Title: Double perovskite materials: From Chern bands to unusual Mott insulators

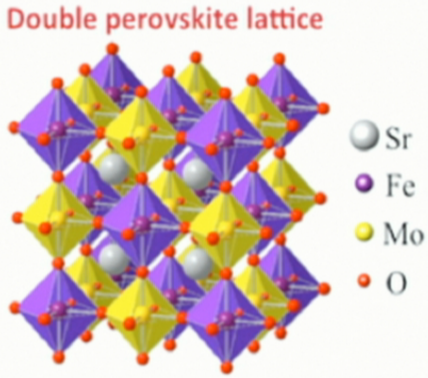
Date: Apr 30, 2015 11:30 AM

URL: http://pirsa.org/15040159

Abstract: Double perovskites, a class of oxide materials with 3d and 5d transition metal ions, can realize a wide variety of interesting phases. Here we focus on our recent theoretical work suggesting the appearance of Chern insulators, and possible emergent nematic phases at Chern transitions in such systems. We will also discuss Mott insulating double perovskites with iridium moments which appear to host unusual magnetic interactions on the 3-dimensional fcc lattice, and present comparisons with experimental data.

Ordered Double Perovskites

General formula: $A_2BB'O_6$ (B,B' = 3d, 4d, 5d)



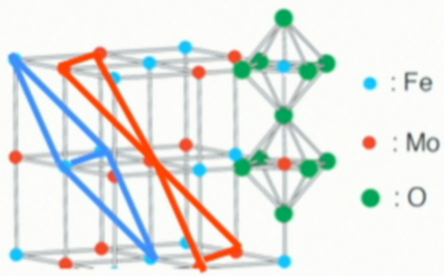
Metallic systems

B: Magnetism and B':Conduction electrons

. Half metallic ferrimagnets (eg:Sr_2FeMoO_6, T_C= 420K)

. Large polarization: good for spin injection

. Interplay of magnetism, **SOC**, metallic transport



Mott insulators

B=magnetism, B'=inert or magnetism

. Get fcc lattice of spins (eg: Ba_2YReO_6)

. Unusual spin-orbit coupled liquids?

. Insulating ferrimagnets (eg: Sr_2CrOsO_6, T_C=725K)

Outline of the talk

I. Bulk metallic double perovskites with SOC
- application to Ba_2FeReO_6

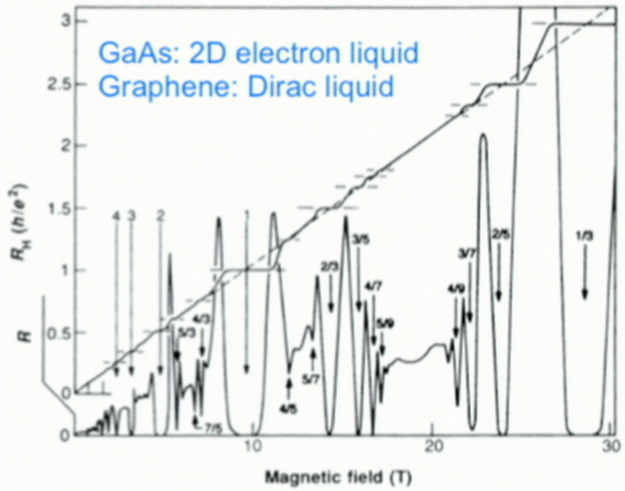
II. Spin dynamics in bulk double perovskites
- application to Ba_2FeReO_6

III. Topological states in "engineered" double perovskite films
- application to Sr_2FeMoO_6

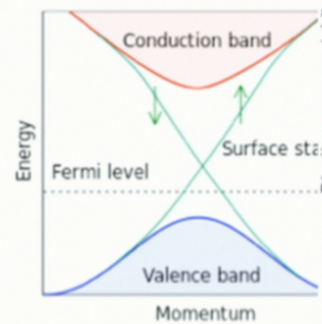
IV. Exotic spin Hamiltonians in Mott insulating double perovskites
- application to La_2MgIrO_6 / La_2ZnIrO_6

