Title: Searching for topological phases in transition metal oxide heterostructures

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Abstract: In this talk I will present our recent investigations on possible topological phases in (111) heterostructures of transition metal oxide. These (111) heterstructures are promising systems to realize many 2D topological phases at high temperatures, even with strong correlations, which is hard to be achieved in conventional materials.

Several examples will be discussed, including high-temperature quantum spin hall effect in LaAlO3/LaAuO3/LaAlO3 bilayer, correlation induced topological phases in LaAlO3/LaNiO3/LaAlO3 multilayer, nearly flat topological band with C=2 (C: Chern number) in SrIrO3 trilayer, and abelian/nonabelian fractional quantum hall effects in the absence of Landau levels (fractional Chern insulators). If time is allowed, I will also briefly introduce our work on classifying wavefunctions of fractional Chern/topological insulators.

Searching for topological phases in transition metal oxide heterostructures

Ying Ran

Boston College

Perimeter Institute Jan 2013

Acknowledgement

- Oak Ridge National Lab: *Di Xiao, Satoshi Okamoto, Wenguang Zhu*
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- Boston College: *Yuan-Ming Lu (→UC Berkeley), Bing Ye, Kaiyu Yang, Andrej Mesaros, Ziqiang Wang*

Refs: *arXiv:1109.3435, arXiv:1109.1551, arXiv:1109.0226, arXiv:1106.4296*

Introduction: Topological phases of matter

- Traditionally, phases of matter are characterized by Landau-Ginzburg symmetry breaking theory.

Examples:

Crystal (breaking translation symmetry in free space)

Nematics (breaking spatial rotational symmetry)

Magnet (breaking time-reversal symmetry)

Superfluid/superconductor (breaking charge conservation)

.....

- Quantum hall states provide striking counter-examples: they are topological phases of matter.

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Topology (geometry)

- In geometry, objects can be characterized by their topology.

Example: Genus of closed 2D orientable surfaces

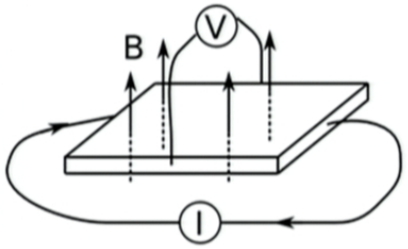
(from Prof. Charles Kane's website)

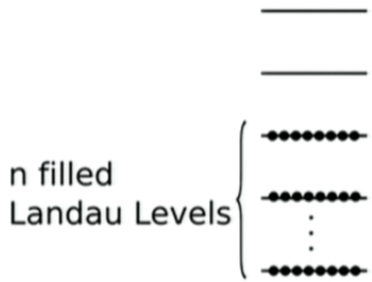
genus is always an integer--- the number of "holes"

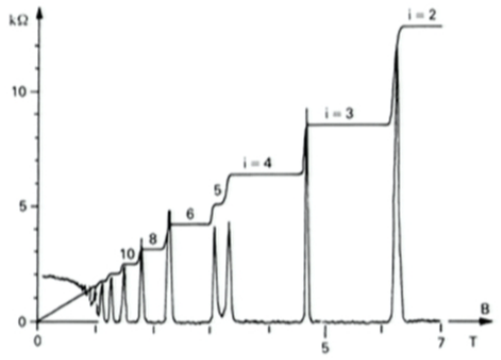
Gauss-Bonnet theorem: $\int_M \text{Curvature} = (2-2g)\cdot 2\pi$

Integer quantum hall effect

- Integer quantum hall Insulators are NOT characterized by symmetry breaking.







Klitzing(1980)

$$\frac{I}{V} = \sigma_{xy} = C \cdot \frac{e^2}{h}$$

(Laughlin 1981)

$$C = 0, \pm 1, \pm 2, \pm 3...$$

C is also an integer, is it some kind of "genus"?

Chern number of a band insulator

- Indeed, IQHE effect can be identified as a topological property of the electronic band structure.

$$\frac{I}{V} = \sigma_{xy} = C \cdot \frac{e^2}{h} \qquad C\text{: TKNN index or Chern number}$$

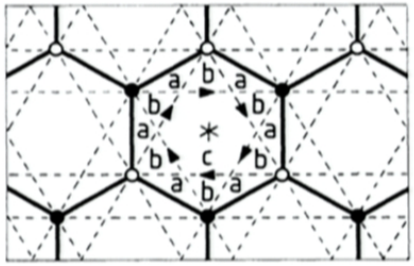
$$2\pi C = \int_{BZ} \mathcal{F}\, dk^2$$

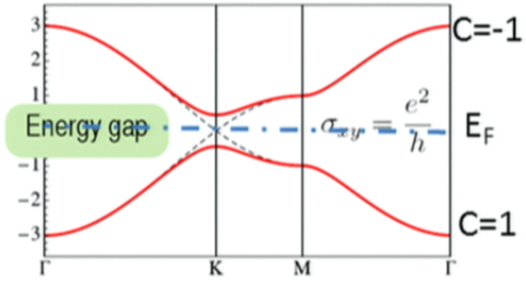
Thouless, Kohmoto, Nightingale, den Nijs (1982)

Berry's curvature of the band structure

- Message: in principle a net external magnetic field is NOT required to realize IQHE
  --- all we need is a band structure involving non-zero Chern numbers

(Called quantum anomalous hall insulators)





Haldane's model
-- spinless fermion
(1988)

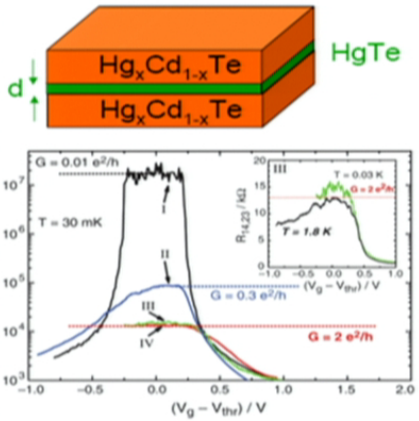
But real electrons have spin....

Topological insulators in 2D and 3D

- A few years ago, time-reversal symmetric topological band structures were theoretically and experimentally identified.

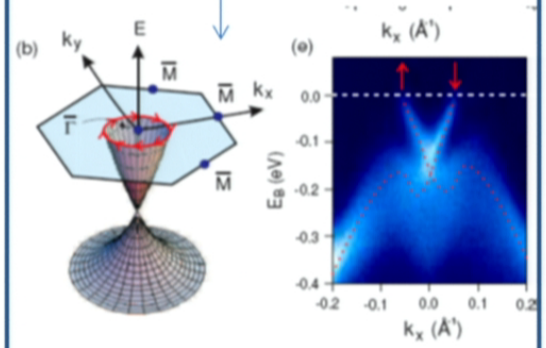
(incomplete: Kane, Mele, Zhang, Bernevig, Molenkamp, Hasan, Fu, Qi, Roy Balents, Moore, Vanderbilt.....)

2D: HgTe quantum well.



Konig et.al. Science 2007

3D: Bi2Se3, Bi2Te3, ...



Hsieh et.al. Nature 2009

Topological insulators in 2D and 3D

- These edge/surface modes can be useful for various purposes. (electric/thermal transports, realizing majorana fermions….)
- Many room-temperature 3D TI materials are found (band gap ~300meV).
- But only ONE 2D TI has been realized with a small band gap (~30meV)

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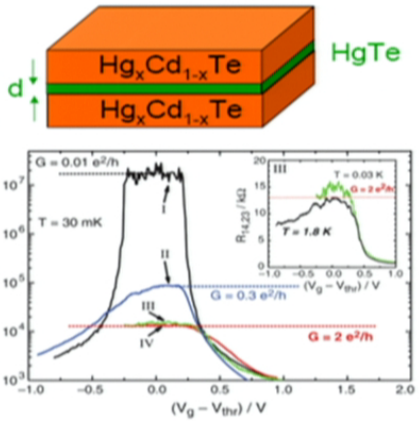

Konig et.al. Science 2007

They have topologically protected edge(surface) metallic modes

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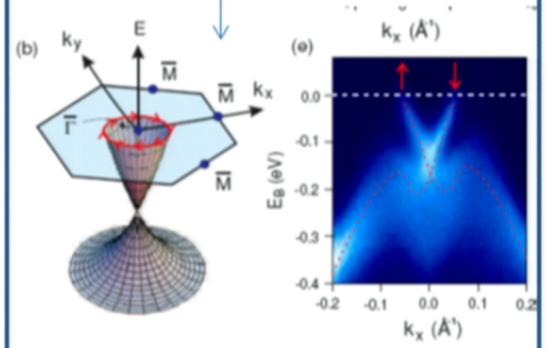

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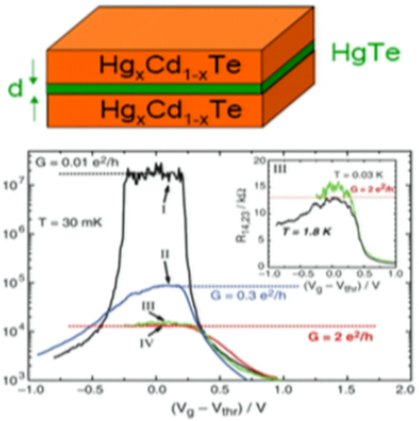

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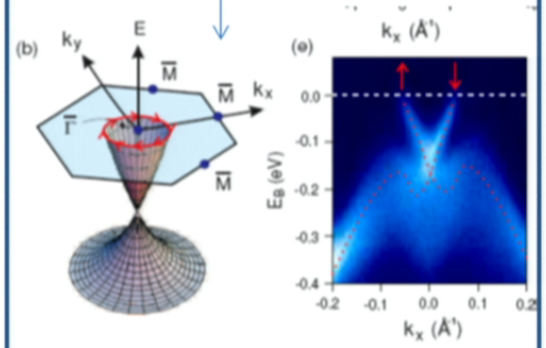

Hsieh et.al. Nature 2009

Topological insulators in 2D and 3D

3D vs. 2D:

- Size of the band gap matters for practical reasons: e.g. detecting new physics experimentally… Larger gap is better.
- However, 2D systems may have a better chance to get a real bulk insulator.

