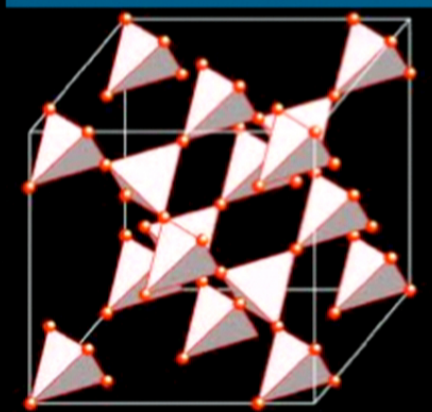
Title: Topological Phases in Transition Metal Oxides

Date: Nov 07, 2013 02:00 PM

URL: http://pirsa.org/13110072

Abstract: Certain varieties of transition metal oxides possess both significant interactions and strong spin-orbit coupling. In this talk I will describe materials-motivated models that predict topological phases in heterostructured and bulk transition metal oxides. We find Z2 topological insulators, Chern insulators, topological crystalline insulators, and interaction-driven topological phases not adiabatically connected to non-interacting topological phases.

Topological Phases in Pyrochlore Oxides: TCI, TCMI, and TI* (and TCI*)



Mehdi Kargarian

Victor Chua

Joseph Maciejko

Gregory A. Fiete

University of Texas at Austin

M. Kargarian and GAF, *Phys. Rev. Lett*. (2013)

J. Maciejko, V. Chua, and GAF arXiv:1307.5566

Outline

- Brief review of predicted topological phases in A_2M_2O7 (mainly M=iridium, A=rare earth)
- Minimal models and band structure considerations
- Topological crystalline insulator (TCI)
  -Interactions can drive a "TCMI", U(1) gauge theory
- The fractionalized TI* phase, Z2 gauge theory
  -Low-energy described by (3+1)D *BF* theory
- Topological phases in oxide thin films:
  -Pyrochlore Iridates and Perovskite Nickelates

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)
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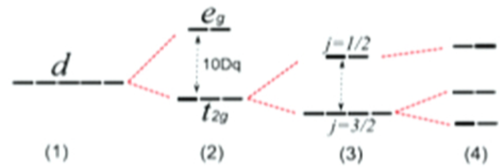
  TI*, SM*

Minimal model for $A_2Ir_2O_7$?

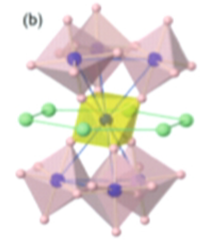
- Key energy scales:

  t~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.

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

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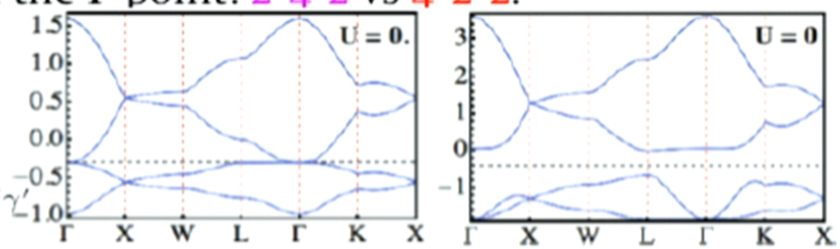

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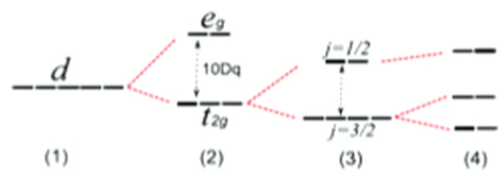

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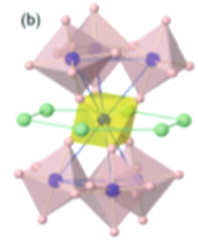

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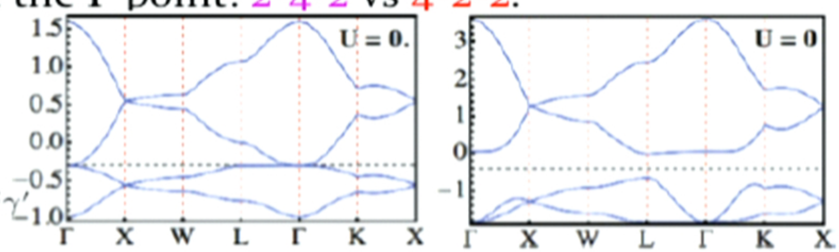

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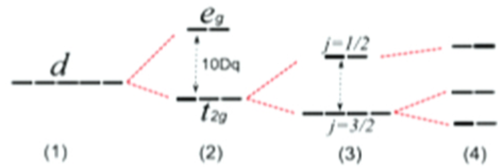

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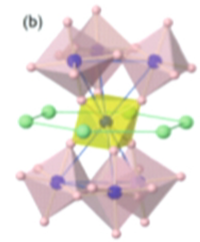

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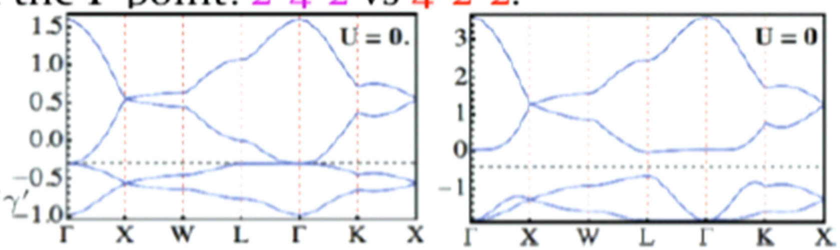

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Topological phases in pyrochlore Iridate systems: $A_2Ir_2O_7$ Hartree-Fock Calculations for j=1/2

