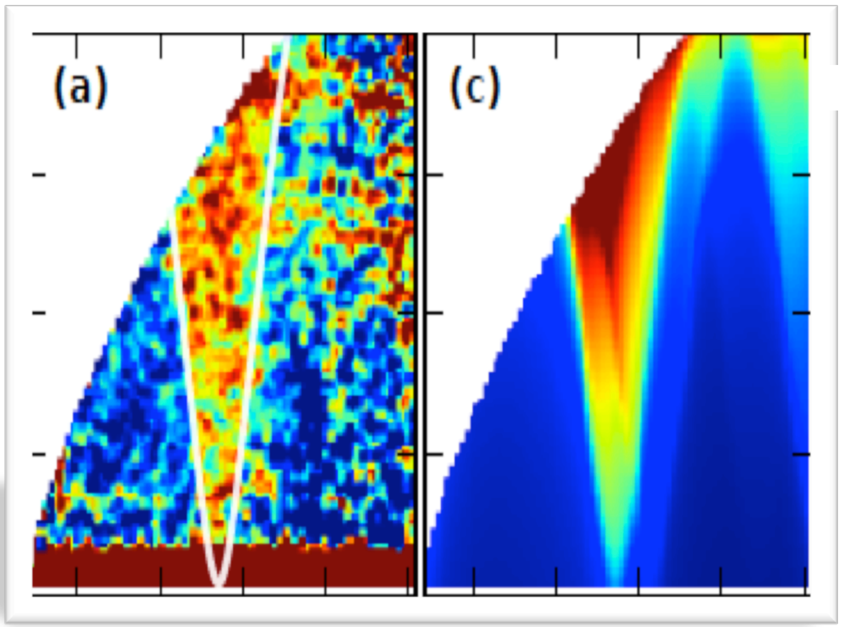
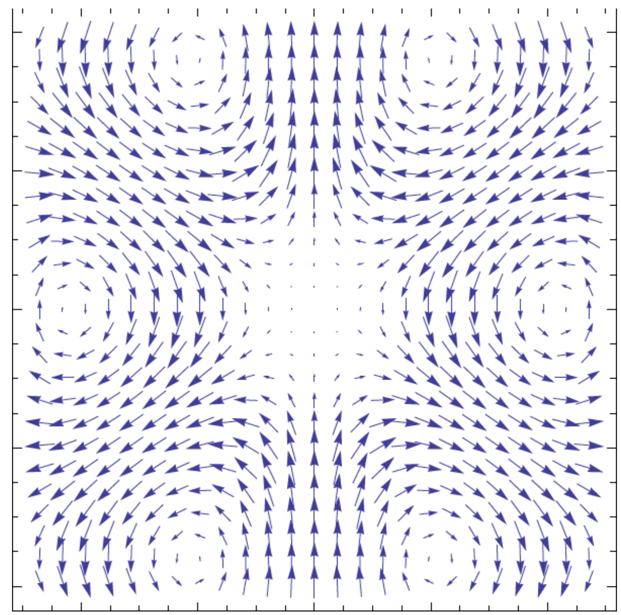
Double Perovskites

Spin-Orbit Coupling, Magnetism, Topological States

Arun Paramekanti

(University of Toronto)





ICTP-JNU workshop on "Current Trends in Frustrated Magnetism"

NSERC CRSNG

CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

Collaborators

Theory

Ashley Cook
(Univ. Toronto)

Ciaran Hickey
(Univ. Toronto)

Stephanie Matern
(Toronto/Koeln)

Neutron scattering and samples

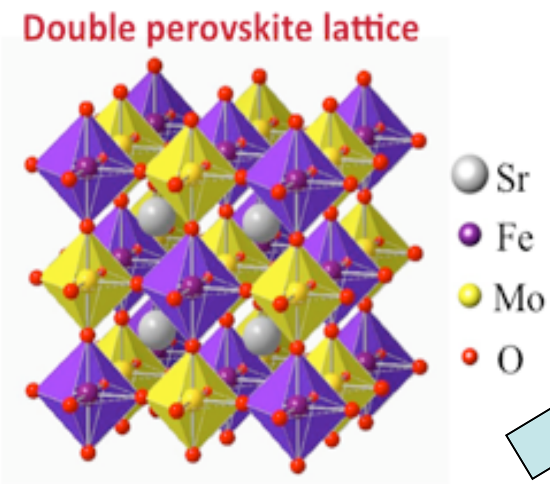
1. Kemp Plumb, Pat Clancy, Y.J. Kim (Toronto), A.Kolesnikov (ORNL)
   B.-C. Jeon, T.-W. Noh (SNU, Korea)

2. Adam Aczel (ORNL), G. Cao (ORNL)

Discussions: Simon Trebst (Koeln)

"Ordered" Double Perovskites

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



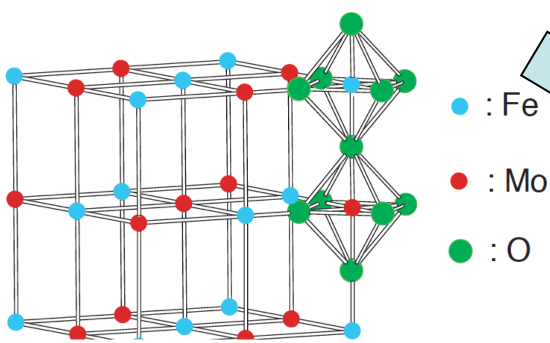
Metallic systems

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

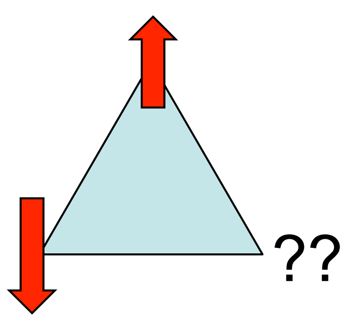
. Get fcc lattice of spins (eg: Ba_2YReO_6)

. Unusual spin-orbit coupled liquids?

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

Outline of the talk

1. Metallic double perovskites with SOC: Ba_2FeReO_6
2. Magnetic fluctuations in metallic DP: Ba_2FeReO_6
3. Magnetism in insulating fcc iridate DPs: La_2MgIrO_6 / La_2ZnIrO_6
4. Topological states in layered double perovskites



I. Metallic DPs with SOC: Bulk physics

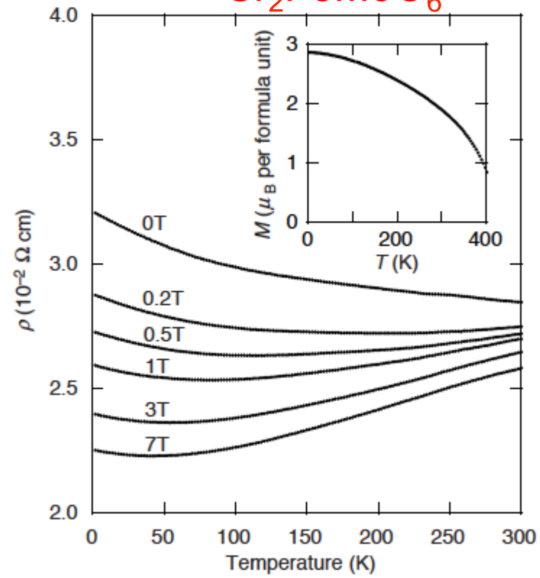
- Metallic, but correlation effects important
  [Ca_2FeReO_6 is insulating]

- Ferrimagnetic T_C (BFRO=315K, SFMO=420K)
- Antiparallel magnetization on Mo/Re and Fe

- Slight tetragonality (c/a < 1) at T_C

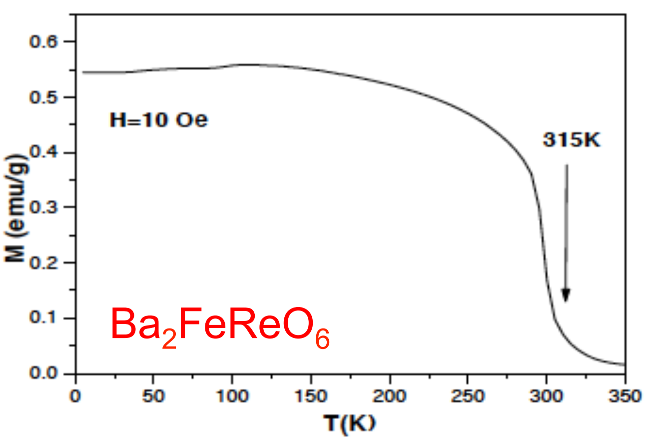
- Low temperature XMCD on BFRO
  Re: Orbital and spin moments
  Fe: Spin moment
  C. Azimonte, et al, PRL **98**, 017204 (2007)

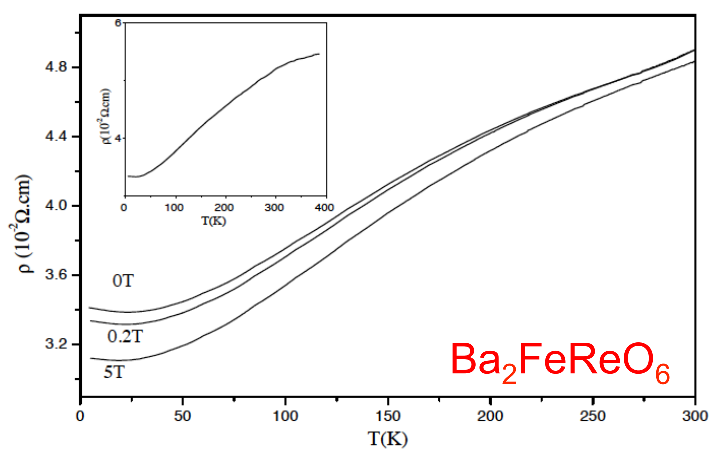
Sr_2FeMoO_6



Tokura group, Nature (1998)

Transport: evidence of half-metallicity?





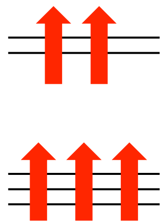
R. L. Greene group
JPCM (2000)

Atomic states

Nominal valence: $Ba_2^{(2+)}Fe^{(3+)}Re^{(5+)}O_6^{(2-)}$
$Sr_2^{(2+)}Fe^{(3+)}Mo^{(5+)}O_6^{(2-)}$

$Fe^{(3+)}$ 3d

e_g



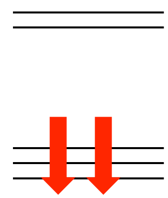
t_{2g}

S=5/2

Hund's coupling dominates over crystal field

$Re^{(5+)}$ 5d

e_g

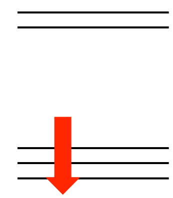


t_{2g}

S.O. λ ~ 500 meV
Hubbard U important

$Mo^{(5+)}$ 4d

e_g



t_{2g}

S.O. λ ~100meV

Re: Spin orbit coupling in t_{2g} (L=1)

$$P_{t_{2g}} \vec{L} P_{t_{2g}} = -\vec{\ell} \qquad (\ell = 1)$$

$$H_{\text{s.o.}} = -\lambda \vec{\ell} \cdot \vec{s}$$

Re: Interactions in t_{2g}

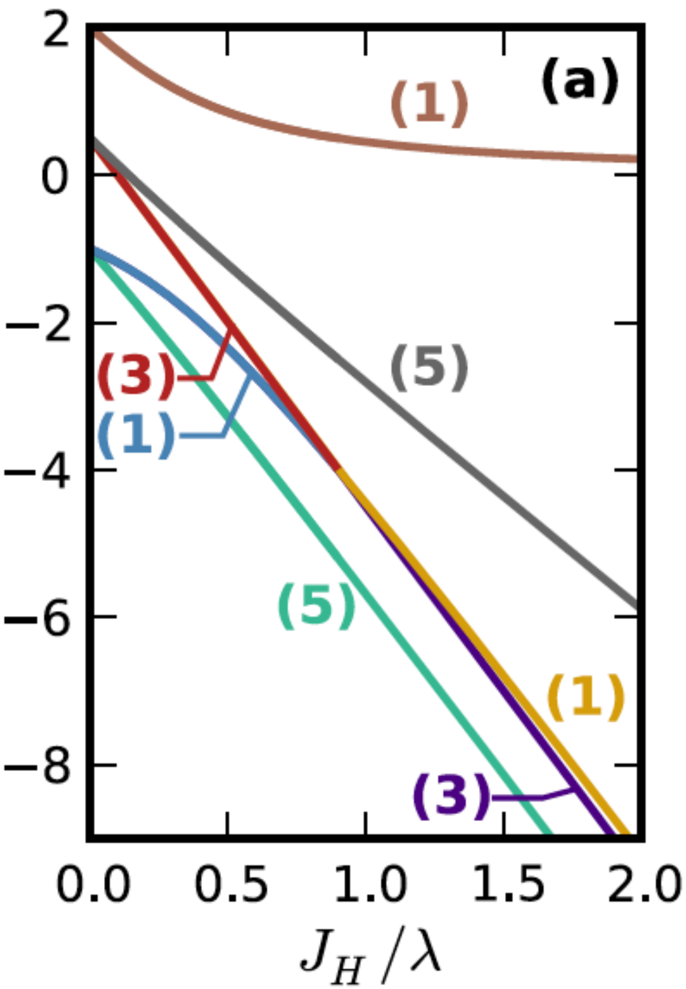
$$H_{\text{int}} = U \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow} + (U - 5\frac{J_H}{2}) \sum_{\alpha<\beta} n_\alpha n_\beta$$
$$-2J_H \sum_{\alpha<\beta} \vec{S}_\alpha \cdot \vec{S}_\beta + J_H \sum_{\alpha\neq\beta} d^\dagger_{\alpha\uparrow} d^\dagger_{\alpha\downarrow} d_{\beta\downarrow} d_{\beta,\uparrow}$$

(Kanamori)

Local atomic states with interactions and SOC

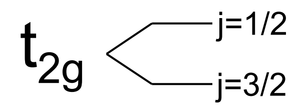
Simplified interaction for d^2

$$H_{\rm at}^{(2)} = -2J_H \vec{S}_{\rm tot}^2 - \frac{J_H}{2}\vec{L}_{\rm tot}^2 - \lambda_0(\vec{L}_1 \cdot \vec{S}_1 + \vec{L}_2 \cdot \vec{S}_2)$$



J_H=0 states

Degeneracy: 6,8,1



Large J_H states simple

L=1,S=1: J=2,1,0

L=2,S=0: No s.o.

