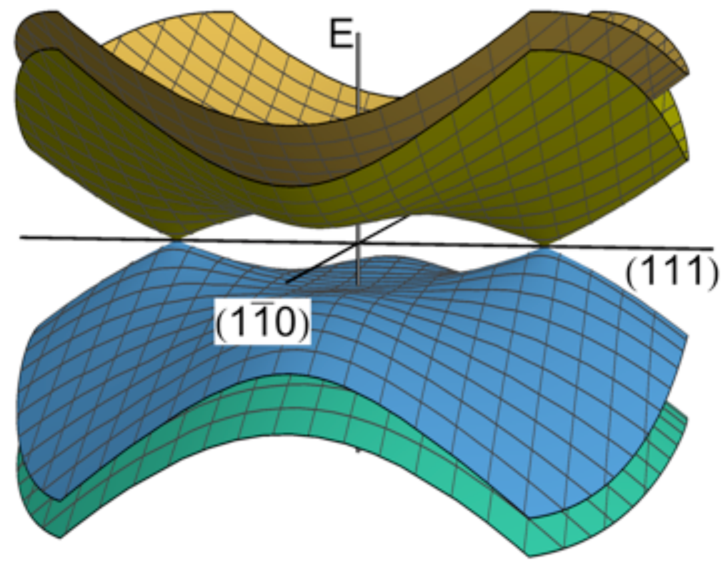


Weyl semimetal





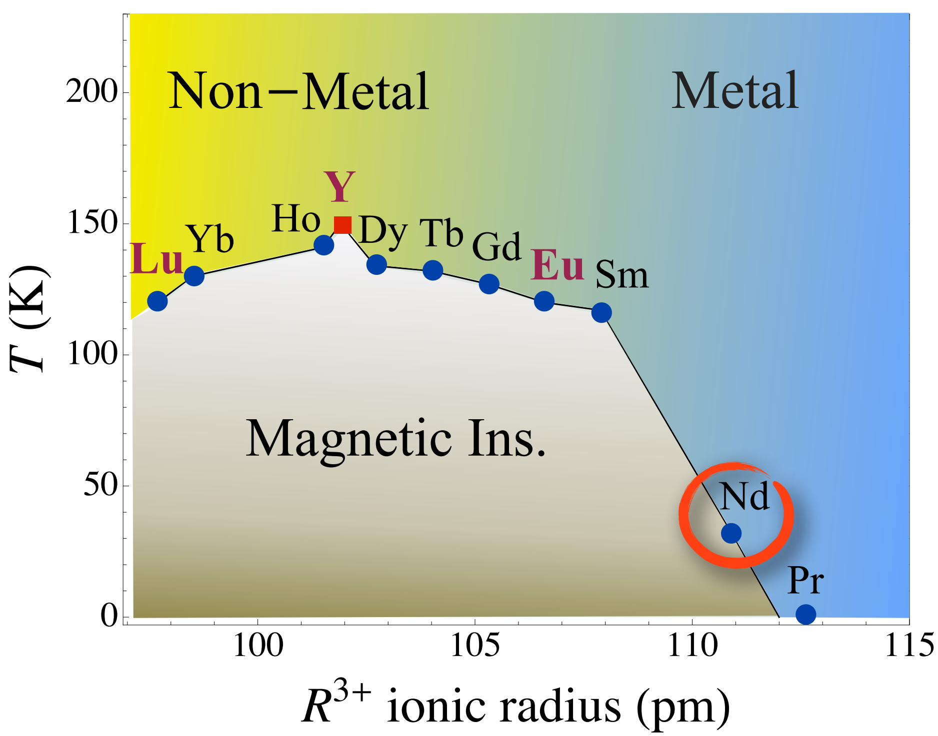




If quasiparticle picture applies at low energy, a *weakly* ordered AIAO state *must* be a Weyl semimetal

Weyl?

- Weyl semimetal?

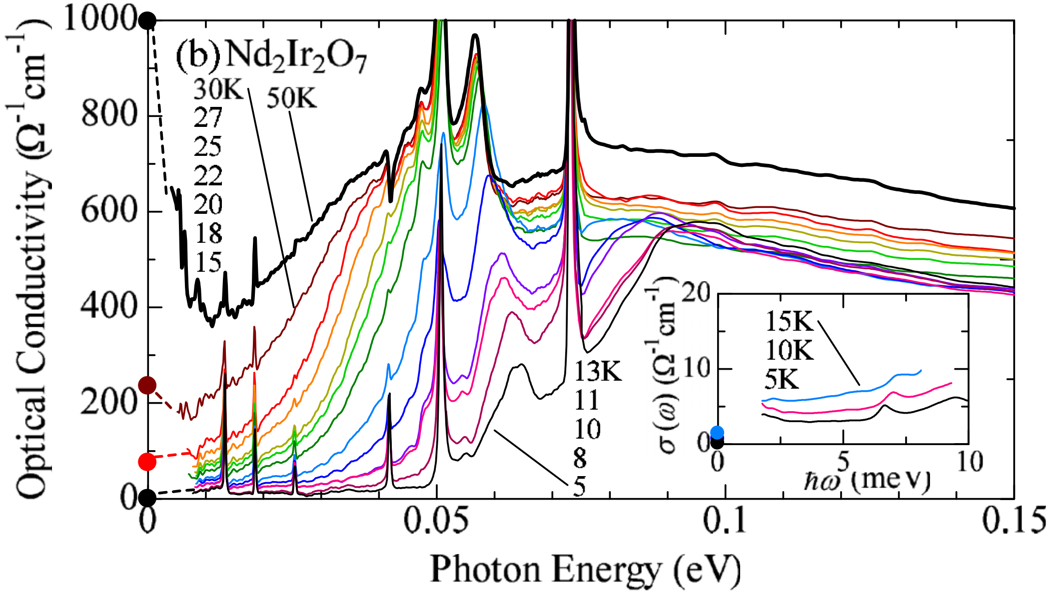


Yanagashima+Maeno, JPSJ 2001
K. Matsuhira et al, JPSJ 2011
W. Witczak-Krempa et al, ARCMP 2013

Best candidate should be $Nd_2Ir_2O_7$

Weyl not?