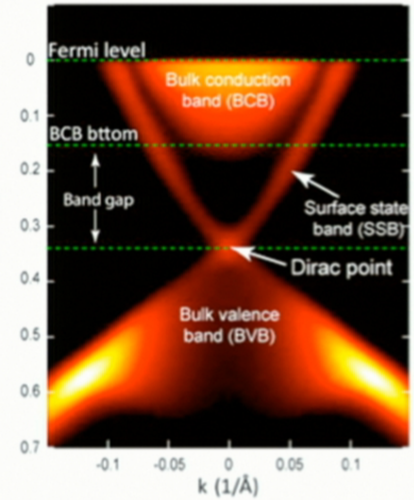
Topological phases of quantum matter

Quantum Hall effects

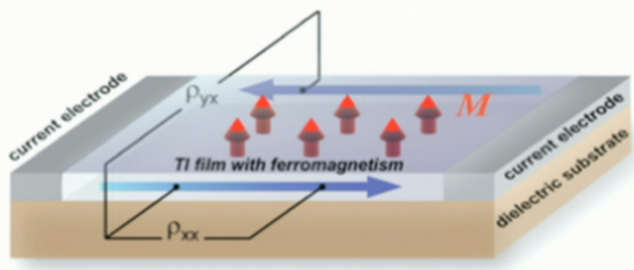


Topological insulators, top. crystalline insulators





Quantum anomalous Hall insulators



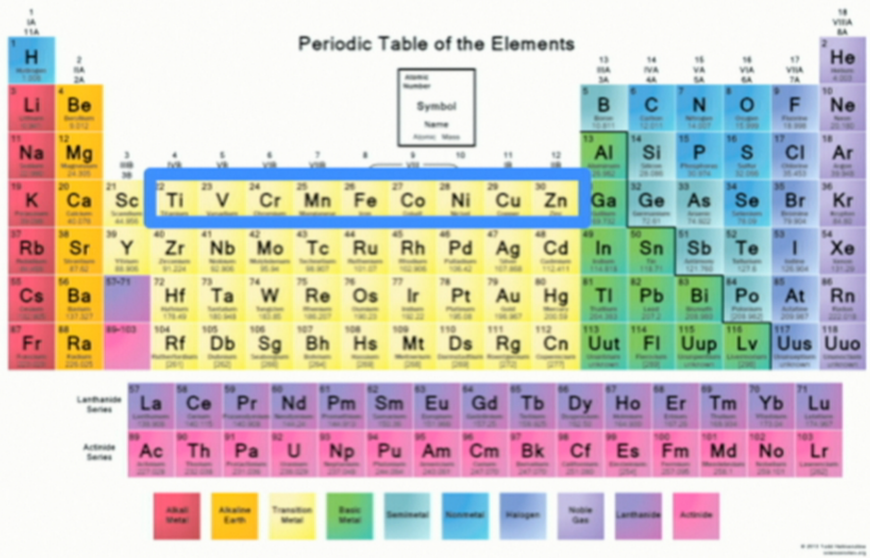
$(Bi,Sb)_2Te_3$ film doped with Cr or V atoms

C.Z. Chang et al, Science 2013 (Xue group, Tsinghua)
C.Z. Chang et al, arXiv (M. Chan + J. Moodera groups, PSU/MIT)
A. J. Bestwick et al, arXiv (Goldhaber-Gordon group, Stanford)
A. Kandala, et al, arXiv (N. Samarth and C.X. Liu groups, PSU)

How to “engineer” correlated topological states in solids?

(1) Strong correlations

- Brink of Mott localization or deep Mott insulator regime
- Common in 3d oxides: Kinetic energy ~ Interactions
- “High” energy/temperature scales for correlations/magnetism



How to "engineer" correlated topological states in solids?

- Q: Can we tie together these two disparate ingredients? Nontrivial topological bands + strong electronic correlations

- Correlated 3d oxides, interaction effects, magnetism, etc strong! Spin orbit coupling ~ 10meV (typically negligible effects)

- Simple 5d oxides - 5d orbitals strongly overlap, SOC large ~ 500 meV ReO_3, IrO_2 (electrocatalyst): metallic (no magnetism, no strong correlations)

- Ternary 5d oxides - 5d atoms further apart Sr_2IrO_4: Magnetism, but Slater-Mott insulator, so no conduction fluid

- Beyond simple and ternary oxides?
- Can we tailor SOC and correlations independently?

“Oxide engineering”

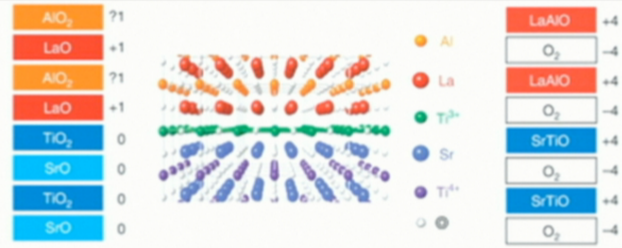
Controlled layer-by-layer growth using MBE/PLD

LaAlO3/SrTiO3 interface [100]

H. Y. Hwang, J.M. Triscone, J. Mannhart,
R. Ashoori, K. A. Moler, ...

Basic physics: Magnetism + Superconductivity

Applications: Write/Erase circuits using electric field



Prediction of topological insulators in simple TMO bilayers

ARTICLE

Received 20 Jun 2011 | Accepted 18 Nov 2011 | Published 20 Dec 2011

Interface engineering of quantum Hall effects in digital transition metal oxide heterostructures