L=0,S=0: No s.o.

Lowest 5 states smooth

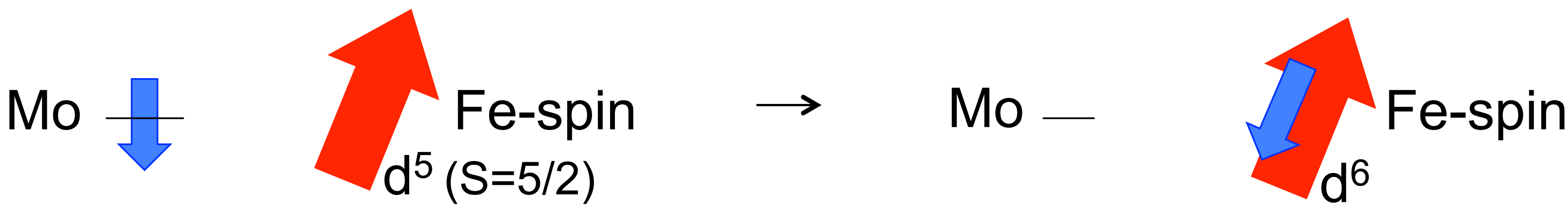
For modest values $J_H > 2\lambda$

L=1 + S=1 giving J=2

K. Plumb, A. Cook, et al, PRB 87,184412 (2013)

Electronic model

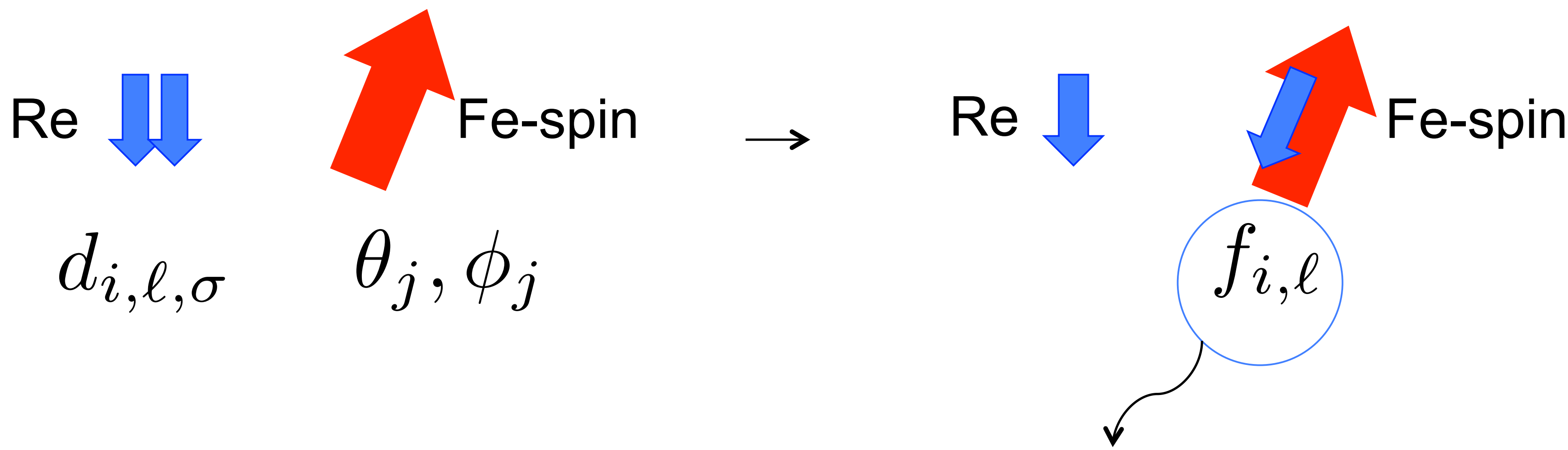
D.D. Sarma, et al (PRL 2000);
S. Di Matteo, G.Jackeli, N.Perkins (PRB 2003); G. Jackeli (PRB 2003);
P. Sanyal, P. Majumdar (PRB 2009);
O. Erten, O. Nganba-Meetei, M. Randeria, N. Trivedi, P. Woodward, (PRL 2011, PRL 2013);



Kinetically stabilized ferromagnetism
Manganites - Double exchange, Hund's coupling: Ferromagnetism
Double perovskite ferrimagnets - Pauli blocking: Ferrimagnetism

Electronic model

Assume a classical underlying Fe moment



Electron spin on Fe is “pinned” to point opposite to underlying Fe moment
Spin degree of freedom is stripped off

$$g_\sigma(\theta_j, \phi_j) d^\dagger_{i\ell\sigma} f_{j,\ell} \quad \left\{ \begin{array}{l} g_\uparrow(\theta_j, \phi_j) = \sin \dfrac{\theta_j}{2} \mathrm{e}^{-i\phi_j/2} \\ g_\downarrow(\theta_j, \phi_j) = -\cos \dfrac{\theta_j}{2} \mathrm{e}^{i\phi_j/2} \end{array} \right.$$

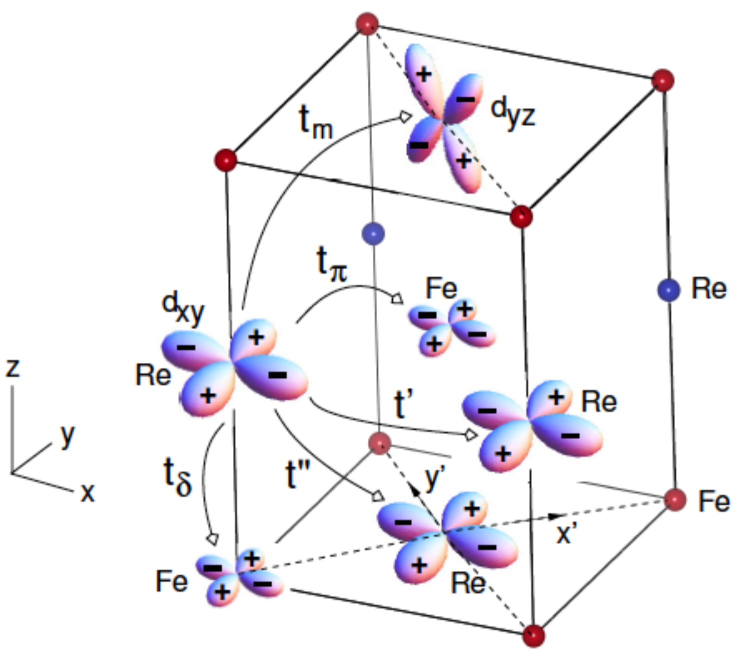
Fluctuations of Fe moments will suppress electron hopping
Lowering conduction electron kinetic energy favors Fe ferromagnetism

Electronic model

Schematic matrix elements

$$\sum_{\mathbf{k}}(\eta_\ell^{rs}(\mathrm{k})g_\sigma(\theta,\phi)d^\dagger_{r\ell\sigma}(\mathrm{k})f_{s\ell}(\mathrm{k}) + \mathrm{h.c.})$$

+ Re-Re hopping
+ Charge transfer
+ SO coupling + Interactions



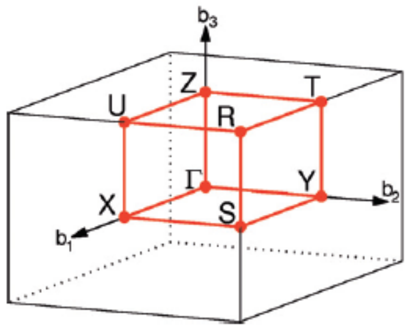
A. Cook, AP, PRB 88, 235102 (2013)

Importance of SO + correlations in "Cr-5d" DPs: H.Das,P.Sanyal,T. Saha-Dasgupta,D.D.Sarma (PRB 2011)

SO coupling: Atomic L.S projected to t_2g orbitals
- "Ferromagnetic" coupling
- Strong ~ 0.5eV

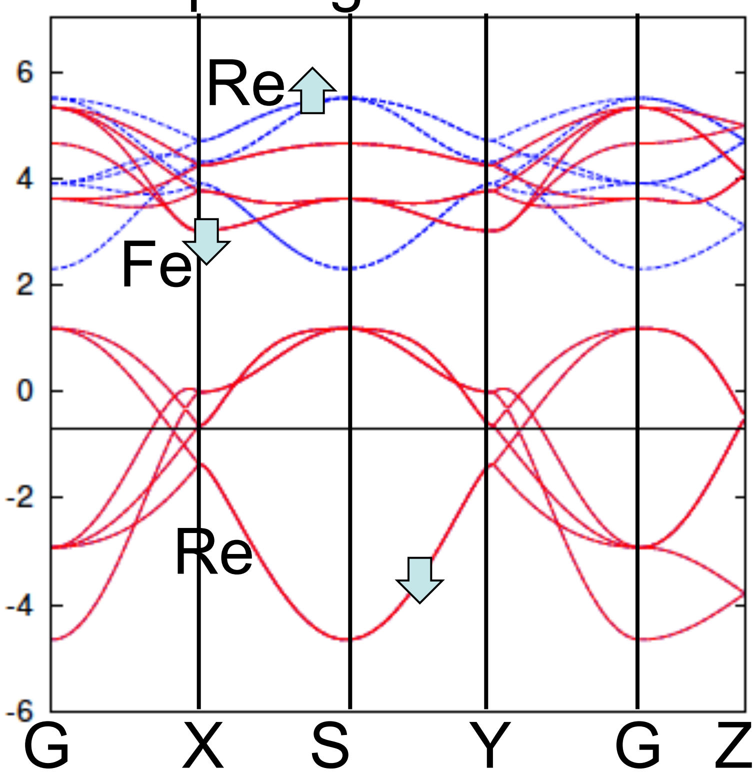
Correlations: Kanamori terms

Electronic model for BFRO: Hartree theory

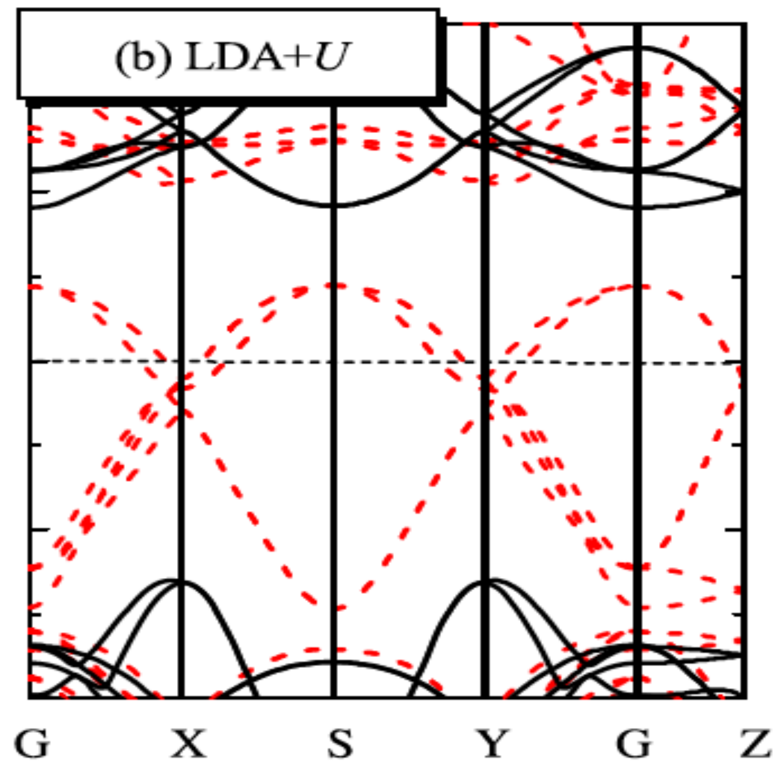


Correlation on Re: Stabilizes half-metallic state
Keep only intra-orbital U
$t_{Fe\text{-}Re}$ ~ 330 meV, U ~ 2.5eV, Δ_{CT} ~ 1 eV
$t_{Re\text{-}Re}$ ~ 100 meV, Other hoppings small < 50 meV

Comparing Hartree-corrected dispersion with LDA+U



A. Cook, AP (PRB 2013)



B.C. Jeon, T.W. Noh, et al, (JPCM, 2010)

