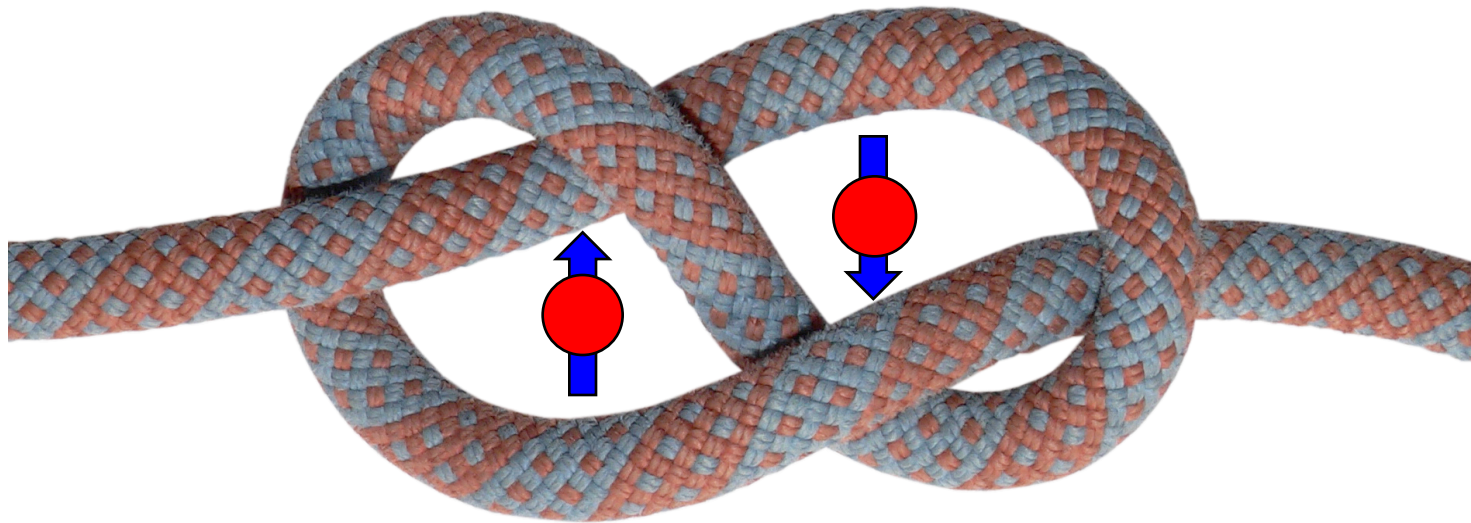


Oxide Heterostructures

A route to engineering topological phases of matter

Arun Paramakanti
(University of Toronto)



Seminar, College de France (Paris, 26 May 2016)

Funding:



UNIVERSITY OF
TORONTO



NSERC
CRSNG



CIFAR
CANADIAN INSTITUTE
for ADVANCED RESEARCH

Topology in Everyday Life

Topology in Everyday Life

Football



Genus = 0

Topology in Everyday Life

Football



Genus = 0

Toronto - Winter travel



Genus = 1

Topology in Everyday Life

Football



Genus = 0

Toronto - Winter travel



Genus = 1

Breakfast



Genus = 1

Topology in Everyday Life

Football



Genus = 0

Toronto - Winter travel



Genus = 1

Breakfast?



Genus = 1

Topology in Everyday Life

Football



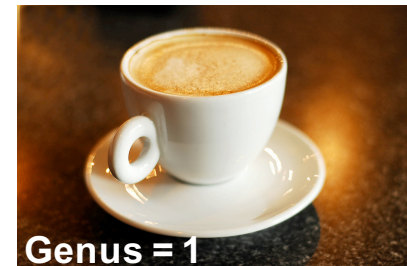
Genus = 0

Toronto - Winter travel



Genus = 1

Breakfast



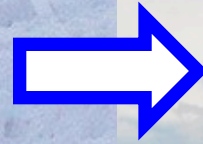
Genus = 1



Genus = 3

Topology in Everyday Life

Toronto in February



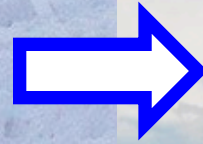
Toronto in May



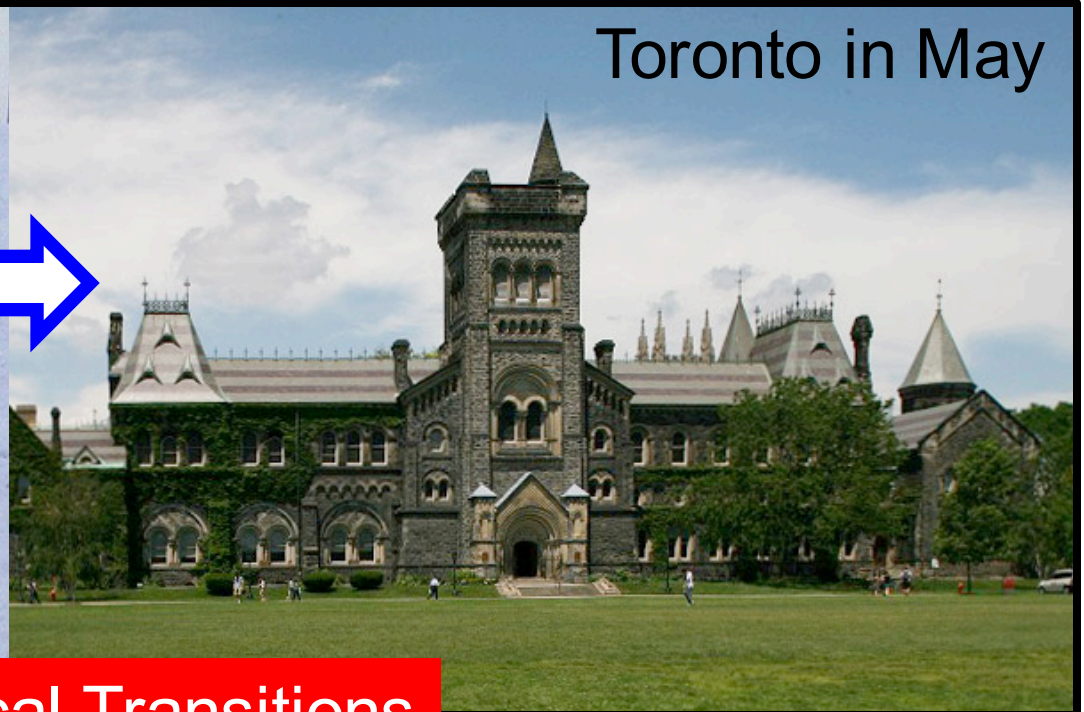
Topological Transitions

Topology in Everyday Life

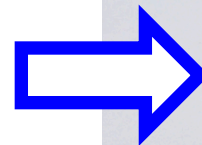
Toronto in February



Toronto in May

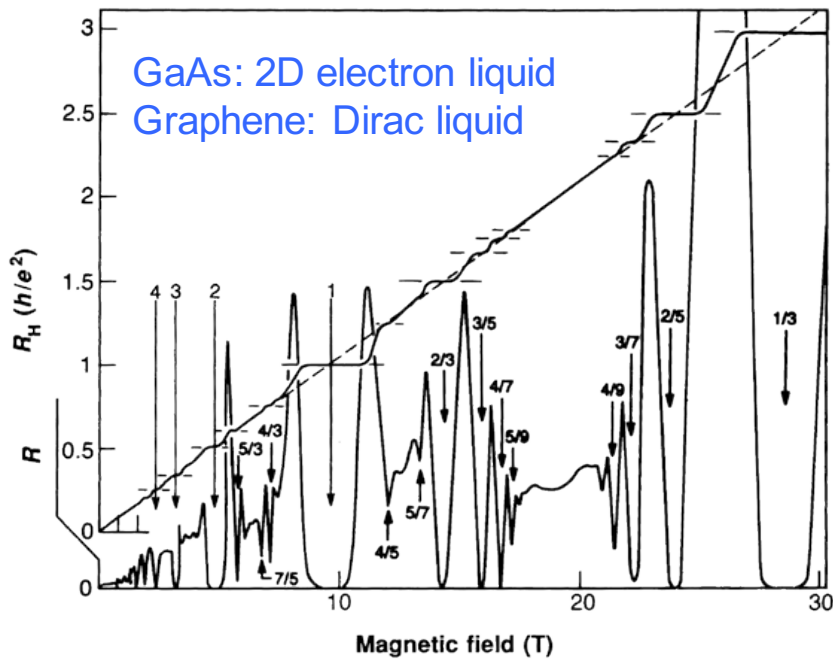


Topological Transitions



Topological phases of quantum matter

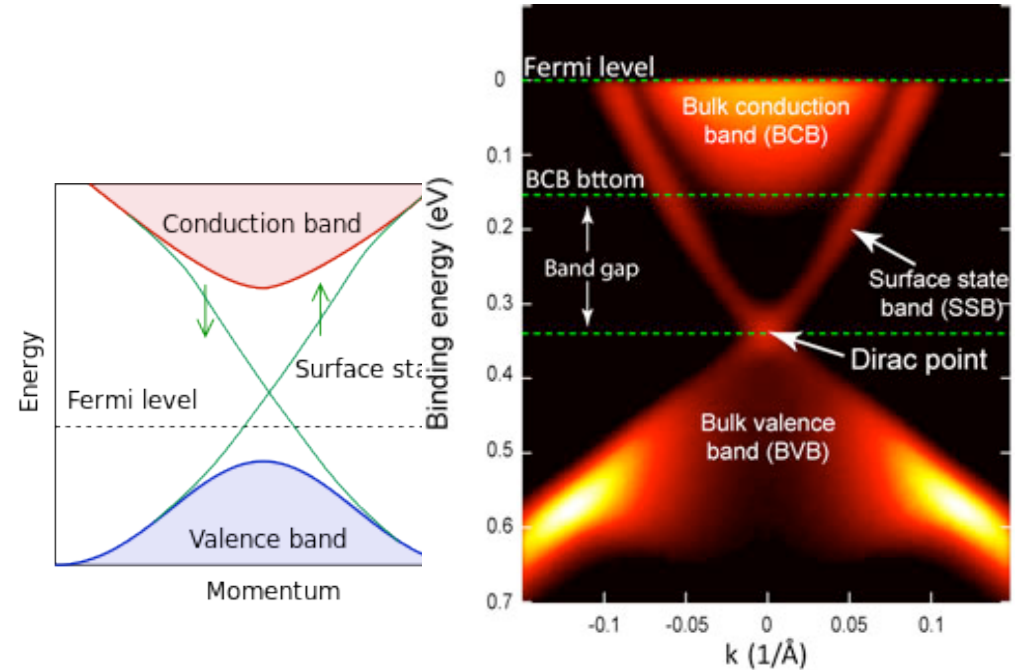
Quantum Hall effects



Quantum Hall effect

- Precise quantization of σ_{xy}
- Chiral edge states

Topological insulators, top. crystalline insulators



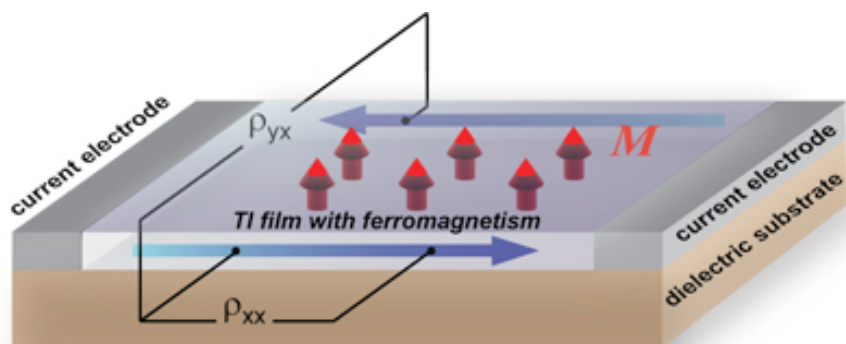
Topological insulators (3d)

- Precise $\vec{E} \cdot \vec{B}$ coefficient $\Theta = \pi$
- Chiral odd-# Dirac surface states

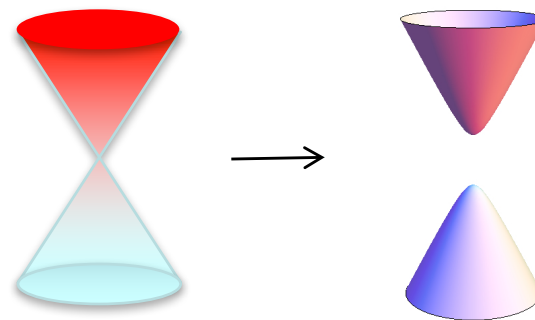
Quantum anomalous Hall effect

Magnetically doped topological insulators

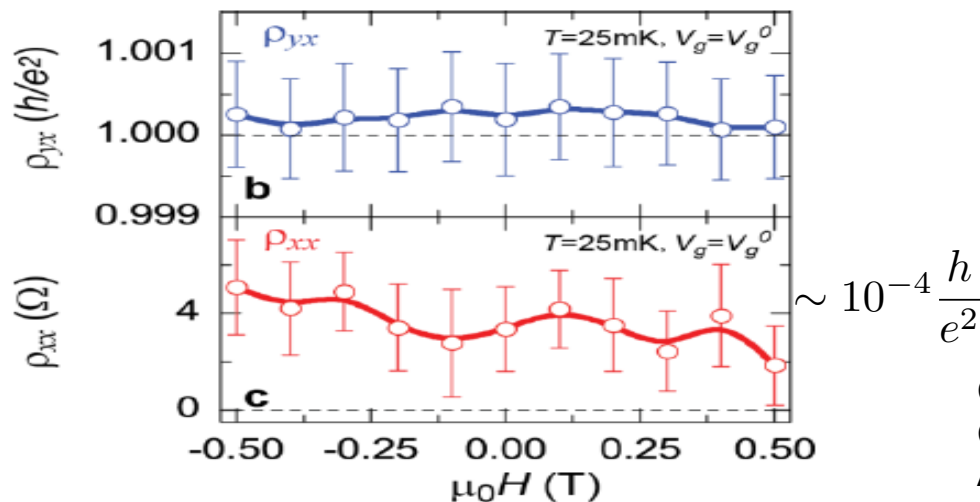
- Consider TIs near a band inversion transition (e.g., thin films)
- Breaking time-reversal strongly with dopant magnetization: QAH effect
- Spin orbit coupling is crucial



R. Yu, et al (Science 2010)



Surface Dirac fermions get gapped

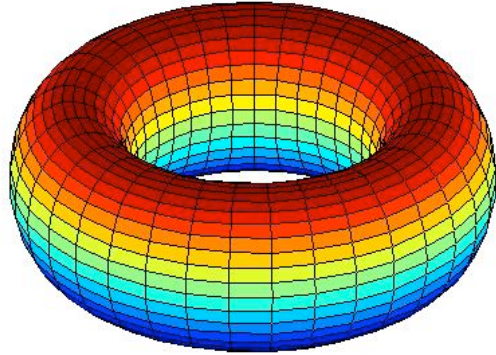


(Bi,Sb)₂Te₃ film doped with Cr or V atoms
 Ferromagnetic T_c ~ 10-15K

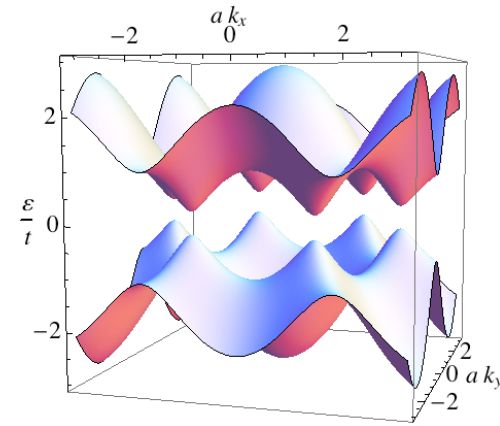
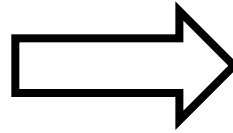
- C.Z. Chang et al, Science 2013 (Xue group, Tsinghua)
- C.Z. Chang et al, arXiv (M. Chan + J. Moodera groups, PSU/MIT)
- A. J. Bestwick et al, arXiv (Goldhaber-Gordon group, Stanford)
- A. Kandala, et al, arXiv (N. Samarth and C.X. Liu groups, PSU)

