Fermi node, Topological Phases and Domain Walls of Pyrochlore Iridates

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KITP , July 30, 2015

Part 1
Fermi node and Topological Phases of Pyrochlore Iridates

UCSB

Leon Balents

Eun-Gook Moon

(now U. Chicago)

Japan

Takeshi Kondo

Satoru Nakatsuji

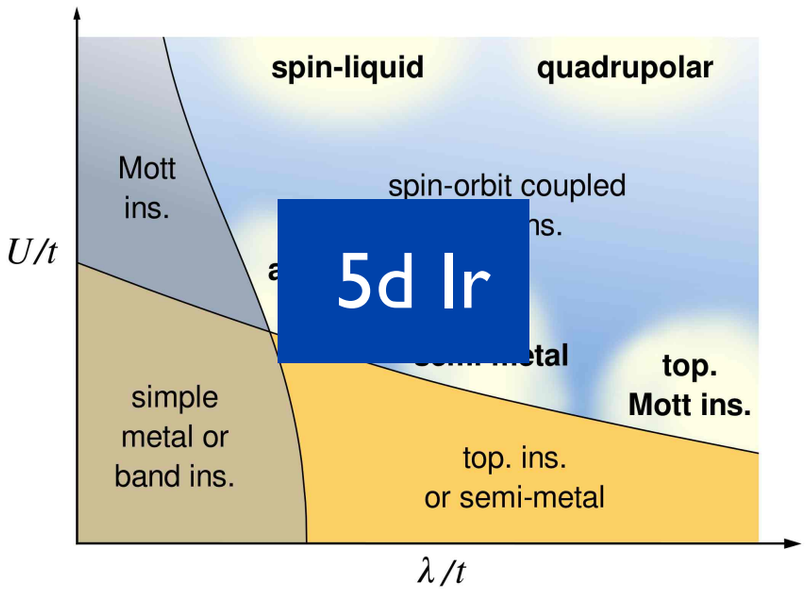
Shik Shin

…

T. Kondo, M. Nakayama, RC, et al, Submitted.

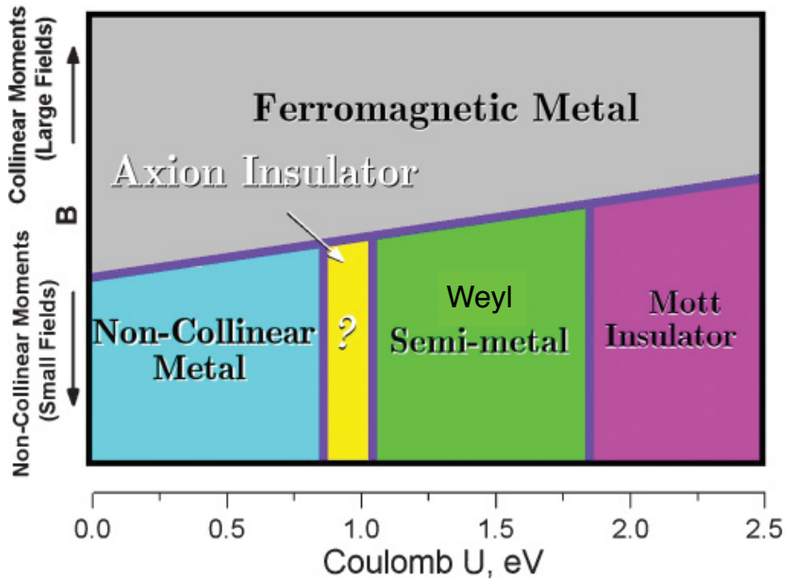
Motivations

- Correlation physics: Mott insulator, superconductivity...
- Spin-orbit coupling: topological insulators, Majorana fermions...
- Coulomb interaction+spin-orbit coupling → new physics?
- Iridates: U(correlation)~W(band width)~λ(spin-orbit)



W. Witczak-Krempa et al, ARCMP 2013

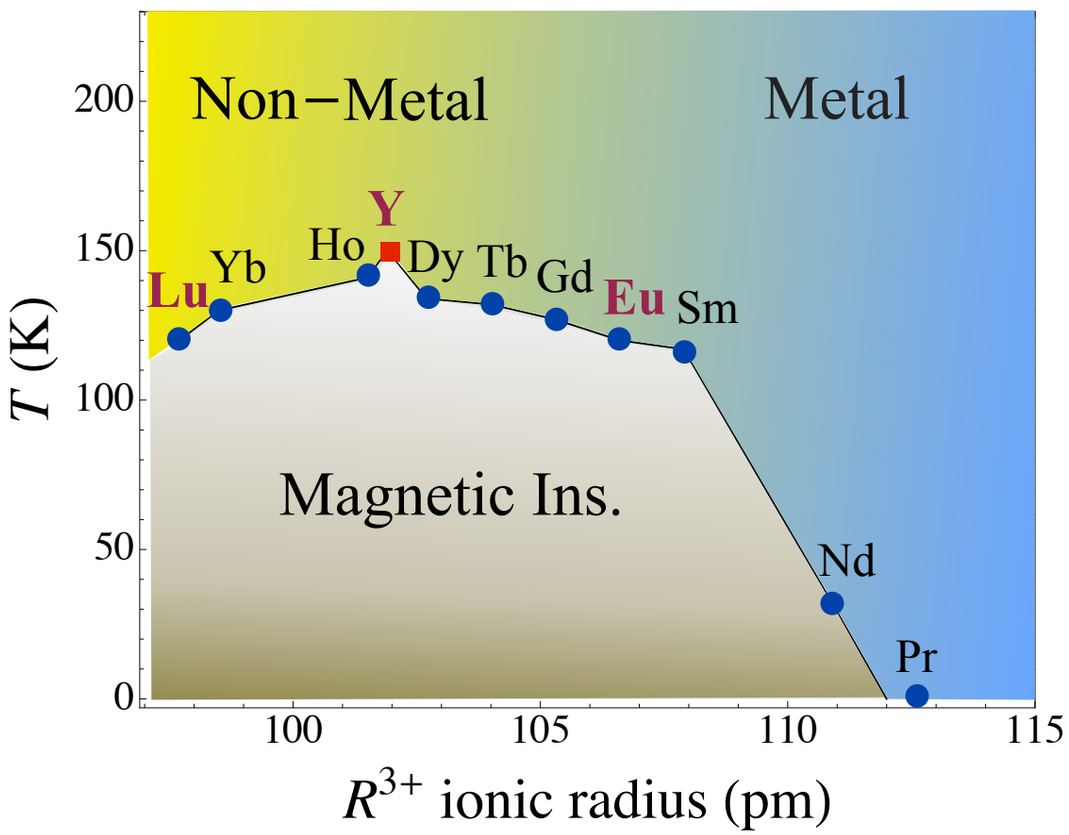
$Y_2Ir_2O_7$



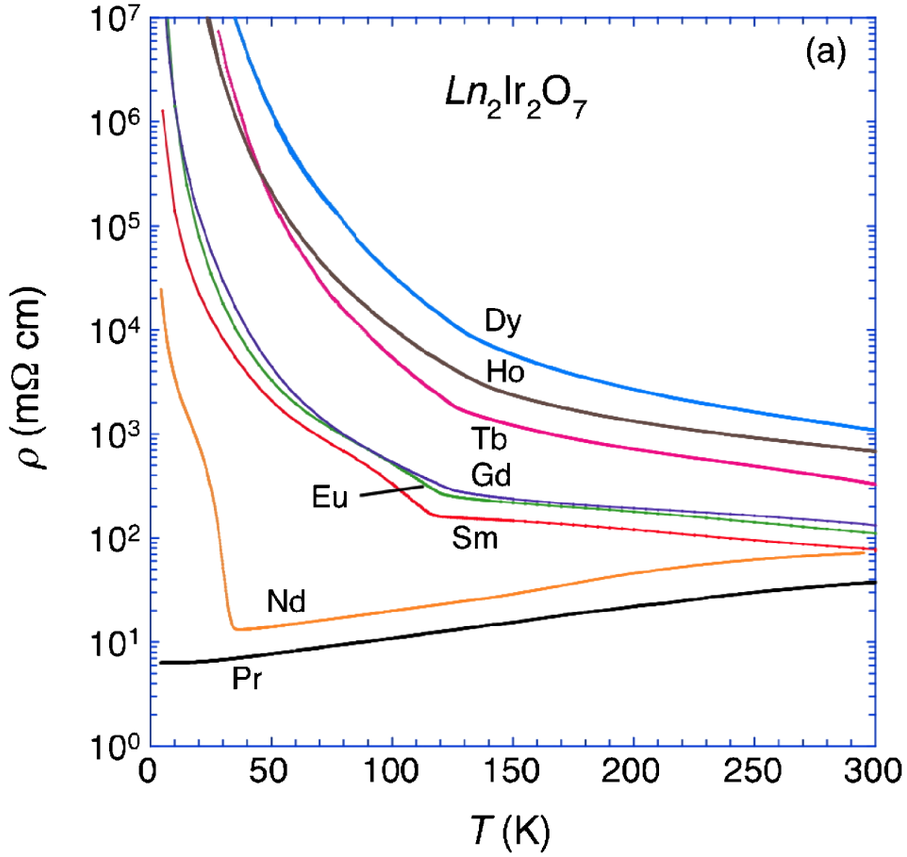
X. Wan et al, PRB 2011

Review on Pyrochlore Iridates $R_2Ir_2O_7$

- Magnetic ordering transition, 2nd order transition
- Magnetic transition and metal-insulator transition coincides for relatively larger rare earth radius compound
- As rare earth ionic radius decreases, T_{MI} increases and gap increases



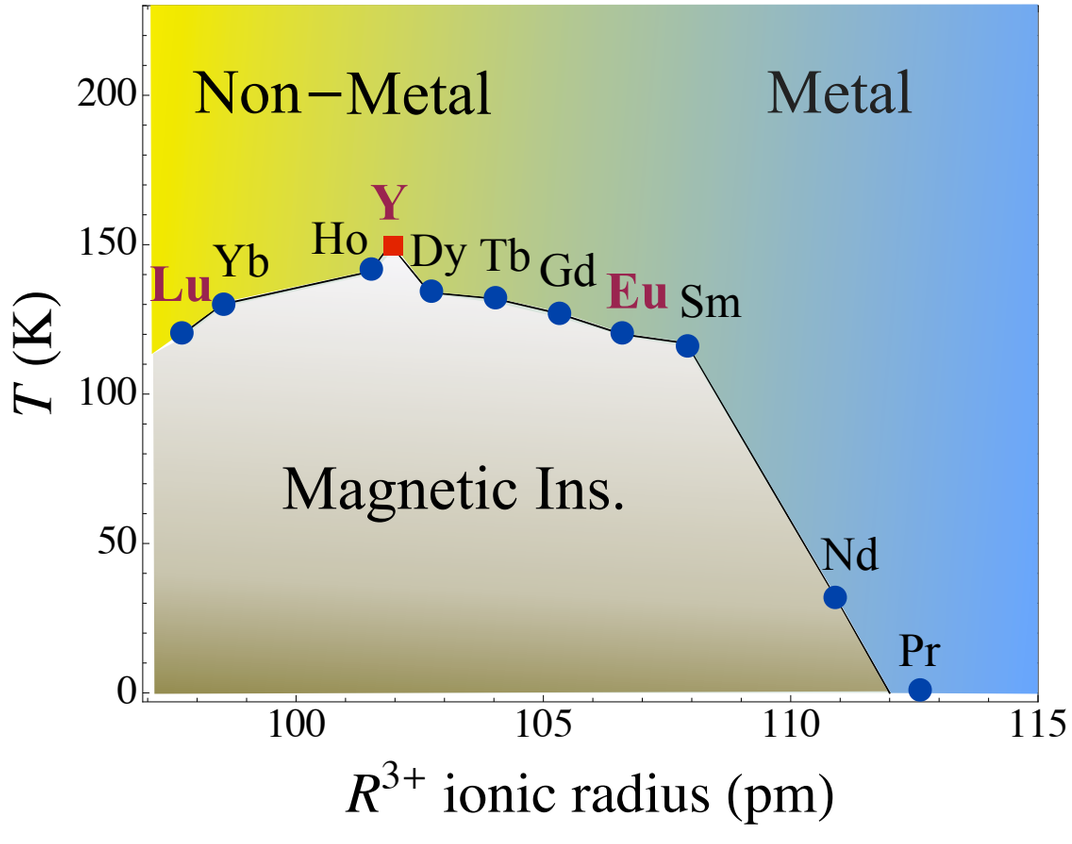
K. Matsuhira et al, JPSJ 2011
W. Witczak-Krempa et al, ARCMP 2013



K.Ueda et al, PRL 2012

Review on Pyrochlore Iridates $R_2Ir_2O_7$

- Magnetic ordering transition, 2nd order transition
- Magnetic transition and metal-insulator transition coincides for relatively larger rare earth radius compound
- As rare earth ionic radius decreases, T_{MI} increases and gap increases
- Energy gap is small comparing to 3d materials



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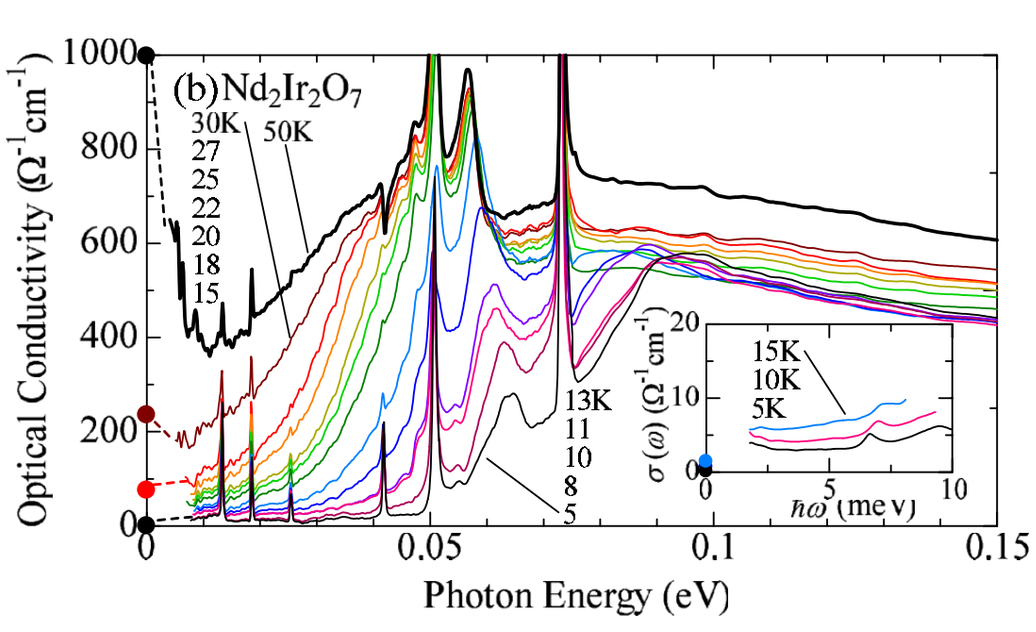
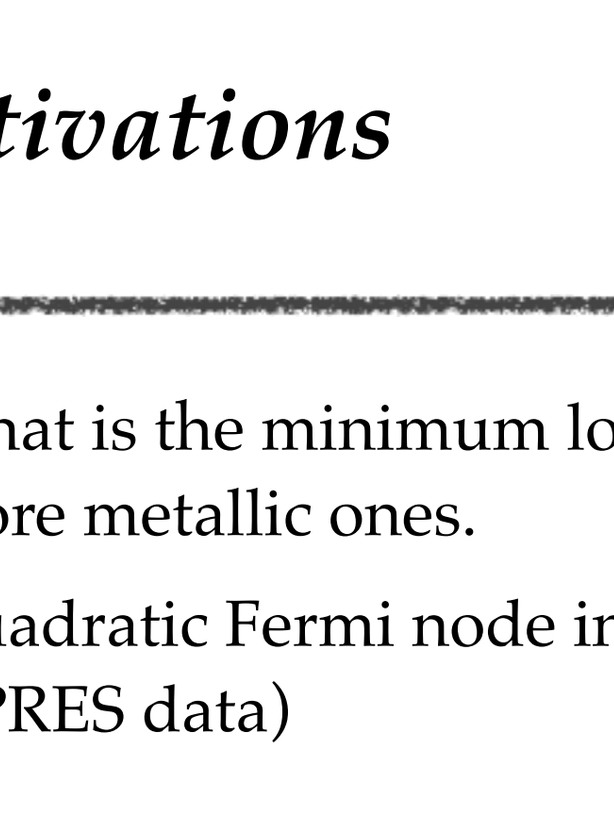


Optical conductivity
gap~0.045eV

K.Ueda et al, PRL 2012

Motivations

- What is the minimum low energy electronic structure of $R_2Ir_2O_7$? Especially for more metallic ones.
- Quadratic Fermi node in $Pr_2Ir_2O_7$ (*ab initio* electronic structure calculation and APRES data)

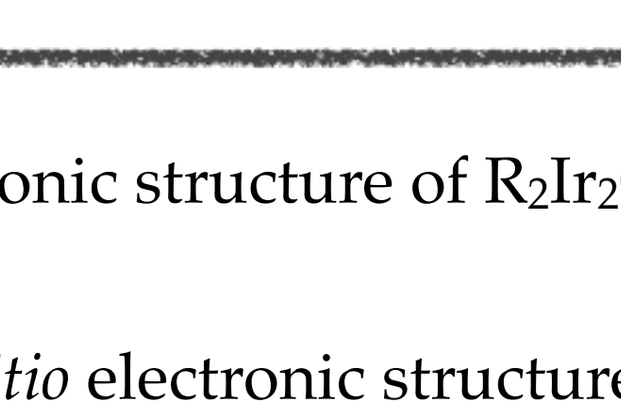


Quadratic band touching:
HgTe

HgTe quantum wells:
Analogy with negligible correlation.

B.A. Bernevig, et al. Science 2006

Strain/Pressure



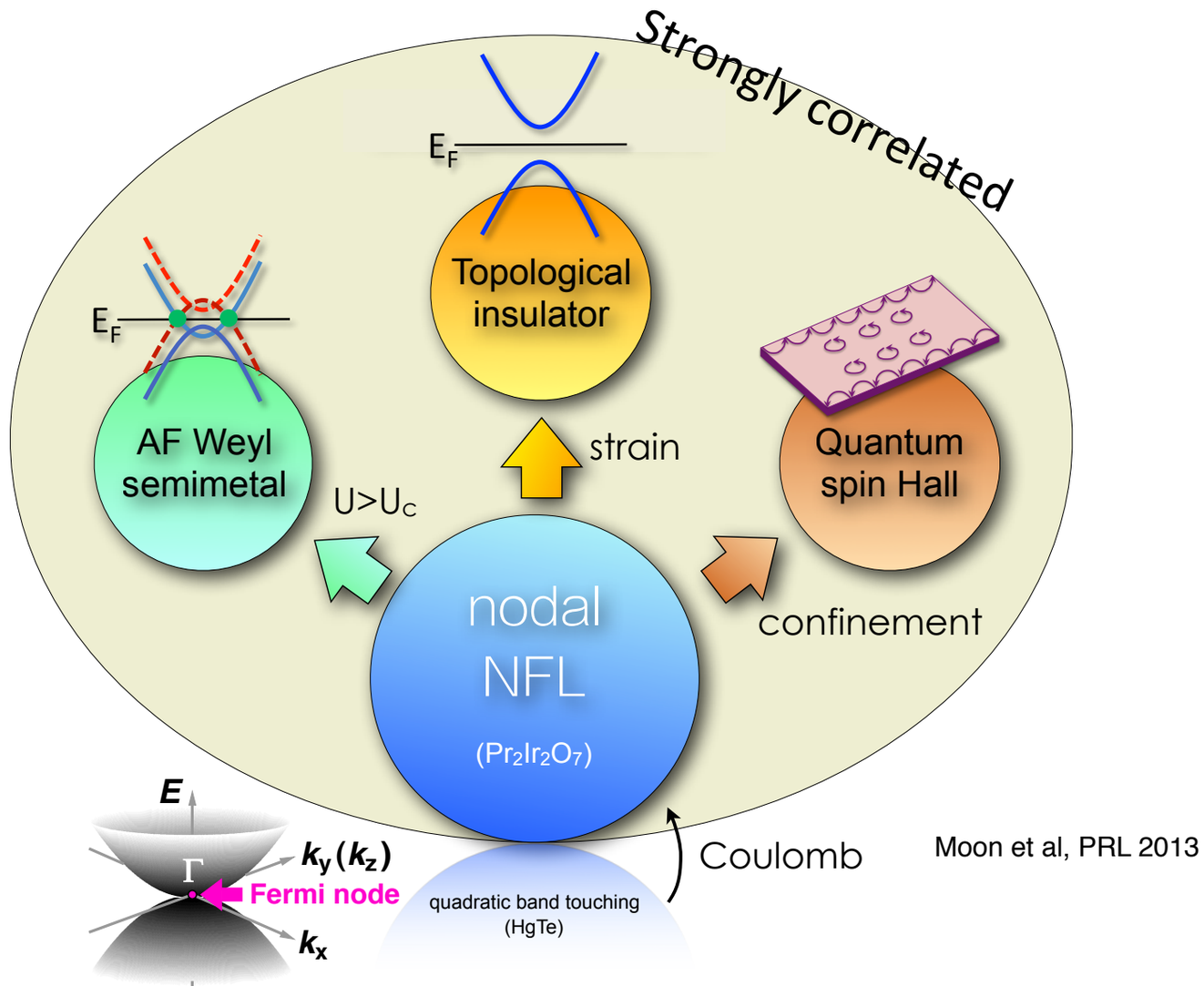
With pressure/strain:
Gapped bulk phase
Gapless HgTe/CdTe interfacial state

Motivations

- Tune the ground state ? If so, how?

  Goal: Topological insulators, quantum anomalous Hall effect, Weyl semimetal

- Growing techniques such as MBE and PLD, magnetic and pressure measurement have made tuning more accessible.

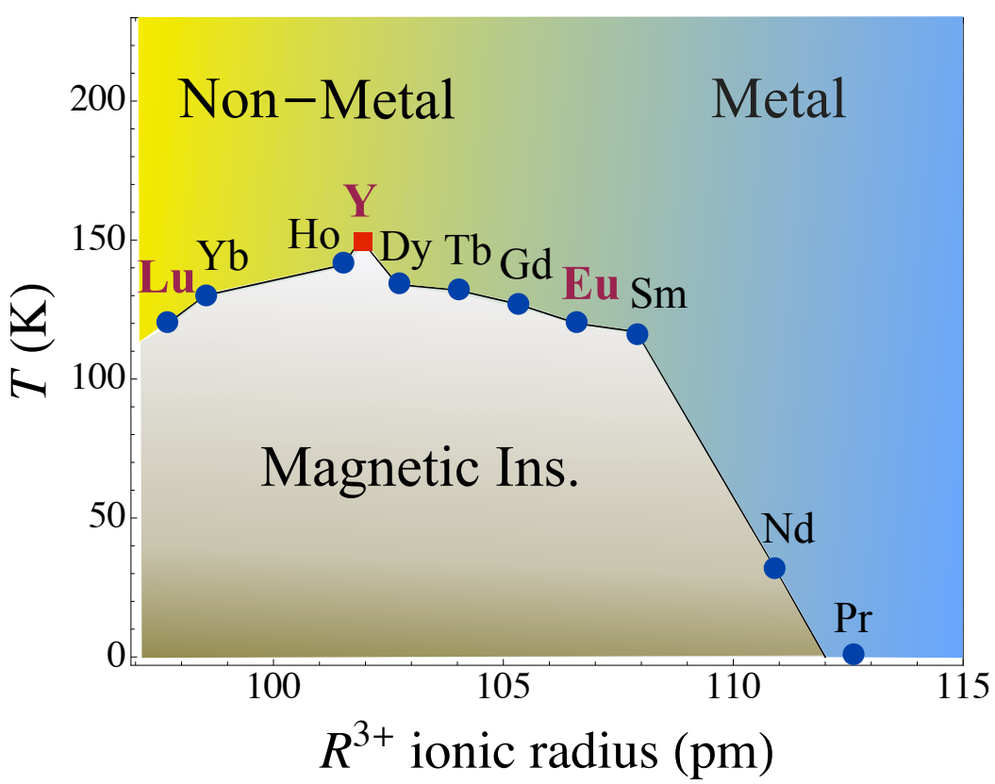


Moon et al, PRL 2013

Motivations

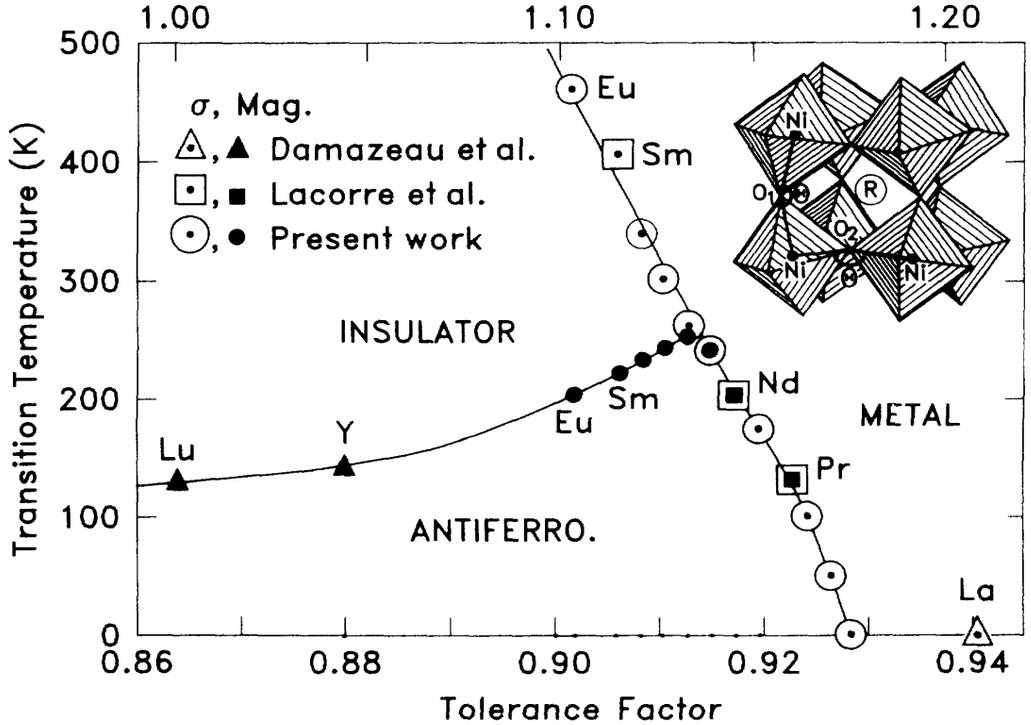
- What are the important microscopic parameters which drive the metal-insulator transition? What drives MIT?

