Topological phases in pyrochlore iridate thin films

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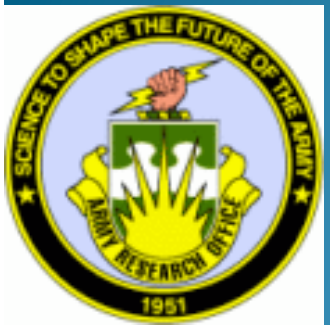


Chief Collaborators on Iridate Films

X. Hu, A. Ruegg, GAF *Phys. Rev. B* **86**, 235141 (2012) [Editor's Suggestion]
X. Hu, Z. Zhong, GAF *Sci. Rep*. **5**, 11072 (2015).
Q. Chen, H.-H. Hung, X. Hu, GAF *Phys. Rev. B* **92**, 085145 (2015)
P. Laurell, GAF (*In preparation*)

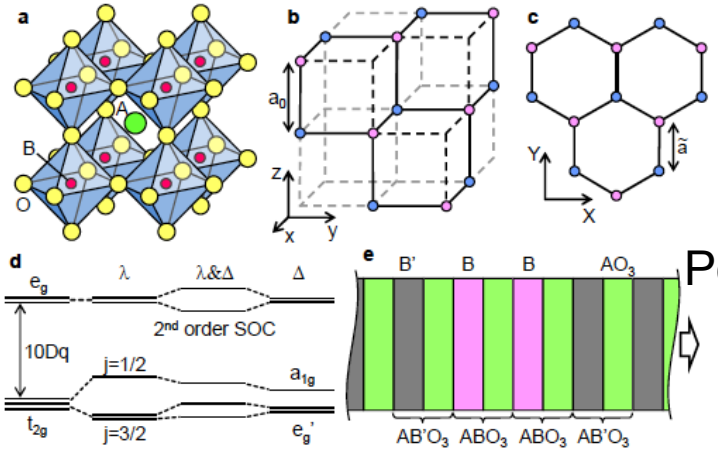
Mini-topical review: GAF and A. Ruegg *J. Appl. Physics* **117**, 172602 (2015). "Topological Phases in Oxide Heterostructures with Light and Heavy Transition Metal ions"

Talk Outline

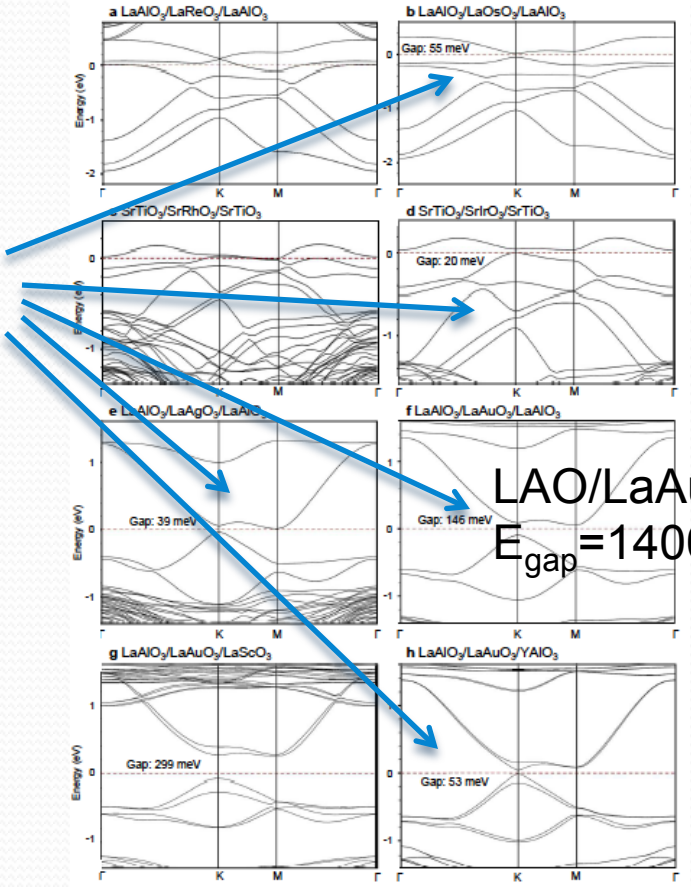
- Film geometry
  - -Bilayer films along [111] direction
  - -Trilayer films along [111] direction
- Weak coupling
  - -Model Hamiltonian+Hartree-Fock
  - -Model Hamiltonian+DMFT
  - -First-principles+Hartree-Fock
- Strong coupling
  - -Spin-wave analysis

An interesting direction for topological phases: oxide heterostructures along [111]: ABO_3 example

D. Xiao, W. Zhu, Y. Ran, N. Nagaosa, and S. Okamoto Nat. Comm. (2011)

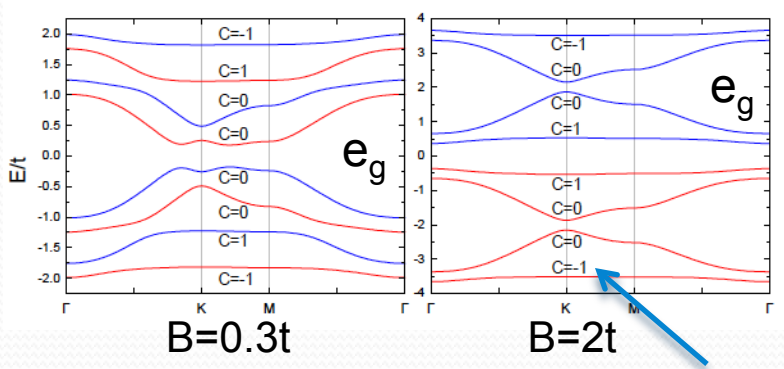


Potential TI



$LAO/LaAuO_3/LAO$

E_{gap}=1400 K



B=0.3t B=2t

Potential fractional quantum Hall states

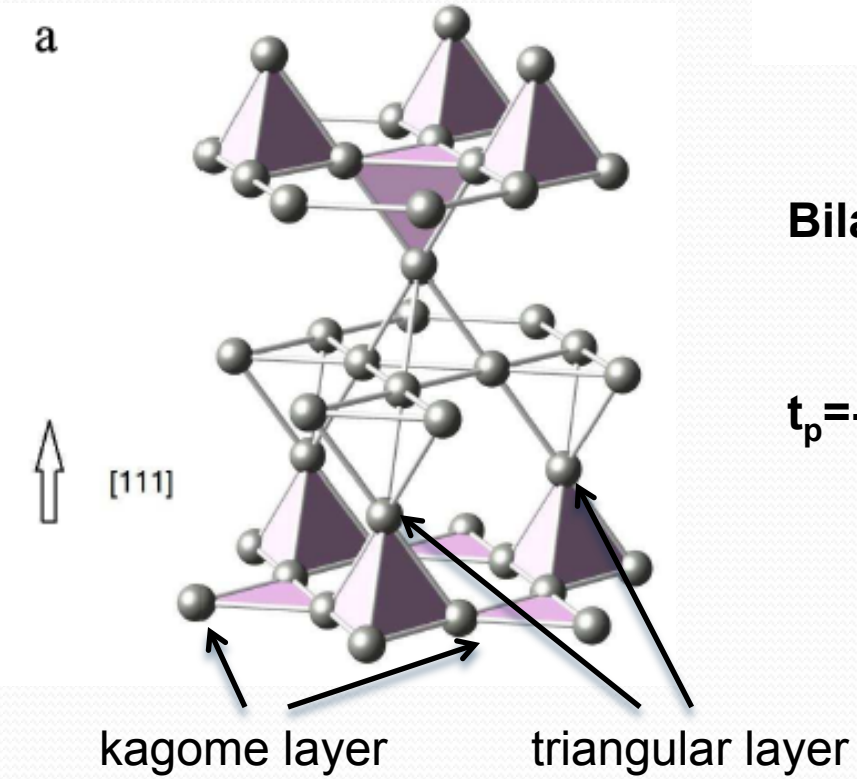
Topological phases in bilayer and trilayer pyrochlore systems along (111): $A_2Ir_2O_7$

Hu, Ruegg, Fiete PRB (2012) Editors' Suggestion

B.-J. Yang and N. Nagaosa, PRL (2014)

$$H_0 = \sum_{\langle i,j\rangle,\alpha,\beta} t_{i\alpha,j\beta} c^{\dagger}_{i\alpha} c_{j\beta} - \lambda \sum_i \mathbf{l}_i \cdot \mathbf{s}_i$$