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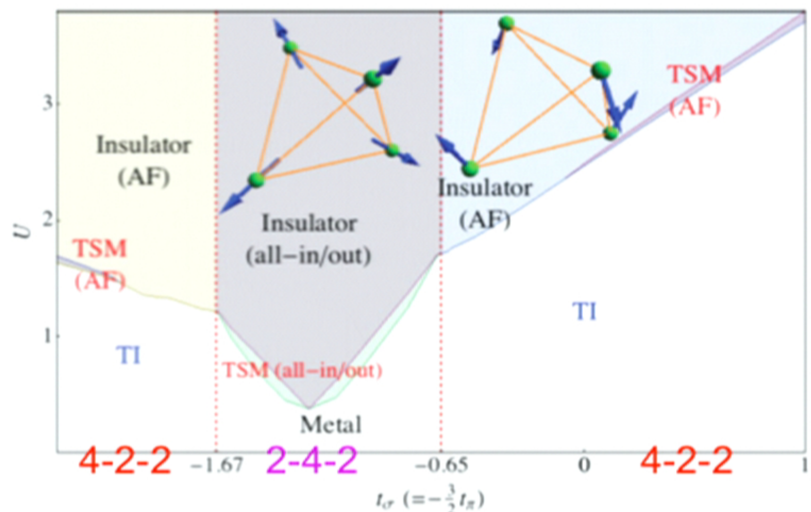

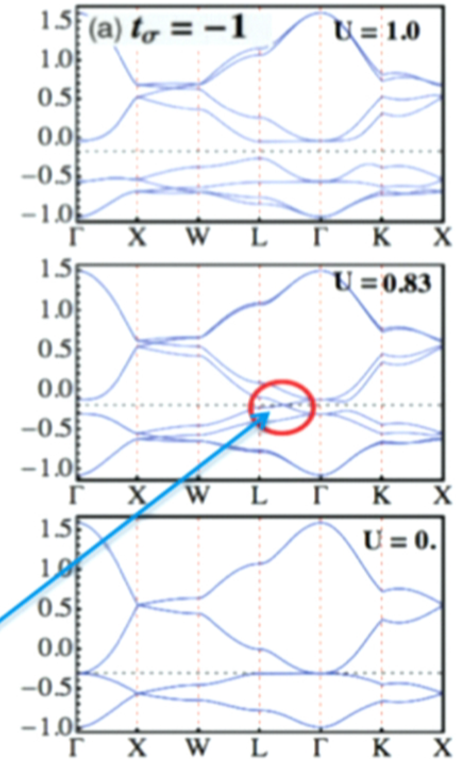

$$H = H_{d-d} + H_{d-o-d} + H_U$$

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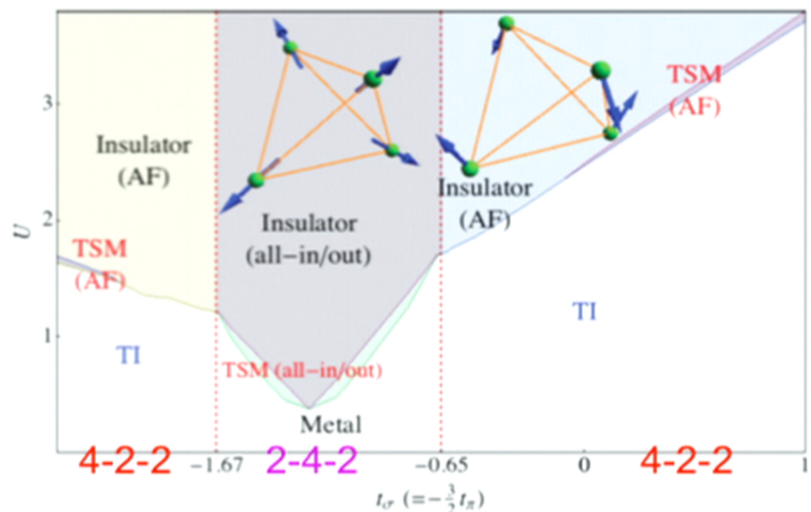

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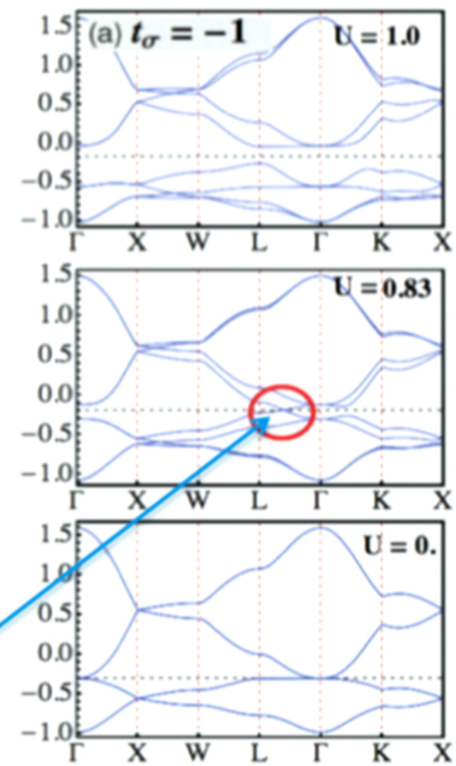
Weyl point



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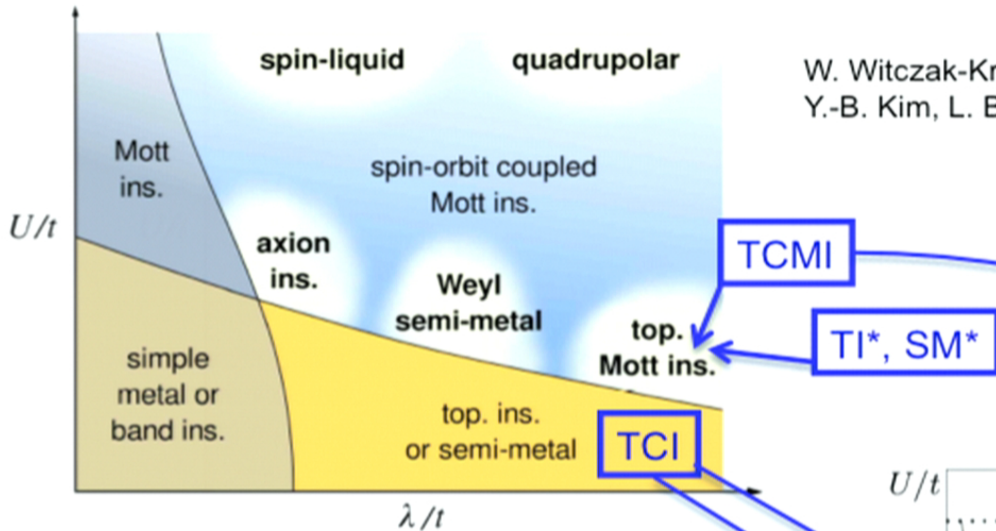
  TI* 4-2-2, SM* 2-4-2