$R_2Ir_2O_7$



K. Matsuhira et al, JPSJ 2011
W. Witczak-Krempa et al, ARCMP 2013

$RNiO_3$
$RTiO_3$

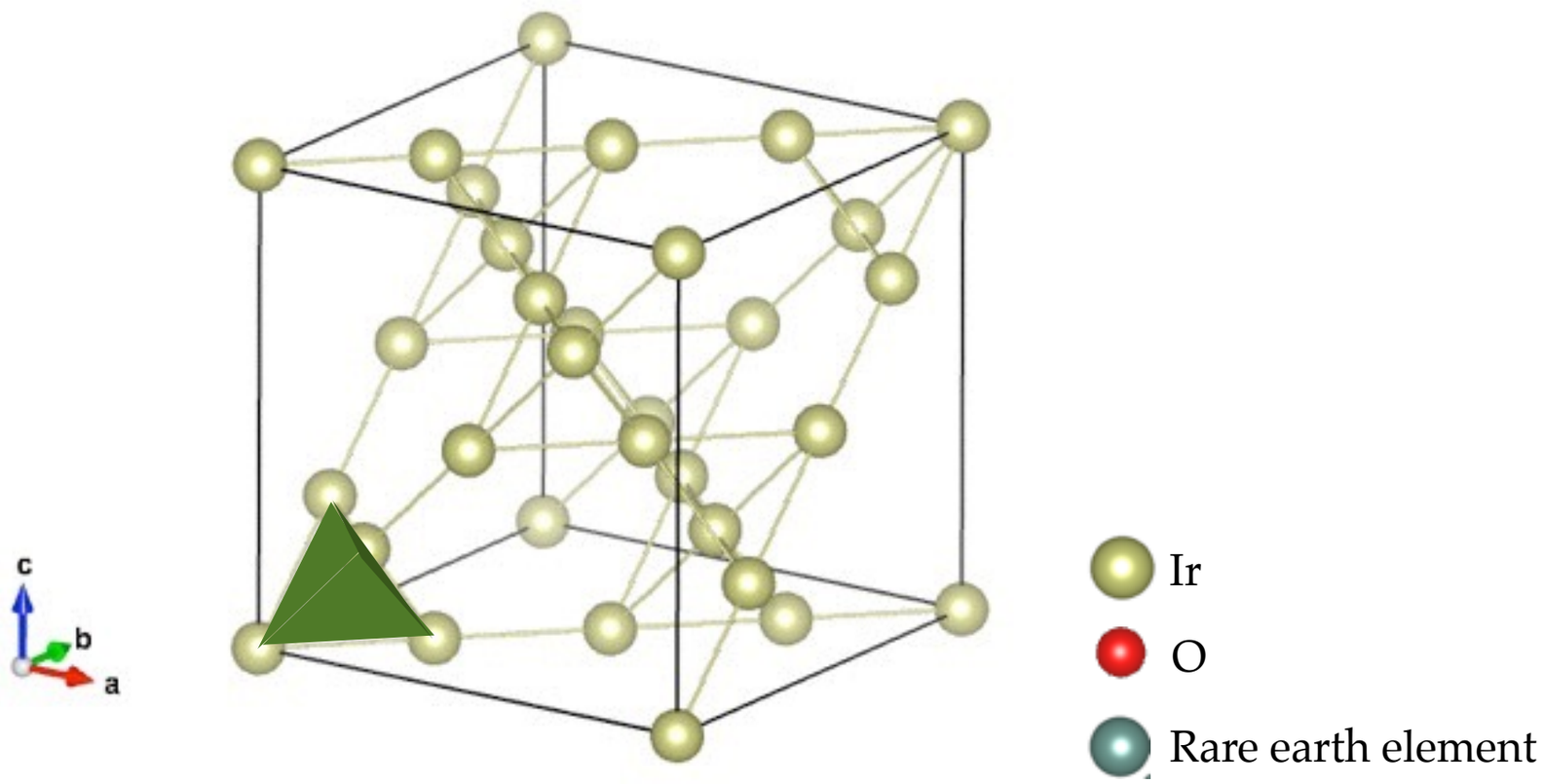


Lacorre et al, PRB 1992

Review on Pyrochlore Iridates $R_2Ir_2O_7$

- Structure of pyrocholre iridate $R_2Ir_2O_7$:

  FCC corner sharing tetrahedra
- Ir-O-Ir bonds are distorted, compressed along 111 direction



Review on Pyrochlore Iridates $R_2Ir_2O_7$

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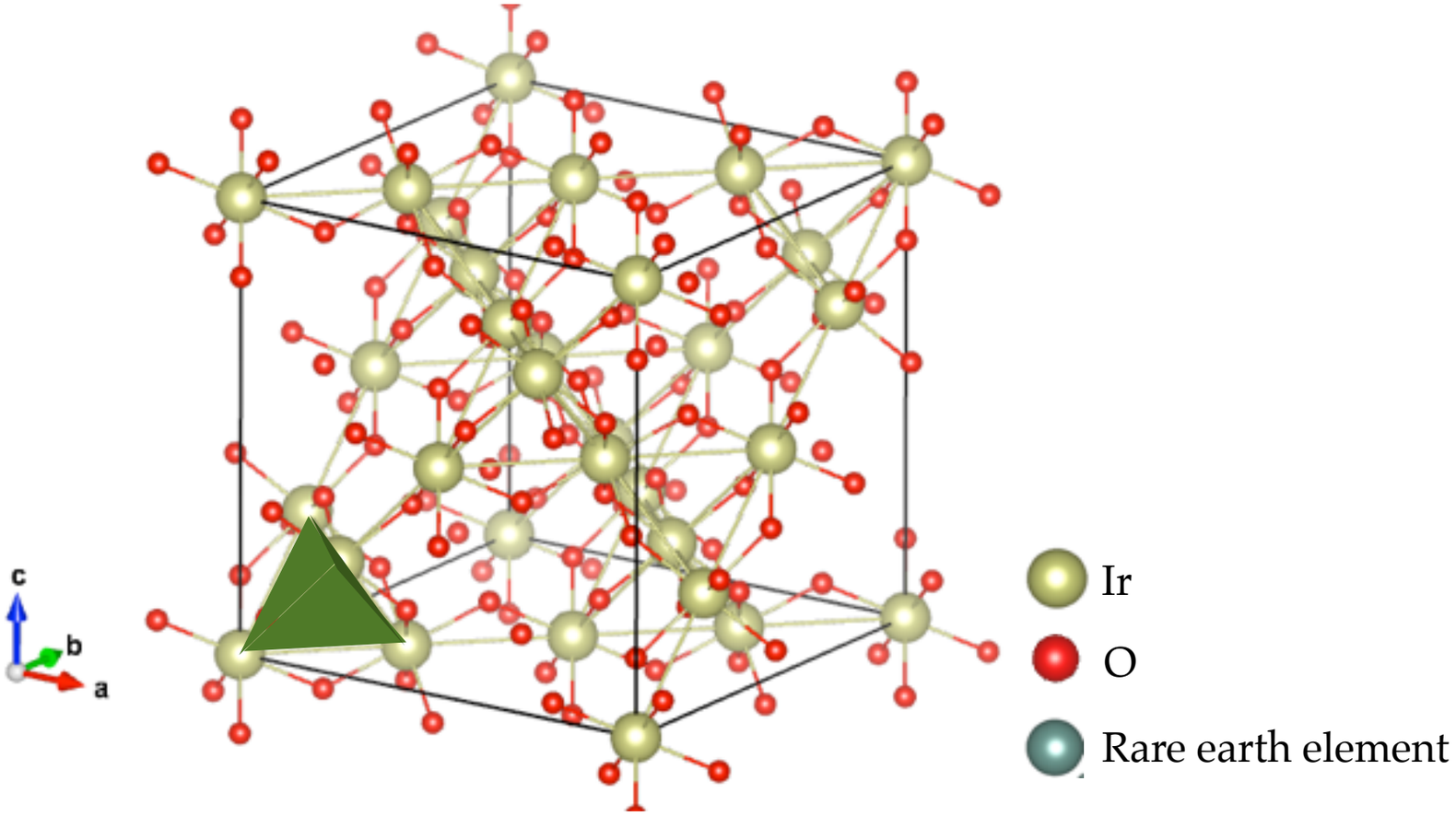

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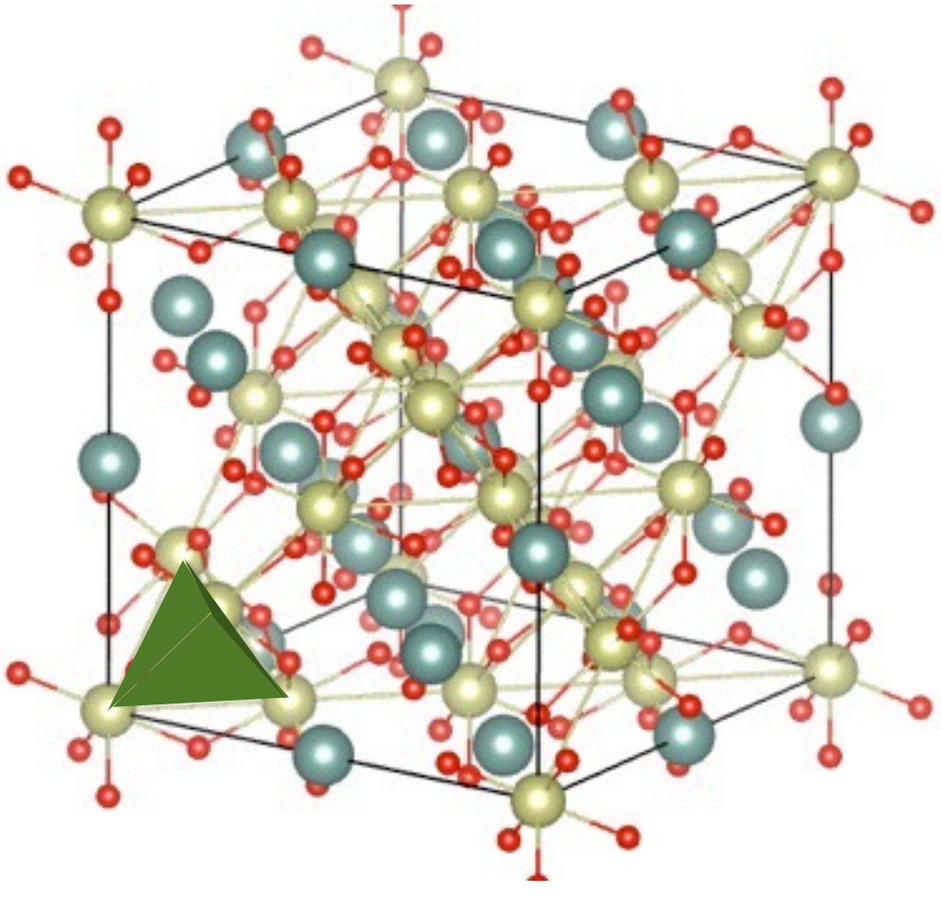
- Ir-O-Ir bond angle Y: ~129˚; Pr: ~132˚

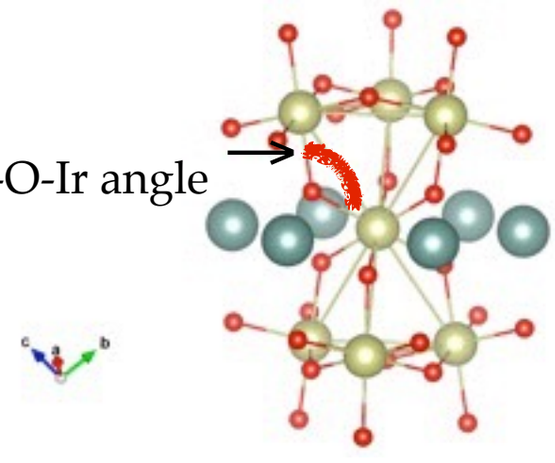


Ir

O

Rare earth element

Ir-O-Ir angle



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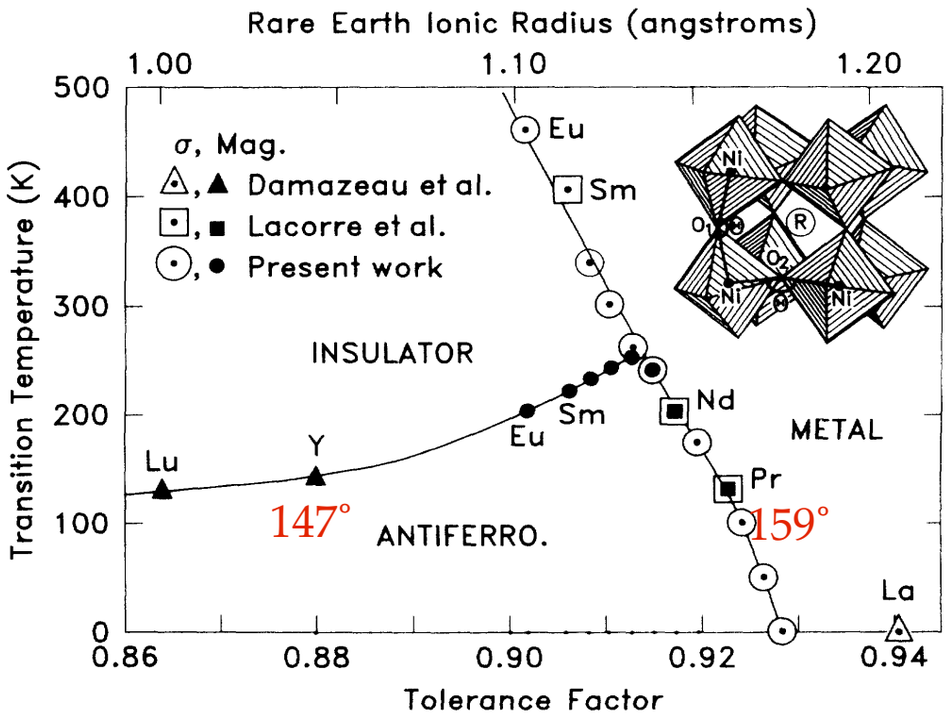
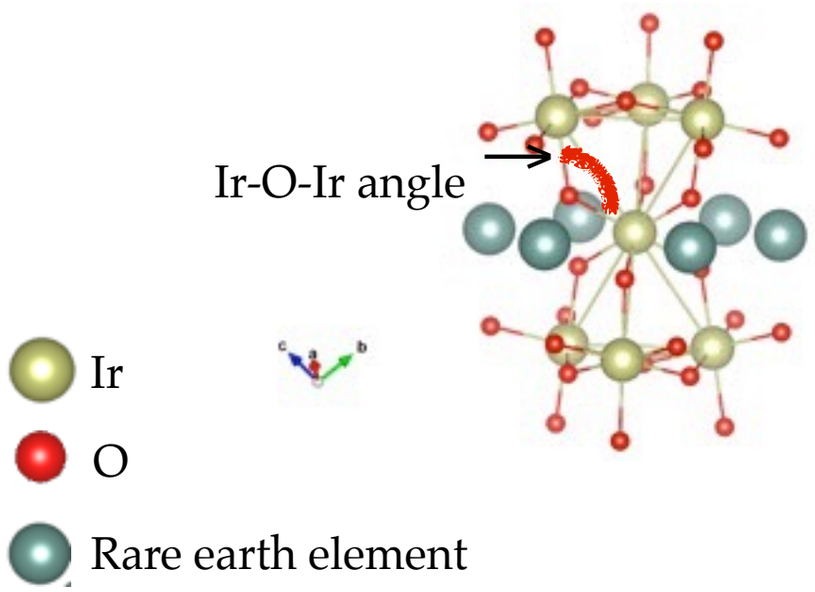


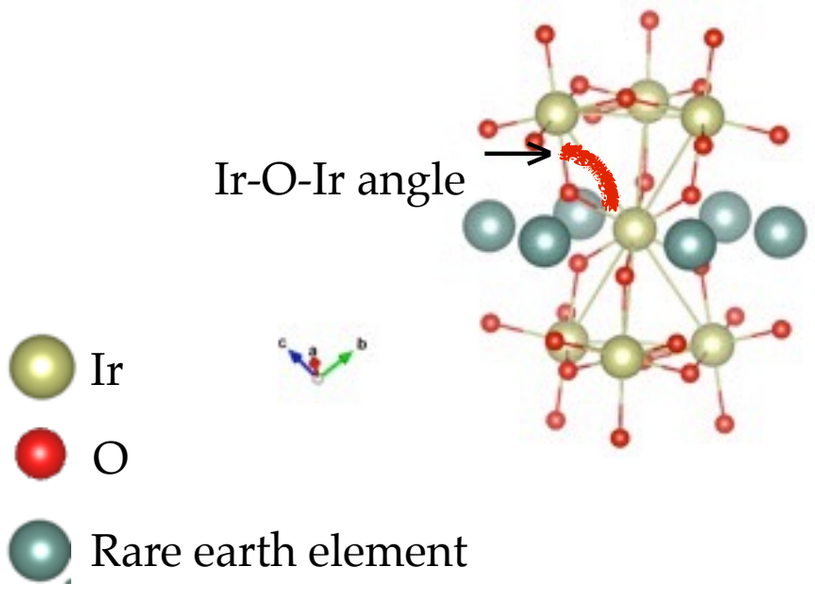
$RNiO_3$



Review on Pyrochlore Iridates $R_2Ir_2O_7$

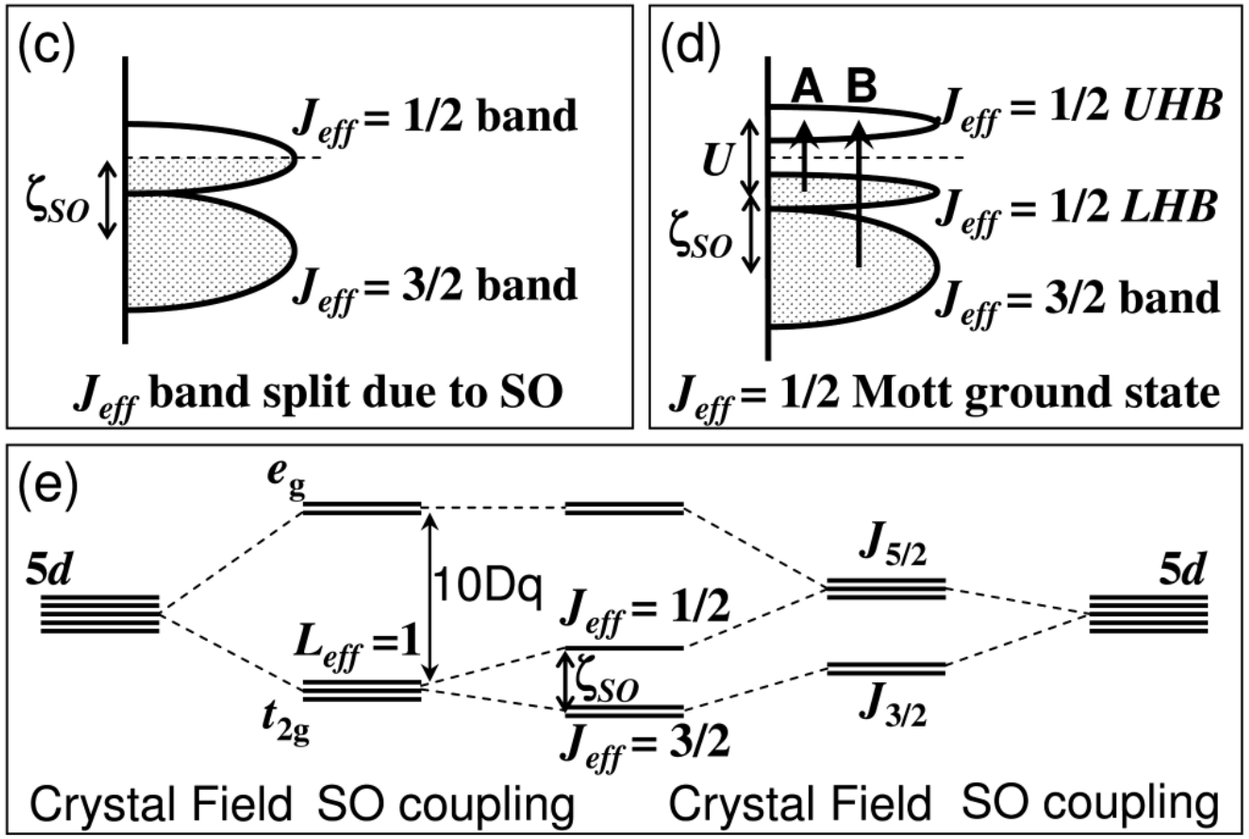
- Structure of pyrocholre iridate $R_2Ir_2O_7$:

  FCC corner sharing tetrahedra
- Ir-O-Ir bond are distorted, compressed along 111 direction
- Ir-O-Ir bond angle Y: ~129˚; Pr: ~132˚
- Ir-O bond length Y: 1.997Å ; Pr: 2.014Å
- Ir-Ir bond length Y: 3.599Å ; Pr: 3.677Å



Review on Pyrochlore Iridates $R_2Ir_2O_7$

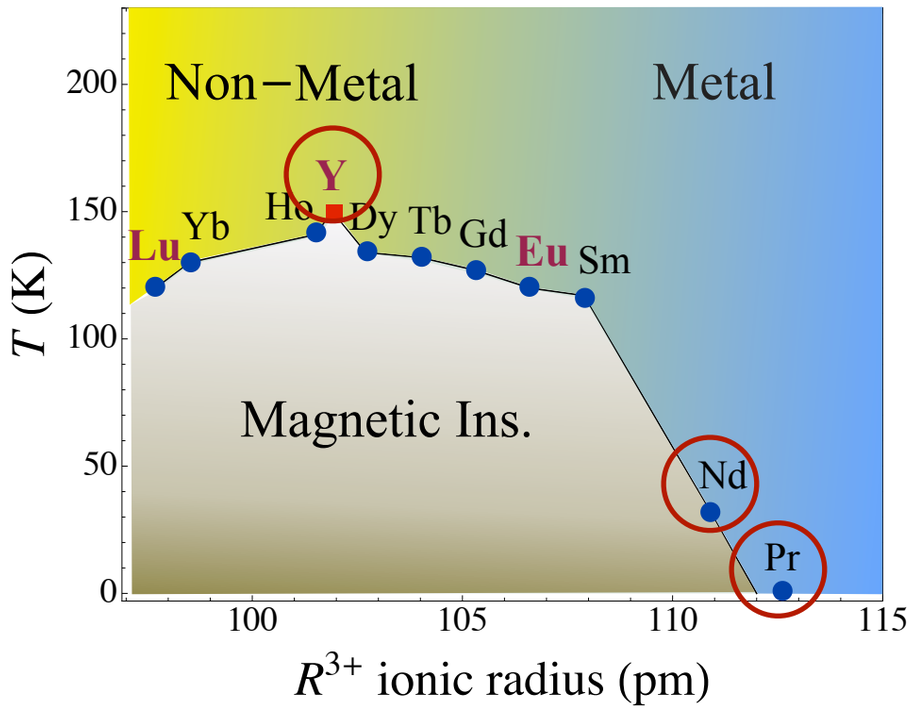
- Ionic picture: Ir^{4+} $5d^5$
- J_{eff}=1/2 doublet



B.J.Kim et al, PRL 2008

Paramagnetic band structure calculation

- Focus on Pr, Nd, Y
- Various functional to explore the trend: GGA+SO, LDA+SO, mBJ+SO
- All electronic potential Wien2k