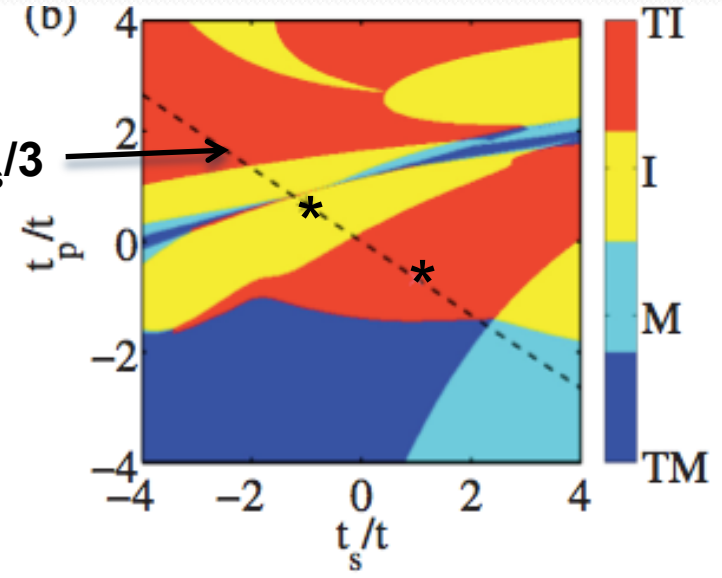
$$t_{i\alpha,j\beta} = t^{\text{in}}_{i\alpha,j\beta} + t^{\text{dir}}_{i\alpha,j\beta}$$



Bilayer, λ=4t (large SOC)

J_{eff}=1/2 only!

t_p=-2t_s/3

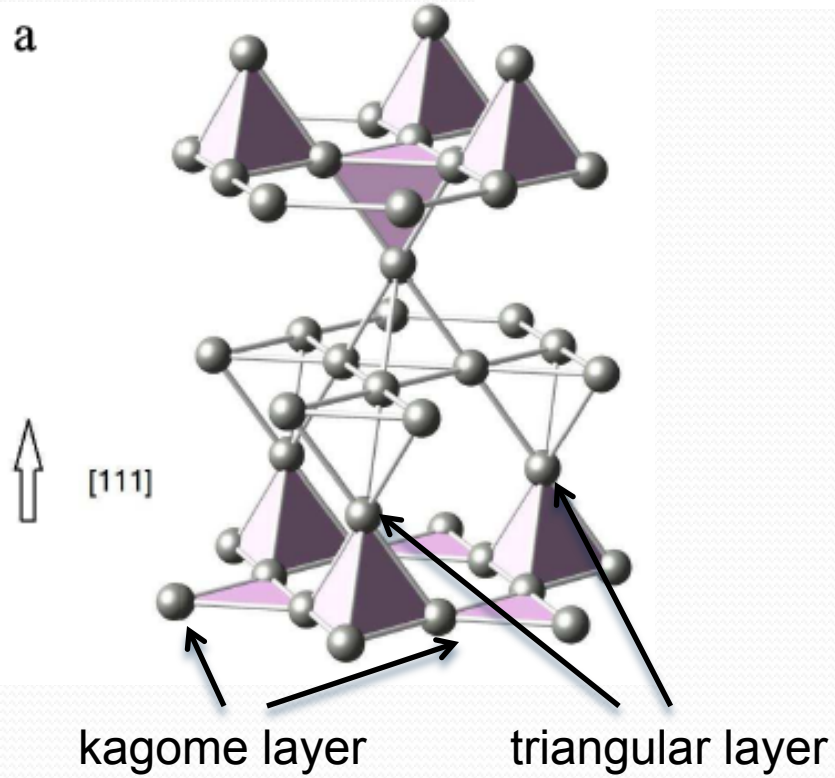


Topological phases in bilayer and trilayer pyrochlore systems along (111): $A_2Ir_2O_7$

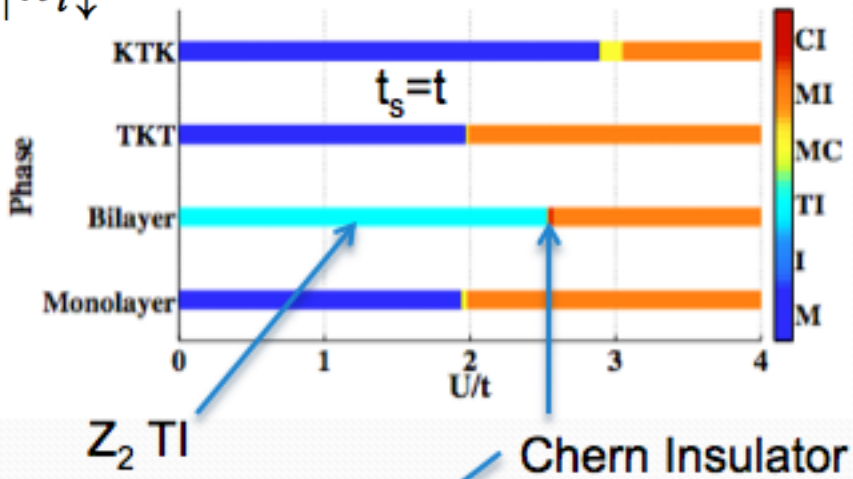
Hu, Ruegg, Fiete PRB (2012) Editors' Suggestion

J_{eff}=1/2 only!

$$H_U = U \sum n_{i\uparrow} n_{i\downarrow}$$

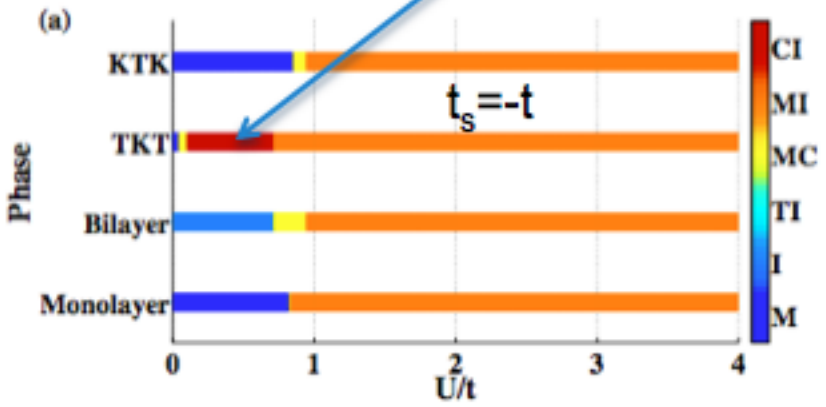


Hartree-Fock Phase Diagram



Z_2 TI

Chern Insulator

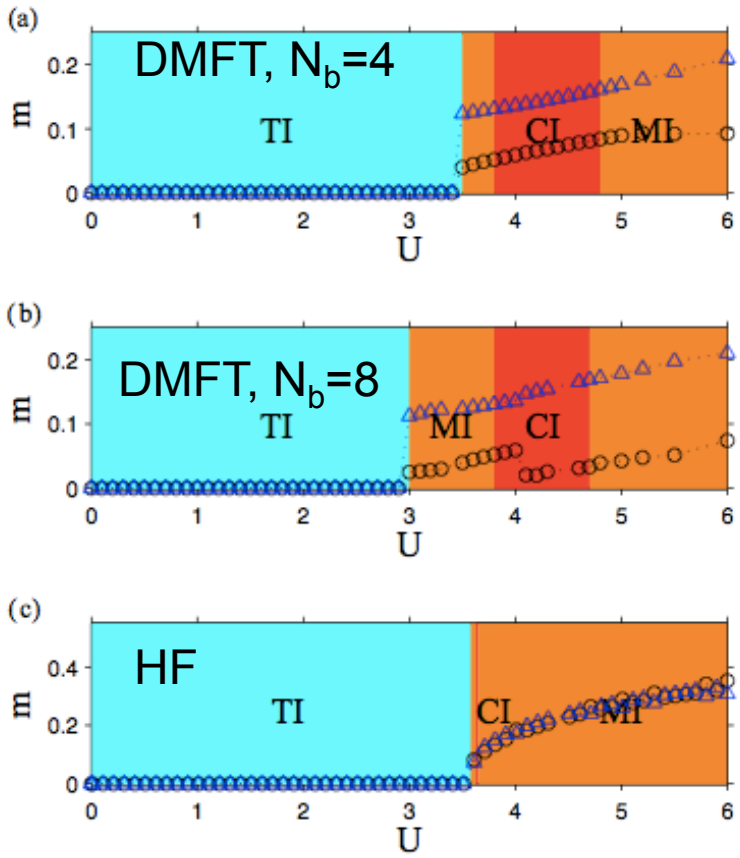


Comparison of DMFT and HF Phase Diagrams

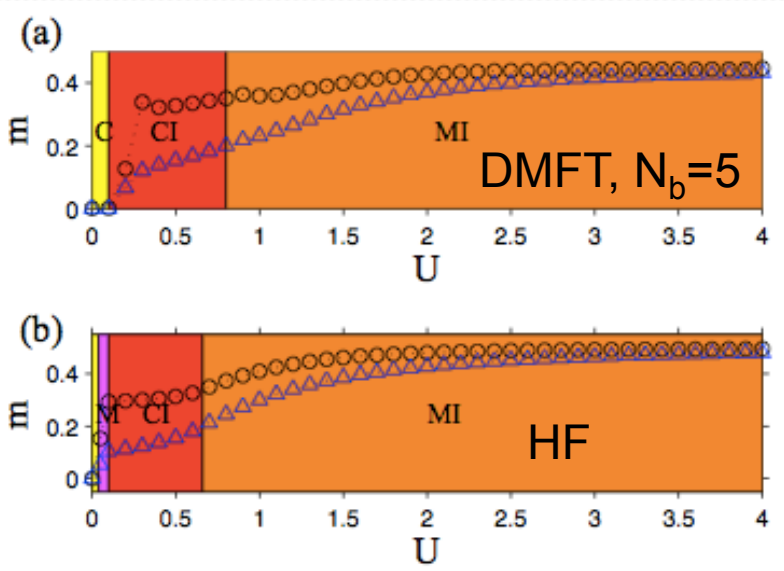
Chen, Hung, Hu, GAF *Phys. Rev. B* **92**, 085145 (2015)

J_{eff}=1/2 only!