(insulating bulk is crucial for both fundamental science and application purposes)

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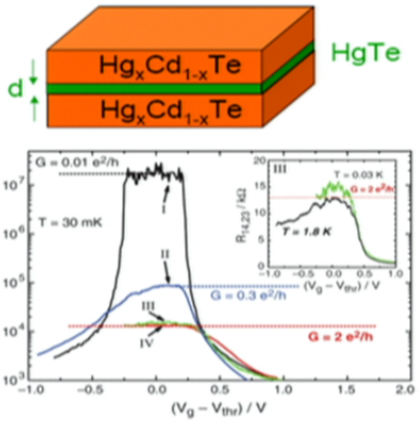

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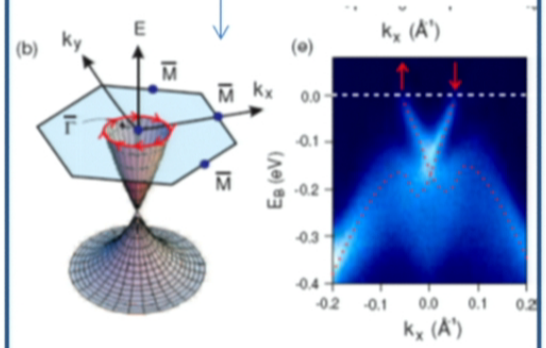

Hsieh et.al. Nature 2009

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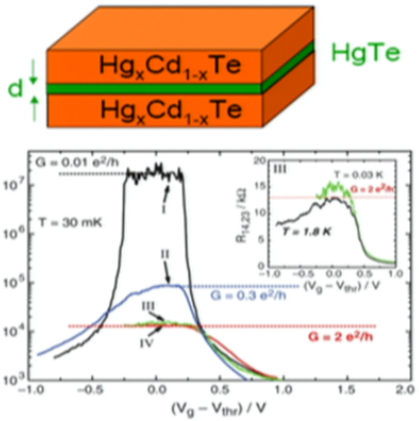

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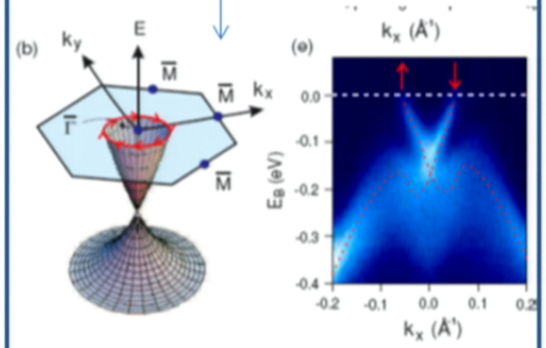

Hsieh et.al. Nature 2009

Can we find more (hopefully high-temperature) 2D TI materials?

What this talk is about:

Certain transition metal oxide heterostructures host:

- room-temperature 2D TI phases.

- And much more than that:

Dirac half-semimetal, quantum anomalous hall insulator, abelian/non-abelian fractional Chern insulators, quantum spin liquids, unconventional superconductivity……

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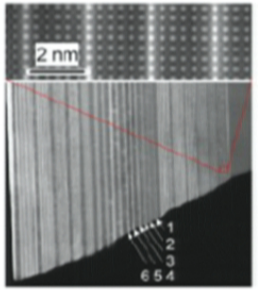
Heterostructures of transition metal oxides

Artificial charge-modulation in atomic-scale perovskite titanate superlattices

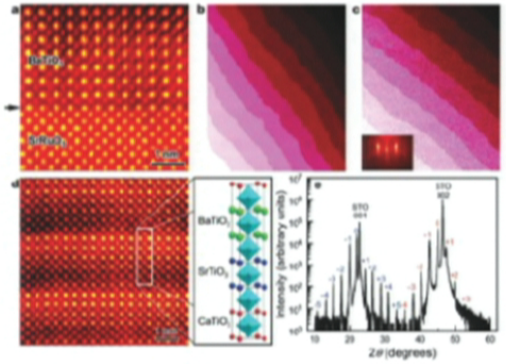
A. Ohtomo, D. A. Muller, J. L. Grazul & H. Y. Hwang



Strong polarization enhancement in asymmetric three-component ferroelectric superlattices

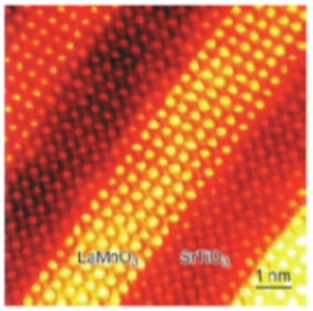
Ho Nyung Lee, Hans M. Christen, Matthew F. Chisholm, Christopher M. Rouleau & Douglas H. Lowndes

Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge,



$[LaMnO_3]_n[SrTiO_3]_m$ superlattice

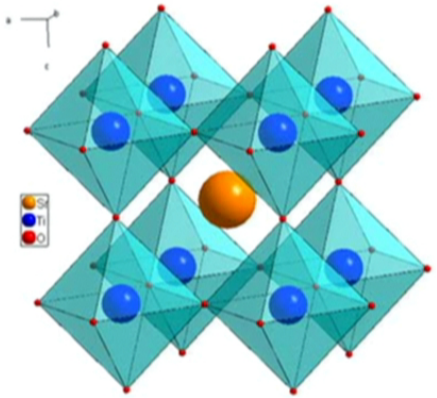
by courtesy of H. N. Lee, ORNL



- Layered structure can be prepared with atomic precision
- Great flexibility: tunable lattice constant, carrier concentration, spin-orbit interaction, correlation strength…
- Correlation physics of d-orbitals: Mott physics, magnetism, superconductivity…

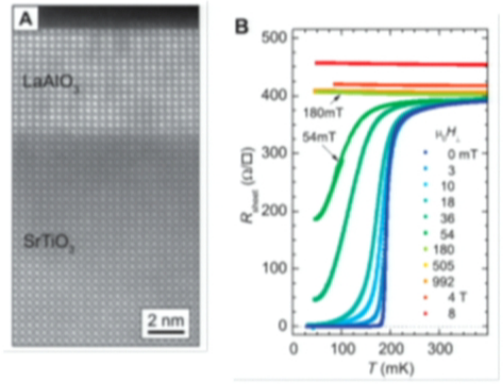
Crystal structure

- Current technology focus on perovskites ABO_3.
- Experimental efforts are mainly on interface/hetero-structures grown along the (001) direction



Perovskite structure of SrTiO3

For example, superconductivity is found on STO/LAO interface



Reyren et al, Science 2007

- So far possible topological phases have not been investigated in TMOH experimentally.
- This is partially because the current efforts are on (001) direction. (square lattice---large fermi surface…)
- I will show that, heterostructures grown along the (111) direction are particularly interesting for topological phases of matter.

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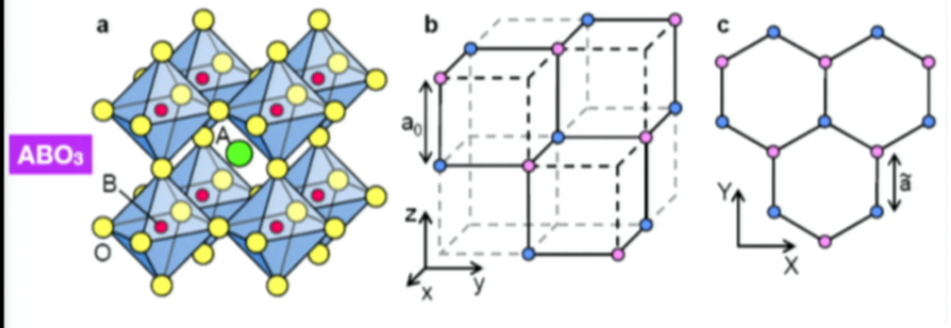
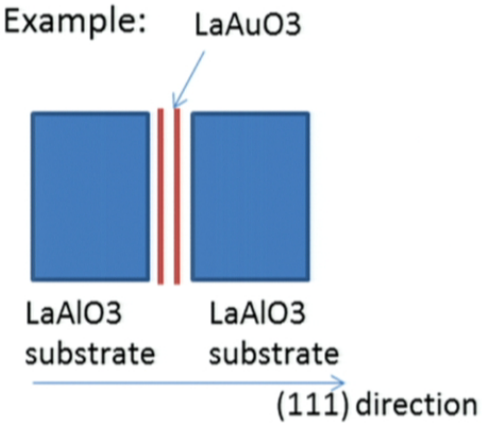
Perovskite (111)-bilayer





- Honeycomb lattice. (Similar physics to graphene? Maybe even "correlated versions" of graphene ?)
- Reduced crystal field symmetry: Octahedral to **Trigonal.**
- Sublattices on different layers: Inversion symmetry breaking can be externally controlled (i.e., gating or asymmetric substrates)

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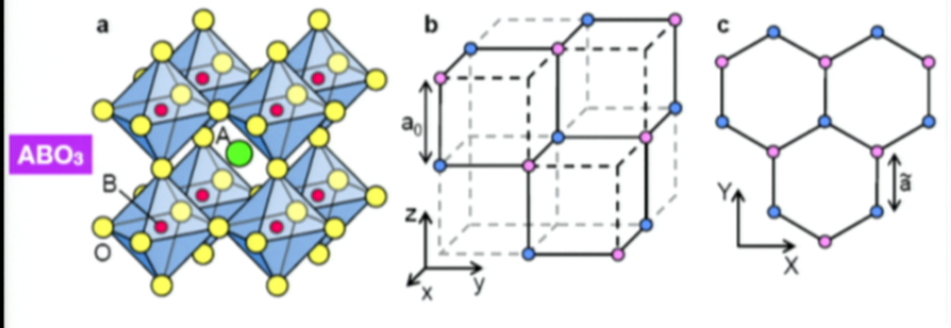

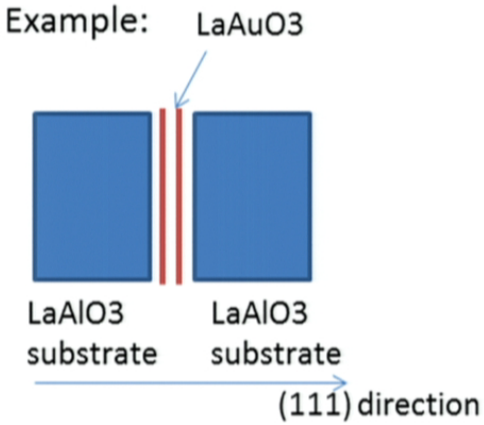

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I will talk about several examples:

- e_g active materials:

  (1)LaAuO3 bilayer

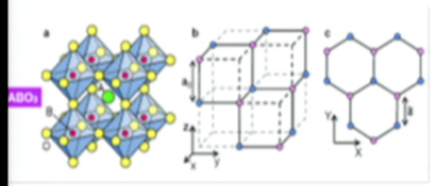
  (2)RNiO3 bilayer (R: rare earth)