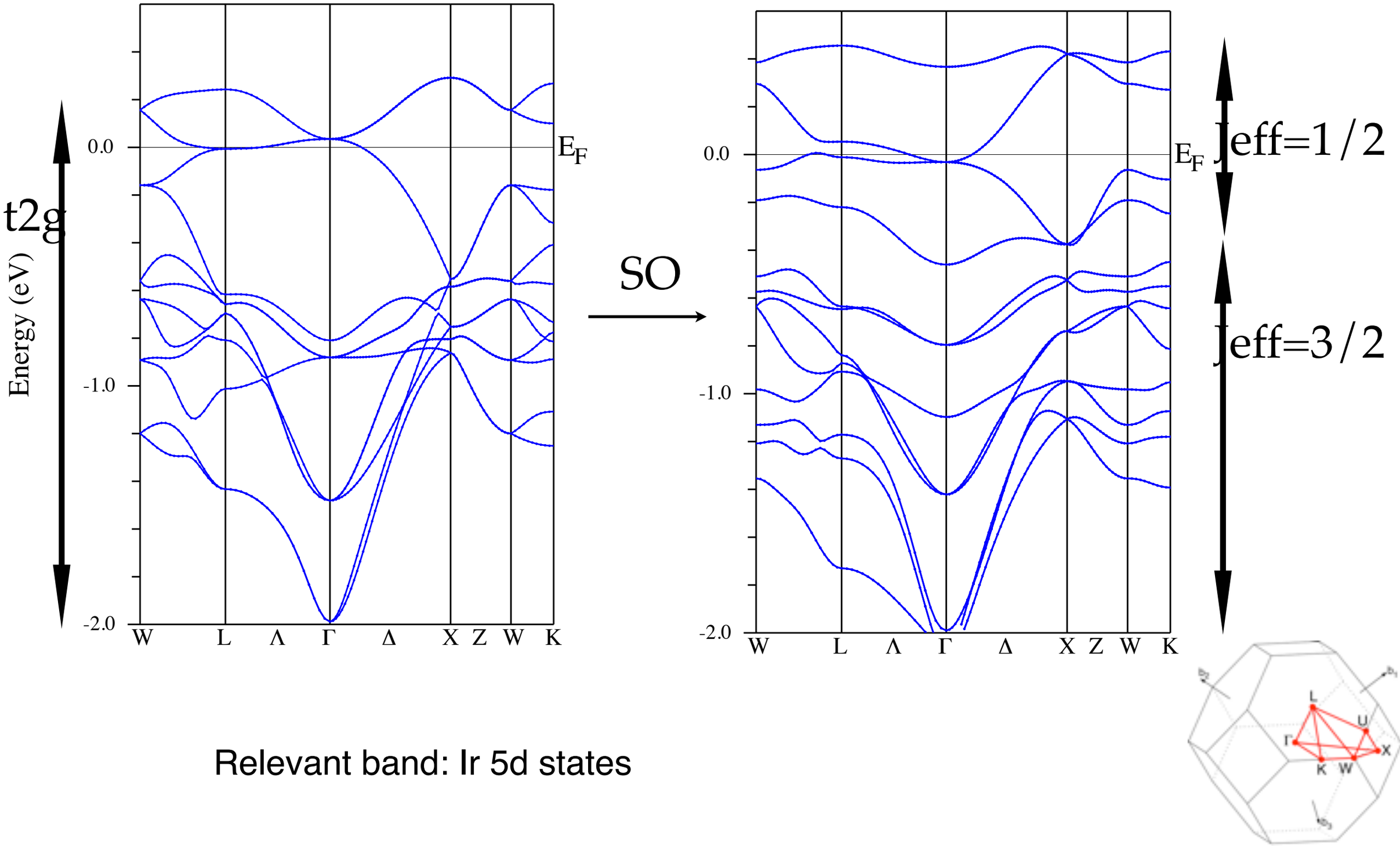


K. Matsuhira et al, JPSJ 2011
W. Witczak-Krempa et al, ARCMP 2013

$Pr_2Ir_2O_7$

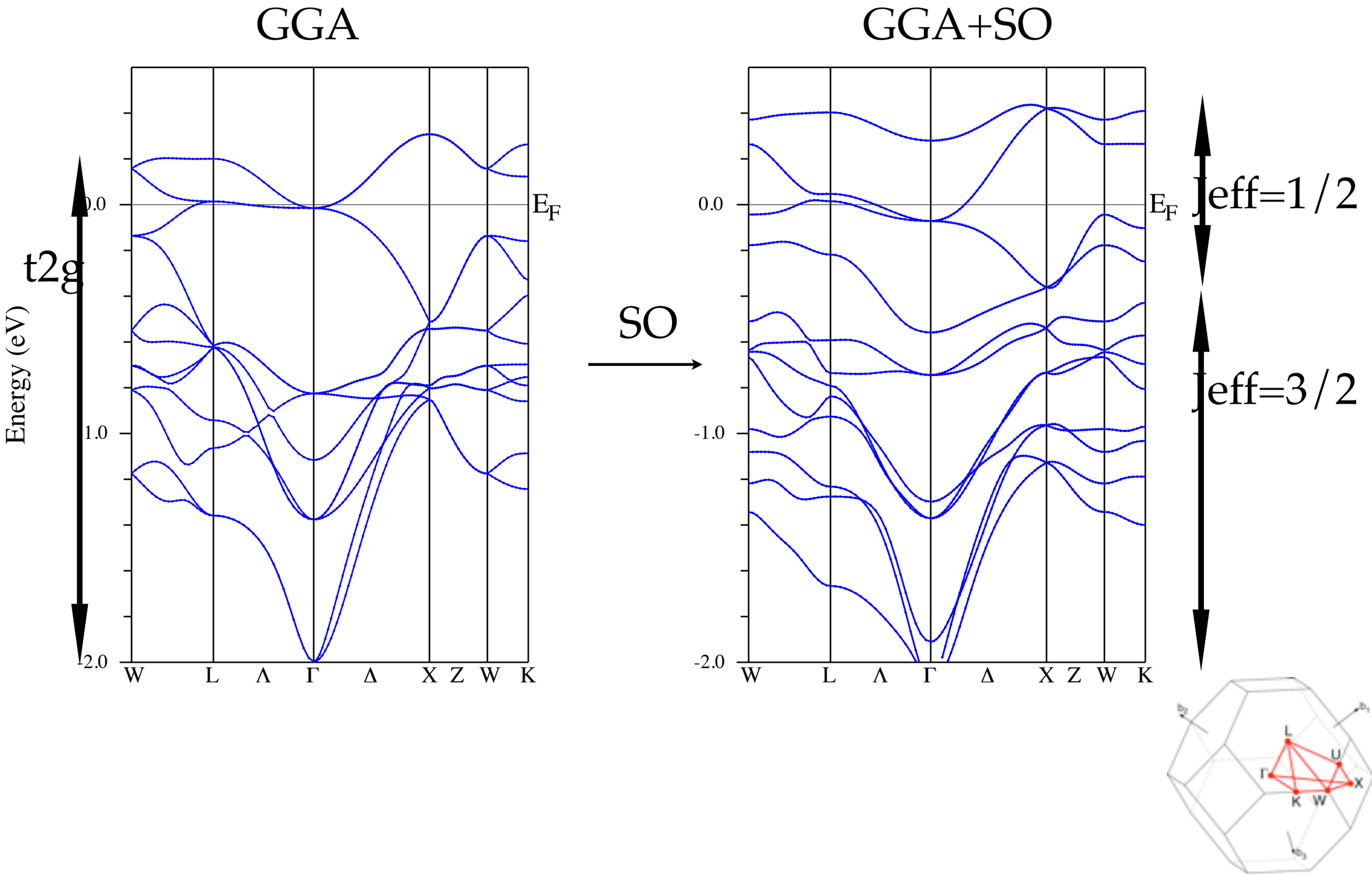
GGA

GGA+SO



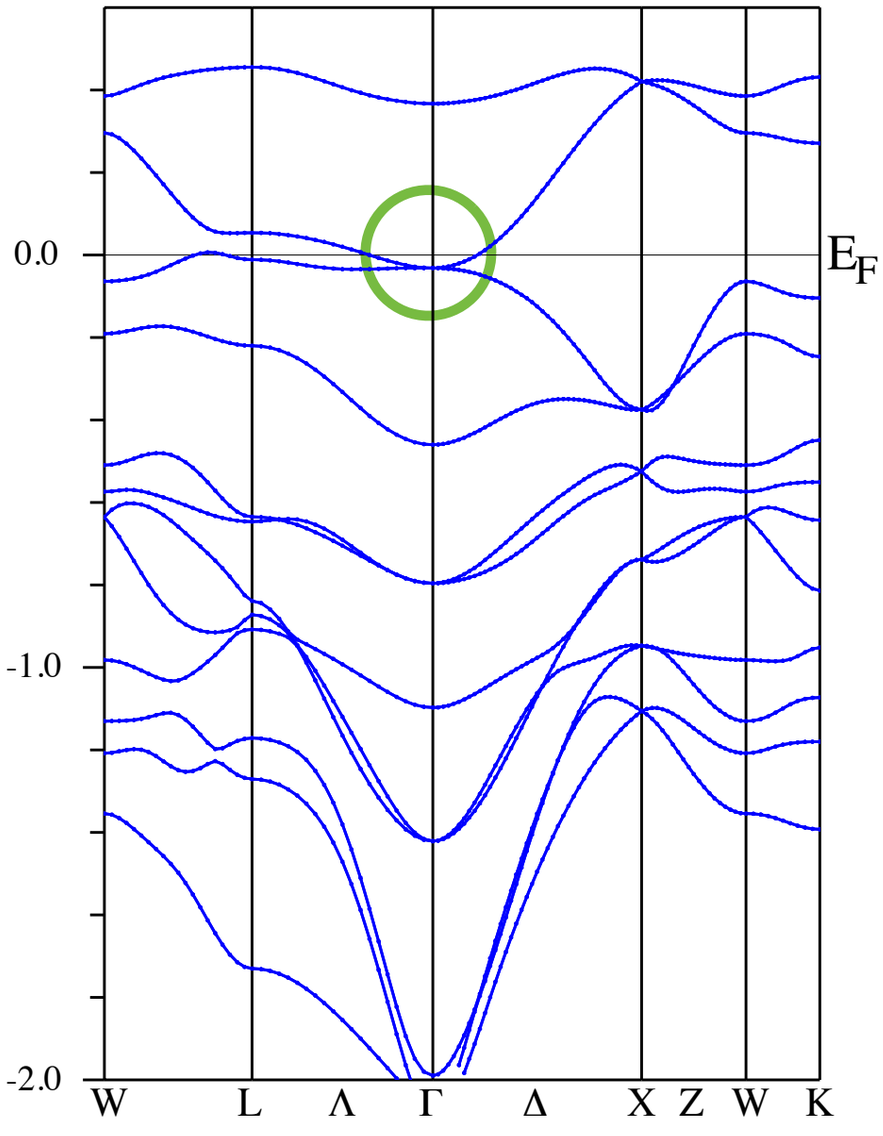
Relevant band: Ir 5d states

$Y_2Ir_2O_7$


GGA
GGA+SO
SO
t2g
Jeff=1/2
Jeff=3/2
Energy (eV)
0.0
1.0
2.0
-1.0
-2.0
E_F
W L Λ Γ Δ X Z W K
L
U
Γ
X
K
W

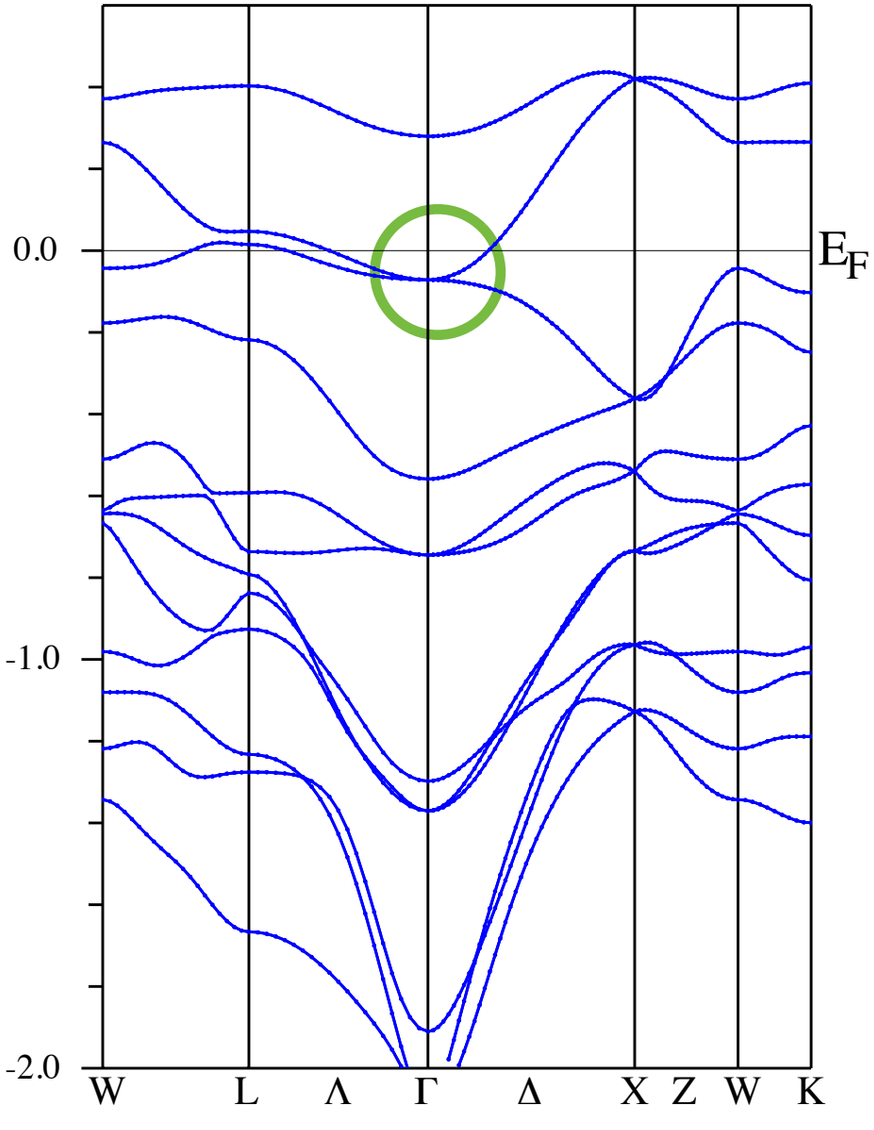
Comparison: $Pr_2Ir_2O_7$ and $Y_2Ir_2O_7$

GGA+SO



Pr2Ir2O7

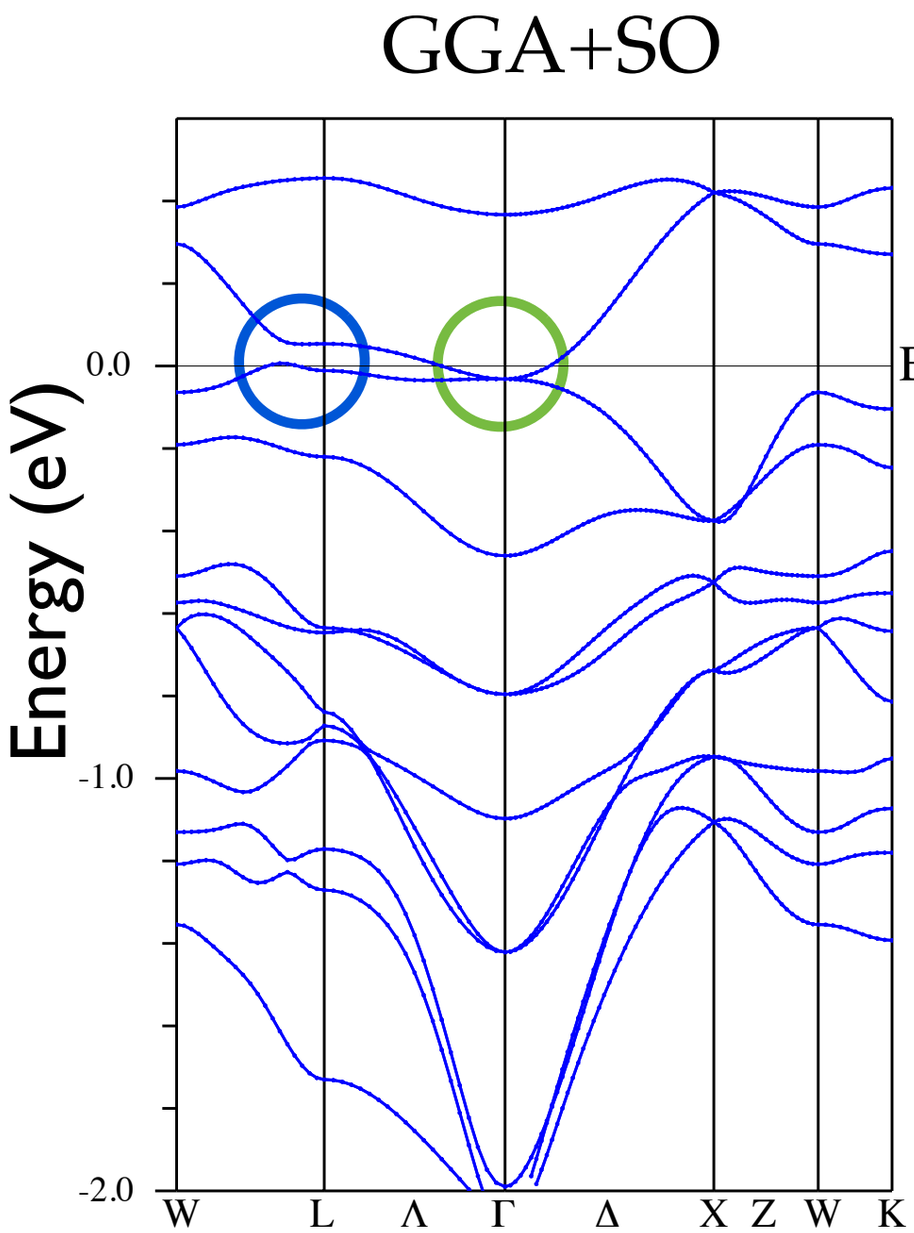
GGA+SO



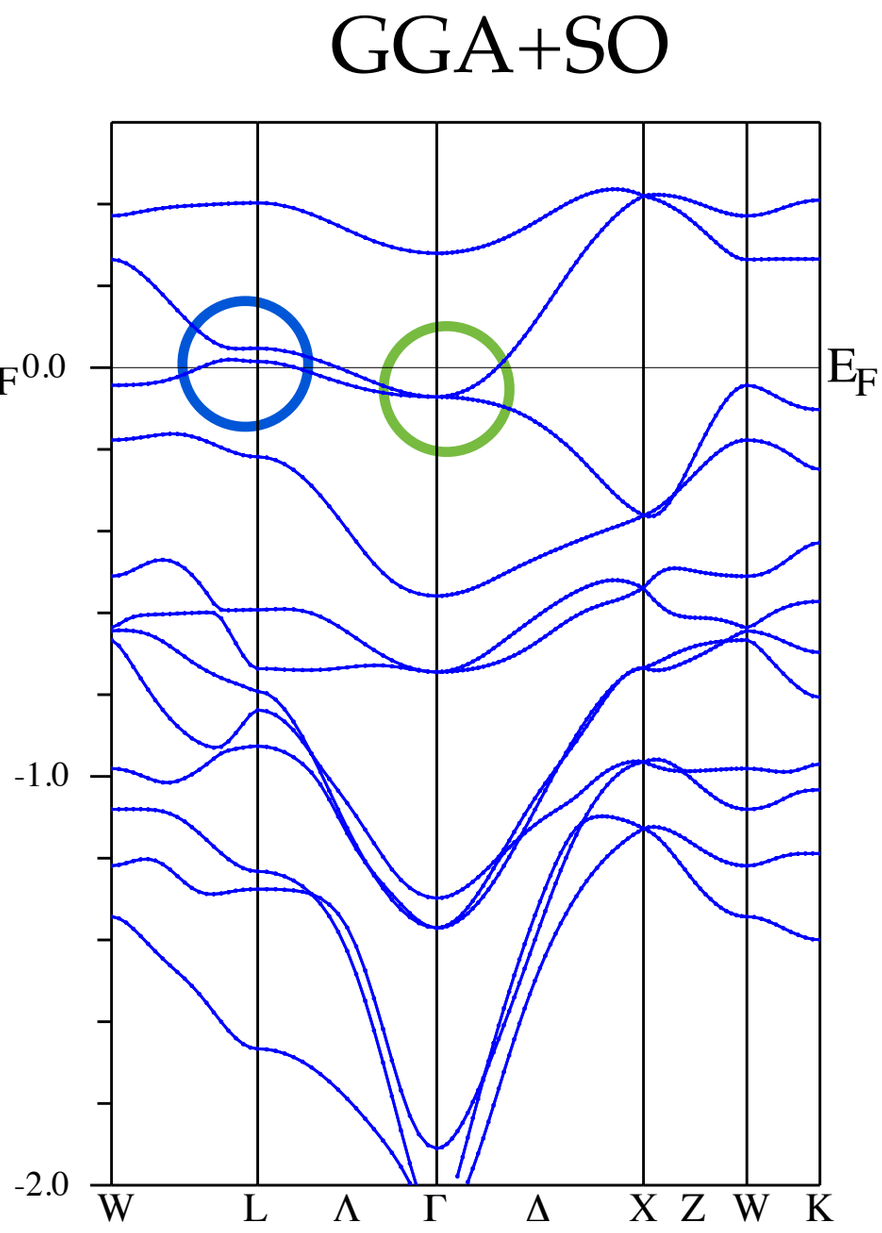
Y2Ir2O7

4-fold quadratic band touching is protected by TR and cubic symmetry.

Comparison: $Pr_2Ir_2O_7$ and $Y_2Ir_2O_7$

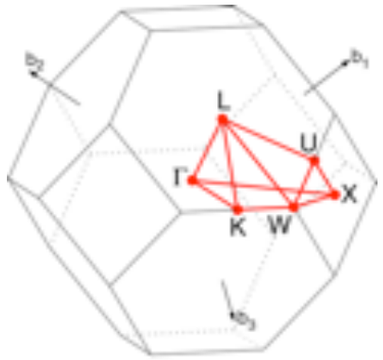


Pr2Ir2O7



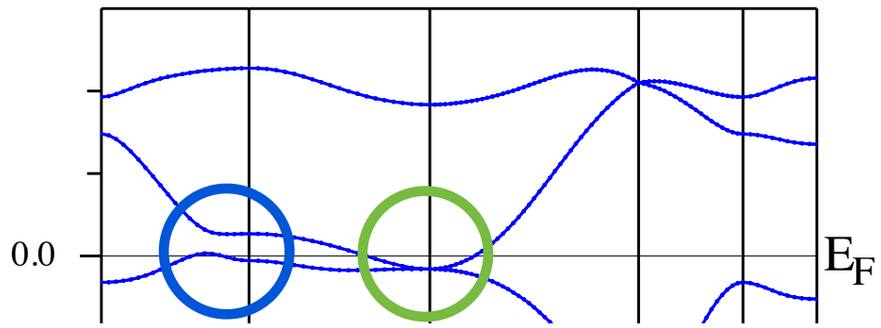
Y2Ir2O7

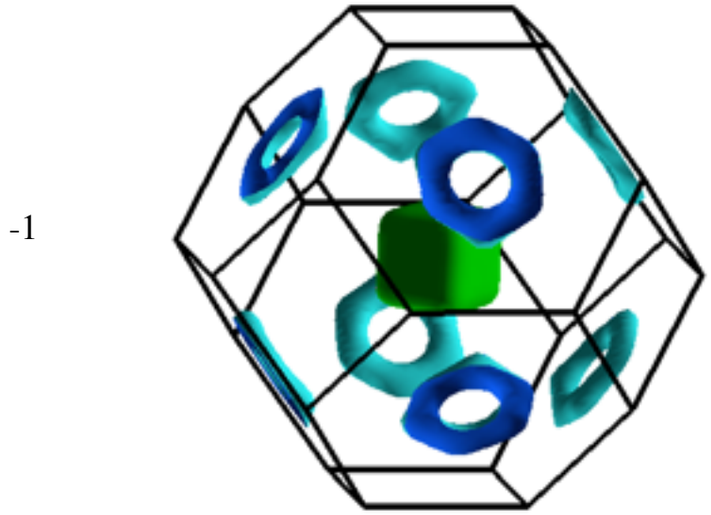
- Not band width tuned (hopping Ir-O-Ir, Ir-Ir competing)
- Very subtle changes near Ef
- Larger R is closer to quadratic band touching at Ef (R=Pr, Nd,Y)

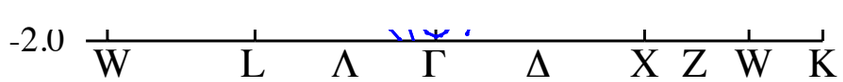


Comparison: $Pr_2Ir_2O_7$ and $Y_2Ir_2O_7$

GGA+SO

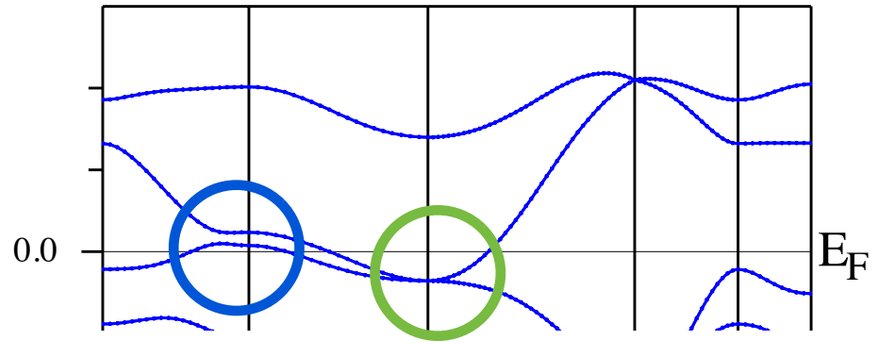


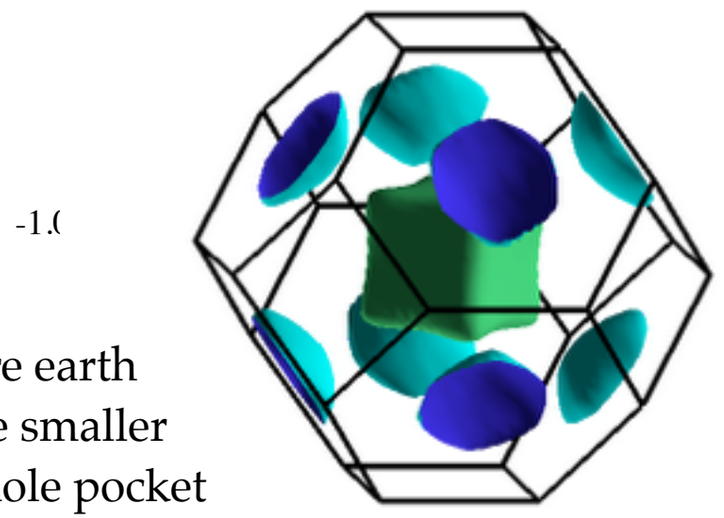


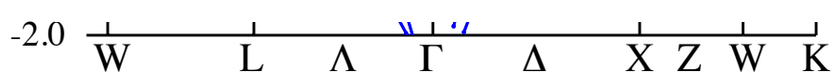


$Pr_2Ir_2O_7$

GGA+SO

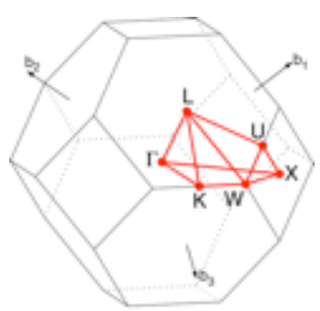






$Y_2Ir_2O_7$

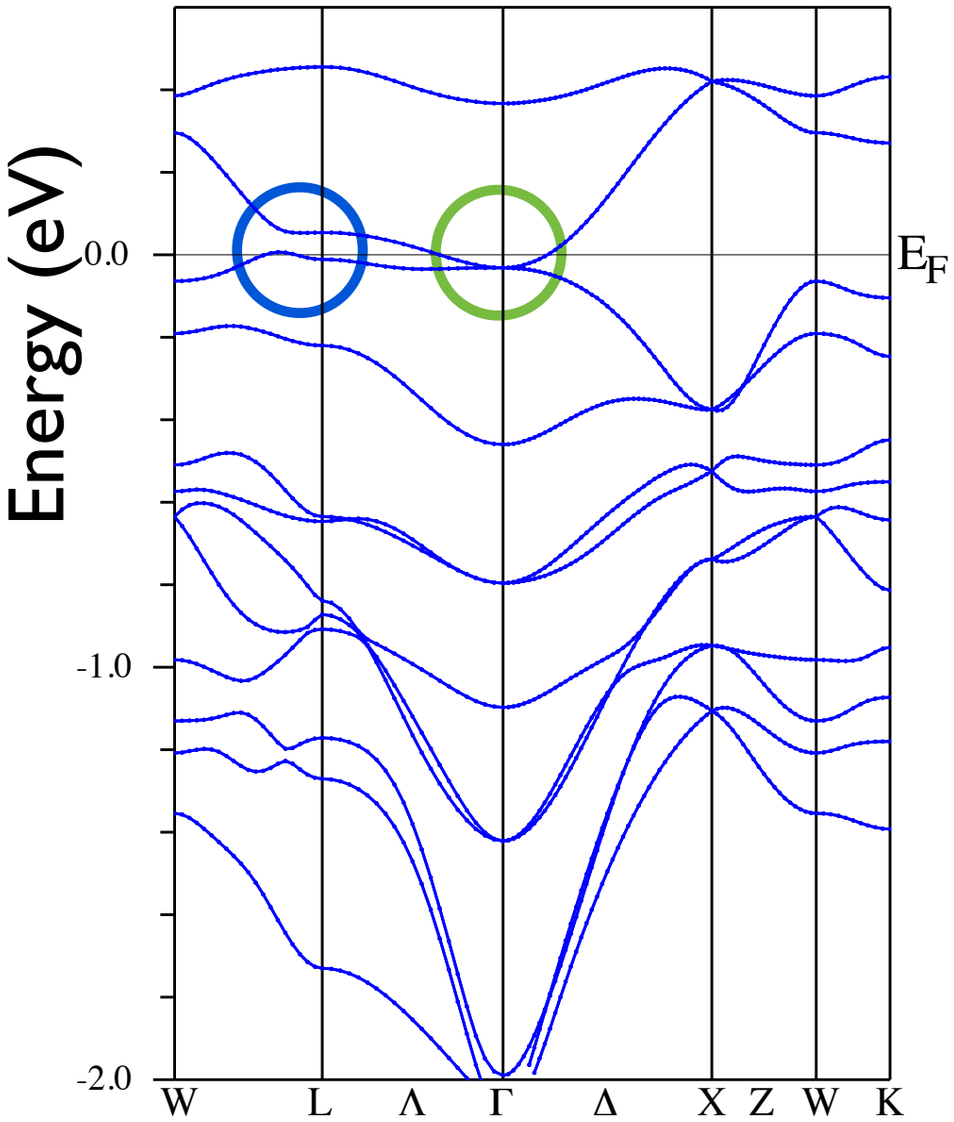
The bigger the rare earth ionic radius is, the smaller the electron and hole pocket Fermi surface is.