Electronic model for BFRO: Correlations and SOC

No correlations

Sz (Fe) ~ +2.40 (i.e., 4.8 μ_B)
Sz (Re) ~ -0.15
Lz (Re) ~ -0.09
(Recall - L flipped in projecting to t_2g)

Ordered J (Re) ~ 0.24

With correlations

Sz (Fe) ~ +2.30 (i.e., 4.6 μ_B)
Sz (Re) ~ -0.78
Lz (Re) ~ -0.48
(Recall - L flipped in projecting to t_2g)

Ordered J (Re) ~ 1.2

Important for correct $m_{sat} = 3.4\ \mu_B$

Comparison with XMCD data

Theory: (μ_{orb}/μ_{spin}) ~ -0.31

XMCD expt: (μ_{orb}/μ_{spin}) ~ -0.29

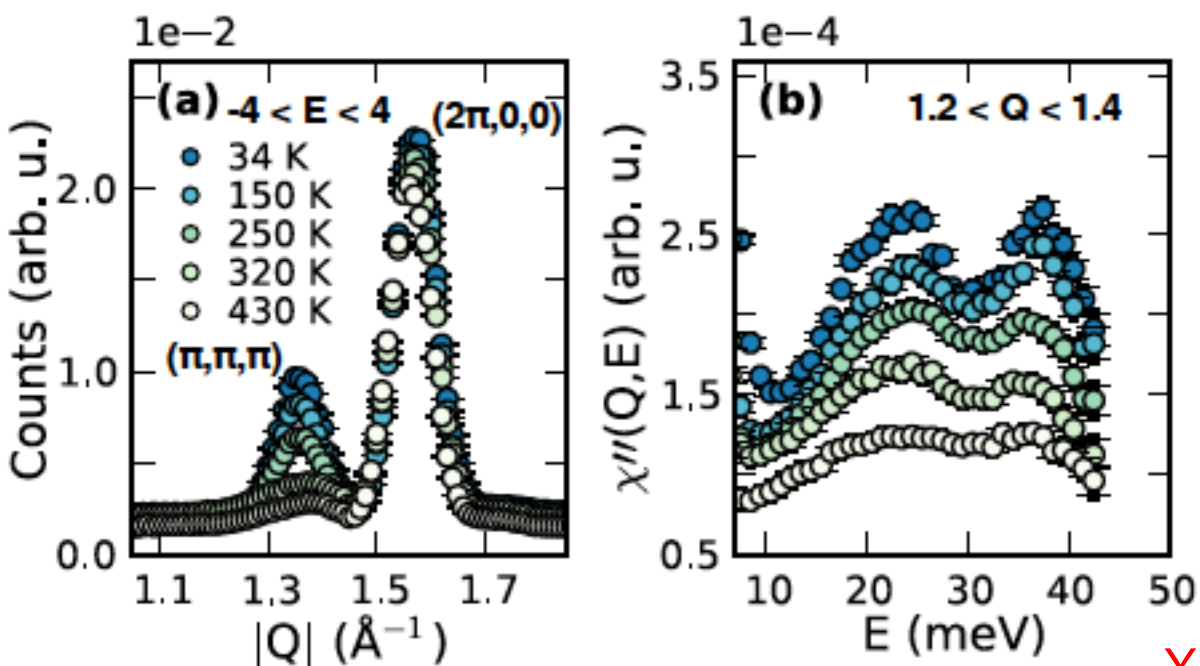
C. Azimonte, et al, PRL **98**, 017204 (2007)

Prediction

Despite SOC, carrier polarization > 90%

II. Magnetic fluctuations in bulk Ba_2FeReO_6

Inelastic neutron spectrum



Y.J. Kim group

- Evidence for scattering at the magnetic Bragg peak
- Evidence for signal disappearing near magnetic Tc
- Confirm with Q-dependence of signal over wider range
  - weaker at large Q, unlike phonons

K. Plumb, A. Cook, et al, PRB 87,184412 (2013)

Local moment Hamiltonian

On symmetry grounds, expect:

$$H = \mathcal{J} \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \vec{S}_{\mathbf{r}} \cdot \vec{\mathcal{F}}_{\mathbf{r}'} - \lambda \sum_{\mathbf{r} \in Re} \vec{L}_{\mathbf{r}} \cdot \vec{S}_{\mathbf{r}}$$

simplify

$\lambda \gg \mathcal{J}$

$$H_{\text{eff}} = \mathcal{J}_{\text{eff}} \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \vec{\mathcal{R}}_{\mathbf{r}} \cdot \vec{\mathcal{F}}_{\mathbf{r}'}$$

<u>2-branch dispersion</u>

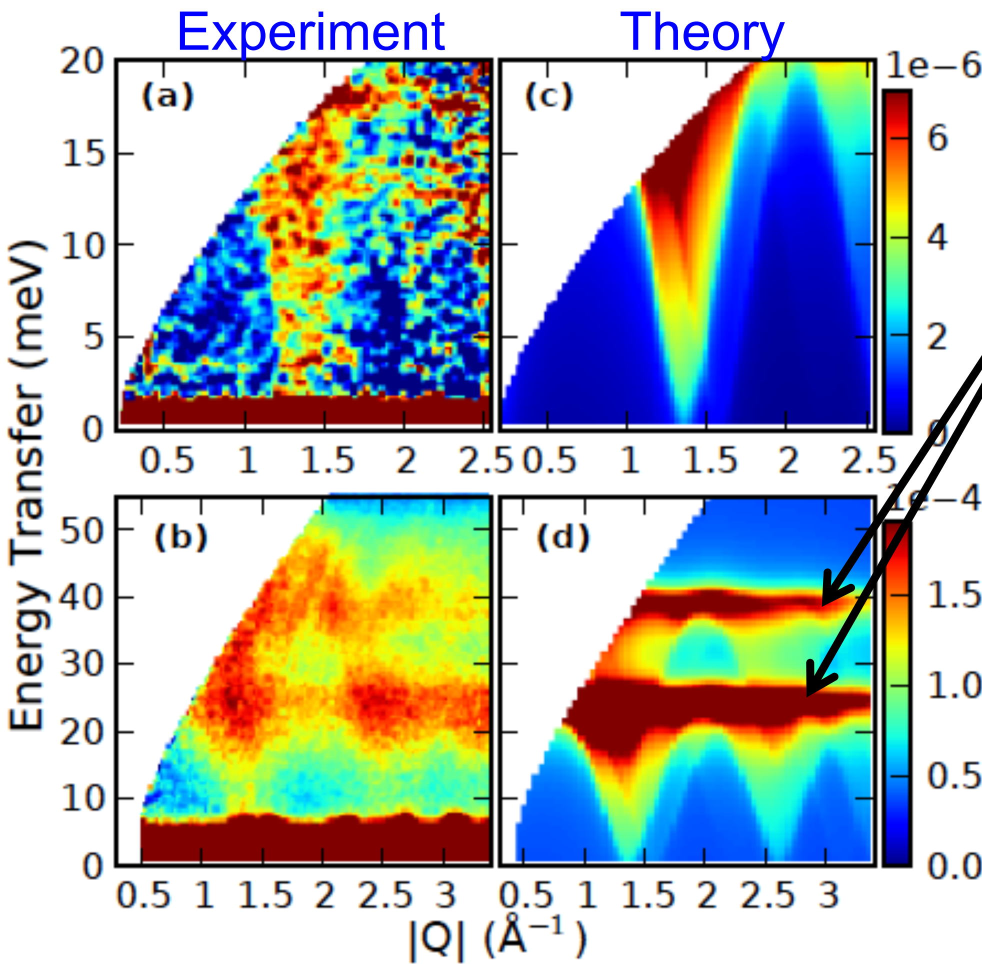
$$\Omega_{\pm}(\mathbf{Q}) = \sqrt{\mathcal{S}_{+}^{2} \gamma_0^2 - \mathcal{F}\mathcal{R}\gamma_{\mathbf{Q}}^{2}} \pm \mathcal{S}_{-}\gamma_0$$

$$\mathcal{S}_{\pm} = (\mathcal{F} \pm \mathcal{R})/2$$

<u>Dynamic structure factor</u>

$$S_{\perp}(\mathbf{Q}, \omega) = 2\pi \sum_{\sigma = \pm} (G_{\mathbf{Q}} - \sigma \mathcal{S}_{-}) \delta(\omega - \Omega_{\sigma}(\mathbf{Q}))$$

Local moment Hamiltonian



Zone boundary energy ratio: $\mathcal{F}/\mathcal{R}$

Experimental estimate
$\mathcal{F}/\mathcal{R} \approx 1.6$

"Mean field" estimate
$\mathcal{F}/\mathcal{R} \approx 1.9$

- Assuming F=2.1-2.3, find R ~ 1.3-1.4 (i.e., R>1)
- Indicative of orbital moments participating in dynamics
- Estimated Re-Fe exchange coupling ~ 3 meV

K. Plumb, A. Cook, et al, PRB 87,184412 (2013)

Rough understanding of other phenomenological aspects

Magnetic transition temperature

Using exch+spin values, estimate magnetic Tc ~ 350K
Experimental value ~ 300K

Weak structural transition

At T<Tc, very weak tetragonality, must imply
weak quartic terms ~ $\left[(L_i^x)^4 + (L_i^y)^4 + (L_i^z)^4\right]$

Nearly gapless spin waves

Weak lattice distortion yields Heisenberg-model
with a tiny gap (from locking to the lattice)

III. Insulating DPs: FCC Lattice Iridates

La_2ZnIrO_6 and La_2MgIrO_6 (in collaboration with A. Aczel, ORNL)

- Ir^{4+} is in $5d^5$ configuration: j=1/2 moment
- Insulating DPs, Zn^{2+}/Mg^{2+} are nonmagnetic

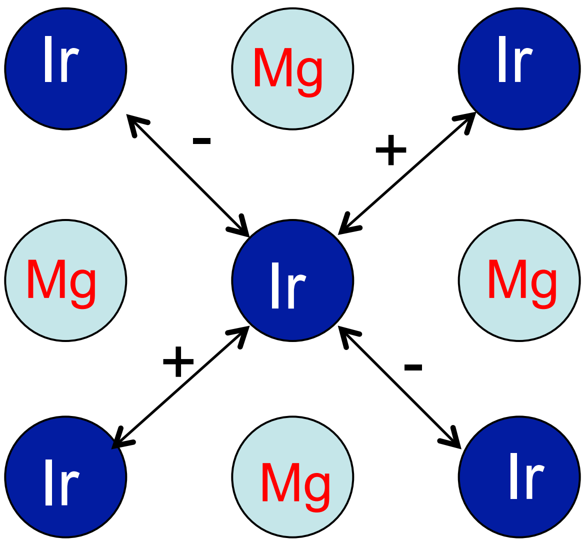
- Small CW temperature, $\Theta_{cw} \sim -24K$ in La_2MgIrO_6
- Deep in the Mott insulator phase: Consistent with larger Ir-Ir spacing compared to perovskites or honeycomb iridates

- A-type magnetic ordering at ~10K (FM layers, AFM stacking)
- Oxygen octahedra nearly perfect, small tilts/rotations
  (G. Cao et al, PRB 2013; Battle and Gore, J. Mater. Chem 1996; Currie et al., J. Sol. St. Chem, 1995)

