

Quantum Hall Effects in Heterostructures of Transition-Metal Oxides

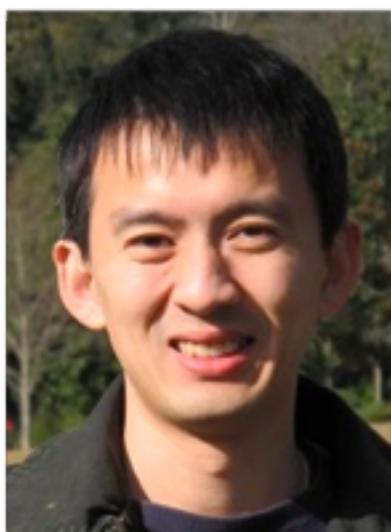
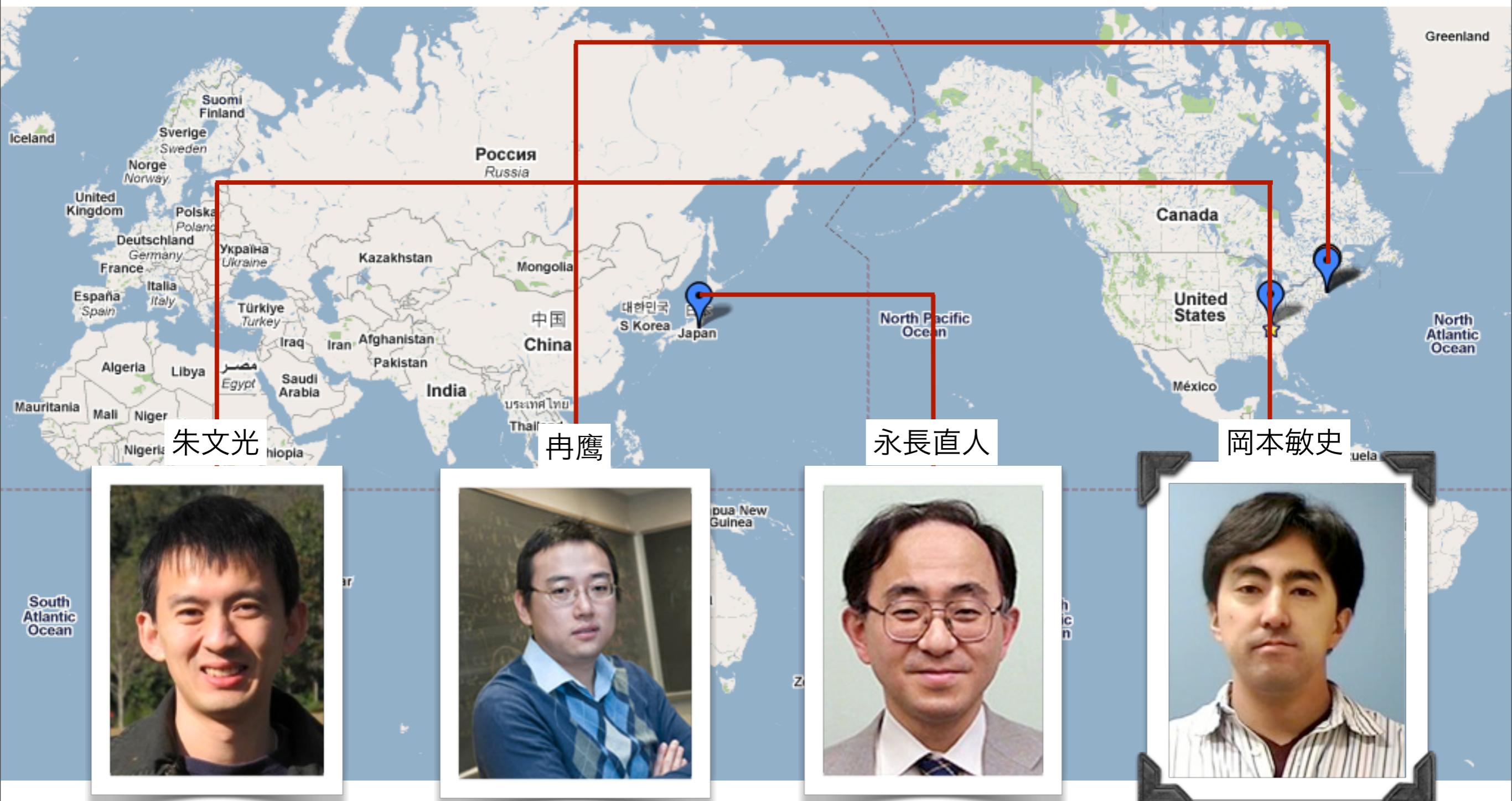
Di Xiao

*Materials Science and Technology Division, Oak Ridge
National Laboratory*



Sponsored by Division of Materials Sciences and Engineering,
Office of Basic Energy Sciences, U.S. Department of Energy

Collaborators



Wenguang Zhu
Knoxville



Ying Ran
Boston



Naoto Nagaosa
Tokyo



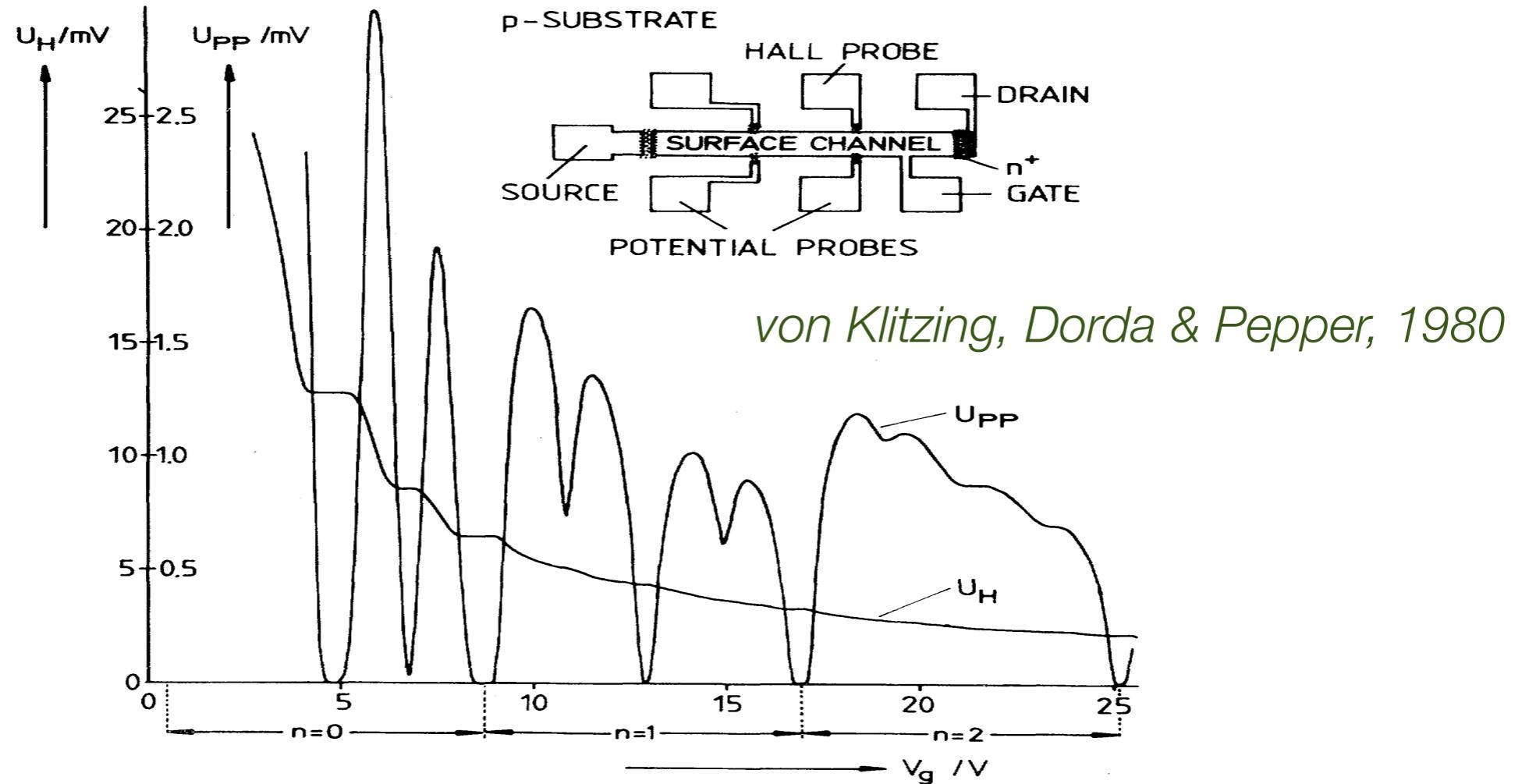
Satoshi Okamoto
Oak Ridge

Outline

- ▶ The quest for topological states of matter
 - Quantum Hall Effect
 - Topological Insulators
- ▶ Heterostructures of transition-metal oxides
 - Quantum spin Hall effect
 - Integer quantum Hall effect
 - Fractional quantum Hall effect
- ▶ Summary

The Quest for Topological States of Matter

The QHE: A Tribute to Materials Advance



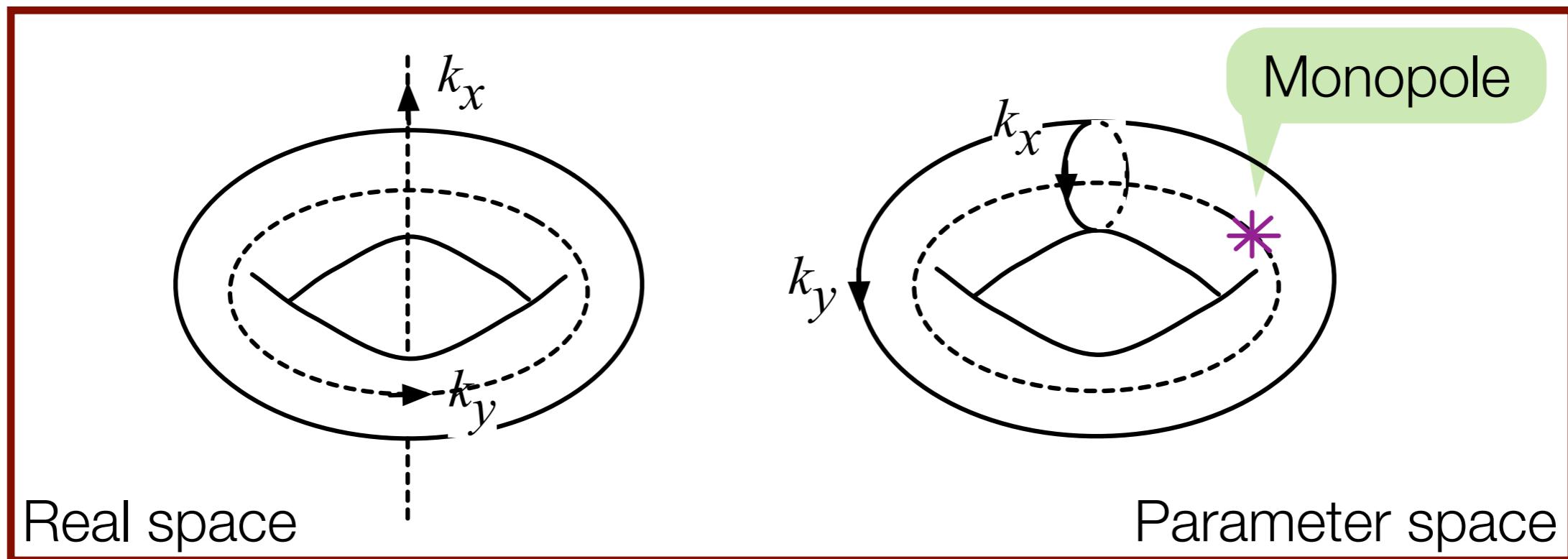
von Klitzing, Dorda & Pepper, 1980

“It should also be mentioned that advances in technology and production methods within semiconductor electronics have played a crucial role in the study of two-dimensional electron systems, and were a precondition for the discovery of the quantised Hall effect.” — *Press Release: The 1985 Nobel Prize in Physics*