Bilayer Film



Trilayer Film

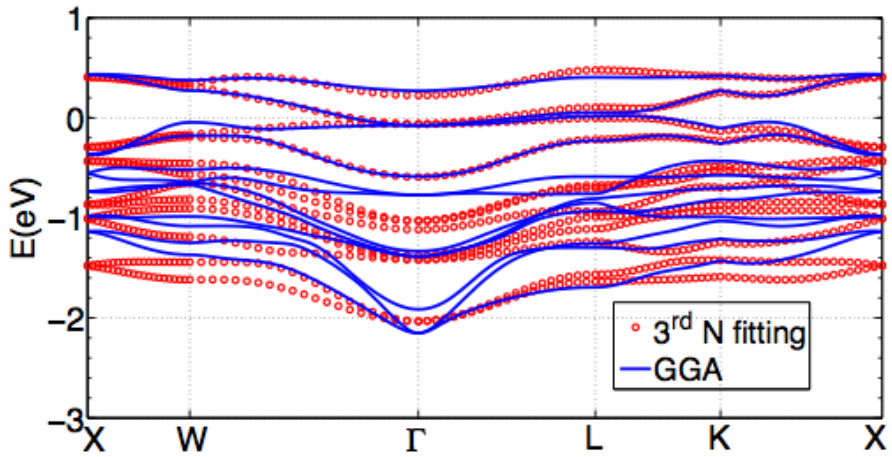


Overall, fairly good agreement. Appears quantum fluctuations may help stabilize CI in bilayer.

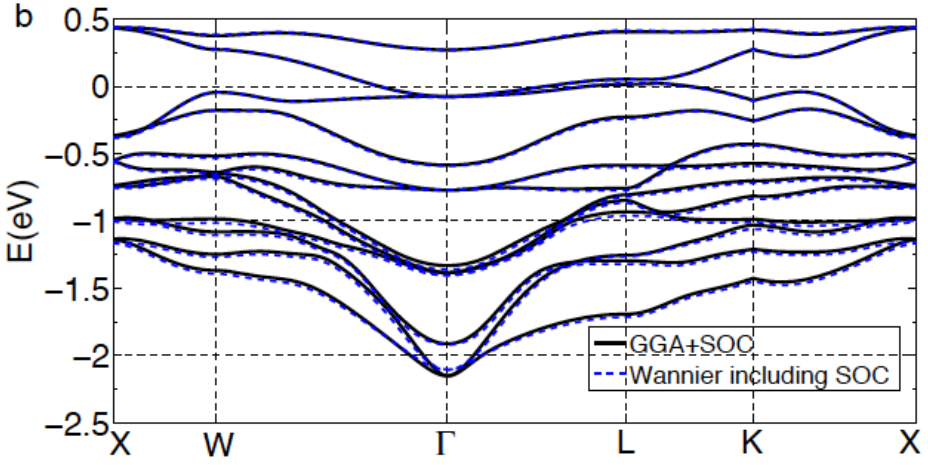
First Principles Study of $Y_2Ir_2O_7$: Fitting the band (bulk) band structure

Hu, Zhong, Fiete Sci. Rep. (2015)

No clear j=1/2 & j=3/2 splitting!



Tight-binding fit

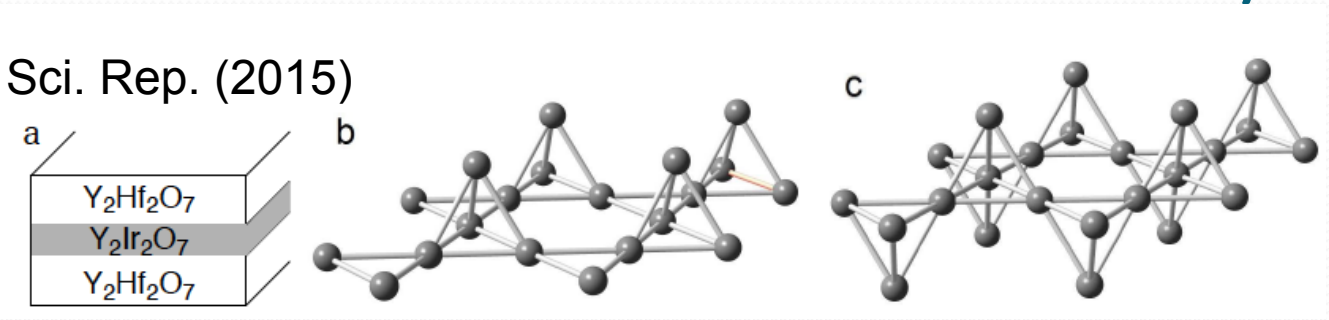


Wannier Fit

More extended 5*d*-orbitals are not well fit by tight binding!

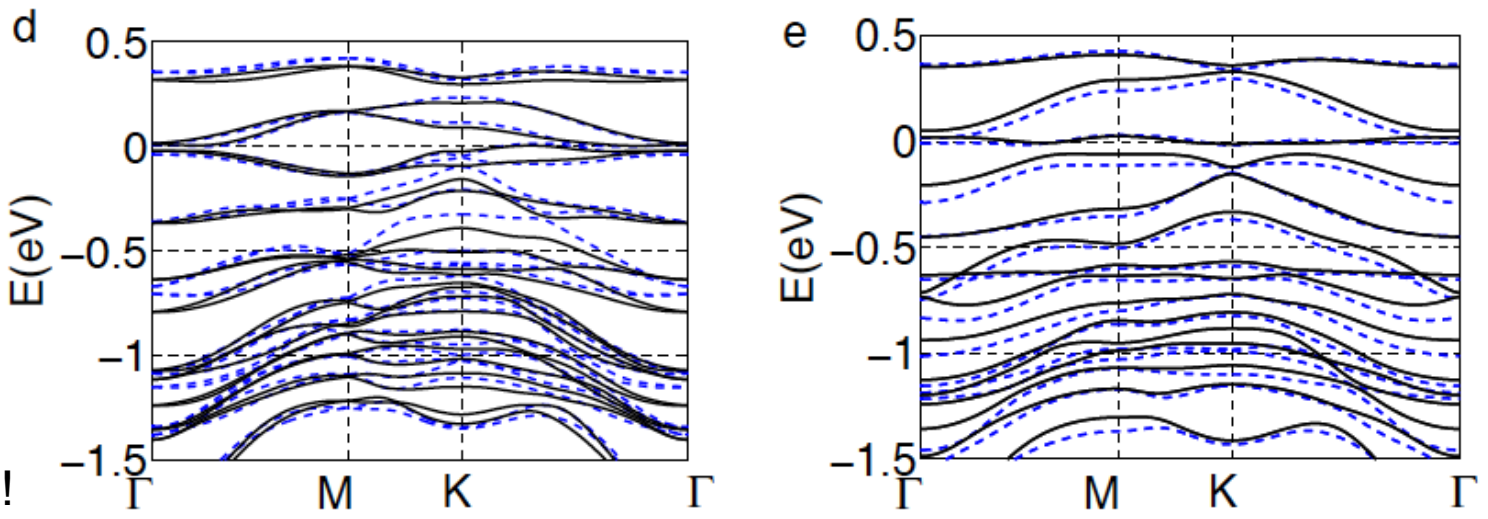
First Principles Study of $Y_2Ir_2O_7$: Fitting the band *thin-film* band structure → Hartree-Fock study

Hu, Zhong, Fiete Sci. Rep. (2015)



Wannier fits

No clear
j=1/2 &
j=3/2 splitting!