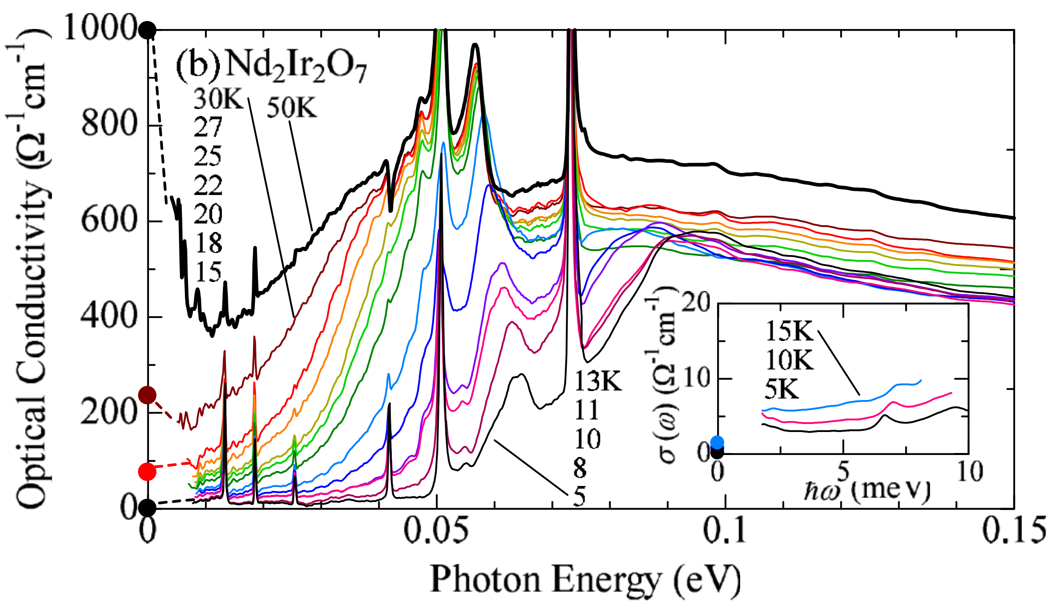
K. Ueda *et al*, 2012



charge gap ~ 45meV

Weyl not?

K. Ueda *et al*, 2012

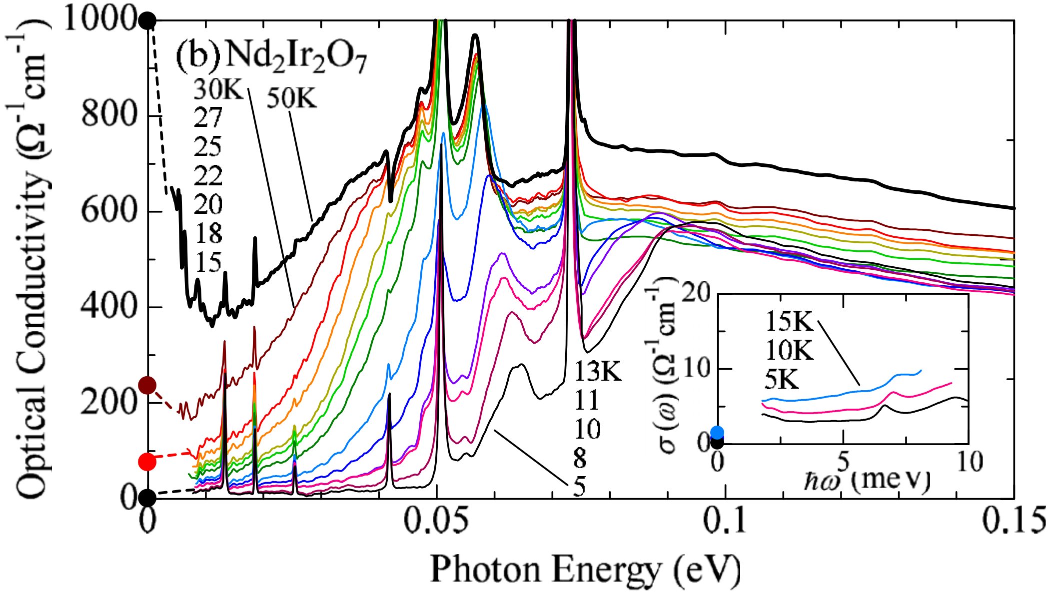


charge gap ~ 45meV

✓Bandwidth reduced by 3-5 from DFT
✓Quasiparticle weight strongly suppressed with temperature
✓Gap ~ 45meV ~ 18 T_c

Weyl not?