- Magnetism of SOC moments on the frustrated fcc lattice

Magnetic Hamiltonian: Symmetry analysis

XY plane



Importance of Kitaev++ interactions

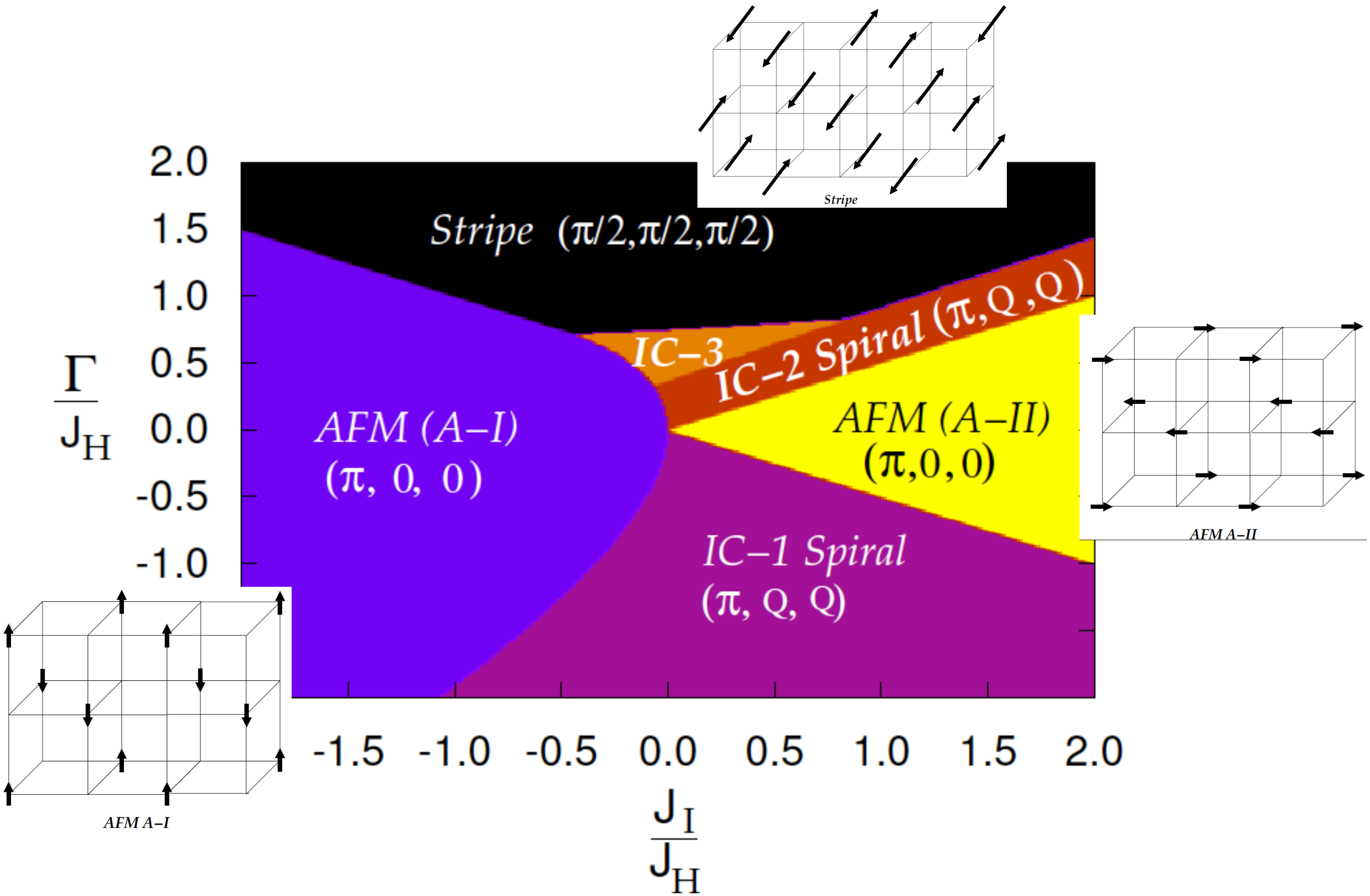
Honeycomb α-Na_2IrO_3/Li_2IrO_3:
Jackeli, Khaliullin, Chaloupka (2011,2012)
J. Rau, H. Y. Kee (PRL+PRB 2014)

Hyper-honeycomb β/γ− Li_2IrO_3:
Takagi (2014), J. Analytis (2014)
I. Kimchi, R. Coldea, A. Vishwanath (2014)
Hyperhoneycomb: E.K.H.Lee, Y.B.Kim (2014)

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

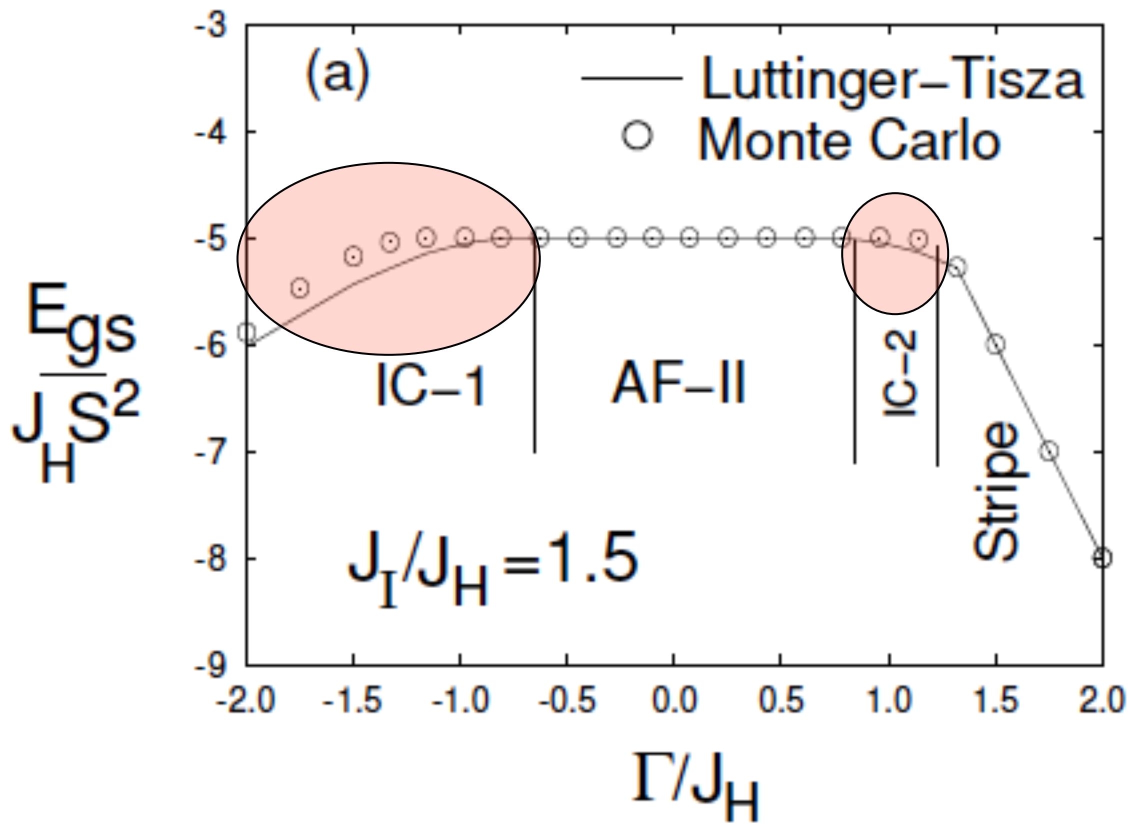
H. Ishizuka, L. Balents (PRB 2014)
A. Cook, S. Matern, C. Hickey, A. A. Aczel, AP (arXiv:1502.01031)

Luttinger-Tisza phase diagram



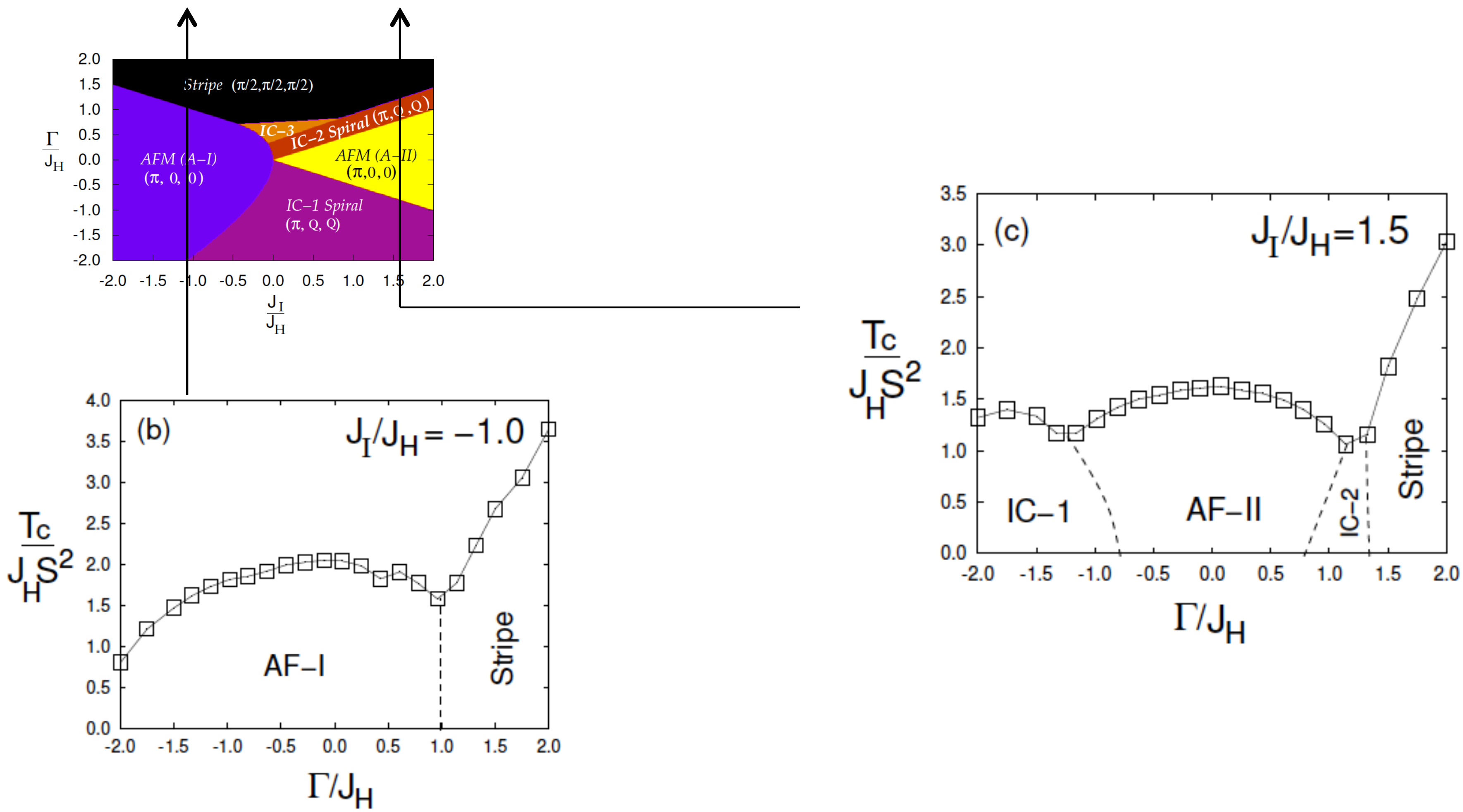
A. Cook, S. Matern, C. Hickey, A. A. Aczel, AP (arXiv:1502.01031)

Luttinger Tisza energy vs numerical simulated annealing



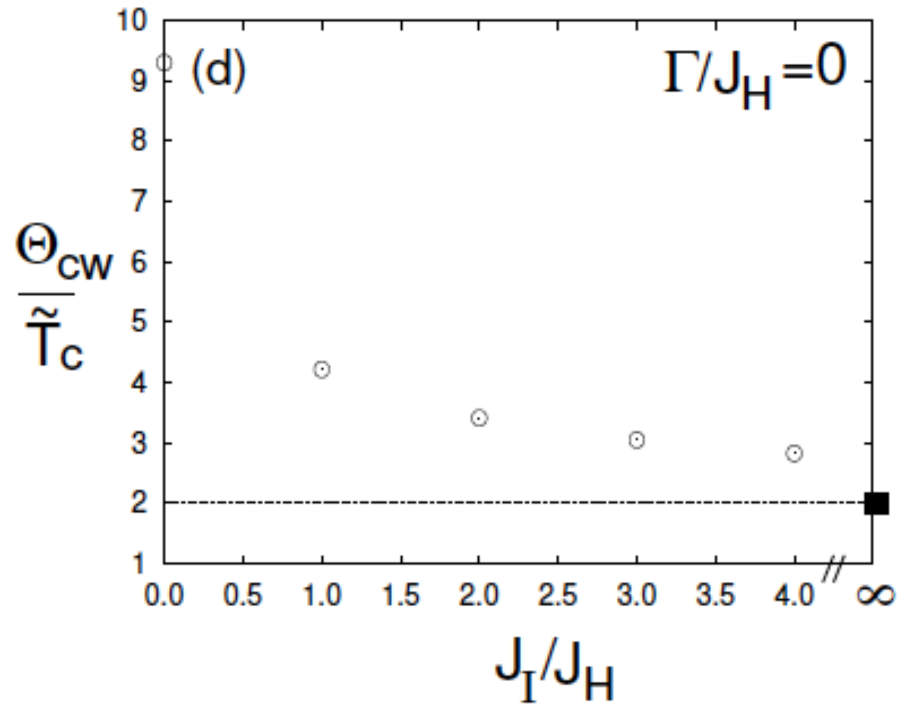
- Small < 2% error in incommensurate spiral phases
- Spirals are multimode noncoplanar states

Thermal transitions



- Heisenberg model $T_c \sim 0.44\, J_H S^2$
- SOC tends to enhance Tc by pinning moment directions
- May suppress spin-liquid phases, and favor ordering?
- Spiral phases may be most promising for melting into spin liquids; how to get big Γ?

Comparison with materials



La_2MgIrO_6

. Θ_{cw} = -24K, orders with Tc = 12K
. Ordering type: A-II
(neutron diffraction + ab initio)
. $\Theta_{cw} = -(3 J_H + J_I)$
. 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)
. Expect dominant J_I and weak FM direct exchange?