bilayer

TKT trilayer

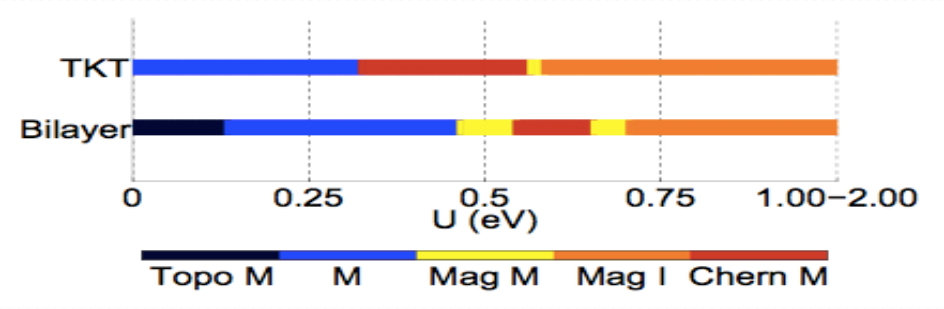
Hartree-Fock study of [111] bilayer and trilayer $Y_2Ir_2O_7$

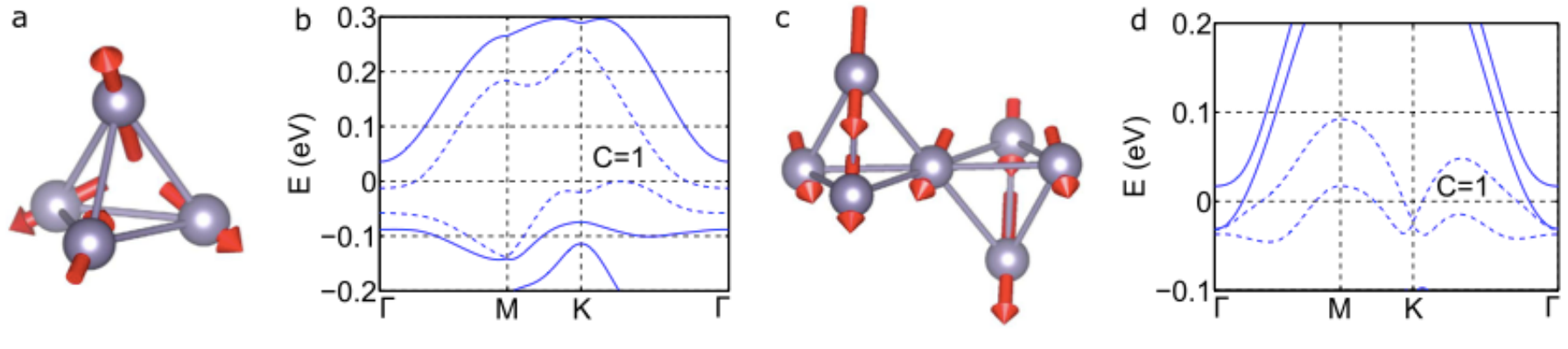
Hu, Zhong, Fiete Sci. Rep. (2015)

$$H = \sum_{i,j,\alpha,\beta} \tilde{t}_{i\alpha,j\beta} c^{\dagger}_{i\alpha} c_{j\beta} + \frac{U}{2} \sum_{i} \left(\sum_{\alpha} \hat{n}_{i\alpha} - 5 \right)^2$$

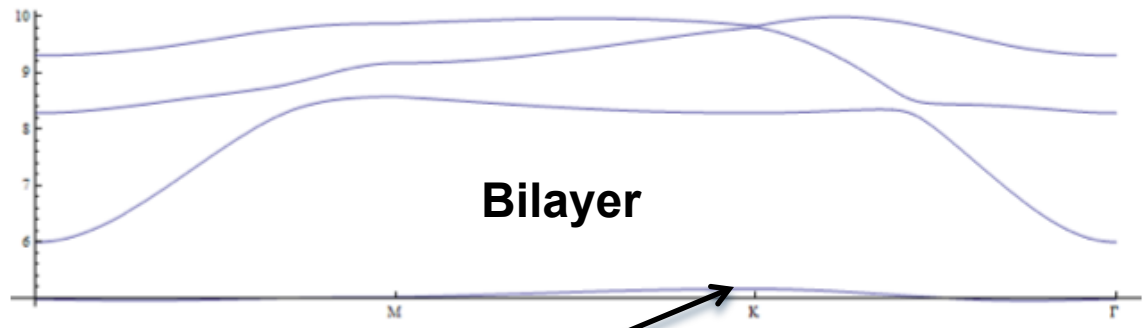
← Full t_{2g} manifold

Hartree-Fock Phase Diagram:





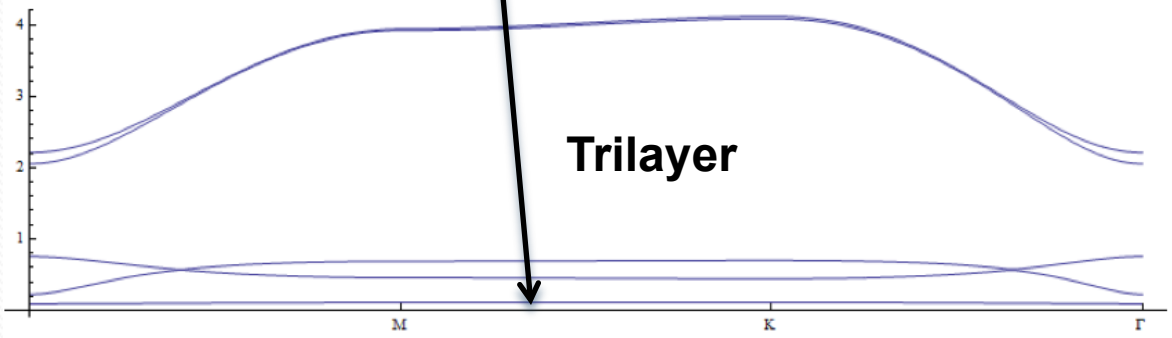
Magnetic excitations in the strong coupling limit:
Flat Magnon Bands with Chern number=1



$$H = \sum_{ij} \left[R_i^T \Lambda_{ij} R_j \right]^{ab} \tilde{S}_i^a \tilde{S}_j^b$$
$$\equiv \sum_{ij} \tilde{\Lambda}_{ij}^{ab} \tilde{S}_i^a \tilde{S}_j^b.$$

$$\Lambda_{ij}^{ab} = J\delta^{ab} + \epsilon^{abc} D_{ij}^c + \Gamma_{ij}^{ab}$$

Flat bands

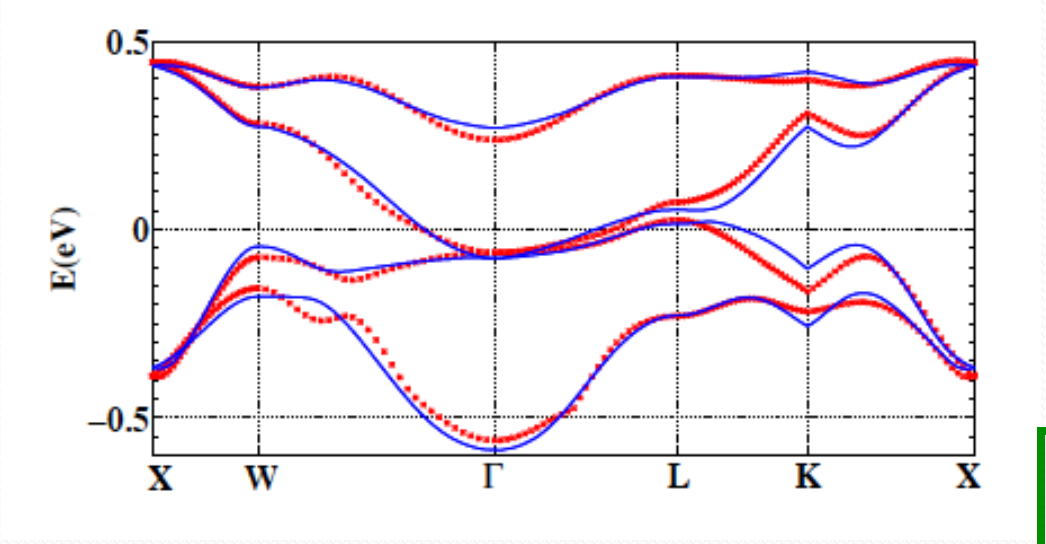


$$J = \frac{4}{U}\left(t^2 - \frac{|\mathbf{v}|^2}{3}\right),$$
$$\mathbf{D}_{ij} = \frac{8}{U} t \mathbf{v}_{ij},$$
$$\Gamma_{ij}^{ab} = \frac{8}{U}\left(v_{ij}^a v_{ij}^b - \delta^{ab}\frac{|\mathbf{v}|^2}{3}\right)$$

Summary

- Studied thin film iridates from both weak and strong coupling limits.
- Topological phases (Chern insulators and Chern metals are possible)
- Magnetic excitations may also show topological properties and interesting interaction effects.

