

# Quantum Hall Effects in Heterostructures of Transition-Metal Oxides

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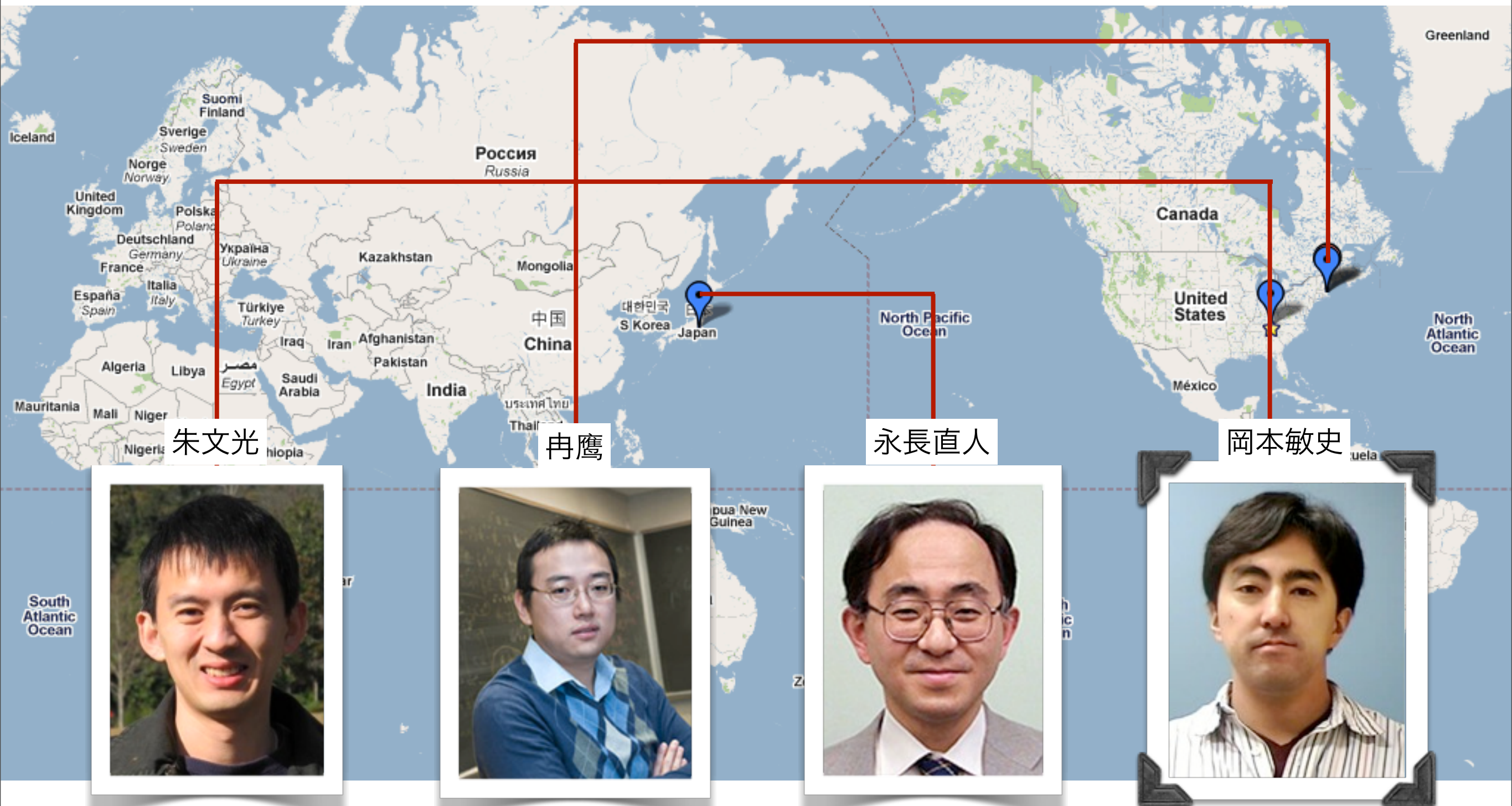
Di Xiao

*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

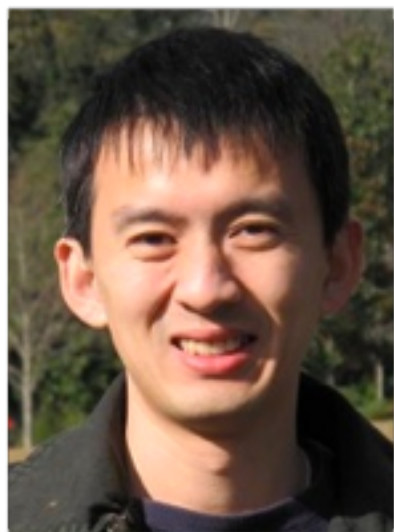


朱文光

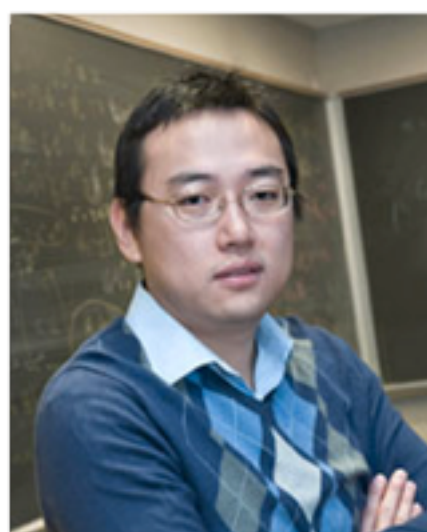
冉鷹

永長直人

岡本敏史



Wenguang Zhu  
Knoxville



Ying Ran  
Boston



Naoto Nagaosa  
Tokyo



Satoshi Okamoto  
Oak Ridge

# Outline

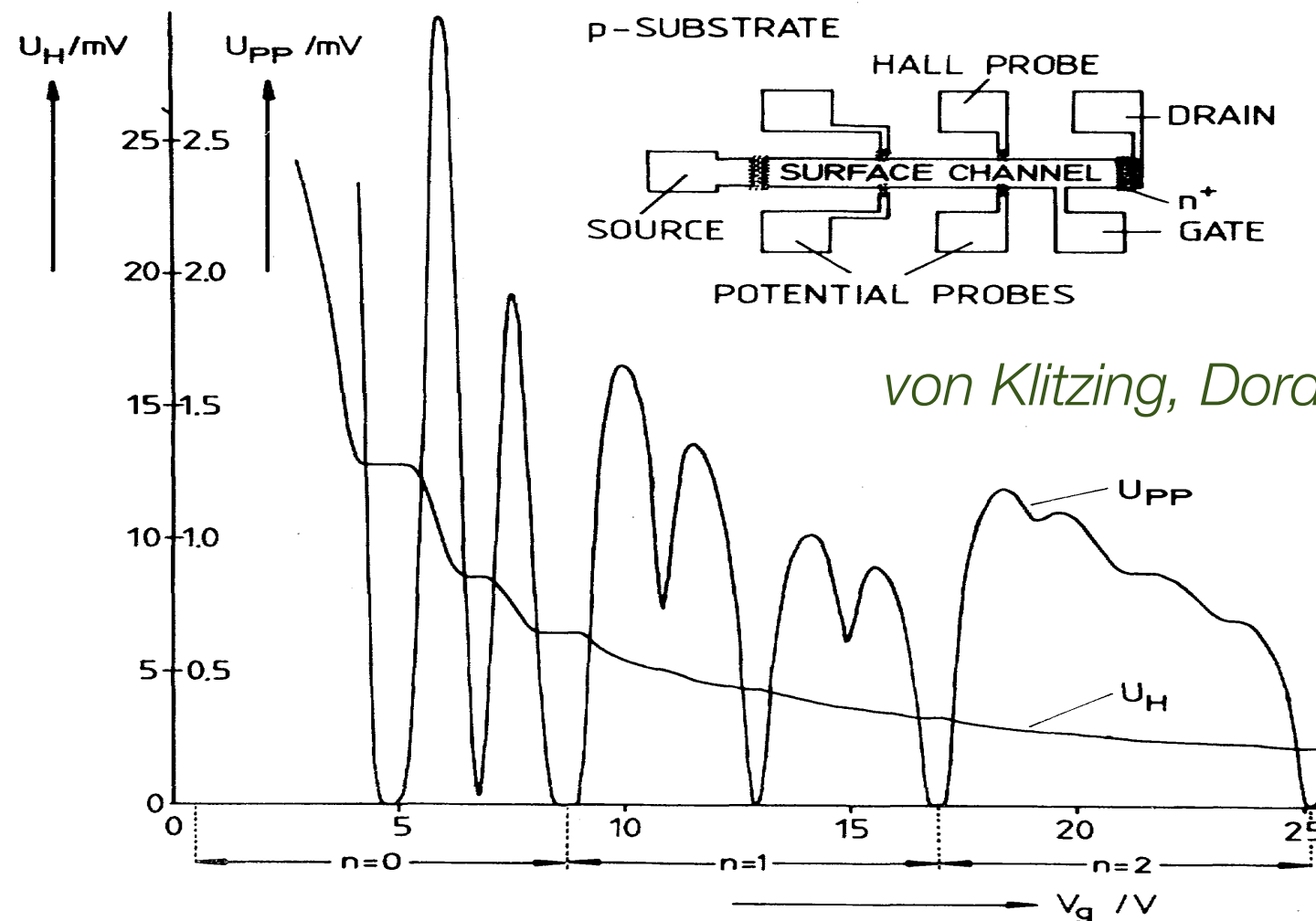
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- ▶ The quest for topological states of matter
  - Quantum Hall Effect
  - Topological Insulators
- ▶ Heterostructures of transition-metal oxides
  - Quantum spin Hall effect
  - Integer quantum Hall effect
  - Fractional quantum Hall effect
- ▶ Summary