Bands in Crystals – Momentum Space Topology

Crystal momentum



2D Brillouin zone: Torus



k-space energy bands: $E_n(\mathbf{k})$
 Bloch wavefunctions: $|\psi_n(\mathbf{k})\rangle$

Two-Band System

$$H(\mathbf{k}) = \vec{d}(\mathbf{k}) \cdot \vec{\sigma} \quad \text{pseudospin}$$

$$E_{\pm}(\mathbf{k}) = \pm |\vec{d}(\mathbf{k})|$$



$\hat{d}(\mathbf{k})$: Information about wavefunction

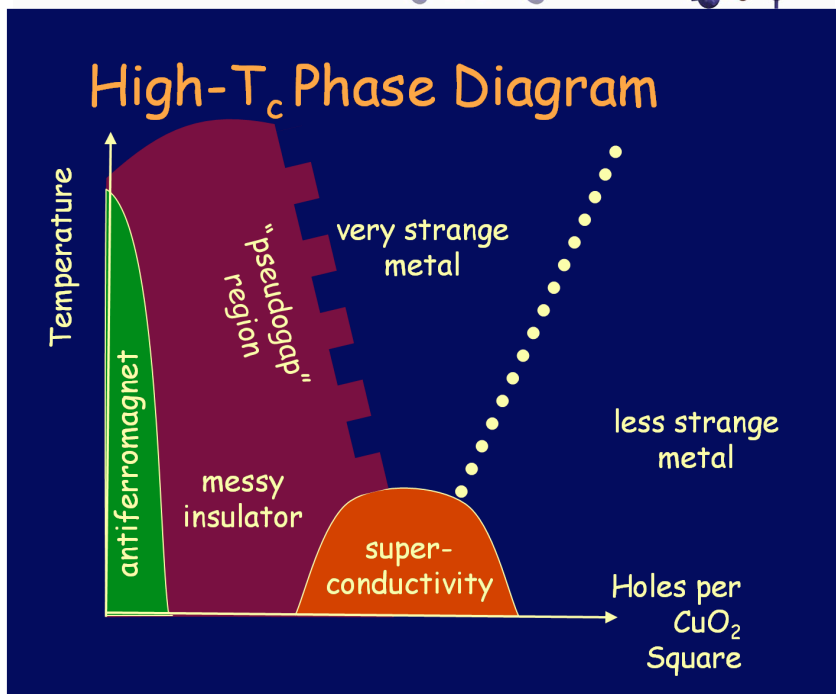
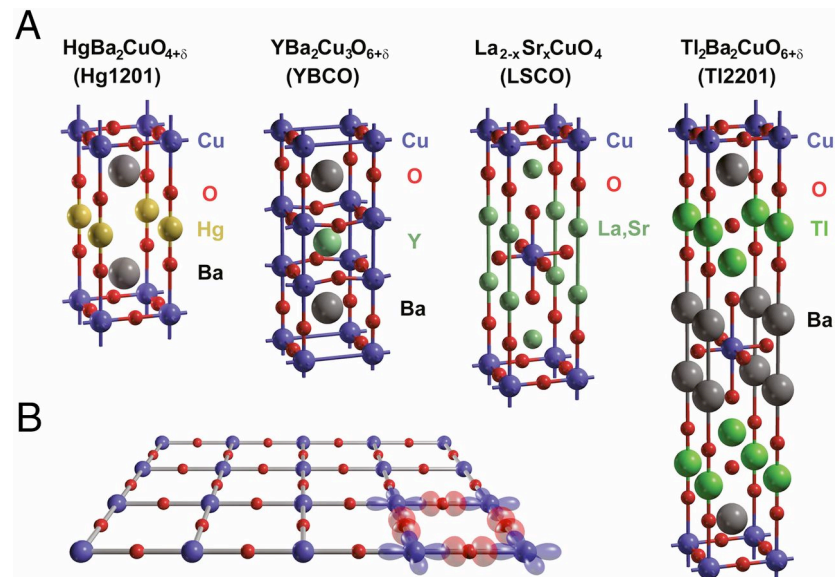
$$\int \frac{dk_x dk_y}{4\pi} \hat{d}(\mathbf{k}) \cdot \partial_x \hat{d}(\mathbf{k}) \times \partial_y \hat{d}(\mathbf{k})$$

→ Topological invariant (Chern number)

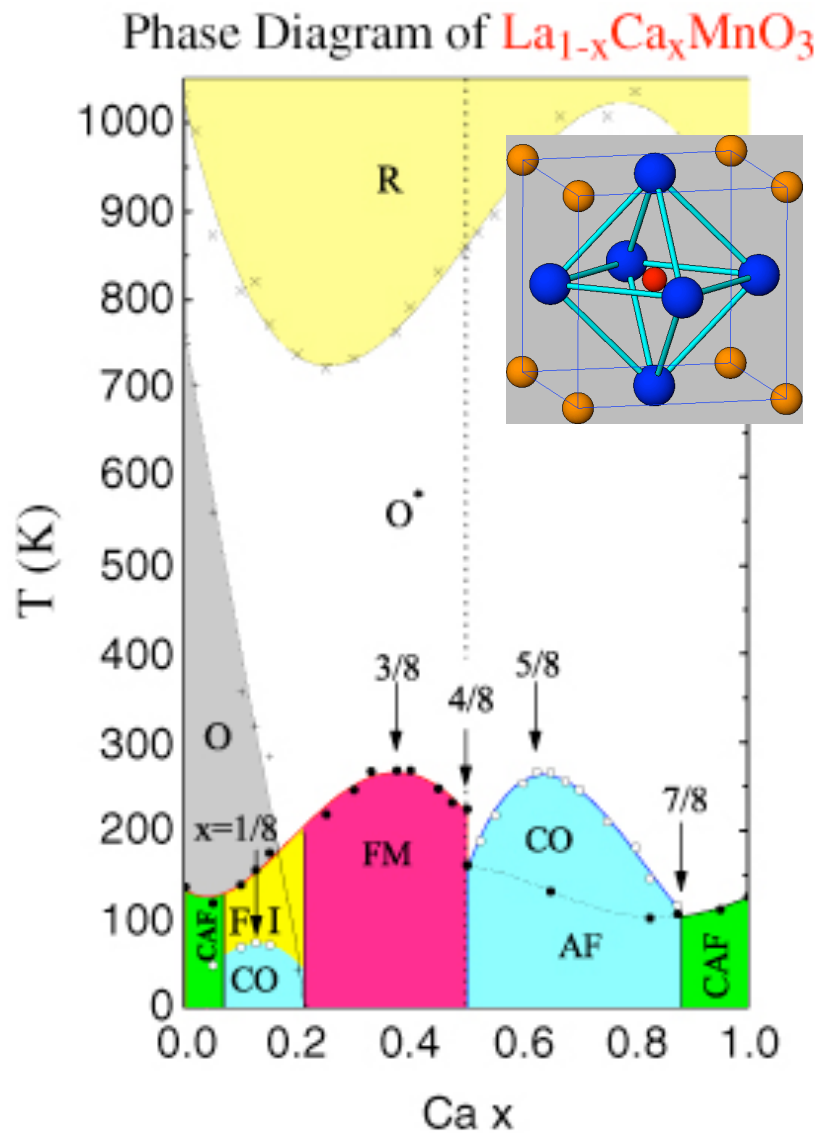
Sample boundary: Change of topology leads to gapless edge states

Strong correlations can drive new phases of matter

High temperature superconductivity



Colossal magnetoresistive oxides

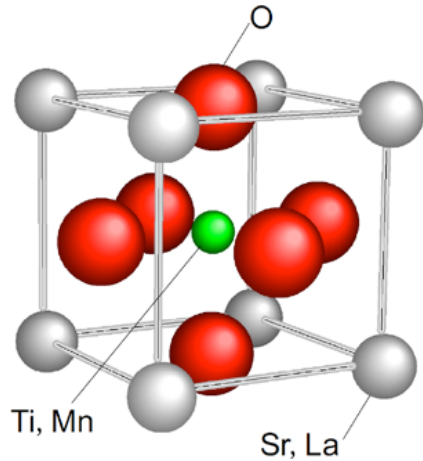


Topology meets Strong Correlations

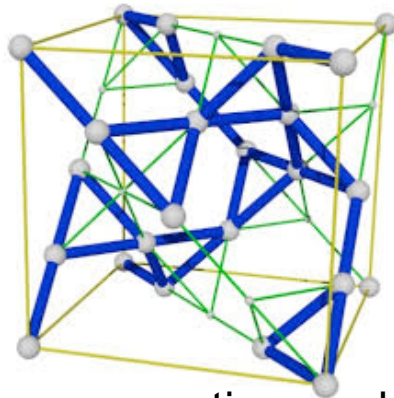
- Band topology - momentum space, global
- Strong correlations - real space, local

- How can we bring together strong correlations and band topology?
- Can strongly correlated materials display topological bands?
- Can we get new types of many-body topological properties?
- Does the interplay lead to new magnetic interactions and phases?
- What happens at an interacting topological transition?

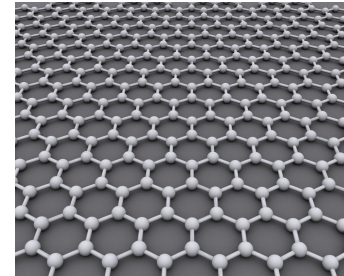
Research interests



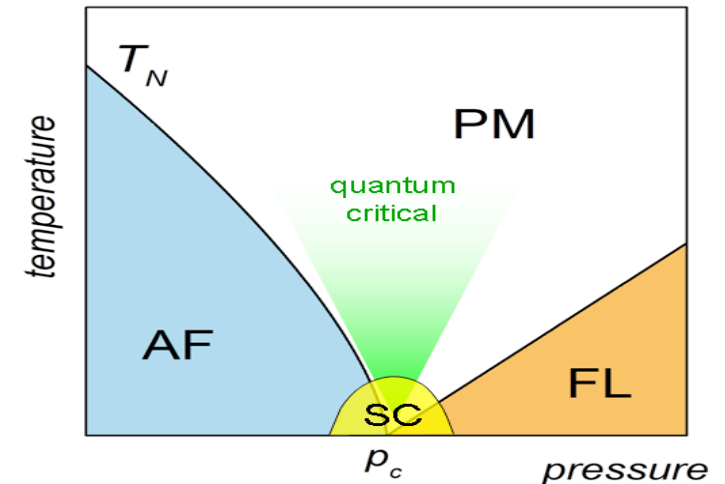
Transition metal oxides and heterostructures:
Can they realize correlated topological phases?



Quantum magnetism and spin liquids:
Are there materials with spin liquid phases and topological order?



Graphene, TM dichalcogenides:
How to endow them with nontrivial topological character?



Quantum phase transitions (QPTs):
What happens at topological phase transitions?

Collaborators



Ashley Cook
(PhD: Toronto -> U. Zurich)



Ciaran Hickey
(PhD: Univ. Toronto)

- Toronto: K. Plumb, J.P. Clancy, **Young-June Kim**
- SNU: B.-C. Jeon, T.-W. Noh
- ORNL: **A.A. Aczel**, G. Cao, T. J. Williams, S. Calder, A. Christianson, D. Mandrus. A. Kolesnikov
- India: Santu Baidya, **Tanusri-Saha Dasgupta**, Umesh Waghmare

Discussions: Bruce Gaulin, John Greedan, , Y. B. Kim, M. Randeria, N. Trivedi, Pat Woodward, S. Trebst, G. Chen, L. Balents, S. Sachdev

(1) Strong correlations

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

Periodic Table of the Elements

Periodic Table of the Elements																							
Legend																							
Alkali Metal	Alkaline Earth	Transition Metal	Basic Metal	Semimetal	Nonmetal	Halogen	Noble Gas	Lanthanide	Actinide														
1 IA 11A H Hydrogen 1.008																			2 18 VIIIA 8A He Helium 4.003				
3 Li Lithium 6.941	4 IIA 2A Be Beryllium 9.012																	5 13 IIIA 3A B Boron 10.811	6 14 IVA 4A C Carbon 12.011	7 15 VA 5A N Nitrogen 14.007	8 16 VIA 6A O Oxygen 15.999	9 17 VIIA 7A F Fluorine 18.998	10 18 VIIIA 8A Ne Neon 20.180
11 Na Sodium 22.990	12 IIA 2A Mg Magnesium 24.305	3 IIIB 3B Sc Scandium 44.956	4 IVB 4B Ti Titanium 47.88	5 VB 5B V Vanadium 50.94	6 VIB 6B Cr Chromium 52.00	7 VIIB 7B Mn Manganese 54.94	8 VIII 8 Fe Iron 55.85	9 VIII 9 Co Cobalt 58.93	10 VIII 10 Ni Nickel 58.71	11 IB 11 Cu Copper 63.55	12 IIB 12 Zn Zinc 65.38	13 IIIA 3A Al Aluminum 26.98	14 IVA 4A Si Silicon 28.09	15 VA 5A P Phosphorus 30.97	16 VIA 6A S Sulfur 32.07	17 VIIA 7A Cl Chlorine 35.45	18 VIIIA 8A Ar Argon 39.95						
19 K Potassium 39.09	20 IIA 2A Ca Calcium 40.08	21 IIIB 3B Sc Scandium 44.96	22 IVB 4B Ti Titanium 47.88	23 VB 5B V Vanadium 50.94	24 VIB 6B Cr Chromium 52.00	25 VIIB 7B Mn Manganese 54.94	26 VIII 8 Fe Iron 55.85	27 VIII 9 Co Cobalt 58.93	28 VIII 10 Ni Nickel 58.71	29 IB 11 Cu Copper 63.55	30 IIB 12 Zn Zinc 65.38	31 IIIA 3A Ga Gallium 69.72	32 IVA 4A Ge Germanium 72.64	33 VA 5A As Arsenic 74.92	34 VIA 6A Se Selenium 78.96	35 VIIA 7A Br Bromine 79.90	36 VIIIA 8A Kr Krypton 83.80						
37 Rb Rubidium 85.47	38 IIA 2A Sr Strontium 87.62	39 IIIB 3B Y Yttrium 88.91	40 IVB 4B Zr Zirconium 91.22	41 VB 5B Nb Niobium 92.91	42 VIB 6B Mo Molybdenum 95.94	43 VIIB 7B Tc Technetium 98.91	44 VIII 8 Ru Ruthenium 101.07	45 VIII 9 Rh Rhodium 102.91	46 VIII 10 Pd Palladium 106.42	47 IB 11 Ag Silver 107.87	48 IIB 12 Cd Cadmium 112.41	49 IIIA 3A In Indium 114.82	50 IVA 4A Sn Tin 118.71	51 VA 5A Sb Antimony 121.76	52 VIA 6A Te Tellurium 127.6	53 VIIA 7A I Iodine 126.90	54 VIIIA 8A Xe Xenon 131.29						
55 Cs Cesium 132.91	56 IIA 2A Ba Barium 137.33	57-71 Lanthanide Series	72 IVB 4B Hf Hafnium 178.49	73 VB 5B Ta Tantalum 180.95	74 VIB 6B W Tungsten 183.85	75 VIIB 7B Re Rhenium 186.21	76 VIII 8 Os Osmium 190.23	77 VIII 9 Ir Iridium 192.22	78 VIII 10 Pt Platinum 195.08	79 IB 11 Au Gold 196.97	80 IIB 12 Hg Mercury 200.59	81 IIIA 3A Tl Thallium 204.38	82 IVA 4A Pb Lead 207.2	83 VA 5A Bi Bismuth 208.98	84 VIA 6A Po Polonium [209]	85 VIIA 7A At Astatine [210]	86 VIIIA 8A Rn Radon [222]						
87 Fr Francium [223]	88 IIA 2A Ra Radium [226]	89-103 Actinide Series	104 IVB 4B Rf Rutherfordium [261]	105 VB 5B Db Dubnium [262]	106 VIB 6B Sg Seaborgium [266]	107 VIIB 7B Bh Bohrium [264]	108 VIII 8 Hs Hassium [269]	109 VIII 9 Mt Meitnerium [268]	110 VIII 10 Ds Darmstadtium [269]	111 IB 11 Rg Roentgenium [272]	112 IIB 12 Cn Copernicium [277]	113 IIIA 3A Uut Ununtrium [278]	114 IVA 4A Fl Flerovium [289]	115 VA 5A Uup Ununpentium [288]	116 VIA 6A Lv Livermorium [293]	117 VIIA 7A Uus Ununseptium [294]	118 VIIIA 8A Uuo Ununoctium [294]						