Pyrochlore Iridate $Y_2Ir_2O_7$ ($La_2Ir_2O_7$) Thin Films



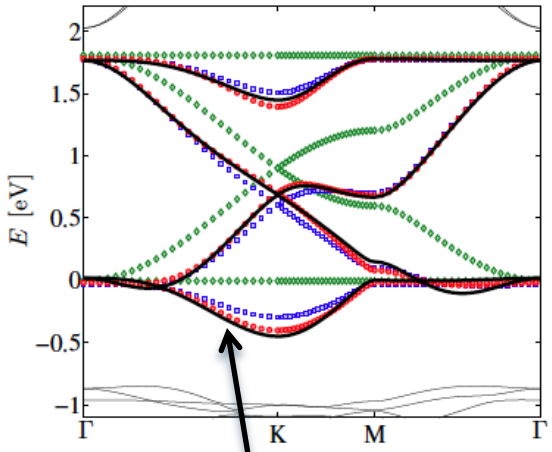
GGA Bandstructure (bulk)

3rd Neighbor tight-binding fit—need further range hoppings

In the end, we did Wannier fits, which are indistinguishable to the eye from DFT.

Extended Phase Diagram for $LaNiO_3$ Bilayer

Ruegg, Mitra, Demkov, Fiete PRB 85, 245131 (2012)



DFT result (LDA)

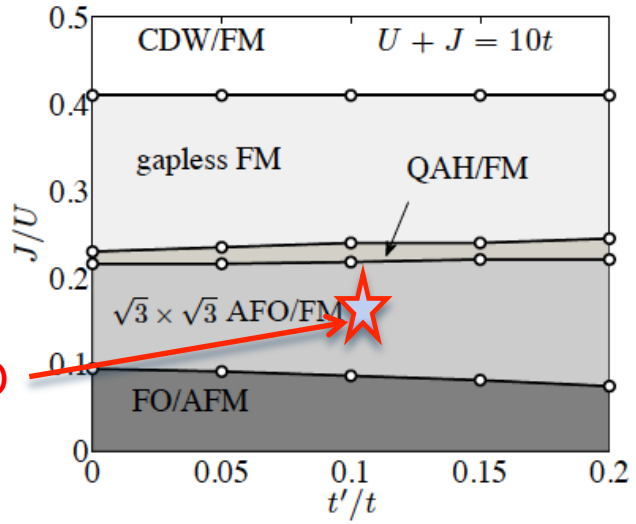
1st neighbor 2nd neighbor

fFt	t (eV)	t' (eV)	Δ (eV)	t_δ (eV)	E_F (eV)
A	0.603	0	0	0	−0.701
B	0.600	0.058	0	0	−0.693
C	0.598	0.062	−0.023	0	−0.693
D	0.598	0.062	−0.023	−0.007	−0.693

$$H_{\text{int}} = \sum_r \Bigg[U \sum_\alpha n_{r\alpha\uparrow} n_{r\alpha\downarrow} + (U' - J) \sum_{\alpha>\beta,\sigma} n_{r\alpha\sigma} n_{r\beta\sigma} + U' \sum_{\alpha\neq\beta} n_{r\alpha\uparrow} n_{r\beta\downarrow} + J \sum_{\alpha\neq\beta} d^\dagger_{r\alpha\uparrow} d_{r\beta\uparrow} d^\dagger_{r\beta\downarrow} d_{r\alpha\downarrow} + I \sum_{\alpha\neq\beta} d^\dagger_{r\alpha\uparrow} d_{r\beta\uparrow} d^\dagger_{r\alpha\downarrow} d_{r\beta\downarrow} \Bigg].$$

U=U' +2J
I=J

(LNO



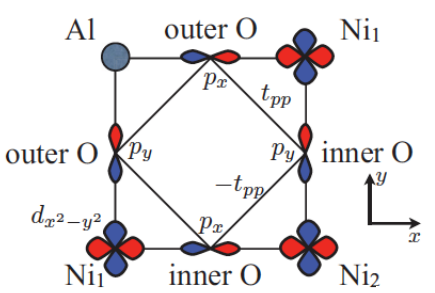
Charge-transfer physics in $LaNiO_3$ Bilayer (Explicitly retain O *p*-orbitals)

Ruegg, Mitra, Demkov, Fiete PRB 85, 245131 (2012)

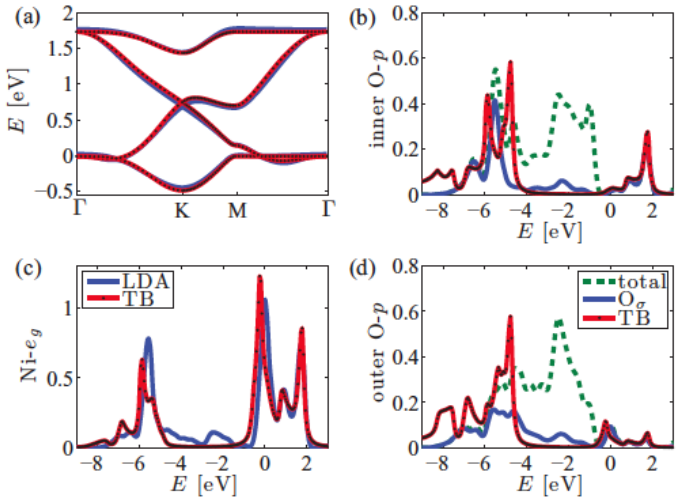
Mean-field (HF)

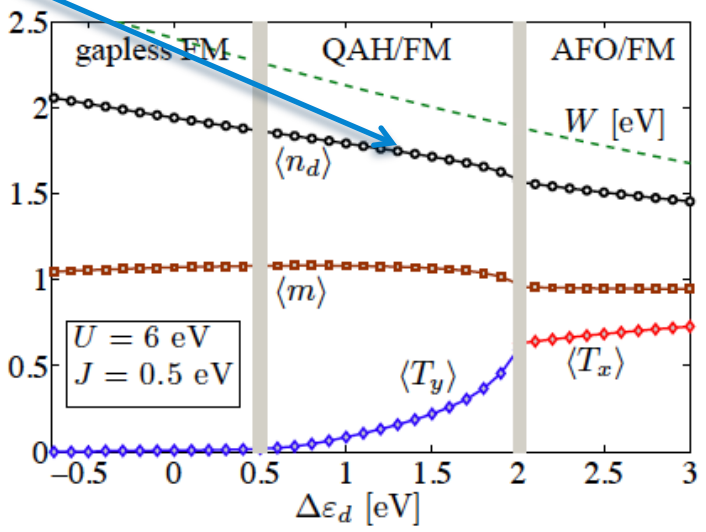
$$H = \sum_{i\sigma} \epsilon_{pi} p^\dagger_{i\sigma} p_{i\sigma} + \sum_{i\alpha\sigma} \epsilon_d d^\dagger_{i\alpha\sigma} d_{i\alpha\sigma} + H_p + H_{\rm hyb} + H_{\rm int} + H_{\rm DC}$$

$$H_{\rm hyb} = \sum_{\langle i,j\rangle} (V^\alpha_{ij} p^\dagger_{i\sigma} d_{j\alpha\sigma} + \text{H.c})$$



Charge-transfer physics

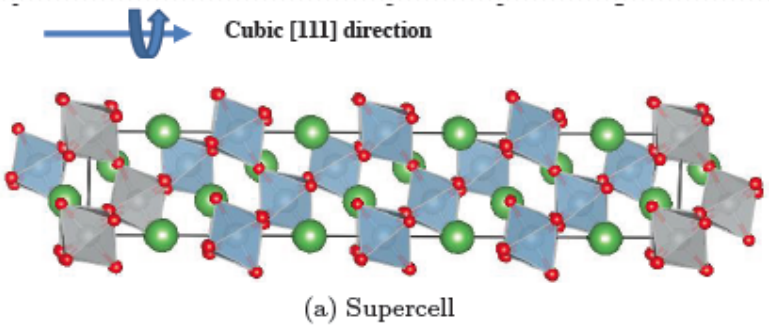


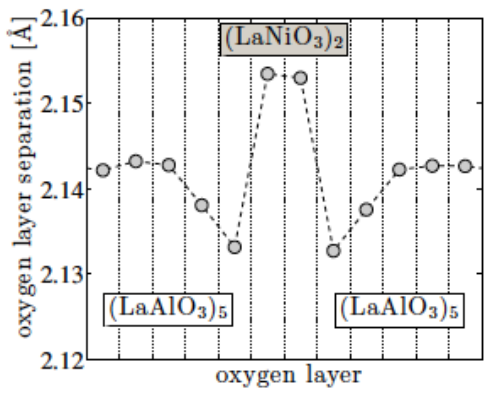


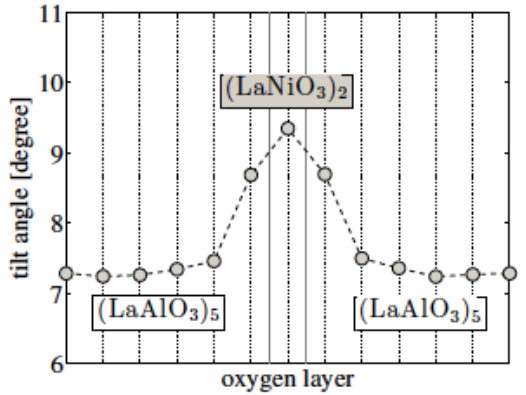
Related work:
Andy Millis Group
(explicit *p*-orbital)