Why is Pr metallic and Y not?

Quadratic Band Touching State

GGA+SO



Pr2Ir2O7

- GGA+SO calculations show Pr2Ir2O7 is very close to quadratic band touching at the Fermi level.

- 4-fold degeneracy at the Γ point is protected by the cubic lattice symmetry, everywhere else gapped.

- GGA/LDA is well known for underestimating gaps.

- Modified Becke-Johnson potential gives band gap very close to experiments/GW calculation.

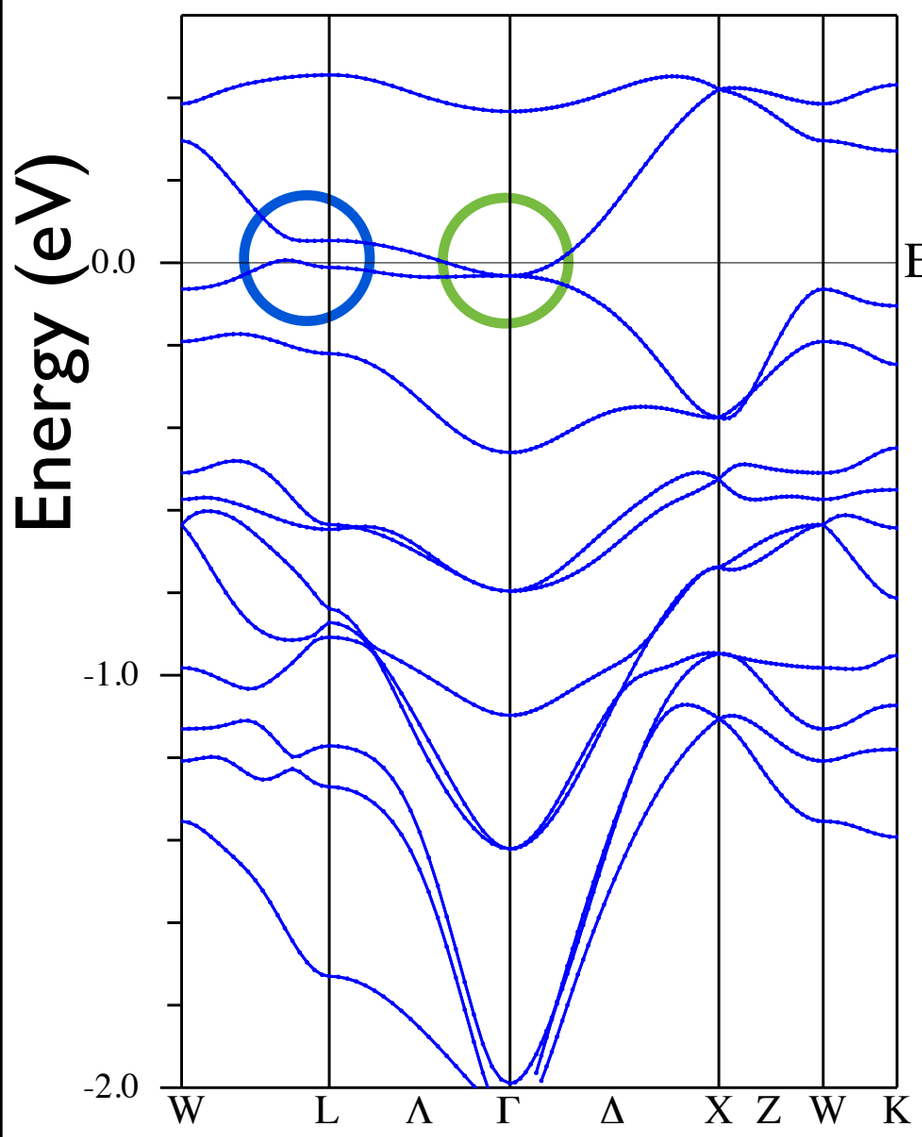
- Widely used for small gap semiconductor, topological insulator.

Quadratic Band Touching State

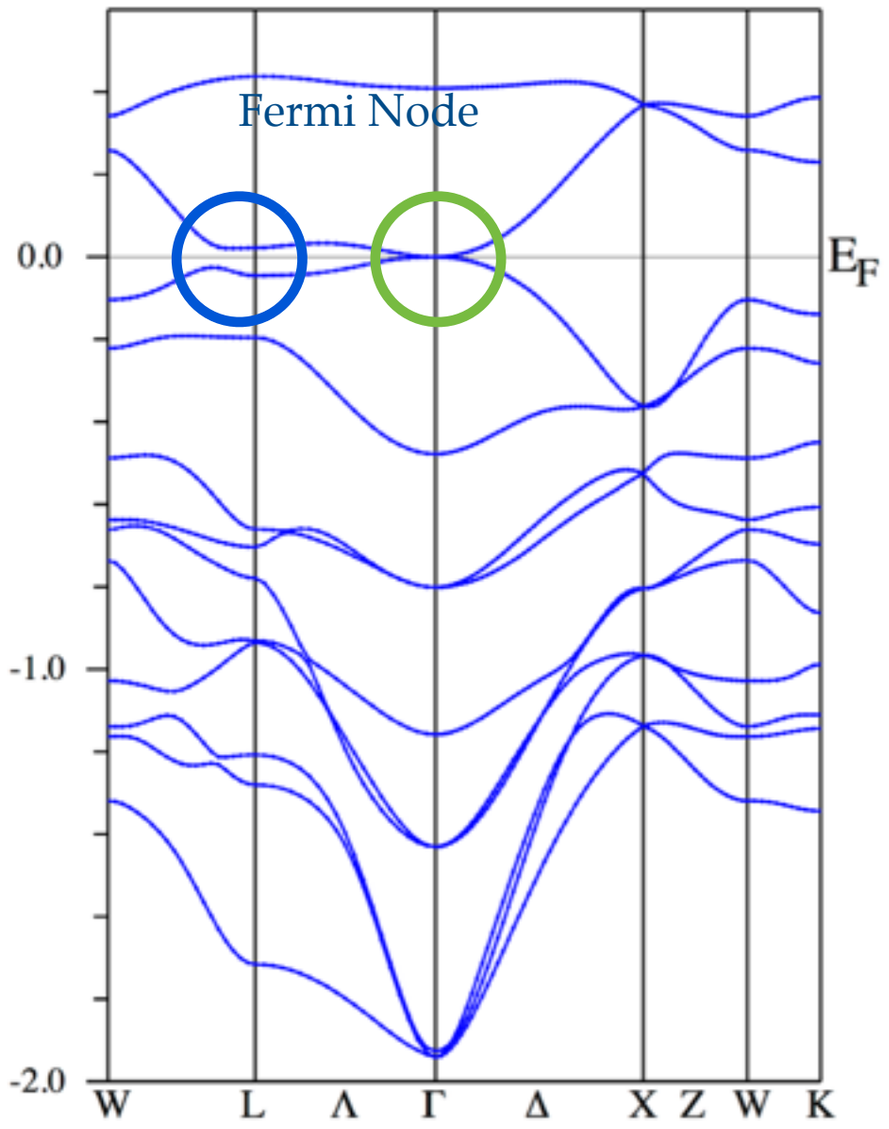
GGA+SO

MBJ+SO

(modified Becke-Johnson potential)



Pr2Ir2O7



Pr2Ir2O7

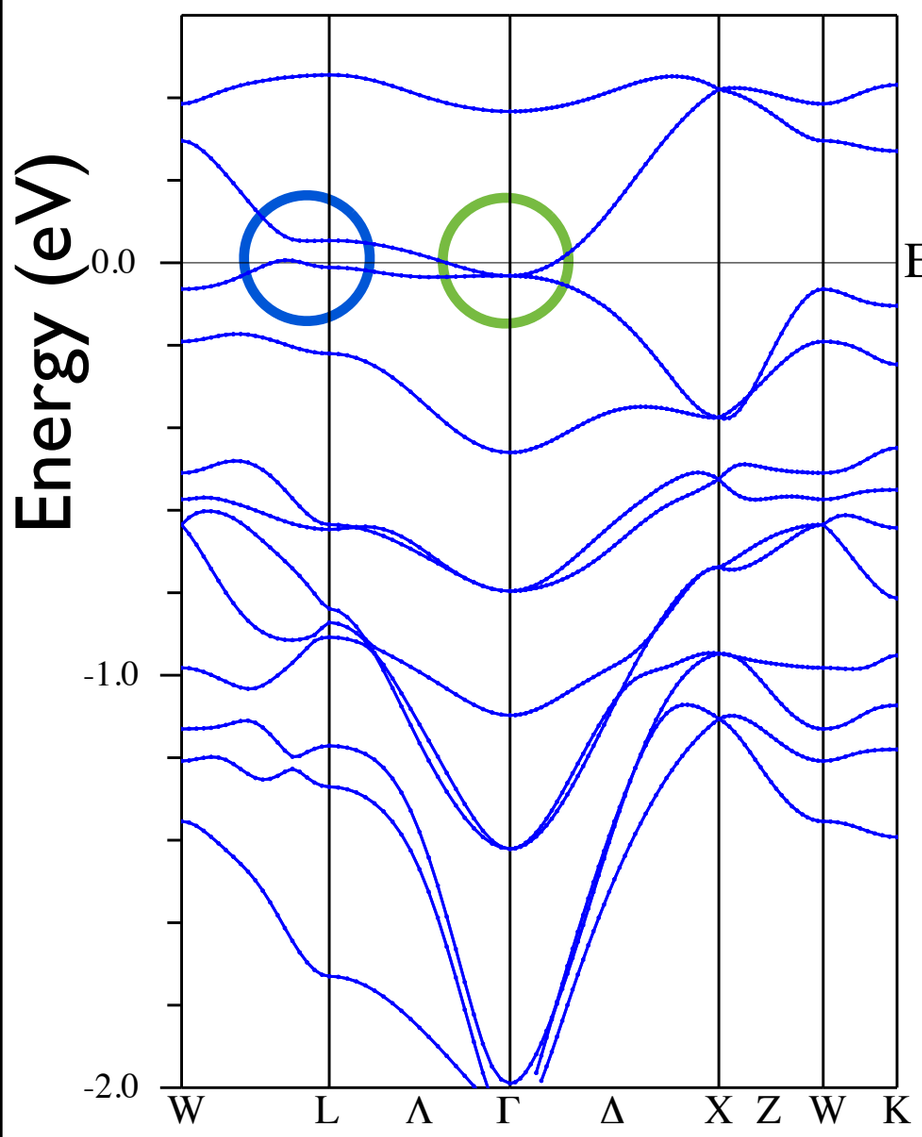
- Quadratic band touching at the Fermi level!
- Universal trend: larger R corresponds to smaller FS and closer to quadratic band touching at Ef regardless of methods

Quadratic Band Touching State

GGA+SO

MBJ+SO

(modified Becke-Johnson potential)



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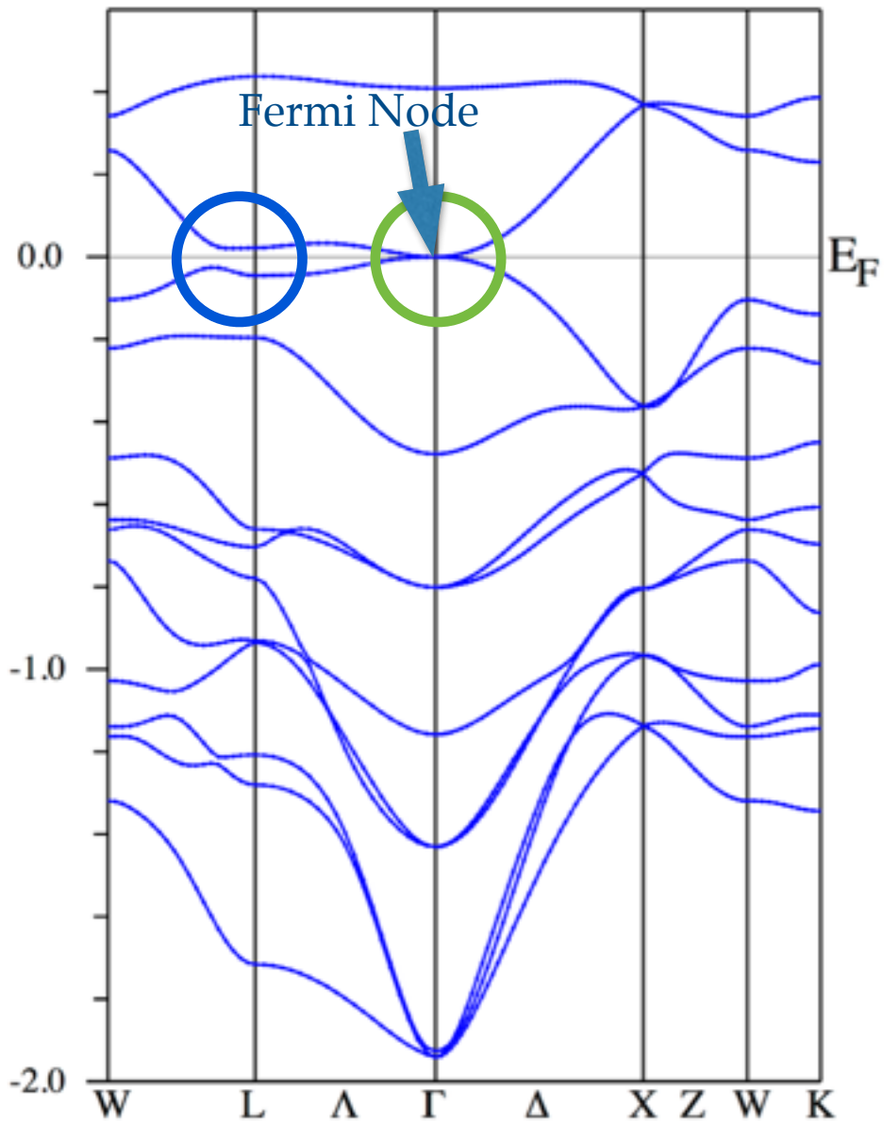

Pr2Ir2O7

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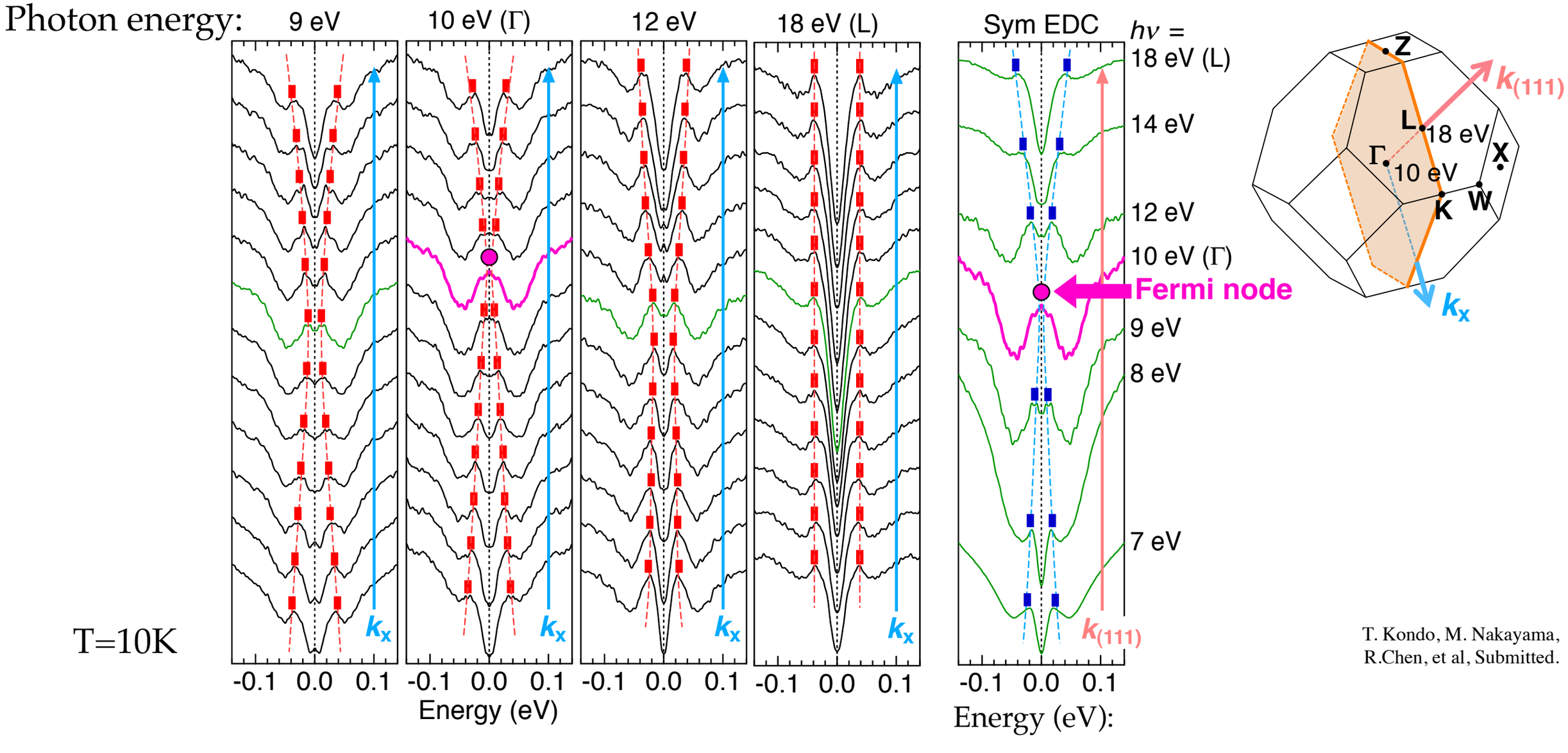
Quadratic Band Touching State

- Direct experimental evidence is strongly desired.
- ARPES result confirms the quadratic Fermi node!



T. Kondo, M. Nakayama, R.Chen, et al, Submitted.

Quadratic Band Touching State

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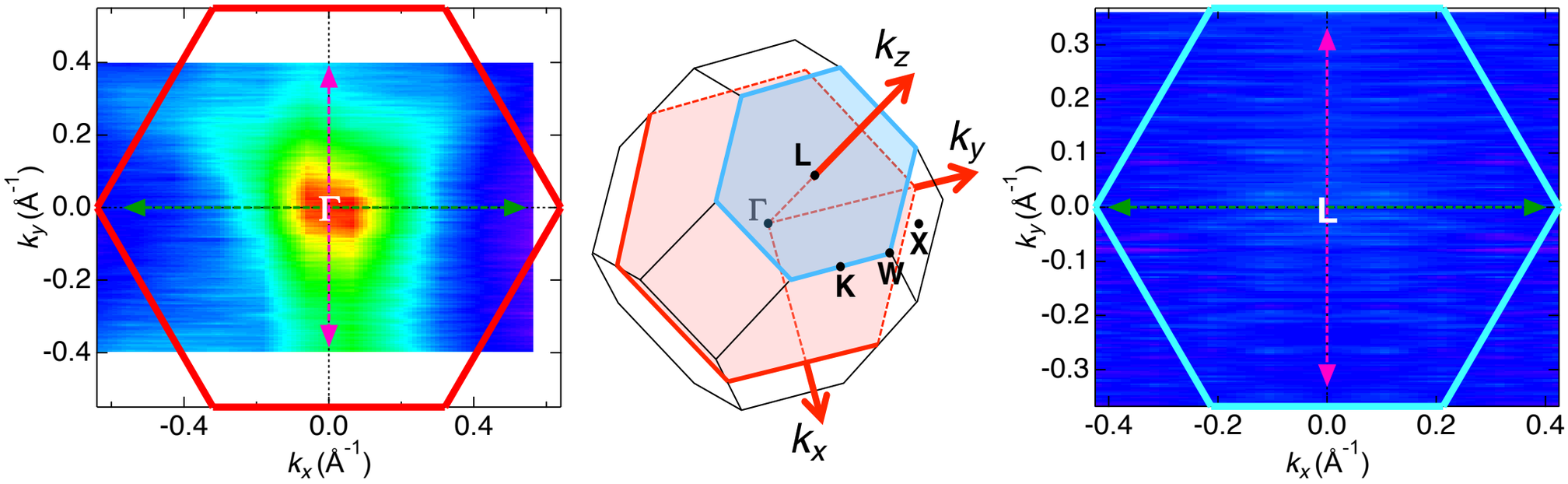


A quadratic band touch only at gamma,
and there is no other FS crossings around L.

Quadratic Band Touching State

- k.p theory, Luttinger Hamiltonian around Γ point with cubic symmetry

$$\mathcal{H}_0(k) = \frac{k^2}{2\tilde{M}_0} + \frac{\frac{5}{4}k^2 - (\vec{k}\cdot\vec{J})^2}{2m} - \frac{(k_x^2 J_x^2 + k_y^2 J_y^2 + k_z^2 J_z^2)}{2M_c}$$

E.-G. Moon et al, PRL 2013

- Jeff= 3/2 matrix
- Similar to electronic structure of semiconductors with diamond structure and zinc blende structure in terms of the k·p perturbation theory
- Effective mass fitting to the band structure:

M_0 = 19.97 me, m = 6.30 me , M_c = 7.44 me

Quadratic Band Touching State

- k.p theory, Luttinger Hamiltonian around Γ point with cubic symmetry

$$\mathcal{H}_0(k) = \frac{k^2}{2\tilde{M}_0} + \frac{\frac{5}{4}k^2 - (\vec{k}\cdot\vec{J})^2}{2m} - \frac{(k_x^2 J_x^2 + k_y^2 J_y^2 + k_z^2 J_z^2)}{2M_c}$$

E.-G. Moon et al, PRL 2013

- Strain/pressure will break the cubic symmetry

$$\mathcal{H}' = -\delta(J_z^2 - \frac{5}{4})$$

- Consider strain/pressure along (111) direction

$$\mathbf{k} = k\hat{n}_{(111)}$$

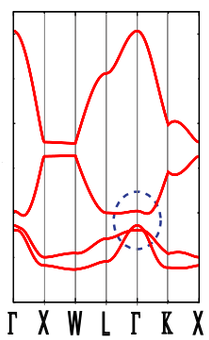
$$E_{\pm}(k) = \frac{k^2}{2M_0} \pm \sqrt{(\frac{k^2(m+M_c)+2\delta m M_c}{2mM_c})^2}$$

- δ>0, opens up a gap at Γ point (topological insulator?)