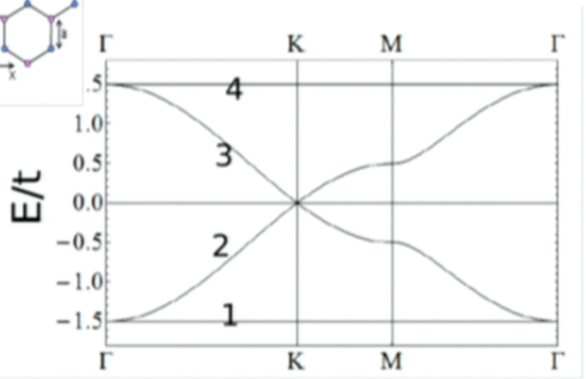
- t_{2g} active materials:

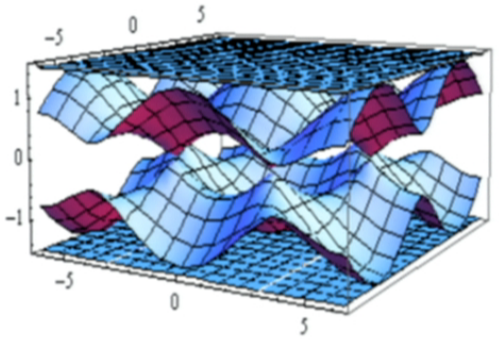
  (3)SrIrO3 bilayer

e_g tight-binding analysis (without SO)

- Consider e_g orbital active systems. If we only include NN ddσ hopping, a single-parameter-bandstructure is obtained:







Interestingly, similar to graphene+2 flat bands.

The exact flatness of these bands are consequence of the NN model. Further neighbor hoppings destroy the exact flatness.

Spin-orbit coupling in e_g orbitals

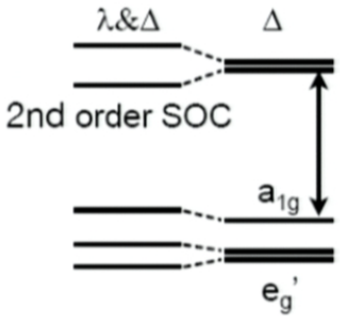
- At the leading order, spin-orbit coupling in e_g vanishes:

$$\lambda \vec{L} \cdot \vec{S}$$

But in d-orbital basis, *L* in e_g is quenched.

$$\vec{L} \sim \left(\begin{array}{c|c} e_g & \\ \hline & t_{2g} \end{array}\right) = \left(\begin{array}{c|c} 0 & \\ \hline & \end{array}\right)_{5\times5}$$

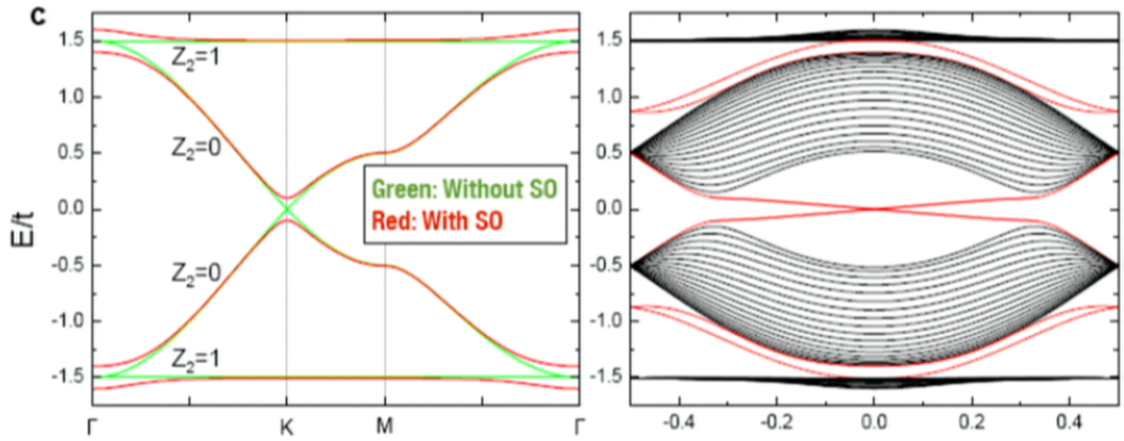
- 2nd order perturbation ➡ non-zero spin-orbit coupling in e_g.



$$H_{\mathrm{SO}}^{lm} = \lambda^2 \sum_{\tau \notin e_g} \frac{\langle l|\vec{L}\cdot\vec{s}|\tau\rangle\langle\tau|\vec{L}\cdot\vec{s}|m\rangle}{E_{eg} - E_{\tau}}$$

For 3d atoms (LaNiO3), 2nd order S-O coupling is tiny (<1meV).
For 5d atoms (LaAuO3), 2nd order S-O coupling is not weak.

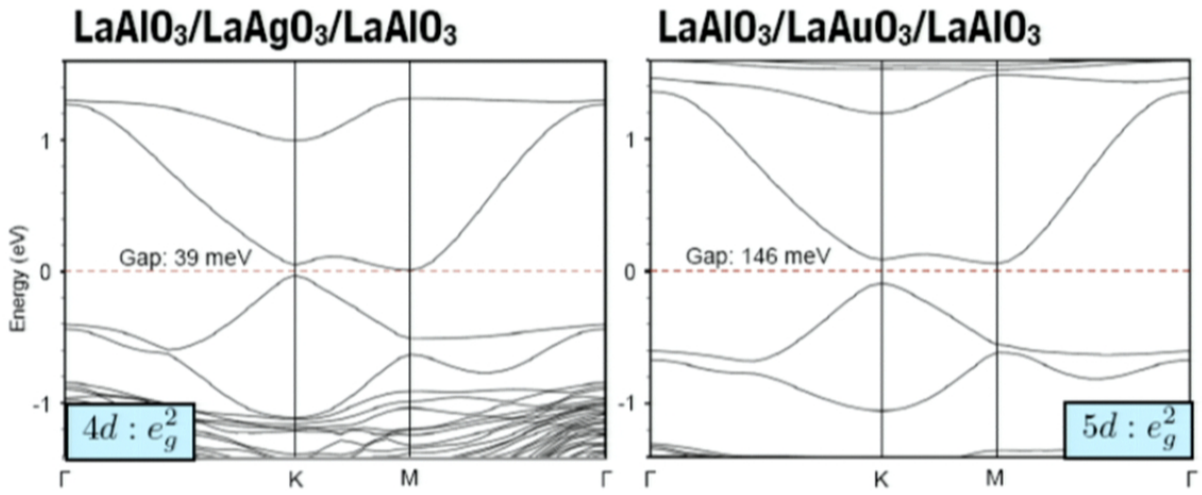
Tight-binding model with H_{SO}



- eg^1, eg^2, eg^3 are all candidate 2D TIs.
- TI phases in eg^2 systems like LaAlO3/LaAuO3/LaAlO3 are particularly stable. (no concern on indirect gap.)
- The non-trivial band topology is carried by the nearly-flat band. (fractional topological phase with partial filling? Will come back later.)

Example 1: LaAuO3 (111) bilayer

Results from LDA:



LaAlO3/LaAuO3/LaAlO3 is a room-temp. 2D TI.

The nearly-flat band is somewhat dispersive, due to further neighbor hoppings

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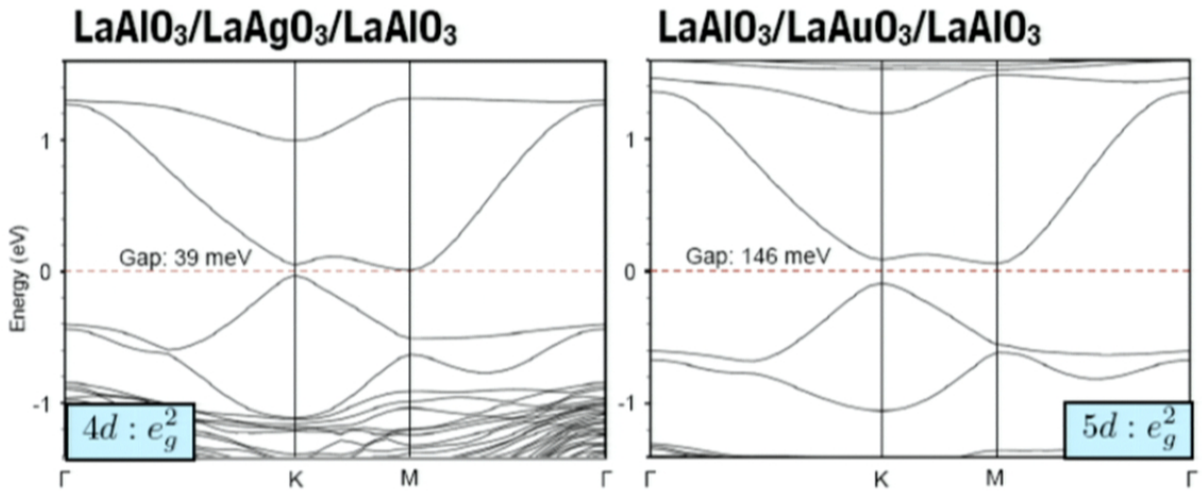

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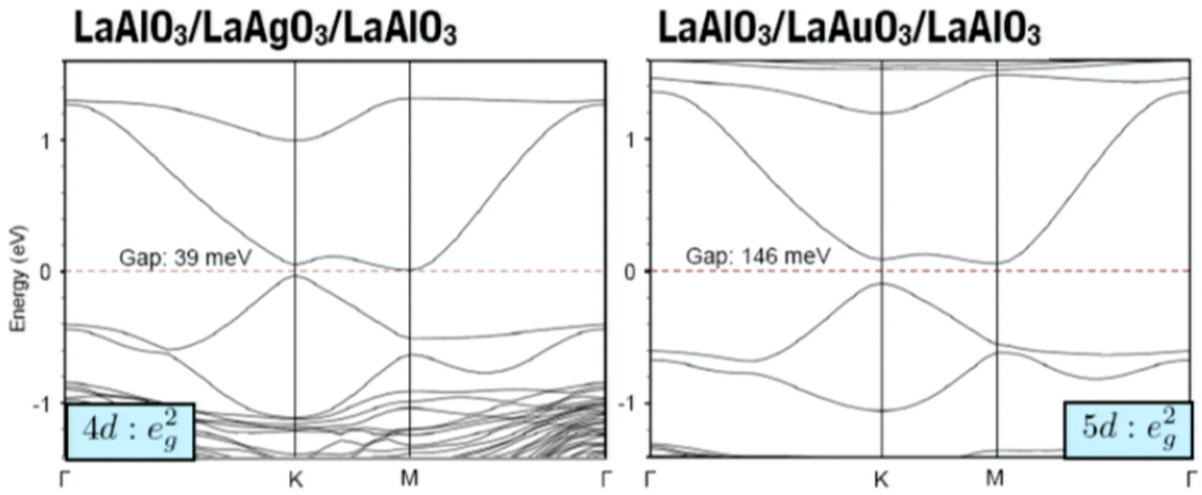

LaAlO3/LaAuO3/LaAlO3 is a room-temp. 2D TI.