Lattice Strain Effects: Internal

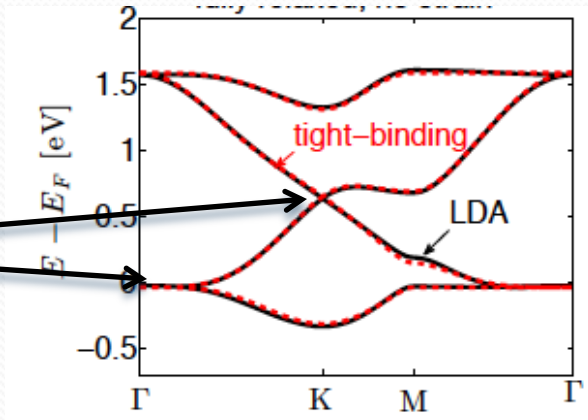
Ruegg, Mitra, Demkov, Fiete PRB (2013)







QBCP & Dirac point intact



Internal lattice strain leaves unstrained picture essentially unchanged, *even quantitatively!*

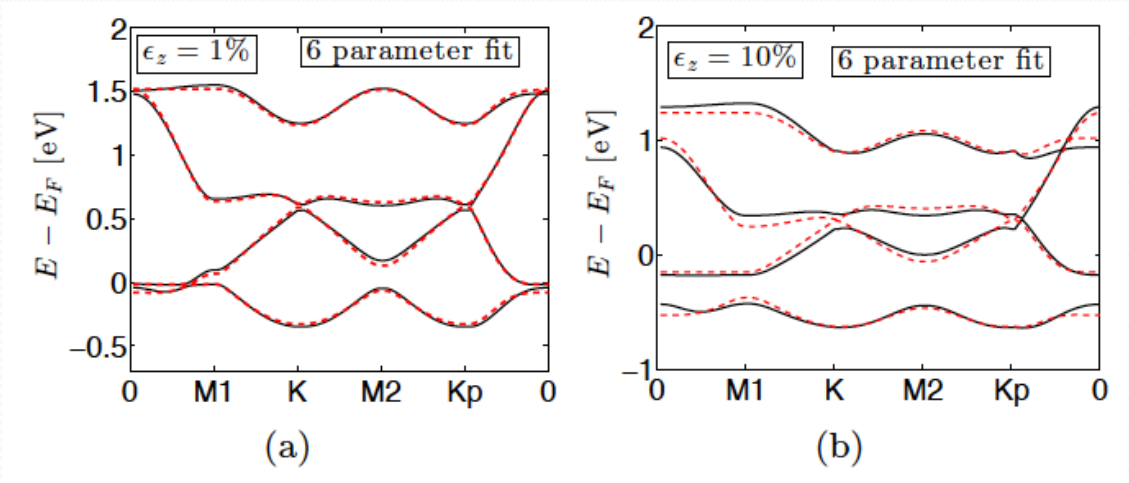
fit	t [eV]	t' [eV]	Δ [eV]	E_F [eV]
unrelaxed	0.598	0.062	-0.023	-0.693
fully relaxed	0.541	0.045	-0.017	-0.641

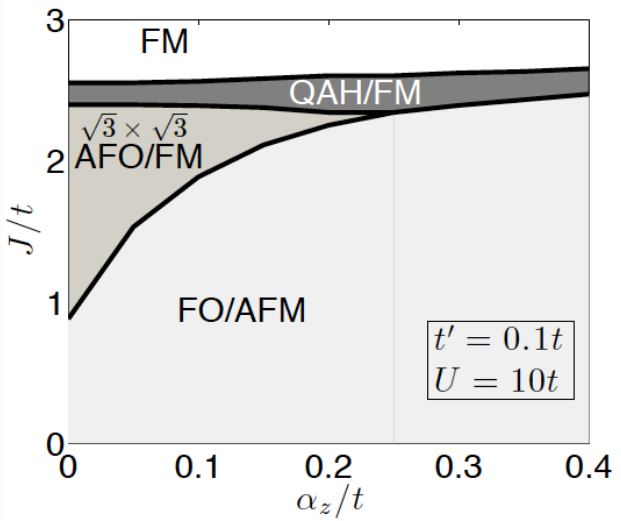
Lattice Strain Effects: External

Ruegg, Mitra, Demkov, Fiete *Phys. Rev. B* (2013)

Apply symmetry-breaking strain along the [001] cubic direction:

$$\mathbf{a_1} = a_0(1-\mu x)\mathbf{i},$$
$$\mathbf{a_2} = a_0(1-\mu x)\mathbf{j},$$
$$\mathbf{a_3} = a_0(1+x)\mathbf{k},$$





Dominant effect is orbital splitting: $H_z = \alpha_z \sum_{\boldsymbol{r}} \left(n_{\boldsymbol{r},x^2-y^2} - n_{\boldsymbol{r},z^2} \right)$

Externally imposed strain along [001] favors FO/AFM order.
Topological phase unaffected.

Predictions for topological phases in pyrochlore iridates (partial)

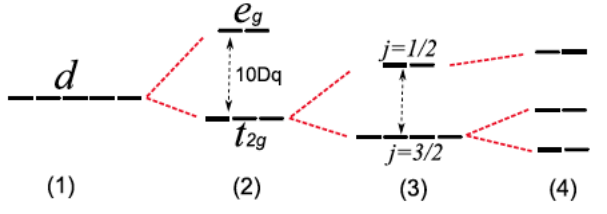
- A_2Ir_2O7 (undistorted): D. Pesin, L. Balents, Nat. Phys. (2010)
  "Topological Mott Insulator" (TMI)
- A_2Ir_2O7 (distorted): B-J. Yang, Y.-B. Kim, PRB (2010)
  Single-particle type TI in non-interacting model
- A_2Ir_2O7 (distorted+interaction): M. Kargarian, J. Wen, GAF PRB (2011)
  "Weak Topological Mott Insulator" (WTMI)
- Y_2Ir_2O7 (magnetically ordered): Wan *et al.* PRB (2011)
  Weyl semi-metal
- A_2Ir_2O7: Go, Witczak-Krempa, Jeon, Park, Y.-B. Kim PRL (2012)
  Axion insulator (found via cellular DMFT)
- A_2Ir_2O7: M. Kargarian, GAF PRL (2013)
  Topological crystalline insulator, TCMI
- A_2Ir_2O7: J. Maciejko, V. Chua, GAF PRL (2014)
  TI*, SM*

Minimal model for $A_2Ir_2O_7$?

- Key energy scales:

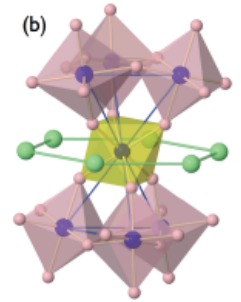
  W~1.5 eV, E_{SOC}~0.5 eV, U~2 eV, $E_{t2g\text{-}eg}$~2 eV

  Δ~0.3-0.5 eV, J_H~0.5 eV



  Moreover, extended 5d orbitals may feel significant crystal fields beyond the local oxygen environment, e.g., Hozio *et al.*, arXiv:1212.4009

  Elements of minimal not entirely clear at present.

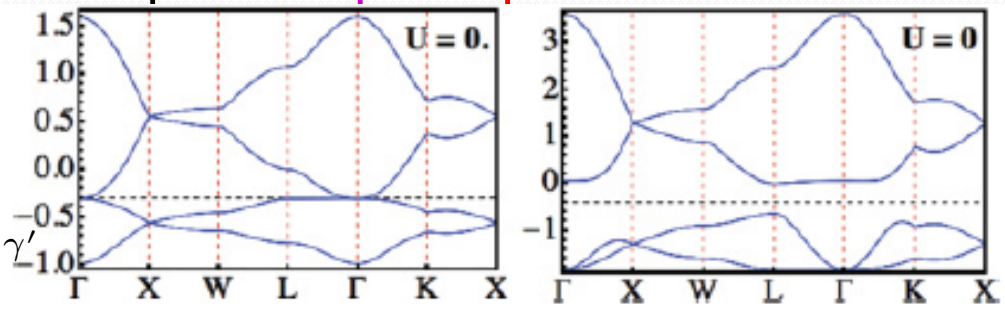


W. Witczak-Krempa, G. Chen, Y.-B. Kim, L. Balents arxiv:1305.2193

- A central issue for topological physics is the j=1/2 band structure, namely order of degeneracies at the Γ point: 2-4-2 vs 4-2-2.

$$H_0 = \sum_{<ij>} (T^{\gamma\gamma'}_{o,ij} + T^{\gamma\gamma'}_{d,ij}) d^\dagger_{i\gamma} d_{j\gamma'}$$