(2) Band topology

- Nontrivial band topology: SOC + conducting electron fluid
- Strong SOC needs heavy elements
- Expected in 4d/5d oxides (eg: Rhenium, Osmium, Iridium)

↓
Increasing
SOC

Periodic Table of the Elements

1 IA 11A																	18 VIIIA 8A						
1 H Hydrogen 1.008																	2 He Helium 4.003						
3 Li Lithium 6.941	4 Be Beryllium 9.012																	5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 9	10 VIII 10	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A						
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.88	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.933	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.723	32 Ge Germanium 72.61	33 As Arsenic 74.922	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 84.80						
37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium [98]	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91	46 Pd Palladium 106.42	47 Ag Silver 107.87	48 Cd Cadmium 112.41	49 In Indium 114.82	50 Sn Tin 118.71	51 Sb Antimony 121.76	52 Te Tellurium 127.6	53 I Iodine 126.90	54 Xe Xenon 131.29						
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87 Fr Francium [223]	88 Ra Radium 226.02	89-103 Actinide Series	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium [284]	114 Fl Flerovium [289]	115 Uup Ununpentium [288]	116 Lv Livermorium [293]	117 Uus Ununseptium [288]	118 Uuo Ununoctium [289]						
		57 La Lanthanum 138.91	58 Ce Cerium 140.12	59 Pr Praseodymium 140.91	60 Nd Neodymium 144.24	61 Pm Promethium [145]	62 Sm Samarium 150.36	63 Eu Europium 151.96	64 Gd Gadolinium 157.25	65 Tb Terbium 158.93	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93	68 Er Erbium 167.26	69 Tm Thulium 168.93	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.96							
		89 Ac Actinium 227.03	90 Th Thorium 232.04	91 Pa Protactinium 231.04	92 U Uranium 238.03	93 Np Neptunium 237.05	94 Pu Plutonium 244.06	95 Am Americium 243.06	96 Cm Curium 247.07	97 Bk Berkelium 247.07	98 Cf Californium 251.08	99 Es Einsteinium [252]	100 Fm Fermium 257.10	101 Md Mendelevium [258]	102 No Nobelium 259.10	103 Lr Lawrencium [260]							

Alkali Metal
Alkaline Earth
Transition Metal
Basic Metal
Semimetal
Nonmetal
Halogen
Noble Gas
Lanthanide
Actinide

Engineering topology + correlations in solids

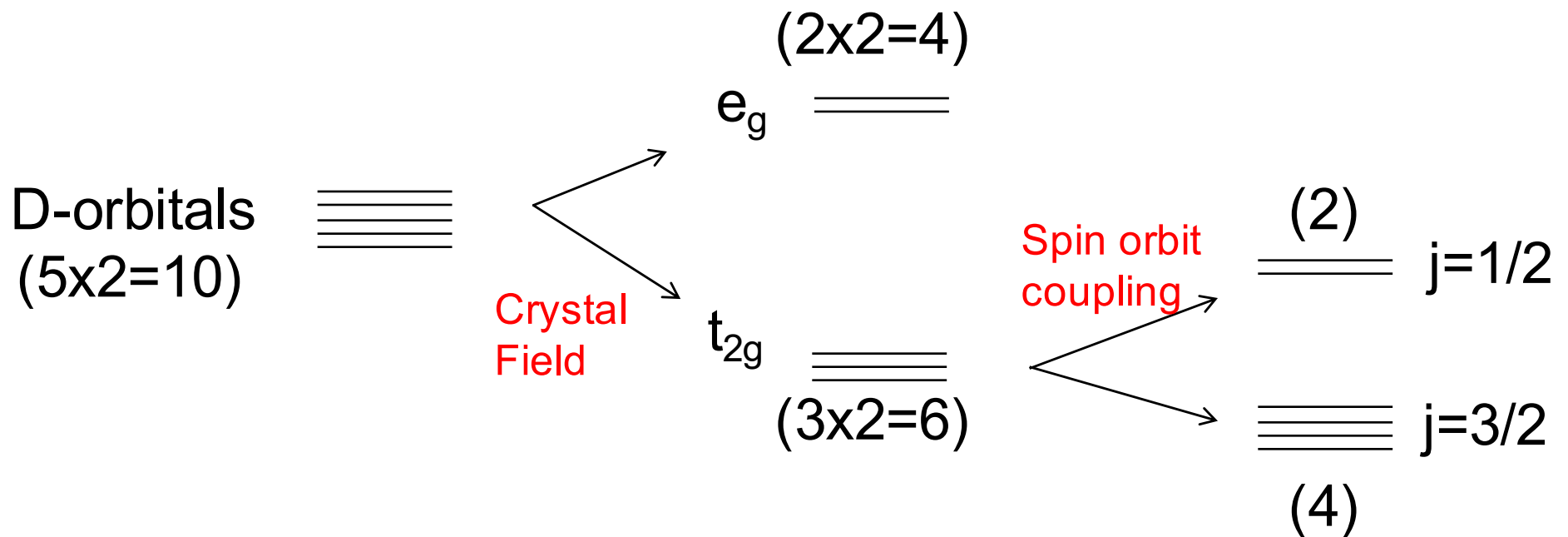
Layered complex oxides of 5d transition metals

Phase-Sensitive Observation of a Spin-Orbital Mott State in Sr_2IrO_4

B. J. Kim,^{1,2*} H. Ohsumi,³ T. Komesu,³ S. Sakai,^{3,4} T. Morita,^{3,5} H. Takagi,^{1,2*} T. Arima^{3,6}

SCIENCE VOL 323 6 MARCH 2009

Strong correlation effects needs narrow bands



Spin orbit coupling can cause band narrowing!

Engineering topology + correlations in solids

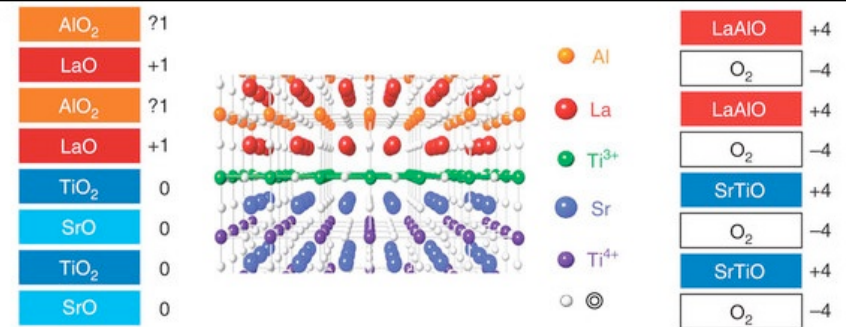
Oxide heterostructures and superlattices

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



3d-3d Superlattices along [111]

nature
materials

LETTERS

PUBLISHED ONLINE 22 JANUARY 2012 | DOI: 10.1038/NMAT3224

Exchange bias in LaNiO₃-LaMnO₃ superlattices

Marta Gibert^{1*}, Pavlo Zubko¹, Raoul Scherwitzl¹, Jorge Íñiguez² and Jean-Marc Triscone¹

3d/5d Superlattices along [111]

H. Takagi group (APL 2015)



Local electronic and magnetic studies of an artificial La₂FeCrO₆ double perovskite

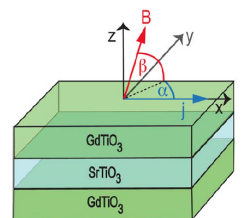
Benjamin Gray, Ho Nyung Lee, Jian Liu, J. Chakhalian, and J. W. Freeland

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

Quantum Wells, Modulation Doping

S. Stemmer group (UCSB)

Confined 2DEGs, high mobilities, magnetism



Prediction of topological insulators in simple TMO bilayers

ARTICLE

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

DOI: 10.1038/ncomms1602

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

Di Xiao¹, Wenguang Zhu^{1,2}, Ying Ran³, Naoto Nagaosa^{4,5} & Satoshi Okamoto¹

Rapid Communication

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

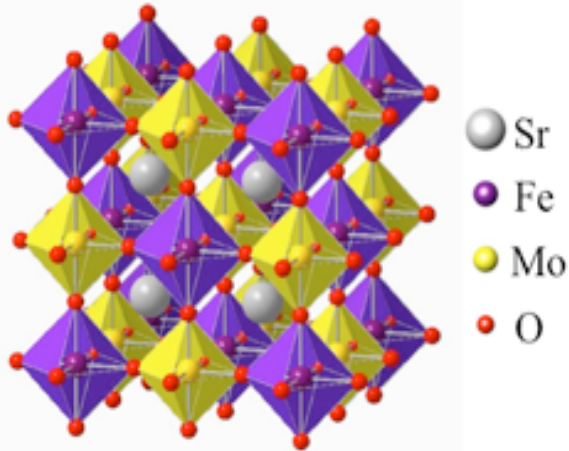
Andreas Rüegg and Gregory A. Fiete

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

Double Perovskites: Mixing correlations and SOC

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

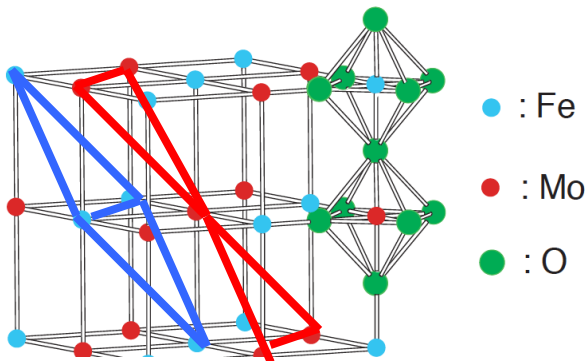
Double perovskite lattice



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, Metallicity**



Layered along [111]

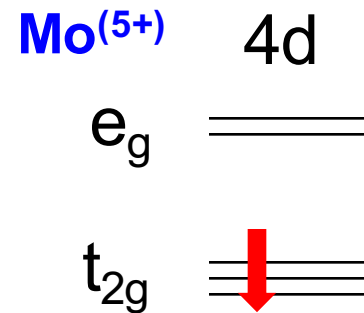
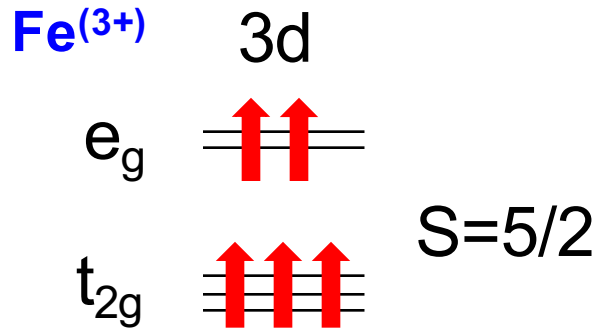
Mott insulators

B=magnetism, B'=inert or magnetism

- . **Well isolated** TM-oxygen octahedra
- . **Frustrated** fcc lattice (eg: Ba_2YReO_6)
- . Unusual spin-orbit coupled liquids?
- . Insulating ferrimagnets (eg: Sr_2CrOsO_6 , $T_C = 725K$)

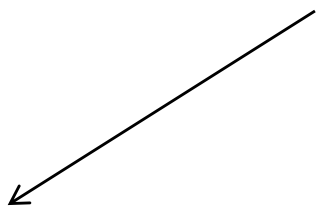
Single atom physics

Nominal valence: $\text{Ba}_2^{(2+)}\text{Fe}^{(3+)}\text{Re}^{(5+)}\text{O}_6^{(2-)}$
 $\text{Sr}_2^{(2+)}\text{Fe}^{(3+)}\text{Mo}^{(5+)}\text{O}_6^{(2-)}$



Hund's coupling > crystal field

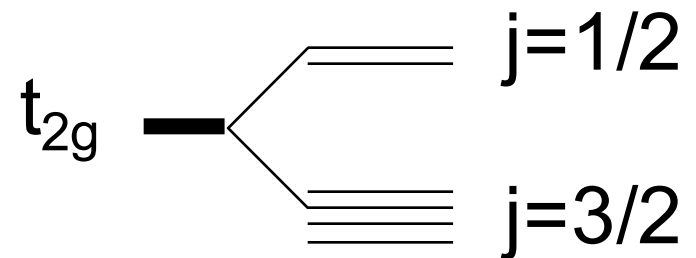
SOC: $\lambda \sim 100\text{meV}$



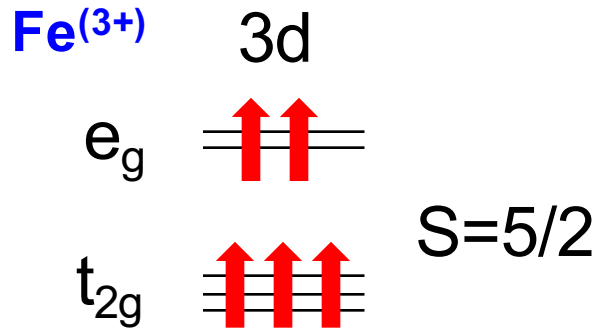
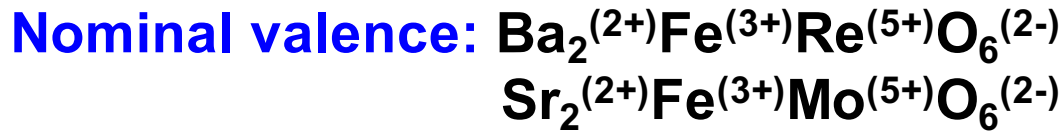
Re: Spin orbit coupling in t_{2g} ($L=1$)

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

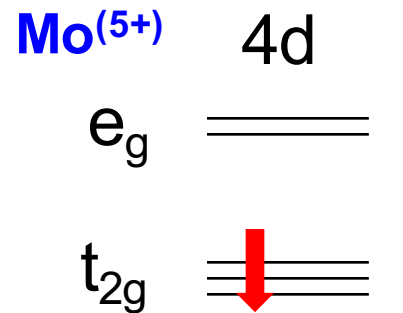
$$H_{\text{s.o.}} = -\lambda \vec{\ell} \cdot \vec{s}$$