Di Xiao[1], Wenguang Zhu[1,2], Ying Ran[3], Naoto Nagaosa[4,5] & Satoshi Okamoto[1]

Rapid Communication

Topological insulators from complex orbital order in transition-metal oxides heterostructures

Andreas Rüegg and Gregory A. Fiete

Phys. Rev. B **84**, 201103(R) – Published 14 November 2011

3d-3d Superlattices along [111]

nature materials LETTERS

PUBLISHED ONLINE: 22 JANUARY 2012 | DOI: 10.1038/NMAT3224

Exchange bias in $LaNiO_3$–$LaMnO_3$ superlattices

Marta Gibert[1]*, Pavlo Zubko[1], Raoul Scherwitzl[1], Jorge Íñiguez[2] and Jean-Marc Triscone[1]

AIP Applied Physics Letters

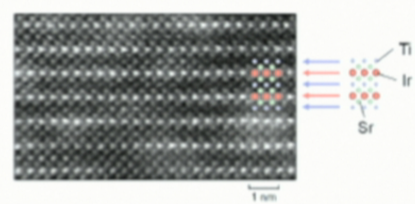
Local electronic and magnetic studies of an artificial La 2 FeCrO 6 double perovskite

Benjamin Gray, Ho Nyung Lee, Jian Liu, J. Chakhalian, and J. W. Freeland

Citation: Applied Physics Letters **97**, 013105 (2010); doi: 10.1063/1.3455323

3d/5d Superlattices

H. Takagi group (2014, 2015)



"Engineering" spin-orbit coupled topological states in solids

nature materials — LETTERS

Exchange bias in $LaNiO_3$-$LaMnO_3$ superlattices

Marta Gibert[1]*, Pavlo Zubko[1], Raoul Scherwitzl[1], Jorge Íñiguez[2] and Jean-Marc Triscone[1]

$(LaNiO3)_m$-$(LaMnO3)_n$ superlattices along {111}
$(LaFeO3)_m$-$(LaCrO3)_n$ superlattices along {111}
Infinite m=1,n=1 superlattice: Double Perovskite

AIP | Applied Physics Letters

Local electronic and magnetic studies of an artificial La 2 FeCrO 6 double perovskite

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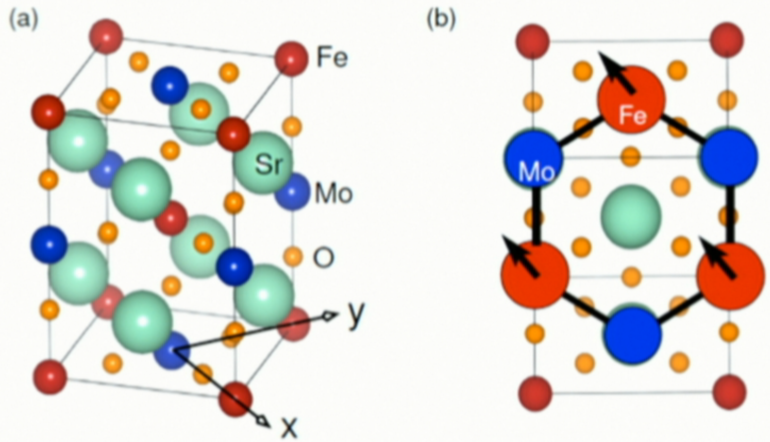
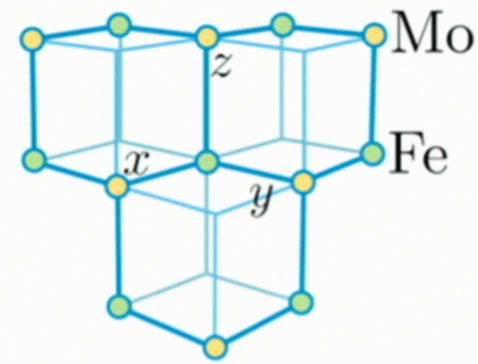
SFMO: {111} bilayer