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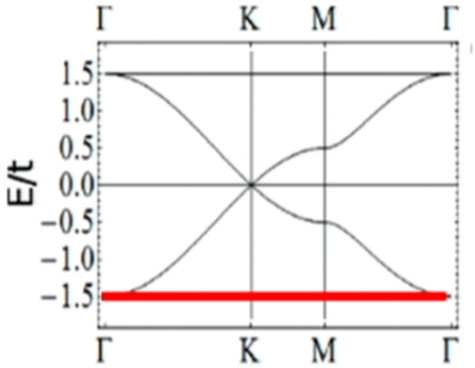
- I was told Au oxides are challenging to grow. (LaAuO3 do exist though.)
- But LaNiO3/LaAlO3 (001) heterostructures were well-studied experimentally. Hopefully the LaNiO3 (111) sample is also relatively easy to grow.
- In fact even the bulk LaNiO3 is interesting, with unusual magnetic-charge ordering.
- This motivates us to study LaNiO3 (111) heterostructures.

Example 2: RNiO3 bilayer

- Bulk LaNiO3 is a metal--- a reasonable starting point:

  tight-binding model



+ multi-orbital Hubbard-interactions.

For RNiO3:

(a) In e_g orbitals: intrinsic spin-orbit coupling<1meV.

(b) ¼ filled. Quadratic band-touching at fermi-level. Unstable in the presence of even weak interactions. (Kai Sun et.al. 2009)

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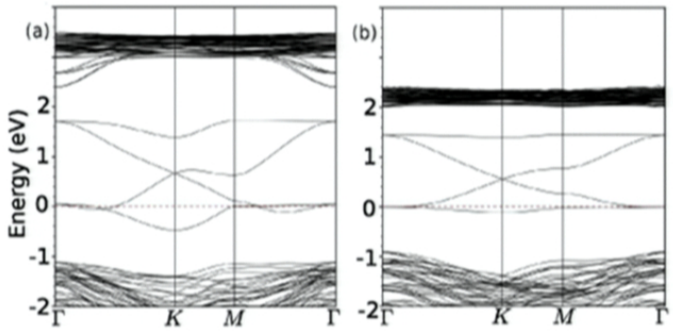
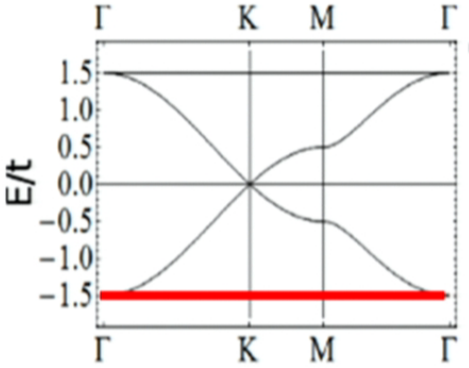


FIG. 3: Results from the non-magnetic LDA+U calculations of the (a) $LaAlO_3/LaNiO_3/LaAlO_3$ and (b) $LaScO_3/LaNiO_3/LaScO_3$ TMOH with lattice relaxation of the $LaNiO_3$ bilayer.

Comparison with non-magnetic LDA+U calculation

≈



What is the phase diagram
as a function of correlation strength?

Example 2: RNiO3 bilayer

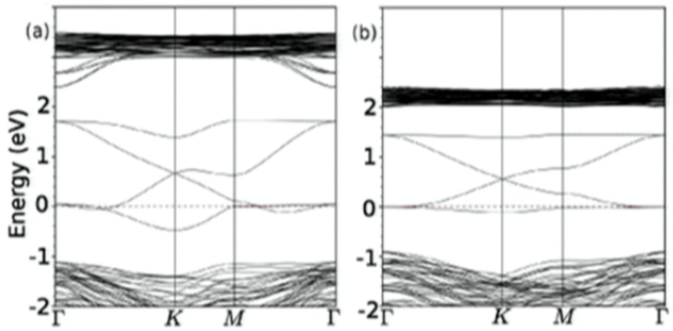
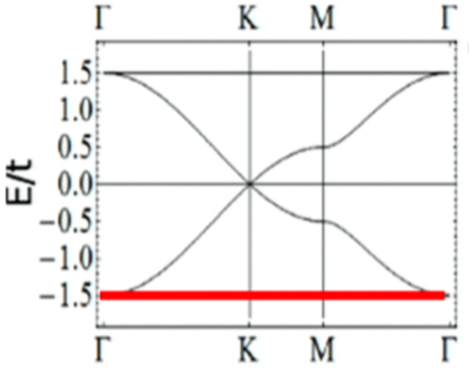


FIG. 3: Results from the non-magnetic LDA+U calculations of the (a) $LaAlO_3/LaNiO_3/LaAlO_3$ and (b) $LaScO_3/LaNiO_3/LaScO_3$ TMOH with lattice relaxation of the $LaNiO_3$ bilayer.

Comparison with non-magnetic LDA+U calculation

≈

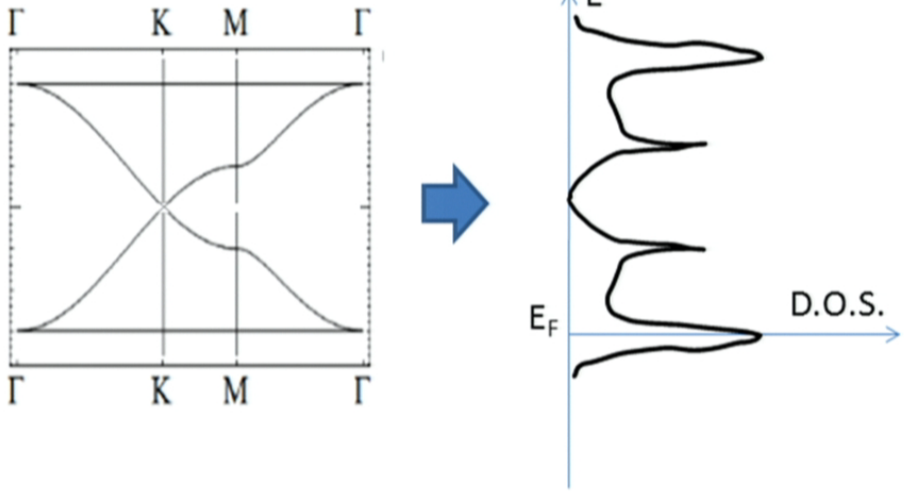


What is the phase diagram
as a function of correlation strength?

An intuitive guess---
Dirac half semi-metal phase ("spinless graphene")

- In reality, the flat-band is slightly dispersive ---fermi level lies in a sharp peak of D.O.S.
- Indicating ferromagnetism is likely to occur.

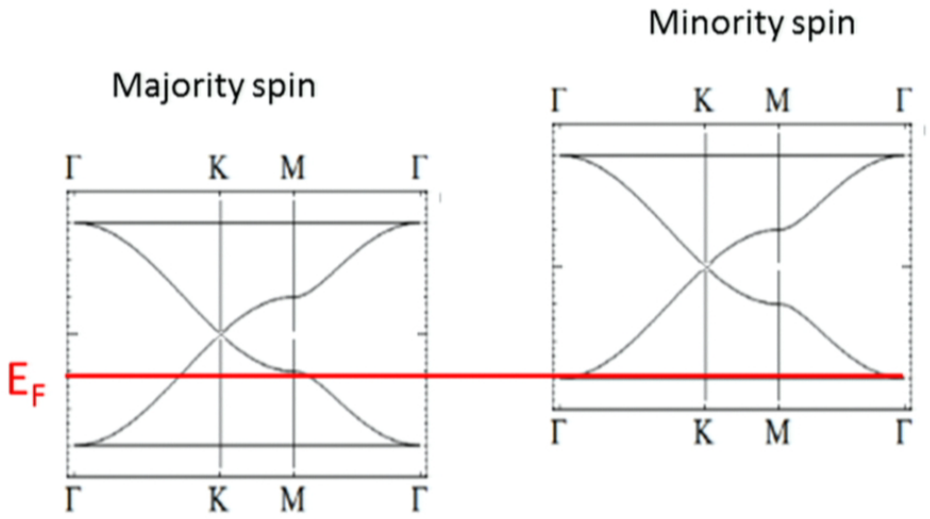
(Stoner's criteria: $U \cdot DOS(E_F) > 1$)



Example 2: RNiO3 bilayer

An intuitive guess---
Dirac half semi-metal phase ("spinless graphene")

- Partially polarized ferromagnetism
  --- partially filled flat band of minority-spin, and disfavored.



Example 2: RNiO3 bilayer

Bulk phenomenology of RNiO3

- Magnetic order, Charge order, and metal-insulator transitions in 3D bulk RNiO3:

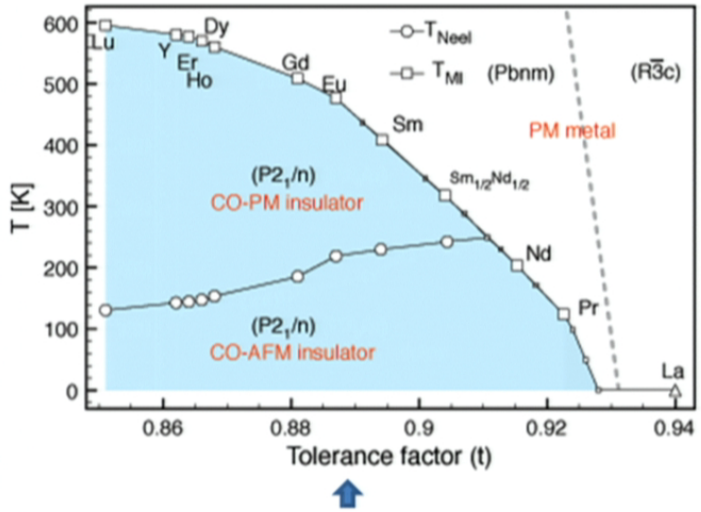
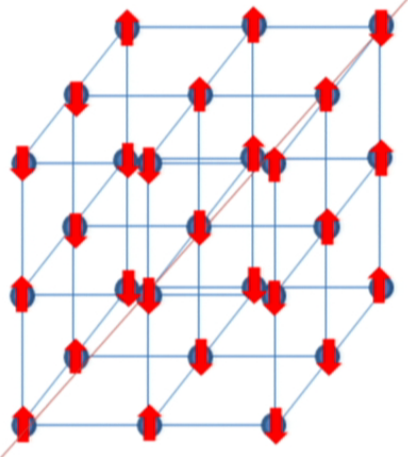


Fig. from Prof. Triscone Group homepage (U. of Geneva)

Magnetic order pattern:
up-up-down-down along (111)
After magnetic ordering, charge order can be understood as a by-product due to symmetry consideration. (Lee&Balents 2011)



This bulk magnetic pattern is consistent with the intuitive guess of bilayer ferromagnetism.