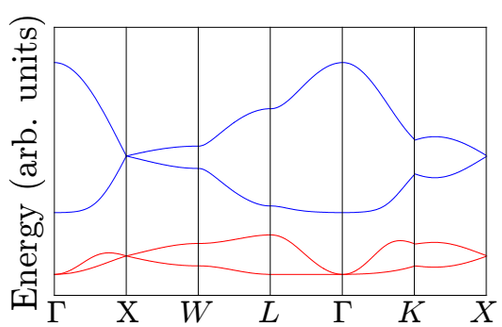
  δ<0, bands crossing along (111) direction

Quadratic Band Touching State

- Several tight-binding studies suggest that pressure would produce topological insulator.



B.-J. Yang et al, PRB2010



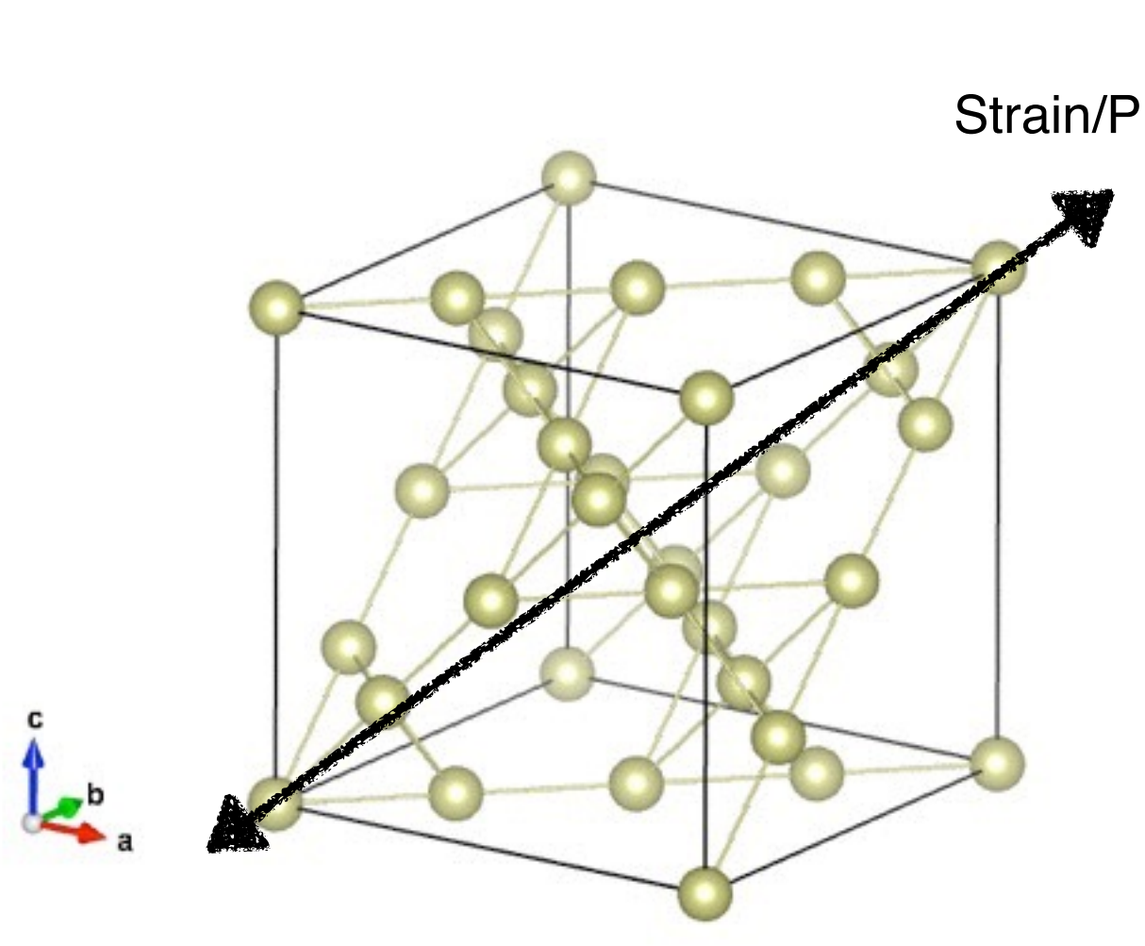
D.A. Pesin et al, Nat phys (2010)

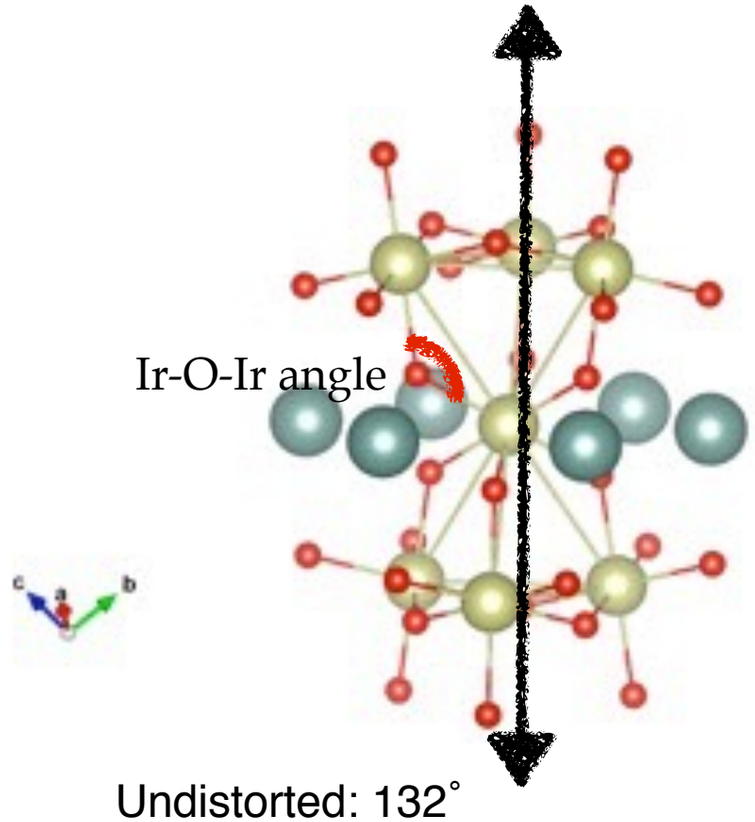
Without pressure, didn't take
Ir-Ir direct hopping into account

- Ir 5d states are quite extended and a tight-binding model will require many parameters for a good fit. It will be interesting to see full ab initio calculation!
- Ab initio results show that $Pr_2Ir_2O_7$ is closest to quadratic band touching at Fermi energy ⟶ it should be very sensitive to strain/pressure!

Pressure/Strain effect on Pyrochlore

- Uniaxial pressure/Strain along (111) direction
- Cubic -> Rhombohedral symmetry
- Full lattice relaxation both on the lattice parameter and the atom positions.



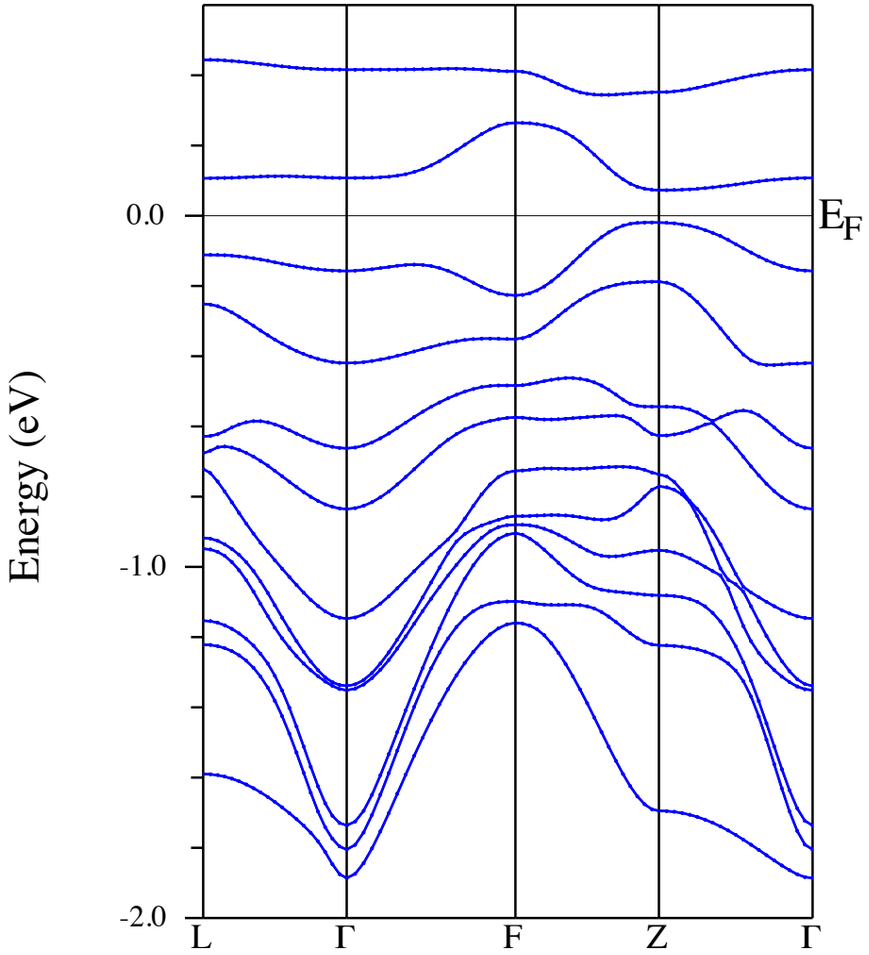


Undistorted: 132˚
Increase pressure: bond angle<132˚
Decrease pressure: bond angle>132˚

Pressure/Strain effect on Pyrochlore

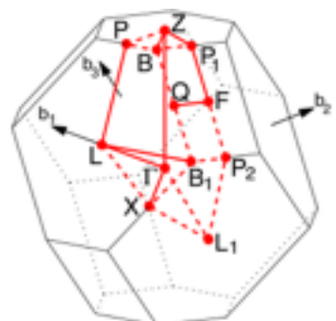
- Pressure/Strain along (111) direction
- Cubic -> Rhombohedral symmetry
- Compressive pressure (in-plane tensile strain)

  $c=0.96c_0$, $a=1.05a_0$



Full lattice relaxation: GGA

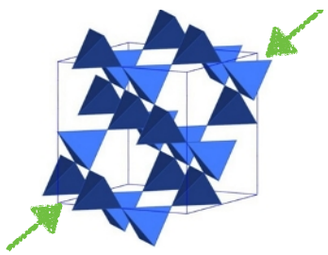
both GGA+SO and mBJ+SO calculation
Insulator
mBJ+SO gap=0.09eV

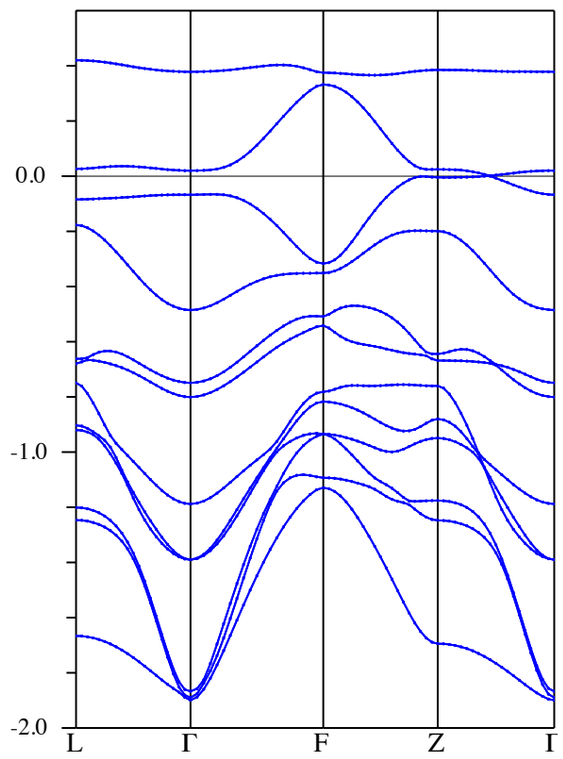


Pressure/Strain effect on Pyrochlore

- Pressure/Strain along (111) direction
- Cubic -> Rhombohedral symmetry
- Compressive pressure (in-plane tensile strain)

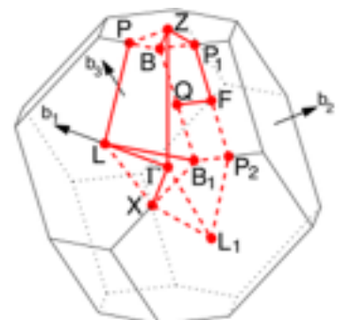
  $c=0.99c_0$, $a=1.01a_0$





Full lattice relaxation: GGA

both GGA+SO and mBJ+SO calculation
Insulator
mBJ+SO gap>0eV



Pressure/Strain effect on Pyrochlore

- Compressive pressure (tensile strain)

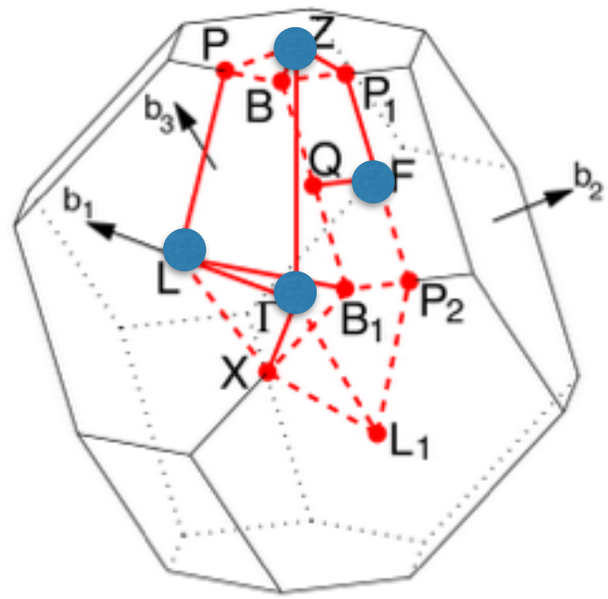
c=0.96c0, a=1.05a0

$$\delta_a = \prod_m \xi_m(\Lambda_a)$$

Parity at time reversal invariant momenta:

Γ	L	Z	F
+	-	-	-

Z_2 invariant (1; 000)

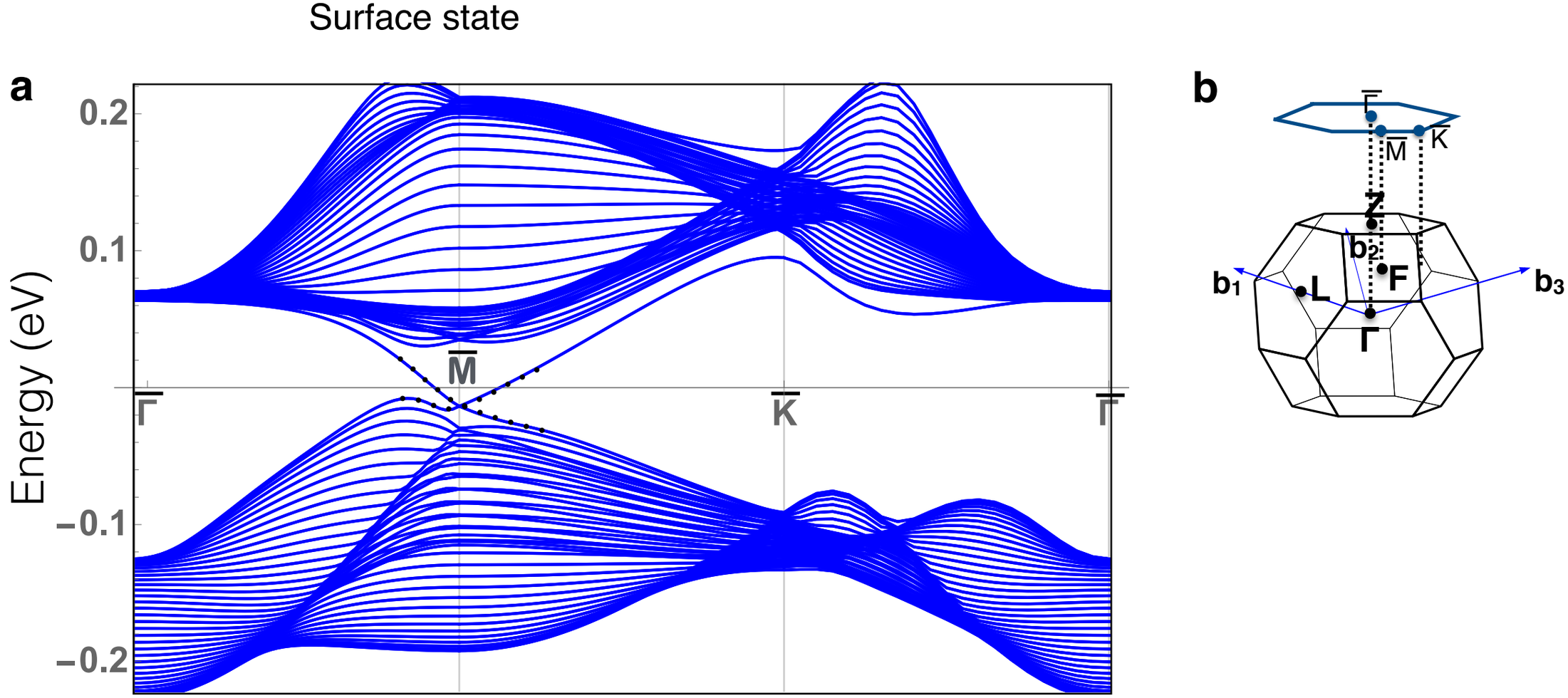


Compressive pressure/ tensile strain along (111) direction will make $Pr_2Ir_2O_7$ a topological insulator!

Pressure/Strain effect on Pyrochlore

- Compressive pressure (tensile strain)

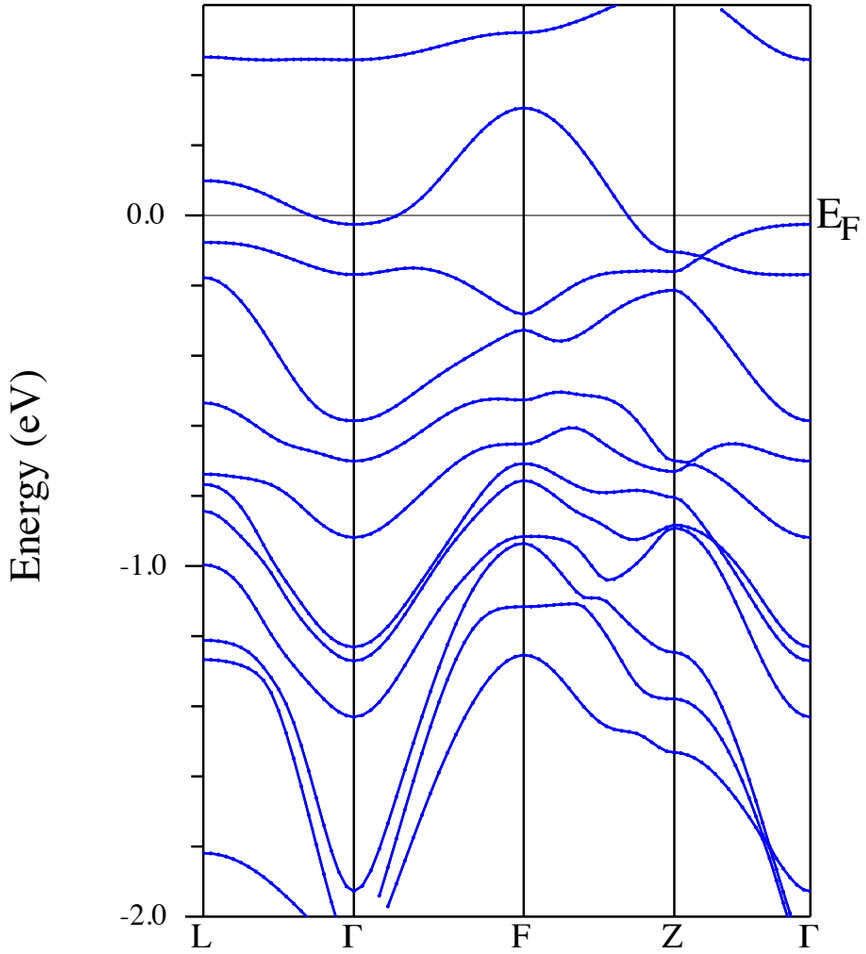
  c=0.96c0, a=1.05a0



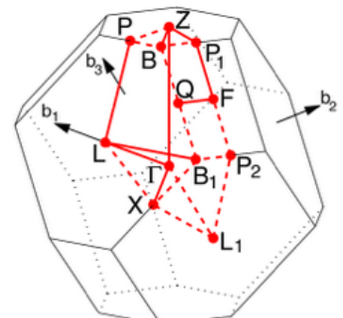
Pressure/Strain effect on Pyrochlore

- Reducing pressure (in-plane compressive strain)

  $c=1.06c_0$, $a=0.95a_0$

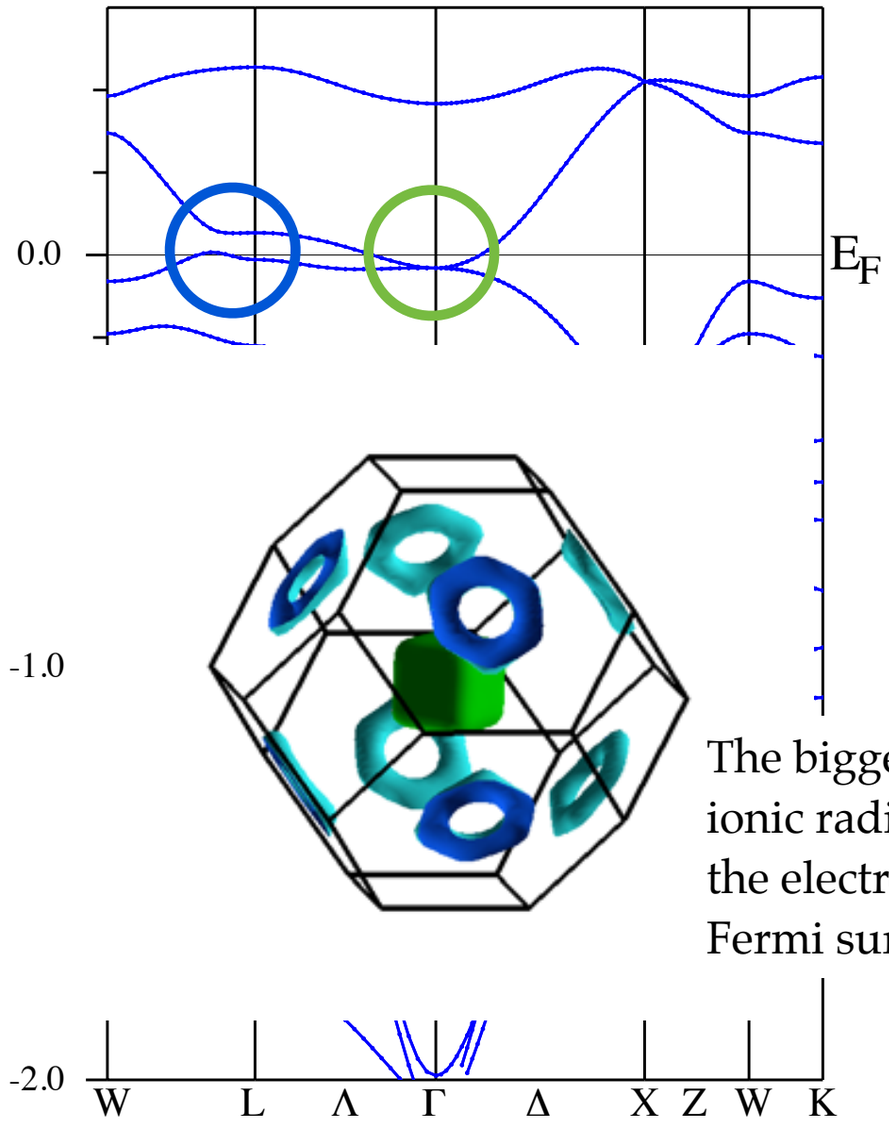


both GGA and mBJ+SO calculation
Metallic
Band crossing along (111) direction

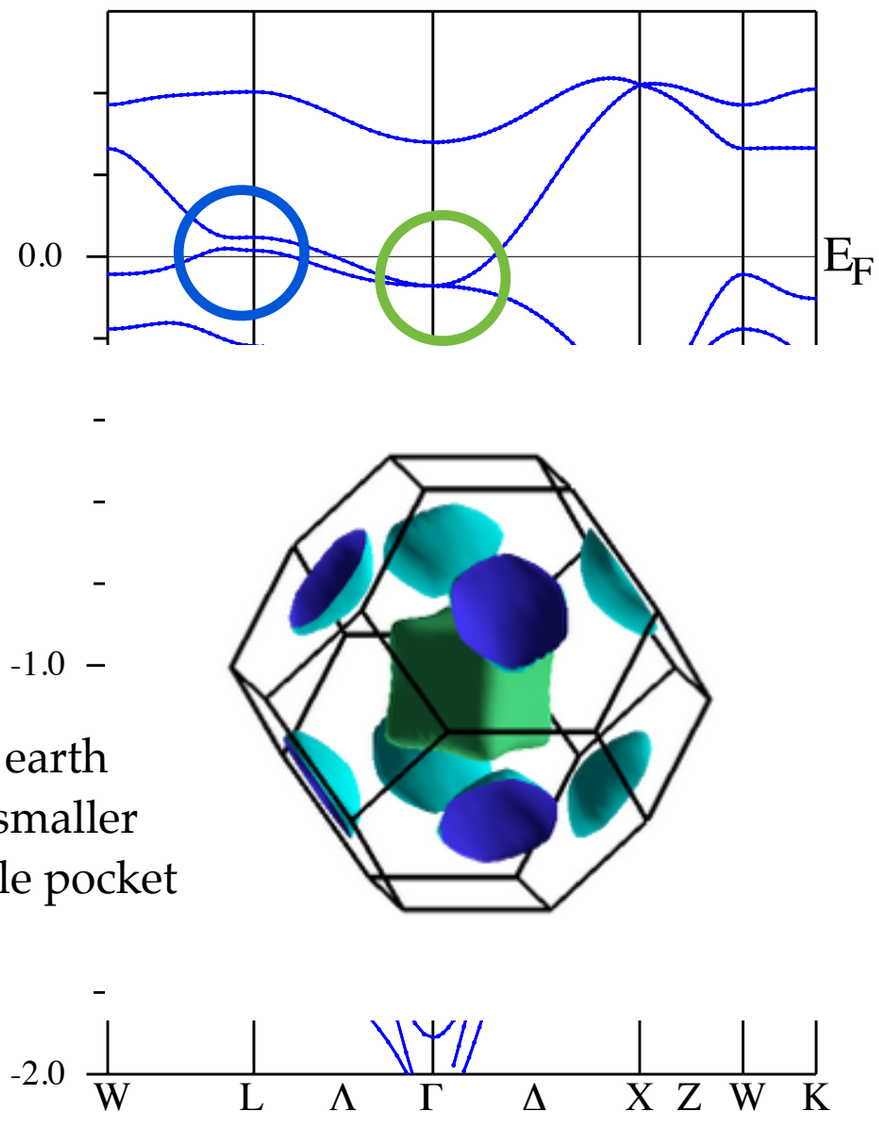


Paramagnetic calculation: $Pr_2Ir_2O_7$ and $Y_2Ir_2O_7$

$Pr_2Ir_2O_7$ GGA+SO



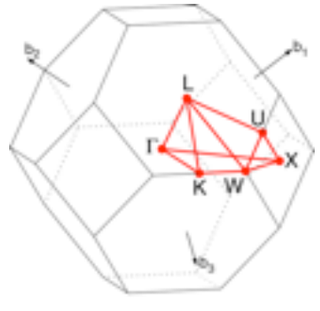
$Y_2Ir_2O_7$ GGA+SO



The bigger the rare earth ionic radius is, the smaller the electron and hole pocket Fermi surface is.