# **The Quest for Topological States of Matter**



# The QHE: A Tribute to Materials Advance

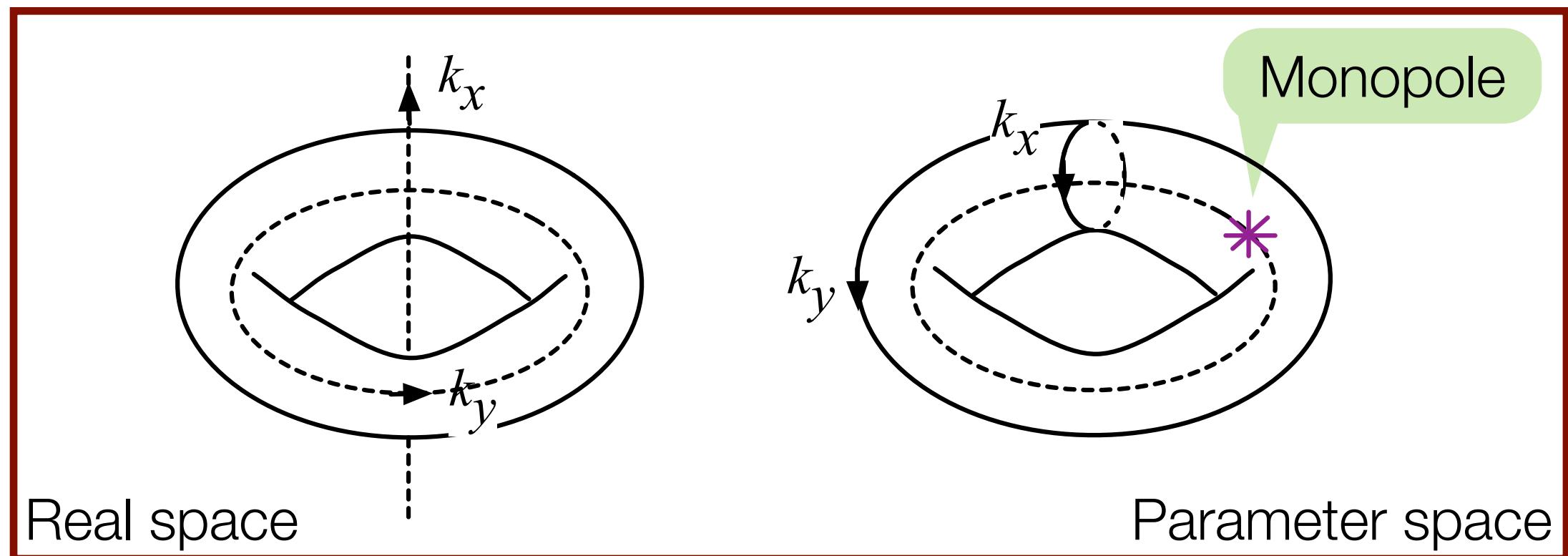


“It should also be mentioned that advances in technology and production methods within semiconductor electronics have played a crucial role in the study of two-dimensional electron systems, and were a precondition for the discovery of the quantised Hall effect.” —*Press Release: The 1985 Nobel Prize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

# Precise Quantization: Topological Origin

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

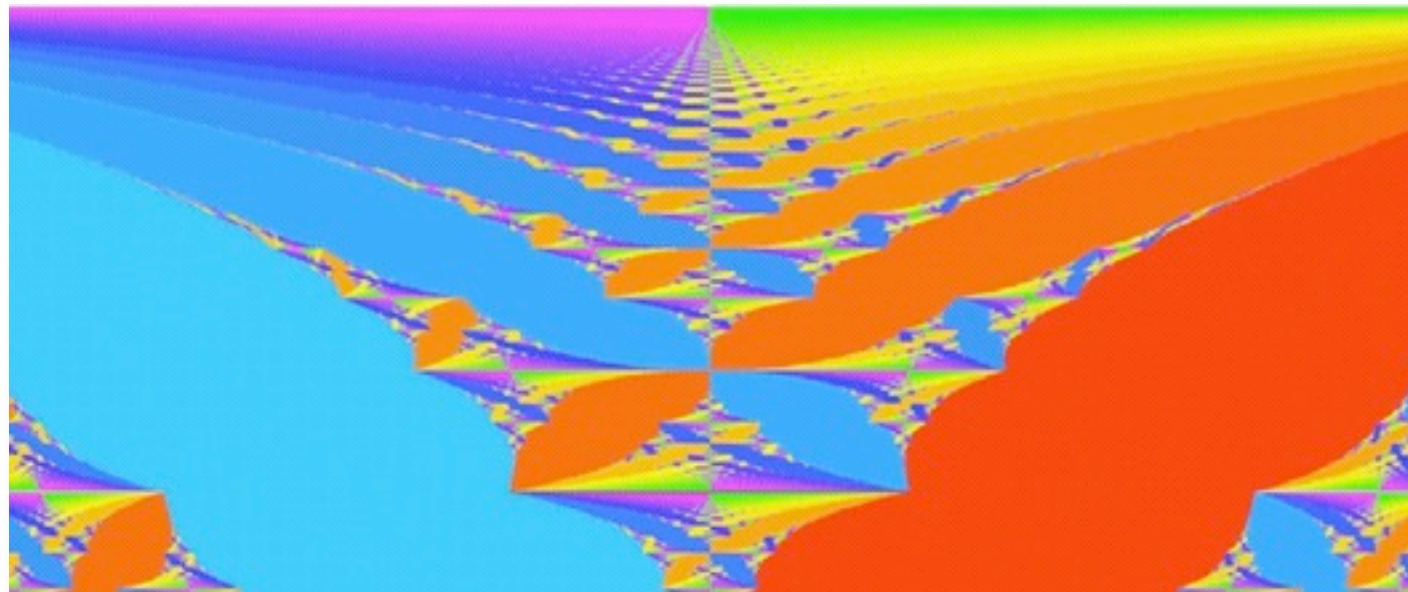
$$\sigma_{xy} = \frac{ie^2}{2\pi h} \int d^2k \left( \left\langle \frac{\partial \Phi_0}{\partial k_x} \middle| \frac{\partial \Phi_0}{\partial k_y} \right\rangle - \left\langle \frac{\partial \Phi_0}{\partial k_y} \middle| \frac{\partial \Phi_0}{\partial k_x} \right\rangle \right)$$



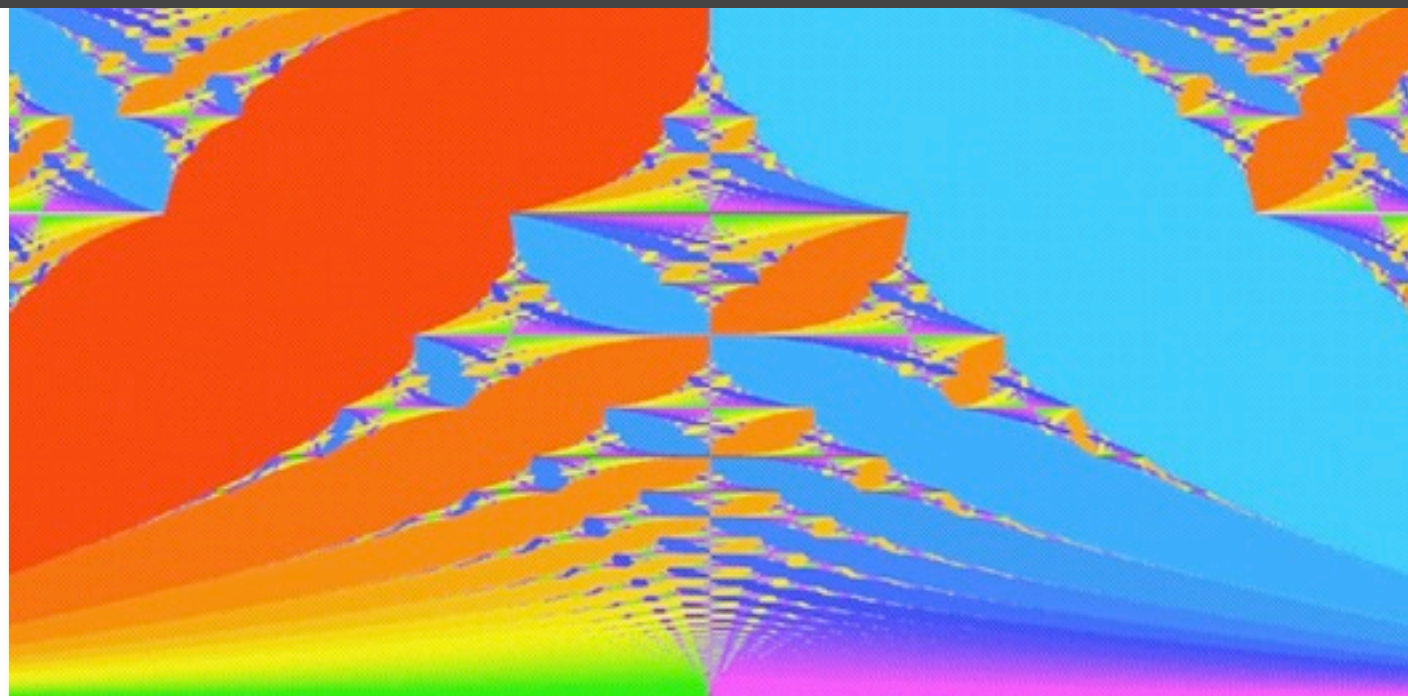
*Thouless et al, 1982; Niu, Wu & Thouless, 1985*