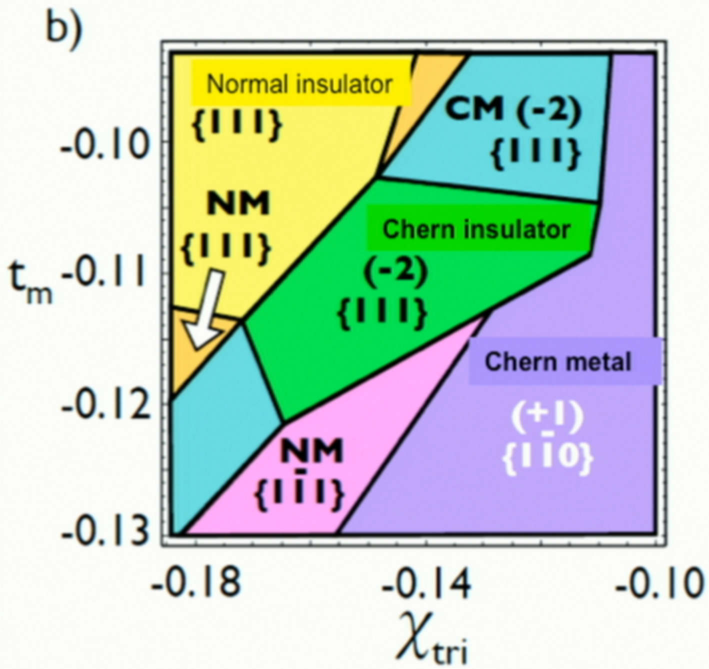


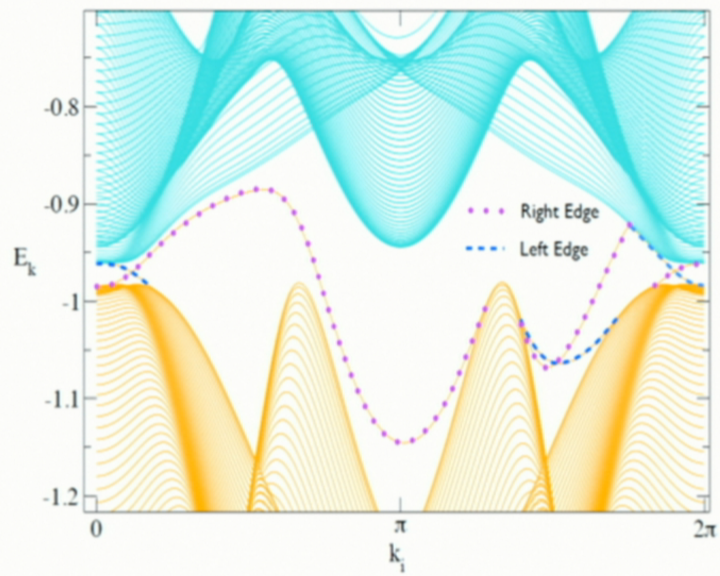
(a) Bulk crystal structure (b) {111} view



Fe and Mo/Re on honeycomb lattice
Fe: Local moments
Mo/Re: Itinerant t_2g electrons

Phase diagram of SFMO in {111} bilayer





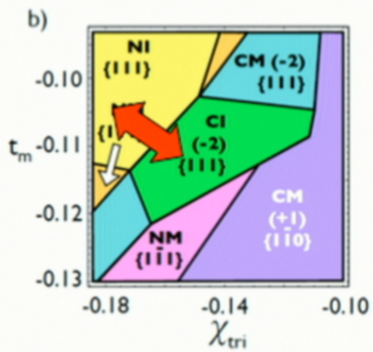
Edge state spectrum in C=2 Chern insulator

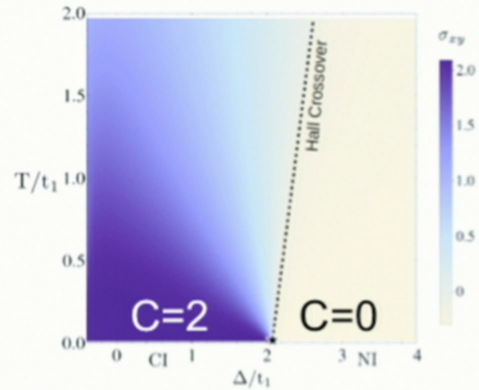
Quantum Hall gap ~ 75K

SFMO bilayer supports topologically nontrivial metals and C=2 Chern insulator

. A. Cook, AP (PRL 2014)

Can interactions drive new phases at topological critical points?