K. Ueda *et al*, 2012

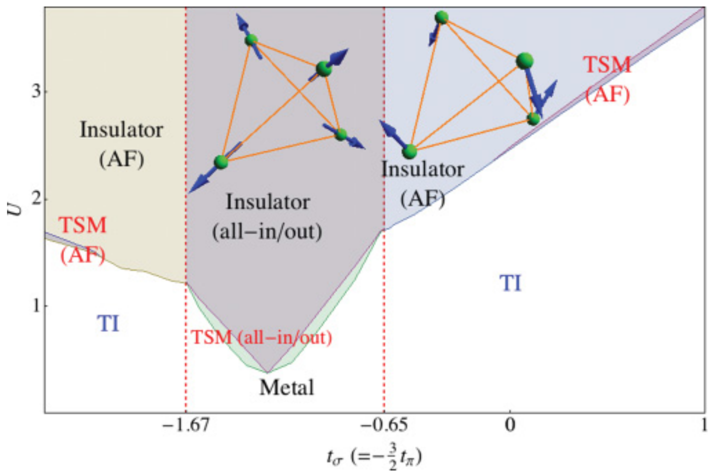


charge gap ~ 45meV

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

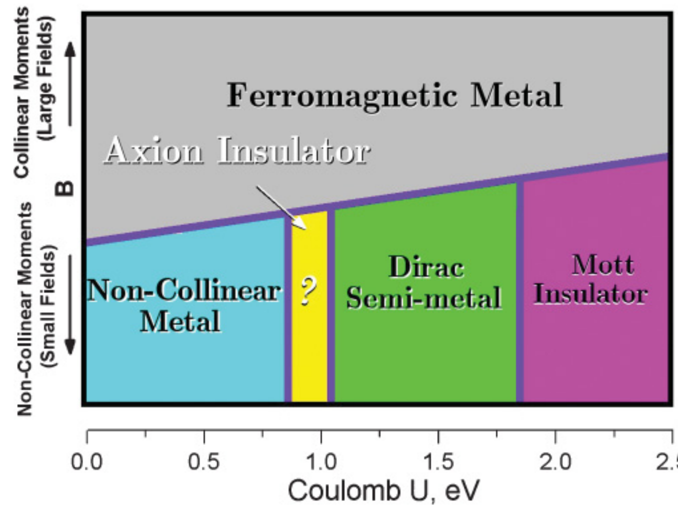
- ✦ Not weakly ordered?
- ✦ No quasiparticles?
- ✦ Weyl with very small DOS?

Weak or not?



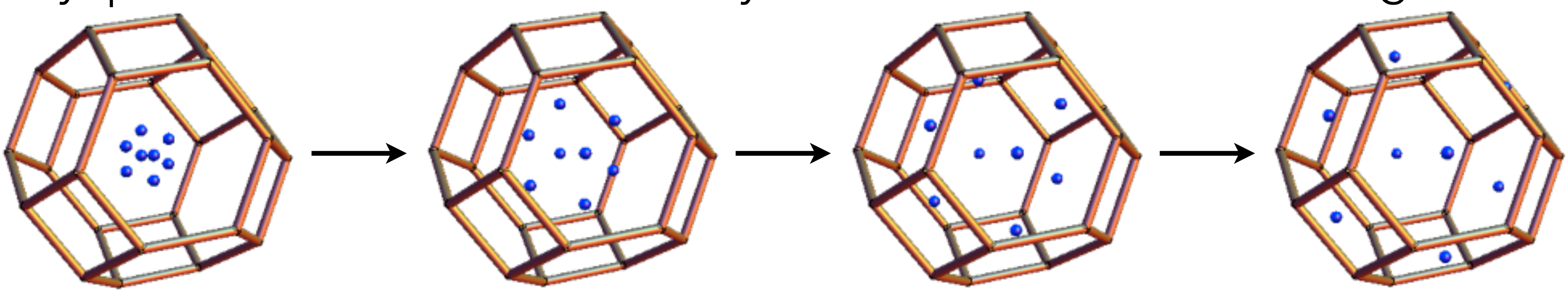
W. Witzak-Krempa + YB Kim, 2012

vs

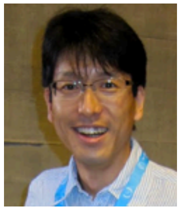


X. Wan *et al*, 2011

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



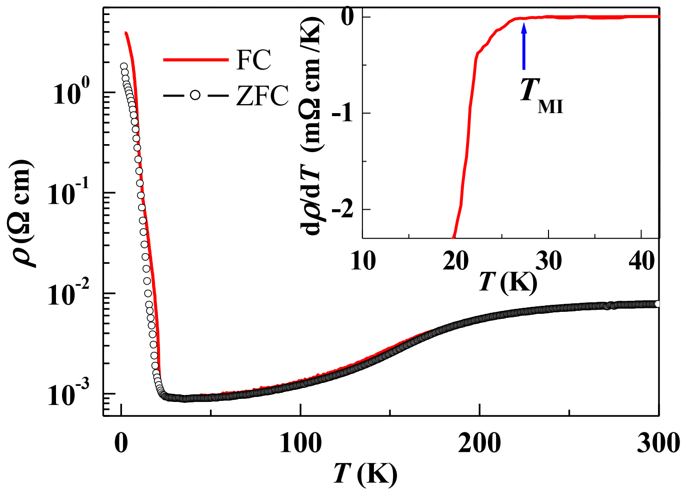
Could this have happened already for Nd?



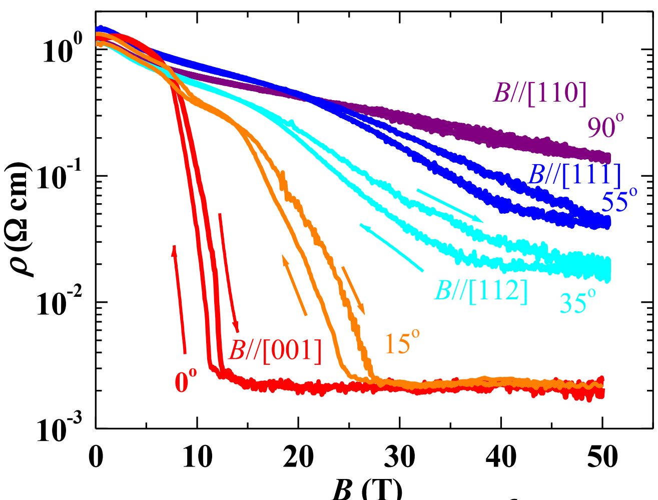
Zhaoming Tian *et al*, Nature Physics, 2015