# The Magnetic Butterfly

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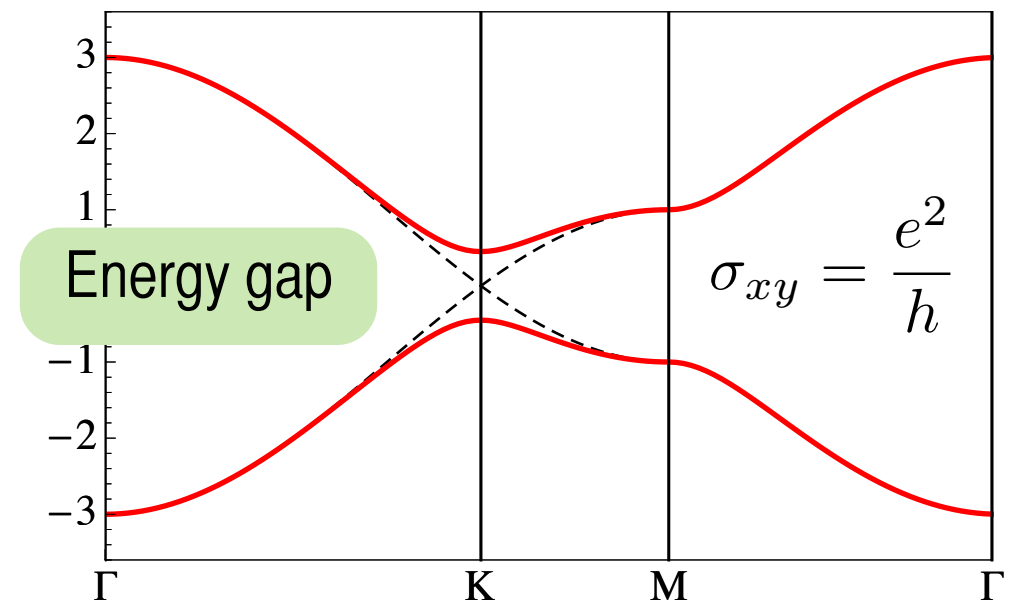
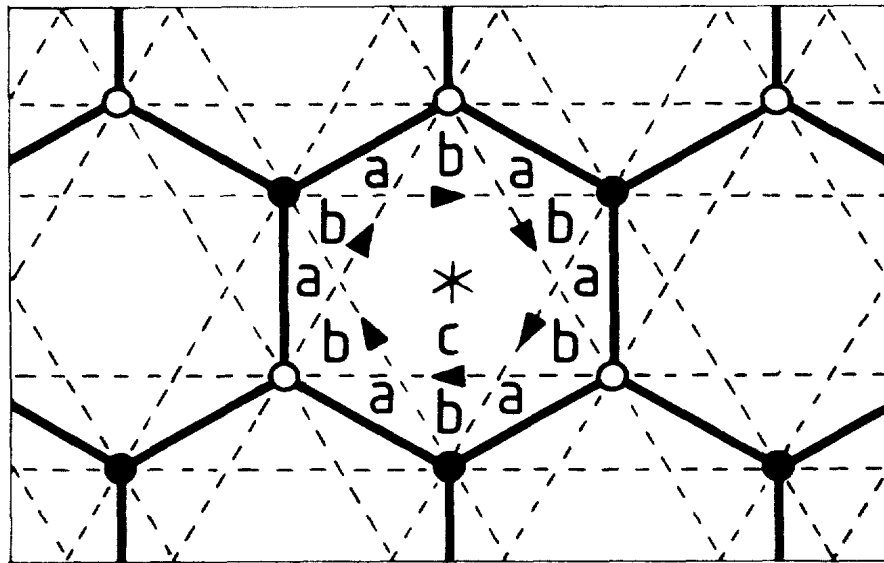
**Is Magnetic Field Necessary?**



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

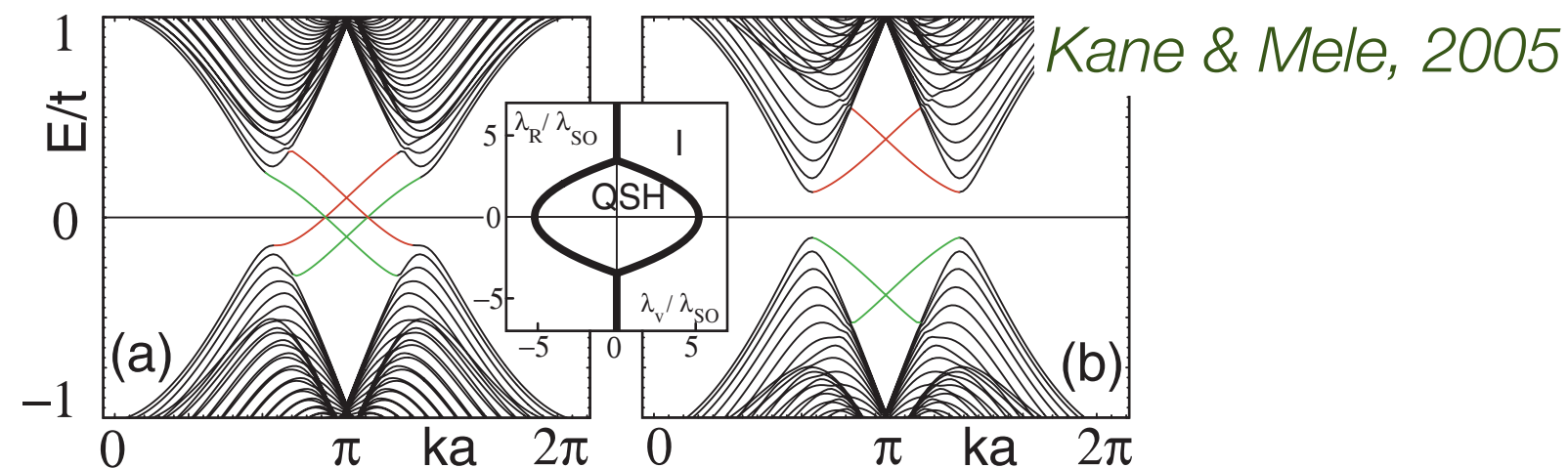
T-symmetry breaking  $\Delta_{\text{Haldane}}\sigma_z\tau_z$

Spin-orbit interaction  $\Delta_{\text{SO}}\sigma_z\tau_zs_z$

$(\sigma_z, \tau_z, s_z) =$

(sublattice, valley, spin)

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



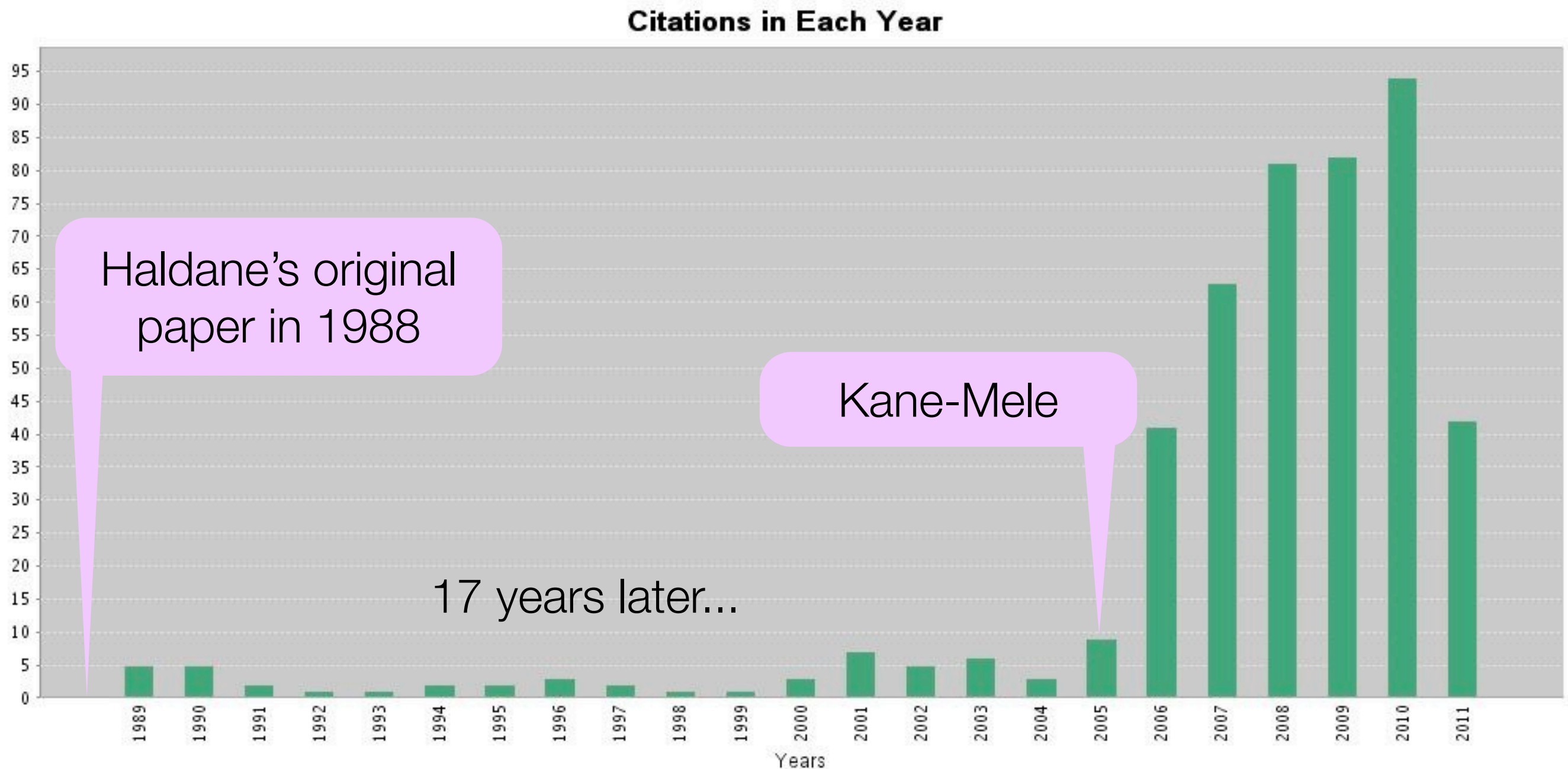
**Topological insulators are characterized by nontrivial band topology ( $Z_2$ ) driven by spin-orbit interaction and support robust “helical” edge/surface states**