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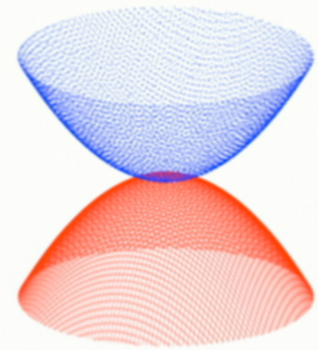


Quadratic band touching critical point

$$H = -\sum_{\langle ij \rangle} t_{ij}^{\alpha\beta} c_{i\alpha}^{\dagger} c_{j\beta} + \Delta \sum_i (n_{i\uparrow} - n_{i\downarrow}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$H_{\Gamma}^{\text{low}} = \begin{pmatrix} \frac{3}{2}(t_2+t_1)\,k^2 + r & \frac{3}{4} t_3 (k_x - i k_y)^2 \\ \frac{3}{4} t_3 (k_x + i k_y)^2 & \frac{3}{2}(t_2 - t_1)\,k^2 - r \end{pmatrix}$$

$$S_{\text{int}} = u \int_0^{\beta} d\tau \sum_i \bar{\psi}_{i\uparrow}(\tau) \bar{\psi}_{i\downarrow}(\tau) \psi_{i\downarrow}(\tau) \psi_{i\uparrow}(\tau)$$

Flow

$$\frac{dr}{d\ell} = 2r + \frac{u\Lambda^2}{4\pi} \frac{t_1}{\sqrt{t_1^2 + t_3^2/4}}$$

$$\frac{du}{d\ell} = \frac{u^2}{6\pi} \frac{1}{\sqrt{t_1^2 + t_3^2/4}}.$$

- Single "hot spot"
- Single marginally relevant coupling

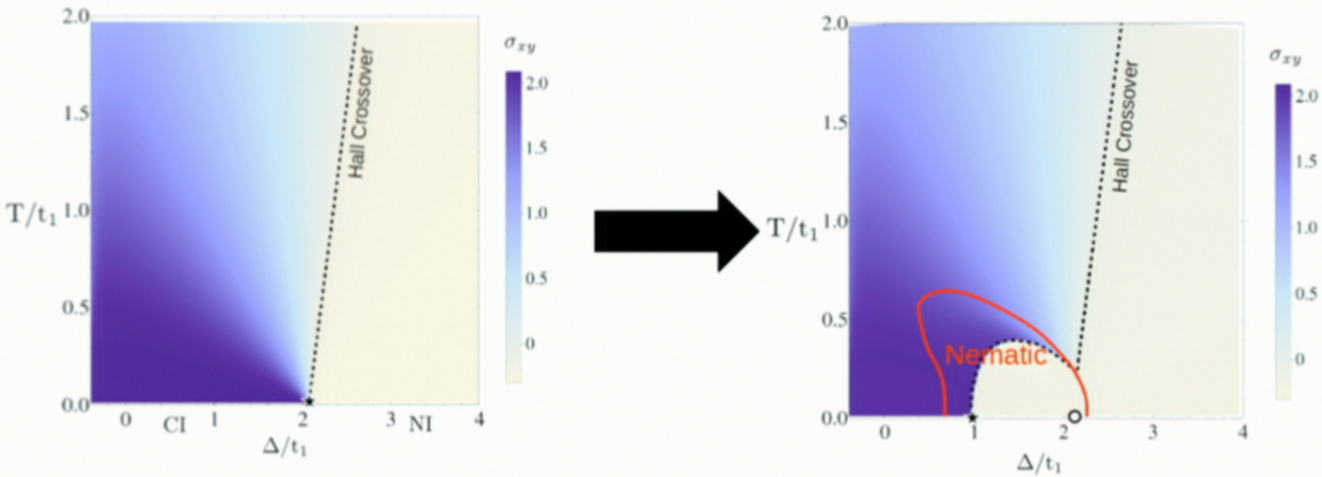
Chern transition: Interactions can drive "emergent" phases

$$\vec{m} = \frac{1}{2N}\sum_{\mathbf{k}}\langle c^{\dagger}_{\mathbf{k}\alpha}\vec{\sigma}_{\alpha\beta}c_{\mathbf{k}\beta}\rangle$$

$$e^{i2\theta_{\mathbf{k}}}$$

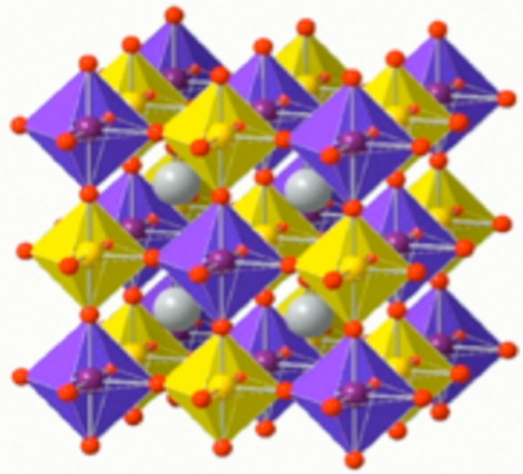
Breaks rotational symmetry
- Emergent "nematic order"

$$H_{\rm mf}(\mathbf{k}) = \begin{pmatrix} A_{\mathbf{k}}-\mu-Um_z & D_{\mathbf{k}}-U(m_x-im_y) \\ D^*_{\mathbf{k}}-U(m_x+im_y) & B_{\mathbf{k}}-\mu+Um_z \end{pmatrix}$$



Can SOC lead to unusual magnetism in Mott insulators?