Example 2: RNiO3 bilayer

Mean-field phase diagram

- Phase diagram as U/t (may be viewed as tuning Lanthanide atoms)
  Note:

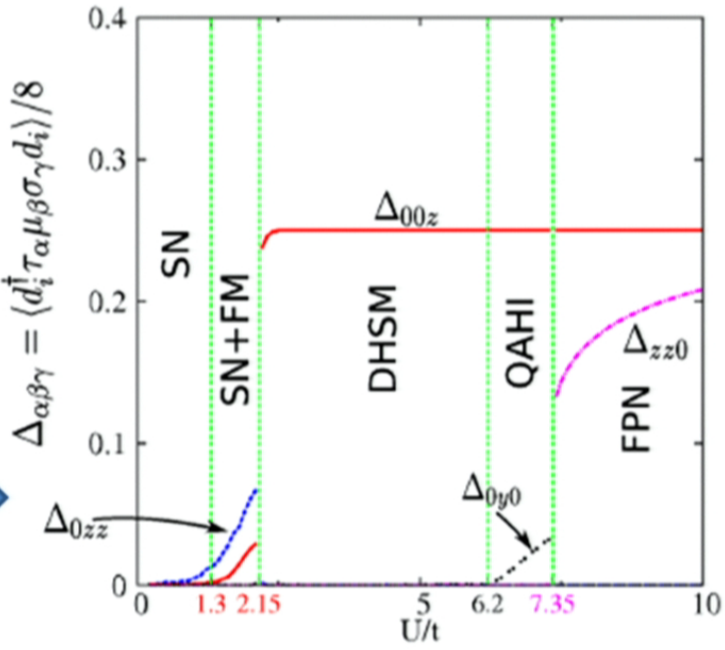
bilayer bandwidth < bulk bandwidth ➡ stronger correlation for bilayer

$$H = H_{TB} + H_I$$

$$H_I = U\sum_{i,a} n_{ia\uparrow}n_{ia\downarrow} + J\sum_{i,a<b}^{\alpha,\beta=\uparrow,\downarrow} d^\dagger_{ia,\alpha}d^\dagger_{ib,\beta}d_{ia,\beta}d_{ib,\alpha}$$
$$+ U'\sum_{i,a<b} n_{ia}n_{ib} + J\sum_{i,a<b}\left(d^\dagger_{ia,\uparrow}d^\dagger_{ia,\downarrow}d_{ib,\downarrow}d_{ib,\uparrow} + h.c.\right)$$

We take $U' = U - 2J$ and $J/U = 0.2$, and vary U/t:

Fully ferro-polarized when U/t>2.15,
DHSM: Dirac half semi-metal
QAHI: Quantum anomalous hall insulator
FPN: Fully polarized nematic phase



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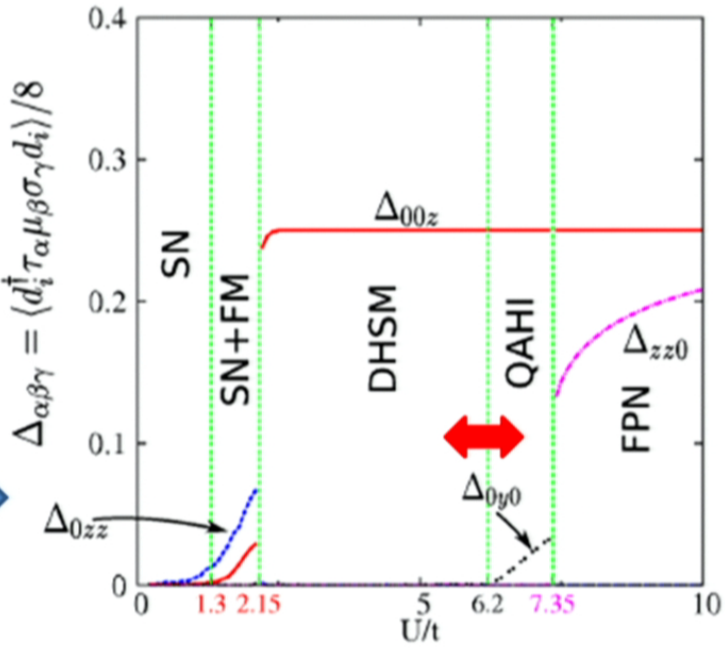
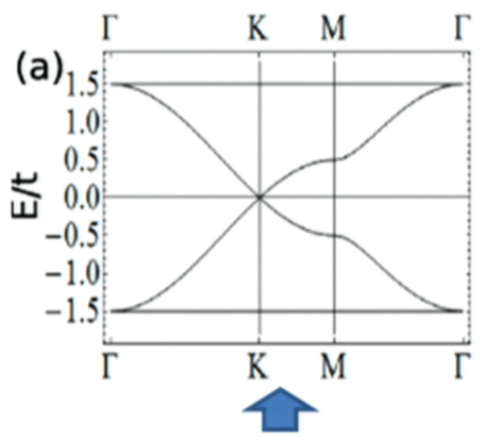


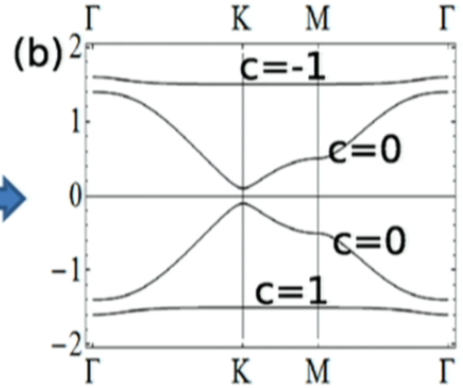
Quantum anomalous hall insulator phase--- spontaneously generated spin-orbit coupling

- Band structure for the majority spin:

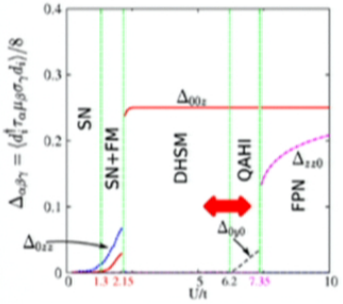


Dirac half semi-metal

Increase U/t



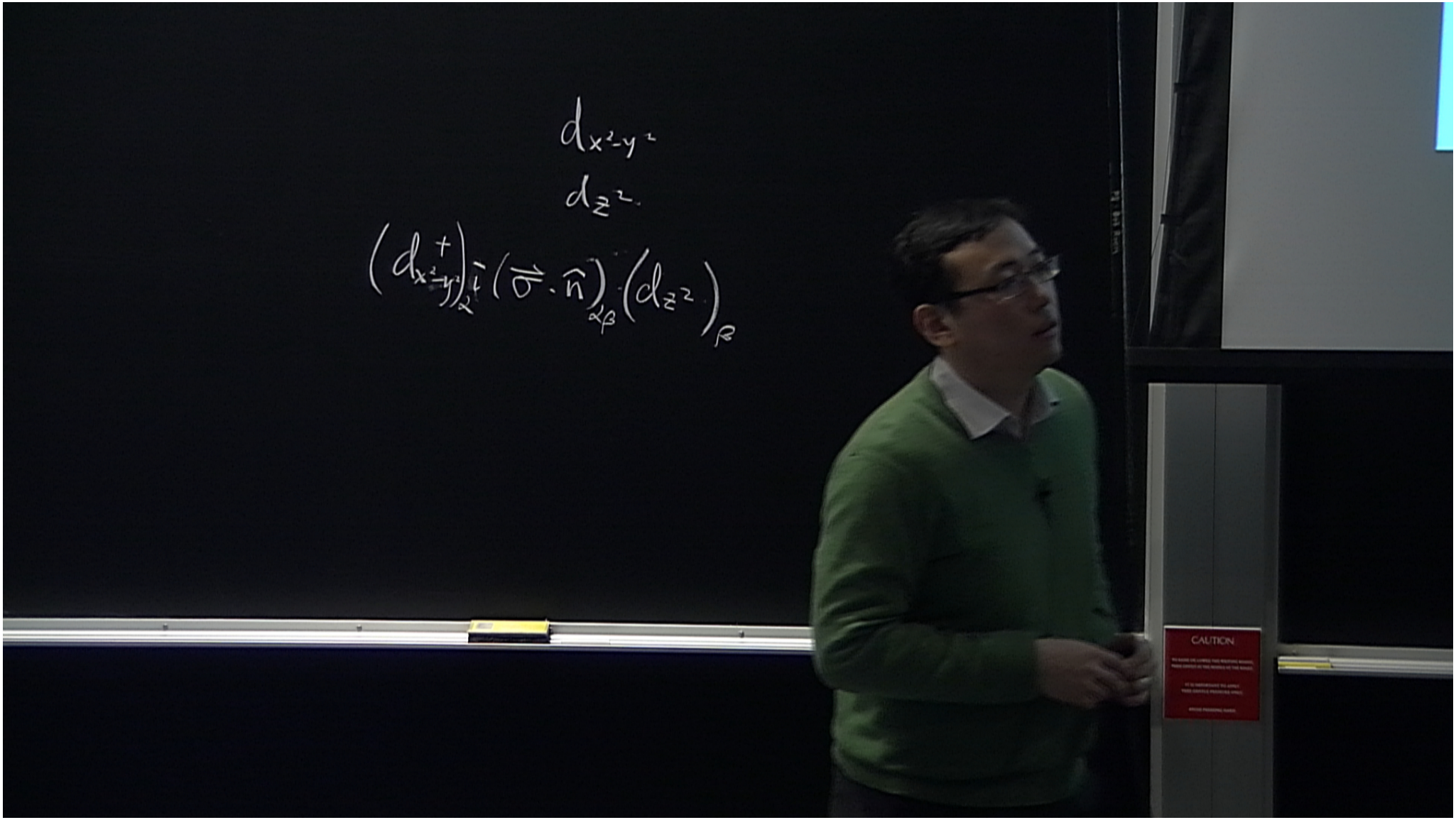
Quantum anomalous hall insulator

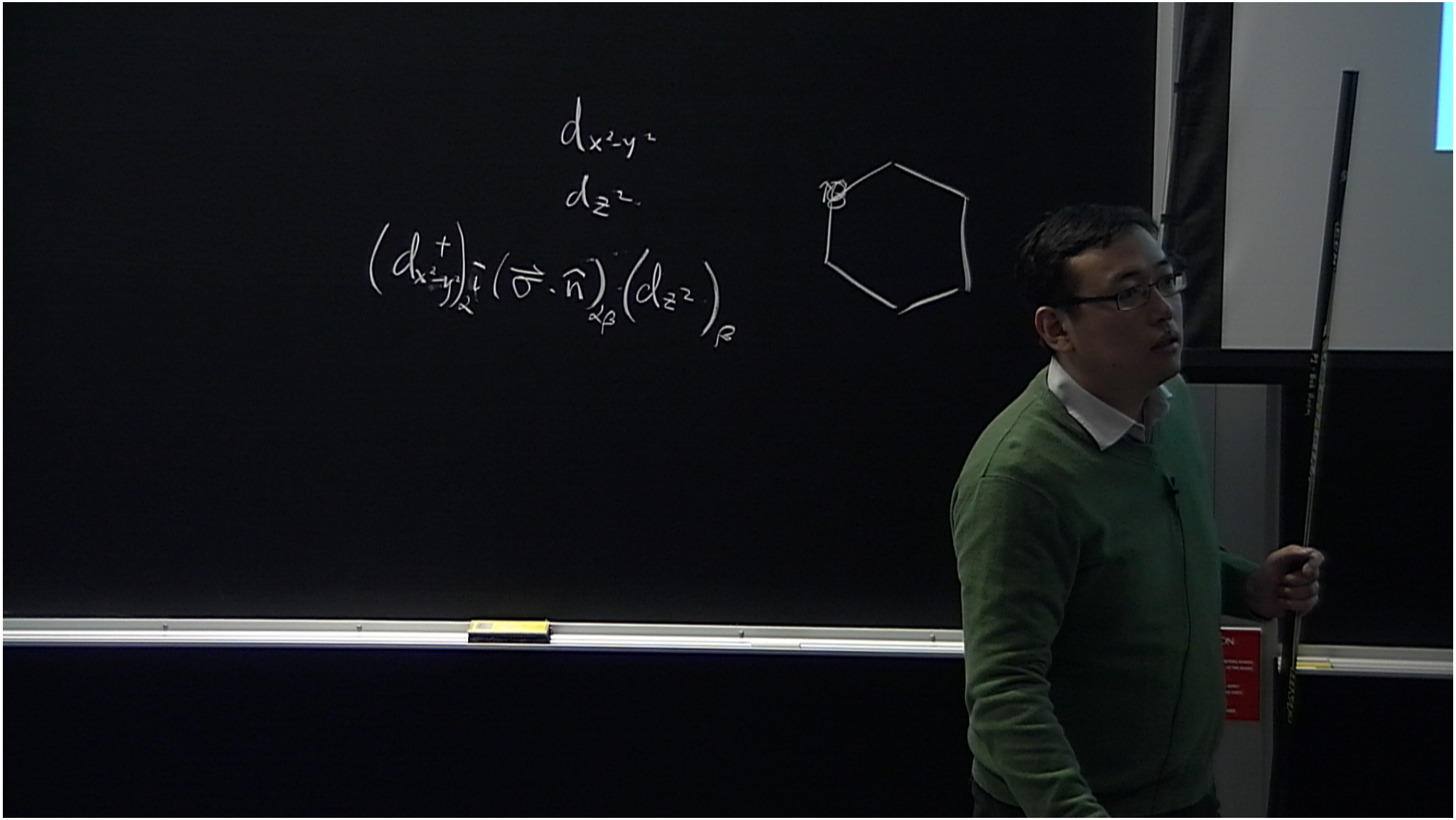


- Energy gap is dynamically generated at band-touching points. (K, K' and Γ).
- Can be viewed as spontaneously generated spin-orbit coupling
- The insulating ground state fills bands with total Chern number=1

➔ $\sigma_{xy} = e^2/h$

(Raghu et.al., 2008 ---QAHI via spontaneous spin-orbit coupling)


$d_{x^2-y^2}$
d_{z^2}
$(d^{\dagger}_{x^2-y^2})_\alpha i(\vec{\sigma}\cdot\hat{n})_{\alpha\beta}(d_{z^2})_\beta$
CAUTION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Several remarks

- Topological solitons/defects in QAHI

Similar to quantum hall ferromagnet, here the skyrmion of the ferromagnetic order carries electric charge *e* and is a fermion.

The domain wall of the spontaneously generated spin-orbit coupling (a Z_2 order parameter here) hosts dissipationless 1D chiral metallic modes.

- Effects of finite temperature

The correlation length of the ferromagnetic order in a spin rotation symmetric system diverges exponentially at low temperature

--- even tiny intrinsic spin-orbit coupling supports finite(large) temperature ferromagnetic phase.

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Experimental progress!

- The successful synthesis of (111) bilayer LaAlO3/LaNiO3/LaAlO3 heterostructure was reported recently:

Dec 2012

Epitaxial growth of (111)-oriented $LaAlO_3/LaNiO_3$ ultra-thin superlattices

S. Middey,[1, a)] D. Meyers,[1] M. Kareev,[1] E. J. Moon,[1] B. A. Gray,[1] X. Liu,[1] J. W. Freeland,[2] and J. Chakhalian[1]
[1)] *Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA*
[2)] *Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA*

The epitaxial stabilization of a single layer or superlattice structures composed of complex oxide materials on polar (111) surfaces is severely burdened by reconstructions at the interface, that commonly arise to neutralize the polarity. We report on the synthesis of high quality $LaNiO_3/mLaAlO_3$ pseudo cubic (111) superlattices on polar (111)-oriented $LaAlO_3$, the proposed complex oxide candidate for a topological insulating behavior. Comprehensive X-Ray diffraction measurements, RHEED, and element specific resonant X-ray absorption spectroscopy affirm their high structural and chemical quality. The study offers an opportunity to fabricate interesting interface and topology controlled (111) oriented superlattices based on ortho-nickelates.

Over the past few years, complex oxide superlattices $CaTiO_3$ on LAO, the epitaxial stabilization is possible

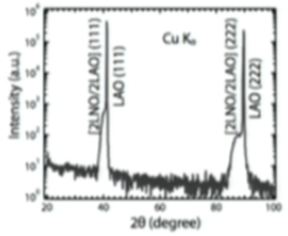

FIG. 2. (color online) 2θ-ω XRD scan for [2LNO/2LAO] superlattice using Cu K_α radiation.

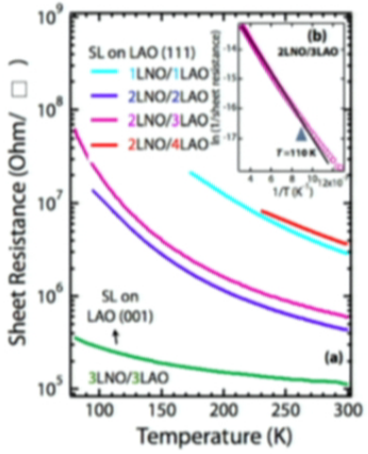

FIG. 4. (color online)(a) Sheet resistance for different superlattices are plotted as a function on temperature. (b) The conductance can be fitted by activated behavior above 110 K.

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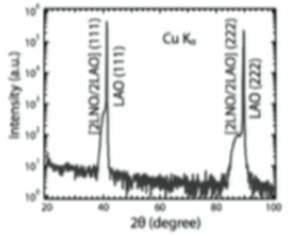

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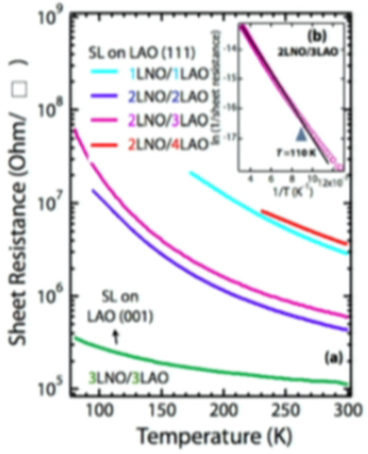

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Example 3: SrIrO3 bilayer

- Iridates with Ir 4+ have attracted a lot of attention:

Sr2IrO4: square-lattice(similar to cuprate), antiferromagnetic Mott insulator, Resonant X-ray: J_{eff}=1/2 system ---B.J.Kim et.al. 2008

Na2IrO3: honeycomb lattice. unusual antiferromagnet. (Kitaev model being relevant? Jackeli&Khaliullin)

R2Ir2O7: pyrochlore lattice. Metal-nonmetal crossover, possible topological phases? (Pesin&Balent, Wan et.al....)

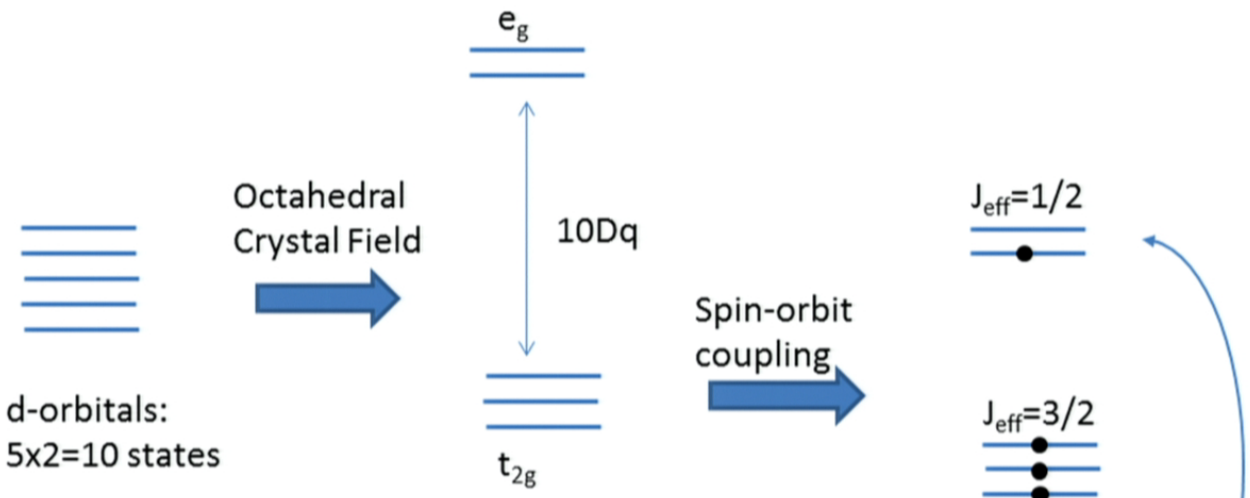
They all have Ir 4+ in the center of the octahedral environment of oxygens.