*2D: Kane & Mele, PRL 2005; Bernevig, Hughes, & Zhang (2006)*

*3D: Fu, Kane & Mele, 2007; Moore & Balents (2007)*



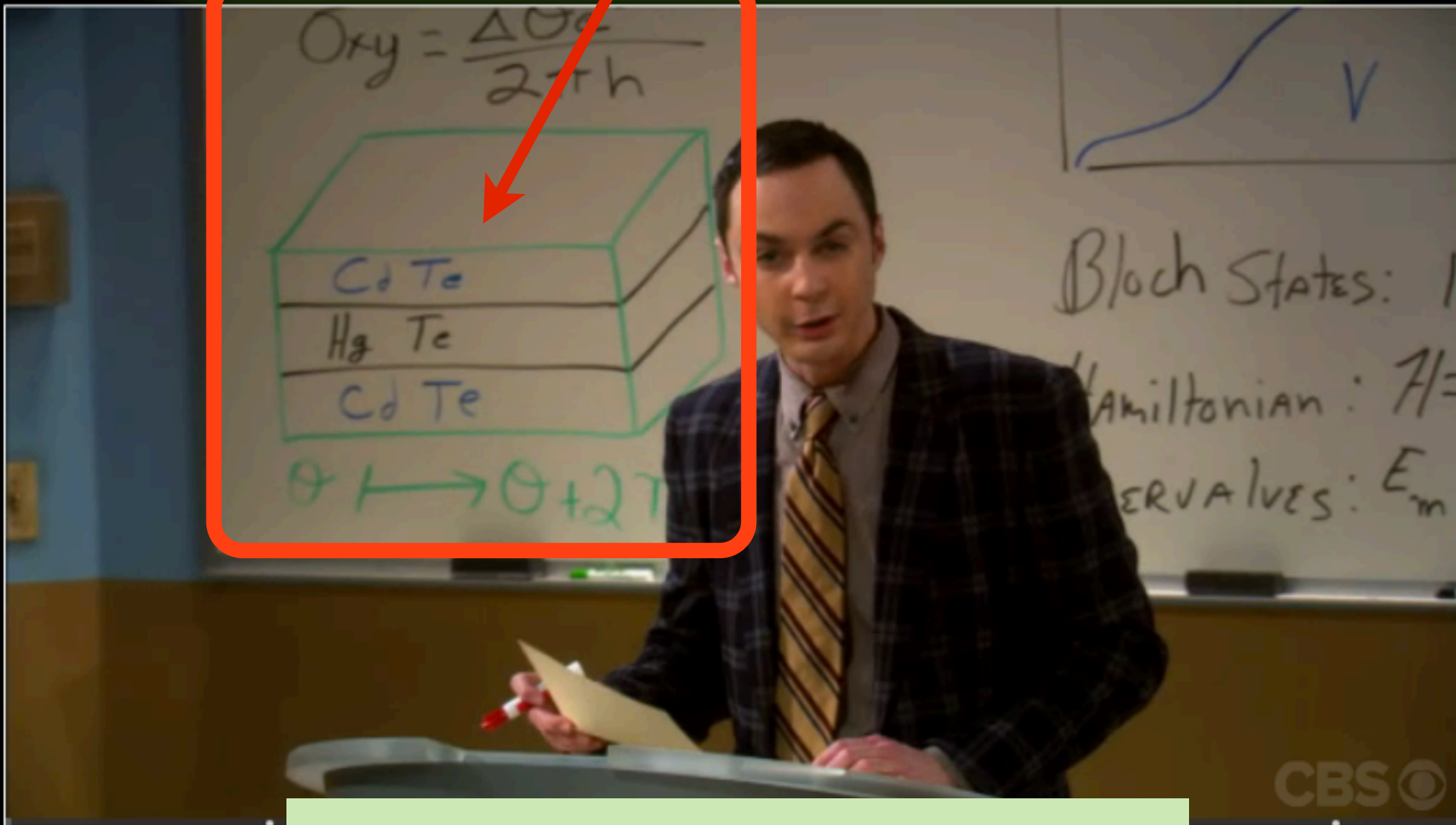
# Haldane: What has Just Happened?





the  
**BIG BANG**  
theory

Thursdays, 8/7c

**This Happened****Material is the key**The Big Bang Theory - The  
Thespian Catalyst

Air Date: 02/03/11

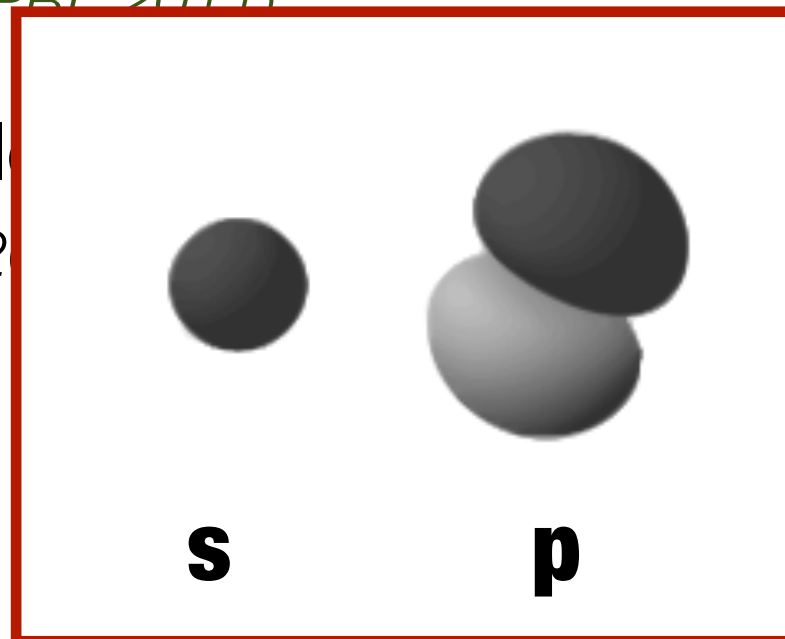
Full Episode 21:39

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

Tweet 7

# Topological Insulators: A Growing Family

- ▶ **CdHgTe/HgTe/CdHgTe** (Bernevig et al, Science 2006, Konig et al, Science 2007)
- ▶ **Bi<sub>1-x</sub>Sb<sub>x</sub>** (Fu and Kane, PRB 2007, Hsieh et al, Nature 2008)
- ▶ **Bi<sub>2</sub>Se<sub>3</sub>, Bi<sub>2</sub>Te<sub>3</sub>, Sb<sub>2</sub>Te<sub>3</sub>** (Zhang et al, Nat Phys 2009, Xia et al, Nat Phys 2009, Chen et al, Science 2009)
- ▶ **TlBiTe<sub>2</sub> and TlBiSe<sub>2</sub>** (Lin et al, PRL 2010, Yan et al, EPL 2010, Sato et al, PRL 2010, Chen et al, PRL 2011)
- ▶ Half-Heuslers, Chalcogenides (Xiao et al, PRL, 2010, Chadov et al, Nat Mat 2010)
- ▶ Many more...