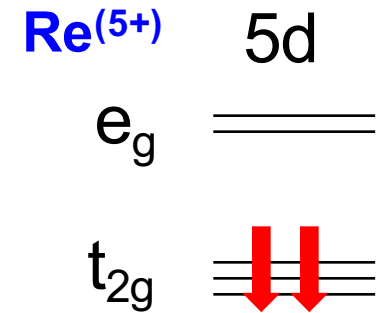
Single atom physics



Hund's coupling > crystal field



SOC: $\lambda \sim 100\text{meV}$



SOC: $\lambda \sim 500\text{meV}$
 Hubbard U
 important

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

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

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

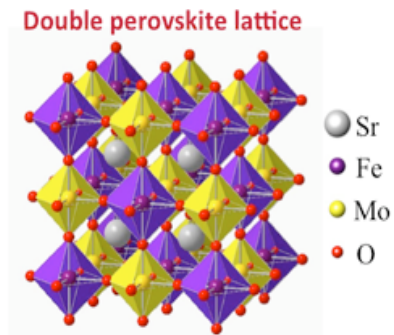
Re: Interactions in t_{2g}

$$H_{\text{int}} = U \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow} + (U - 5 \frac{J_H}{2}) \sum_{\alpha < \beta} n_{\alpha} n_{\beta}$$

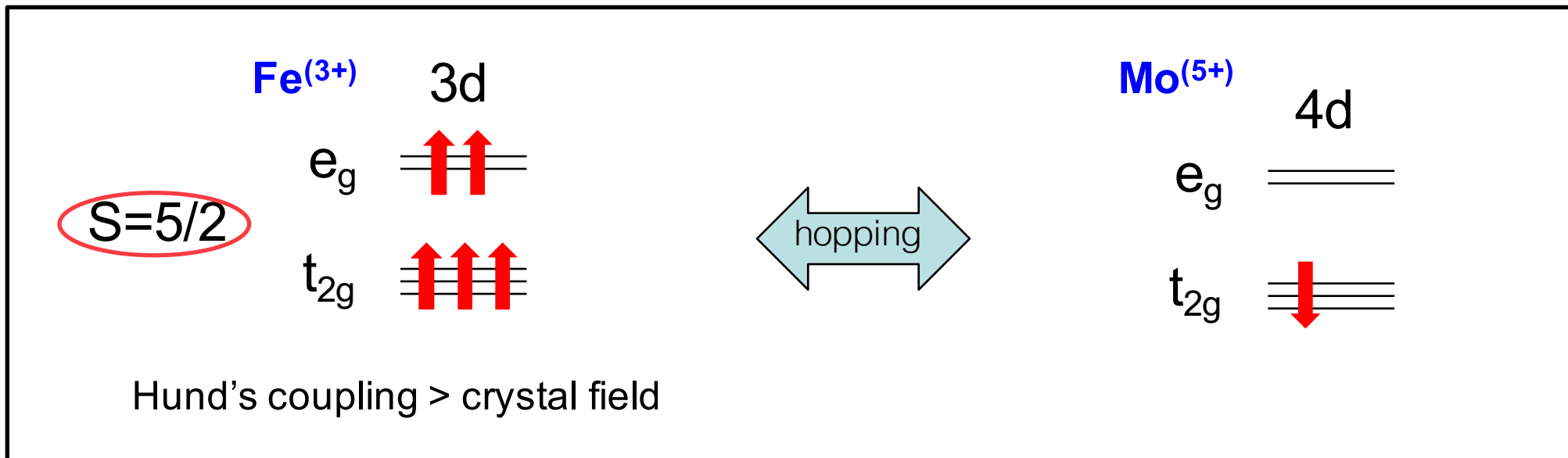
$$-2J_H \sum_{\alpha < \beta} \vec{S}_{\alpha} \cdot \vec{S}_{\beta} + J_H \sum_{\alpha \neq \beta} d_{\alpha\uparrow}^{\dagger} d_{\alpha\downarrow}^{\dagger} d_{\beta\downarrow} d_{\beta\uparrow}$$

(Kanamori)

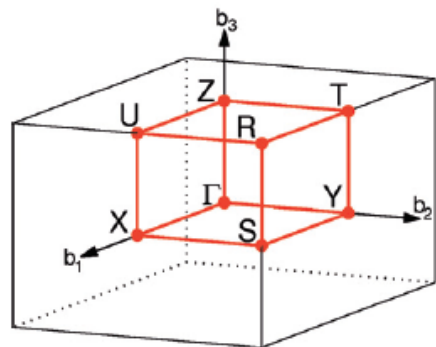
Double perovskites: Itinerant perspective



Origin of half-metallicity



Electronic model for $\text{Ba}_2\text{FeReO}_6$: Hartree theory



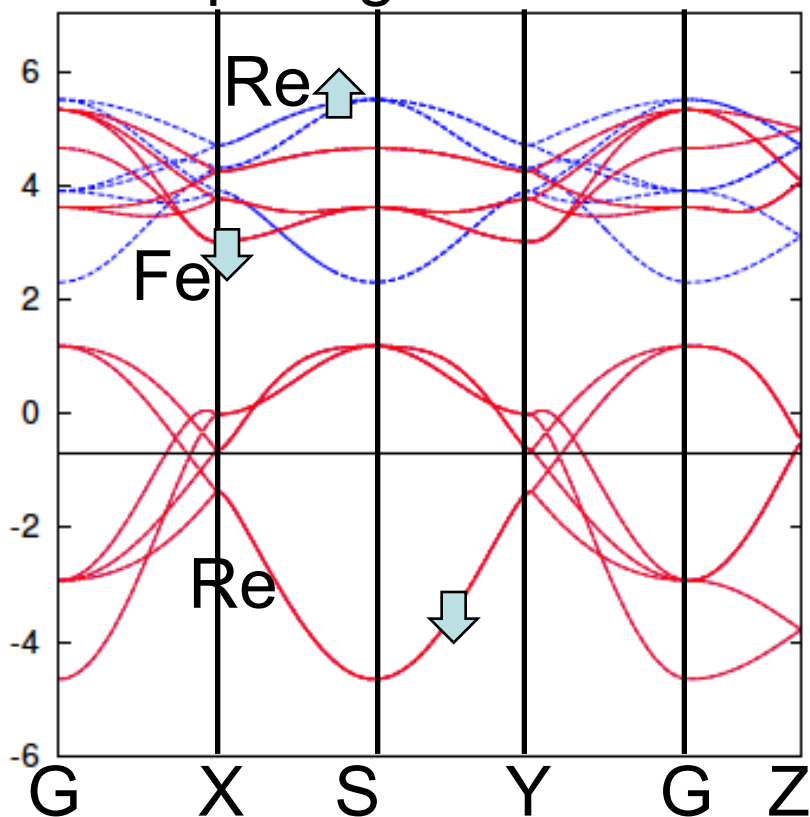
Correlation on Re: Stabilizes half-metallic state

Keep only intra-orbital U

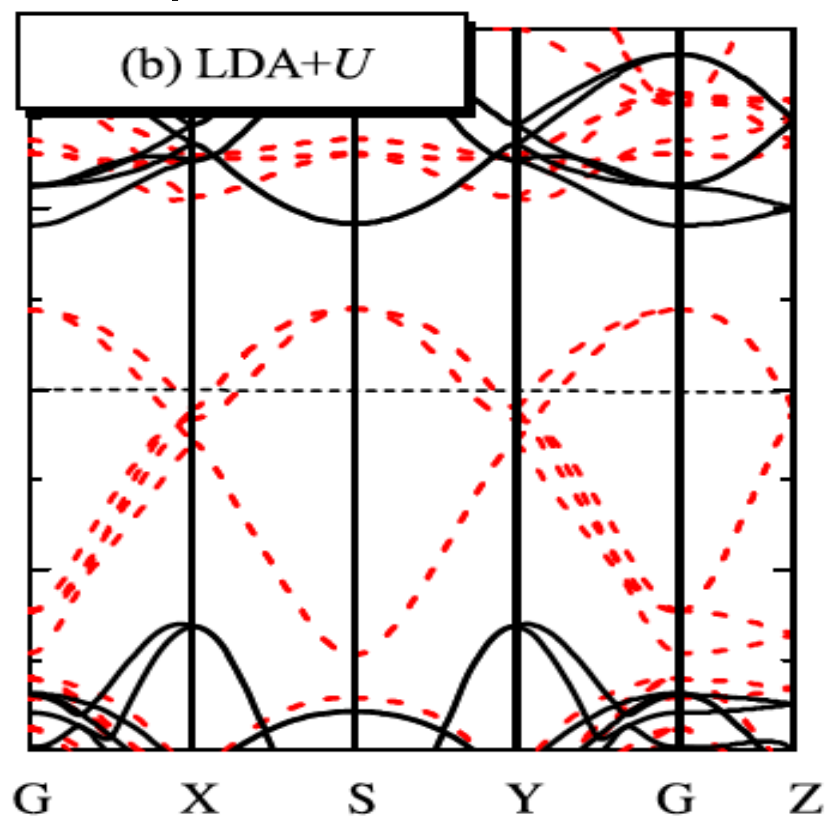
$t_{\text{Fe-Re}} \sim 330 \text{ meV}$, $U \sim 2.5 \text{ eV}$, $\Delta_{\text{CT}} \sim 1 \text{ eV}$

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

Comparing **Hartree-corrected** dispersion with LDA+U



A. Cook, AP (PRB 2013)



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

Incorporating SOC and Hartree Mean Field Interactions

Non-Interacting

$$S_z(\text{Fe}) \sim +2.40 \quad (\text{i.e., } 4.8 \mu_B)$$

$$S_z(\text{Re}) \sim -0.15$$

$$L_z(\text{Re}) \sim -0.09$$

(Recall - L flipped in projecting to t_{2g})

$$\text{Ordered } J(\text{Re}) \sim 0.24$$

With Hartree

$$S_z(\text{Fe}) \sim +2.30 \quad (\text{i.e., } 4.6 \mu_B)$$

$$S_z(\text{Re}) \sim -0.78$$

$$L_z(\text{Re}) \sim -0.48$$

(Recall - L flipped in projecting to t_{2g})

$$\text{Ordered } J(\text{Re}) \sim 1.2$$

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

Comparison with XMCD data

$$\text{Theory: } (\mu_{\text{orb}}/\mu_{\text{spin}}) \sim -0.31$$

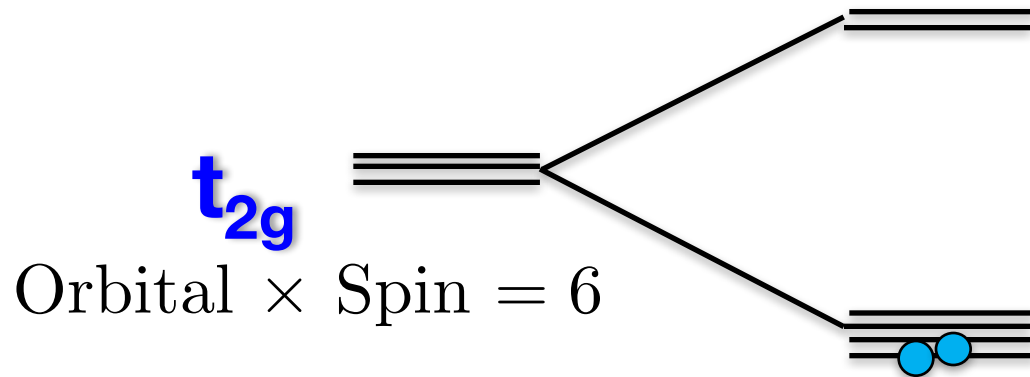
$$\text{XMCD expt: } (\mu_{\text{orb}}/\mu_{\text{spin}}) \sim -0.29$$

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

A. Cook, AP (PRB 2013)

Single atom physics: Hund's coupling and SOC

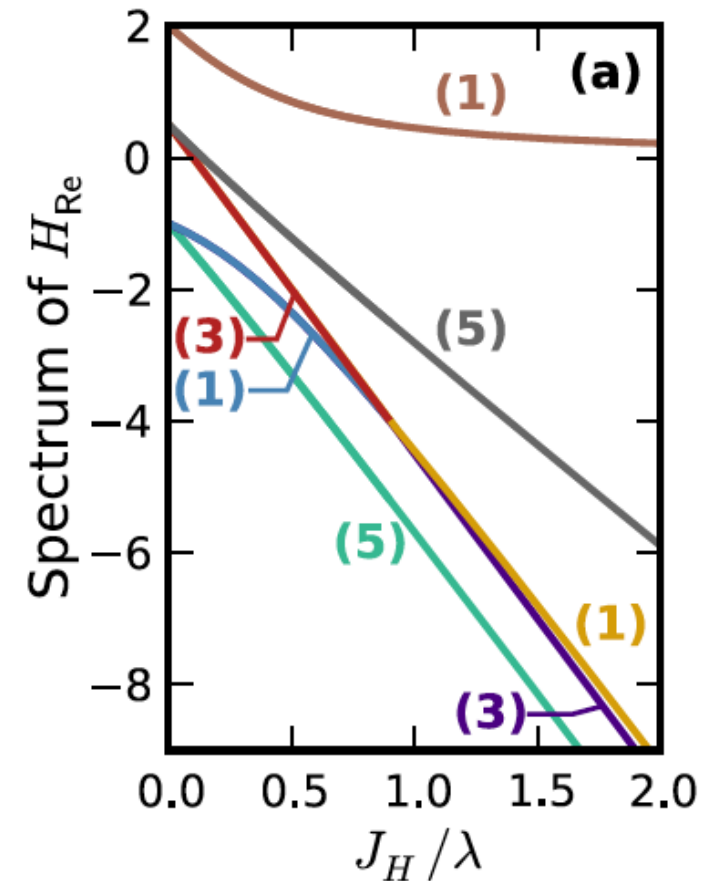
Consider rhenates $5d^2$



Solve “atomic” Kanamori interaction

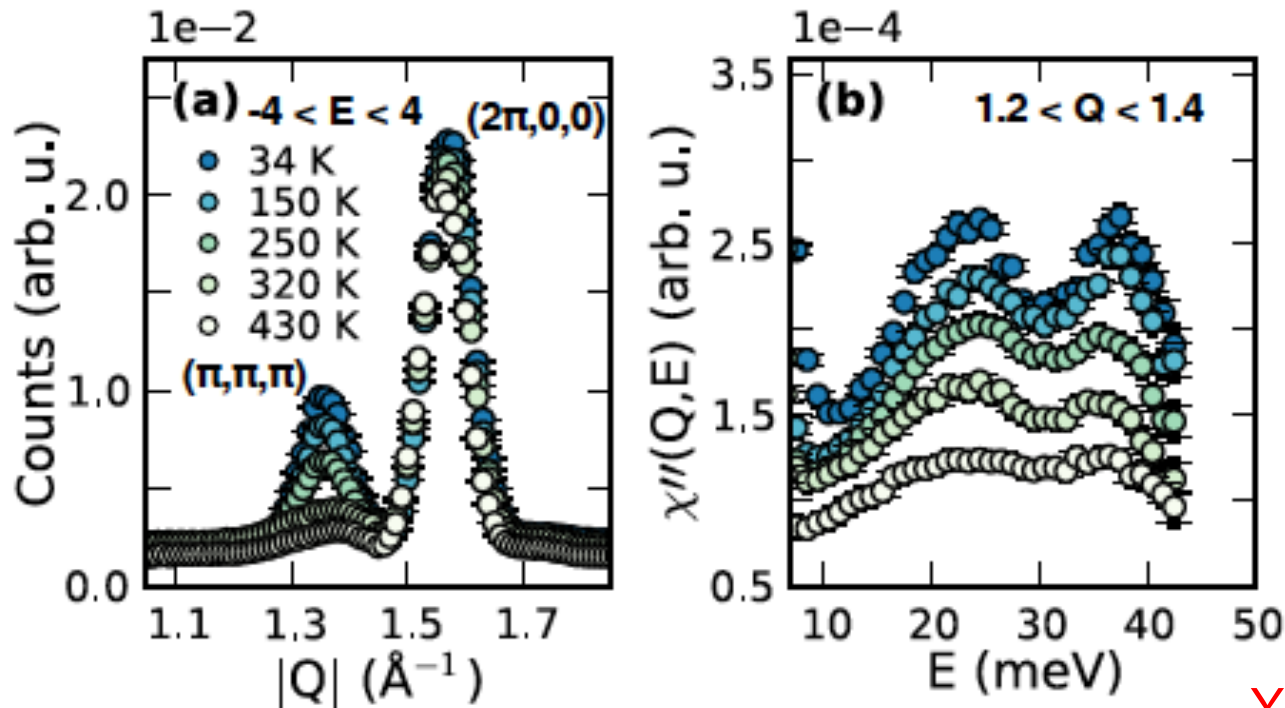
$$H_{\text{int}} = \frac{U - 3J_H}{2} n_{\text{tot}}^2 - 2J_H \vec{S}_{\text{tot}}^2 - \frac{J_H}{2} \vec{L}_{\text{tot}}^2$$