Precise Quantization: Topological Origin

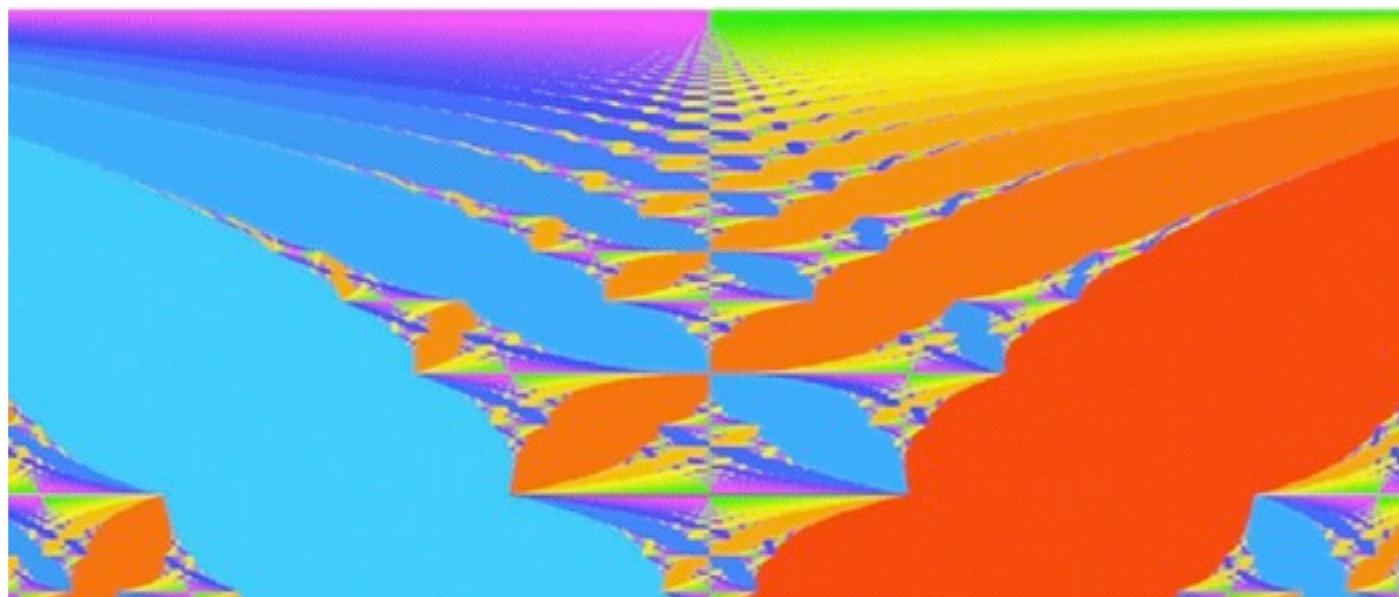
- ▶ Hall plateau: Localization physics
- ▶ Precise quantization: Nontrivial topology

$$\sigma_{xy} = \frac{ie^2}{2\pi h} \int d^2k \left(\left\langle \frac{\partial \Phi_0}{\partial k_x} \middle| \frac{\partial \Phi_0}{\partial k_y} \right\rangle - \left\langle \frac{\partial \Phi_0}{\partial k_y} \middle| \frac{\partial \Phi_0}{\partial k_x} \right\rangle \right)$$

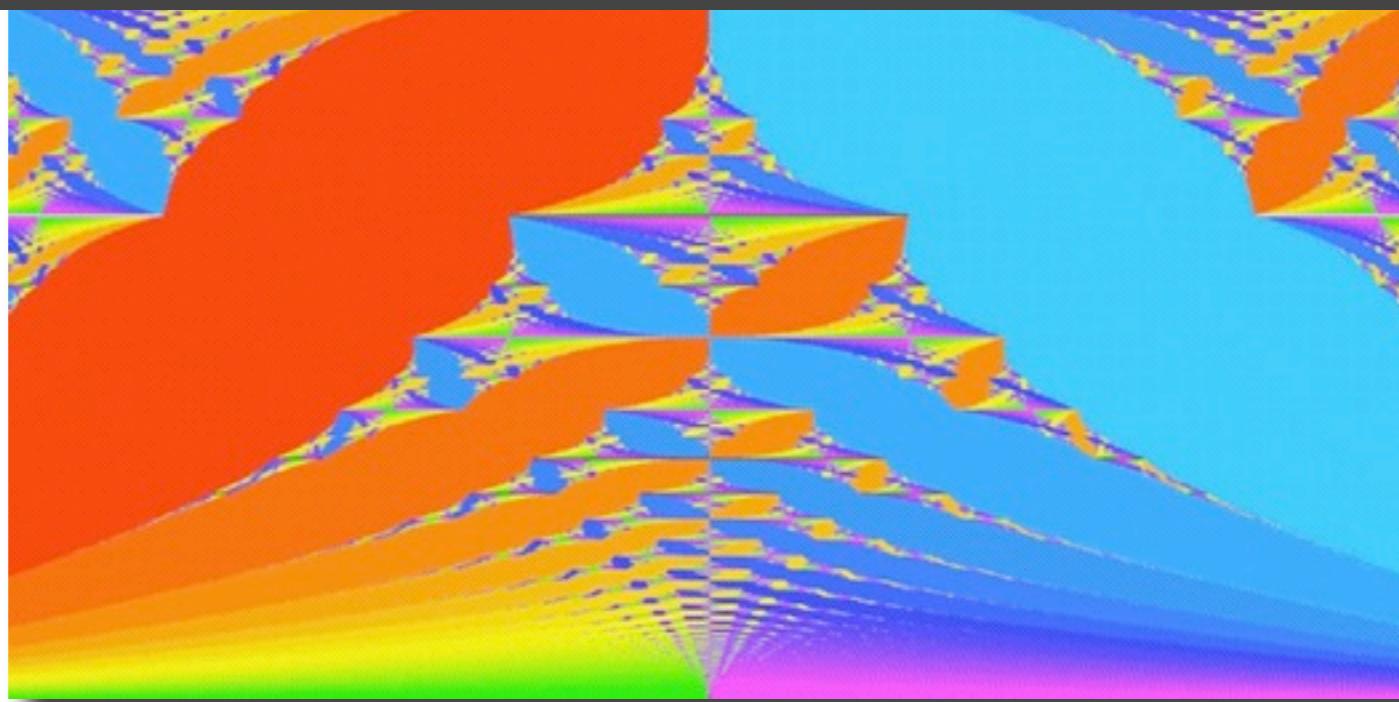


Thouless et al, 1982; Niu, Wu & Thouless, 1985

The Magnetic Butterfly



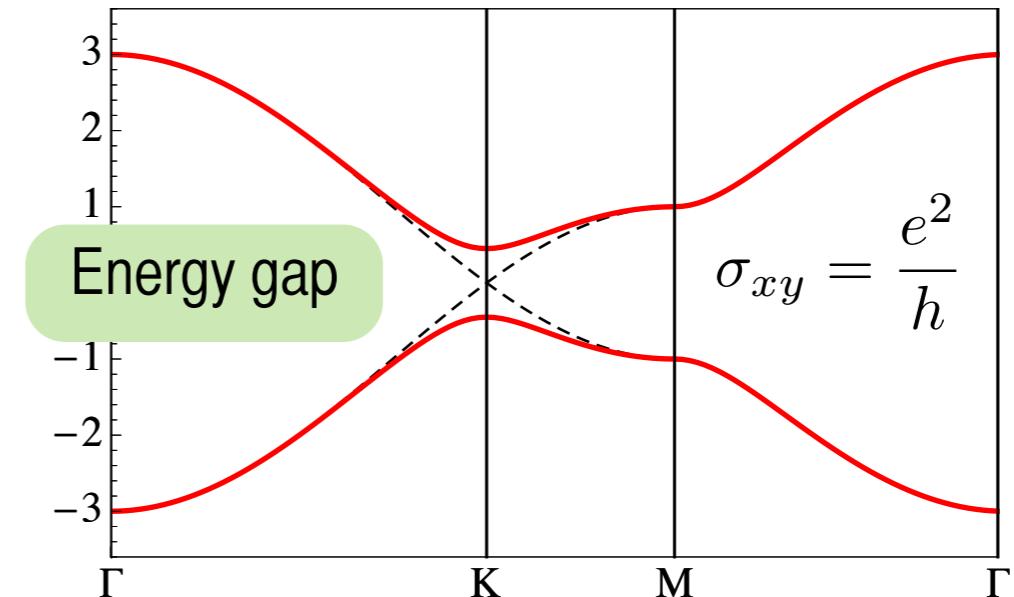
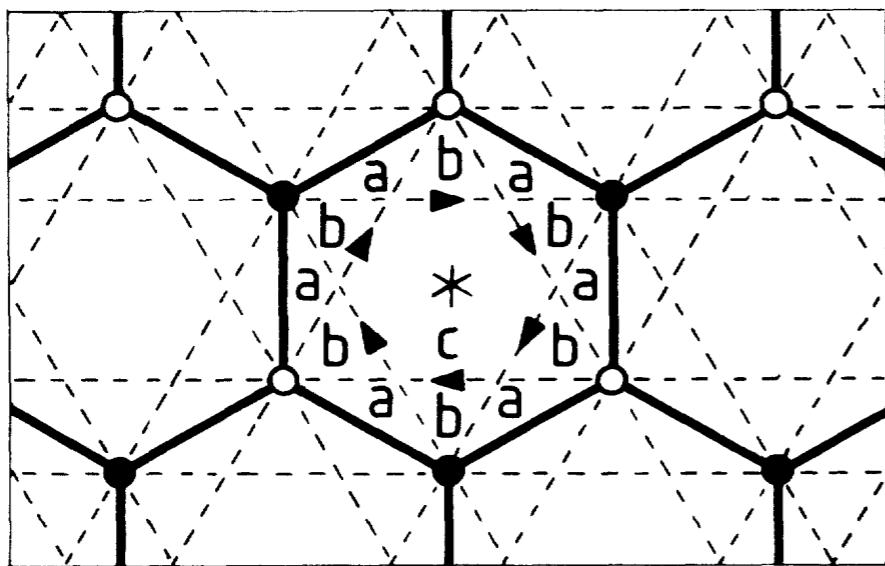
Is Magnetic Field Necessary?



Hofstadter's Butterfly. Credit: J.E. Avron

QHE without Landau Levels

Haldane, 1988



- ▶ Periodic magnetic field with zero total flux through the unit cell
- ▶ Next nearest neighbor hopping becomes complex, opens a band gap

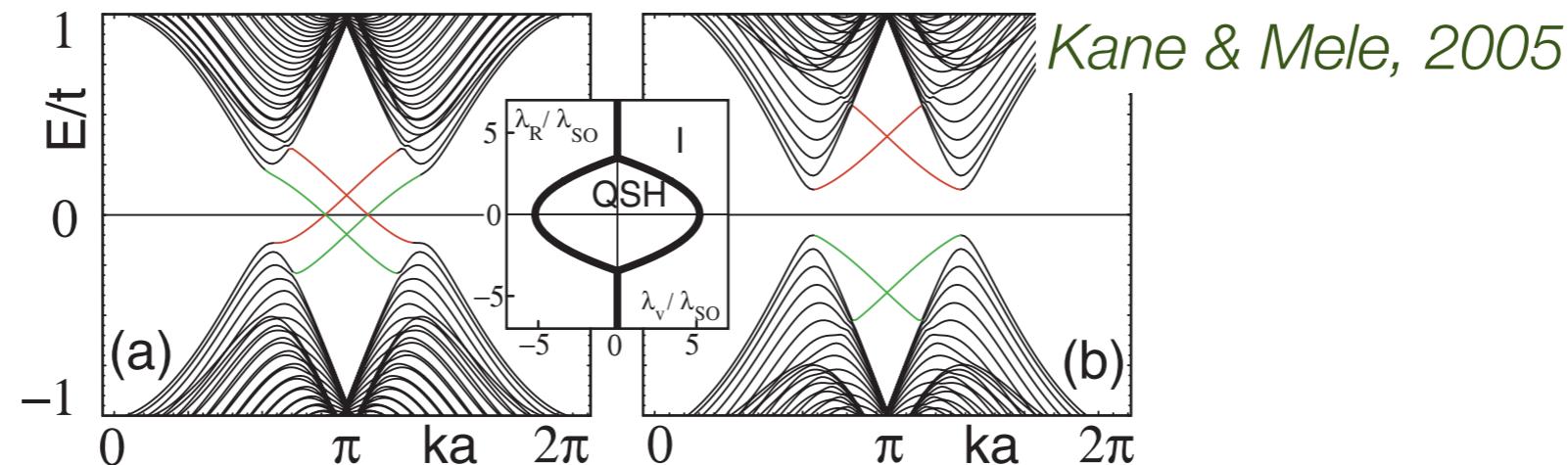
Nontrivial topology in simple band insulators

QSHE driven by Spin-Orbit Interaction

T-symmetry breaking	$\Delta_{\text{Haldane}} \sigma_z \tau_z$
Spin-orbit interaction	$\Delta_{\text{SO}} \sigma_z \tau_z s_z$

$(\sigma_z, \tau_z, s_z) =$
(sublattice, valley, spin)