- These iridates are interesting mainly because:

(1) Coexistence of strong spin-orbit coupling & strong correlation

(2) Effective J_{eff}=1/2 system --- potentially a single band Hubbard system.

Where the J_{eff}=1/2 comes from?



Ir 4+ has $5d^5$ configuration --- one hole in t_{2g}

$$|J_z = 1/2\rangle = \frac{1}{\sqrt{3}}(+i|xy,\uparrow\rangle - |xz,\downarrow\rangle + i|yz,\downarrow\rangle)$$

$|J_z = -1/2\rangle$ is the time-reversal partner

Experimentally confirmed by B.J.Kim et.al. in Sr2IrO4 2008 2009.

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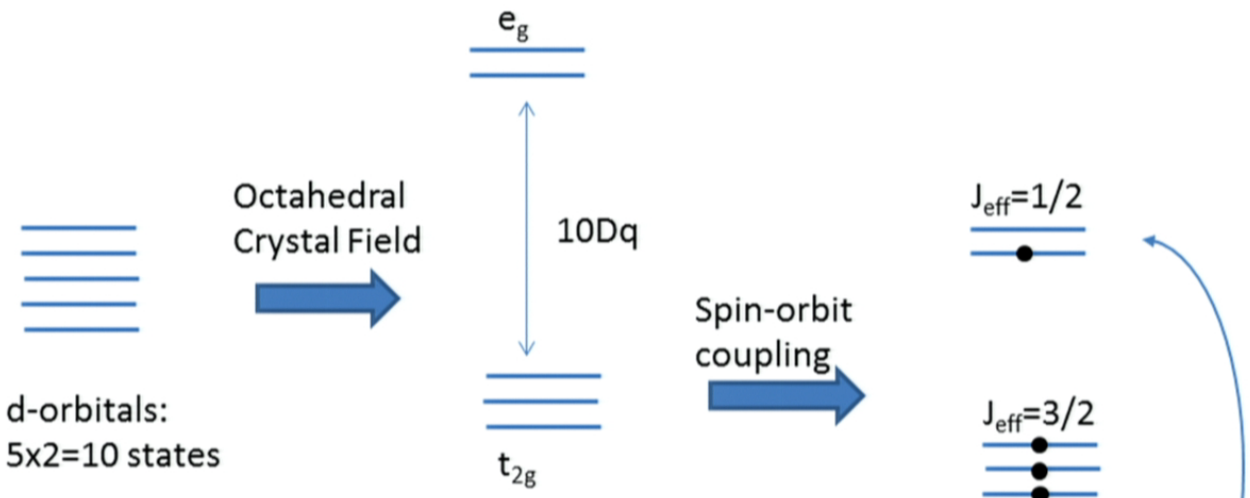

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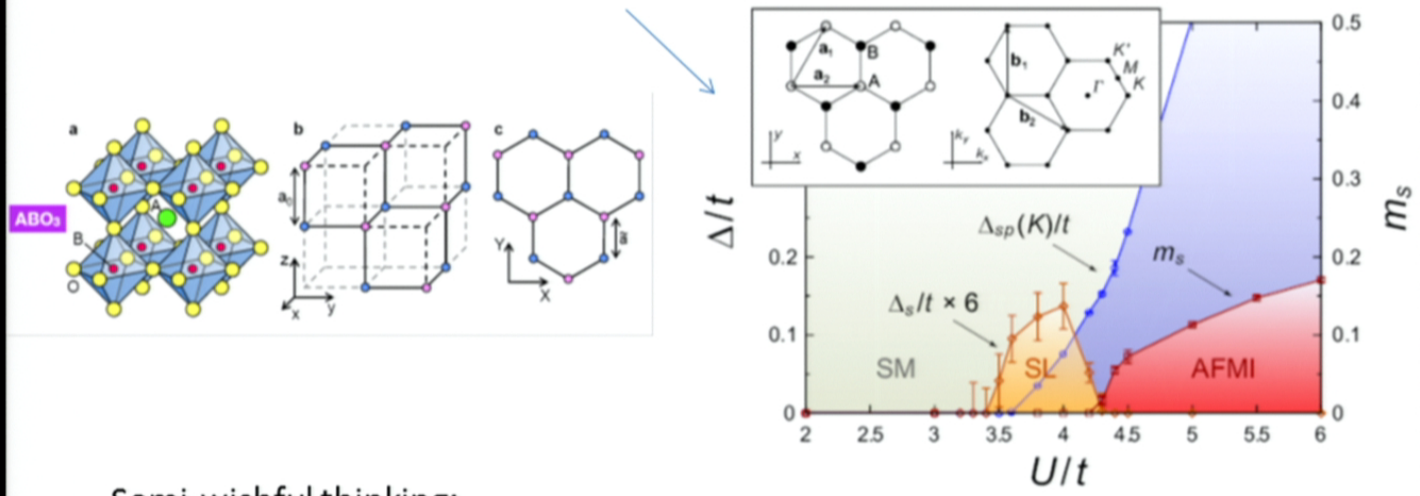
SrTiO3/SrIrO3/SrTiO3 (111) bilayer

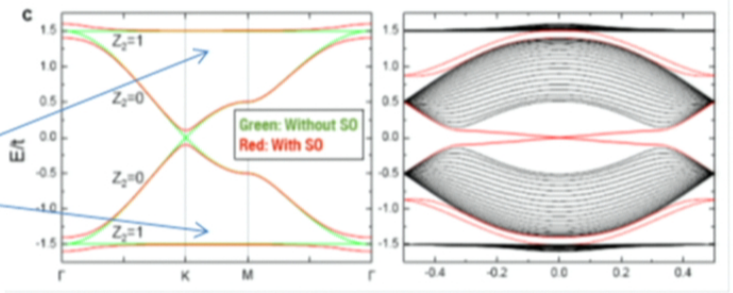
- At the leading order, this is exactly a realization of the single band Hubbard model on the honeycomb lattice, in the vicinity of the Mott transition.
- A truly correlated version of graphene. (This is interesting enough.)
- A possible quantum spin liquid has been revealed exactly in this regime by quantum Monte Carlo simulation (Meng et.al. Nature 2010)!



Semi-wishful thinking:

- if one plugs in t~0.25 eV(typical LDA value for Sr2IrO4), and U~1eV ---U/t~4.
- Doping --- unconventional high-temperature superconductivity ?

Finally, let's come back to these flat bands



- When nearly flat topological band is partially filled:

Short-range Coulomb repulsion lifts the many-body degeneracy.

--- abelian/nonabelian Fractional Chern insulators

high temperature fractional quantum hall effect without an external magnetic field.

(Incomplete list: Mudry, Chamon,Tang, Wen, Sun, Sheng, Gu,Bernevig, Fiete….2011)

Stoner's instability

- One very likely consequence of correlation for flat bands is ferromagnetism:

Stoner's criteria: U >1/DOS(E_F) is satisfied in an extreme way, due to the flatness of the band.

- If this happens: MF hamiltonian $H = H_{eg} + \vec{h} \cdot \vec{\sigma}$

- Of course, the same MF hamiltonian can come from extrinsic ferromagnetic coupling (FM substrates). Our discussion is not limited to spontaneous ferromagnetism.

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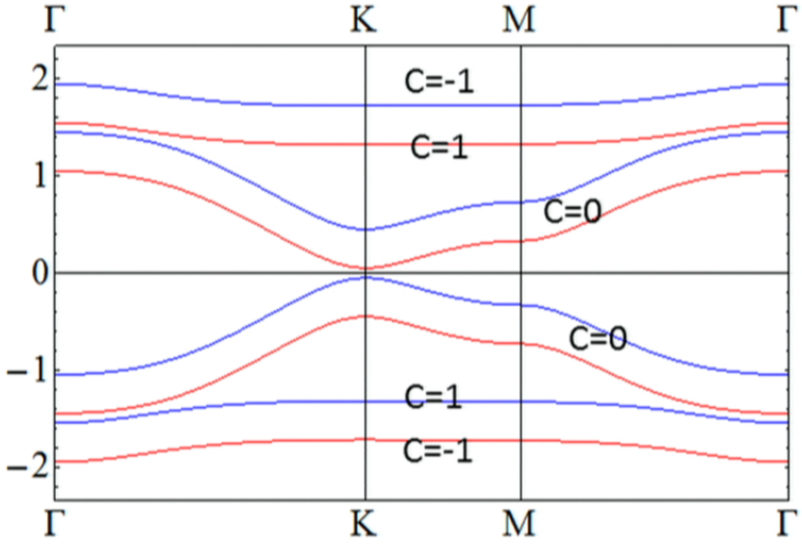
Quantized anomalous hall phase



- After turning on FM, bands carry Chern numbers.
- At fillings $eg^{0.5}$, $eg^{3.5}$, we expect QAHE, could be a high-temp. effect (depends on indirect gap).
- What will happen if a Chern band is partially filled?
  (FCI?)

Exact diagonalization study

- The model:

$$H = H_{eg} + h\sigma_z + H_I$$

$$H_I = U \sum_{i,\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + U' \sum_{i,\alpha>\beta} n_{i\alpha} n_{i\beta} + V_{\langle ij \rangle} n_i n_j$$

multi-orbital Hubbard-type model

- *U=U'=t, V=0.5t* (*t* ~ 1eV for LaAuO3)
- 1/3 fill the top flat Chern band.
- To reduce the dimension of Hilbert space, we project the interaction in the flat band. (i.e., band mixing is not considered)

What is the ground state?