Schematic Phase Diagram



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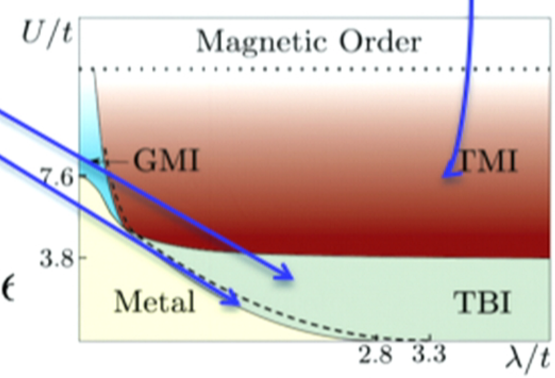

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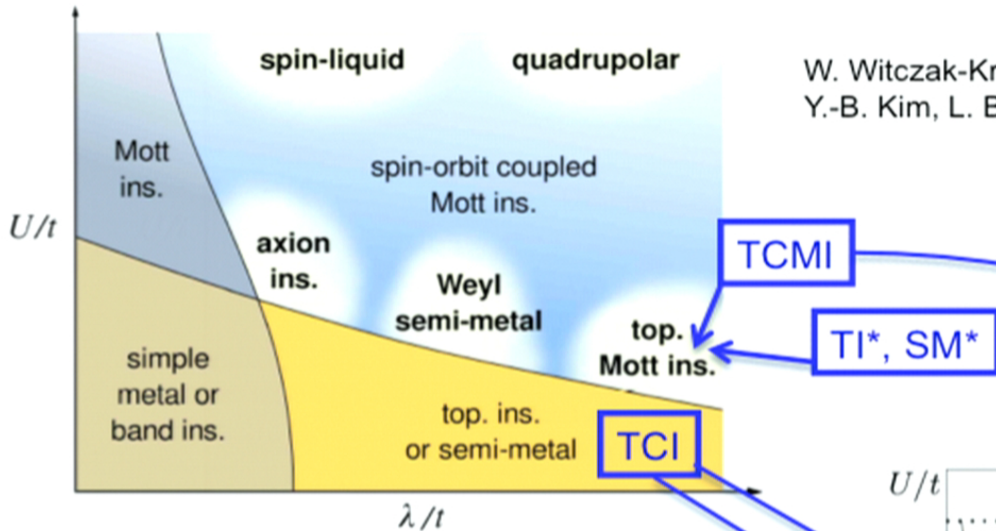

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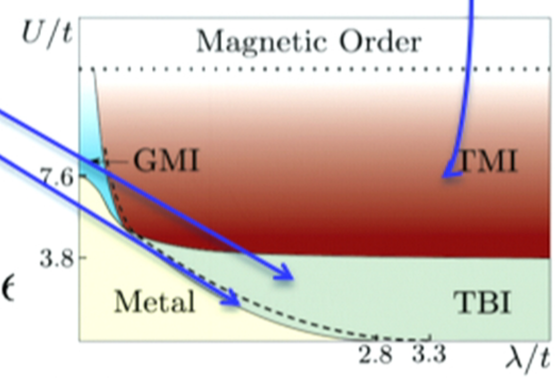

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Topological Crystalline Insulators: Mirror Chern Number

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  --Also recent, J. Liu, W. Duan, L. Fu arXiv:1304.0430. IV-VI semiconductors

- Realized essentially simultaneously by three groups:

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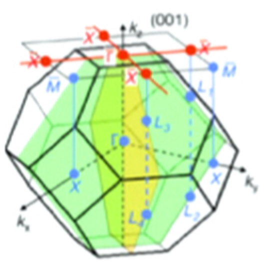

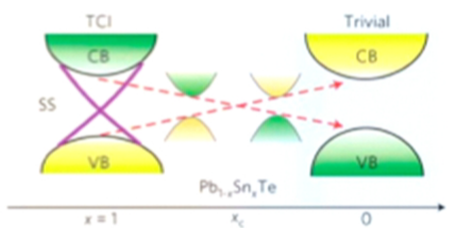

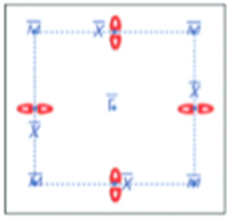

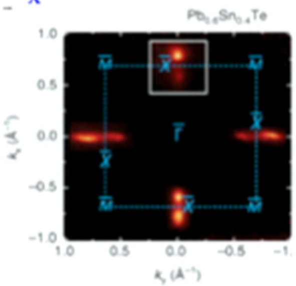

Topological Crystalline Insulators: Mirror Chern Number

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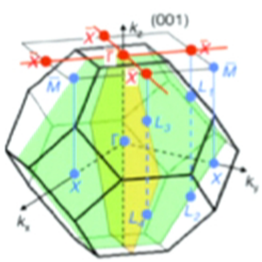
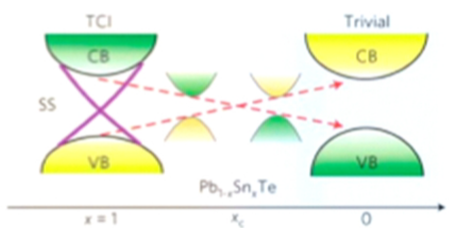
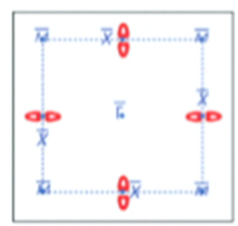
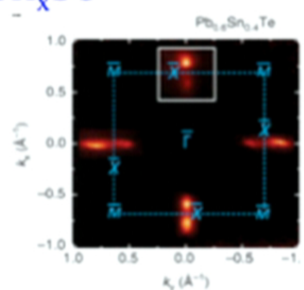