# What About d-Orbitals?

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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

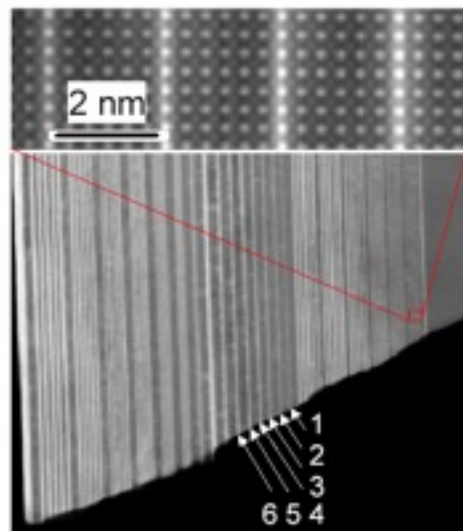
*Shitade et al, 2009; Pesin & Balents, 2010*

# **Heterostructures of Transition-Metal Oxides**

# Heterostructures of Transition-Metal Oxides

## Artificial charge-modulation in atomic-scale perovskite titanate superlattices

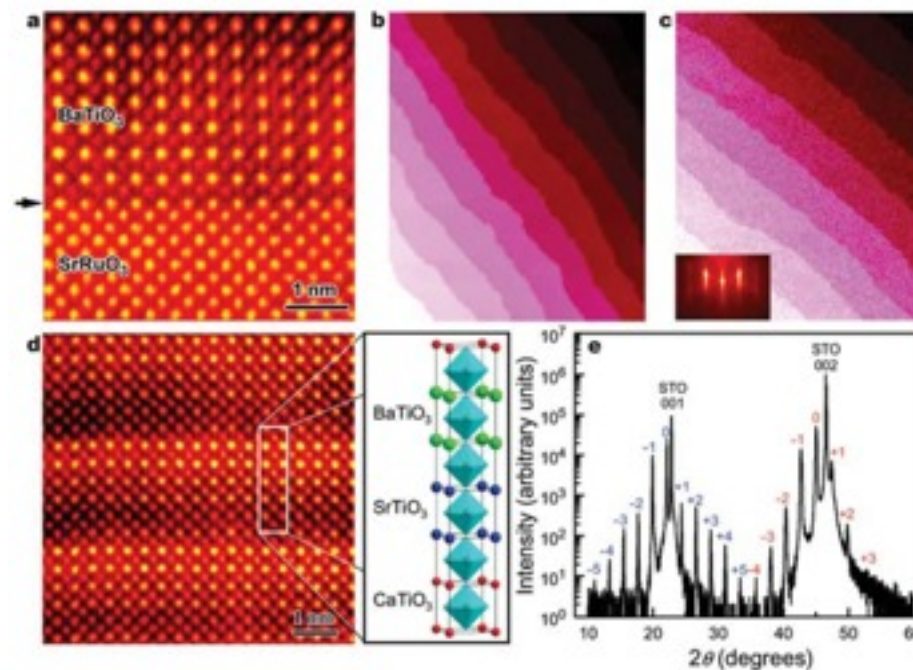
A. Ohtomo, D. A. Muller, J. L. Grazul & H. Y. Hwang



## Strong polarization enhancement in asymmetric three-component ferroelectric superlattices

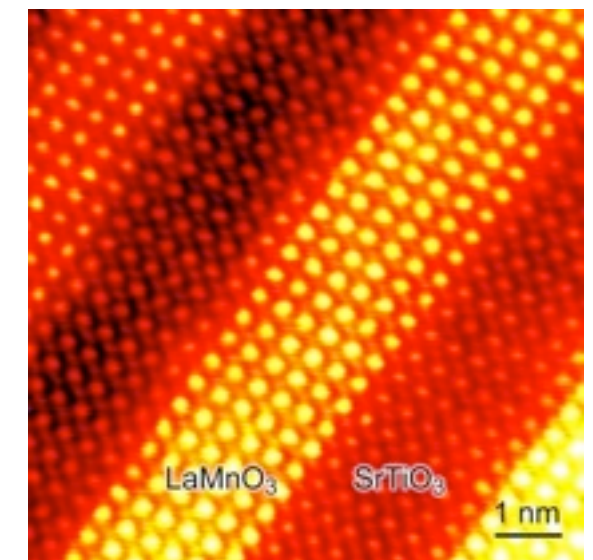
Ho Nyung Lee, Hans M. Christen, Matthew F. Chisholm, Christopher M. Rouleau & Douglas H. Lowndes

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

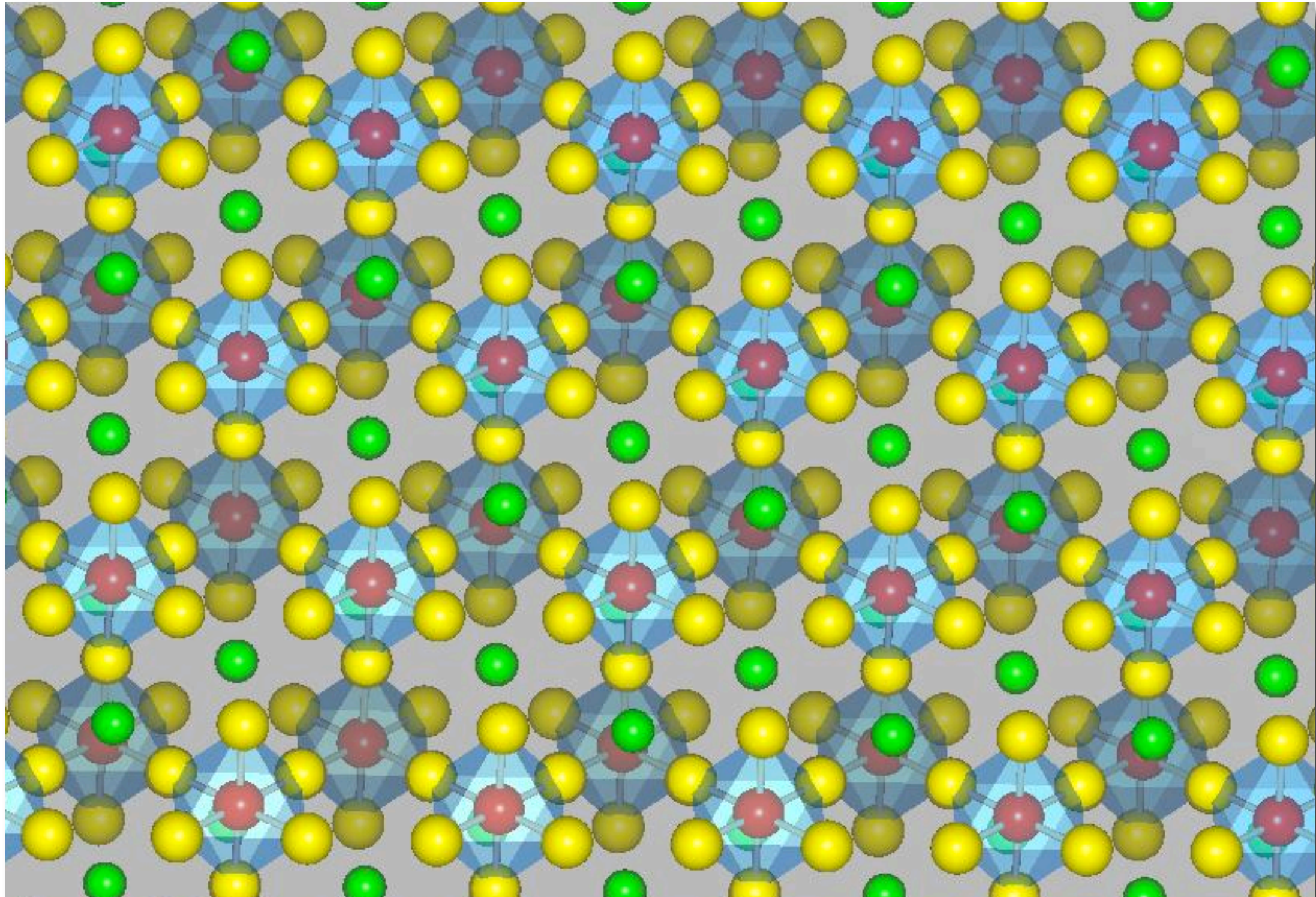


- ▶ Layered structure can be prepared with atomic precision
- ▶ Great flexibility: tunable lattice constant, carrier concentration, spin-orbit interaction, correlation strength



# Perovskite (111)-bilayer

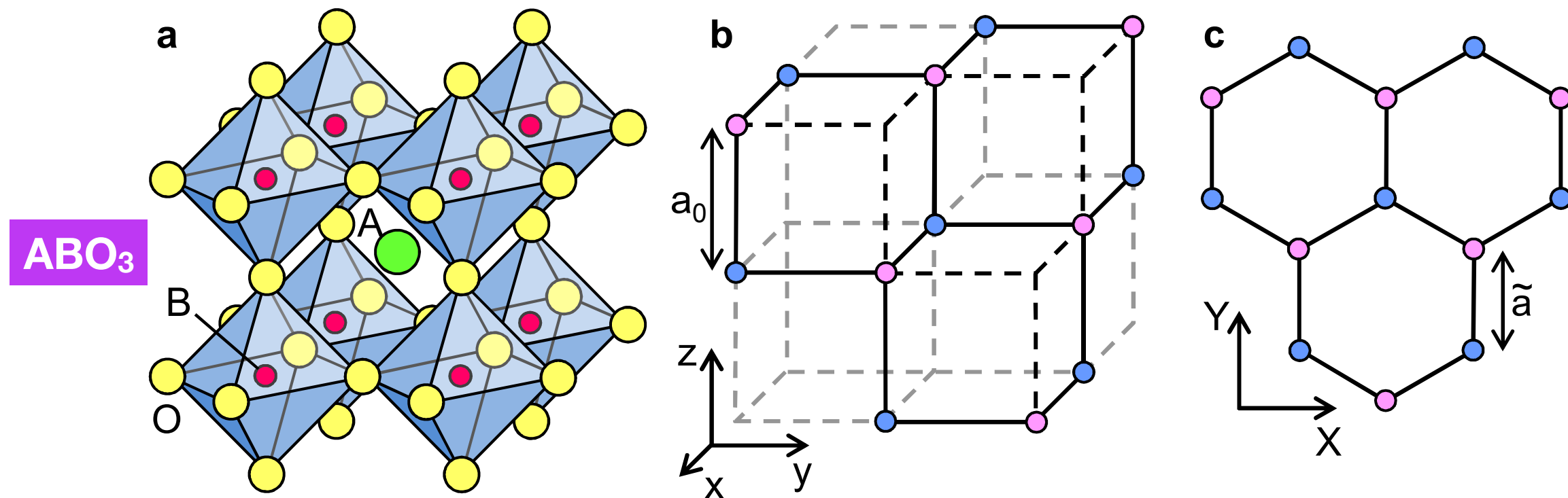
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*Credit: Satoshi Okamoto*