- Weak interactions: Fill up j-manifold
- Strong interactions: Effective $j=2$ “spin”



Magnetic fluctuations in bulk $\text{Ba}_2\text{FeReO}_6$

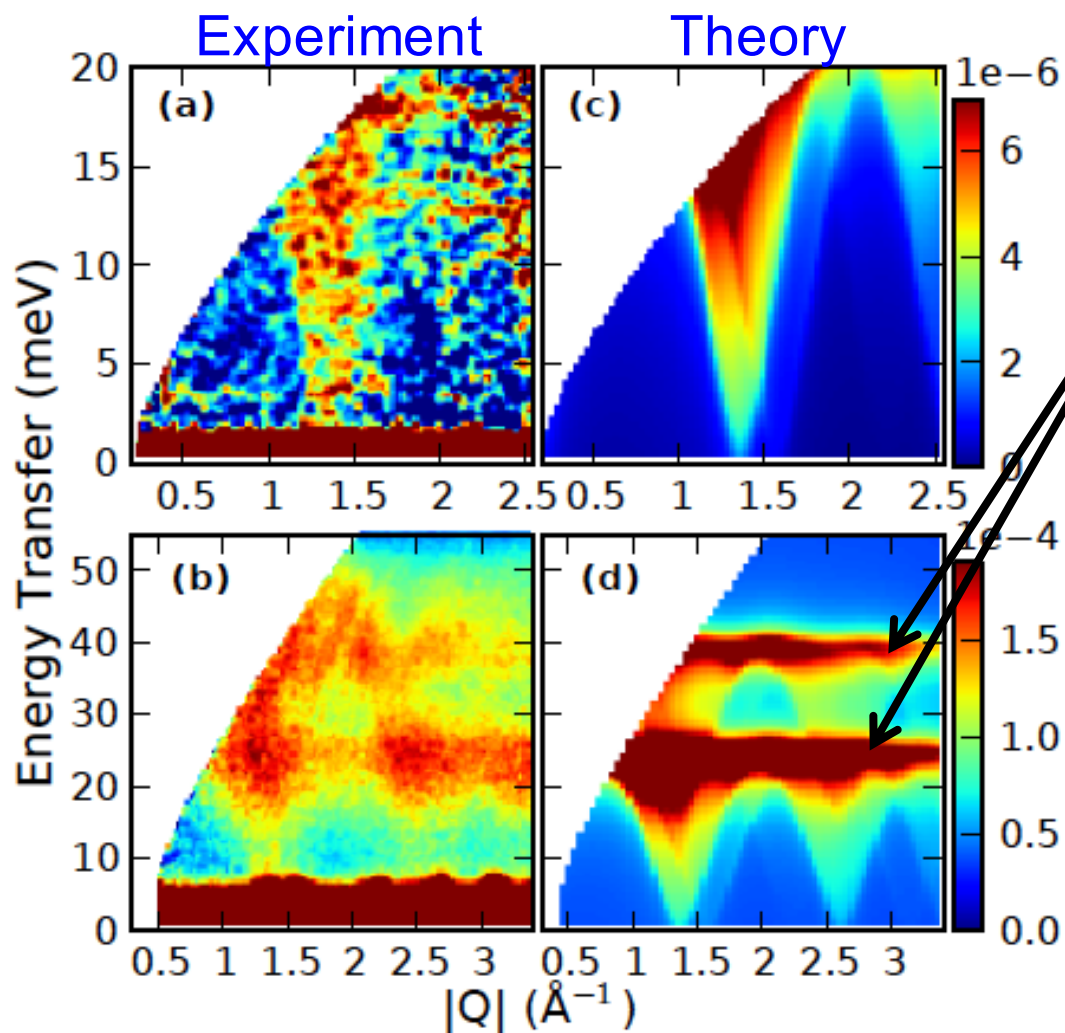
Inelastic neutron spectrum



Y.J. Kim group

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

Magnetic fluctuations in bulk $\text{Ba}_2\text{FeReO}_6$: Local moment perspective



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

Experimental estimate

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

“Mean field” estimate

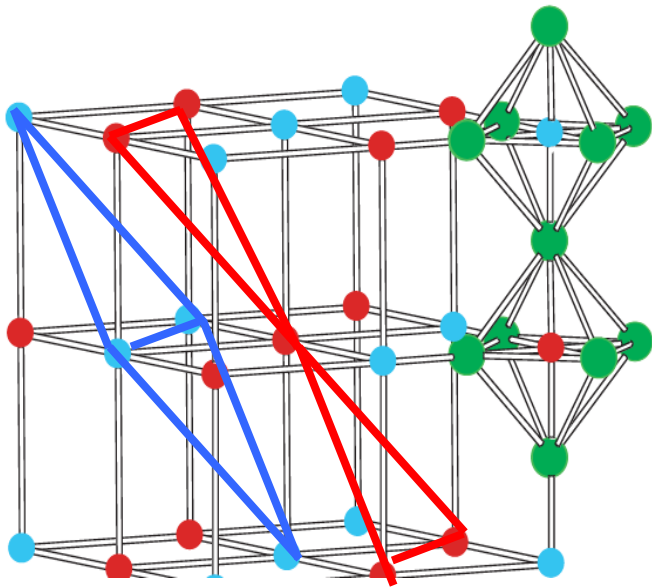
$$\mathcal{F}/\mathcal{R} \approx 1.9$$

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

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

Ultrathin double perovskite films

- What if we dimensionally confine the half-metal to 2D?



Exchange bias in $\text{LaNiO}_3\text{-LaMnO}_3$ superlattices

Marta Gibert^{1*}, Pavlo Zubko¹, Raoul Scherwitzl¹, Jorge Íñiguez² and Jean-Marc Triscone¹

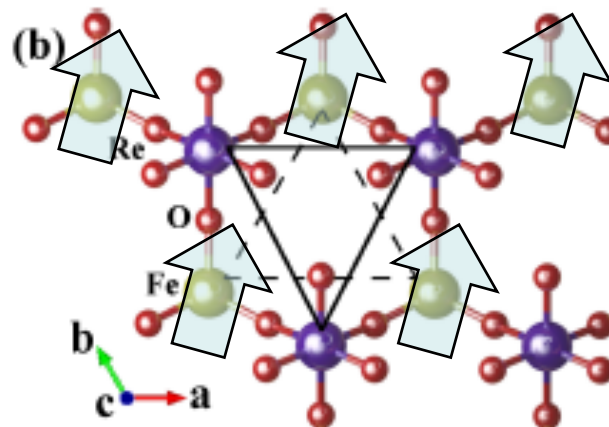
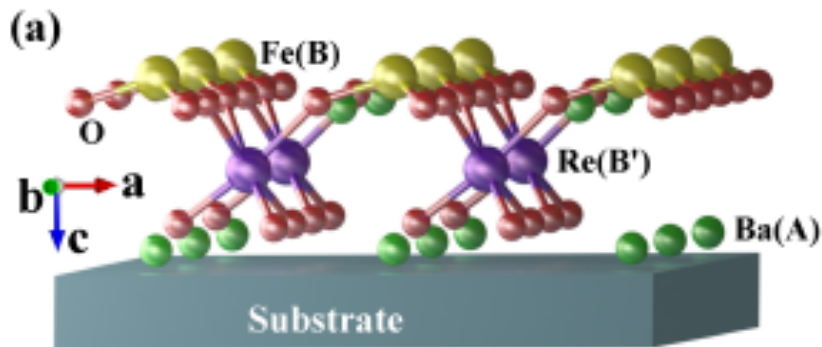


Local electronic and magnetic studies of an artificial $\text{La}_2\text{FeCrO}_6$ double perovskite

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

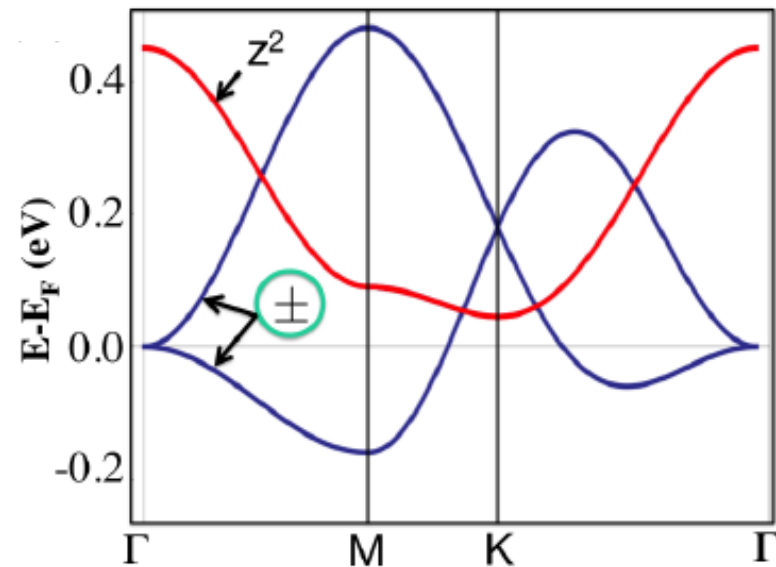
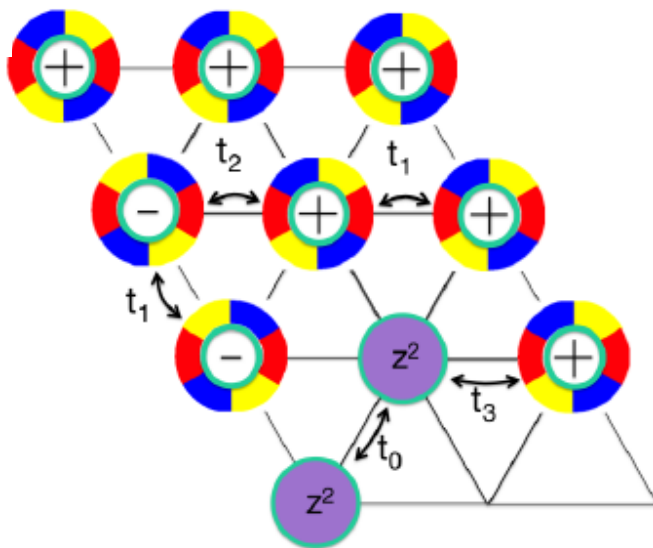
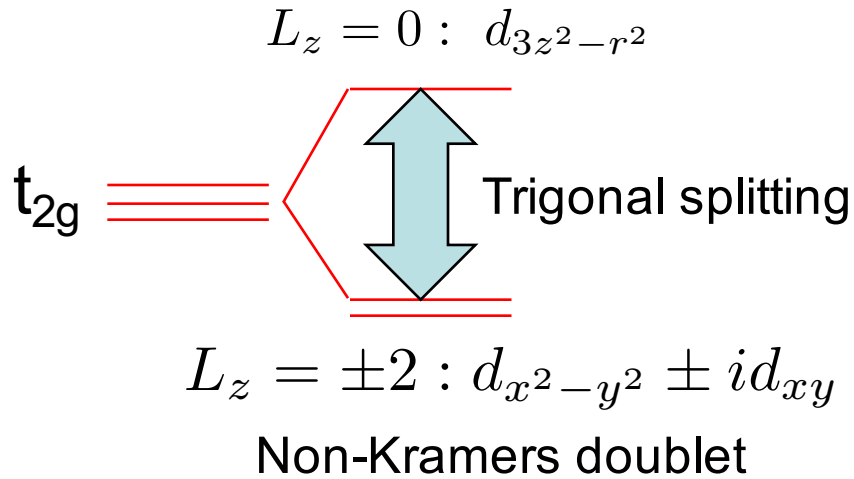
- Bilayer: Buckled honeycomb lattice