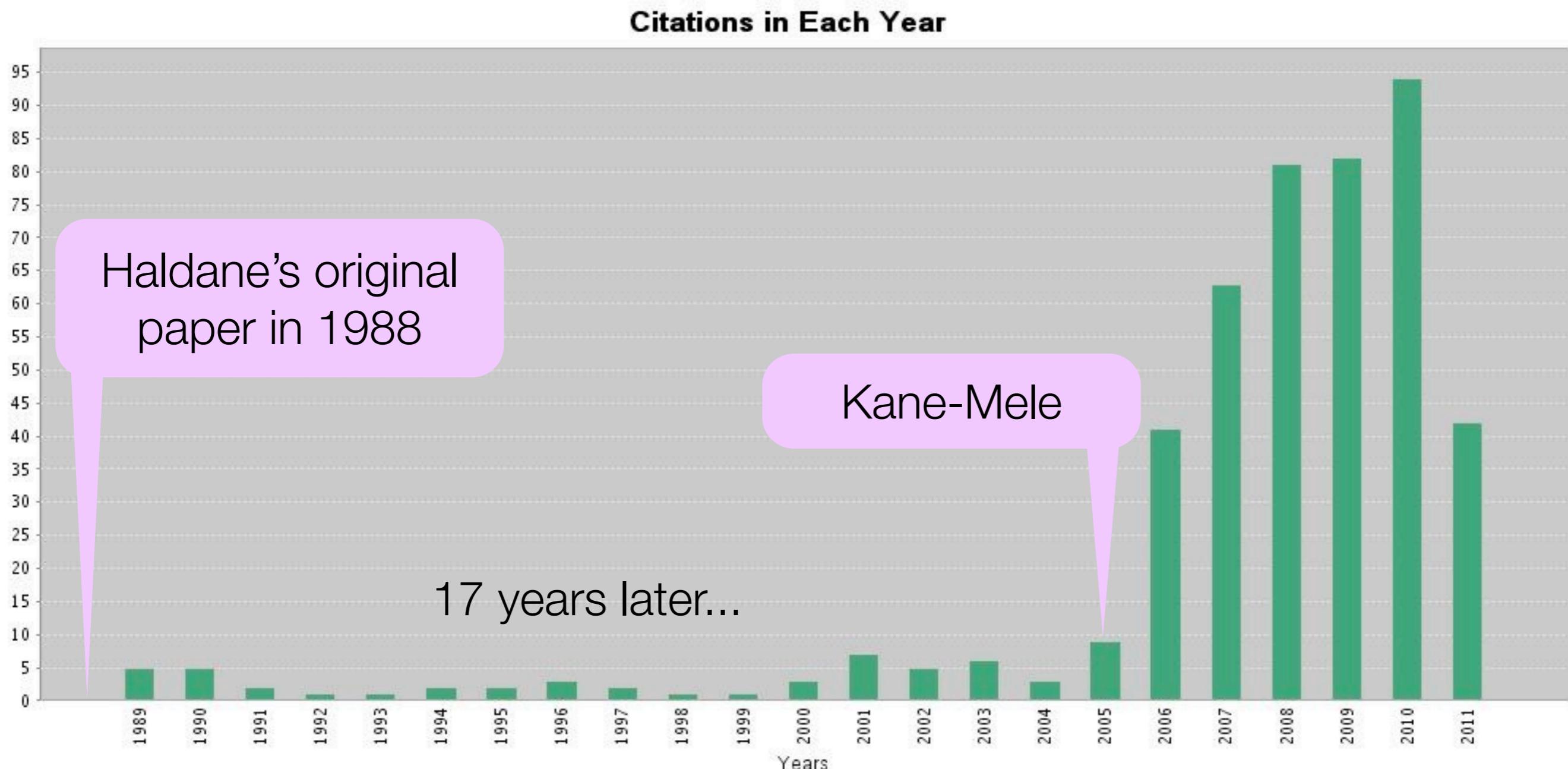
- ▶ s_z conserved: Two copies of Haldane model
- ▶ s_z not conserved: Edge states **still** protected by T-symmetry



Topological insulators are characterized by nontrivial band topology (Z_2) driven by spin-orbit interaction and support robust “helical” edge/surface states

2D: Kane & Mele, PRL 2005; Bernevig, Hughes, & Zhang (2006)
3D: Fu, Kane & Mele, 2007; Moore & Balents (2007)

Haldane: What has Just Happened?



[Shows](#) [Videos](#) [Schedule](#)**the
BIG BANG
theory**

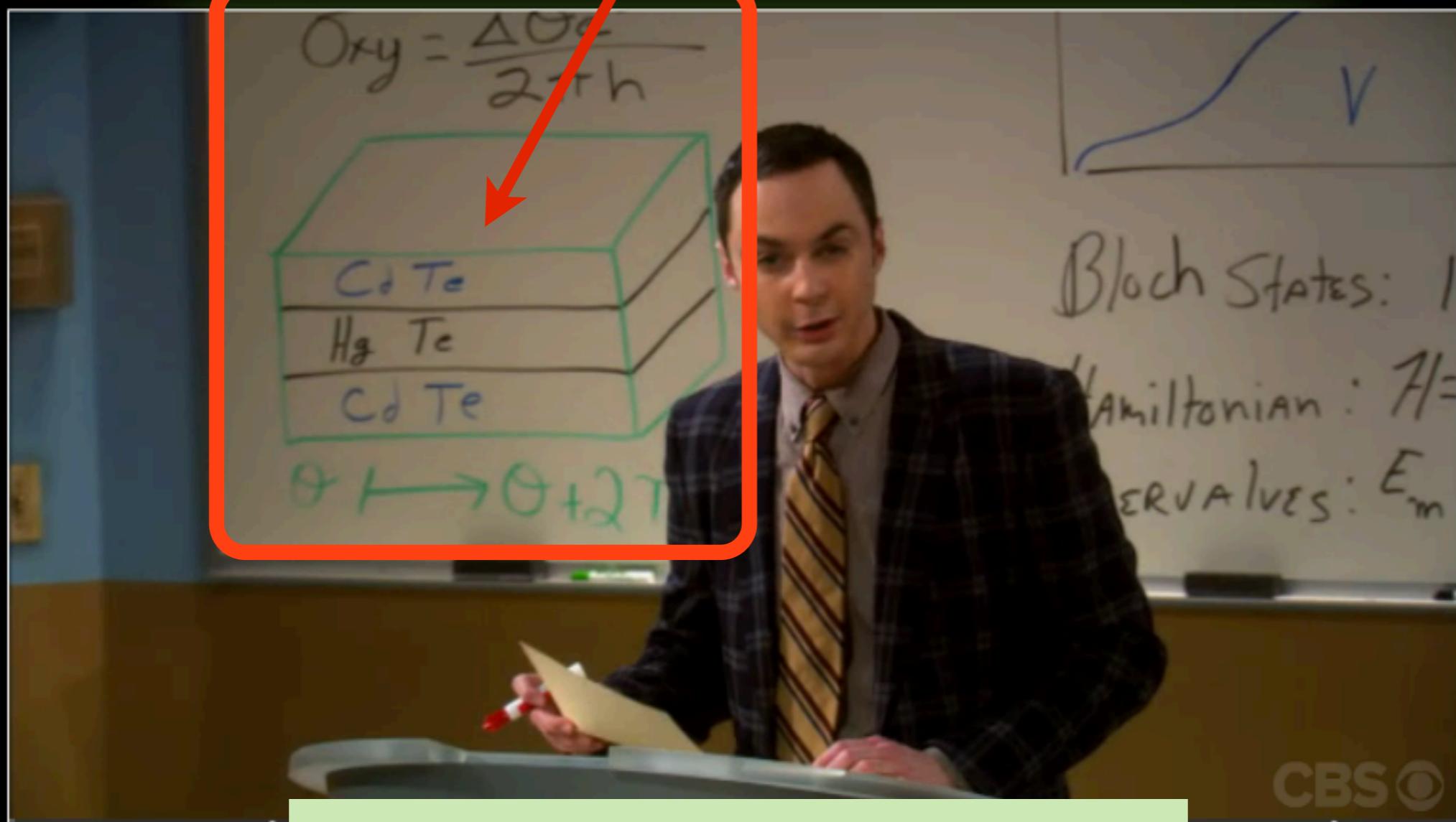
Thursdays, 8/7c

[Login](#) | [Join Us](#)

Search CBS



This Happened



Material is the key

[Tweet](#) 7

The Big Bang Theory - The
Thespian Catalyst

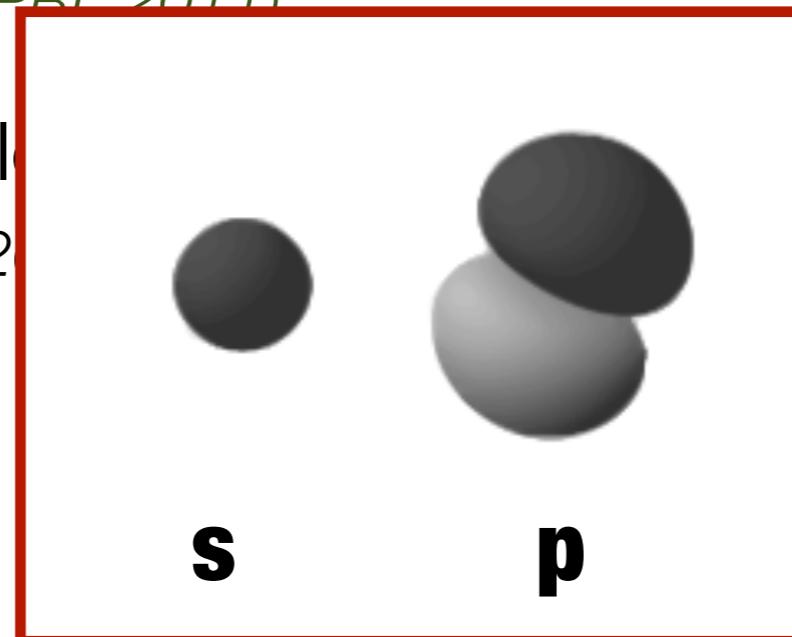
Air Date: 02/03/11

Full Episode 21:39

help him become a better teacher. Meanwhile, Koothrappali fantasizes about his best friend's girlfriend.

Topological Insulators: A Growing Family

- ▶ **CdHgTe/HgTe/CdHgTe** (*Bernevig et al, Science 2006, König et al, Science 2007*)
- ▶ **Bi_{1-x}Sb_x** (*Fu and Kane, PRB 2007, Hsieh et al, Nature 2008*)
- ▶ **Bi₂Se₃, Bi₂Te₃, Sb₂Te₃** (*Zhang et al, Nat Phys 2009, Xia et al, Nat Phys 2009, Chen et al, Science 2009*)
- ▶ **TlBiTe₂ and TlBiSe₂** (*Lin et al, PRL 2010, Yan et al, EPL 2010, Sato et al, PRL 2010, Chen et al, PRL 2011*)
- ▶ Half-heuslers, Chalcopyrites, *et. 2010, Chadov et al, Nat Mat 2010, Xiao et al, PRL, 2010*
- ▶ Many more...



What About d-Orbitals?



Specialize in **superconductivity**,
magnetism, **ferroelectricity**, **Mott**
insulating, etc.

+

Topological order

- ▶ Proximity effects between TIs and symmetry-breaking states, (magnetoelectric effects, Majorana fermions)
- ▶ Competing phases: Mott vs. TI

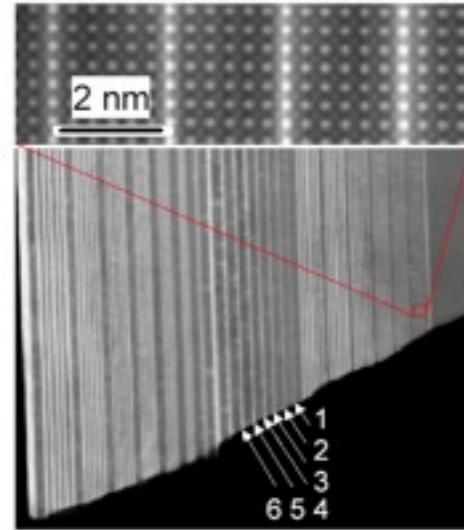
Shitade et al, 2009; Pesin & Balents, 2010