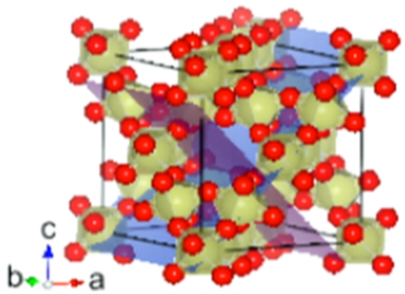


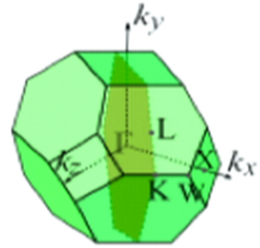




Computing TCI invariant for $A_2Ir_2O_7$

M. Kargarian and GAF PRL (2013)





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4-2-2

$$n_M = (n_{+i} - n_{-i})/2$$

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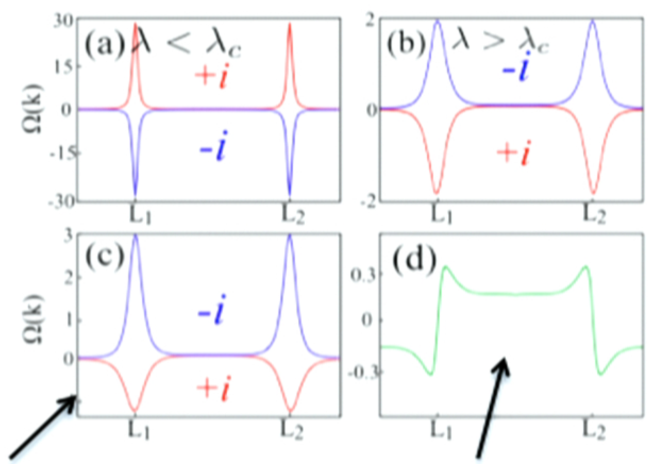

TRS Breaking, Mirror Preserved

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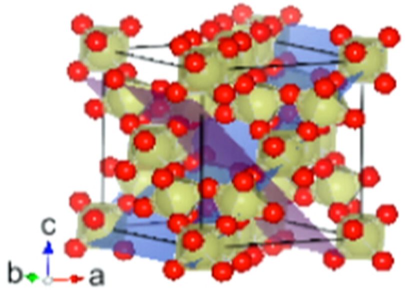

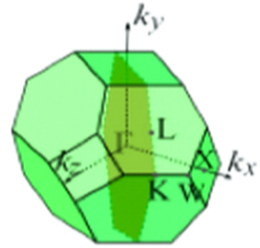

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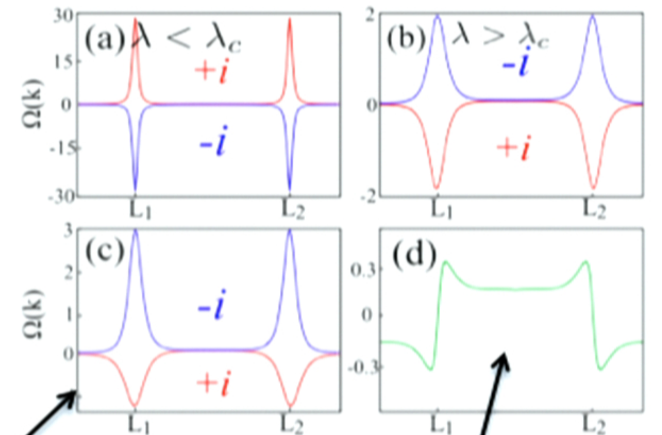
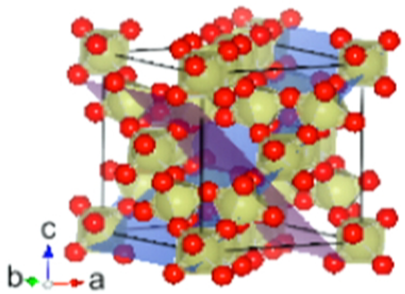
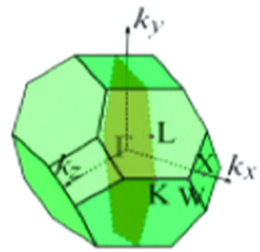


TCI edge states for $A_2Ir_2O_7$: Slab geometry [010] Direction
Mirror Planes: (101) and (10<u>1</u>)

M. Kargarian and GAF PRL (2013)





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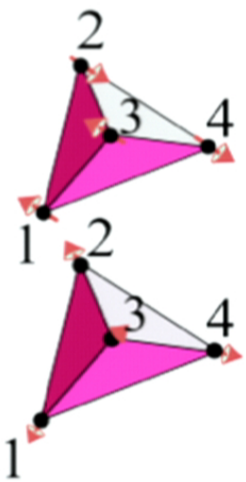