Double perovskite lattice



Mott insulating double perovskites

A sublattice: Inert closed shell atom

B sublattice: Magnetic ion

- Atoms farther apart, suppresses delocalization
- Rich variety of fcc lattice Mott insulators

Ba_2Y**Mo**O_6, Sr_2Y**Re**O_6, Sr_2Y**Ir**O_6, Ba_2Y**Ru**O_6,…

T. Aharen et al, Phys. Rev. B 81, 224409 (2010)
J. P. Carlo, et al, Phys. Rev. B 88, 024418 (2013)
G. Cao, et al, Phys. Rev. B 87, 155136 (2013)
G. Chen, L. Balents, PRB 84, 094420 (2011)
T. Dodds, T.P.Choy, Y.B. Kim, PRB 84, 104439 (2011)

Iridate double perovskites

La_2ZnIrO_6 , La_2MgIrO_6 [G. Cao, et al, PRB 2013]

- Small CW temperature, Θ_{cw} ~ -24K in La_2MgIrO_6
- Deep in the Mott insulator phase: Consistent with larger Ir-Ir spacing compared to perovskites or honeycomb iridates
- A-type magnetic ordering at ~10K (FM layers, AFM stacking)
- Opportunity to explore magnetism of SOC moments on the frustrated fcc lattice

Magnetic Hamiltonian: Symmetry analysis

Honeycomb α-Na_2IrO_3/Li_2IrO_3

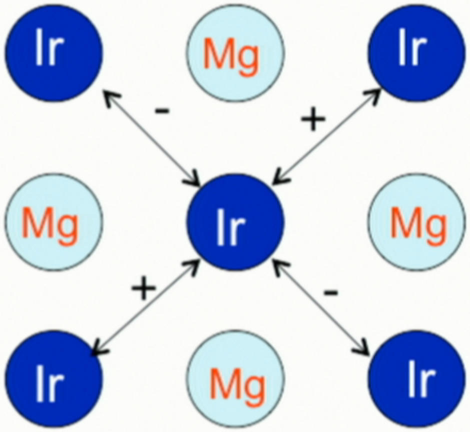
Jackeli, Khaliullin, Chaloupka (2011,2012) – **Kitaev Hamiltonian**

J. Rau, H. Y. Kee (PRL+PRB 2014) – **Beyond Kitaev**

Hyper-honeycomb β/γ– Li_2IrO_3

Takagi group (2014), J. Analytis group (2014) – **3D Kitaev generalization**

I.Kimchi, R. Coldea, A. Vishwanath (2014); E.K.H.Lee, Y.B.Kim (2014)



$$H_{xy} = J\vec{S}_1 \cdot \vec{S}_2 + J_I S_1^z S_2^z \pm \Gamma(S_1^x S_2^y + S_1^y S_2^x)$$