Do we expect a ferromagnetic moment in the ordered state?
Experimentally – observed in La_2ZnIrO_6 but not in La_2MgIrO_6
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)

IV. {111} Superlattices: topological states

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

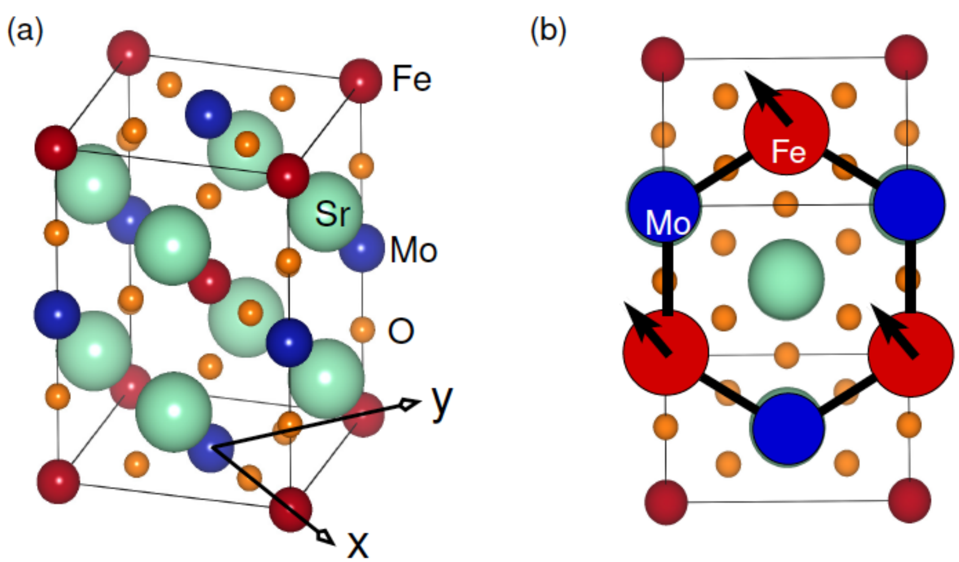
Local electronic and magnetic studies of an artificial La 2 FeCrO 6 double perovskite

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

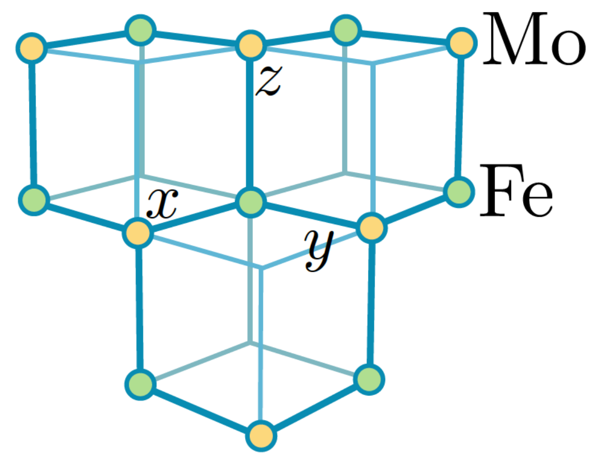
$(LaNiO3)_m$-$(LaMnO3)_n$ superlattices along {111}
$(LaFeO3)_m$-$(LaCrO3)_n$ superlattices along {111}
Infinite m=1,n=1 superlattice: Double Perovskite

SFMO: {111} bilayer



Bulk crystal structure

{111} view



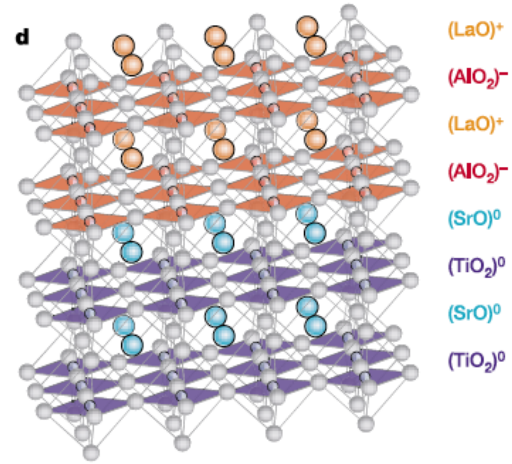
Fe and Mo/Re on honeycomb lattice
Fe: Local moments
Mo/Re: Itinerant t_2g electrons

Broader interest in oxide heterostructures

A high-mobility electron gas at the $LaAlO_3/SrTiO_3$ heterointerface

A. Ohtomo[1,2,3] & H. Y. Hwang[1,3,4]

NATURE | VOL 427 | 29 JANUARY 2004 | www.nature.com/nature



ARTICLE
Received 19 Mar 2013 | Accepted 24 Jul 2013 | Published 22 Aug 2013
DOI: 10.1038/ncomms3351

$LaAlO_3$ stoichiometry is key to electron liquid formation at $LaAlO_3/SrTiO_3$ interfaces

M.P. Warusawithana[1], C. Richter[2,3], J.A. Mundy[4], P. Roy[1], J. Ludwig[1], S. Paetel[2], T. Heeg[5], A.A. Pawlicki[1], L.F. Kourkoutis[4,6], M. Zheng[7], M. Lee[1], B. Mulcahy[7], W. Zander[8], Y. Zhu[4], J. Schubert[8], J.N. Eckstein[7], D.A. Muller[4,6], C. Stephen Hellberg[9], J. Mannhart[3] & D.G. Schlom[5,6]

nature physics
LETTERS
PUBLISHED ONLINE: 4 SEPTEMBER 2011 | DOI: 10.1038/NPHYS2079

Direct imaging of the coexistence of ferromagnetism and superconductivity at the $LaAlO_3/SrTiO_3$ interface

Julie A. Bert[1], Beena Kalisky[1], Christopher Bell[1], Minu Kim[1,2], Yasuyuki Hikita[1], Harold Y. Hwang[1,2] and Kathryn A. Moler[1]*

ARTICLE
Received 18 Jul 2012 | Accepted 25 Mar 2013 | Published 14 May 2013
DOI: 10.1038/ncomms2804
OPEN

Anisotropic two-dimensional electron gas at the $LaAlO_3/SrTiO_3$ (110) interface

A. Annadi[1,2], Q. Zhang[3,4,5], X. Renshaw Wang[1,2], N. Tuzla[6], K. Gopinadhan[1,7], W.M. Lü[1,7], A. Roy Barman[1,2], Z.Q. Liu[1,2], A. Srivastava[1,2], S. Saha[1,2], Y.L. Zhao[1,2], S.W. Zeng[1,2], S. Dhar[1,7], E. Olsson[6], B. Gu[5,8], S. Yunoki[4,5,9,10], S. Maekawa[5,8], H. Hilgenkamp[11,12], T. Venkatesan[1,2,7] & Ariando[1,2]

LETTERS
PUBLISHED ONLINE: 4 SEPTEMBER 2011 | DOI: 10.1038/NPHYS2080
nature physics

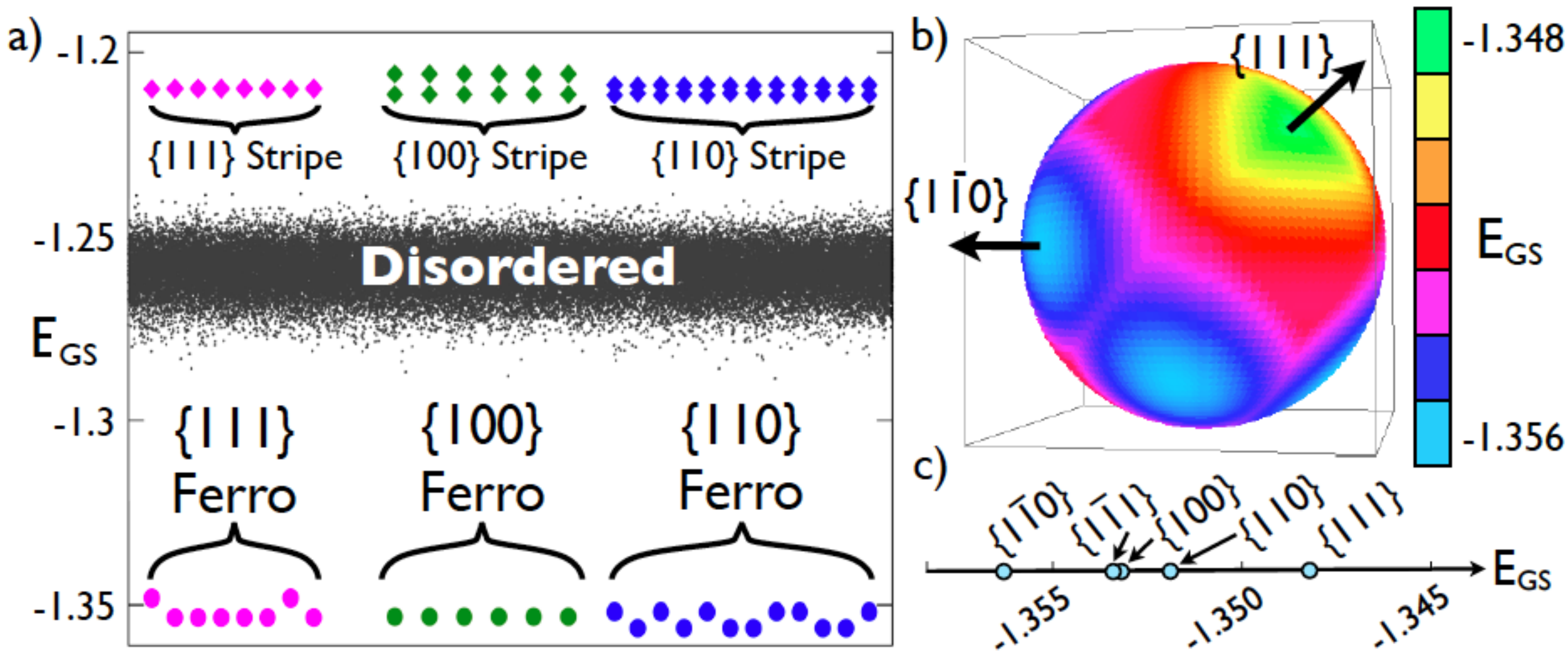
Coexistence of magnetic order and two-dimensional superconductivity at $LaAlO_3/SrTiO_3$ interfaces

Lu Li[1], C. Richter[2], J. Mannhart[3] and R. C. Ashoori[1]*

Magnetism of SFMO in {111} Thin Film Geometry

<u>Adapt spins+fermions model to bilayer</u>

Ferro orientation

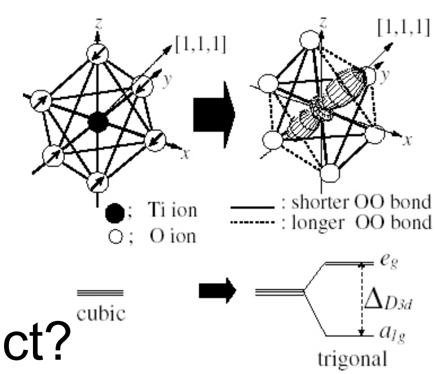


Lowest energy: Ferromagnetic orientation of Fe moments

Exchange energy between Fe (S=5/2) moments ~ 1.5meV

Ising-like anisotropy due to SOC

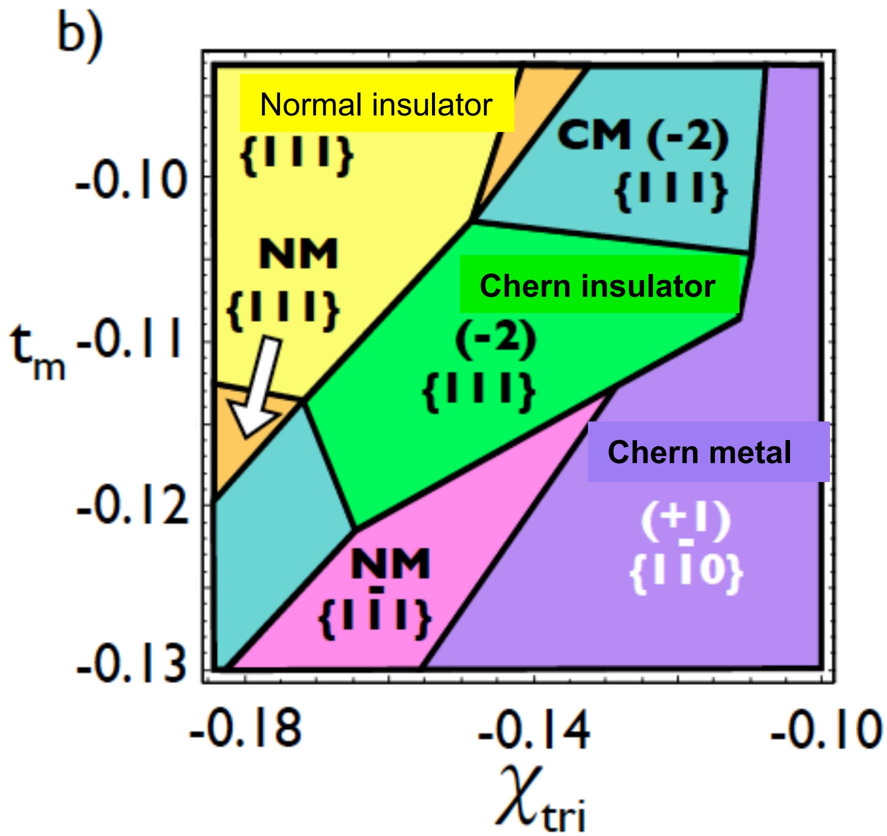
Estimated Tc ~ 200 K

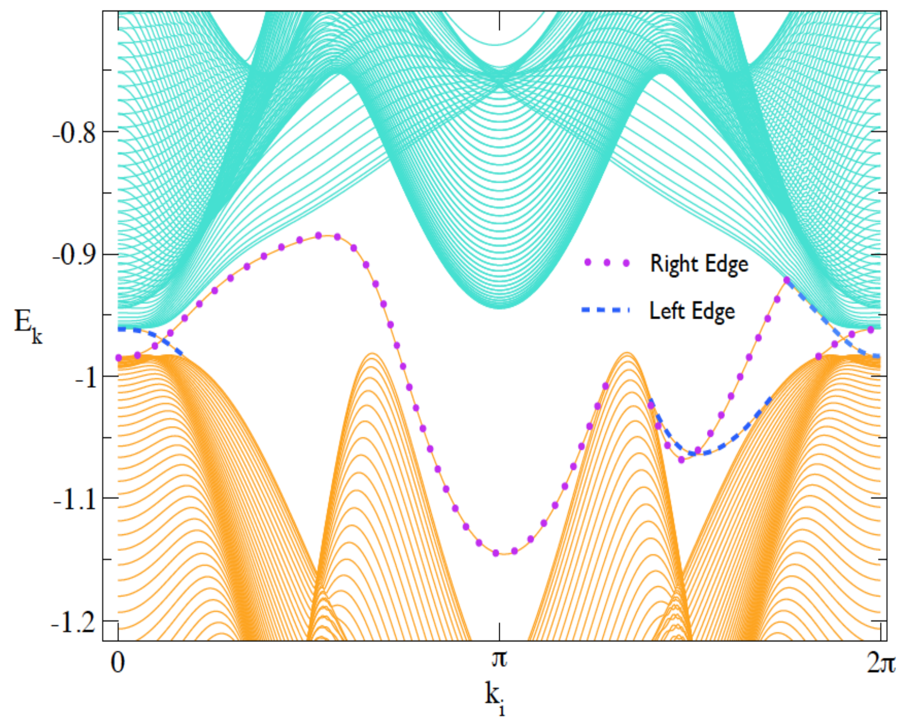


. A. Cook, AP (PRL 2014)

Trigonal distortion effect?