Heterostructures of Transition-Metal Oxides

Heterostructures of Transition-Metal Oxides

Artificial charge-modulation in atomic-scale perovskite titanate superlattices

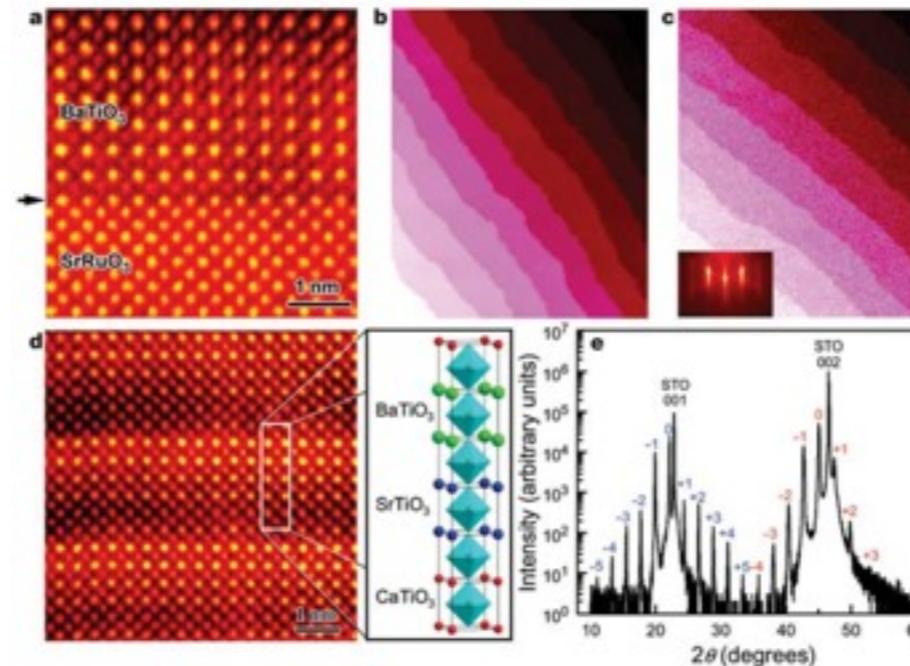
A. Ohtomo, D. A. Muller, J. L. Grazul & H. Y. Hwang



Strong polarization enhancement in asymmetric three-component ferroelectric superlattices

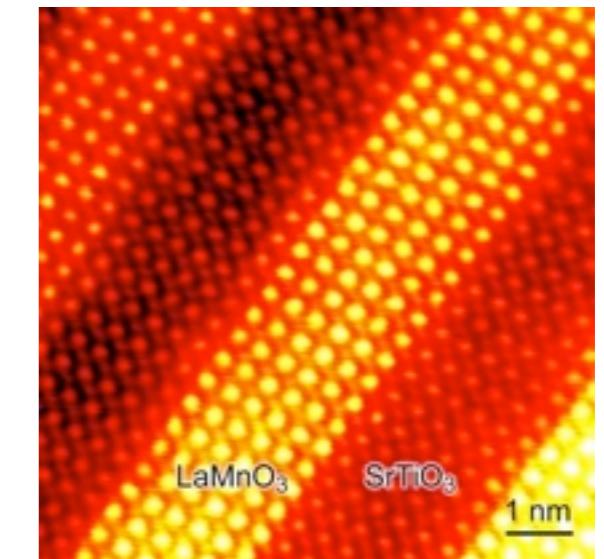
Ho Nyung Lee, Hans M. Christen, Matthew F. Chisholm, Christopher M. Rouleau & Douglas H. Lowndes

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



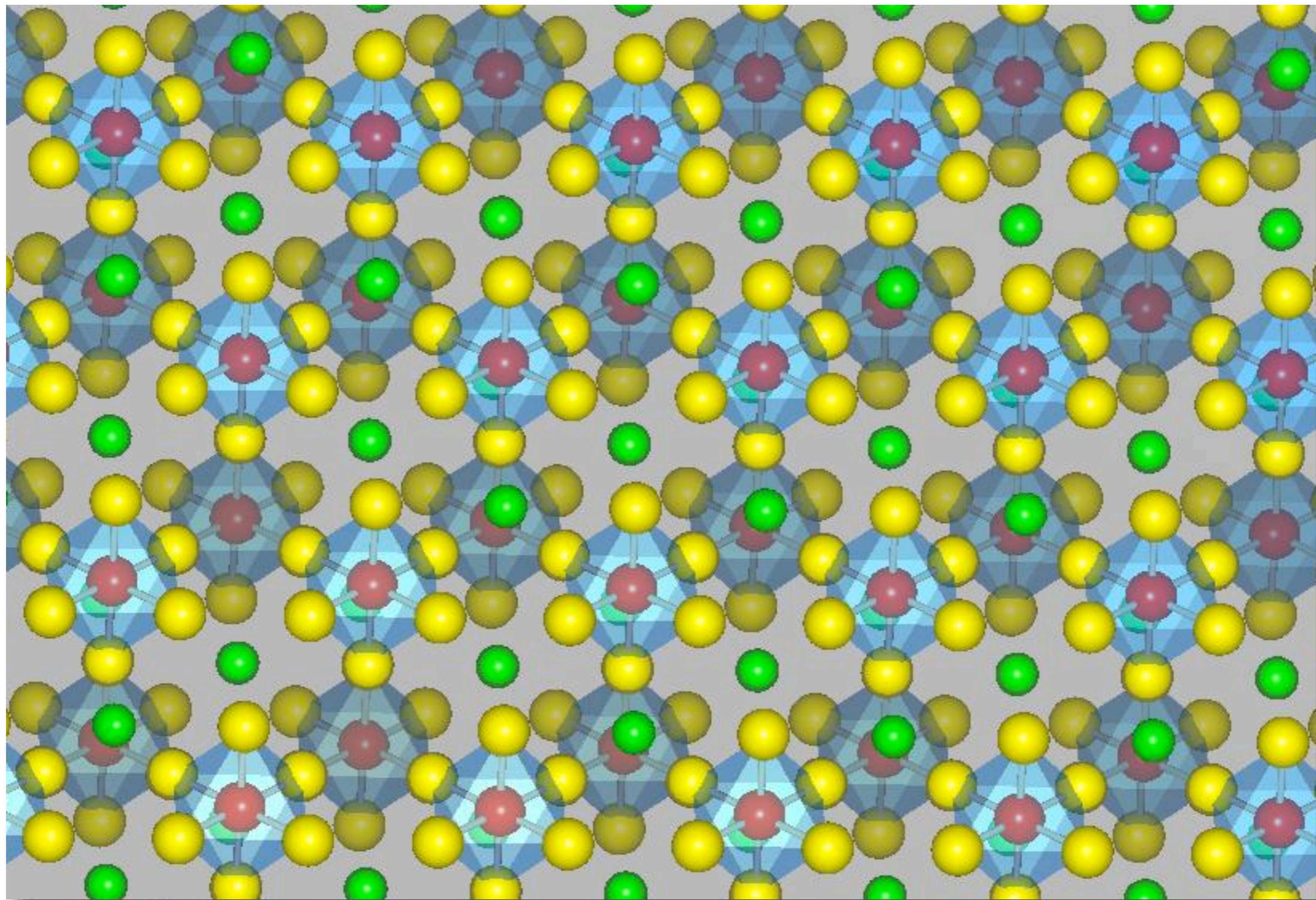
$[\text{LaMnO}_3]_n[\text{SrTiO}_3]_m$ superlattice

by courtesy of H. N. Lee, ORNL



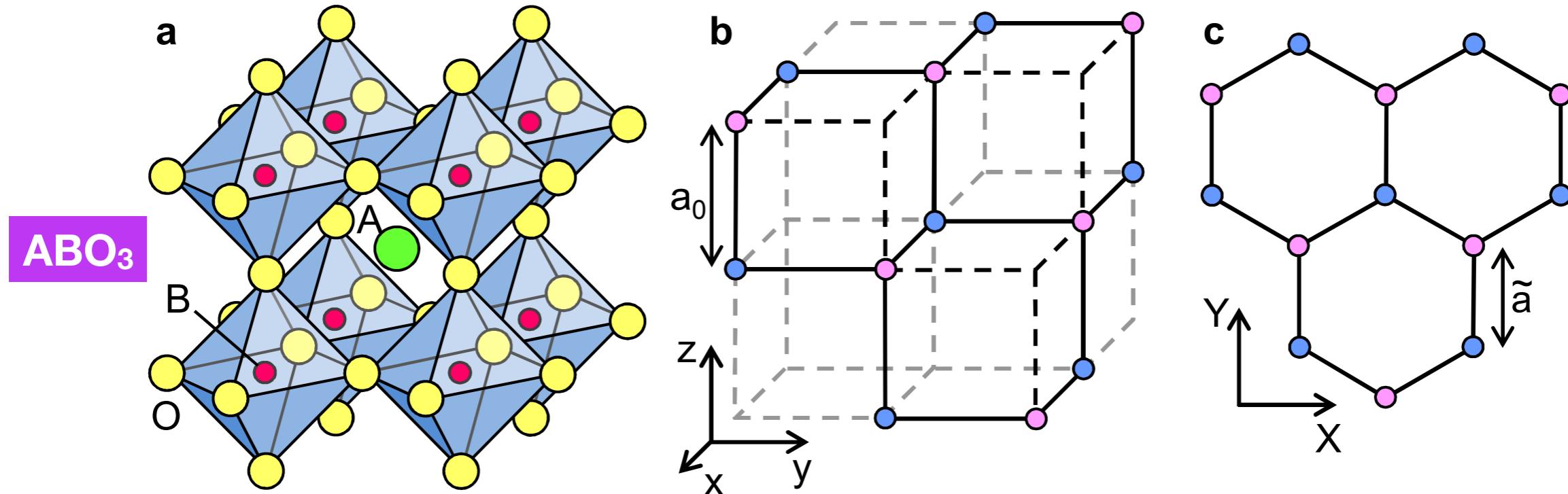
- ▶ Layered structure can be prepared with atomic precision
- ▶ Great flexibility: tunable lattice constant, carrier concentration, spin-orbit interaction, correlation strength

Perovskite (111)-bilayer



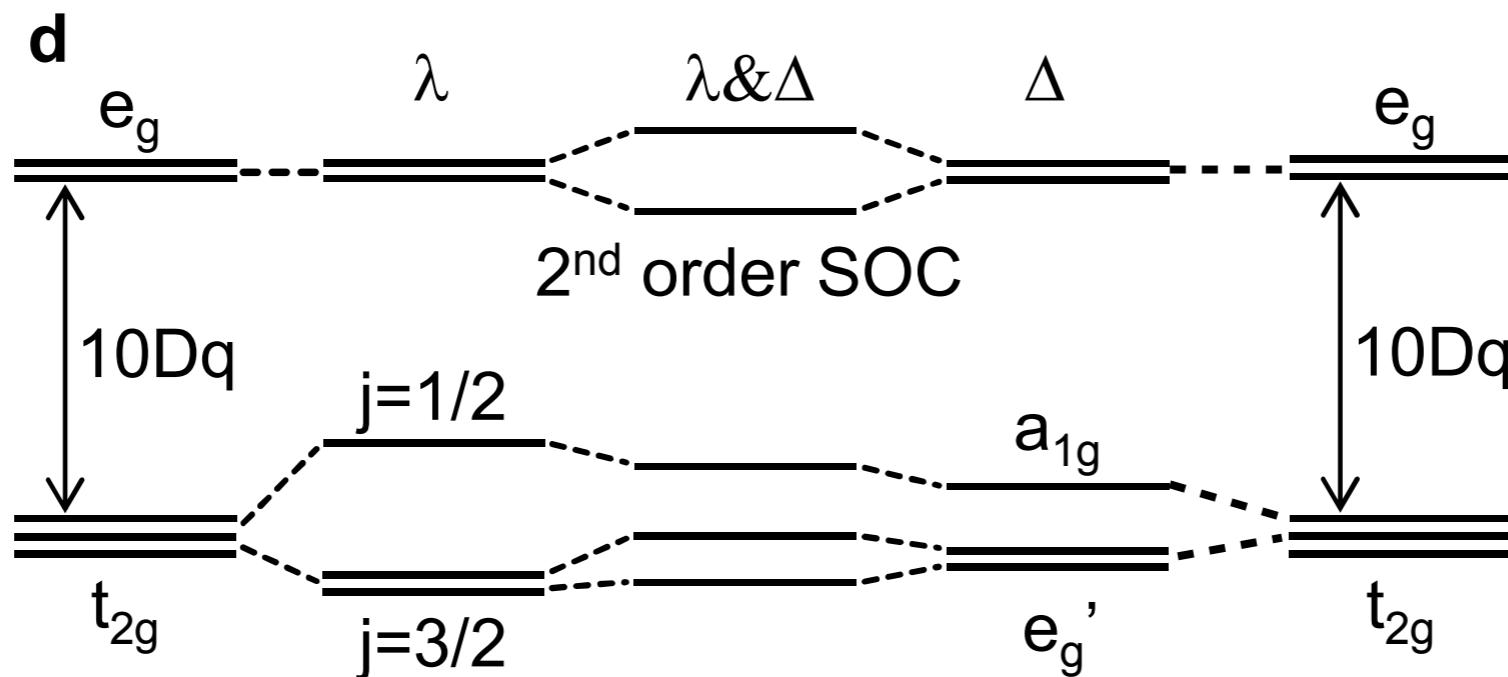
Credit: Satoshi Okamoto

Perovskite (111)-bilayer



- ▶ Honeycomb lattice: Similar physics to graphene is expected
- ▶ Sublattices on different layer: Inversion symmetry breaking can be externally controlled (i.e., gating or asymmetric substrates)
- ▶ Reduced crystal field symmetry: Octahedral to **trigonal**