- Ir-O-Ir bond angle Y: ~129˚; Pr: ~132˚
- Ir-O bond length Y: 1.997Å ; Pr: 2.014Å
- Ir-Ir bond length Y: 3.599Å ; Pr: 3.677Å

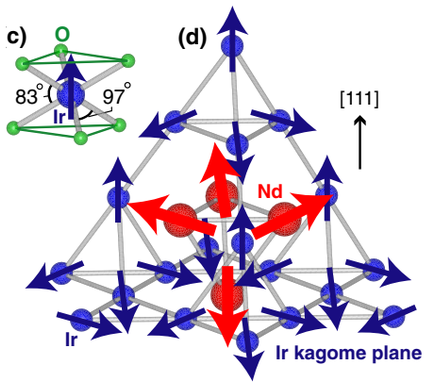
Why is Pr metallic and Y not?



Magnetic band structure calculation

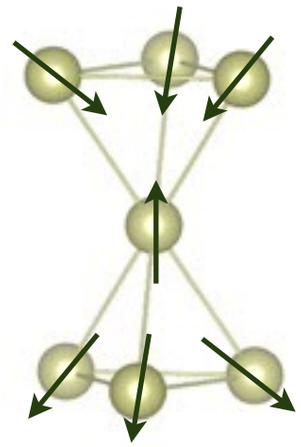
- Focus on Pr, Nd, Y
- GGA+SO+U, U=2eV since 5d are more extended
- Magnetism in R 4f electrons and in Ir 5d electrons → Magnetic ground state can be complicated!
- non-collinear magnetism :Wien2k+WIENNCM

$Nd_2Ir_2O_7$



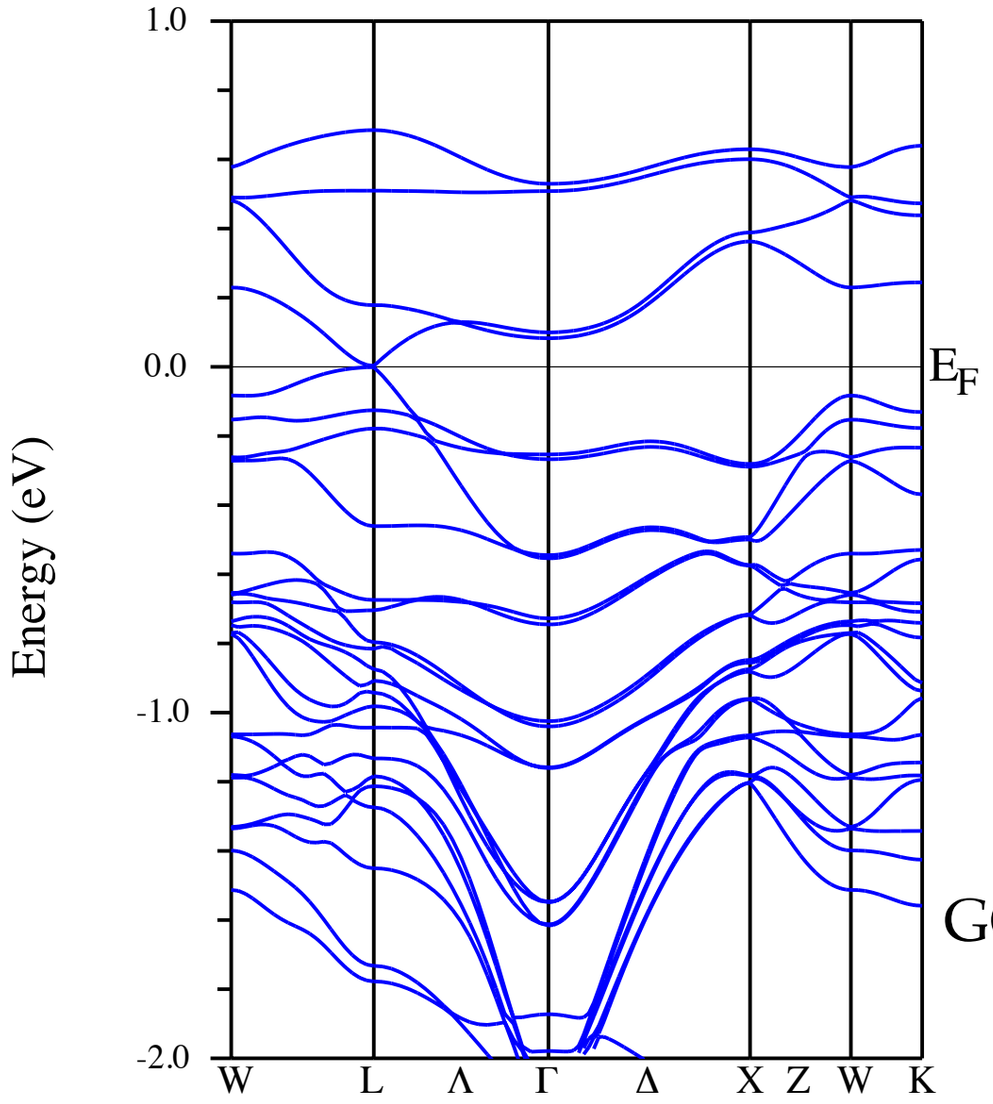
Neutron diffraction and
inelastic scattering measurement
$\mathbf{q}_0=(0,0,0)$

magnetic state:
all-in all-out state



Pr2Ir2O7

- Metallic/paramagnetic down to 0.3K
- Experimental: Pr 4f: 2-in 2-out Ir: paramagnetic
- Try both Pr and Ir all-in all-out order

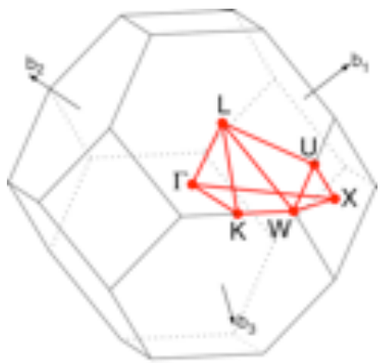


GGA+SO+U

U_{Ir}=2eV

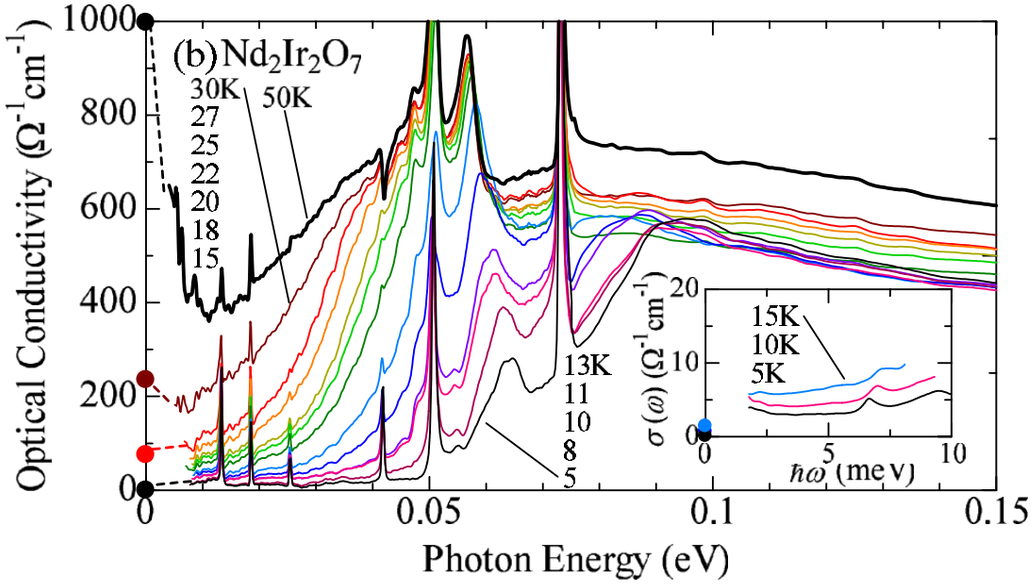
U_{Pr}=6eV

The gap barely closes at the L point
In proximity to Weyl semimetal
GGA/LDA+U may overestimate magnetism



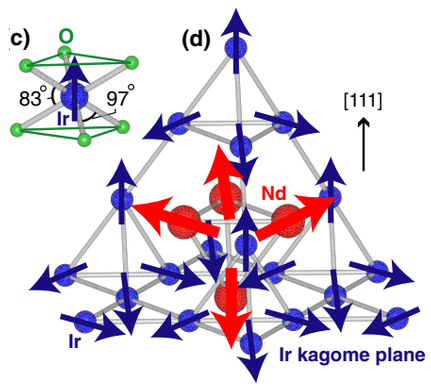
$Nd_2Ir_2O_7$

- T_{MI}~33K, optical conductivity measurement infers the full opening of the charge gap.
- Experiment suggesting both Nd and Ir are all-in all-out



Optical conductivity
gap~0.045eV

K.Ueda et al, PRL 2012

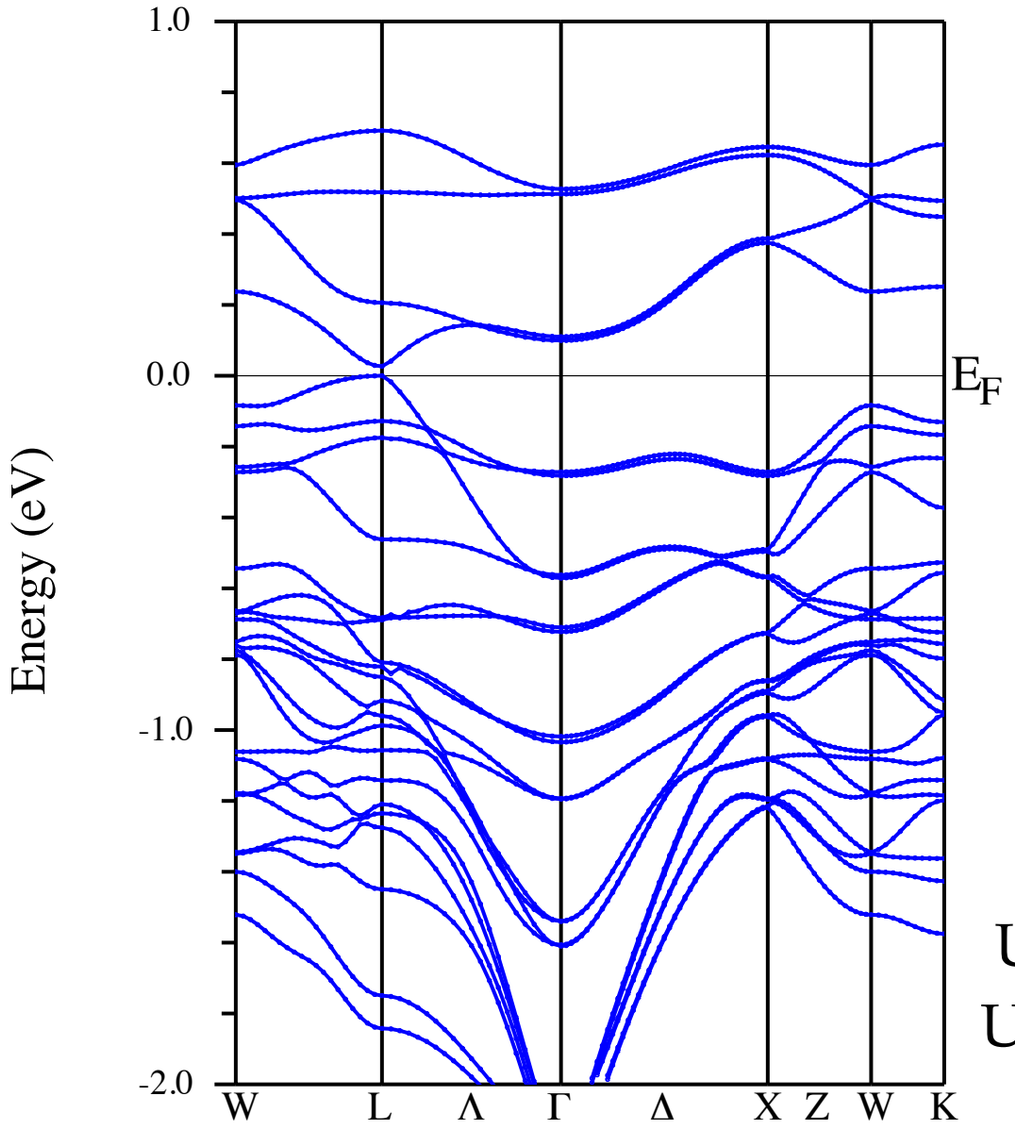


Neutron diffraction and
inelastic scattering measurement
$\mathbf{q}_0$=(0,0,0)

Keisuke Tomiyasu et al, JPSJ 2012

$Nd_2Ir_2O_7$

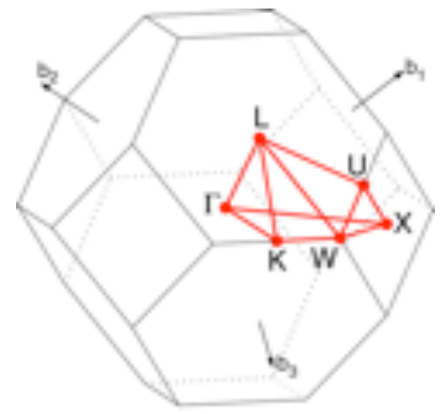
- T_{MI}~33K, optical conductivity measurement infers the full opening of the charge gap.
- Experiment suggesting both Nd and Ir are all-in all-out



GGA+SO+U calculation
all-in all-out magnetic

Mott insulator
Gap~0.03eV

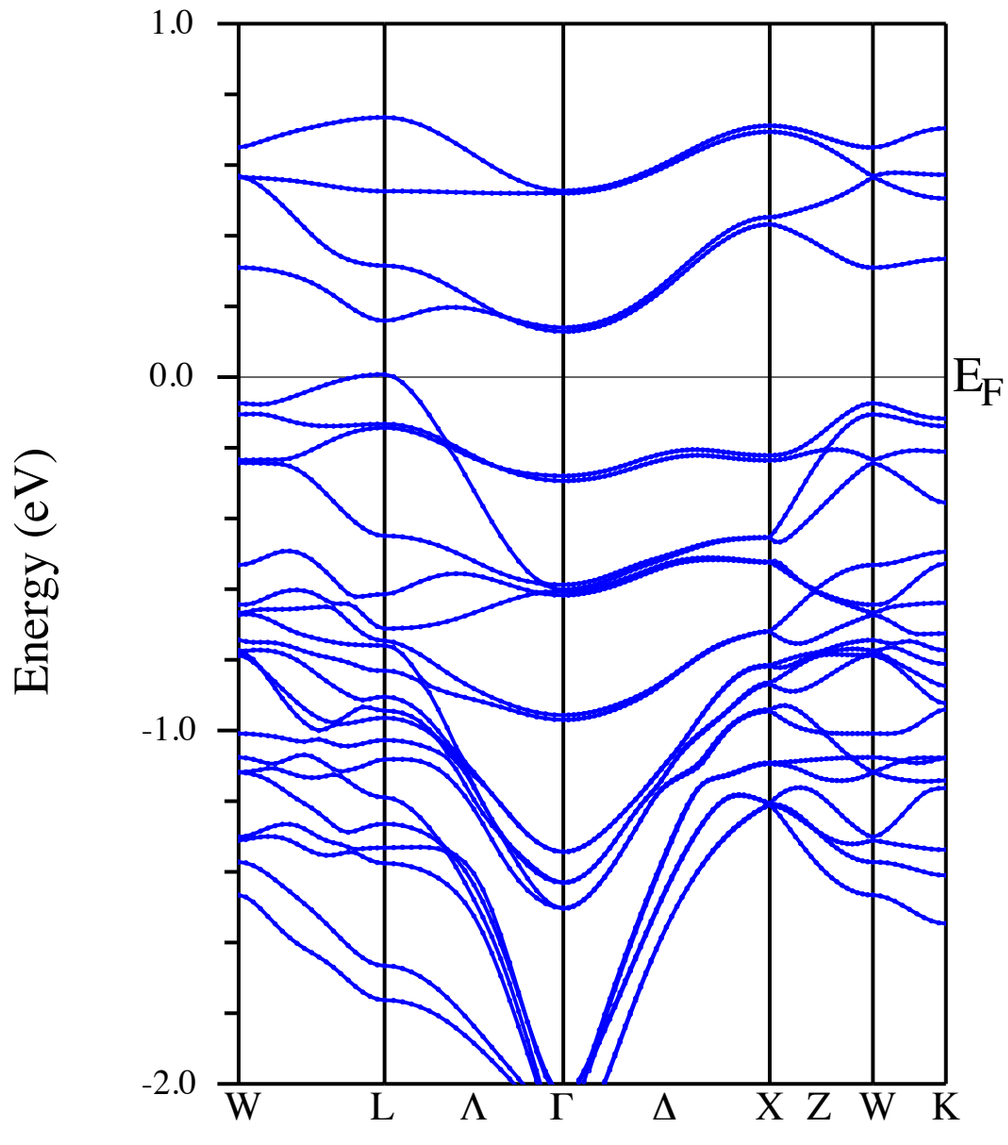
U_{Ir}=2eV
U_{Nd}=6eV



$Y_2Ir_2O_7$

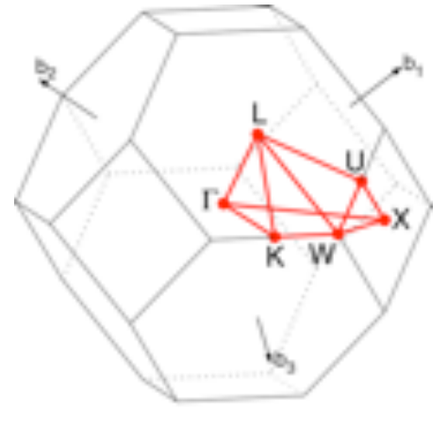
- T_{MI}~150K
- Y: no f electron
- Theory and experiment: all-in all-out state

X. Wan et al, PRB 2011



GGA+SO+U
all-in all-out magnetic
Mott insulator
Gap~0.12eV

U_{Ir}=2eV



Summary for Part 1

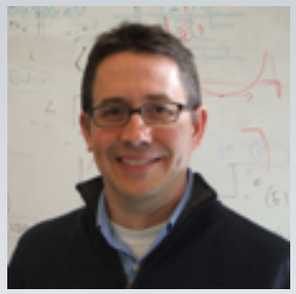
- $Pr_2Ir_2O_7$: Quadratic Fermi node
- Strain/pressure along (111) direction make $Pr_2Ir_2O_7$ a strong topological insulator with correlation.
- Systematic gap decrease trend as rare earth ionic radius increases.

Part 2
Domain walls in the insulating state of Pyrochlore Iridates

UCB & LBNL

Ashvin Vishwanath

Jeffrey Neaton



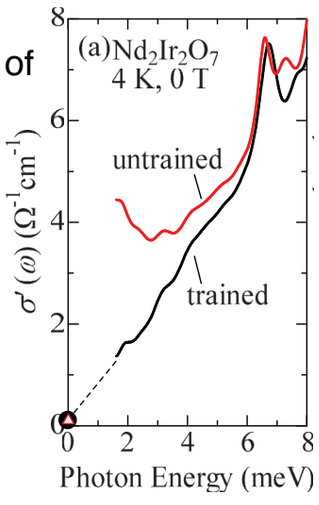
Domain wall states in pyrochlore Iridates

Conducting metallic domain wall even at the gapped bulk state!

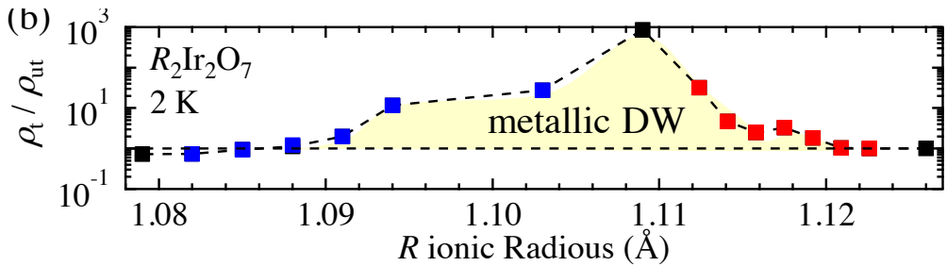
Theory and experiments:

Yamaji & Imada Phys. Rev. X 2014, arXiv: 1507.04153
Ueda, Fujioka, Nagaosa, et al. arXiv: 1506.07336, arXiv:1507.04804
Fujita et al. Scientific Reports 2015
many others…

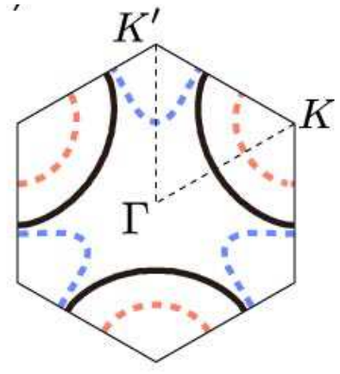
Magnetic tuning of domain wall



K. Ueda et al., Phys. Rev. B 89, 075127 (2014)



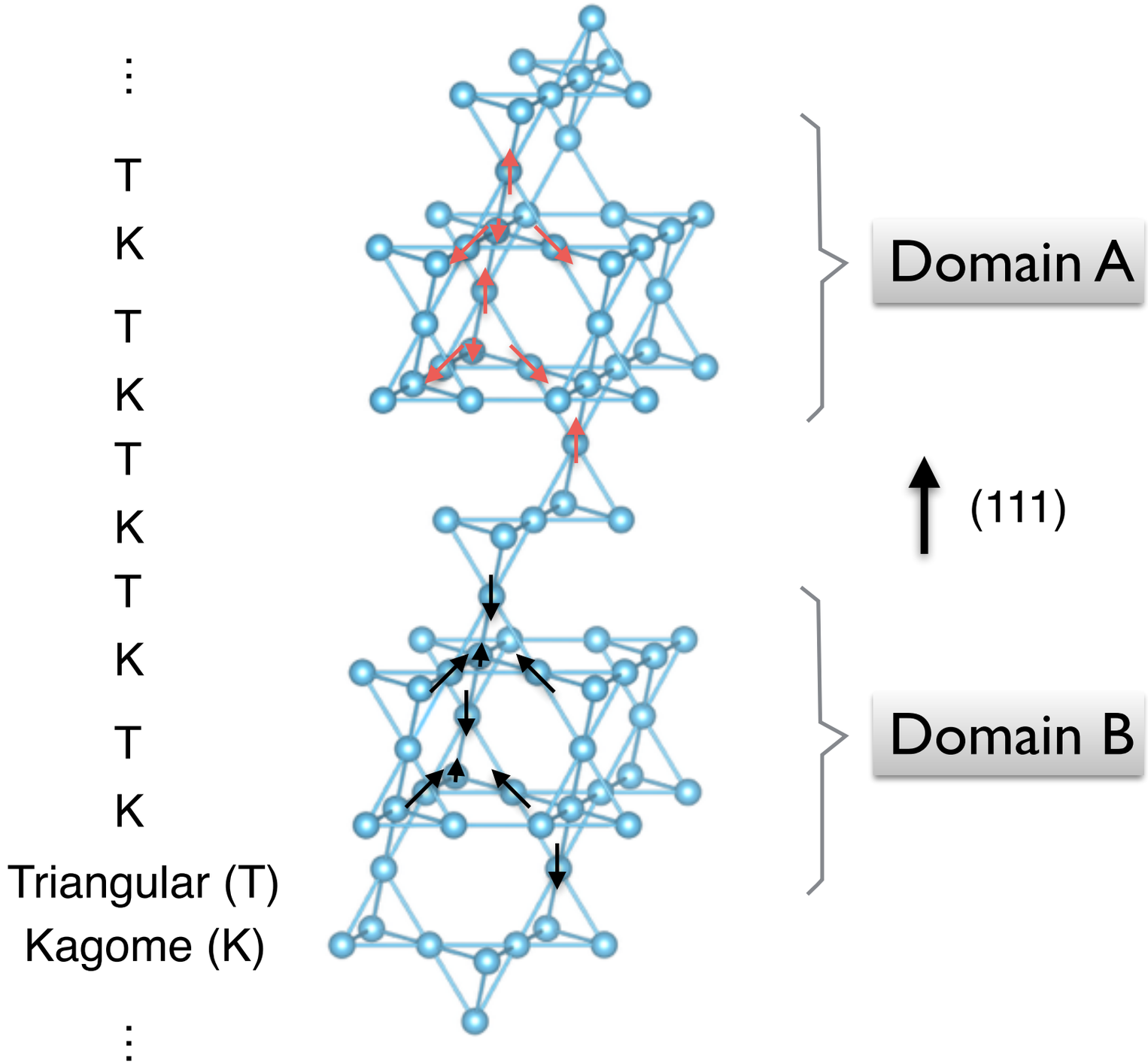
Ueda, et al. arXiv:1507.04804



Yamaji & Imada arXiv: 1507.04153

A full ab initio calculation is desirable.