Re: Triangular lattice

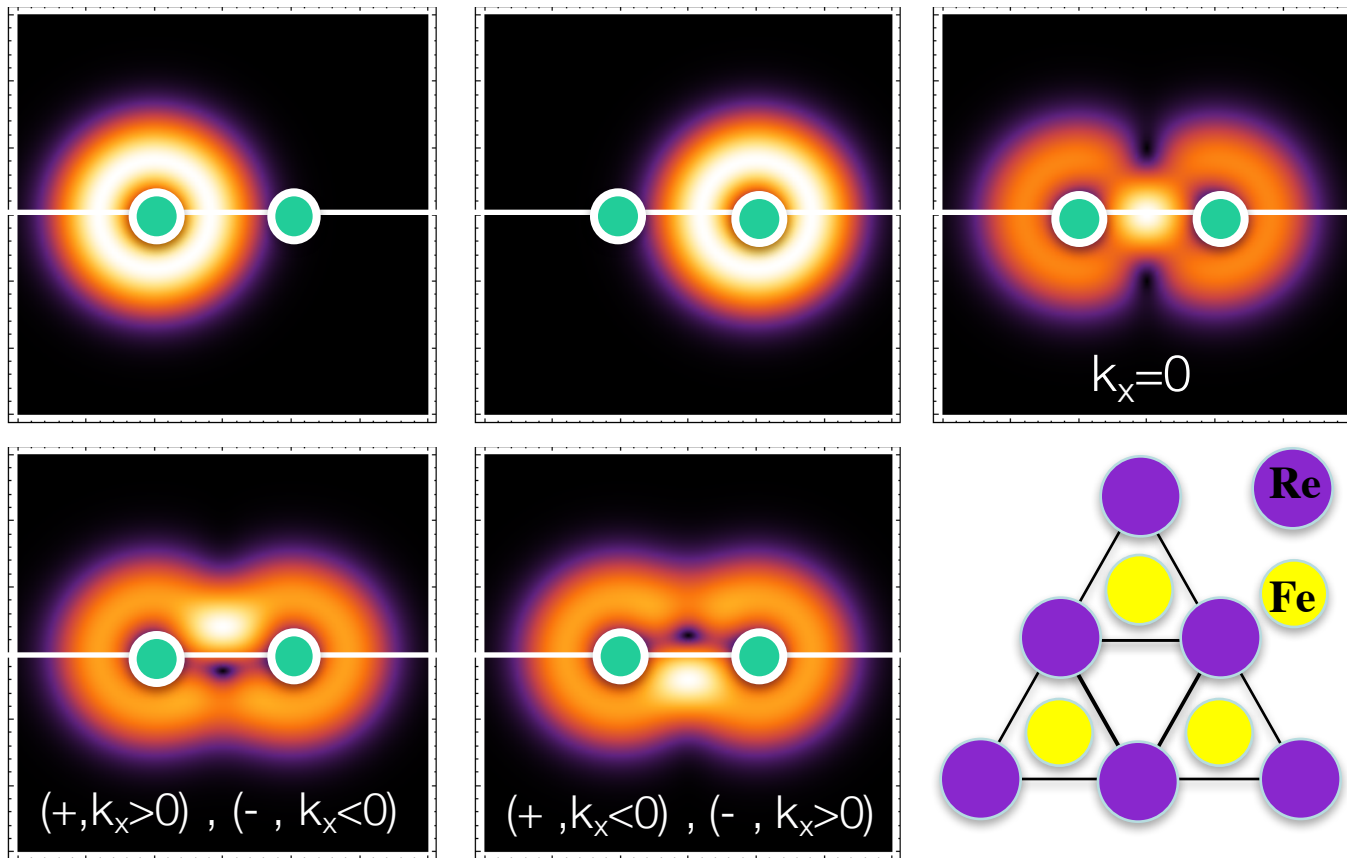
Ultrathin double perovskite films

- Triangular half-metal



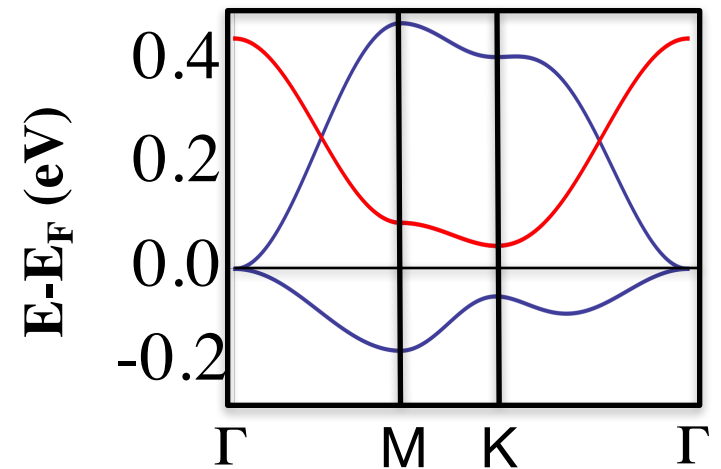
Dirac points at K: Inversion + “Time-reversal”
 Quadratic band touching at Γ : C3 + “Time reversal”

“Orbital Dipoles” and the “Orbital Rashba effect”

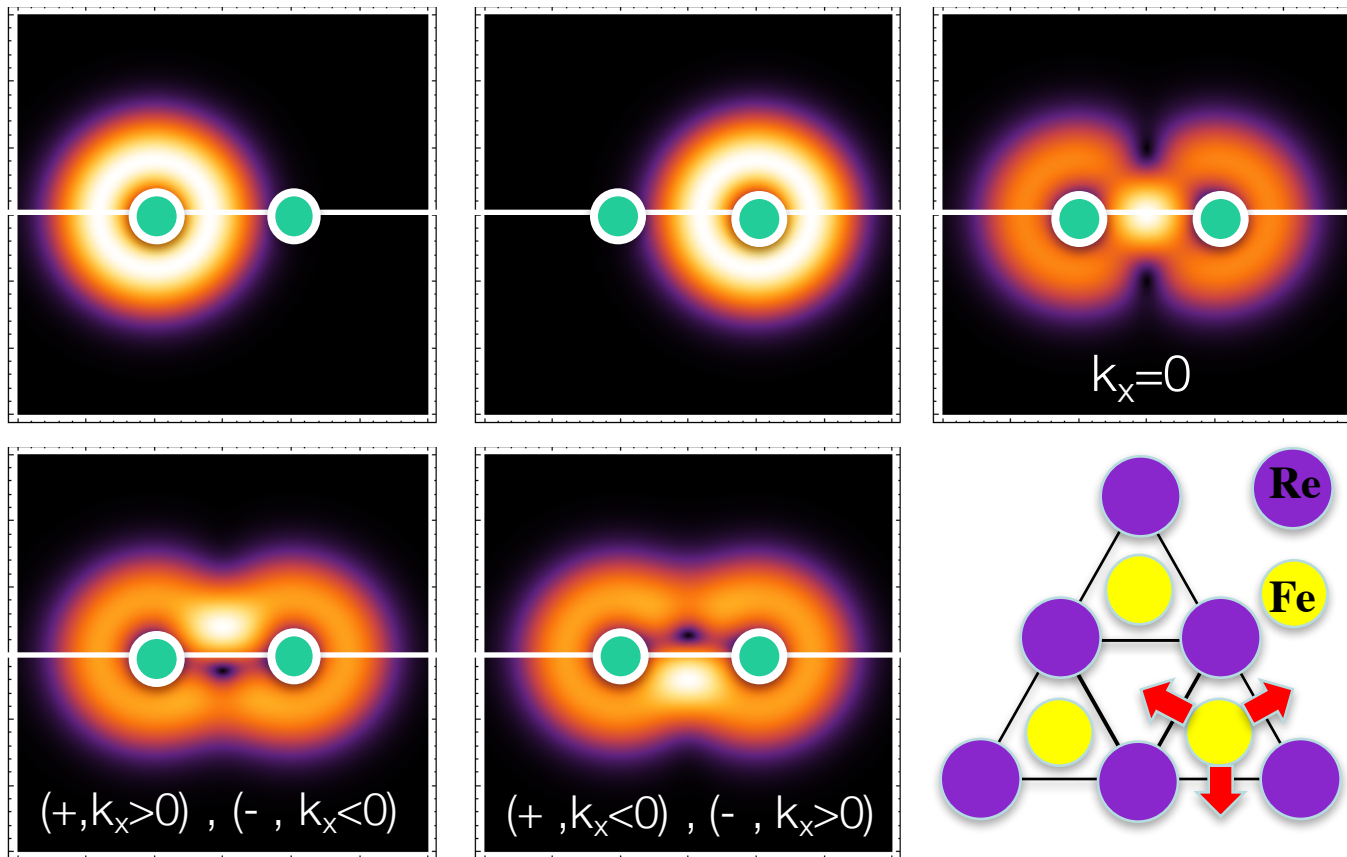


Inversion-symmetry breaking

- “Orbital Rashba” effect gaps out K Dirac point
- Half-semimetal

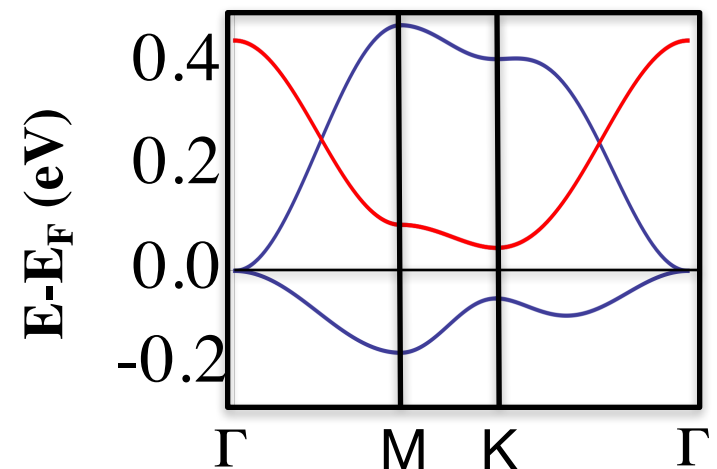


“Orbital Dipoles” and the “Orbital Rashba effect”

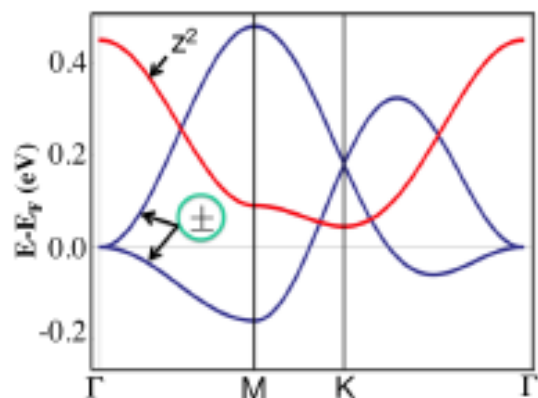


Inversion-symmetry breaking

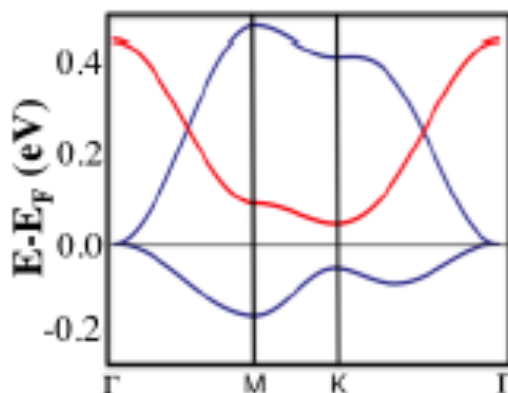
- “Orbital Rashba” effect gaps out K Dirac point
- Half-semimetal



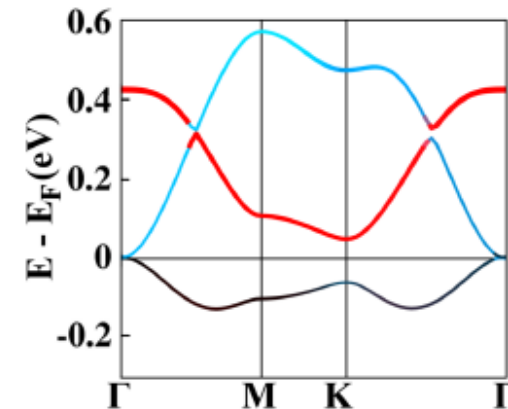
Large gap quantum anomalous Hall insulator



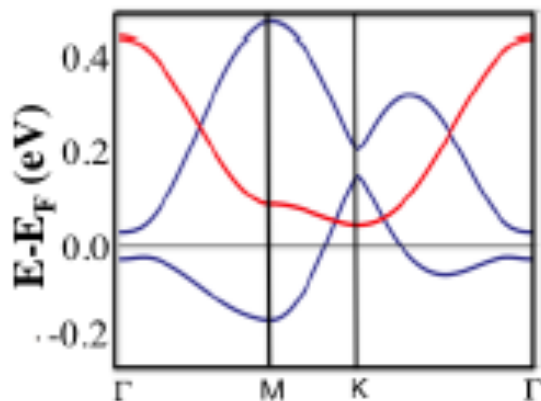
“Orbital Rashba”
→



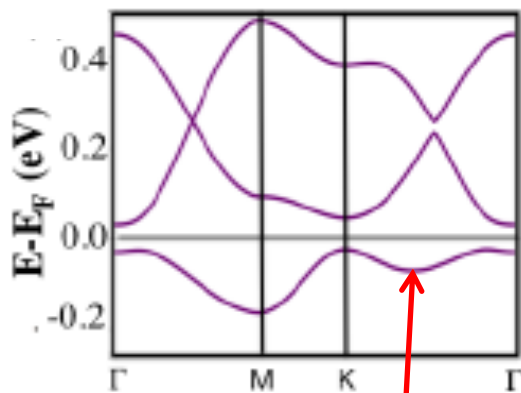
DFT calculations



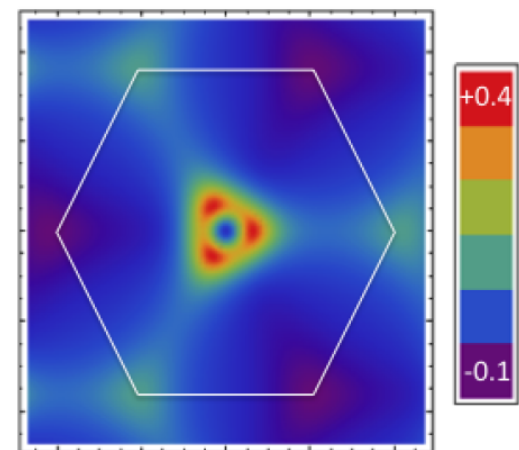
↓ SOC



↓ SOC



Chern band C=1



Berry curvature

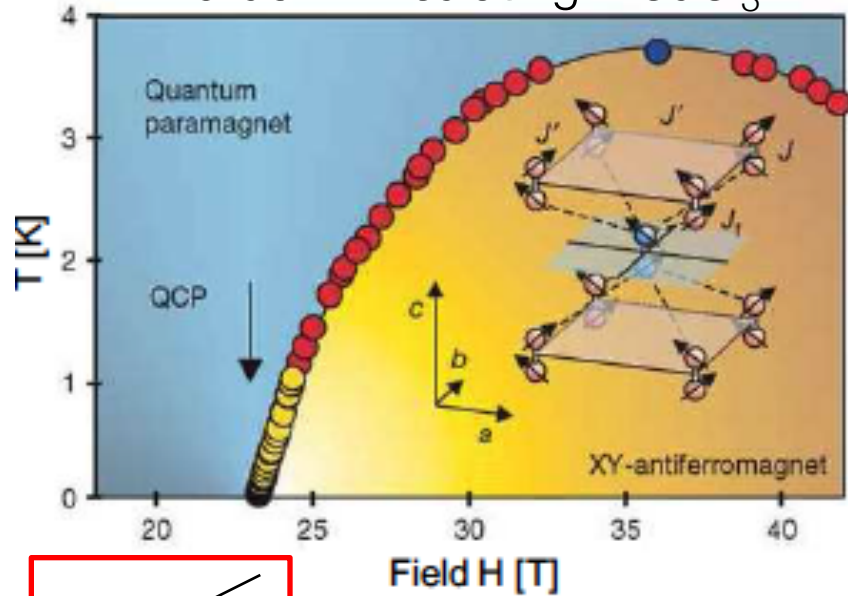
QAH gap ~ 100 meV
 Ferromagnetic $T_c \sim 250-300$ K

Can interactions drive new phases at **topological** critical points?