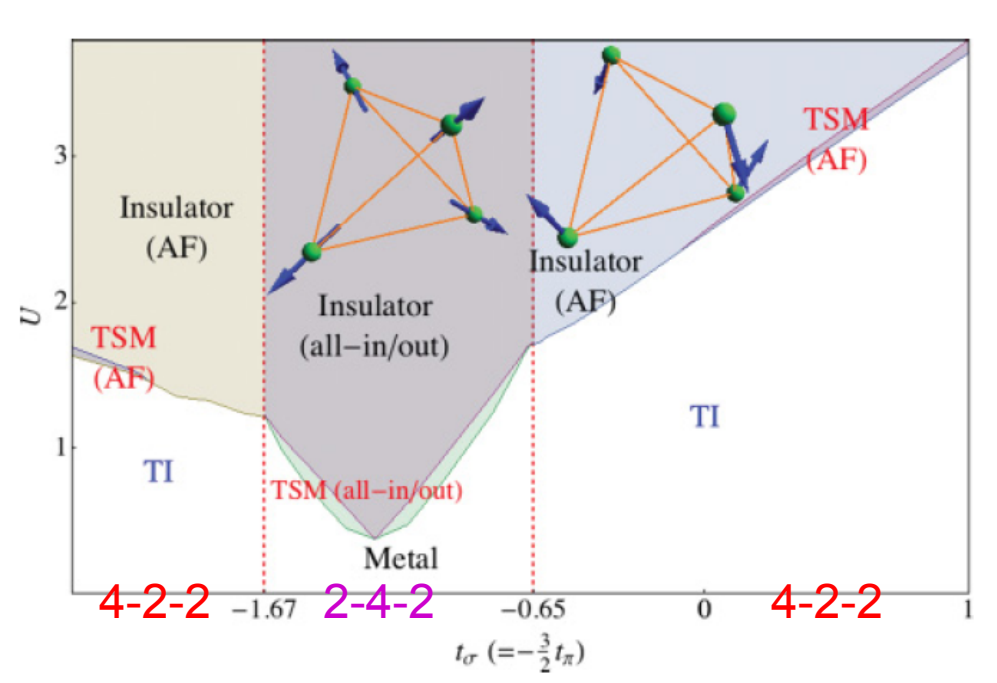
$$= \sum_{<ij>} (t_1 \delta_{\gamma\gamma'} + i t_2 \mathbf{d}_{ij} \cdot \vec{\sigma}_{\gamma\gamma'}) d^\dagger_{i\gamma} d_{j\gamma'}$$



W. Witczak-Krempa and Y.-B. Kim, PRB (2012)

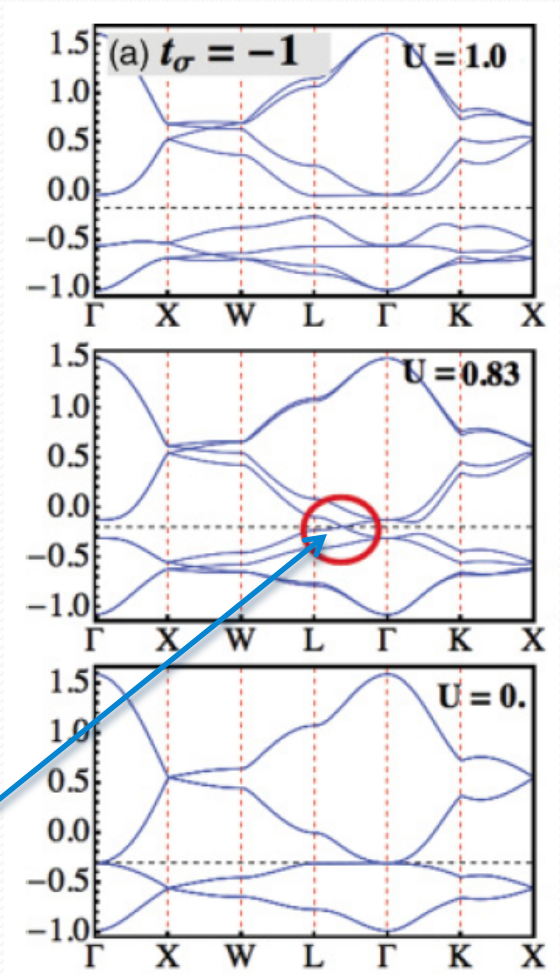
Topological phases in pyrochlore Iridate systems: $A_2Ir_2O_7$ Hartree-Fock Calculations for j=1/2

Witczak-Krempa and Kim, PRB (2012)

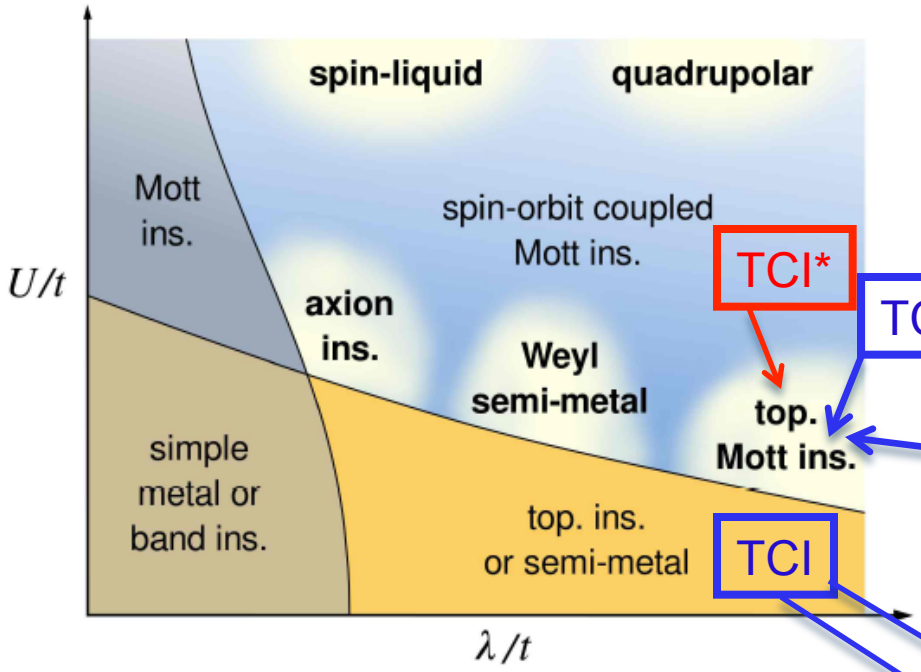


$$H = H_{d-d} + H_{d-o-d} + H_U$$

Weyl point



Summary



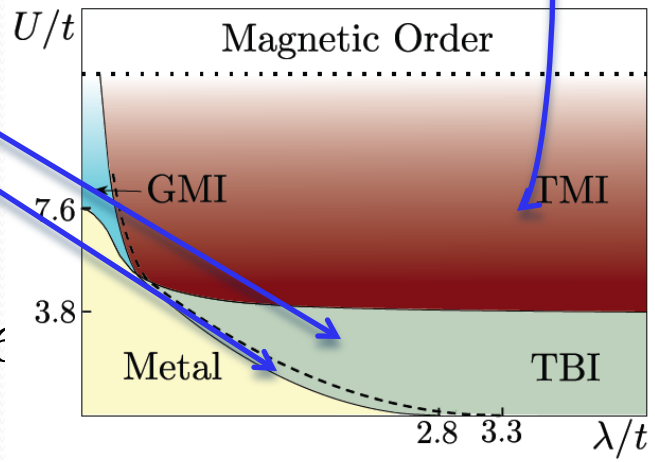
W. Witczak-Krempa, G. Chen,
Y.-B. Kim, L. Balents arxiv:1305.2193