Transport

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

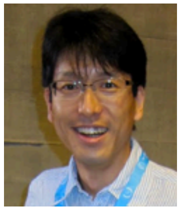


- Seems to b … with hard gap
- thermal tra… continuous



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

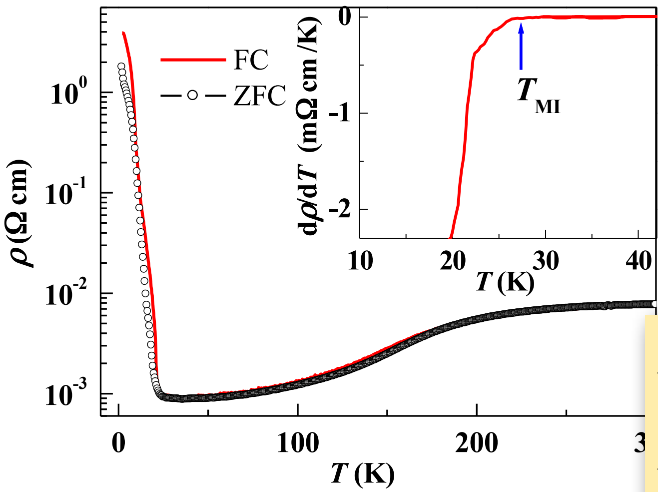
c.f. K. Ueda *et al*, 2015



Zhaoming Tian *et al*, Nature Physics, 2015

Transport

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



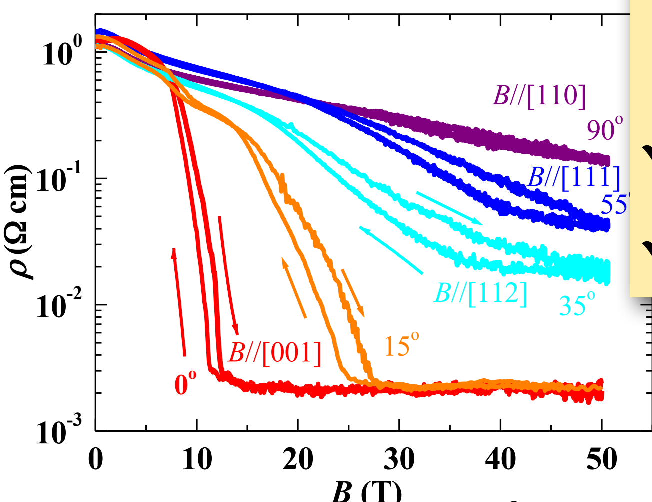
- Seems to b… with hard gap
- thermal tra… continuous

✓Bandwidth reduced by 3-5 from DFT

✓Quasiparticle weight strongly suppressed with temperature

✓Gap ~ 45meV ~ 18 T_c

✓MIT driven by (tiny) 12T field

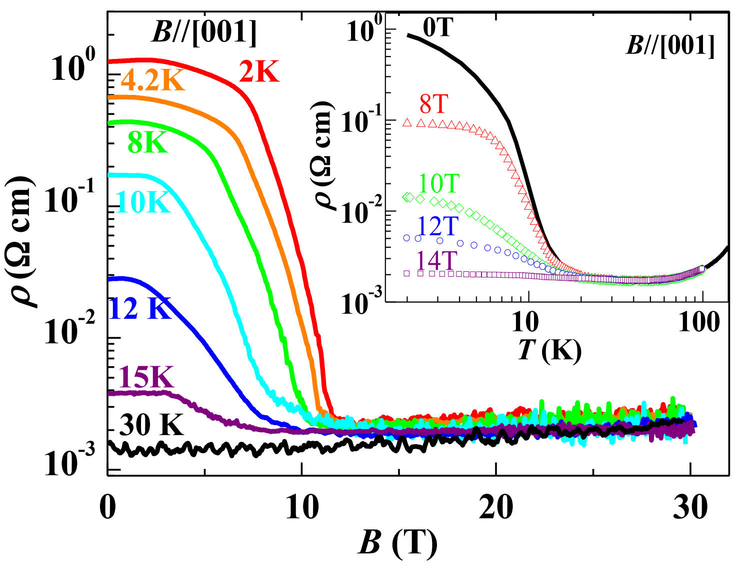


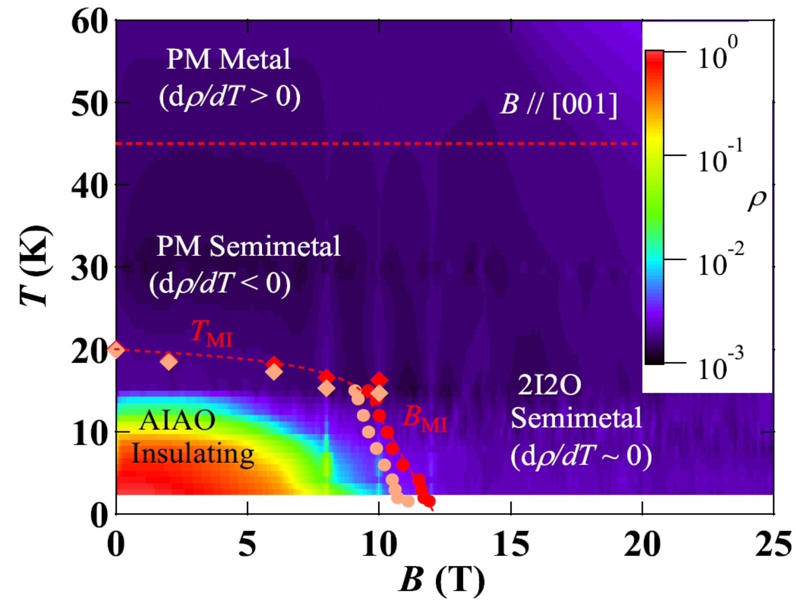
fields along (100)