Exact diagonalization study

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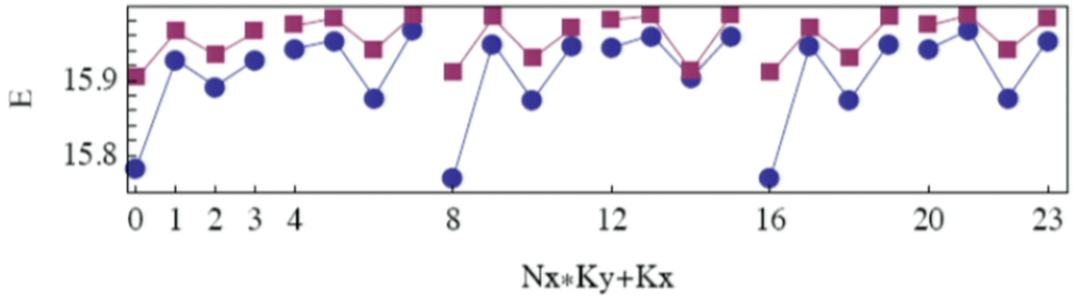
Results of exact diagonalization

- 3-fold ground state degeneracy on torus (6x4 unit cells).



- Many-particle Chern number

$$\sigma_{xy} = \frac{e^2}{hg} \sum_{K=1}^{g} \int_0^{2\pi} \int_0^{2\pi} d\phi_1 d\phi_2 \left(\left\langle \frac{\partial \Phi_0}{\partial \phi_1} \middle| \frac{\partial \Phi_0}{\partial \phi_2} \right\rangle - \left\langle \frac{\partial \Phi_0}{\partial \phi_2} \middle| \frac{\partial \Phi_0}{\partial \phi_1} \right\rangle \right)$$

g=3, C_1=0.3344, C_2=0.3311, C_3=0.3344

This explicitly show that we are in a $\sigma_{xy} = 1/3e^2/h$ FQH phase.

Likely in the same universality class as Laughlin's 1/3 state.

Nearly flat Chern band with C=2?

- This is an intrinsically new regime of quantum hall physics (unlikely realizable in the magnetic field case)

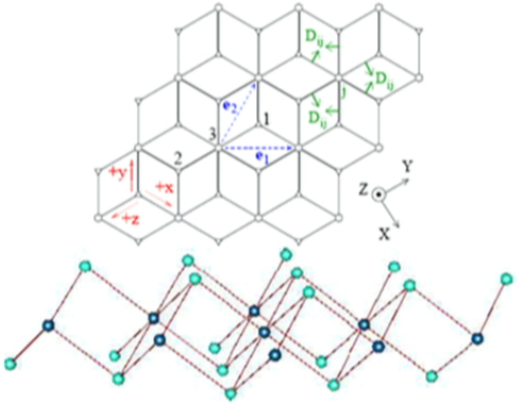
- From low energy theory, one finds the counter part of the Laughlin's 1/3 state with C=2 is a non-abelian state.

(SU(3) level-2 Chern-Simons theory, can be used for universal quantum computation.)

Are there nearly flat C=2 band in practical materials?

A potential realization of C=2 nearly flat band: SrIrO3 (111) trilayer

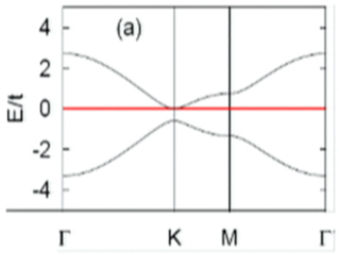
- Trilayer: metal atoms form a Dice-lattice.



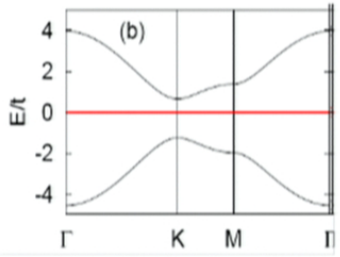
To the leading order, same as s-orbitals hopping on a Dice lattice + Rashba-type S-O coupling .

Dice lattice is well-know to support flat band. (one of the many Lieb's theorems)

The two-fold degenerate flat band is half-filled.



Without S-O



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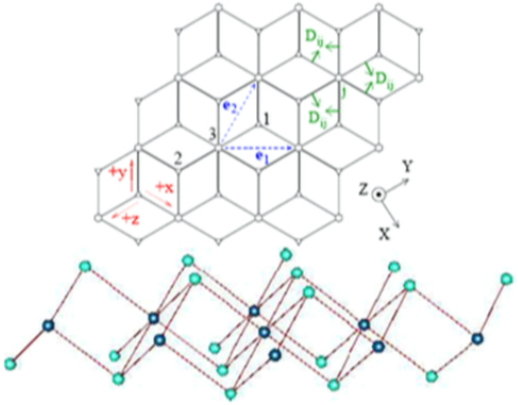

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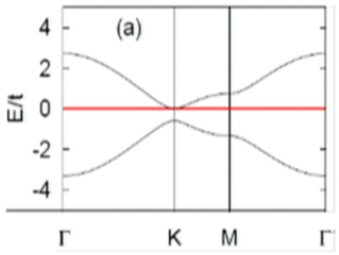
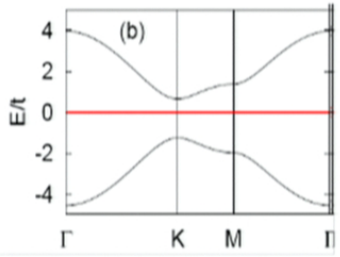


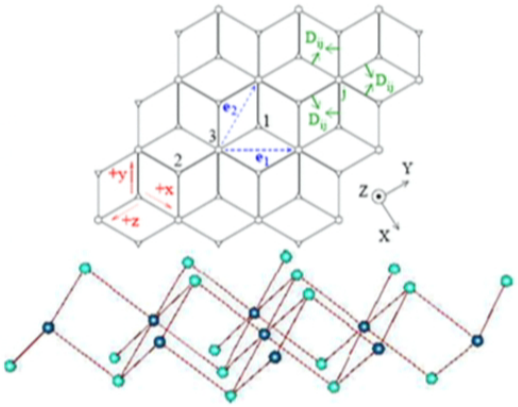
Without S-O



With S-O

A potential realization of C=2 nearly flat band: SrIrO3 (111) trilayer

- Trilayer: metal atoms form a Dice-lattice.

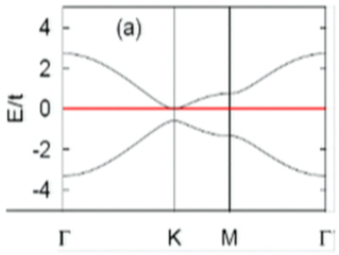


+ Hubbard interaction

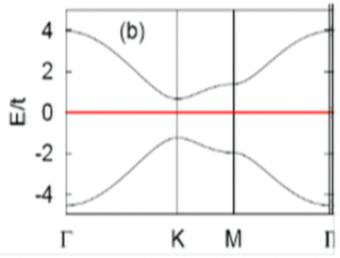
(111) Ferromgnetism (consistent with Lieb's theorem in the absence of S-O coupling) in mean-field calculation

➔ Quantum anomalous hall insulator with C=2.

Fermi level close to Chern=2 flat bands....
(partially filled C=2 band --- non-abelian states?)

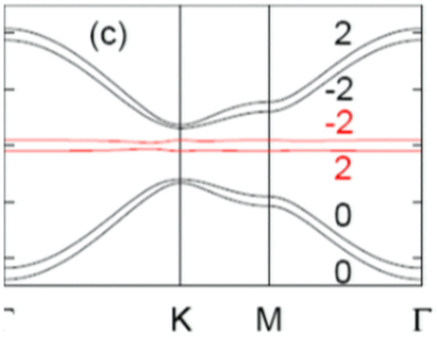


Without S-O



With S-O

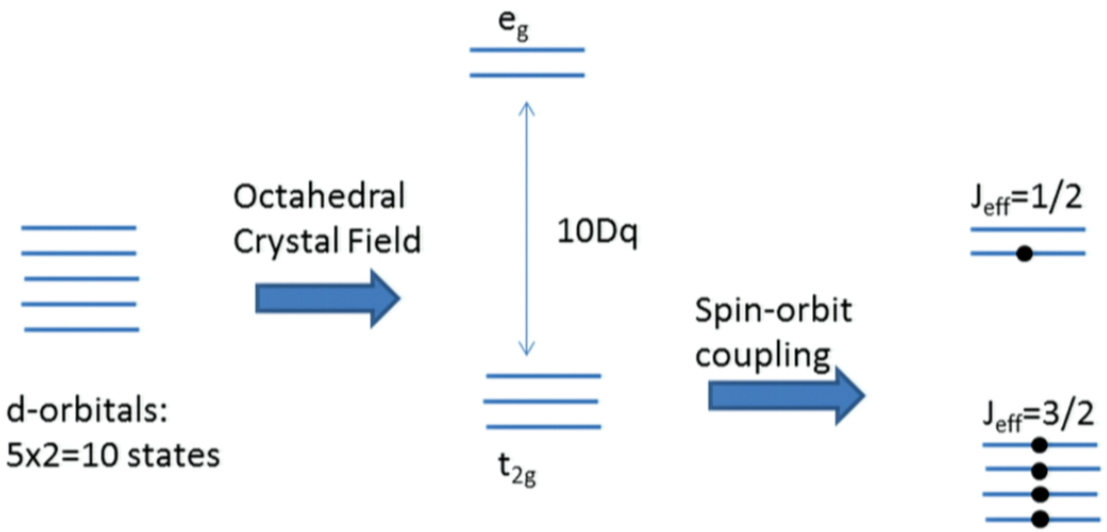
Hubbard U



Summary and Future directions:

- Transition metal oxides (111) heterostructures are promising materials to realize many 2D topological phases. (e.g., $RNiO_3$, $LaAuO_3$, $SrIrO_3$…., TI, quantum anomalous hall insulator, fractional Chern insulator, quantum spin liquid….)
- Many practical issues need to be investigated: lattice reconstruction, trigonal splitting…..
- Experimental synthesis/characterization of these materials will be the true driving force for this new area.

Where the J_{eff}=1/2 comes from?



Ir 4+ has $5d^5$ configuration --- one hole in t_{2g}

This gives a narrow bandwidth ~ 1eV for J_{eff}=1/2, comparable with hubbard U.

In fact, most iridates are either Mott insulators or metals,
and among them a lot are in the vincinity of the Mott transition.
(metal-nonmetal crossover in pyrochlores R2Ir2O7,
Na4Ir3O8 becomes metallic under moderate pressure...)