Domain wall states in pyrochlore Iridates



Domain wall states in pyrochlore Iridates

⋮

T

K

T

K

T

K

T

K

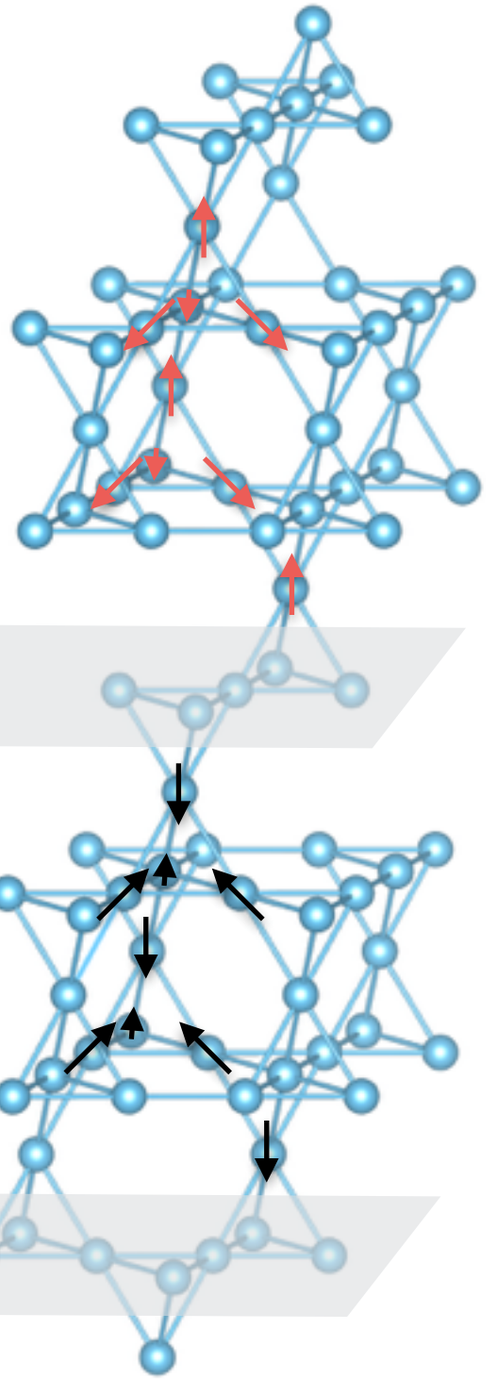
T

K

Triangular (T)

Kagome (K)

⋮



(111)

Domain wall states in pyrochlore Iridates

⋮

T

K

T

K

T

K

T

K

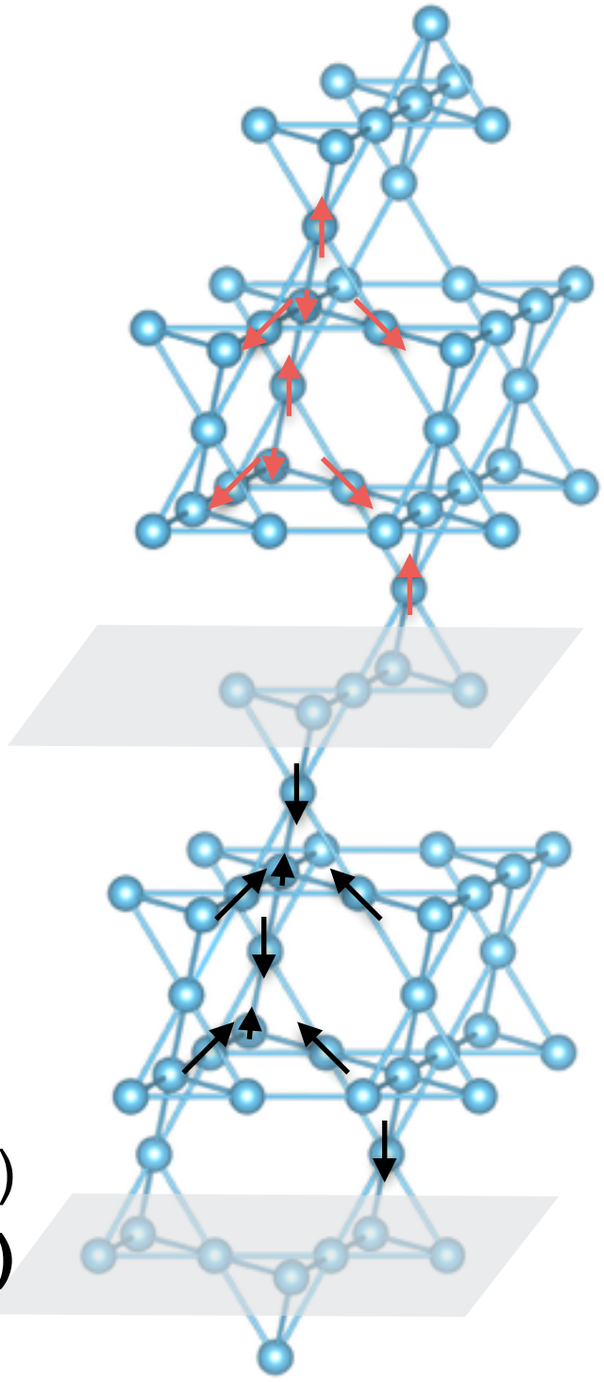
T

K

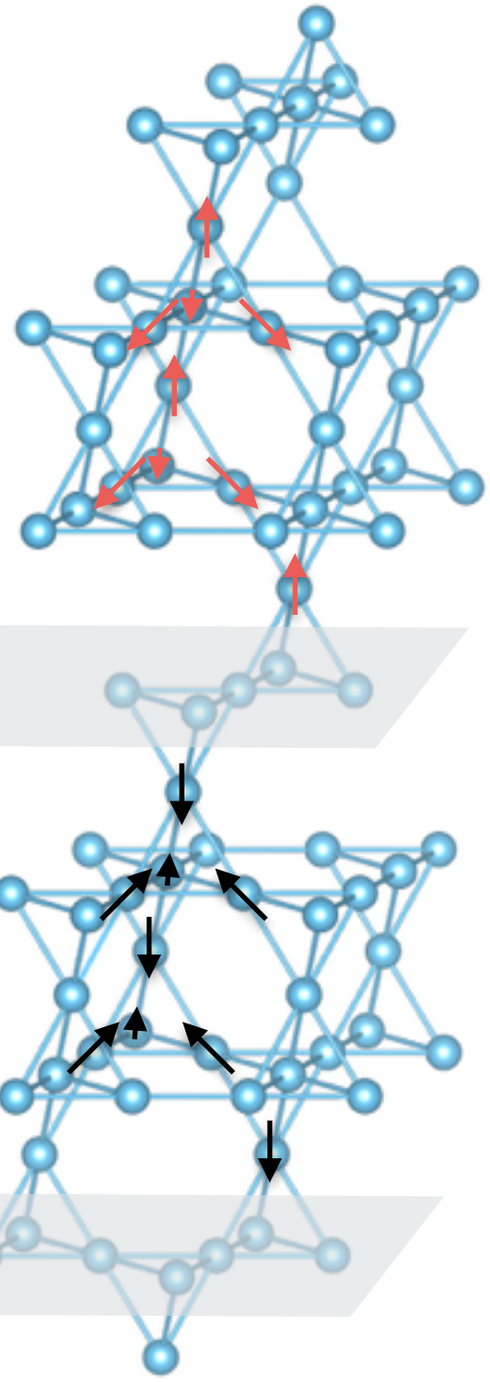
Triangular (T)

Kagome (K)

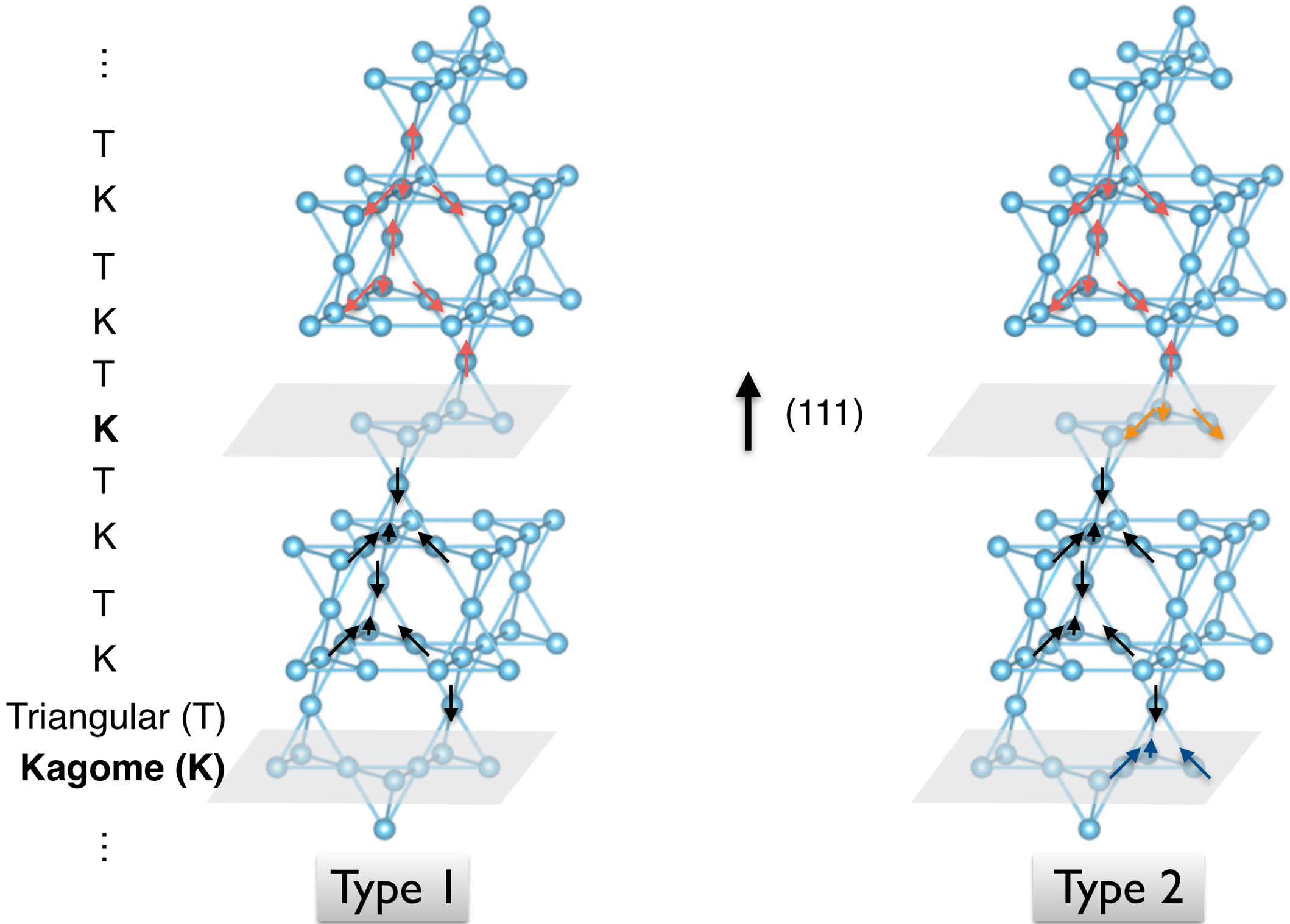
⋮



(111)



Domain wall states in pyrochlore Iridates



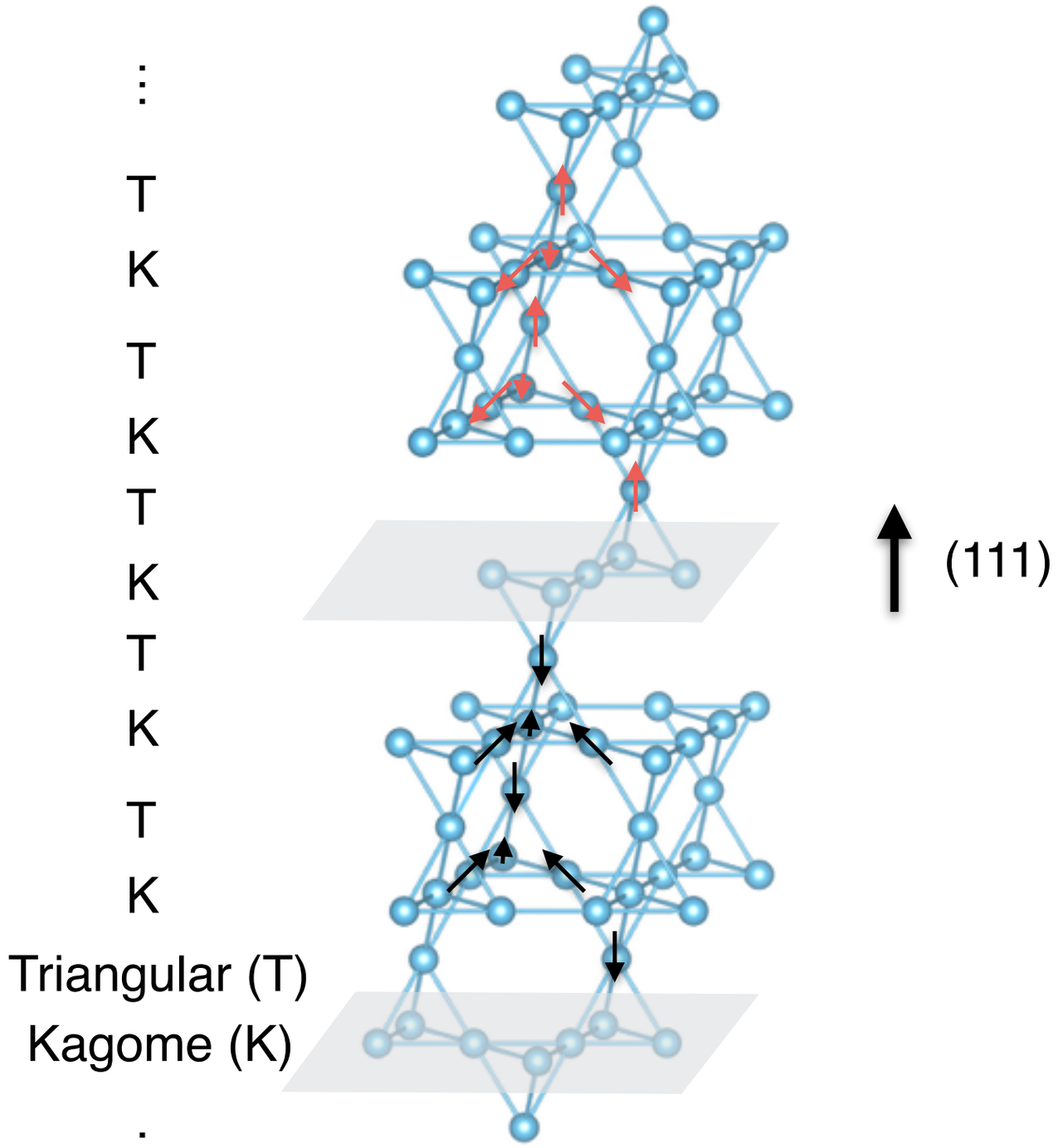
Domain wall states in $Y_2Ir_2O_7$

Method

- Vasp
- GGA+U+SOC
- Periodic domain wall condition
- Magnetic moment is fully relaxed.
- Convergence test:

  number of k points

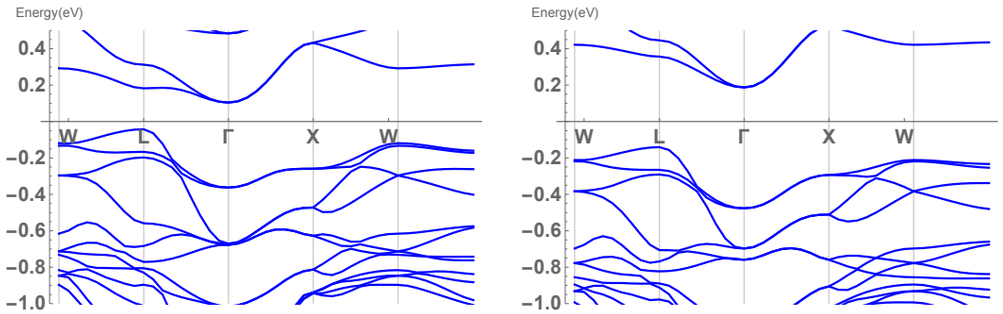
  How big is domain region
- Type 1 and 2 domain wall as local minima, different initial magnetic moments.



Domain wall states in $Y_2Ir_2O_7$

Method:
Band structure at different U deviates a little from different program.
Overall qualitatively agrees.

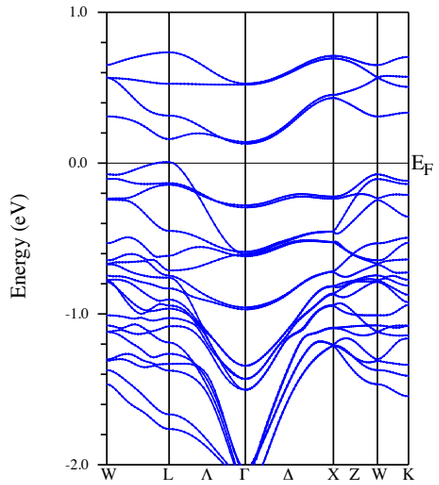
Vasp



U=1.5eV
gap~0.08eV

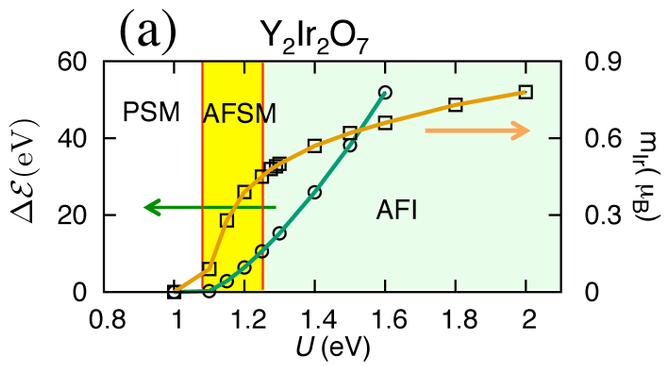
U=2eV
gap ~ 0.2eV

Wien2k



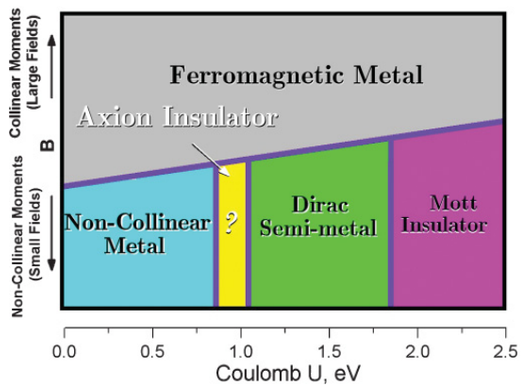
U=2eV
gap ~ 0.12eV

openMX



Onoda, et al. J. Phys. Soc. Jpn. 84, 073703 (2015)

LmtART



X. Wan et al, PRB 2011

Domain wall states in $Y_2Ir_2O_7$

Method:
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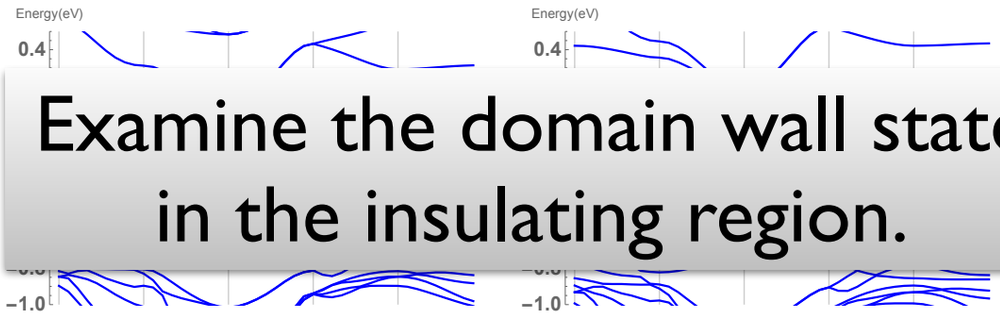
Vasp

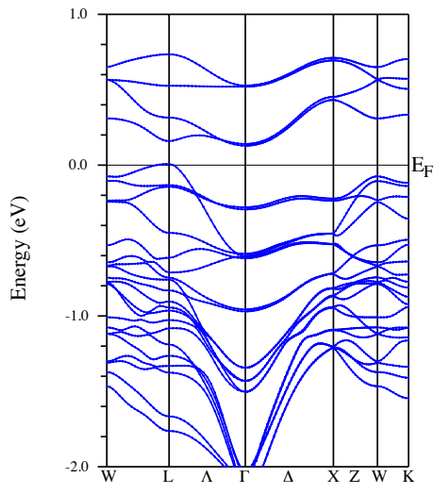


Examine the domain wall state in the insulating region.

U=1.5eV
gap~0.08eV

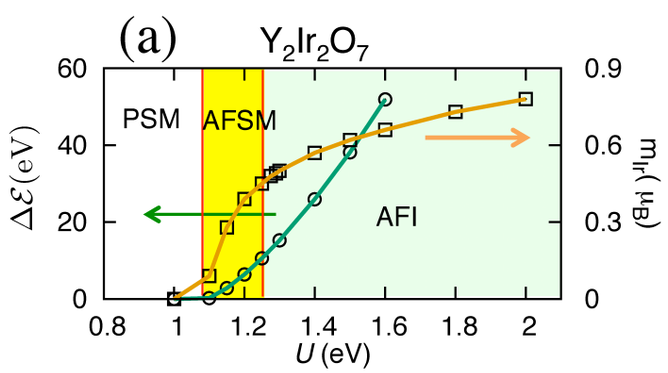
U=2eV
gap ~ 0.2eV

Wien2k



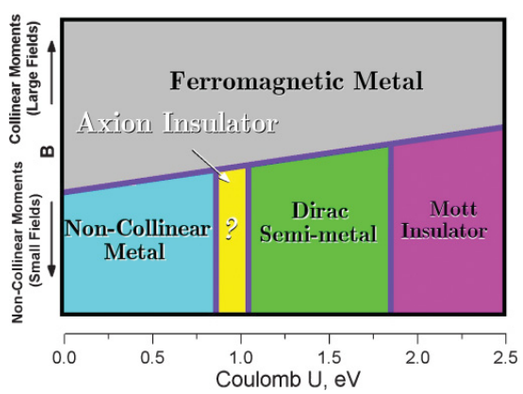
U=2eV
gap ~ 0.12eV

openMX



Onoda, et al. J. Phys. Soc. Jpn. 84, 073703 (2015)