c.f. K. Ueda *et al*, 2015

Zhaoming Tian *et al*, Nature Physics, 2015

Metal-Insulator Transition

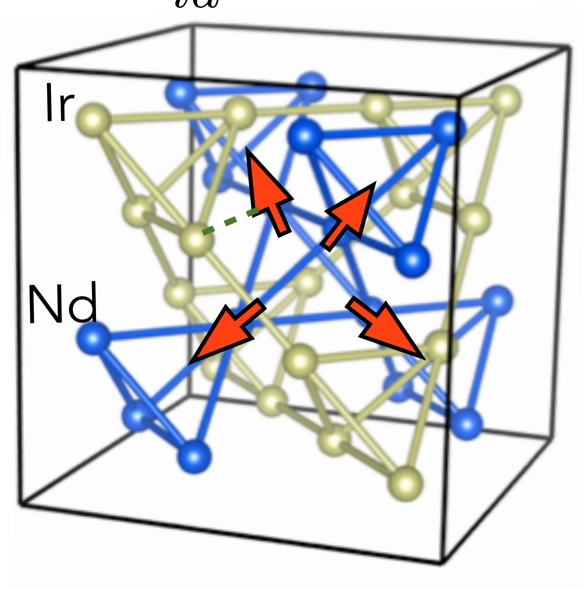




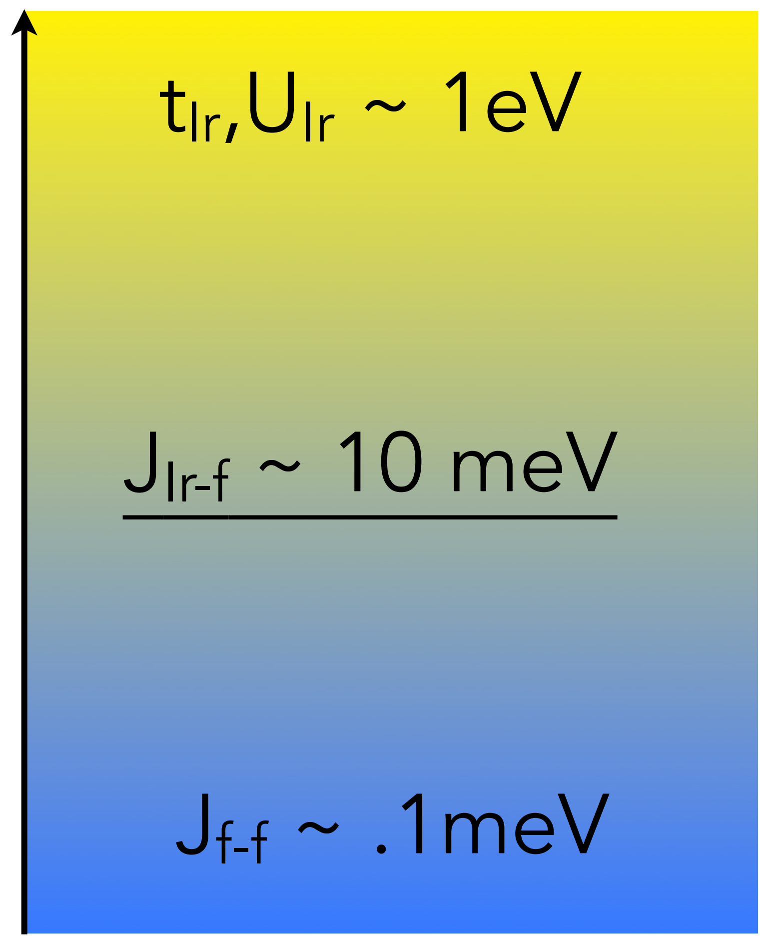
- First order transition at low temperature: mechanism of MIT is vanishing of condensation energy, not gap closing.
- Anisotropy: clear indication that Nd plays a direct role in the MIT - probably this is a unique feature for R=Nd

Nd physics

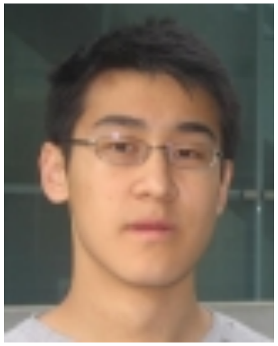
$$H_K = \sum_{ia} \vec{S}_i \cdot \mathsf{J}_{ia} \cdot \vec{\tau}_a$$



- 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

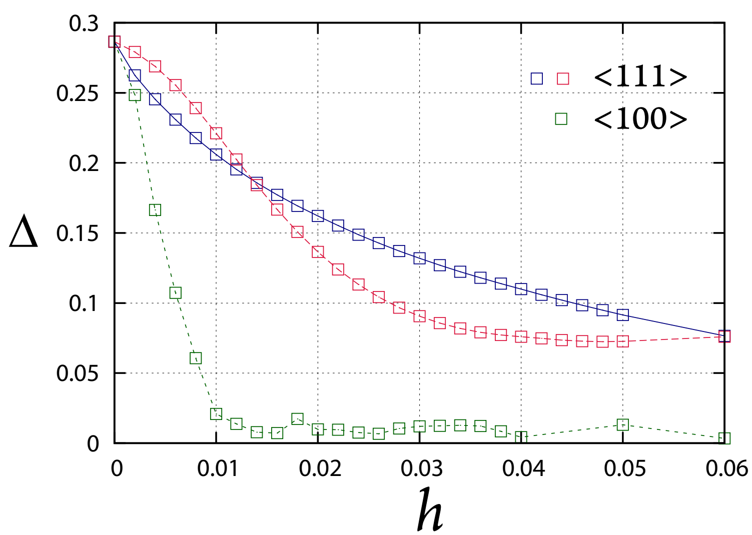


Anisotropy

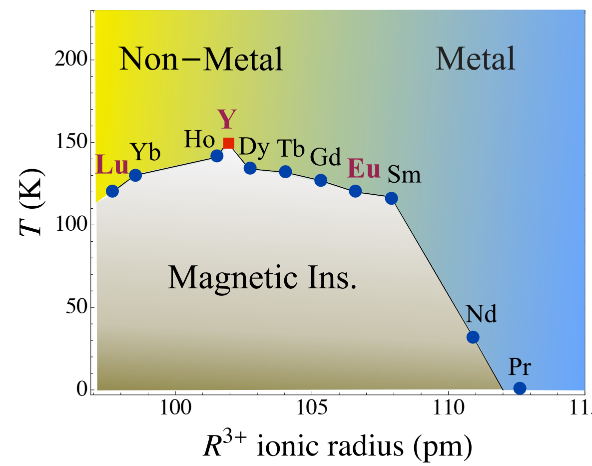
- Nd sensitivity to direction is transferred to Ir