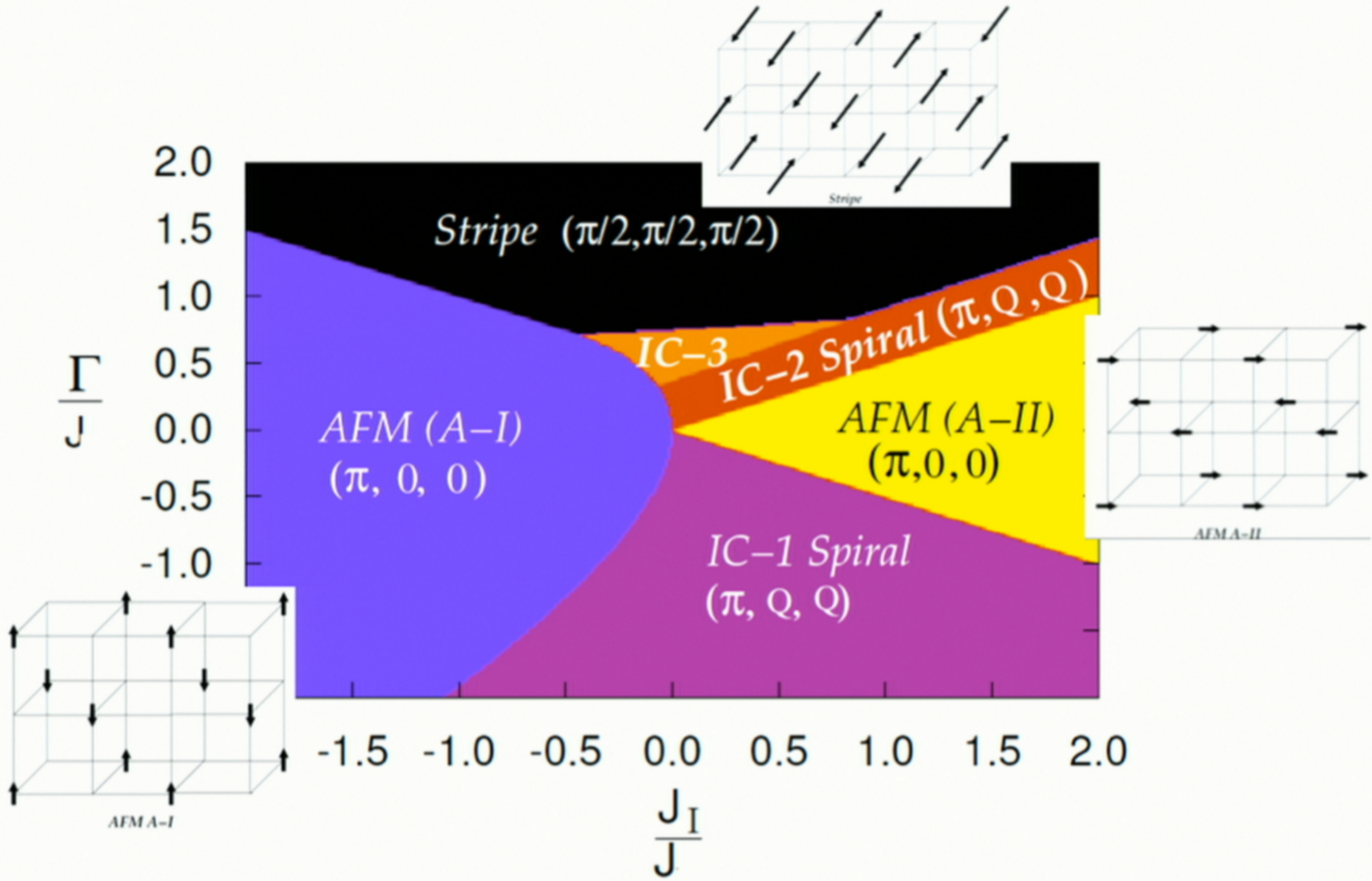
$$H_{yz} = J\vec{S}_1 \cdot \vec{S}_2 + J_I S_1^x S_2^x \pm \Gamma(S_1^y S_2^z + S_1^z S_2^y)$$

$$H_{xz} = J\vec{S}_1 \cdot \vec{S}_2 + J_I S_1^y S_2^y \pm \Gamma(S_1^x S_2^z + S_1^z S_2^x)$$

H. Ishizuka, L. Balents (PRB 2014)

A. Cook, S. Matern, C. Hickey, A. A. Aczel, AP (arXiv:1502.01031)

Luttinger-Tisza phase diagram

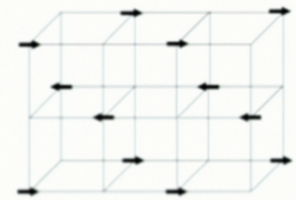


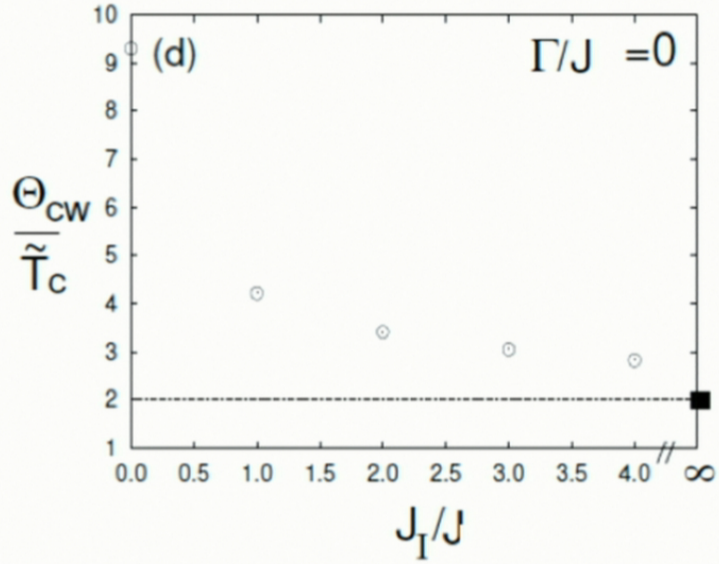
A. Cook, S. Matern, C. Hickey, A. A. Aczel, AP (arXiv:1502.01031)

Comparison with materials

La_2MgIrO_6
. Θ_{cw} = -24K, orders with Tc = 12K
. Ordering type: A-II
(neutron diffraction + ab initio)
. $\Theta_{cw} = -(3J + J_I)$
. Getting Θ_{cw}/Tc to be small needs big SOC – expect J_I dominant

La_2ZnIrO_6
. Θ_{cw} = -5K, orders with Tc = 7.5K
. Ordering type: A-II
(neutron diffraction + ab initio)
. Experimental uncertainties in Θ_{cw}?