Phase diagram of SFMO in {111} bilayer





Edge state spectrum in C=2 Chern insulator

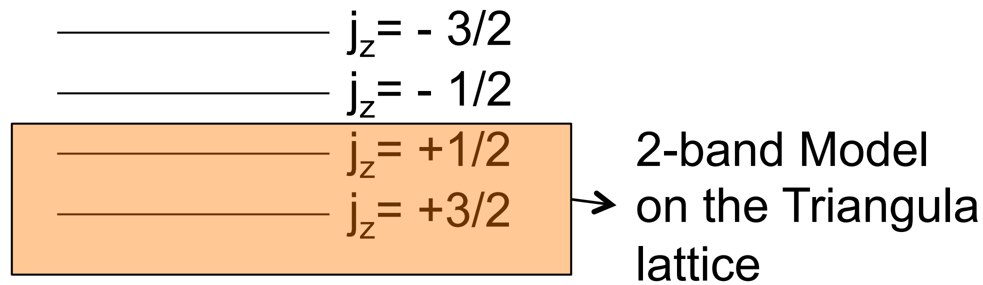
SFMO bilayer supports topologically nontrivial metals and C=2 Chern insulator

Quantum Hall gap ~ 75K

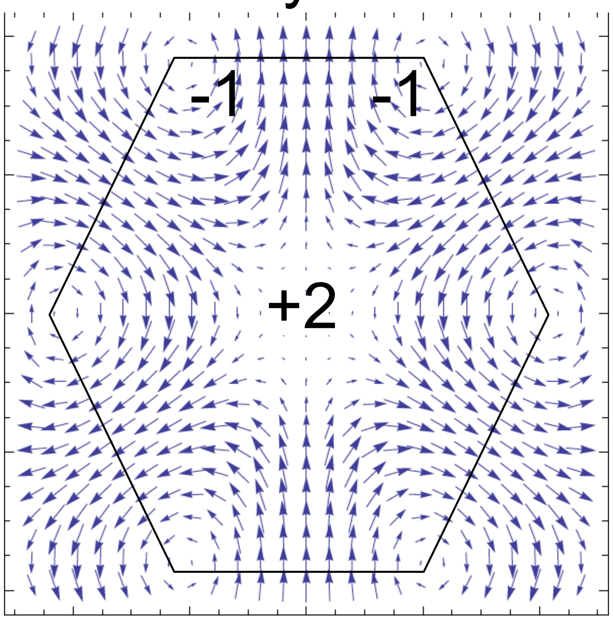
. A. Cook, AP (PRL 2014)

Emergence of C=2 Chern bands in the {111} ferromagnet

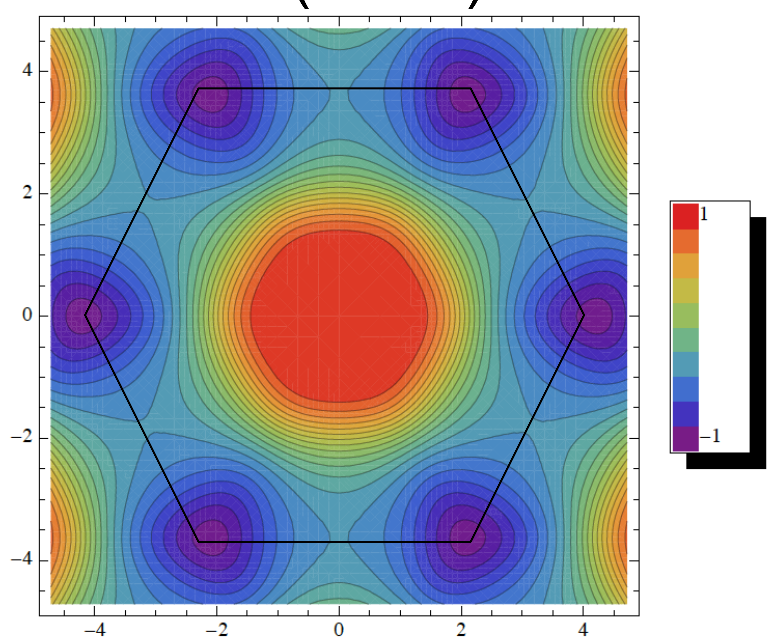
“Kinetic” Zeeman split j=3/2 states on Mo due to Fe ferromagnetism



xy



z (mass)



Skyrmion number = +/- 2

Summary

- 3D Bulk complex oxide: Ba_2FeReO_6
  - band structure with Weyl nodes
  - spin and orbital magnetization from strong correlations
  - spin dynamics in agreement with neutron data

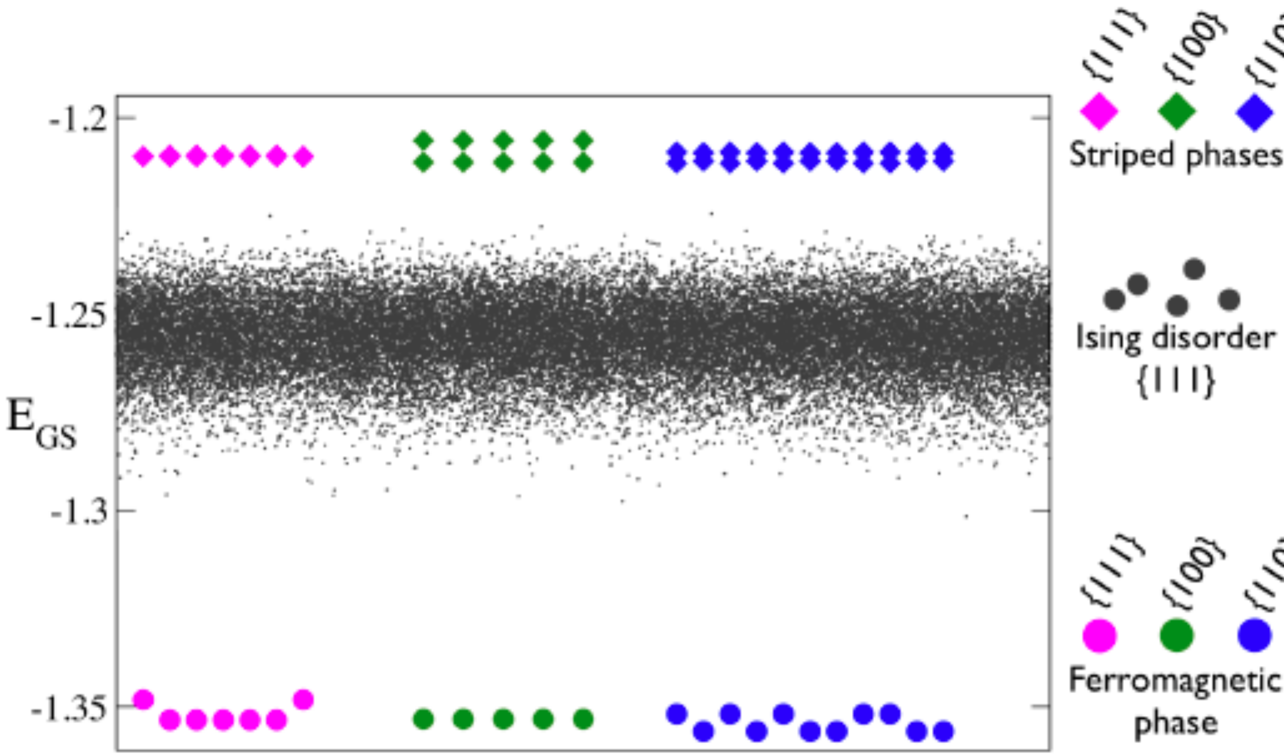
- Magnetism in insulating DPs: La_2ZnIrO_6, La_2MgIrO_6
  - magnetic order in agreement with data
  - resolve differences between Zn vs Mg

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

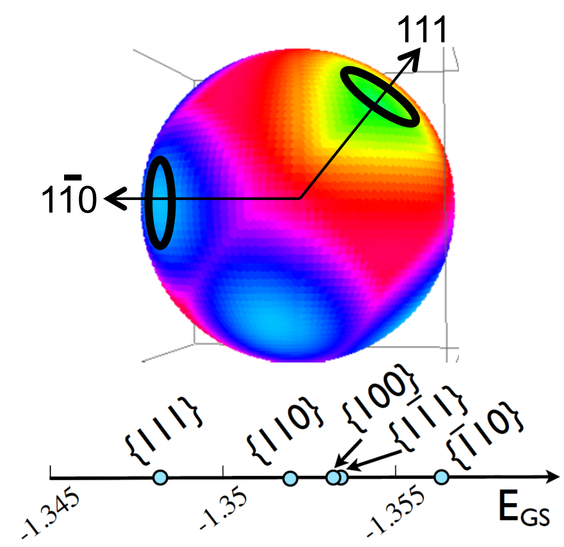
References

1. K. Plumb, A.Cook, J.P.Clancy, A.Kolesnikov, B.C.Jeon,T.W.Noh, AP, Y.J.Kim, PRB 87,184412 (2013)
2. A. Cook, AP, PRB 88, 235102 (2013)
3. A. Cook, AP, PRL 113, 077203 (2014)
4. A. Cook, C. Hickey, AP Phys. Rev. B 90, 085145 (2014)
5. A. Cook, S. Matern, C. Hickey, A. A. Aczel (arXiv:1502.01031)

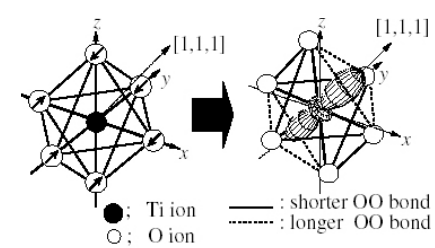
Magnetism of SFMO in {111} Thin Film Geometry