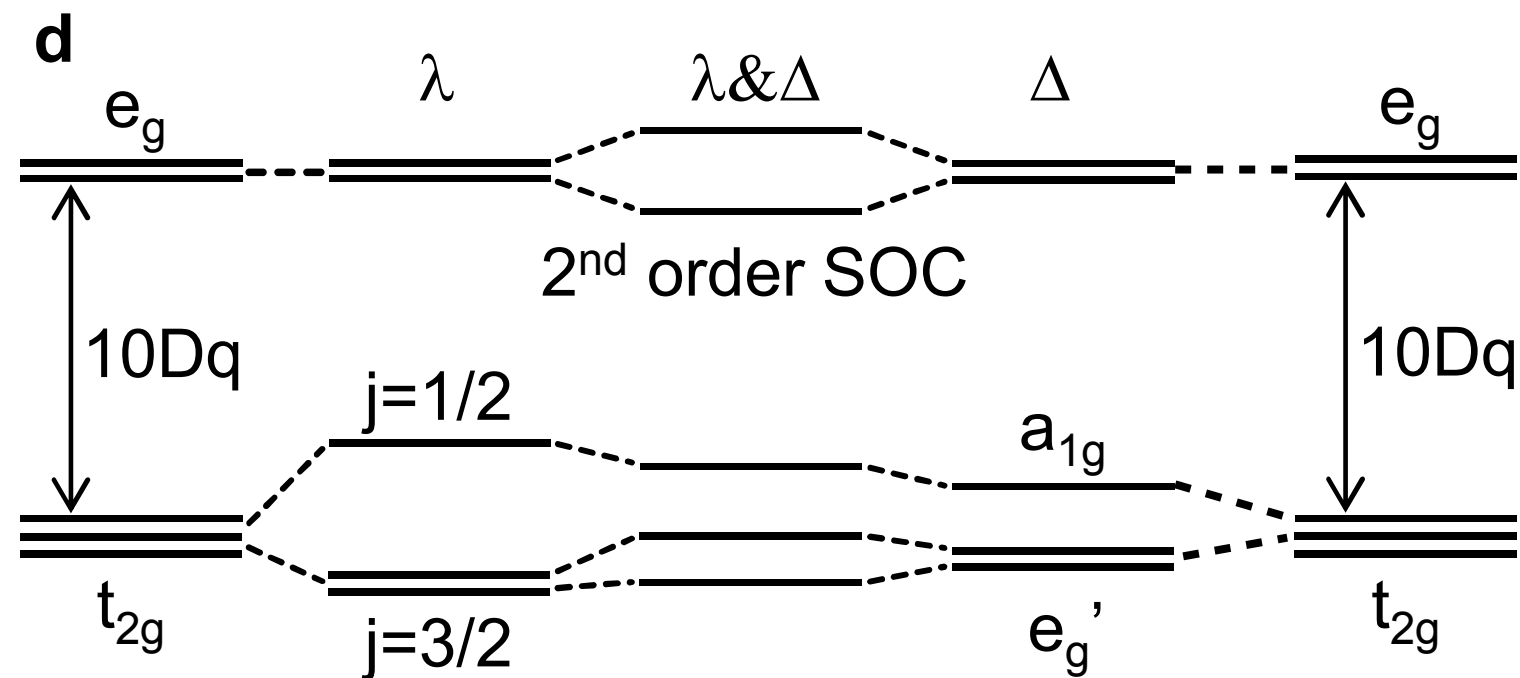


# Perovskite (111)-bilayer



- ▶ 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**

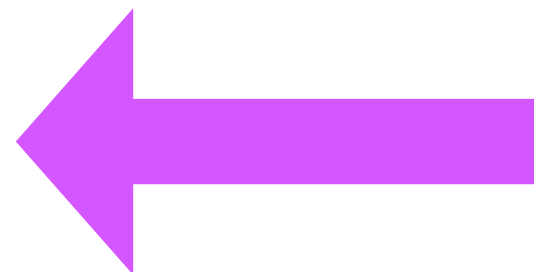
# Atomic Orbitals in Crystal Field + SO



## Spin-orbit interaction

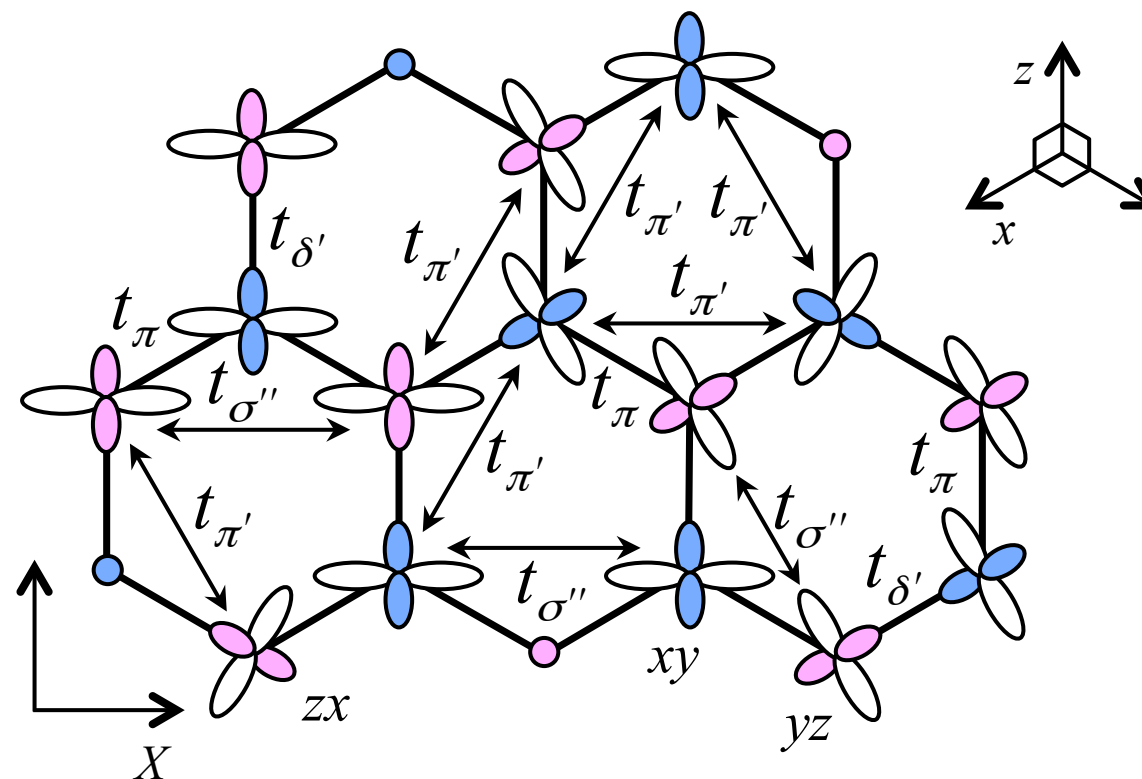
+

## Trigonal symmetry



# **t<sub>2g</sub> orbitals**

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

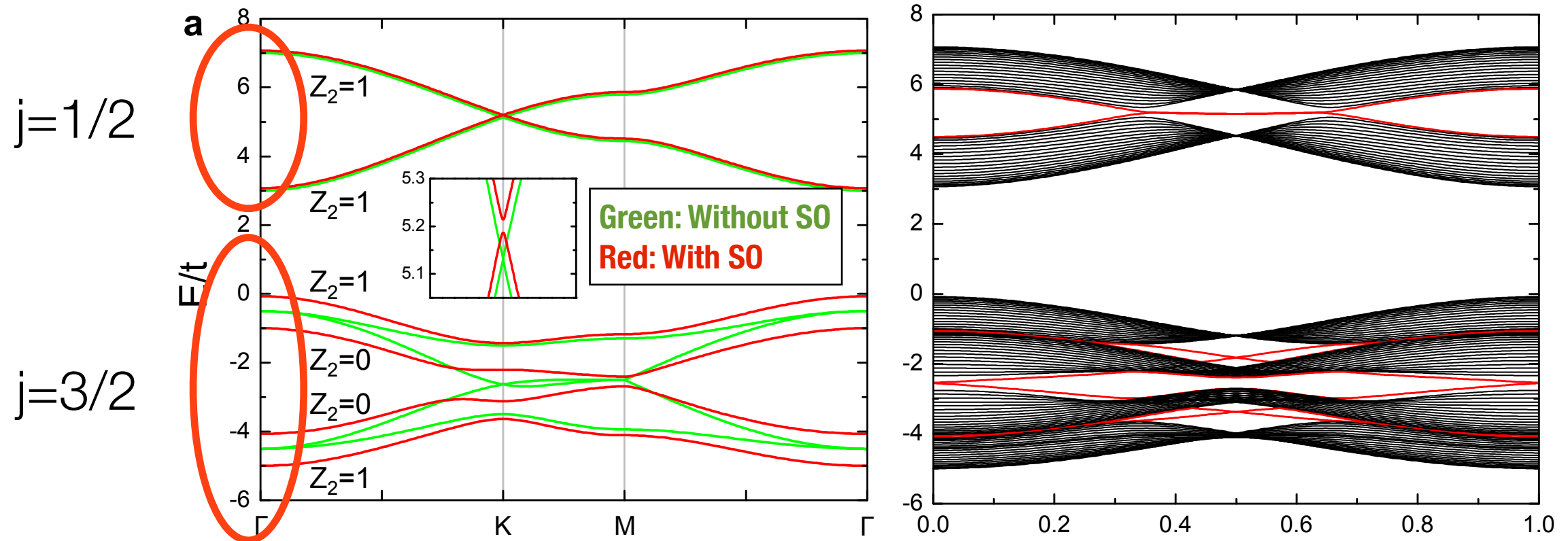


# $t_{2g}$ Orbitals - Strong SOC

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

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