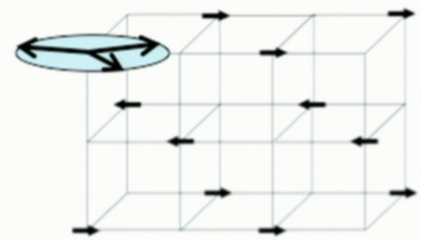
Material has octahedral rotations which are staggered between layers
Do we expect a ferromagnetic moment in the ordered AFM state?
Experiment: Observed in La_2ZnIrO_6 (ok) but not in La_2MgIrO_6 (puzzle)
Prediction: Staggered octahedral rotations do not coincide with stacking direction in La_2MgIrO_6 – test using Xrays

A. Cook, S. Matern, C. Hickey, A. A. Aczel, AP (arXiv:1502.01031)

Spin dynamics

- Minimal Hamiltonian: "Quantum Ising model"

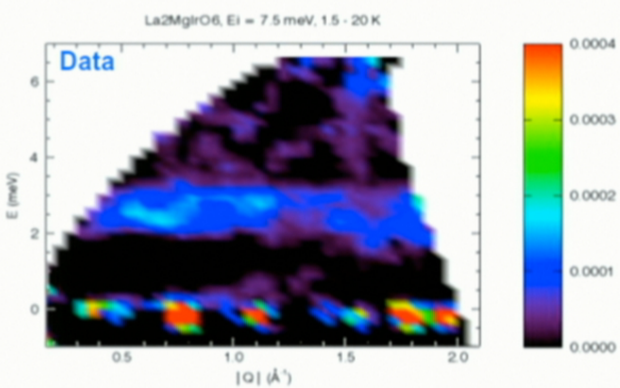
$$H = J_I \sum_{\langle ij \rangle_{\mathrm{XY}}} S_i^z S_j^z + J_I \sum_{\langle ij \rangle_{\mathrm{YZ}}} S_i^x S_j^x + J_I \sum_{\langle ij \rangle_{\mathrm{XZ}}} S_i^y S_j^y$$



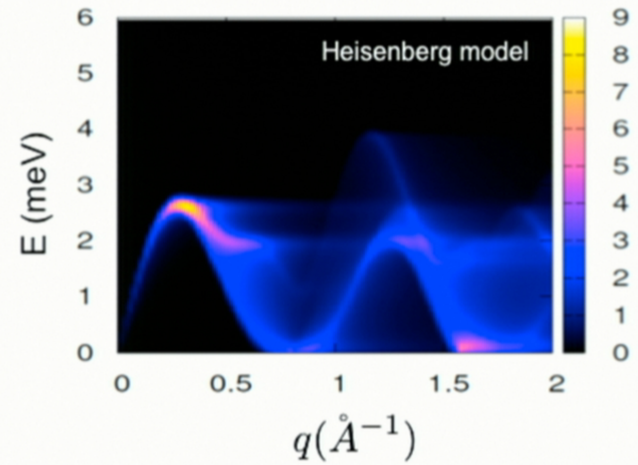
Classically: Spins can point anywhere in XY plane

- Thermodynamic studies: $J_I \sim 24\mathrm{K}$

- **Quantum order by disorder**
- **Pins moments** to point along Ir-O bond direction
- **Leads to a gap** in the spin wave spectrum



Note: Ir is a strong neutron absorber



- Data much less dispersive, lower in energy
- Impurity physics? Spin-phonon coupling?

A. A. Aczel, A. Cook, AP (manuscript in preparation)

Summary

- 3D metallic double perovskites: Ba_2FeReO_6
  - band structure with Weyl nodes
  - spin and orbital magnetization from strong correlations
  - spin dynamics in agreement with neutron data

- 2D double perovskite films along {111}: Sr_2FeMoO_6
  - Topological phases including emergent Chern bands
  - C=2 quantum anomalous Hall insulators

- Mott insulating double perovskites: La_2ZnIrO_6, La_2MgIrO_6
  - Spin Hamiltonian with exotic non-Heisenberg interactions
  - magnetic order in agreement with experimental data
  - resolve differences between La_2ZnIrO_6 and La_2MgIrO_6
  - Qualitative understanding of spin dynamics

References

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5. A. Cook, S. Matern, C. Hickey, A. A. Aczel (arXiv:1502.01031)

THANK YOU!