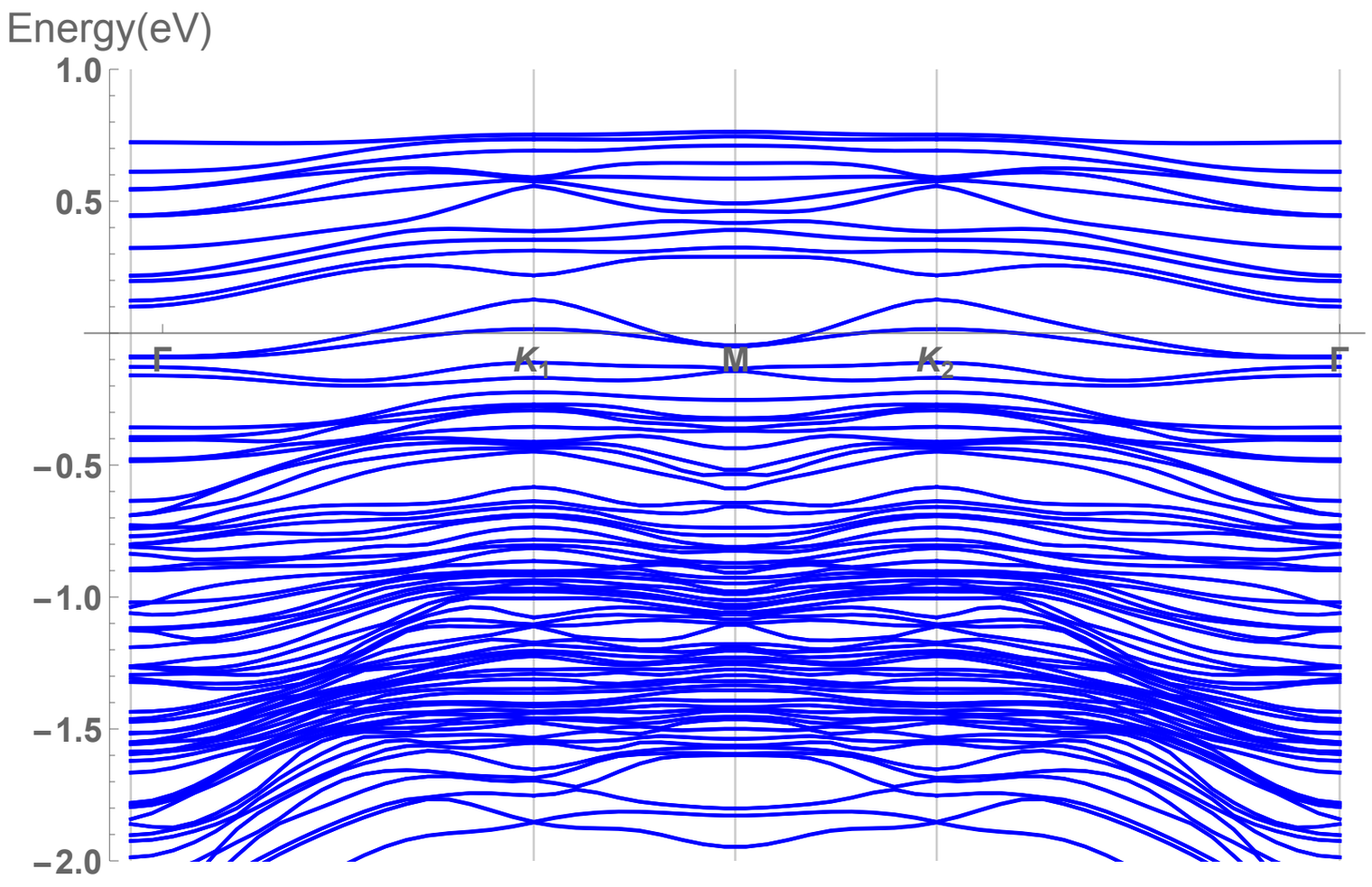
LmtART



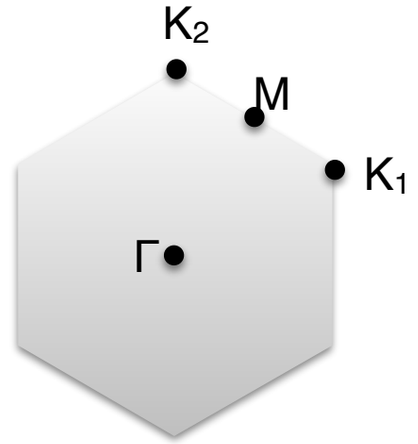
X. Wan et al, PRB 2011

Domain wall states in $Y_2Ir_2O_7$

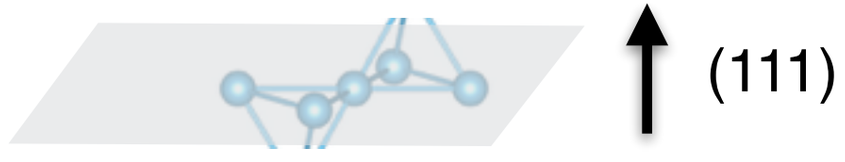
Type 1 Domain walls



6 K & 6 T layers
GGA+SO+U
U_{Ir}=2eV

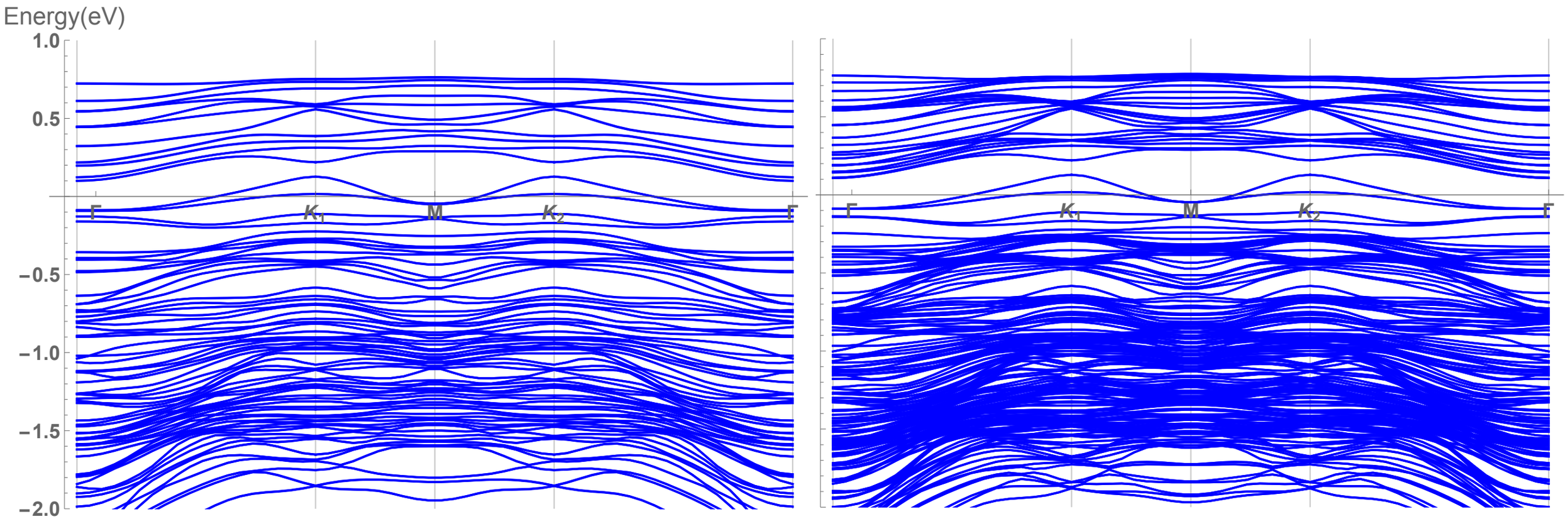


2D Brillouin zone



Domain wall states in $Y_2Ir_2O_7$

Is 6K & 6T superlattice large enough?

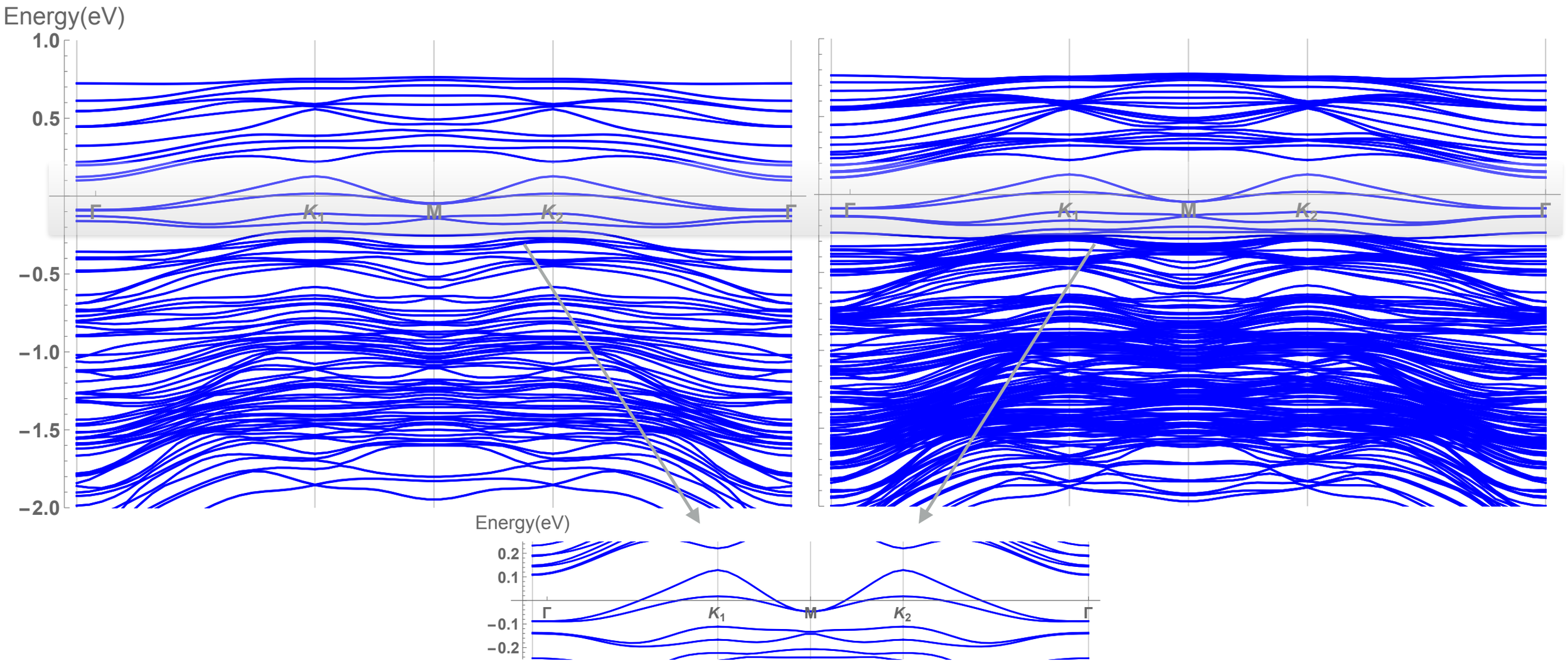


6 K & 6 T layers

12 K & 12 T layers

Domain wall states in $Y_2Ir_2O_7$

Is 6K & 6T superlattice large enough? Yes for both type 1 and 2 domain walls.

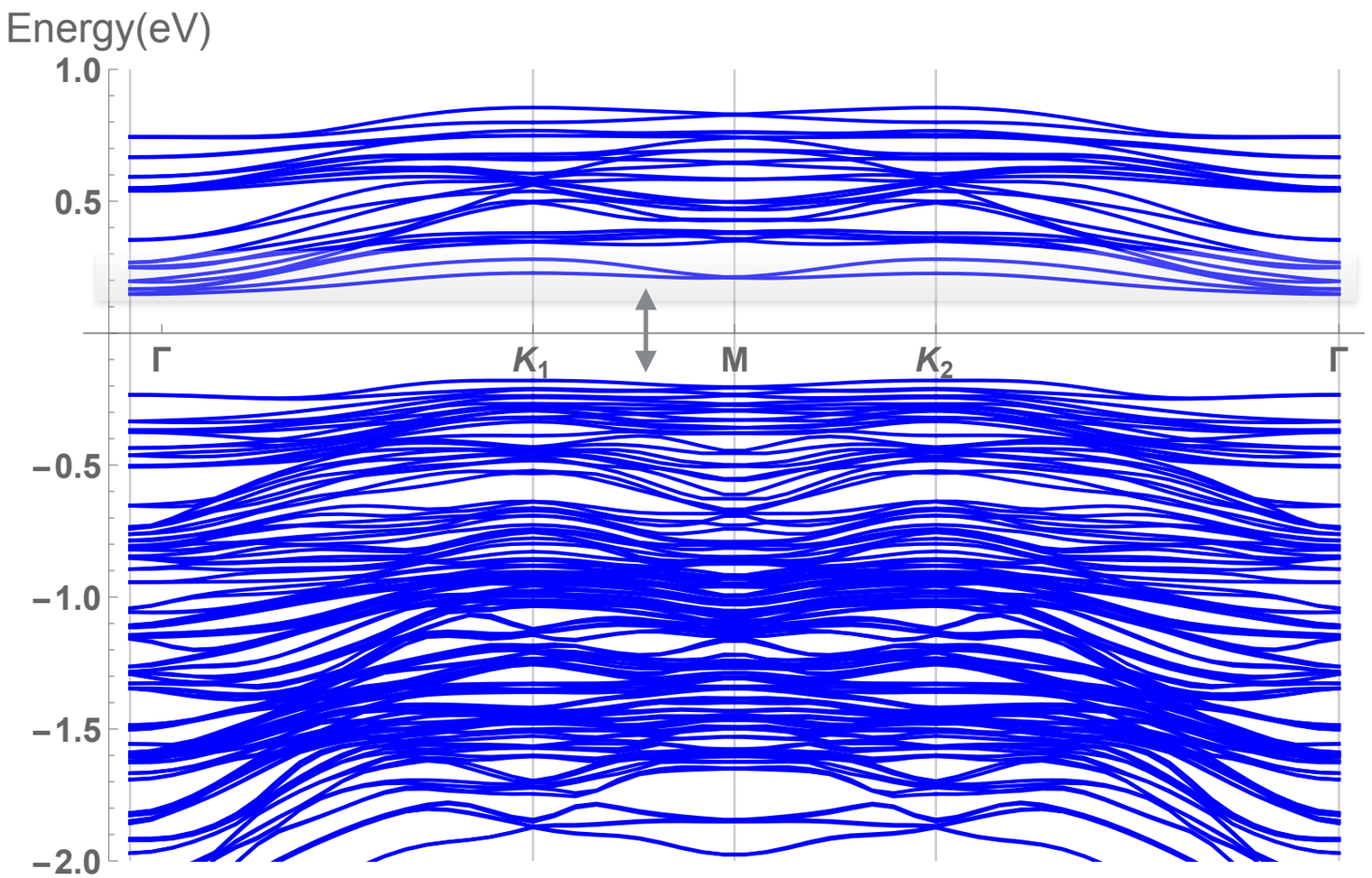


6 K & 6 T layers

12 K & 12 T layers

Domain wall states in $Y_2Ir_2O_7$

Type 2 Domain walls

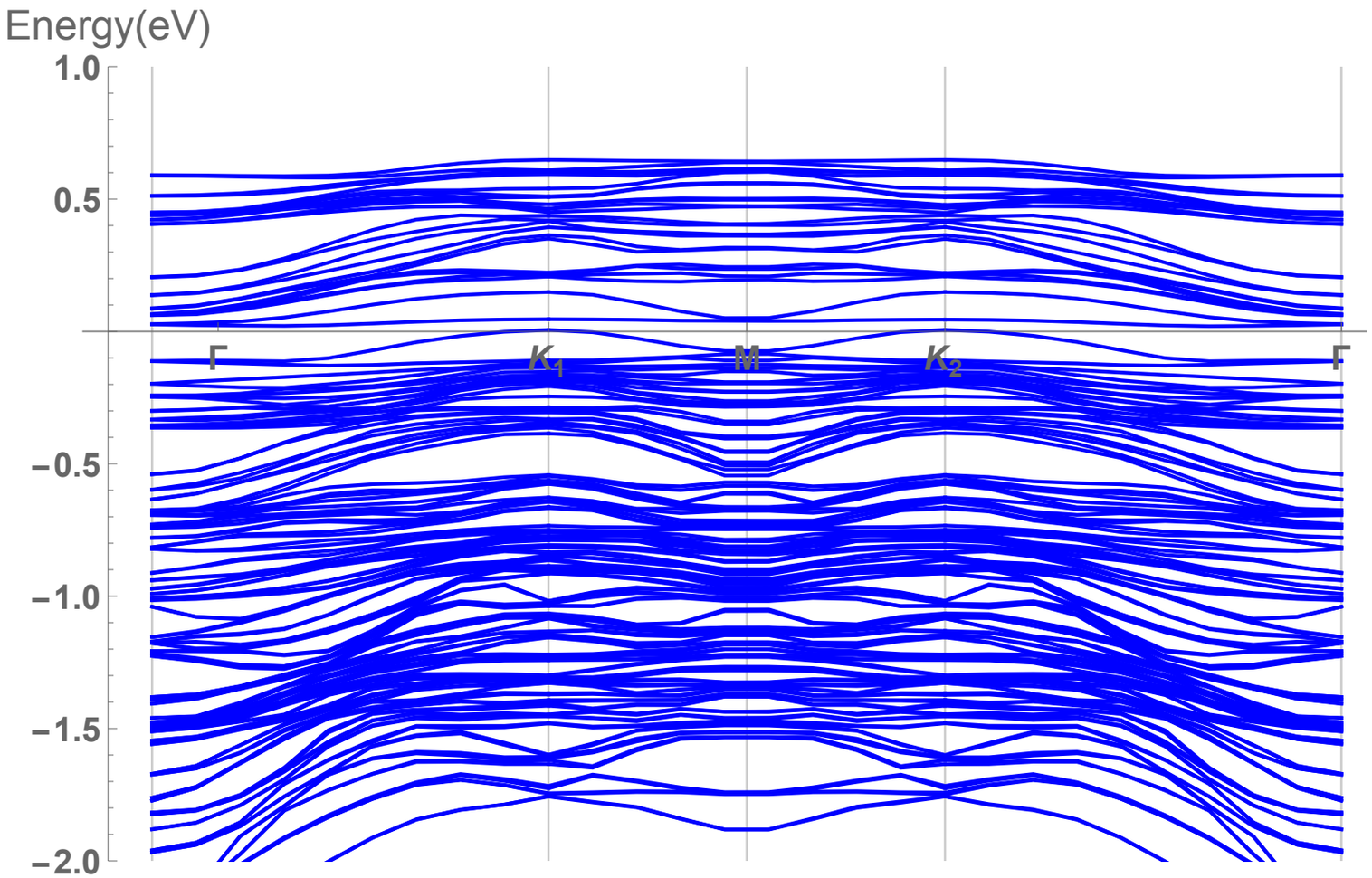


6 K & 6 T layers
GGA+SO+U
U_{Ir}=2eV

Gapped out domain wall states

Domain wall states in $Y_2Ir_2O_7$

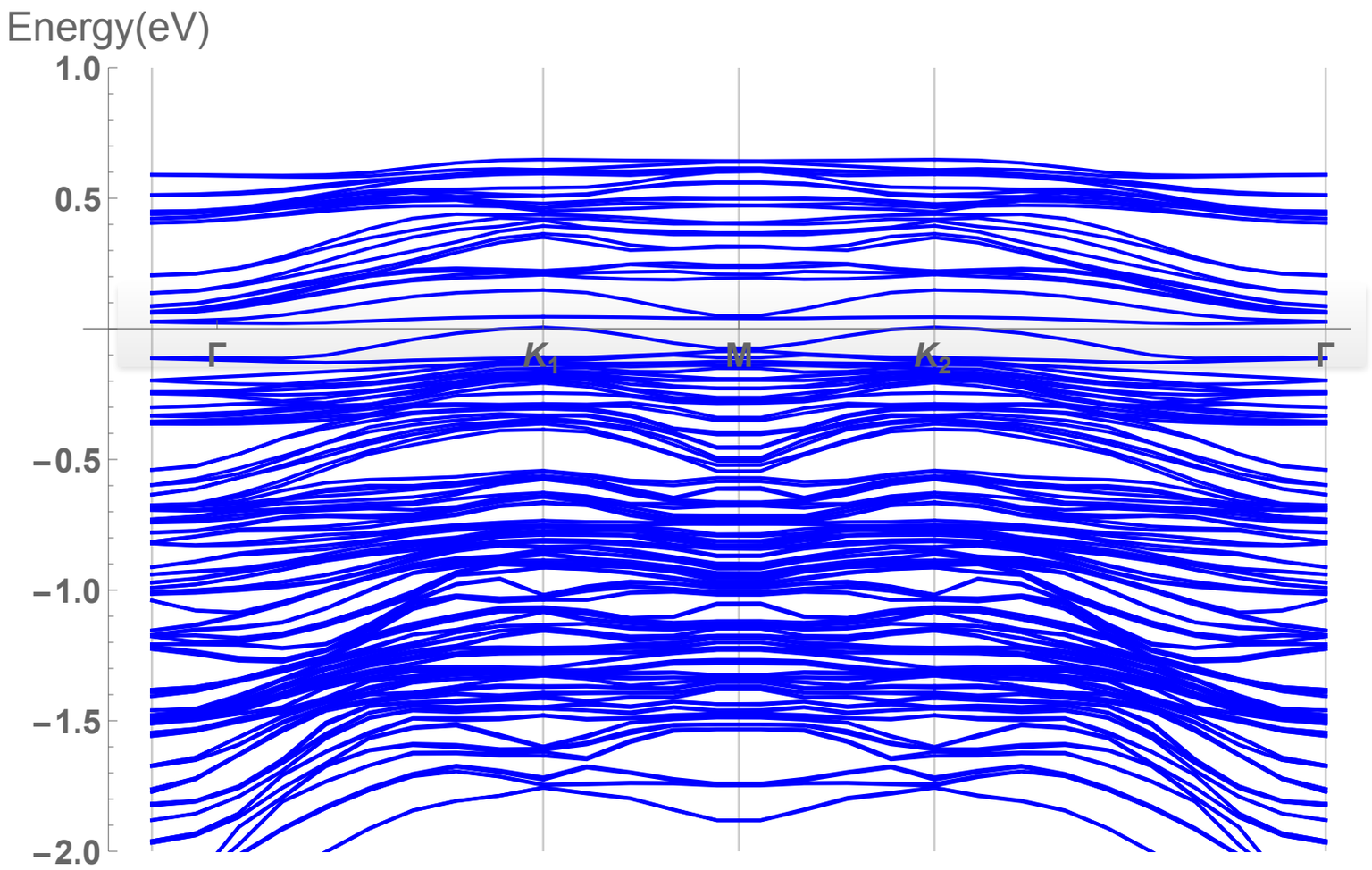
Type 2 Domain walls



6 K & 6 T layers
GGA+SO+U
U_{Ir}=1.5eV

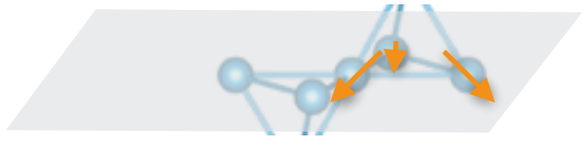
Domain wall states in $Y_2Ir_2O_7$

Type 2 Domain walls



Metallic magnetic domain wall states

6 K & 6 T layers
GGA+SO+U
U_{Ir}=1.5eV



(111)

Domain wall states in $Y_2Ir_2O_7$

Total energy per domain wall (2D Kagome plane)	**U = 1.5 eV**	**U = 2 eV**
Type 1 Domain walls	**0.05eV**	**0.25eV**
Type 2 Domain walls	**0**	**0**

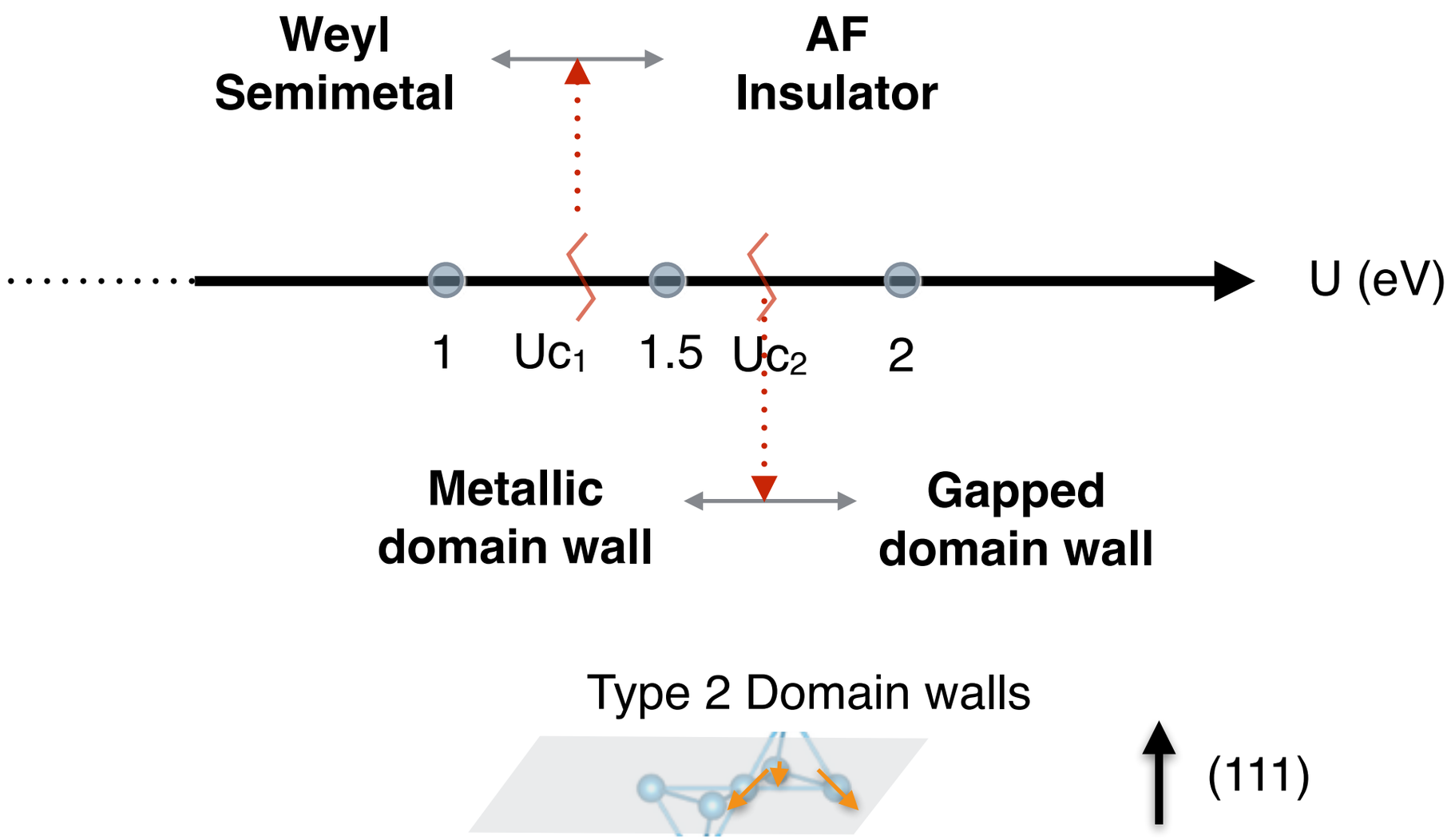
Domain wall states in $Y_2Ir_2O_7$

Total energy per domain wall (2D Kagome plane)	**U = 1.5 eV**	**U = 2 eV**
Type 1 Domain walls	**0.05eV**	**0.25eV**
Type 2 Domain walls	**0**	**0**

energetically favorable!

Domain wall states in $Y_2Ir_2O_7$

Tentative DFT phase diagram



Summary for Part 2

- From ab initio calculation, type 2 domain wall (magnetic) is energetically favored
- Within the AF insulating phase of $Y_2Ir_2O_7$, there're two phases, one with conducting domain wall, with stronger correlation, the conducting domain wall is gapped out.