$$H_K = \sum_{ia} \vec{S}_i \cdot \mathrm{J}_{ia} \cdot \vec{\tau}_a$$

acts like h_{eff} ~10meV local field on Ir



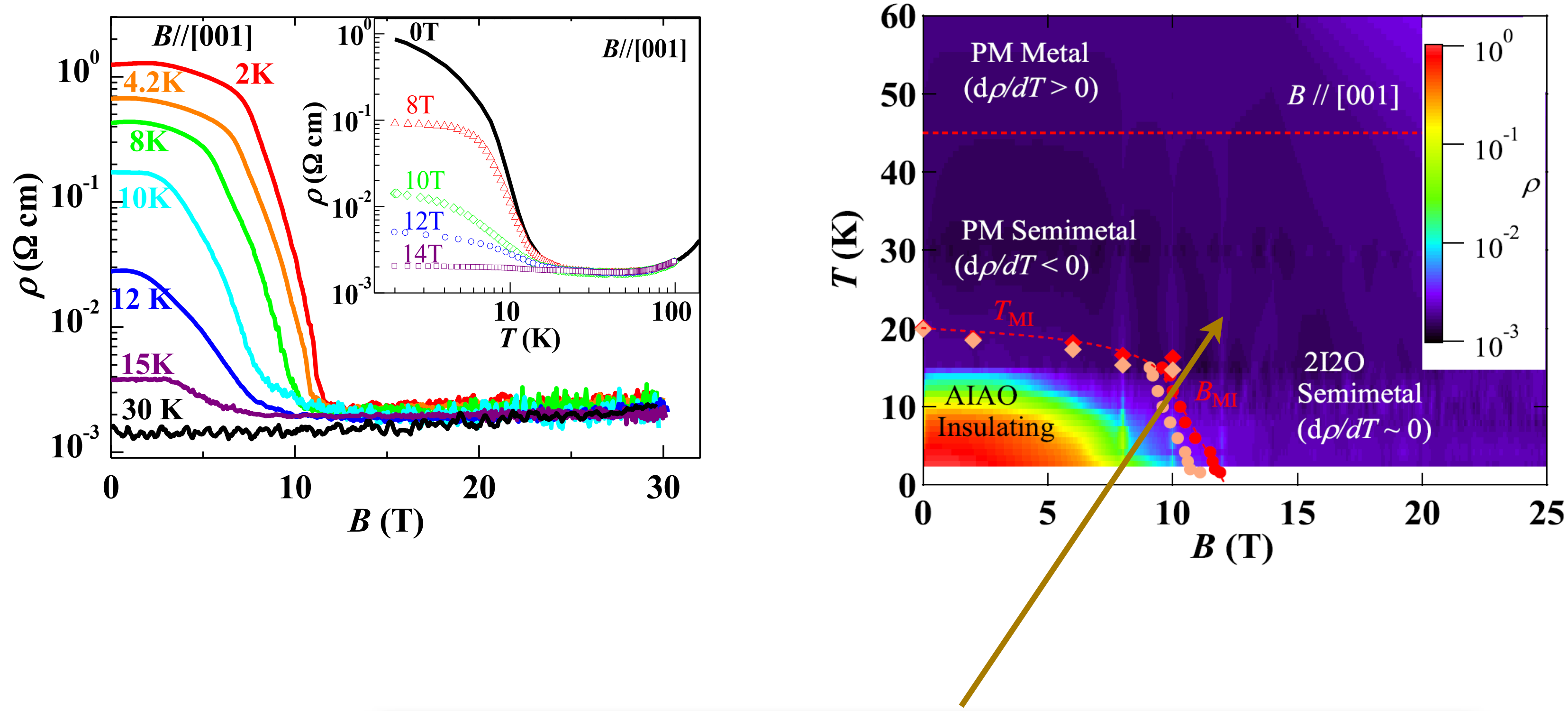
Hartree-Fock on Hubbard +Kondo lattice model



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

Zhaoming Tian *et al*, Nature Physics, 2015

Metal-Insulator Transition

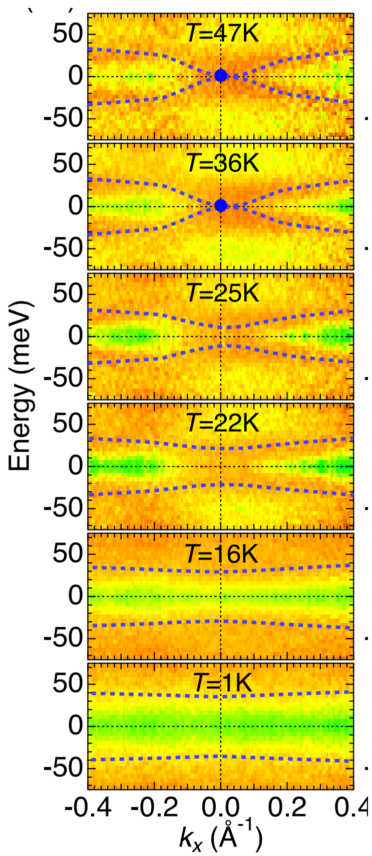


Nd moments are 2in-2out here, but no evidence that Ir is 2in-2out, or even has substantial local moments here

M. Nakayama *et al*, unpublished-- coming soon!

Quasiparticles?

- Already observed bandwidth reduction in $Pr_2Ir_2O_7$ - what happens for Nd?



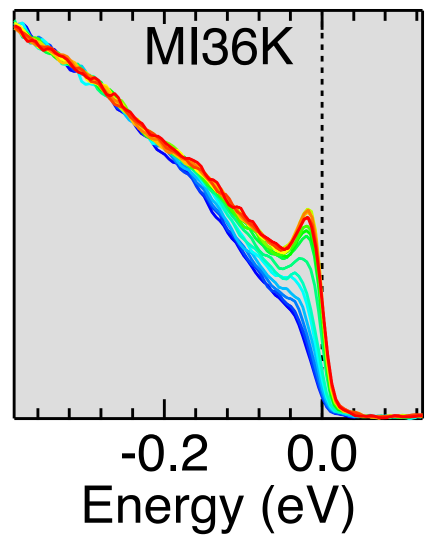
T>T_c: like Pr

T=T_c: no precursor - Slater

T < T_c: gap developing

Slater to Mott crossover?

T << T_c: remarkably flat



loss of quasiparticle peak

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

M. Nakayama *et al*, unpublished-- coming soon!

Quasiparticles?