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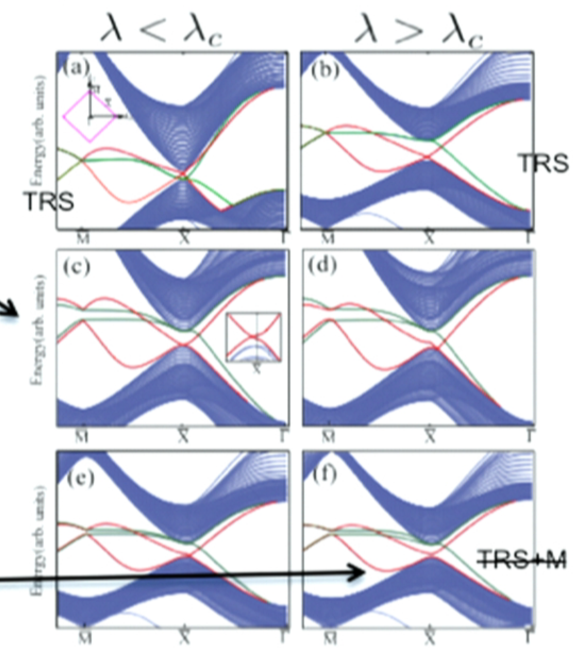

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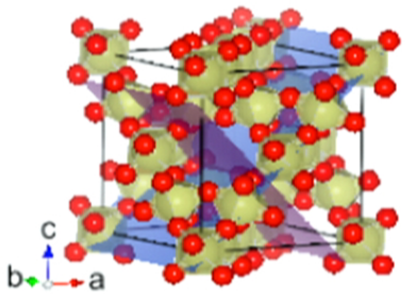

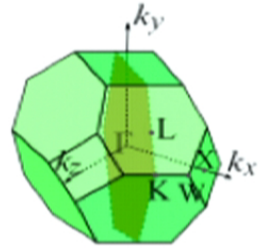

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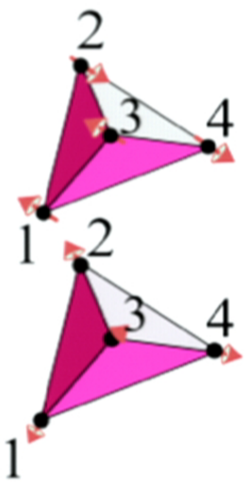

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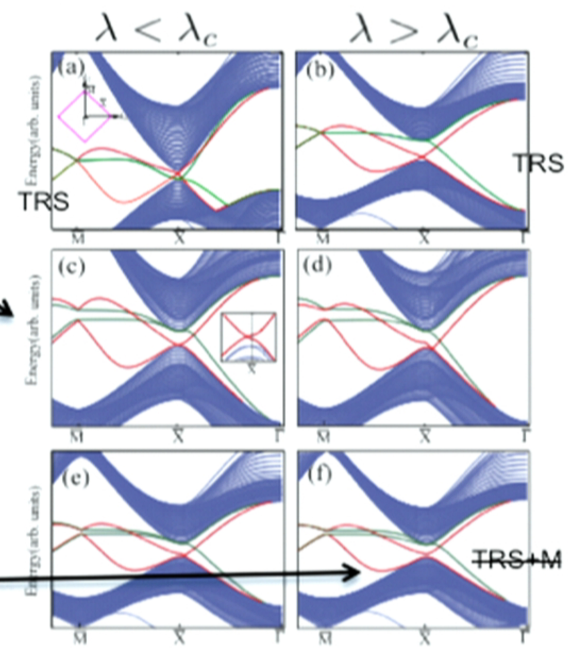
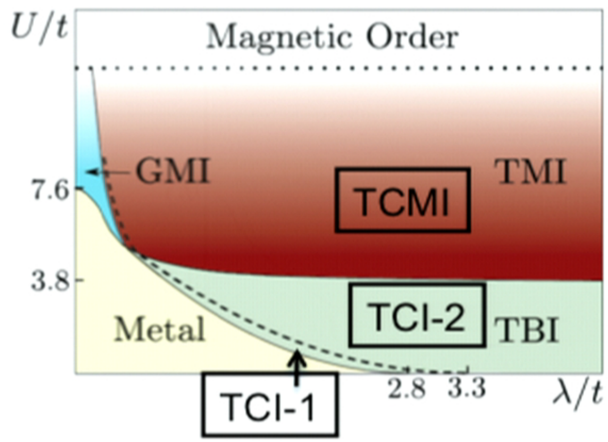


"TCMI" from slave rotors: Refined Phase Diagram

M. Kargarian and GAF PRL (2013)



Pesin and Balents Nat. Phys. (2010)