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

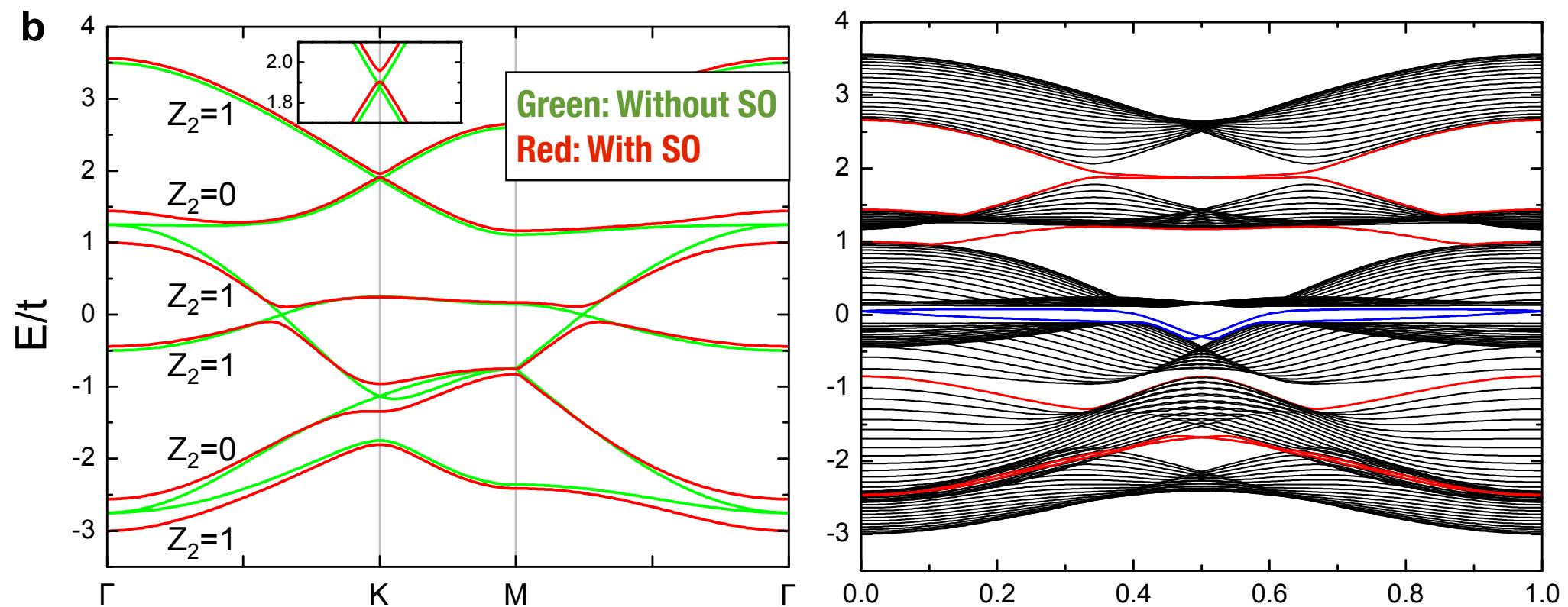


# $t_{2g}$ Orbitals - Weak SOC

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

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

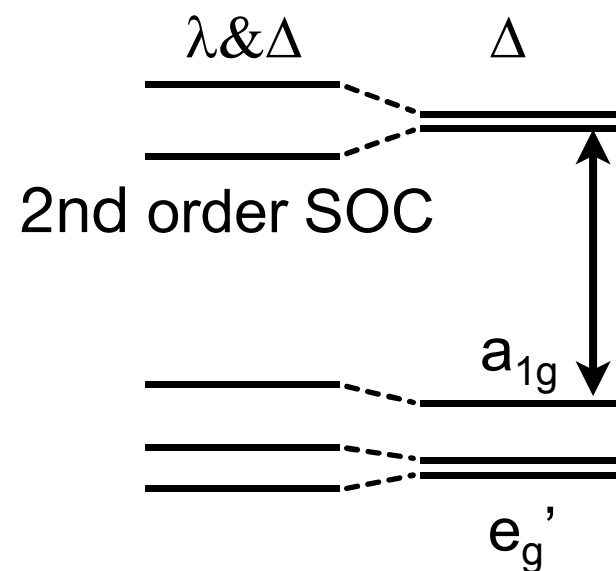
$t_{2g}^2, t_{2g}^4, t_{2g}^5$  are possible candidates



# e<sub>g</sub> Orbitals

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

Allowed by trigonal symmetry



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

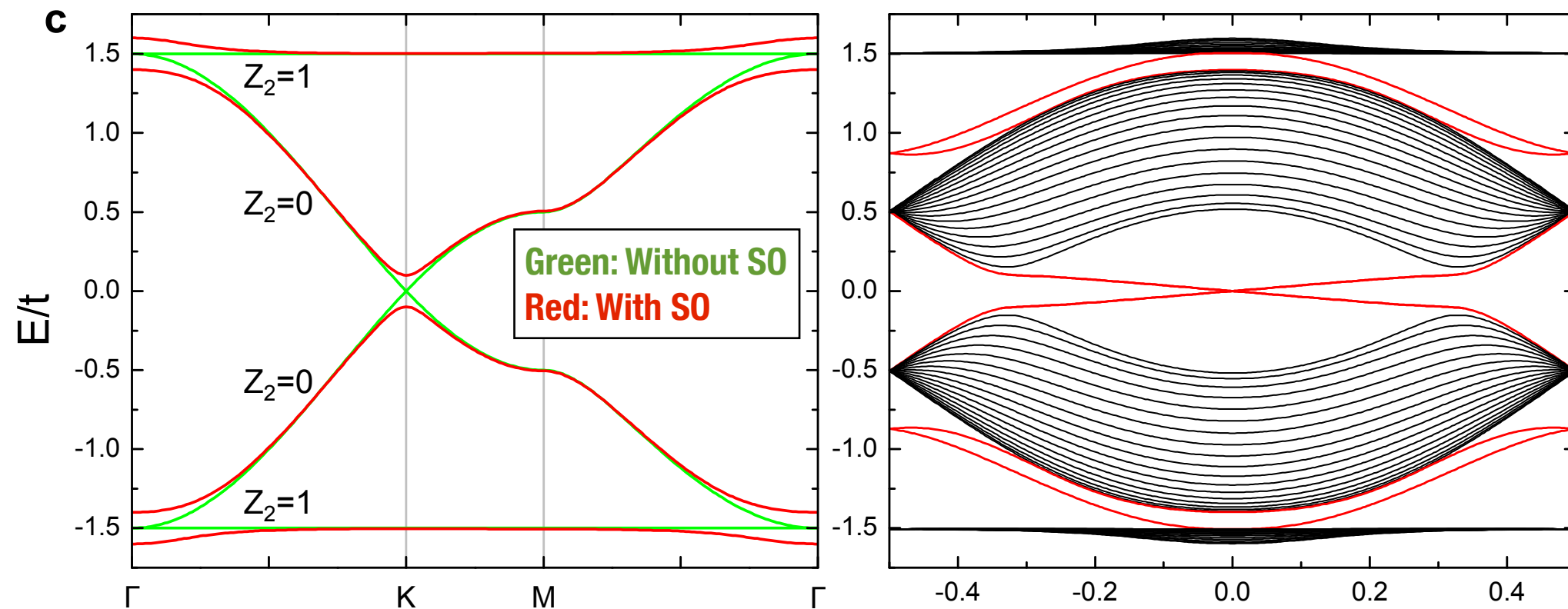
Vanishes in the limit of  $\Delta \rightarrow 0$