Atomic Orbitals in Crystal Field + SO

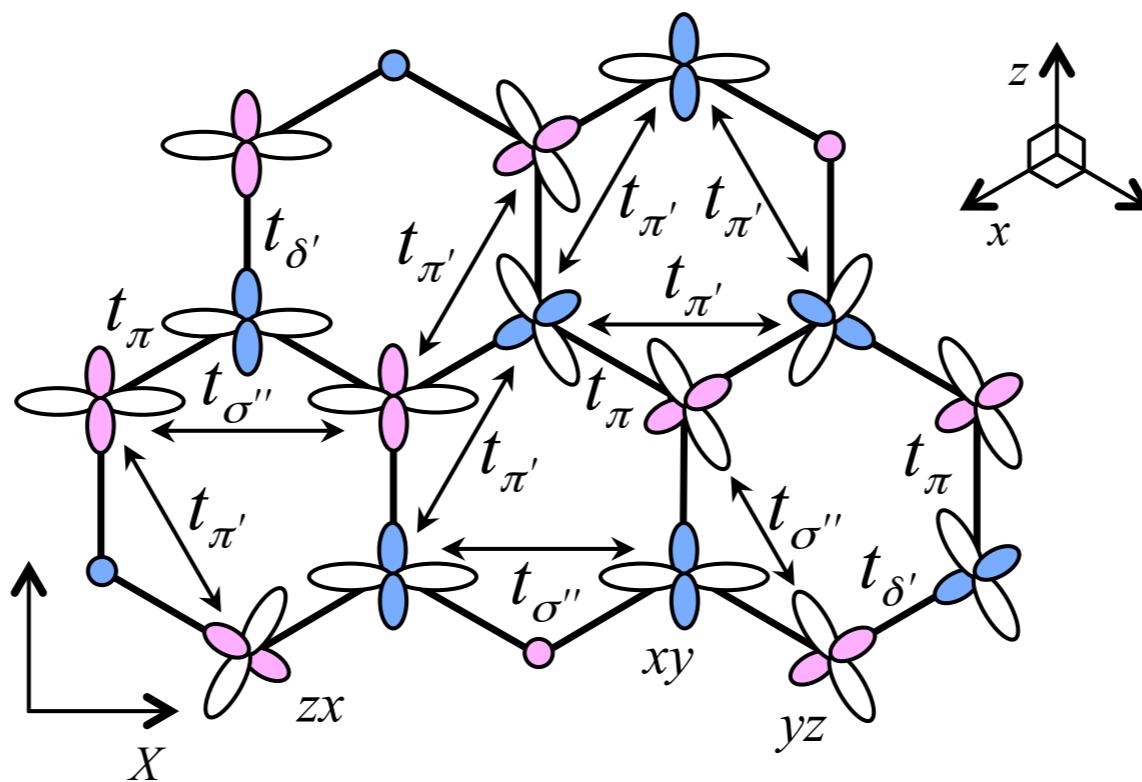


Spin-orbit interaction + Trigonal symmetry



t_{2g} orbitals

$$H = H_{\text{hop}} + \lambda \sum_i \vec{L}_i \cdot \vec{s}_i + H_{\text{crystal}} + \frac{V}{2} \sum_i \xi_i c_i^\dagger c_i$$

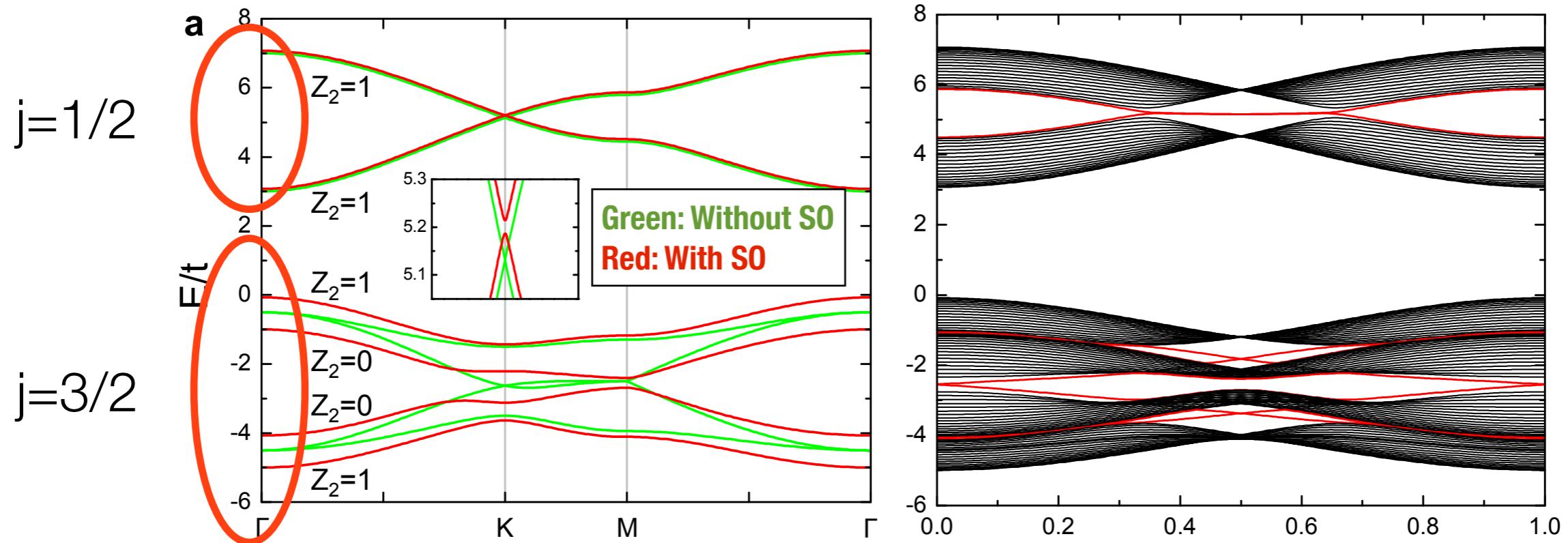


t_{2g} Orbitals - Strong SOC

$$\frac{\lambda}{t} > \frac{8}{3}$$

$j=1/2$ and $j=3/2$ manifolds are completely separated

t_{2g}^2, t_{2g}^5 are possible candidates

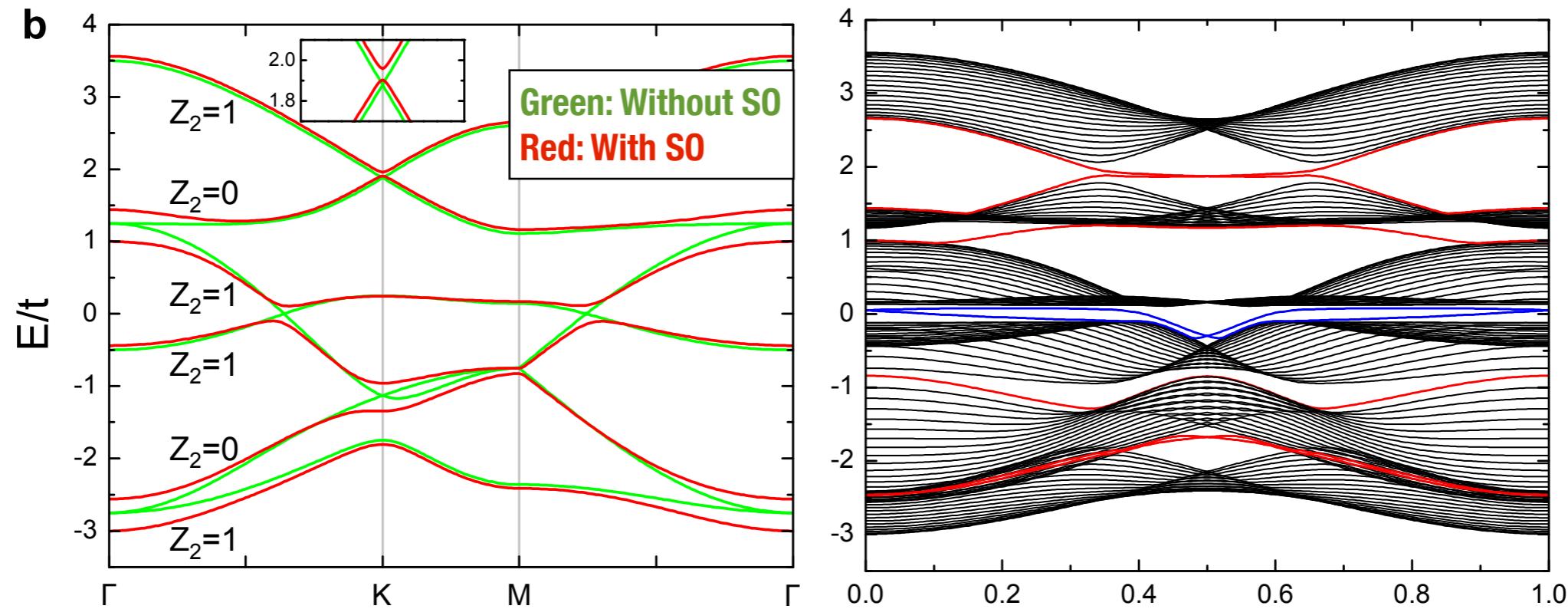


t_{2g} Orbitals - Weak SOC

$$\frac{\lambda}{t} < \frac{8}{3}$$

$j=1/2$ and $j=3/2$ manifolds are mixed away from Gamma

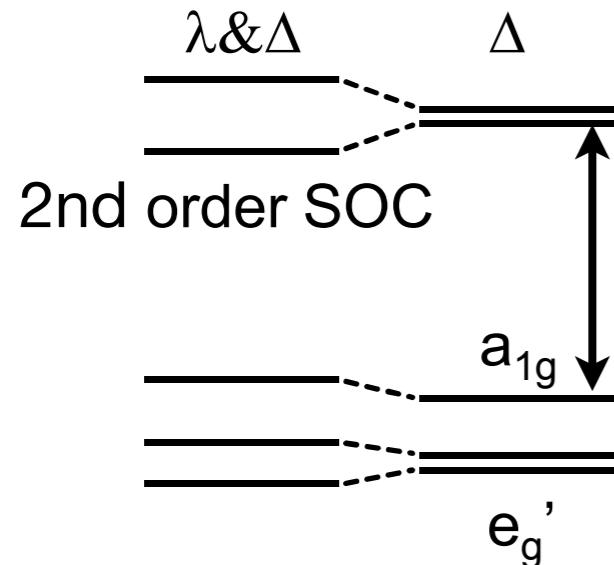
$t_{2g}^2, t_{2g}^4, t_{2g}^5$ are possible candidates



e_g Orbitals

$$H = H_{\text{hop}} + H_{\text{SO}} + \frac{V}{2} \sum_i \xi_i c_i^\dagger c_i$$

Allowed by trigonal symmetry



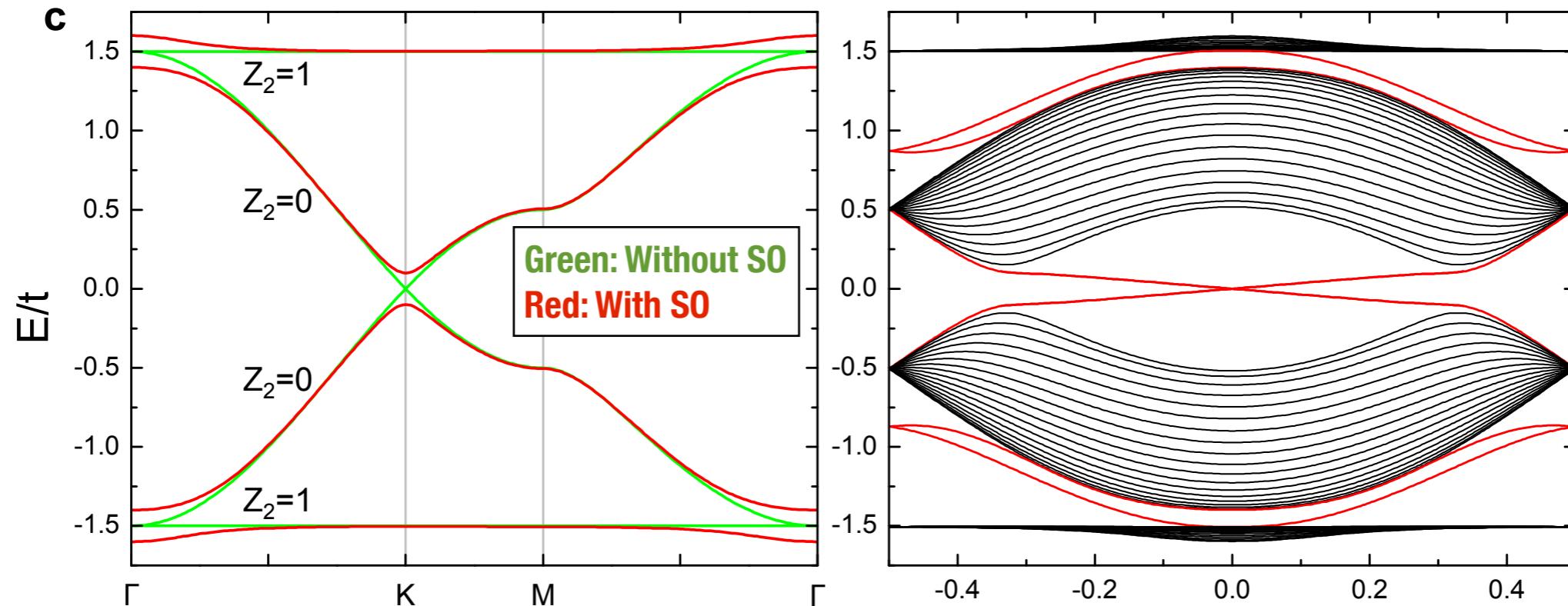
$$H_{\text{SO}}^{lm} = \lambda^2 \sum_{\tau \notin e_g} \frac{\langle l | \vec{L} \cdot \vec{s} | \tau \rangle \langle \tau | \vec{L} \cdot \vec{s} | m \rangle}{E_{eg} - E_\tau}$$