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

$$t_i = \varepsilon_d - \lambda l \cdot s$$

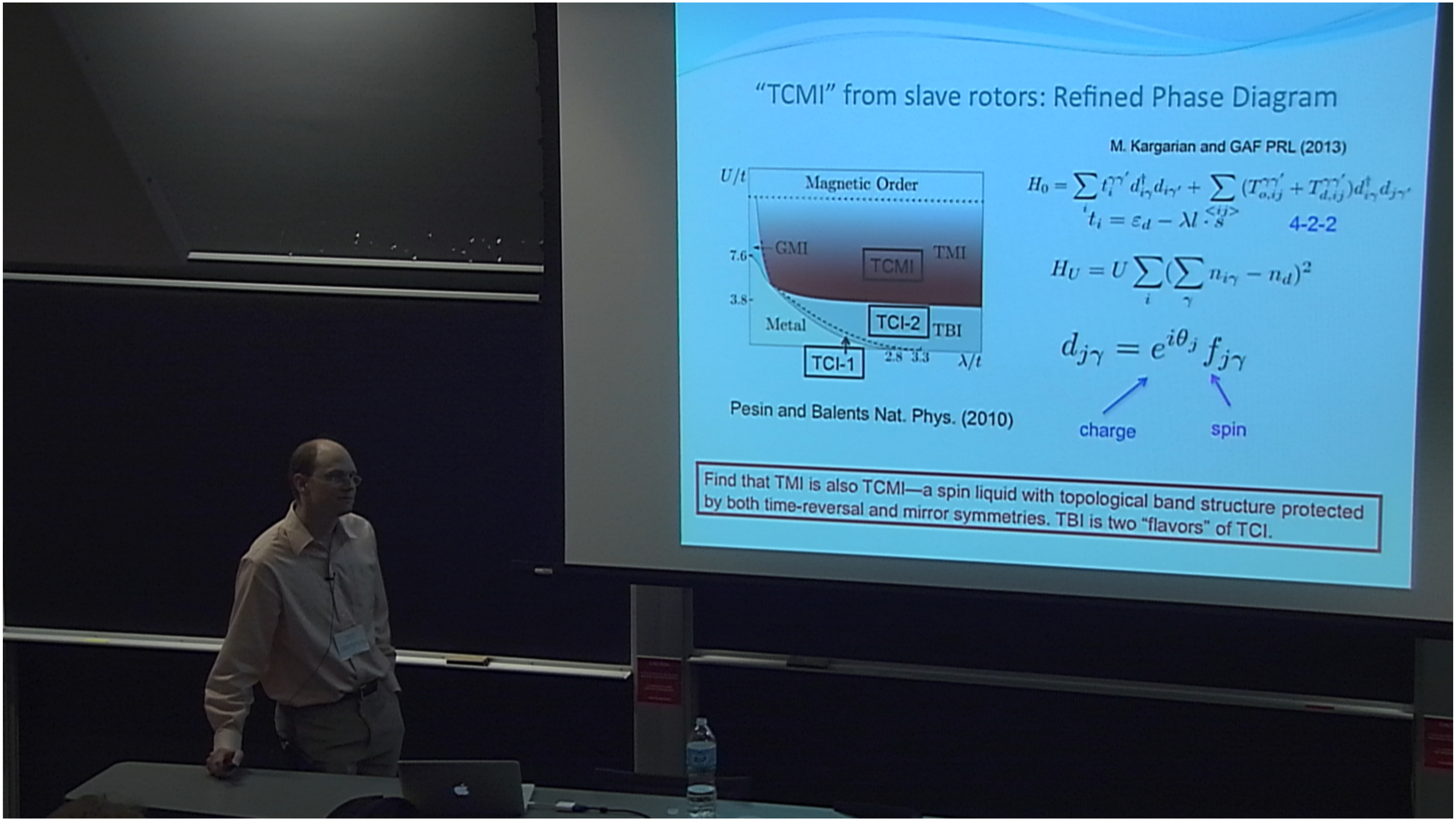
4-2-2

$$H_U = U \sum_i (\sum_\gamma n_{i\gamma} - n_d)^2$$

$$d_{j\gamma} = e^{i\theta_j} f_{j\gamma}$$

charge spin

Find that TMI is also TCMI—a spin liquid with topological band structure protected by both time-reversal and mirror symmetries. TBI is two "flavors" of TCI.


"TCMI" from slave rotors: Refined Phase Diagram
M. Kargarian and GAF PRL (2013)
U/t
Magnetic Order
7.6
3.8
GMI
TMI
TCMI
TCI-2
TBI
Metal
TCI-1
2.8
3.3
λ/t
4-2-2
$H_U = U \sum_i (\sum_\gamma n_{i\gamma} - n_d)^2$
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charge
spin
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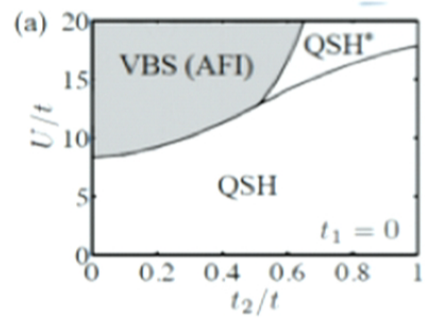
TI* from slave spins: Topological Field Theory & Mean-field Theory

J. Maciejko, V. Chua, GAF arXiv:1307.5566

- Idea is to generalize QSH* phase to three-dimensions

  A. Ruegg and GAF PRL (2012)

$$H = \sum_{rr'} \sum_{\alpha\beta} t^{rr'}_{\alpha\beta} c^\dagger_{r\alpha} c_{r'\beta} + \frac{U}{2} \sum_r \left(\sum_{\alpha=\uparrow,\downarrow} n_{r\alpha} - 1 \right)^2$$



S. Huber and A. Ruegg PRL (2009)
A. Ruegg, S. Huber, M. Sigrist PRB (2010)

$$c_{r\alpha} = f_{r\alpha} \tau^x_r$$

R. Nandkishore, M. A. Metliski, T. Senthil PRB (2012)
Zhong, Wang, Luo arXiv:1304.2099
-Exactly solvable models

**J. Maciejko and A. Ruegg arXiv:1305.1290 CI* Phase

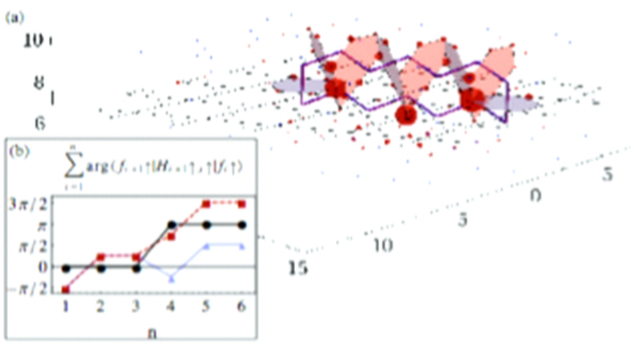
Mean-Field Theory for TI*: Phase Diagram and Braiding