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✓Bandwidth reduced by 3-5 from DFT

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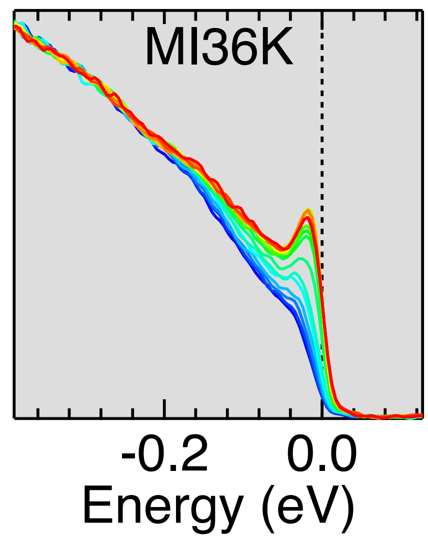
✓MIT driven by (tiny) 12T field

✓Extreme band flattening and reduction of QP peak at *low* T



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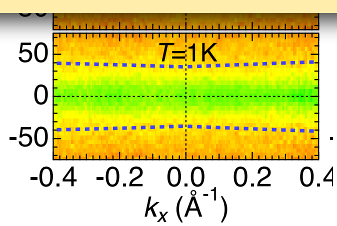
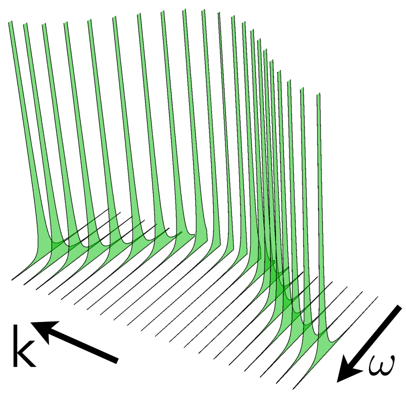


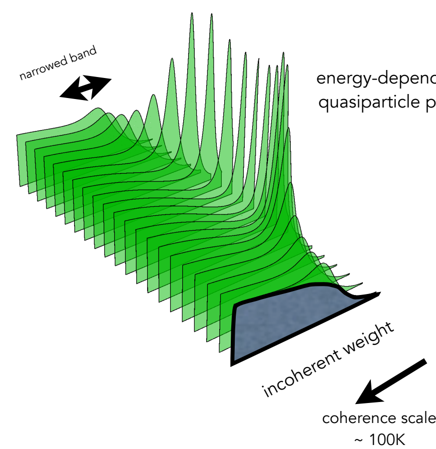
T << T_c: remarkably flat

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

Energy regimes

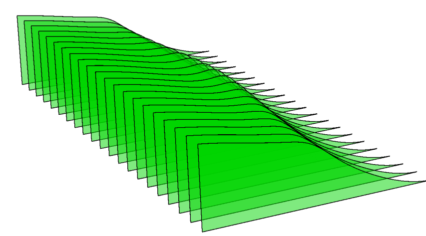


bare (DFT)
quasiparticle



highly
renormalized
"Fermi liquid"

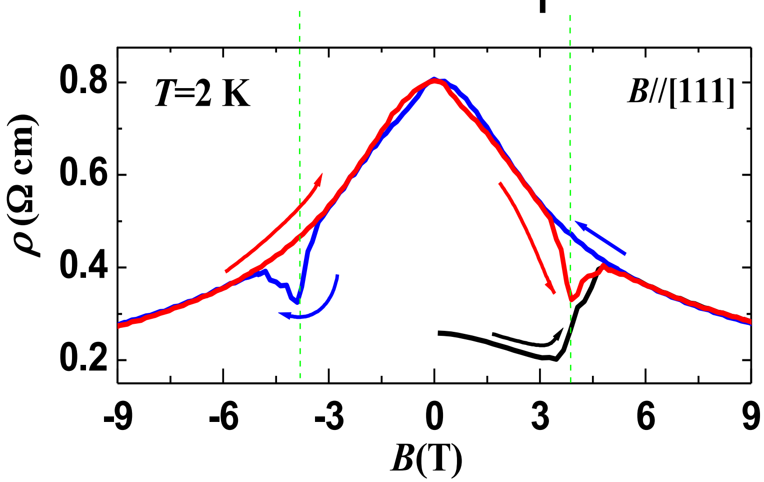
mean-field onset



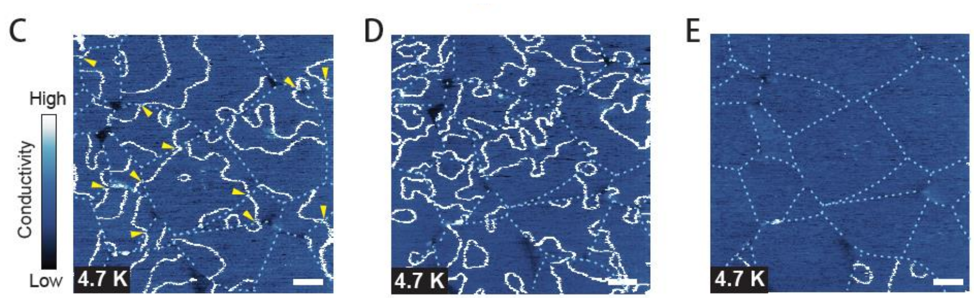
Mott-like low T limit?