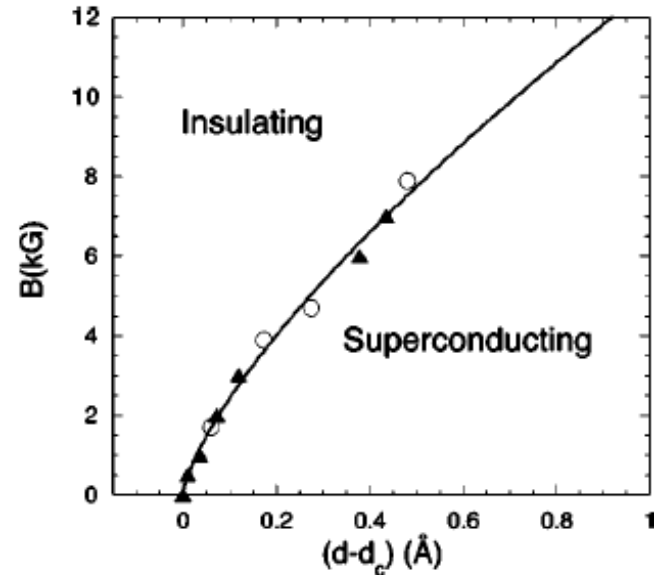
Quantum critical points in “gapped” systems

Quantum phase transitions

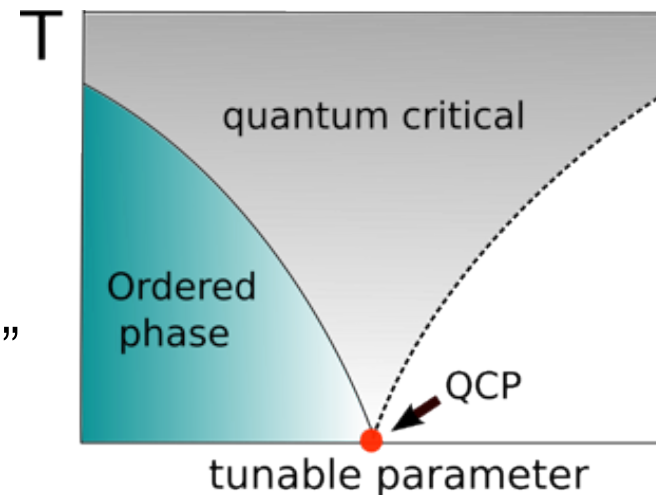
B-field induced magnetic order in insulating TlCuCl_3



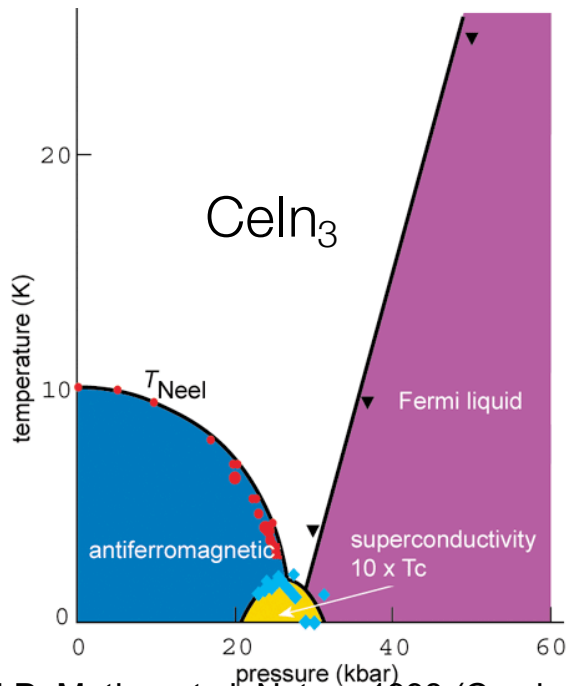
Disorder tuned or B-field tuned Superconductor-insulator transition



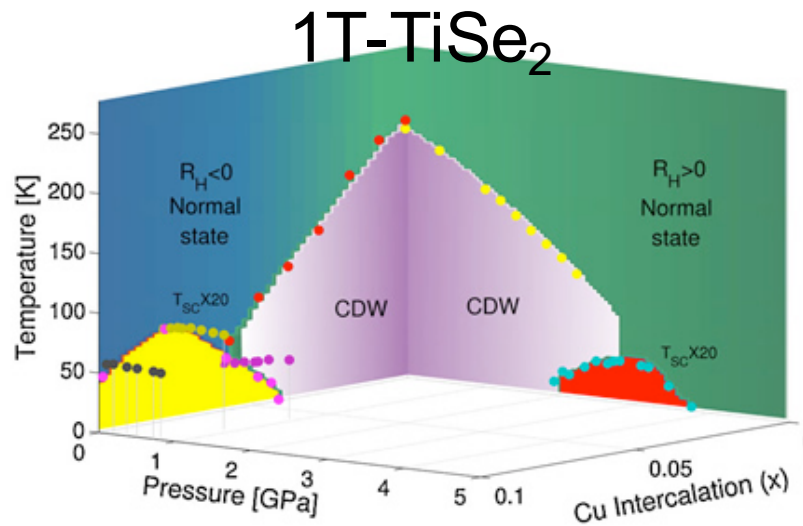
- Sharp change in ground state with tuning parameter at $T=0$
- Finite T crossovers: “critical fan”



Quantum critical points in metals - “emergent” phases



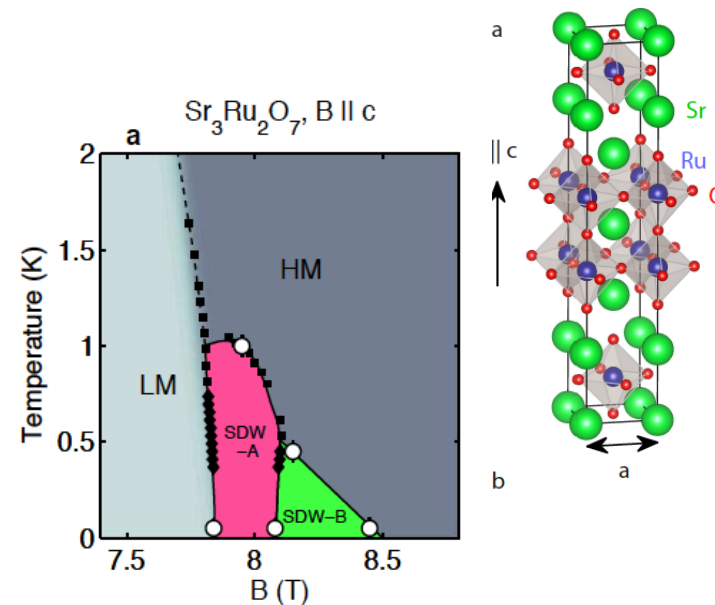
N.D. Mathur et al, Nature 1998 (Cambridge)
+ Grenoble group results



A.F. Kusmartseva, et al, PRL 2009

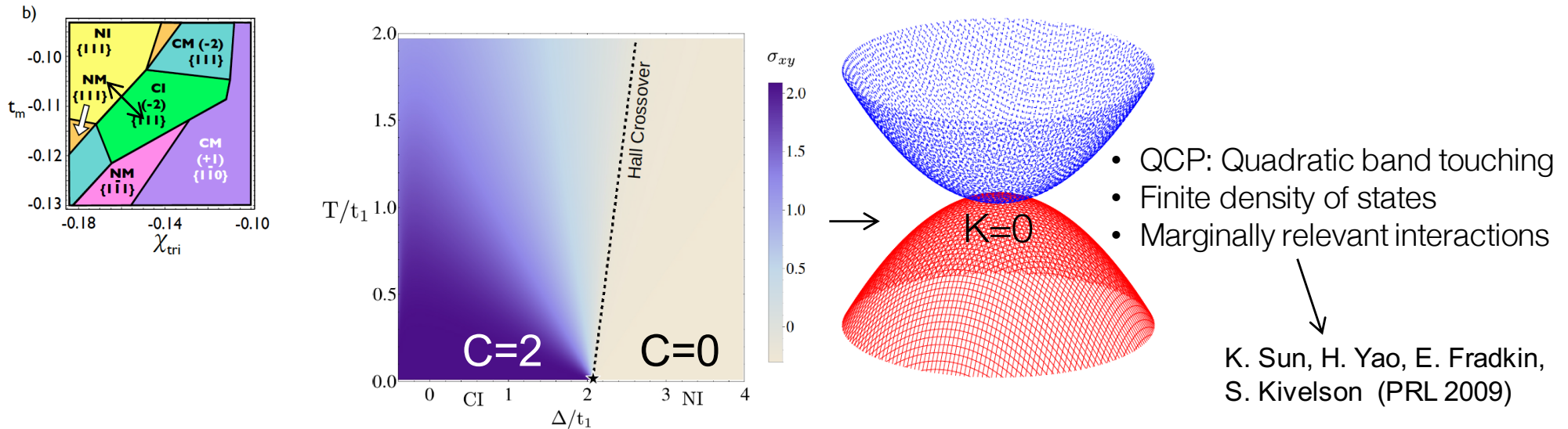
- Critical point involves Fermi surface reconstruction
- General overview: “Hot spots” on the Fermi surface could lead to new instabilities

(Metlitski, Sachdev, 2010; Berg, Metlitski, Sachdev, 2011)



C.Lester, et al, Nat. Mat. 2015

Can interactions drive new phases at **topological** critical points?



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

$$H_\Gamma^{\text{low}} = \left(\begin{array}{cc} \frac{3}{2} (t_2 + t_1) k^2 + r & \frac{3}{4} t_3 (k_x - ik_y)^2 \\ \frac{3}{4} t_3 (k_x + ik_y)^2 & \frac{3}{2} (t_2 - t_1) k^2 - r \end{array} \right)$$

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

RG flow

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

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

- Single “hot spot”
- Single marginally relevant coupling

Chern transition and “emergent” phases

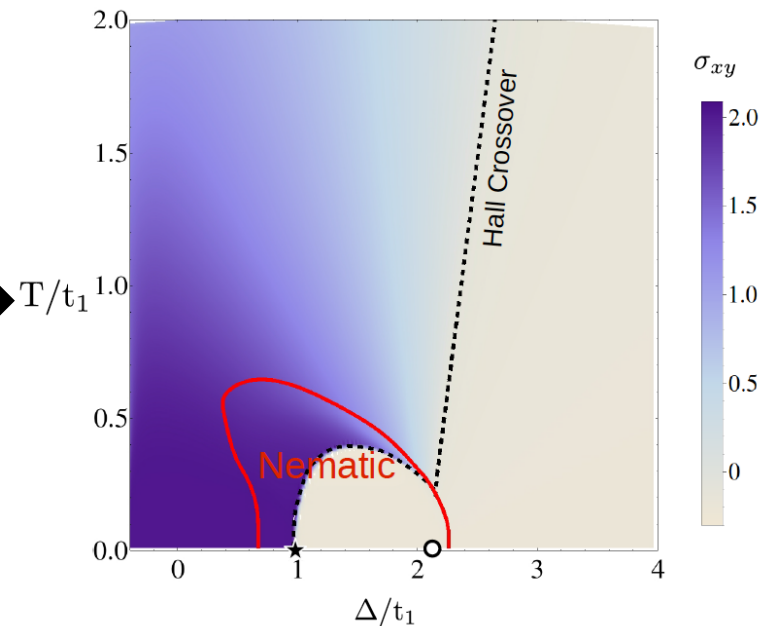
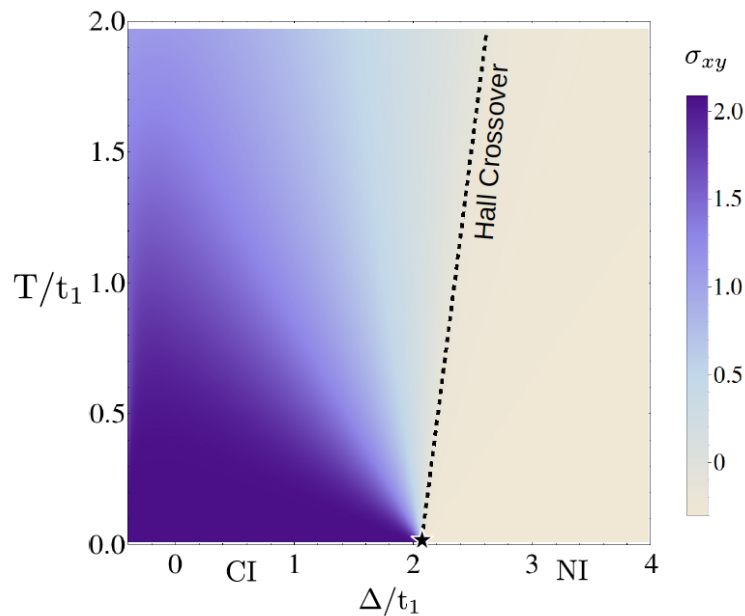
$$\vec{m} = \frac{1}{2N} \sum_{\mathbf{k}} \langle c_{\mathbf{k}\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{\mathbf{k}\beta} \rangle$$

$$H_{\text{mf}}(\mathbf{k}) = \begin{pmatrix} A_{\mathbf{k}} - \mu - U m_z & D_{\mathbf{k}} - U(m_x - i m_y) \\ D_{\mathbf{k}}^* - U(m_x + i m_y) & B_{\mathbf{k}} - \mu + U m_z \end{pmatrix}$$

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

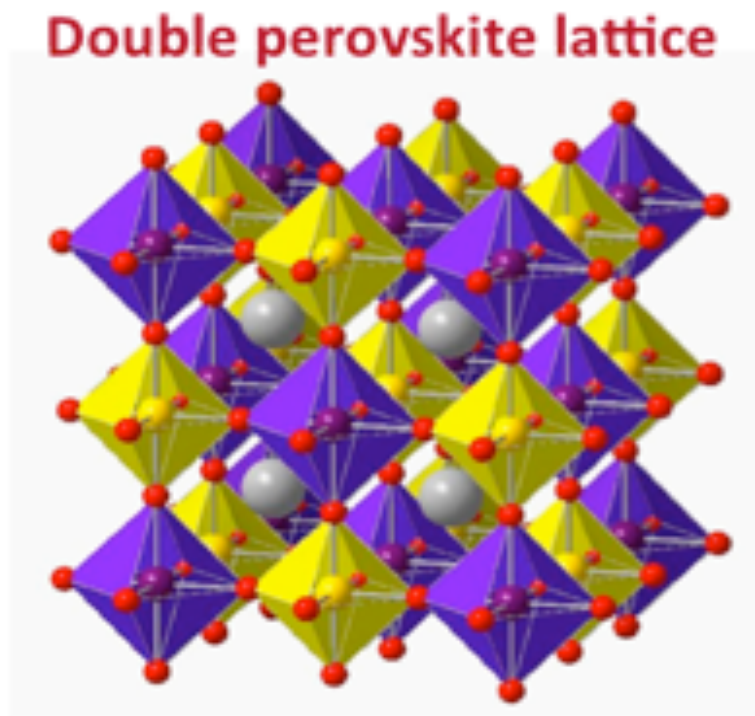
Breaks rotational symmetry
- Emergent “nematic order”

Quadratic band touching point splits into two Dirac nodes



Interactions give rise to an emergent liquid crystal!

Mott insulating double perovskites: FCC lattice iridates



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

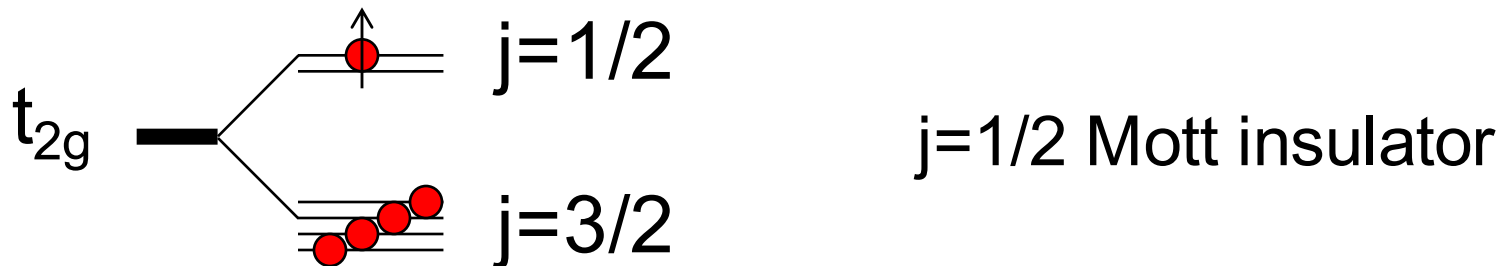
Ba_2YMoO_6 , Sr_2YReO_6 , Sr_2YIrO_6 , $\text{La}_2\text{MgIrO}_6$, ...