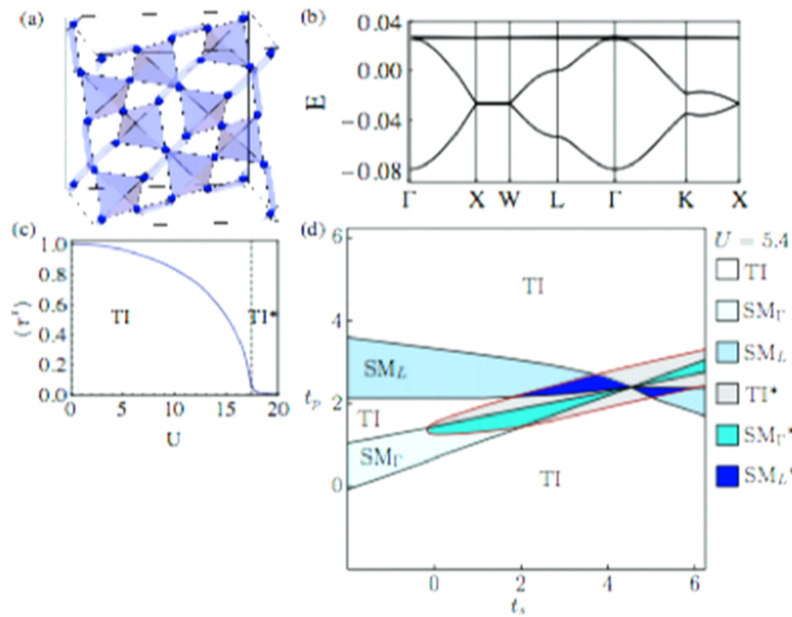
J. Maciejko, V. Chua, GAF arXiv:1307.5566

$$H_{\mathrm{MF}} = \sum_{rr'} \sum_{\alpha\beta} \chi_{\alpha\beta}^{rr'} \sigma_{rr'} f_{r\alpha}^{\dagger} f_{r'\beta} + \sum_{rr'} J_{rr'} \sigma_{rr'} \tau_r^x \tau_{r'}^x + \frac{U}{4} \sum_r (\tau_r^z + 1)$$

$$\chi_{\alpha\beta}^{rr'} = t_{\alpha\beta}^{rr'} \sigma_{rr'} \langle \tau_r^x \tau_{r'}^x \rangle_{\mathrm{MF}},$$

$$J_{rr'} = \sum_{\alpha\beta} t_{\alpha\beta}^{rr'} \sigma_{rr'} \langle f_{r\alpha}^{\dagger} f_{r'\beta} \rangle_{\mathrm{MF}}$$





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J. Maciejko, V. Chua, GAF arXiv:1307.5566

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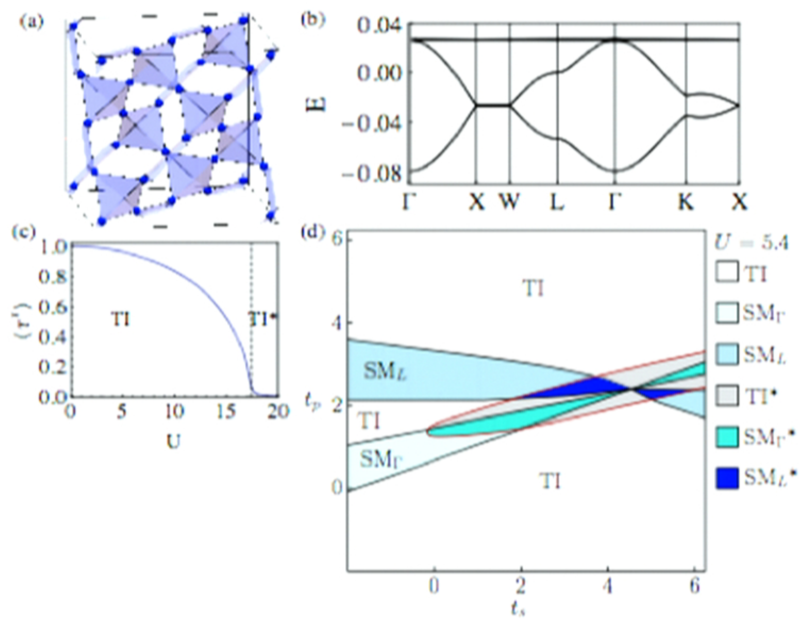