TCI*

TCMI

TI*, SM*

TCI



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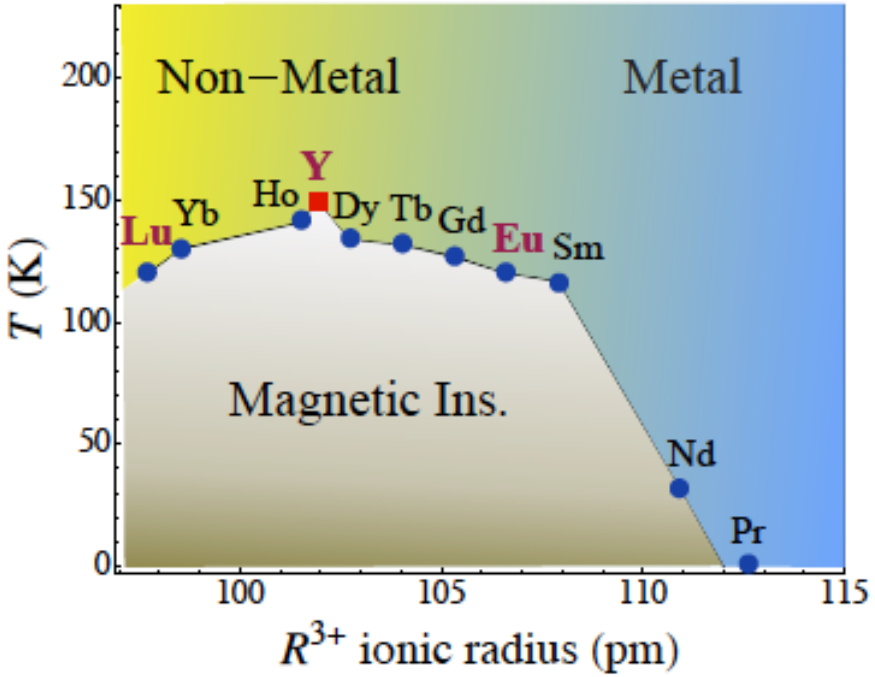
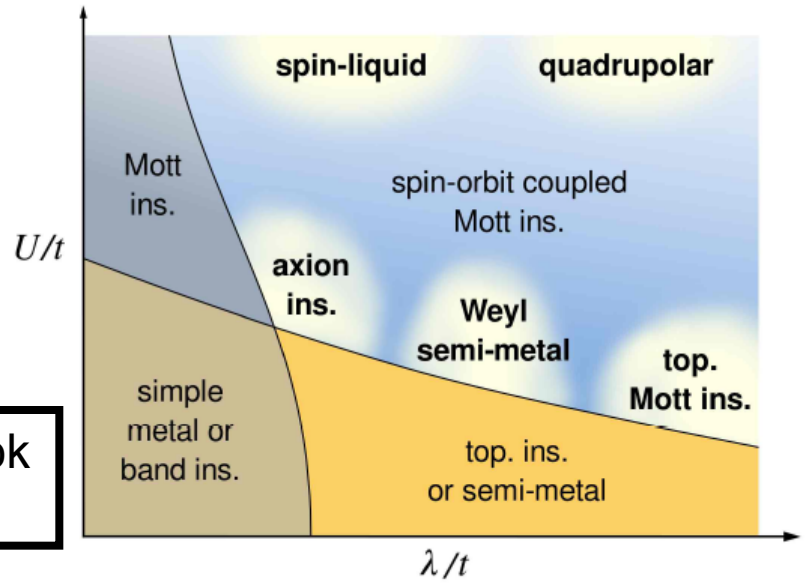
- $A_2Ir_2O_7$: M. Kargarian, GAF PRL (2013)
  Topological crystalline insulator, TCMI 4-2-2
- $A_2Ir_2O_7$: J. Maciejko, V. Chua,GAF arXiv:1307.5566
  TI* 4-2-2, SM* 2-4-2

Experimental Phase Diagram for Bulk Pyrochlore Iridates

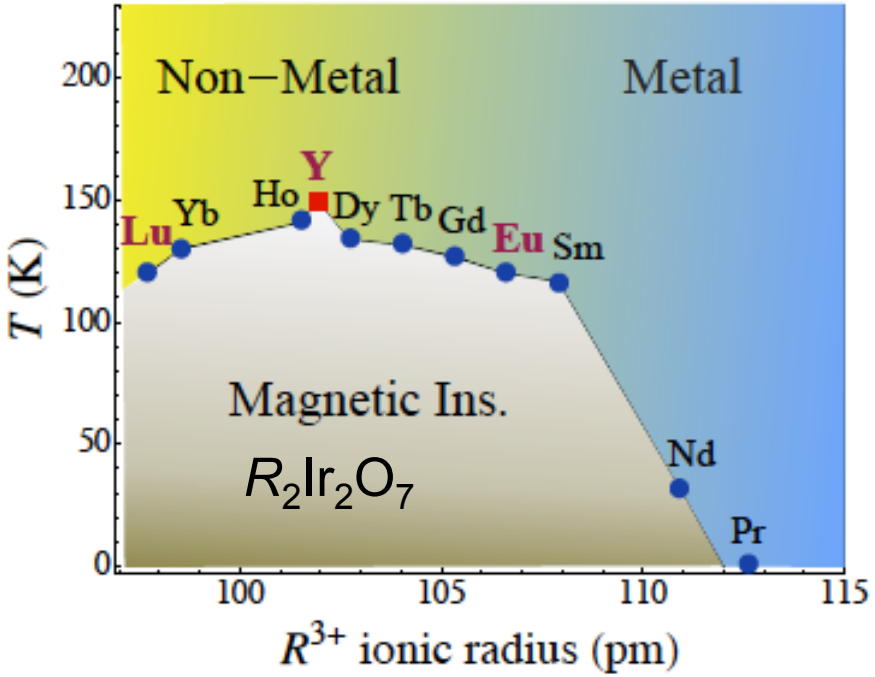


W. Witczak-Krempa, G. Chen,
Y.-B. Kim, L. Balents arxiv:1305.2193

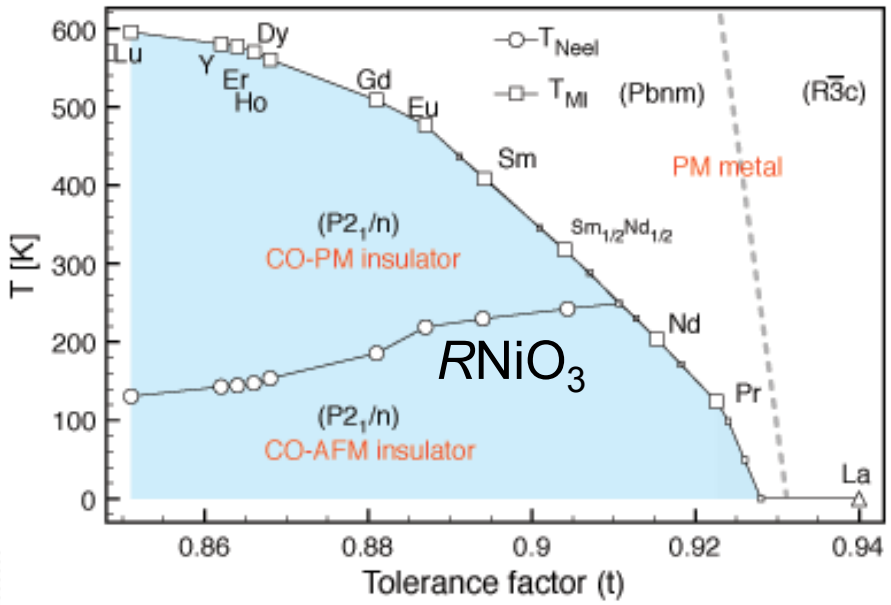


Overall, these particular materials do not look promising for topological phases.

Experimental Phase Diagram for Bulk Pyrochlore Iridates and Bulk Perovksite Nickelates



W. Witczak-Krempa, G. Chen, Y.-B. Kim, L. Balents arxiv:1305.2193

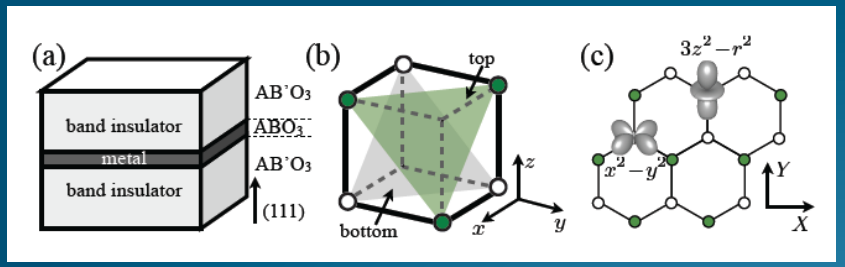


Overall, these particular materials do not look promising for topological phases.

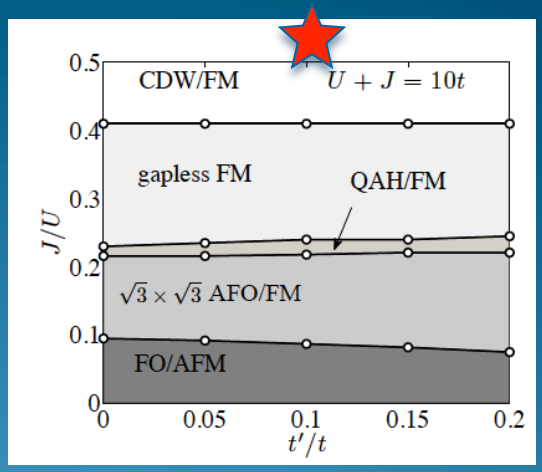
From Triscone Group Website

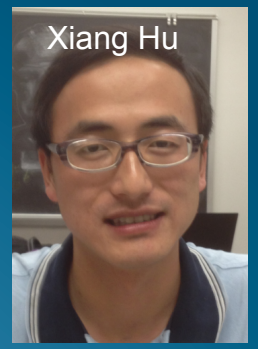
But thin films are a different story!

Topological Phases in Perovskite Heterostructures



$LaAlO_3/LaNiO_3/LaAlO_3$





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