Mott insulating double perovskites: FCC lattice iridates

La₂ZnIrO₆ , La₂MgIrO₆ [G. Cao, et al, PRB 2013]

- Insulating DPs, Zn²⁺/Mg²⁺ are nonmagnetic
- Ir⁴⁺ is in 5d⁵ configuration: j=1/2 moment
- 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)



Other well studied examples of j=1/2 Mott insulators

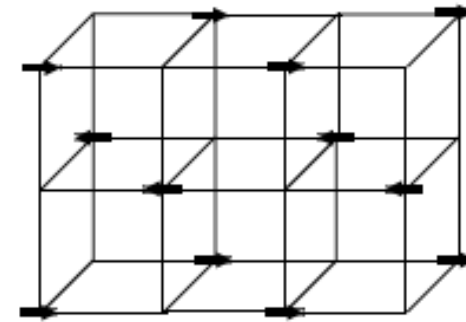
Perovskite, Sr₂IrO₄ - B. J. Kim, et al, Science 2009

Honeycomb, Na₂IrO₃ - Y. Singh and P. Gegenwart PRB 2010 (“**Kitaev material**”)

Opportunity to explore magnetism of SOC moments on the frustrated fcc lattice

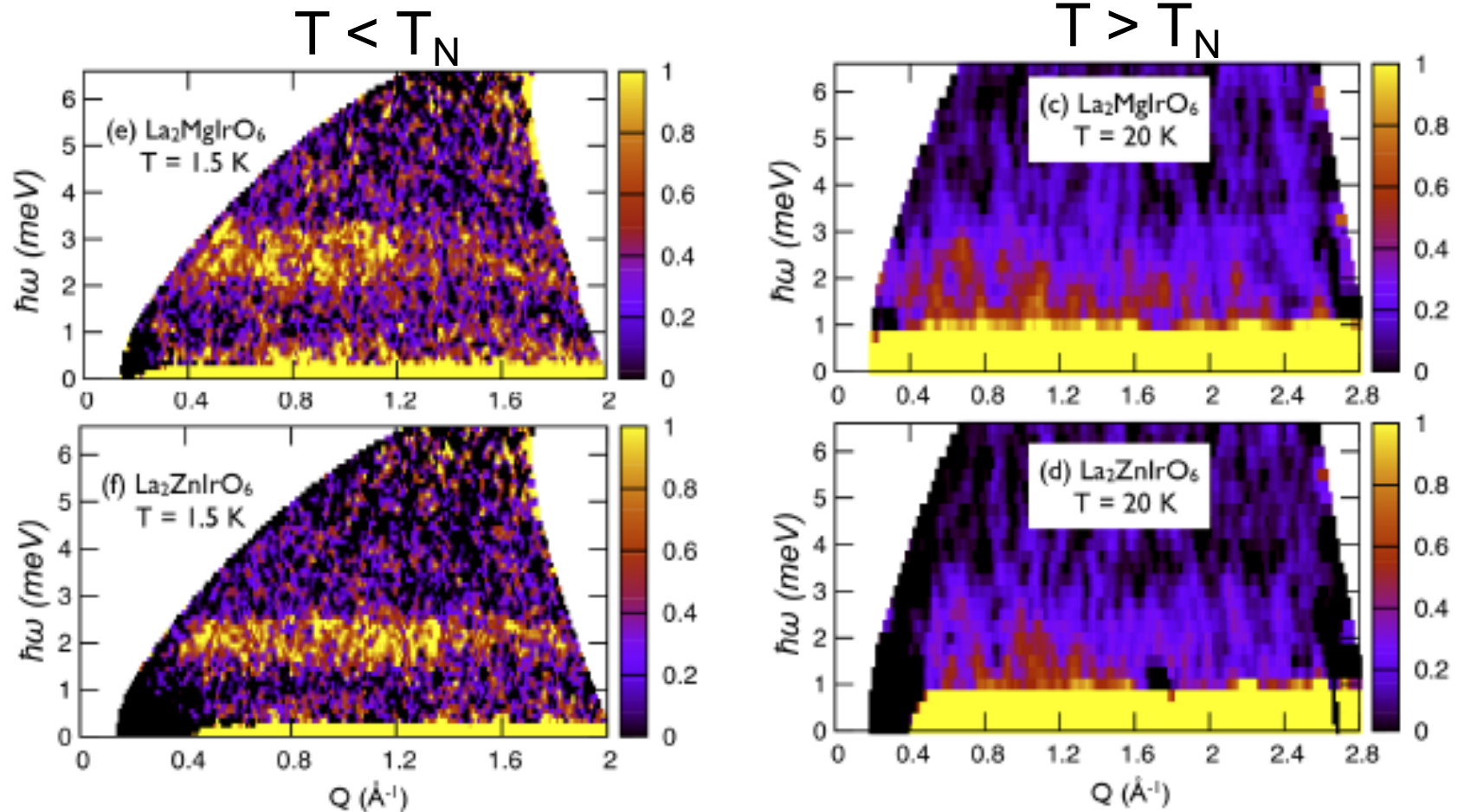
Magnetic order and spin dynamics

Magnetic order: Type I AFM
 $\Theta/T_N < 2$ (weak frustration)



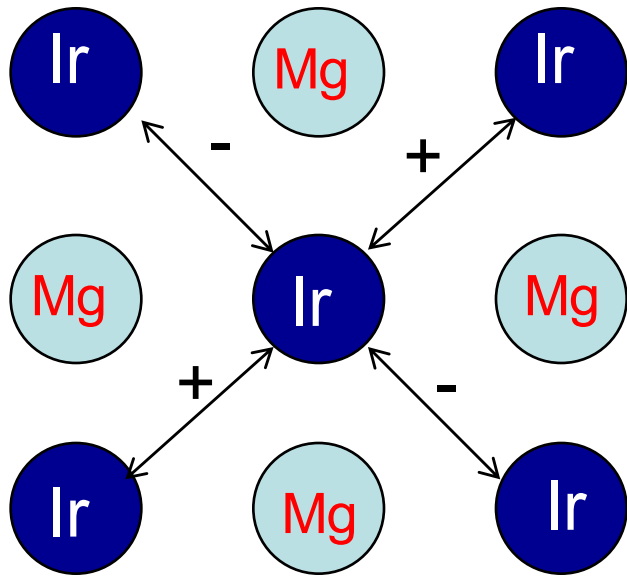
AFM A-II

Inelastic neutron scattering (ORNL)



Band of gapped magnon excitations - Is this just a boring “Ising” model?

Magnetic Hamiltonian: Symmetry analysis of ideal fcc lattice



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

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

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

H. Ishizuka, L. Balents (PRB 2014)

A. Cook, S. Matern, C. Hickey, A. A. Aczel, AP (PRB 2015)

Important conclusion:

Uniaxial Ising interaction forbidden on ideal fcc lattice

2d/3d Honeycomb lattice:
Kitaev model leads to a
quantum spin liquid with
topological order

Kitaev++ models in iridate materials

Honeycomb α - $\text{Na}_2\text{IrO}_3/\text{Li}_2\text{IrO}_3$

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

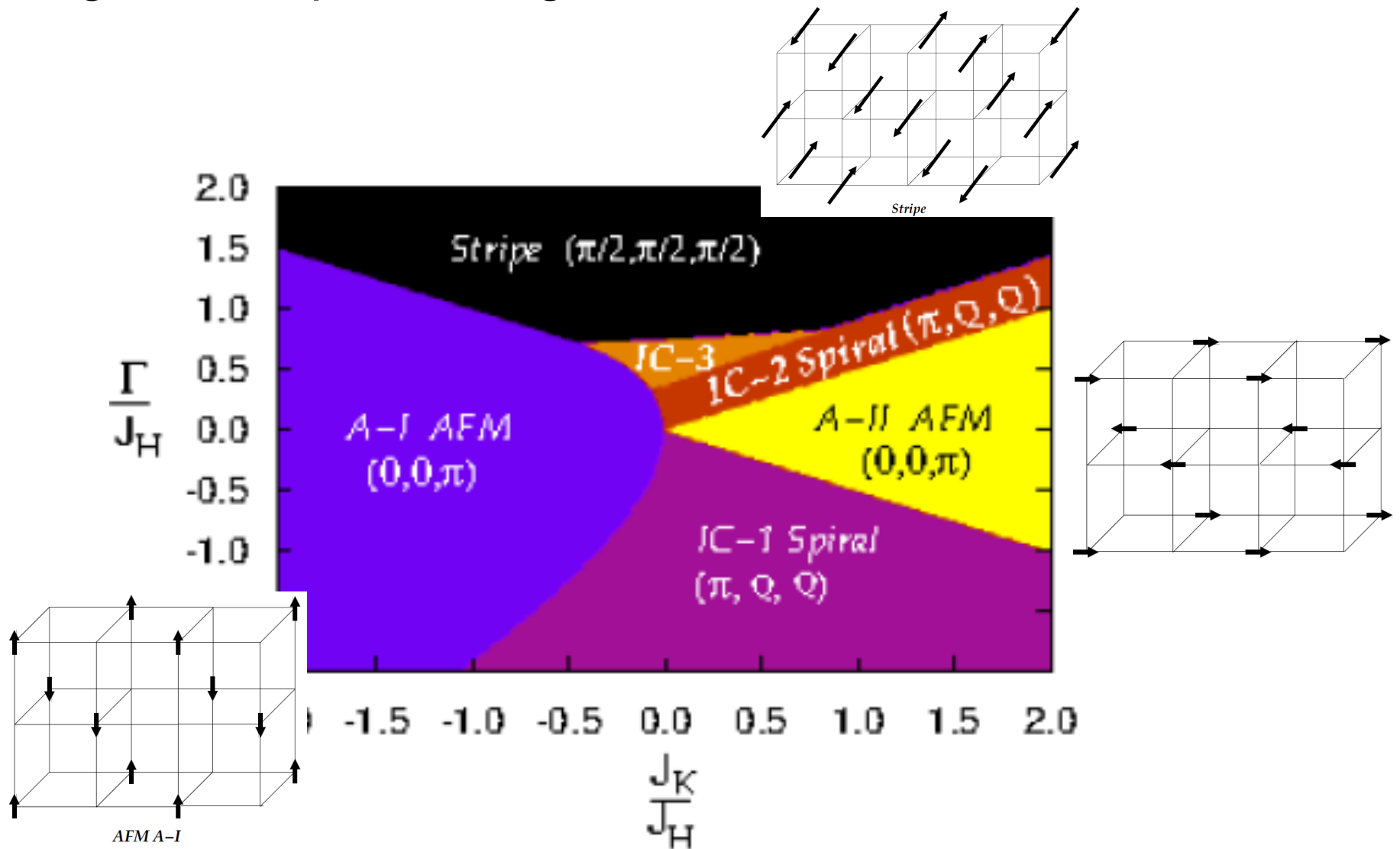
J. Rau, H. Y. Kee (PRL+PRB 2014) – **Beyond Kitaev**

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)

Luttinger-Tisza phase diagram

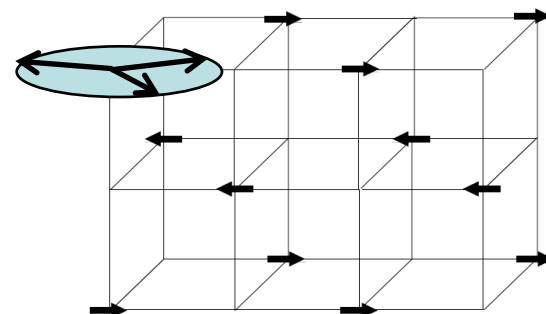


Small frustration parameter and measured order A-II suggests large $J_K > 0$

Spin dynamics

- Minimal Hamiltonian: “Kitaev model”

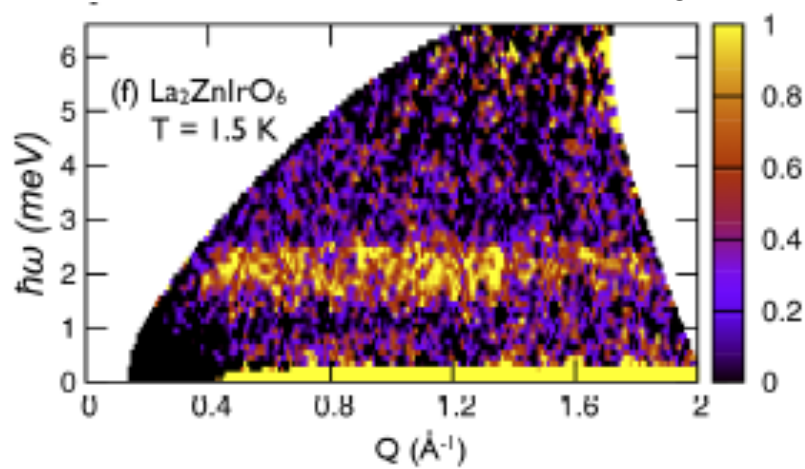
$$H_K = J_K \sum_{\langle \mathbf{r}\mathbf{r}' \rangle_{xy}} S_{\mathbf{r}}^z S_{\mathbf{r}'}^z + J_K \sum_{\langle \mathbf{r}\mathbf{r}' \rangle_{yz}} S_{\mathbf{r}}^x S_{\mathbf{r}'}^x + J_K \sum_{\langle \mathbf{r}\mathbf{r}' \rangle_{xz}} S_{\mathbf{r}}^y S_{\mathbf{r}'}^y$$



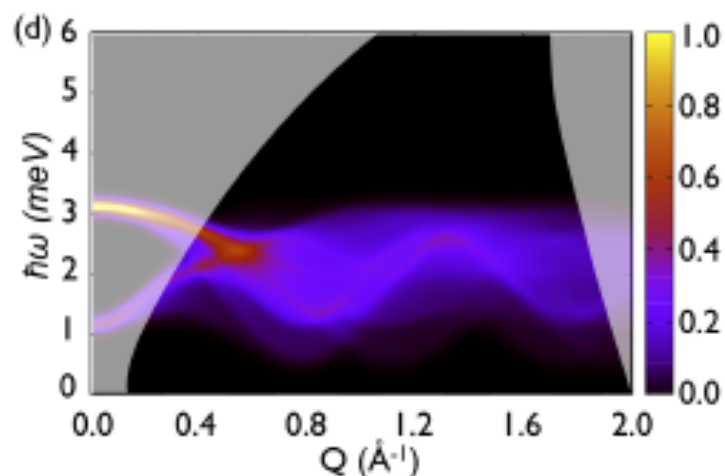
Classically: Spins can point anywhere in XY plane

- Thermodynamic studies: $J_K \sim 24\text{K}$
- Quantum order by disorder:** Pins moments to point along Ir-O bond direction
- Magnon interactions important:** Leads to a gap in the spin wave spectrum
- Incorporate weak second neighbor ferromagnetism

Data for $\text{La}_2\text{ZnIrO}_6$



Theory for $\text{La}_2\text{ZnIrO}_6$



$$J_K \sim +0.7 \text{ meV}; J_2 \sim -0.2 J_K$$

Heterostructures could realize engineered topological 2D Kitaev models

Summary

- 2D/3D double perovskites: $\text{Sr}_2\text{FeMoO}_6$, $\text{Ba}_2\text{FeReO}_6$
 - Topological phases including emergent Chern bands
 - $C=1$ quantum anomalous Hall insulators
- Emergent nematic order at topological quantum critical points
- Mott insulating double perovskites: $\text{La}_2\text{ZnIrO}_6$, $\text{La}_2\text{MgIrO}_6$
 - Spin Hamiltonian with unusual non-Heisenberg interactions
 - Heterostructures might realize 2D Kitaev models: Topological physics?