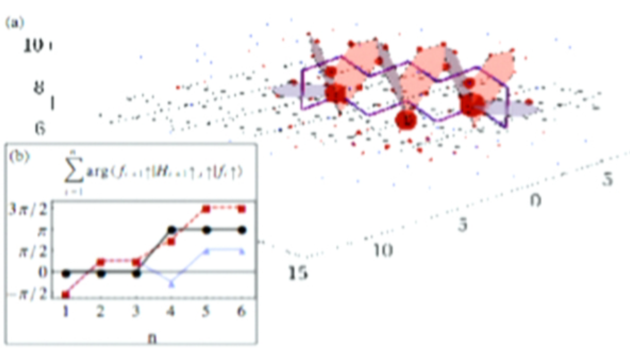

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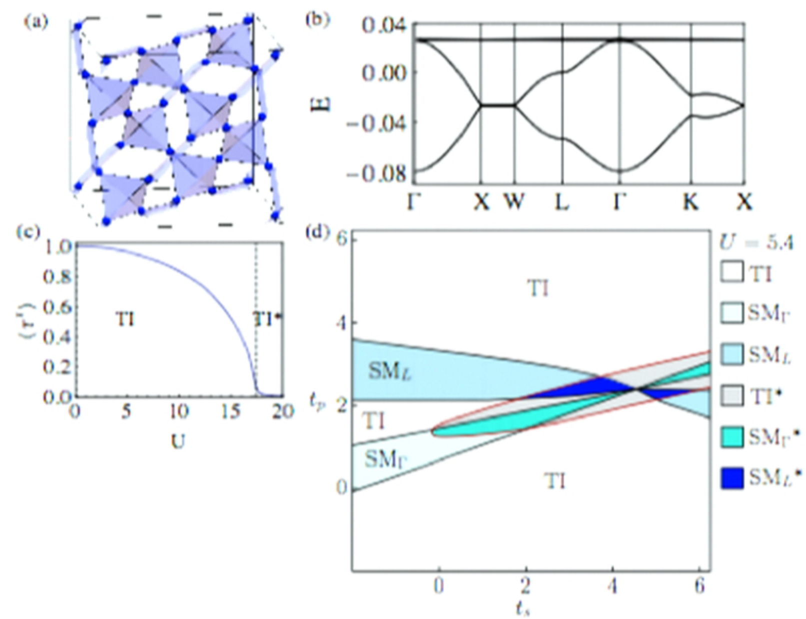
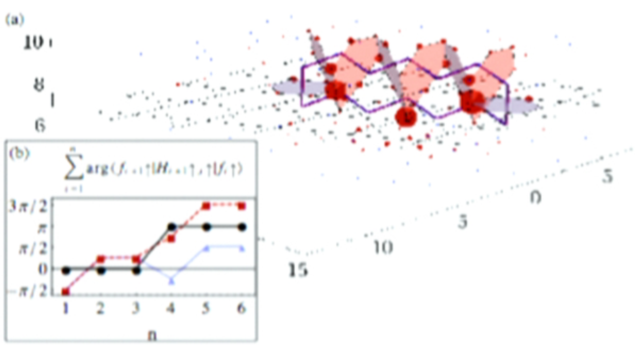
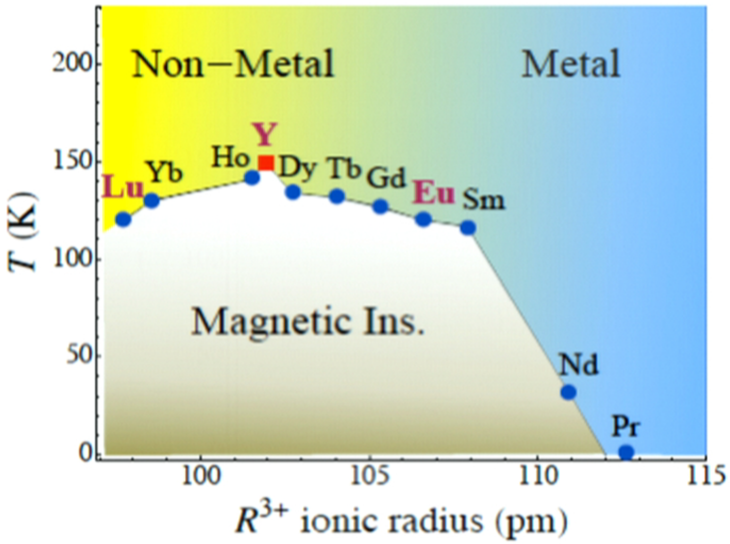
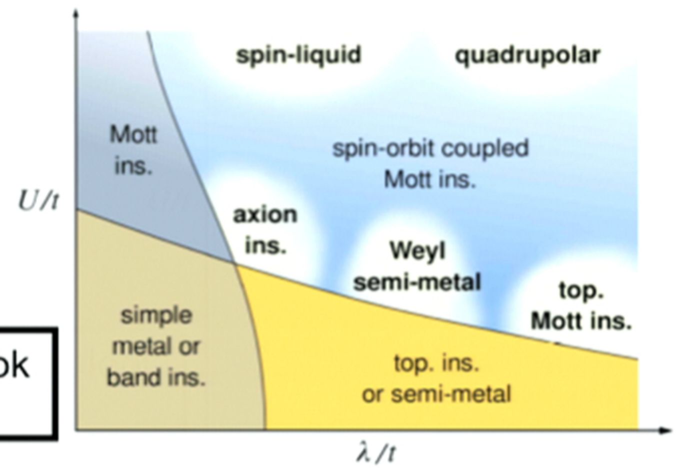




Experimental Phase Diagram for Bulk Pyrochlore Iridates

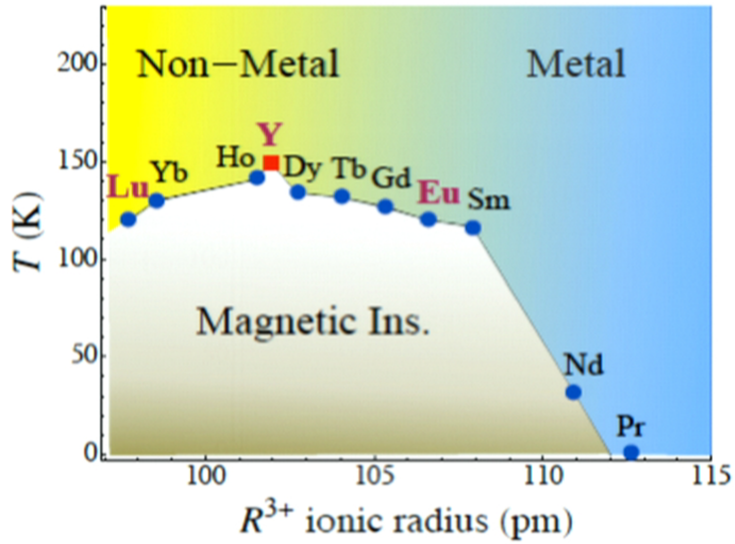


W. Witczak-Krempa, G. Chen, Y.-B. Kim, L. Balents arxiv:1305.2193



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

Experimental Phase Diagram for Bulk Pyrochlore Iridates



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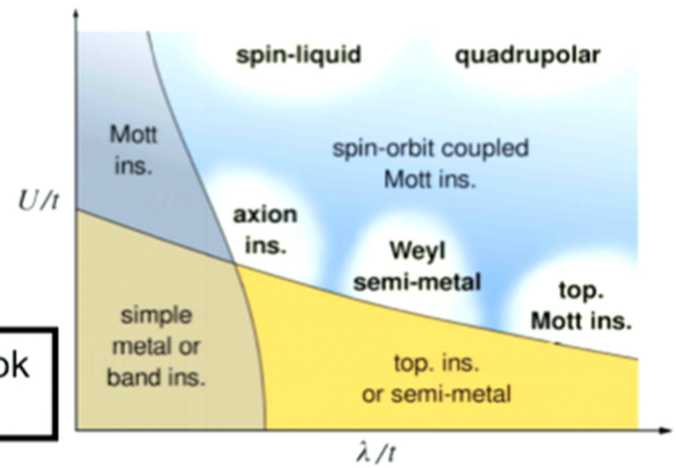

Overall, these particular materials do not look promising for topological phases.