Vanishes in the limit of $\Delta \rightarrow 0$

Similar to graphene, see *Min et al, PRB 2006*

e_g Orbitals

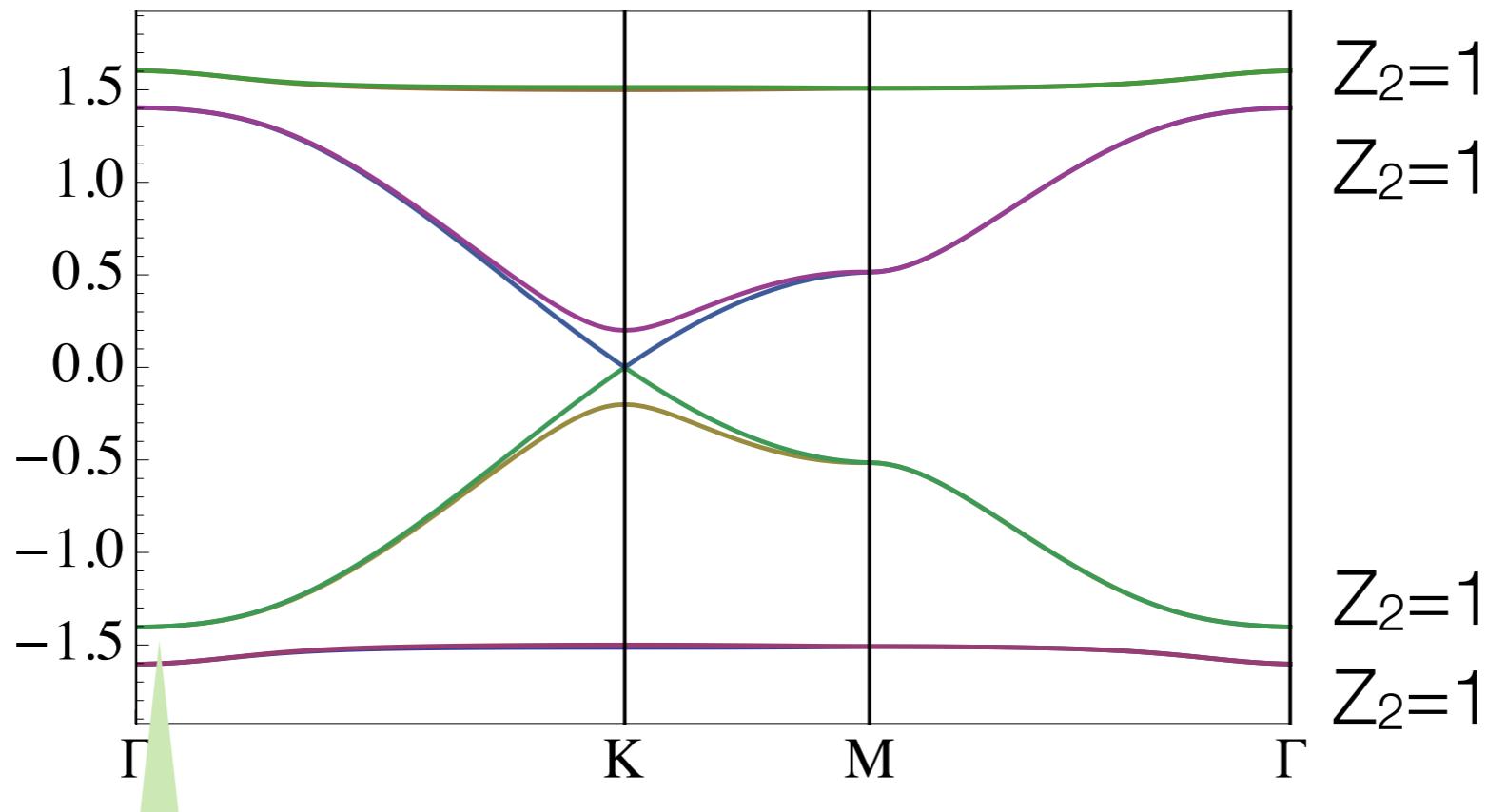
e_g^1, e_g^2, e_g^3 are possible candidates



Nearly flat Z_2 band obtained if $V_{dd\delta}/V_{dd\sigma} \sim 0$

Control of Topological Order

- Topological order can be destroyed by inversion symmetry breaking



This gap is robust against inversion symmetry breaking, closes if the Jahn-Teller effect is strong

Materials Consideration

Periodic Table of the Elements

© www.elementsdatabase.com

■ hydrogen

■ alkali metals

■ alkali earth metals

■ transition metals

■ poor metals

■ nonmetals

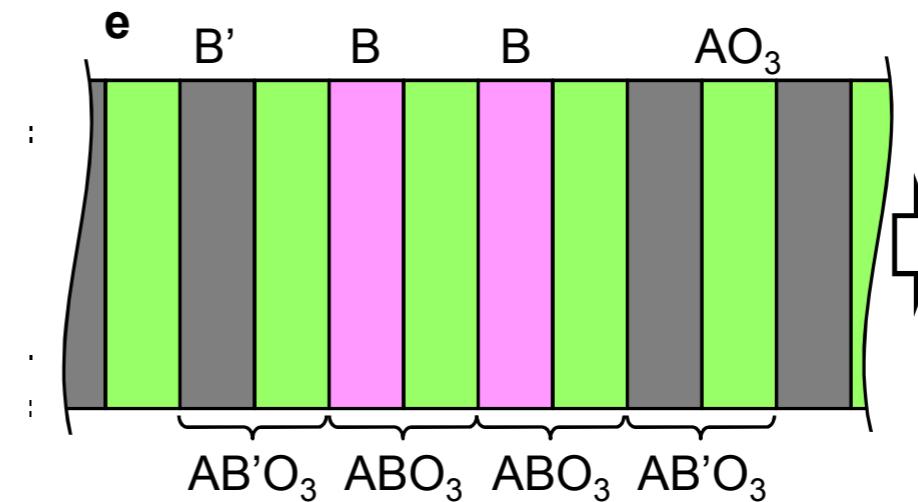
■ noble gases

■ rare earth metals

H	1	He	2																								
Li	3	Be	4																								
Na	11	Mg	12																								
K	19	Ca	20																								
Rb	37	Sr	38																								
Cs	55	Ba	56																								
Fr	87	Ac	88																								
Pr	59	Unq	89																								
Pa	91	Unp	104																								
U	92	Unh	105																								
Np	93	Uns	106																								
Pu	94	Uno	107																								
Am	95	Une	108																								
Cm	96	Unn	109																								
Bk	97		110																								
Cf	98																										
Es	99																										
Fm	100																										
Md	101																										
No	102																										
Lr	103																										
Ce	58	Pr	59	Nd	60	Pm	61	Sm	62	Eu	63	Gd	64	Tb	65	Dy	66	Ho	67	Er	68	Tm	69	Yb	70	Lu	71
Th	90	Pa	91	U	92	Np	93	Pu	94	Am	95	Cm	96	Bk	97	Cf	98	Es	99	Fm	100	Md	101	No	102	Lr	103

Materials Consideration

$A=La^{3+}, Sr^{2+}$
 $LaBO_3 \rightarrow B^{3+}$
 $SrBO_3 \rightarrow B^{4+}$



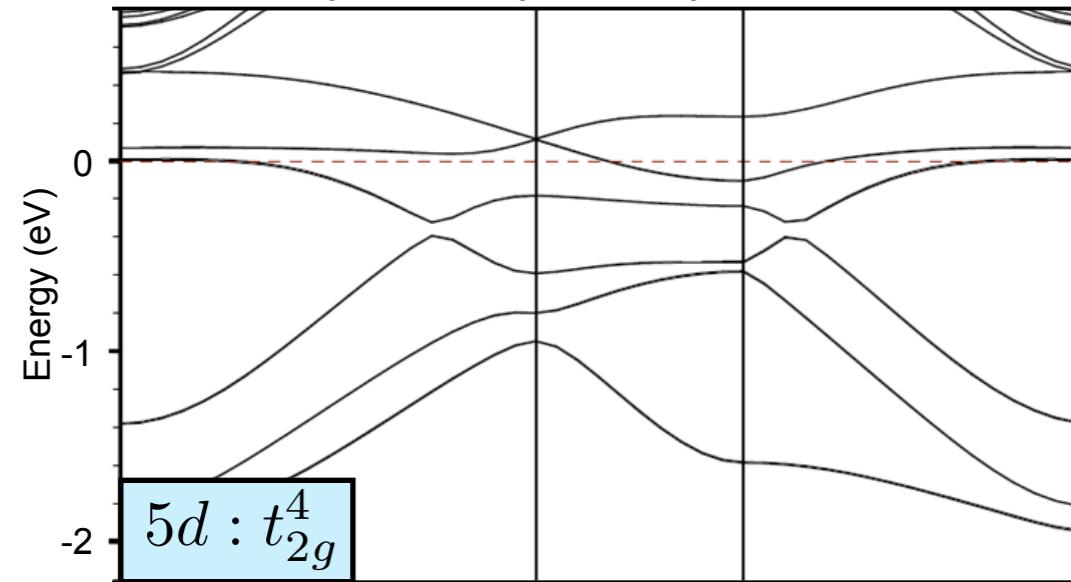
AB'O₃: LaAlO₃ and SrTiO₃

TABLE SI: List of candidate materials

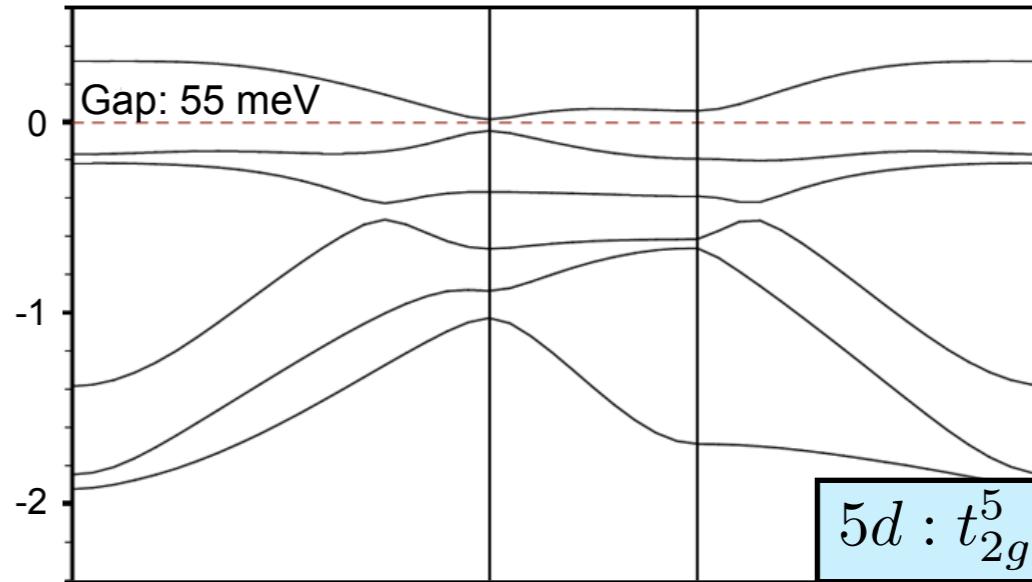
	Configuration	Bulk	Superlattice
LaReO ₃	t_{2g}^4	—	—
LaRuO ₃	t_{2g}^5	metallic Ref. [2]	—
SrRhO ₃	t_{2g}^5	metallic Ref. [3]	Ref. [4]
SrIrO ₃	t_{2g}^5	metallic Refs. [5, 6]	metallic Ref. [7]
LaOsO ₃	t_{2g}^5	—	—
LaAgO ₃	e_g^2	metallic (band calc.) Ref. [8]	—
LaAuO ₃	e_g^2	Refs. [9, 10]	—