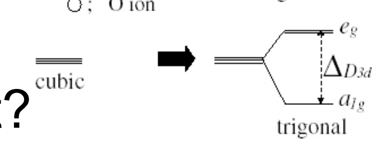


Ferro orientation



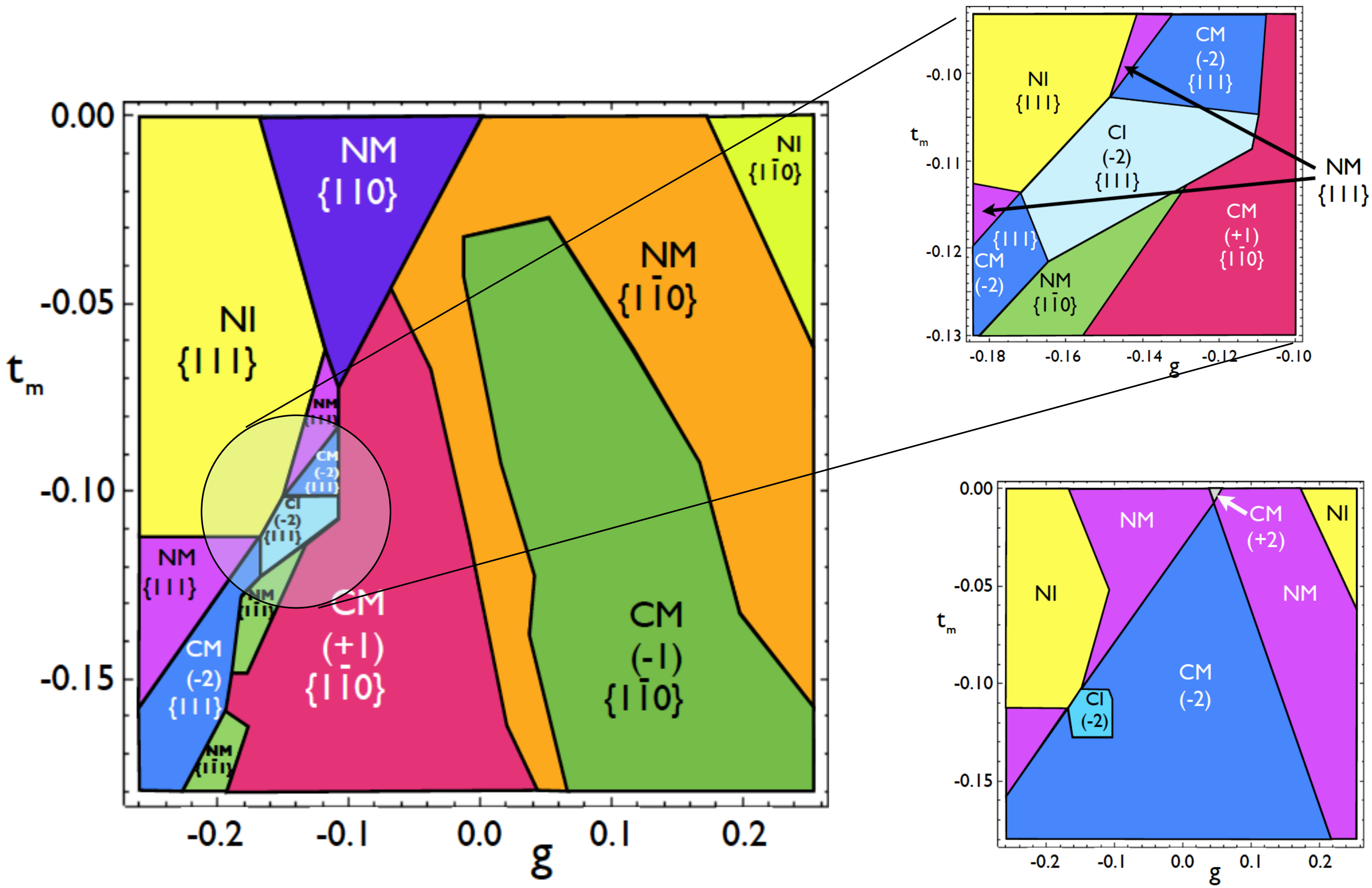
Lowest energy: Ferromagnetic orientation of Fe moments
Exchange energy between Fe (S=5/2) moments ~ 1meV
Ising-like anisotropy due to SOC
Mean field Tc ~ 100 K





Trigonal distortion effect?

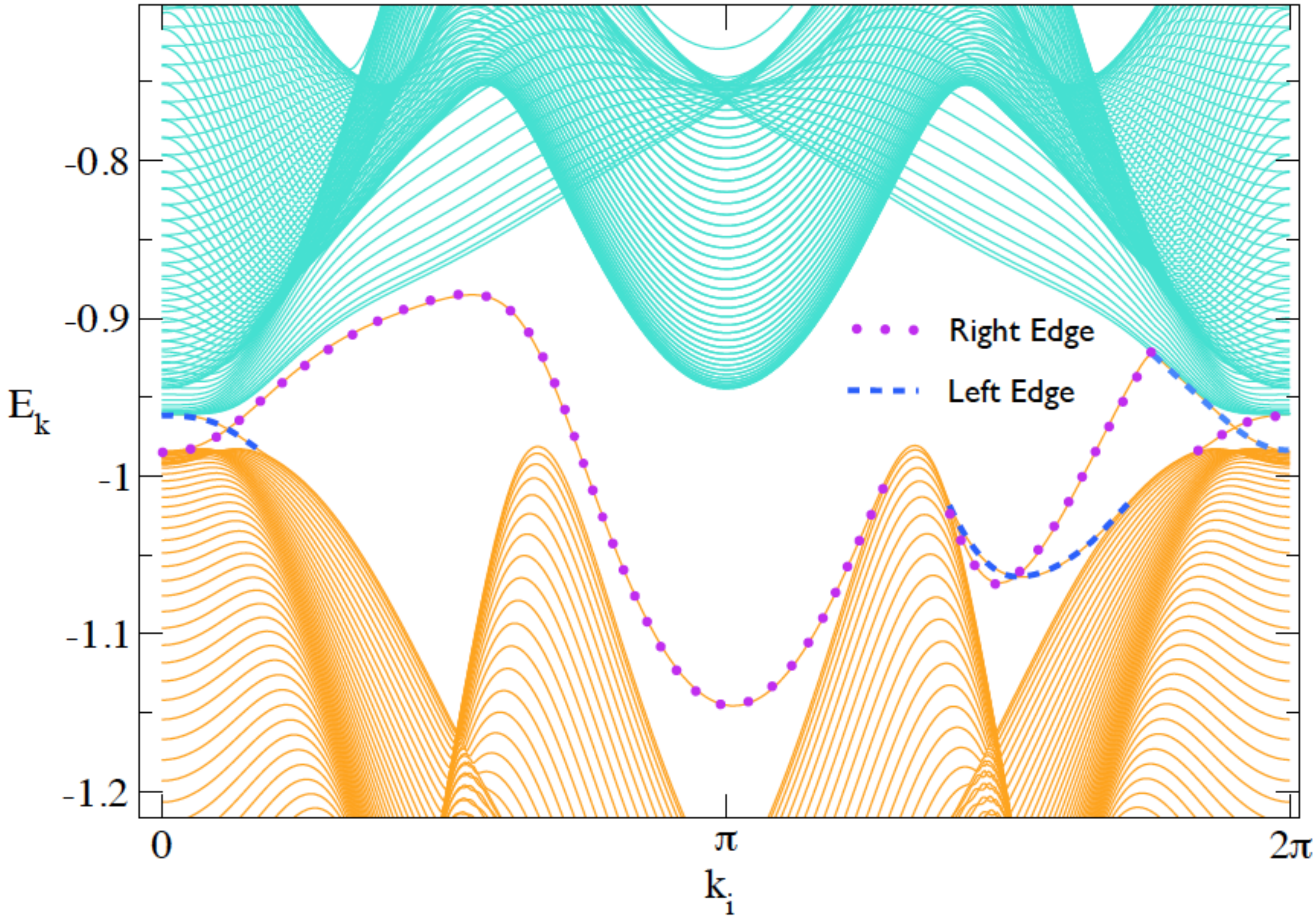
Phase diagram of SFMO in {111} bilayer



Ferro {111}

How can we understand the emergence of C=2 Chern bands?

Edge states in the C=2 quantum anomalous Hall state



2 topologically protected chiral edge modes

Summary

- Double perovskites:
  Applications to spintronics + Quantum spin liquid physics

- Strong correlations and SO effects:
  - band structure
  - spin and orbital magnetizations
  - spin dynamics

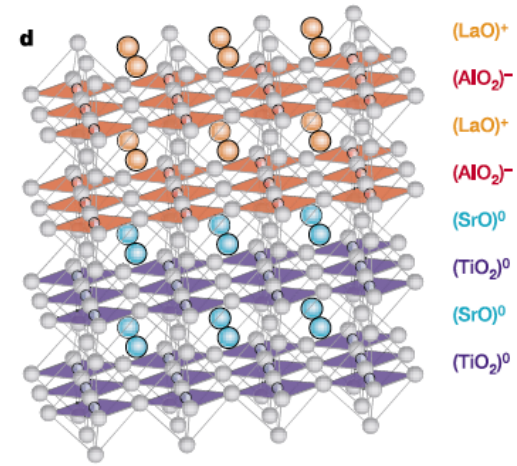
- Heterostructures:
  Rich phase diagram including emergent Chern bands and quantum anomalous Hall insulators
  Can Mott correlations drive unusual chiral spin liquids?

Oxide heterostructures

A high-mobility electron gas at the $LaAlO_3/SrTiO_3$ heterointerface

A. Ohtomo[1,2,3] & H. Y. Hwang[1,3,4]

NATURE | VOL 427 | 29 JANUARY 2004 | www.nature.com/nature



ARTICLE

Received 19 Mar 2013 | Accepted 24 Jul 2013 | Published 22 Aug 2013 DOI: 10.1038/ncomms3351

$LaAlO_3$ stoichiometry is key to electron liquid formation at $LaAlO_3/SrTiO_3$ interfaces

M.P. Warusawithana[1], C. Richter[2,3], J.A. Mundy[4], P. Roy[1], J. Ludwig[1], S. Paetel[2], T. Heeg[5], A.A. Pawlicki[1], L.F. Kourkoutis[4,6], M. Zheng[7], M. Lee[1], B. Mulcahy[7], W. Zander[8], Y. Zhu[4], J. Schubert[8], J.N. Eckstein[7], D.A. Muller[4,6], C. Stephen Hellberg[9], J. Mannhart[3] & D.G. Schlom[5,6]

nature physics LETTERS
PUBLISHED ONLINE: 4 SEPTEMBER 2011 | DOI: 10.1038/NPHYS2079

Direct imaging of the coexistence of ferromagnetism and superconductivity at the $LaAlO_3/SrTiO_3$ interface

Julie A. Bert[1], Beena Kalisky[1], Christopher Bell[1], Minu Kim[1,2], Yasuyuki Hikita[1], Harold Y. Hwang[1,2] and Kathryn A. Moler[1]*

ARTICLE

Received 18 Jul 2012 | Accepted 25 Mar 2013 | Published 14 May 2013 DOI: 10.1038/ncomms2804 OPEN

Anisotropic two-dimensional electron gas at the $LaAlO_3/SrTiO_3$ (110) interface

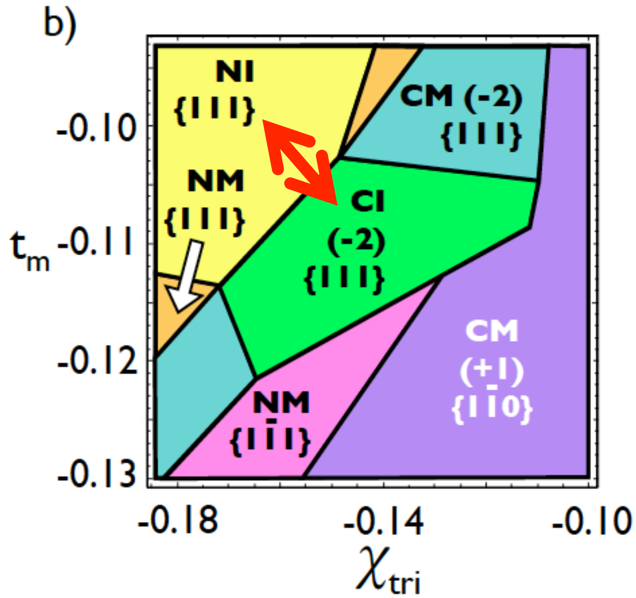
A. Annadi[1,2], Q. Zhang[3,4,5], X. Renshaw Wang[1,2], N. Tuzla[6], K. Gopinadhan[1,7], W.M. Lü[1,7], A. Roy Barman[1,2], Z.Q. Liu[1,2], A. Srivastava[1,2], S. Saha[1,2], Y.L. Zhao[1,2], S.W. Zeng[1,2], S. Dhar[1,7], E. Olsson[6], B. Gu[5,8], S. Yunoki[4,5,9,10], S. Maekawa[5,8], H. Hilgenkamp[11,12], T. Venkatesan[1,2,7] & Ariando[1,2]

LETTERS nature physics
PUBLISHED ONLINE: 4 SEPTEMBER 2011 | DOI: 10.1038/NPHYS2080

Coexistence of magnetic order and two-dimensional superconductivity at $LaAlO_3/SrTiO_3$ interfaces

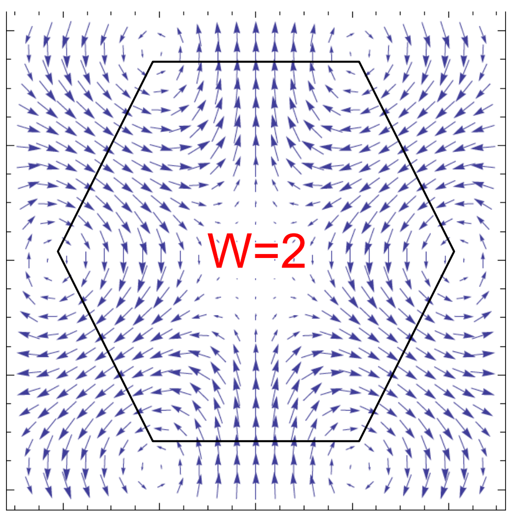
Lu Li[1], C. Richter[2], J. Mannhart[3] and R. C. Ashoori[1]*

C=2 Chern insulator to Normal insulator transition

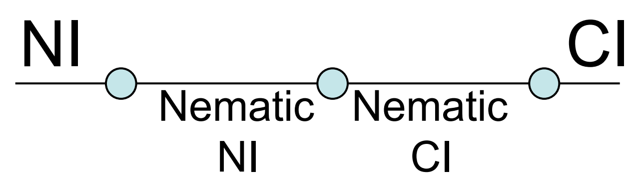


Haldane model: Chern number changes by "1".