Domains

- Large magnetic moment of Nd allows manipulation of domains



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

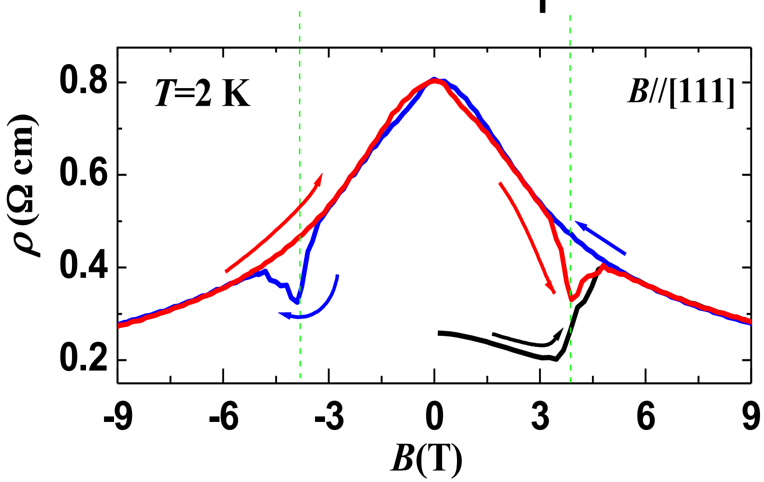


local conductivity
E. Y. Ma *et al*, 2015

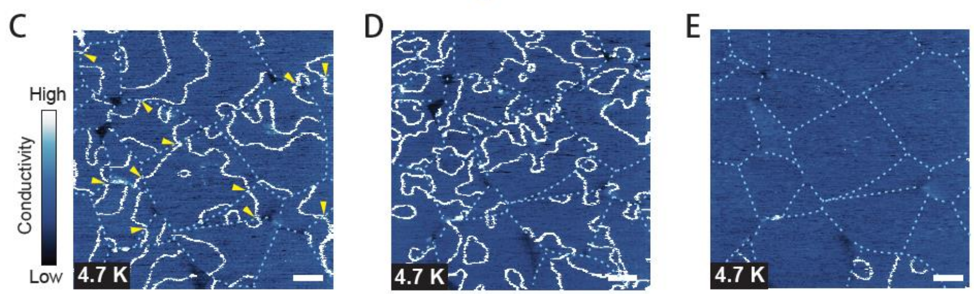
conducting domain walls! c.f. previous talks

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

may be evidence for correctness of Slater picture?

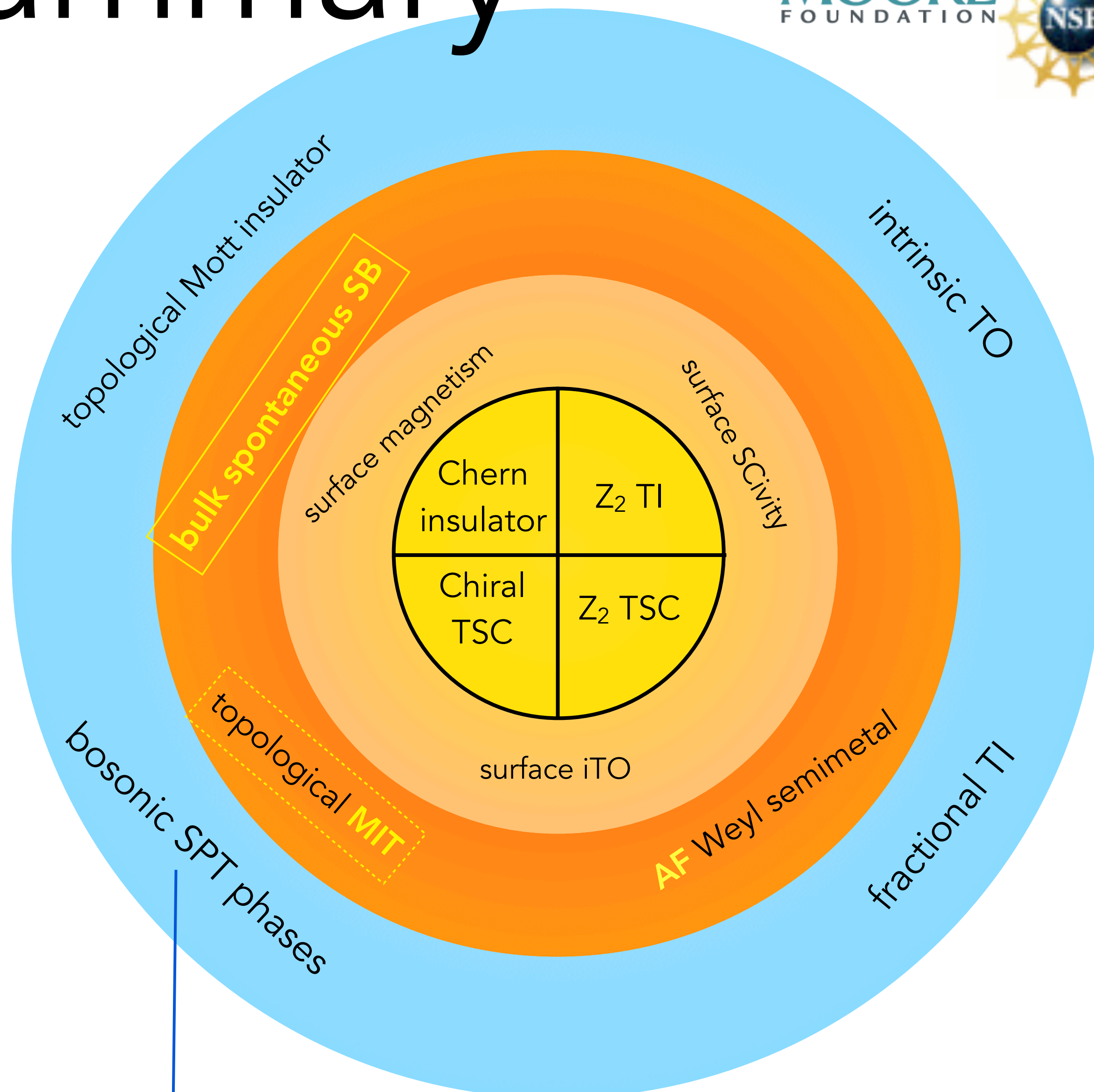
estimate $d \sim \rho_{\mathrm{metal},3d}/\rho_{\Box} \sim (1m\Omega \cdot cm)/(1k\Omega)$ ~ 10nm

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. Challenge: can we recover them? (c.f. K. Ueda talk?)

- Quite a bit still to explore! Correlated materials prove surprising and challenging



Advertisement: Zhen Bi *et al*, arXiv:1602.03190