t_{2g} Systems

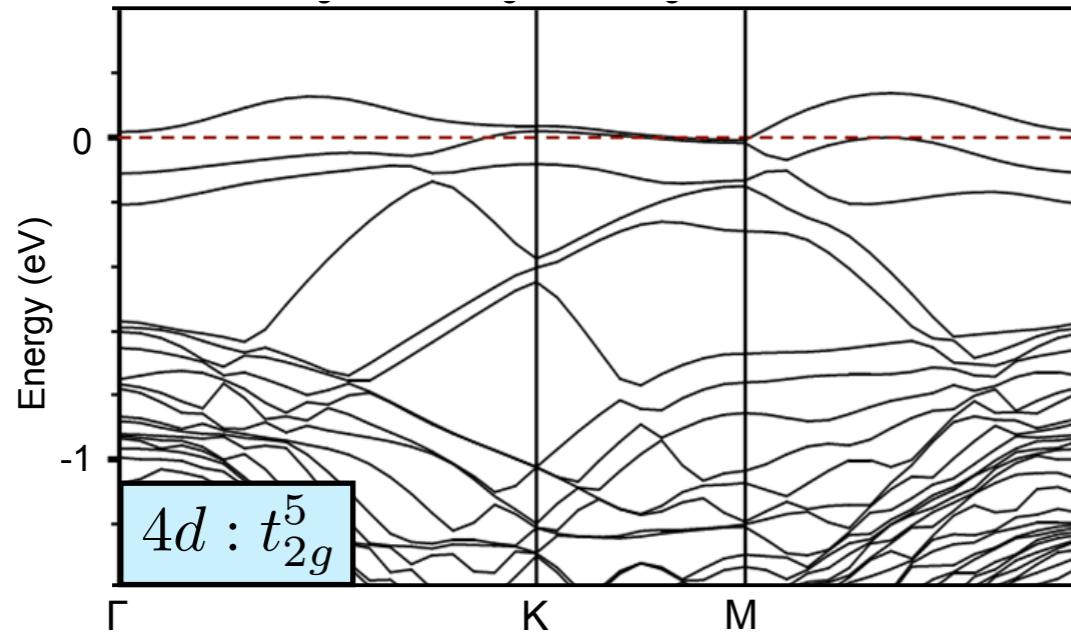
$\text{LaAlO}_3/\text{LaReO}_3/\text{LaAlO}_3$



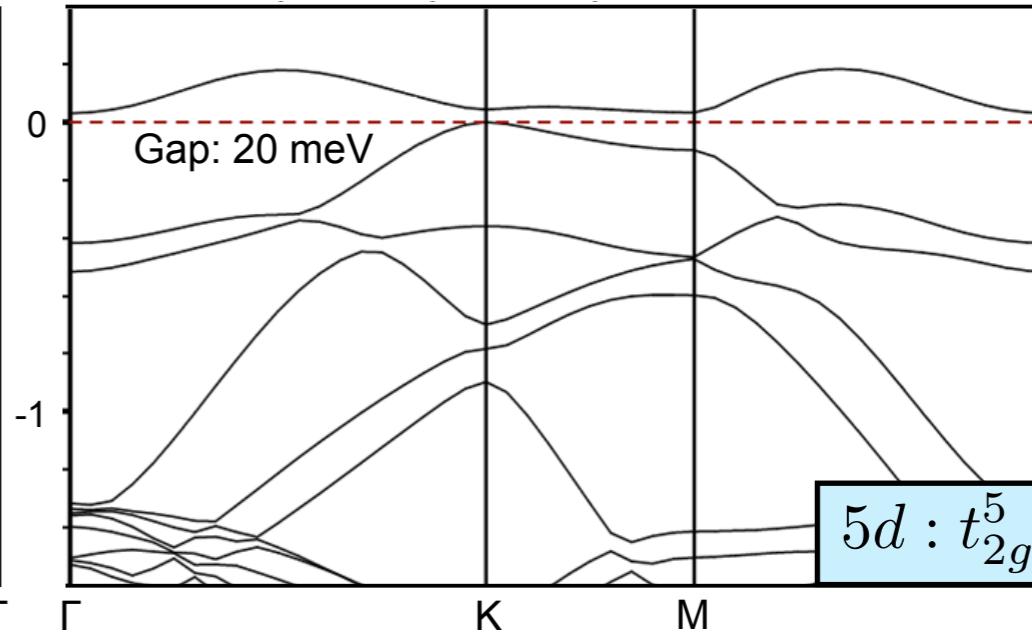
$\text{LaAlO}_3/\text{LaOsO}_3/\text{LaAlO}_3$



$\text{SrTiO}_3/\text{SrRhO}_3/\text{SrTiO}_3$

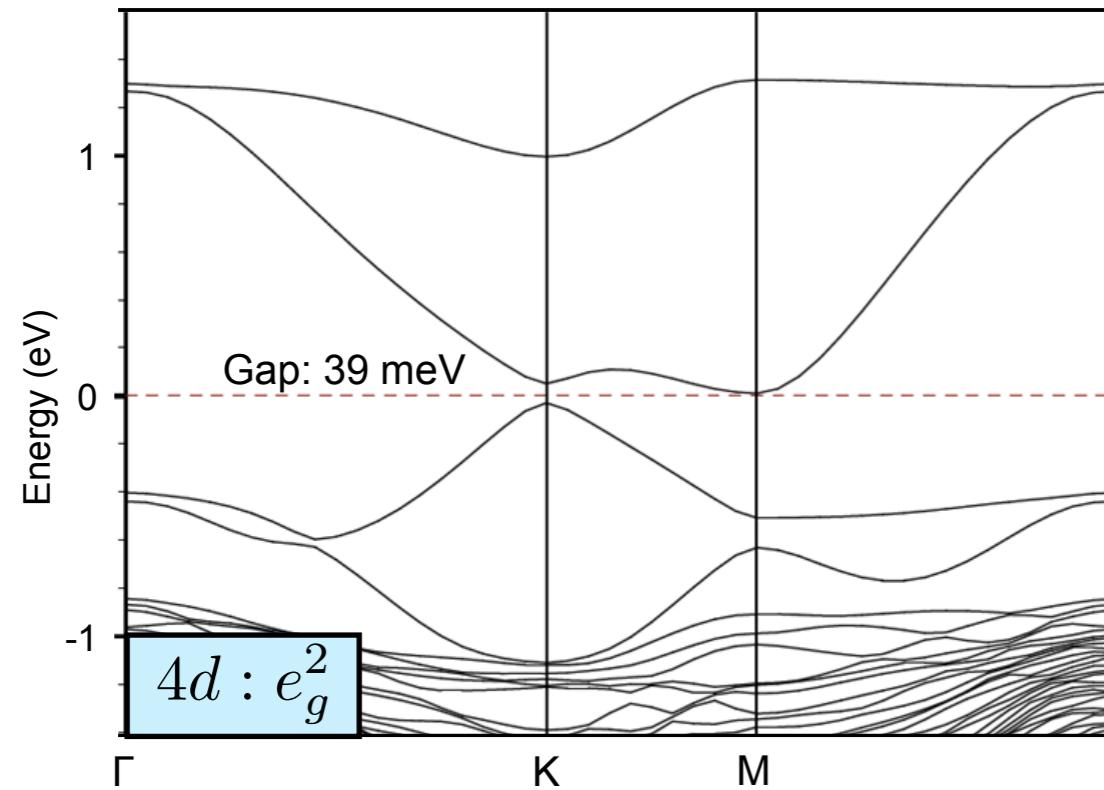


$\text{SrTiO}_3/\text{SrIrO}_3/\text{SrTiO}_3$

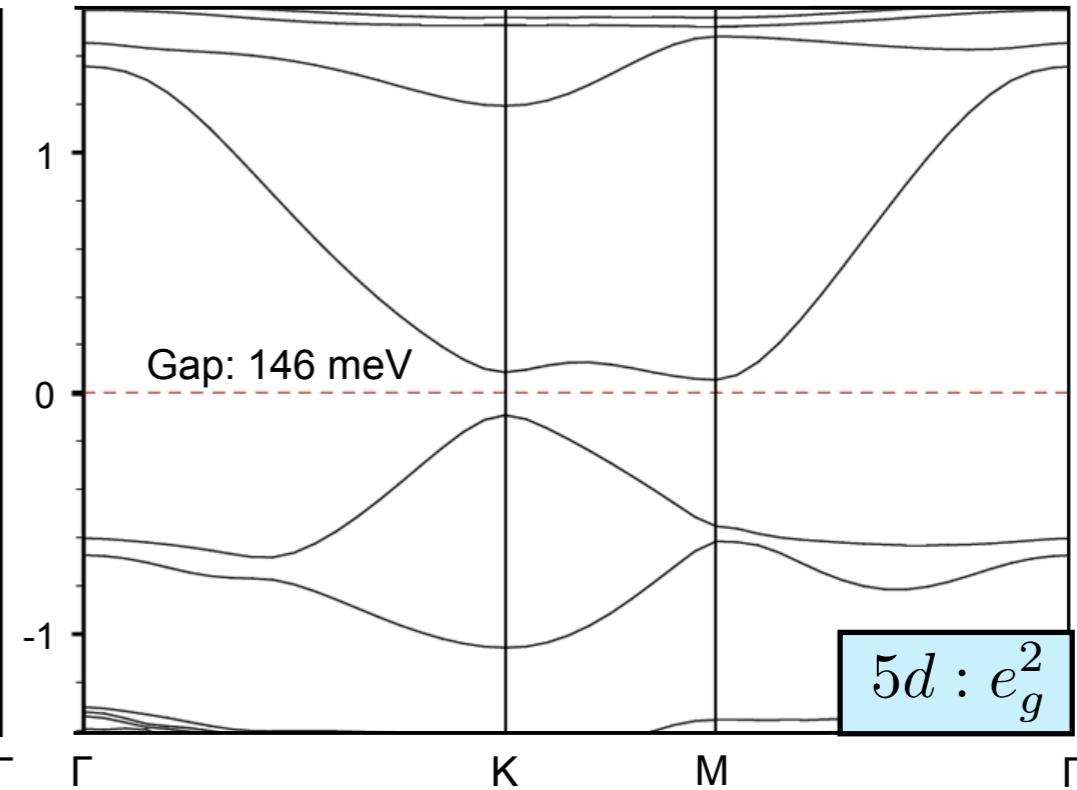


e_g Systems

$\text{LaAlO}_3/\text{LaAgO}_3/\text{LaAlO}_3$



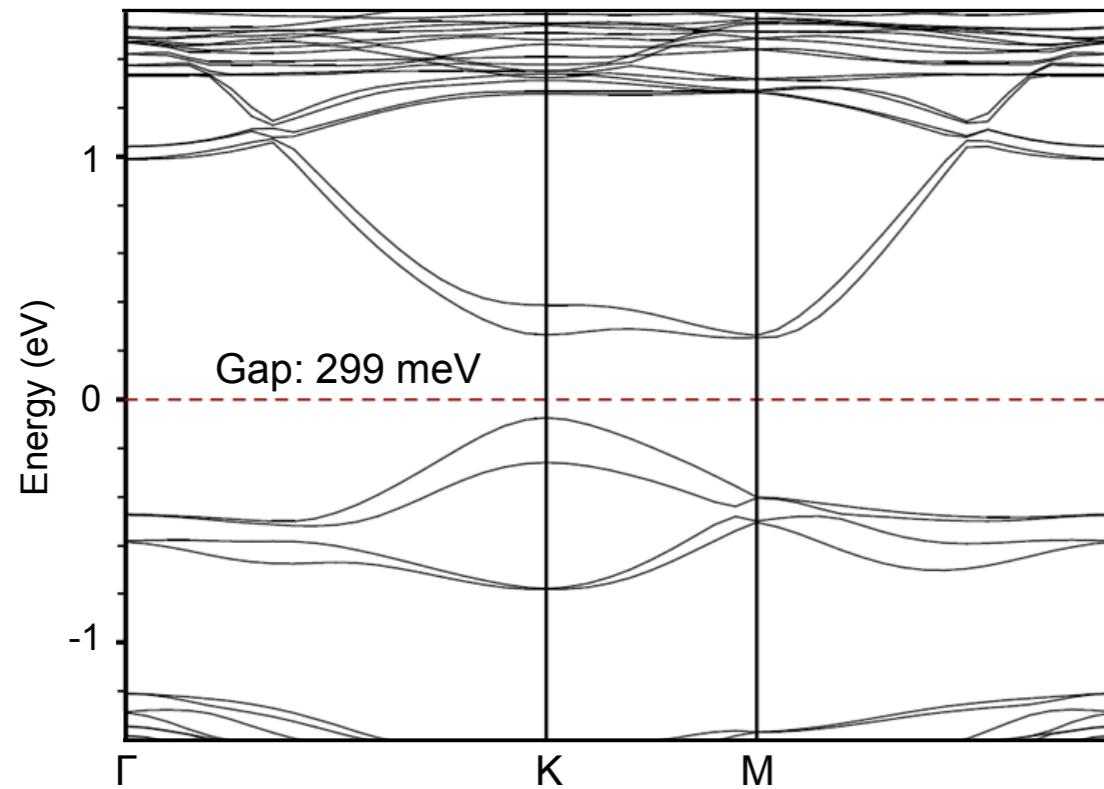
$\text{LaAlO}_3/\text{LaAuO}_3/\text{LaAlO}_3$