Chern number change by "2" is unusual: Symmetry protection needed (inversion or C_6 of Mo triangular lattice)



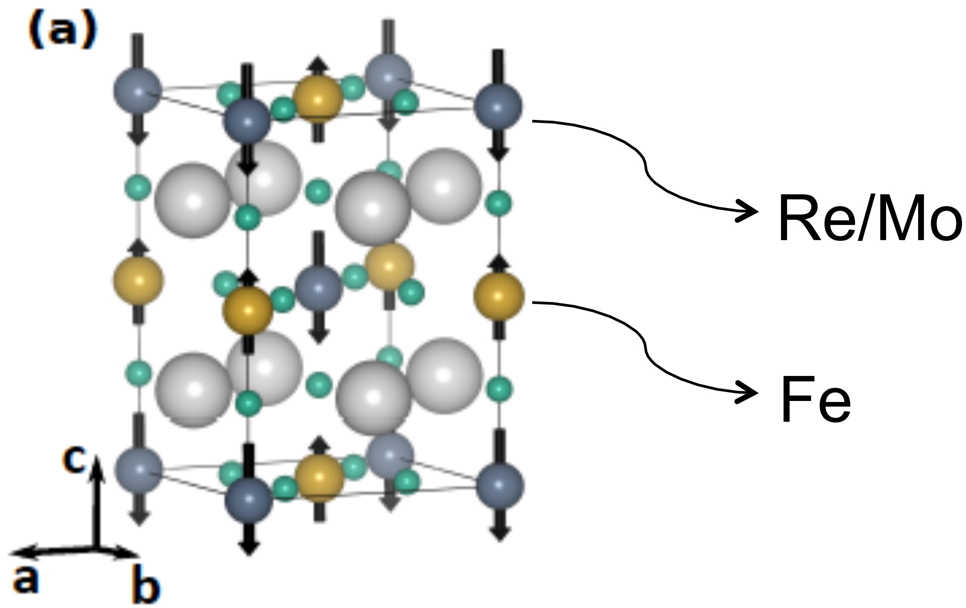
- Quadratic band touching at Γ-point with skyrmion texture having winding number=2
- Marginally relevant interactions drive nematic order around the putative critical point



A. Cook, C. Hickey, AP (PRB 2014)

Double Perovskites

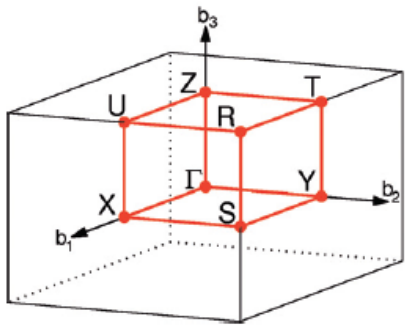
General formula: $A_2BB'O_6$ (B,B' = 3d, 4d, 5d)



Ba_2FeReO_6, Sr_2FeMoO_6: Half-metallic with strong spin orbit coupling

- Understand interplay of SO coupling, magnetism, and transport
- Interplay of Hund's coupling + spin-orbit interactions
- Typically low anti-site disorder for 3d/5d DPs (<1%)

Electronic model for BFRO: Tight binding

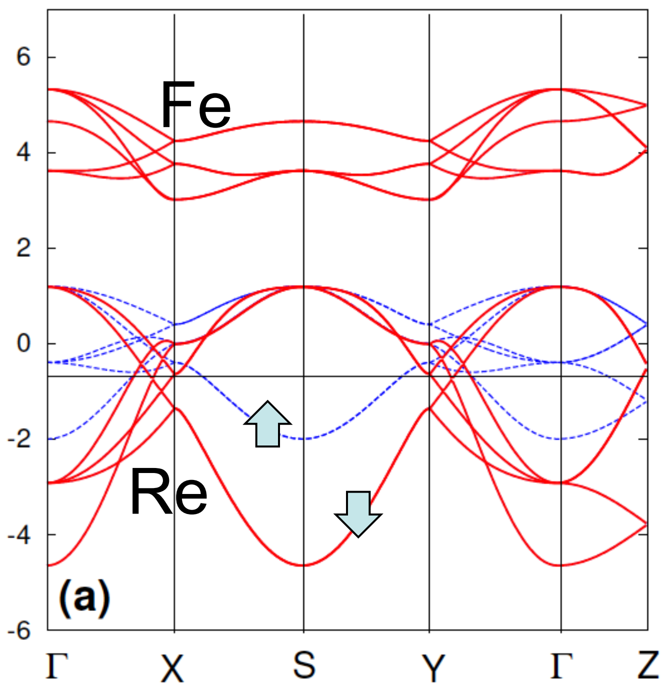


Parameters

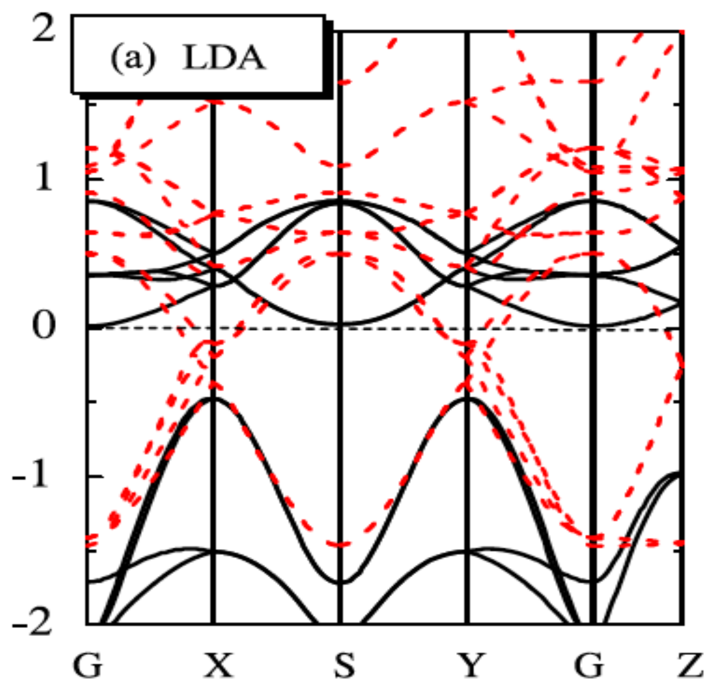
$t_{Fe\text{-}Re}$ ~ 330 meV, Δ_{CT} ~ 1 eV

$t_{Re\text{-}Re}$ ~ 100 meV, Other hoppings small < 50 meV

Comparing uncorrelated (U=0) dispersion with LDA



A. Cook, AP (PRB 2013)



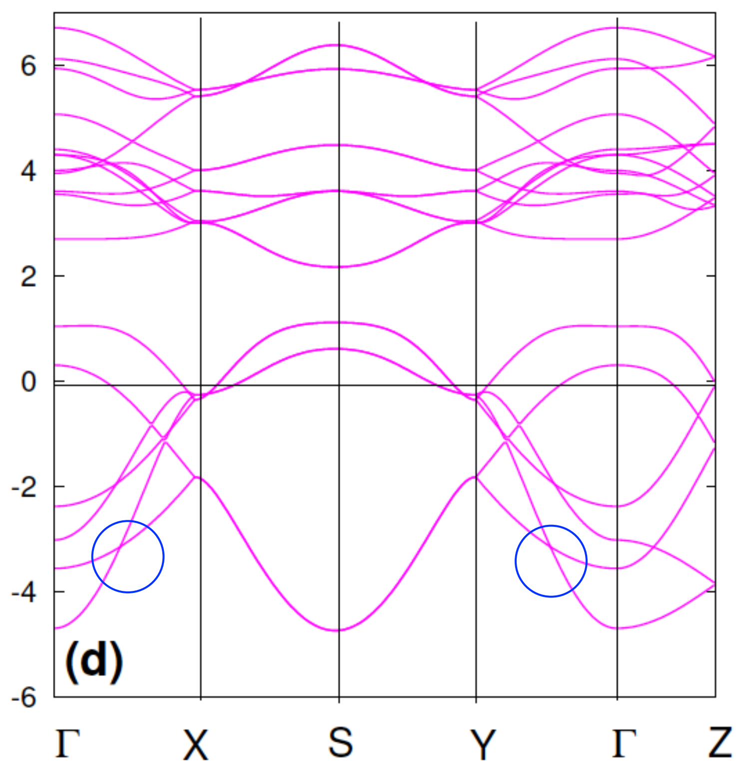
B.C. Jeon, T.W. Noh, et al, (JPCM, 2010)

Electronic model for BFRO: Correlations and SOC

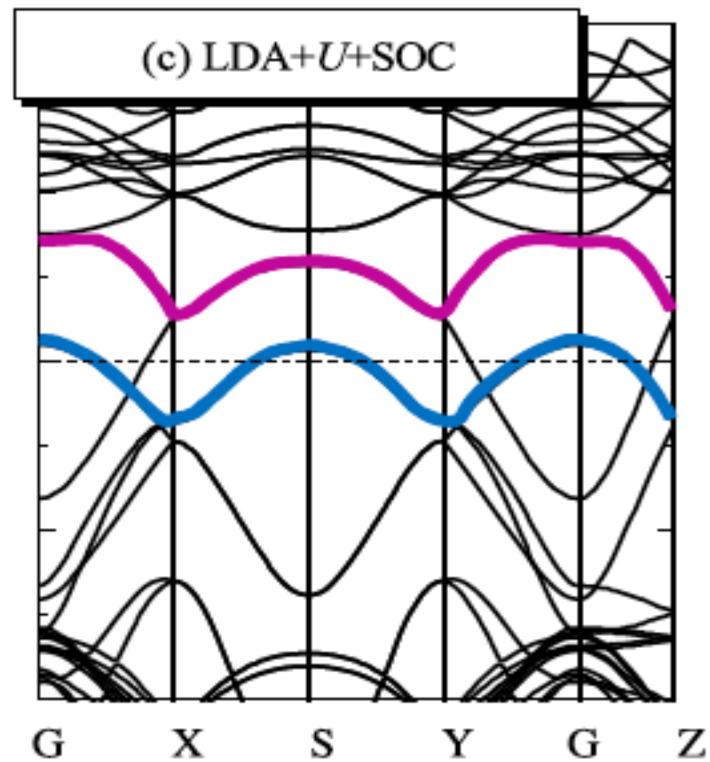
Spin-orbit coupling lifts many degeneracies
Weyl nodes: Discrete band touching points with topological properties

[X.Wan, et al (PRB 2011); A. Burkov, L. Balents (PRL 2012), W.Witczak-Krempa, Y.B. Kim (PRB 2012)]

Comparing Hartree + SO dispersion with LDA+U+SOC



A. Cook, AP (PRB 2013)

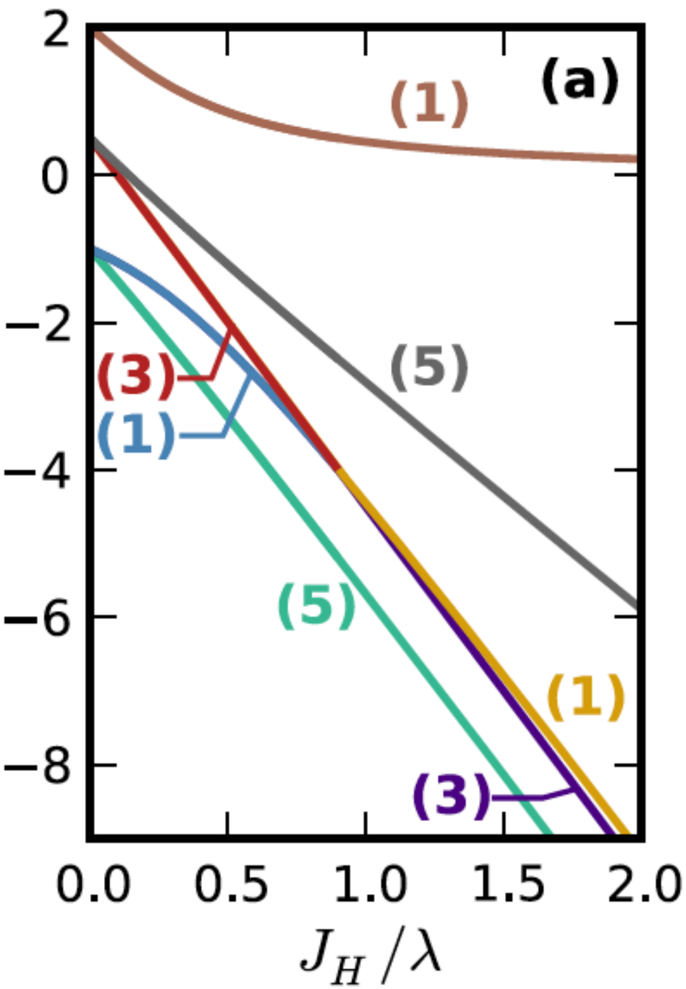


B.C. Jeon, T.W. Noh, et al, (JPCM, 2010)

Local moment starting point: Atomic states

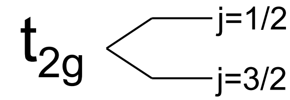
Simplified interaction for d^2

$$H_{\rm at}^{(2)} = -2J_H \vec{S}_{\rm tot}^2 - \frac{J_H}{2}\vec{L}_{\rm tot}^2 - \lambda_0(\vec{L}_1 \cdot \vec{S}_1 + \vec{L}_2 \cdot \vec{S}_2)$$



J_H=0 states

Degeneracy: 6,8,1



Large J_H states simple

L=1,S=1: J=2,1,0

L=2,S=0: No s.o.

L=0,S=0: No s.o.

Lowest 5 states smooth

For modest values $J_H > 2\lambda$

L=1 + S=1 giving J=2

K. Plumb, A. Cook, et al, PRB 87,184412 (2013)