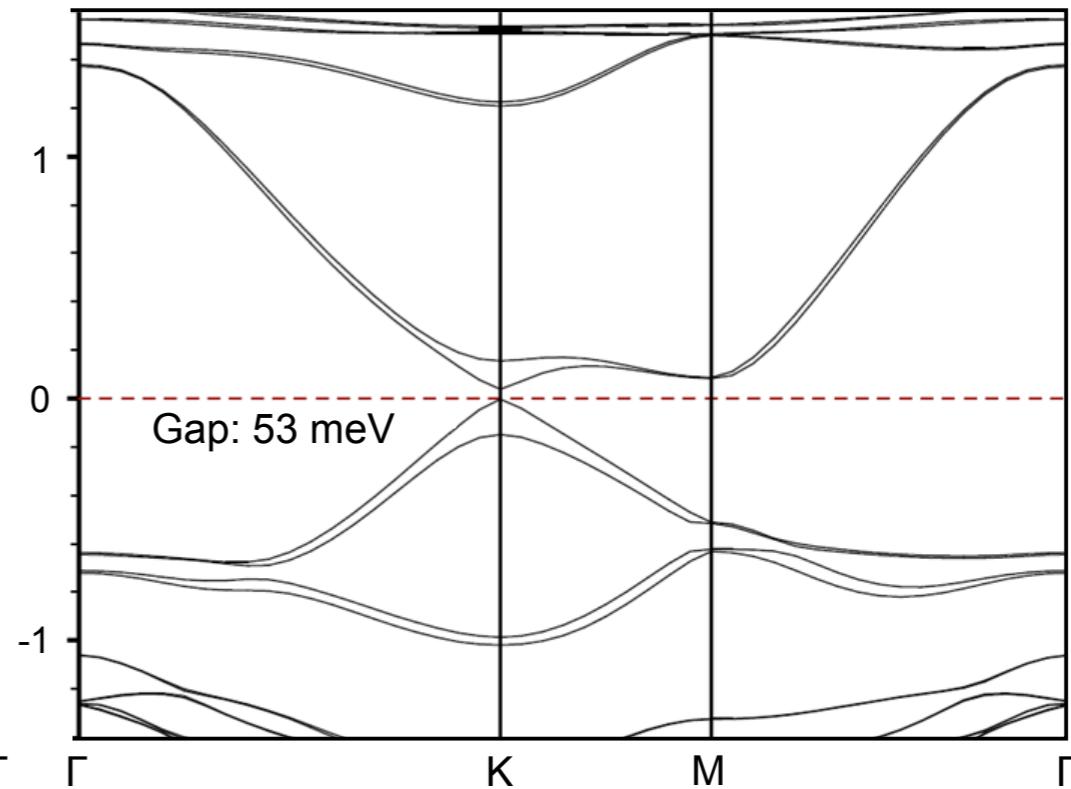
LaAuO₃ bilayer has an energy gap ~ 2000 K

Asymmetric Substrates

LaAlO₃/LaAuO₃/LaScO₃



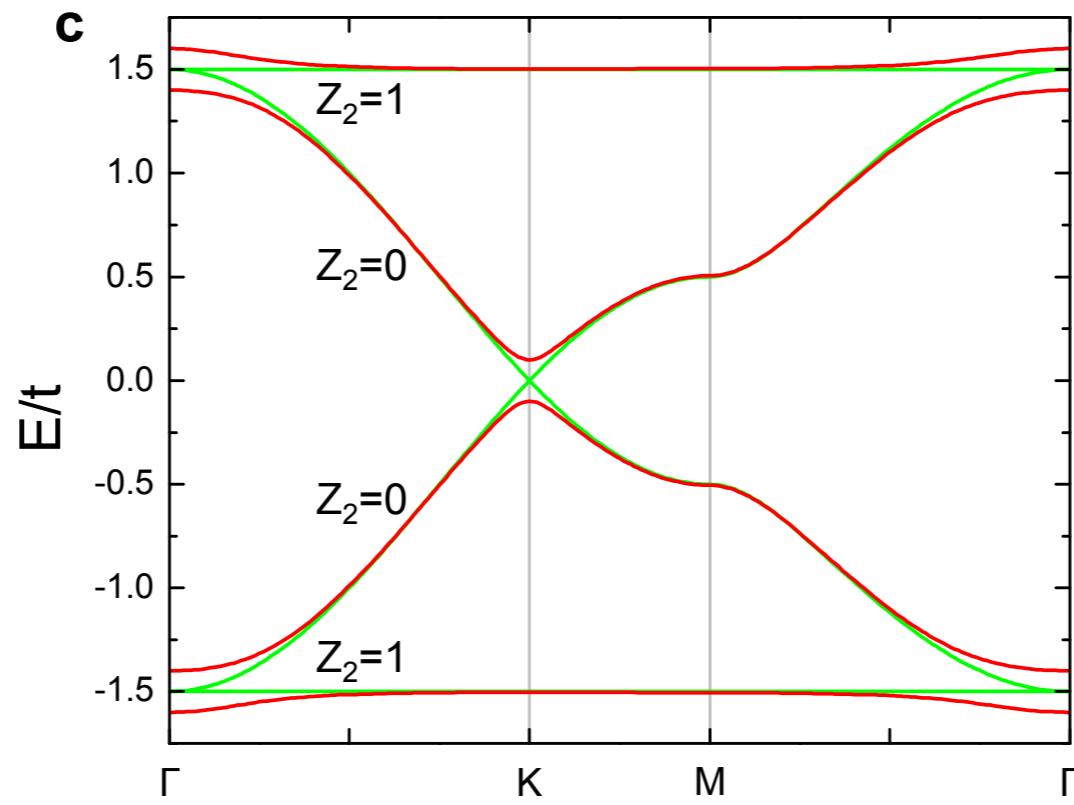
LaAlO₃/LaAuO₃/YAlO₃



Trivial insulator

Topological insulator

Physics inside Flat Z_2 Bands

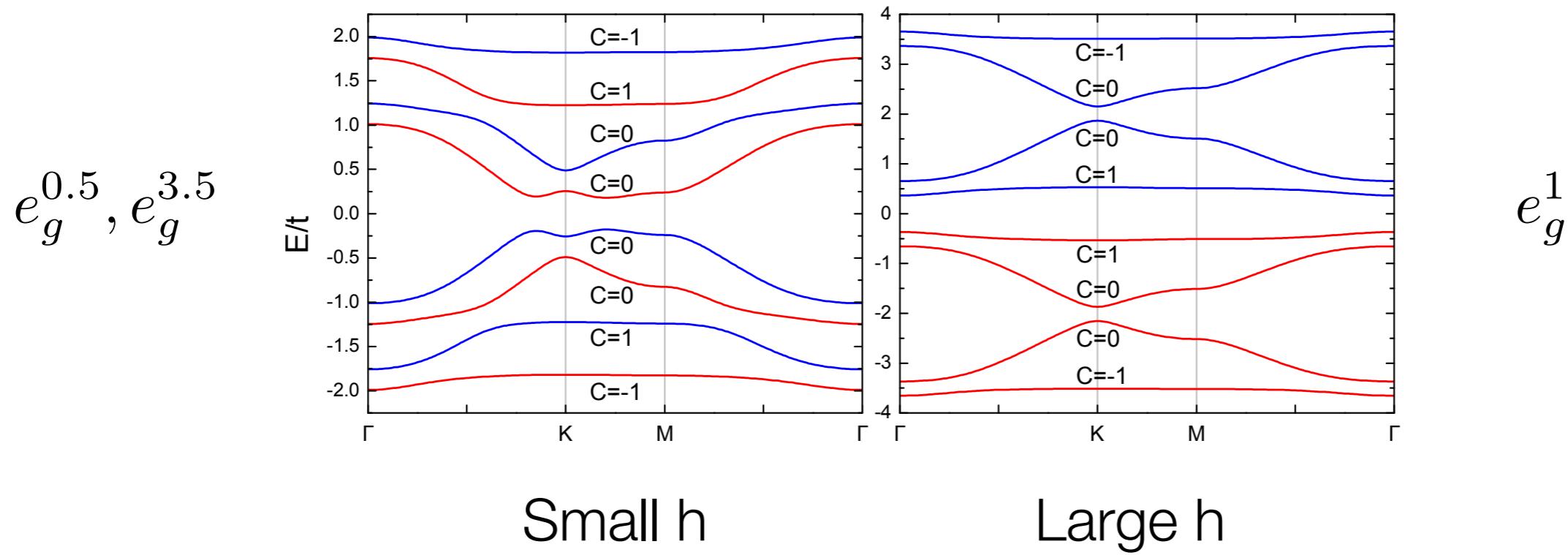


Integer Quantum Hall Effect

How to break time-reversal symmetry?

- ▶ External: Ferromagnetic or G-type antiferromagnetic substrate
- ▶ Internal: Stoner instability ($U/\text{Bandwidth} \gg 1$)

Mean field Hamiltonian $H = H_{eg} + \vec{h} \cdot \vec{\sigma}$



Fractional Quantum Hall Effect

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

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

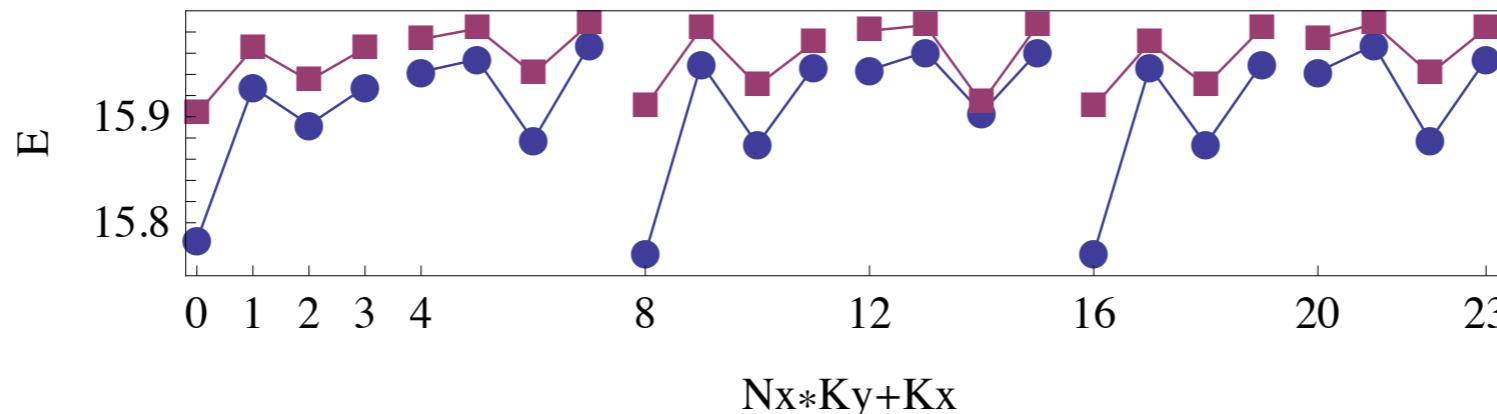
U: Onsite intra-orbital repulsion
U': On-site inter-orbital repulsion
V: Nearest-neighbor repulsion

$$U = U' = t, V = 0.5t$$

What is the Hall conductance for a 1/3 filled nearly flat band

Fractional Quantum Hall Effect

- ▶ 3-fold degenerate GS



- ▶ Chern number

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

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

Other proposals, see Tang et al PRL; Neupert et al PRL; Sun et al PRL, 2011

What is Next?

- ▶ Competition between Jahn-Teller effect and TI phase
- ▶ Detailed adjustment of the band dispersion
- ▶ Complete phase diagram (multi-orbital Kane-Mele-Hubbard model)
- ▶ Identification of materials suitable for IQHE and FQHE
- ▶ The nature of the FQHE state in the absence of LL

Actually grow the sample

LaAuO₃

Summary

- ▶ Heterostructures of transition metal oxides provide an exciting platform for topological electronics
- ▶ Lots of perovskite (111)-bilayers are possible candidates for topological insulators. In particular, LaAuO_3 has a band gap $\sim 200\text{meV}$
- ▶ Lots of possibilities for realizing novel quantum phases, such as IQHE and FQHE
- ▶ Lots to be done...

Manuscript can be found on arXiv