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



# $e_g$ Orbitals

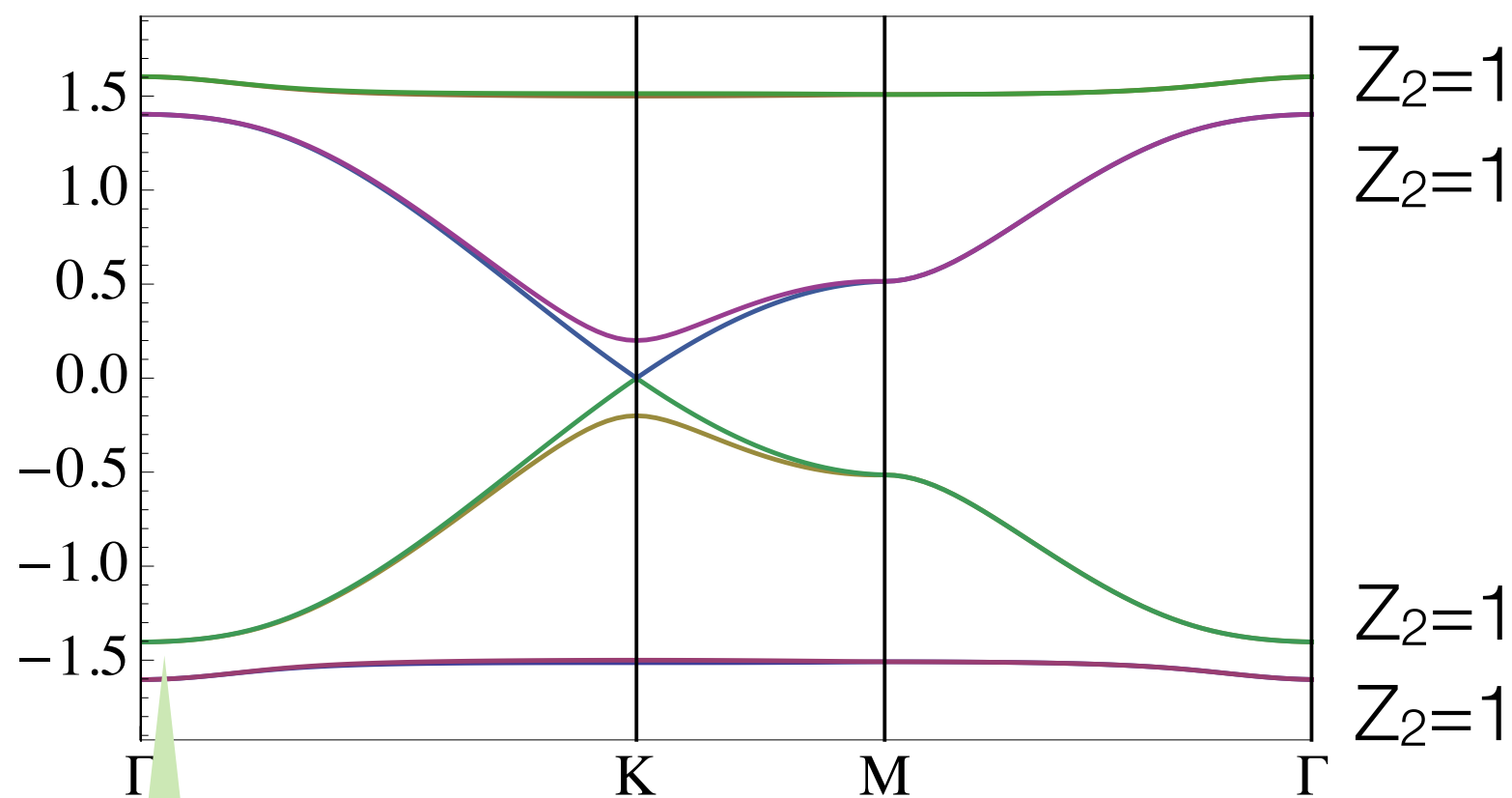
$e_g^1, e_g^2, e_g^3$  are possible candidates



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

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Unq	105 Unp	106 Unh	107 Uns	108 Uno	109 Une	110 Unn								

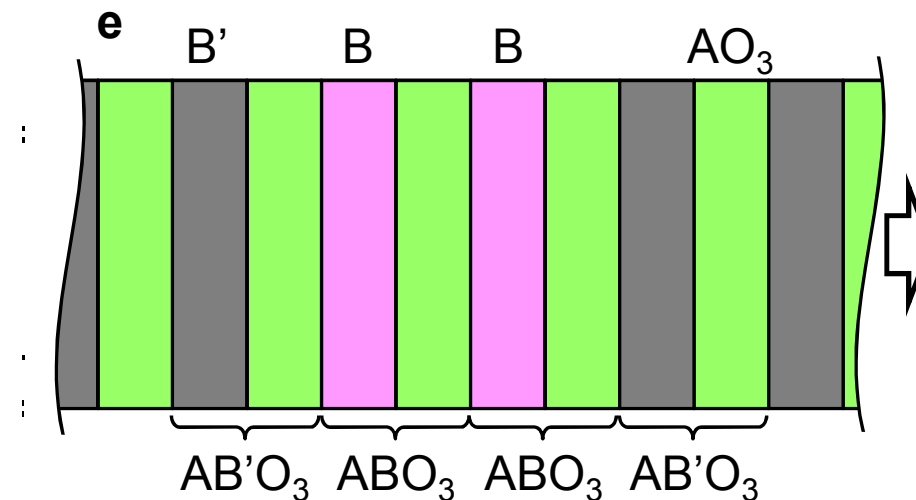
  

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

**Legend:**

- hydrogen (black)
- alkali metals (yellow)
- alkali earth metals (red)
- transition metals (purple)
- poor metals (green)
- nonmetals (blue)
- noble gases (pink)
- rare earth metals (teal)

# Materials Consideration



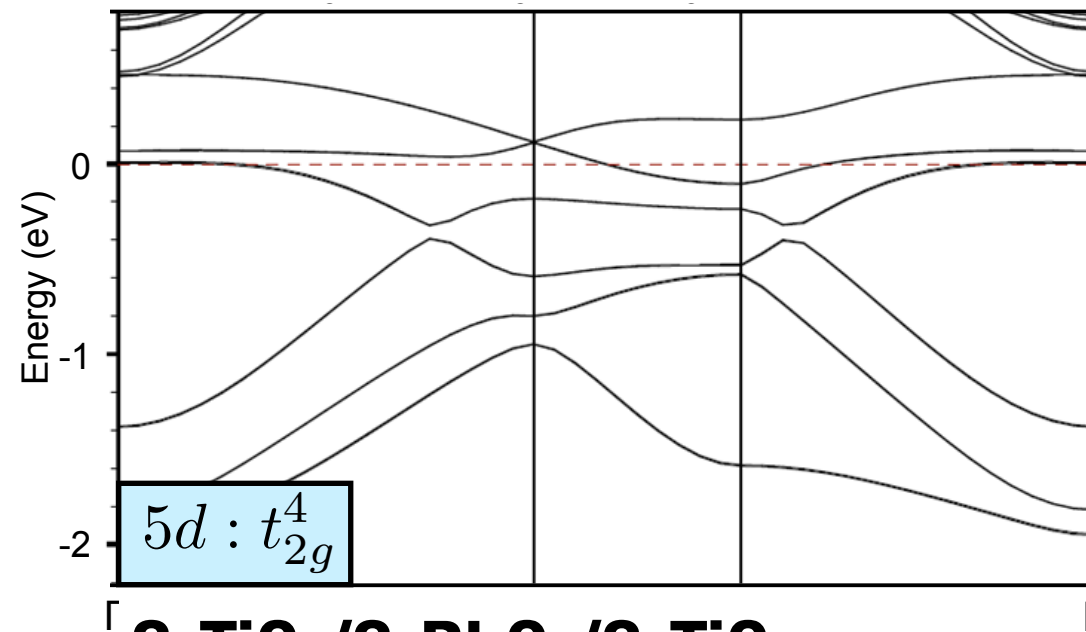
## **AB'O<sub>3</sub>: LaAlO<sub>3</sub> and SrTiO<sub>3</sub>**

TABLE SI: List of candidate materials

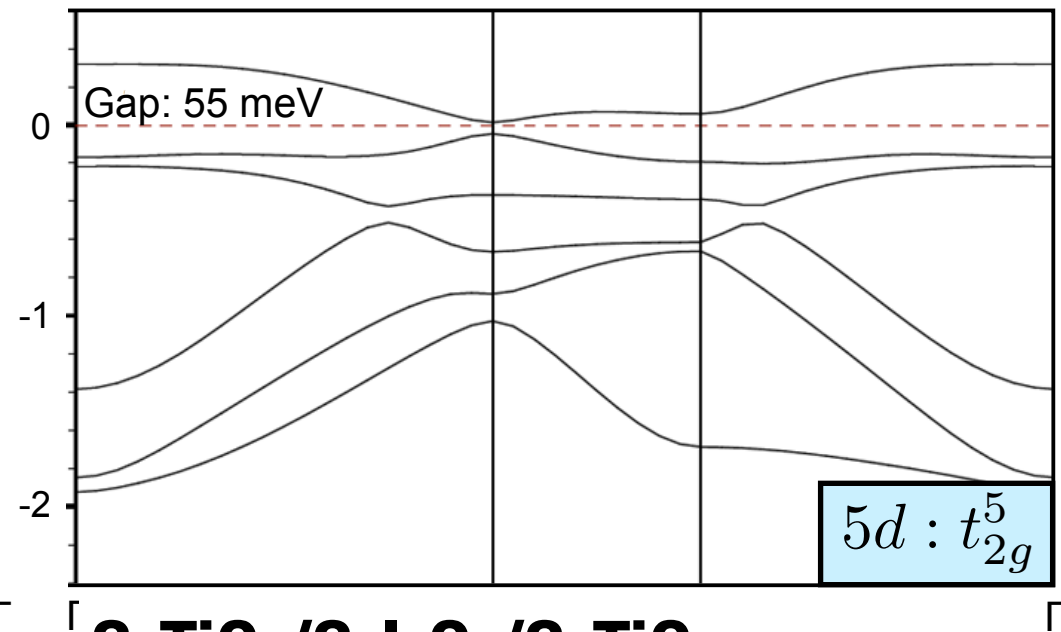
Configuration		Bulk	Superlattice
LaReO <sub>3</sub>	$t_{2g}^4$	—	—
LaRuO <sub>3</sub>	$t_{2g}^5$	metallic Ref. [2]	—
SrRhO <sub>3</sub>	$t_{2g}^5$	metallic Ref. [3]	Ref. [4]
SrIrO <sub>3</sub>	$t_{2g}^5$	metallic Refs. [5, 6]	metallic Ref. [7]
LaOsO <sub>3</sub>	$t_{2g}^5$	—	—
LaAgO <sub>3</sub>	$e_g^2$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

# $t_{2g}$ Systems

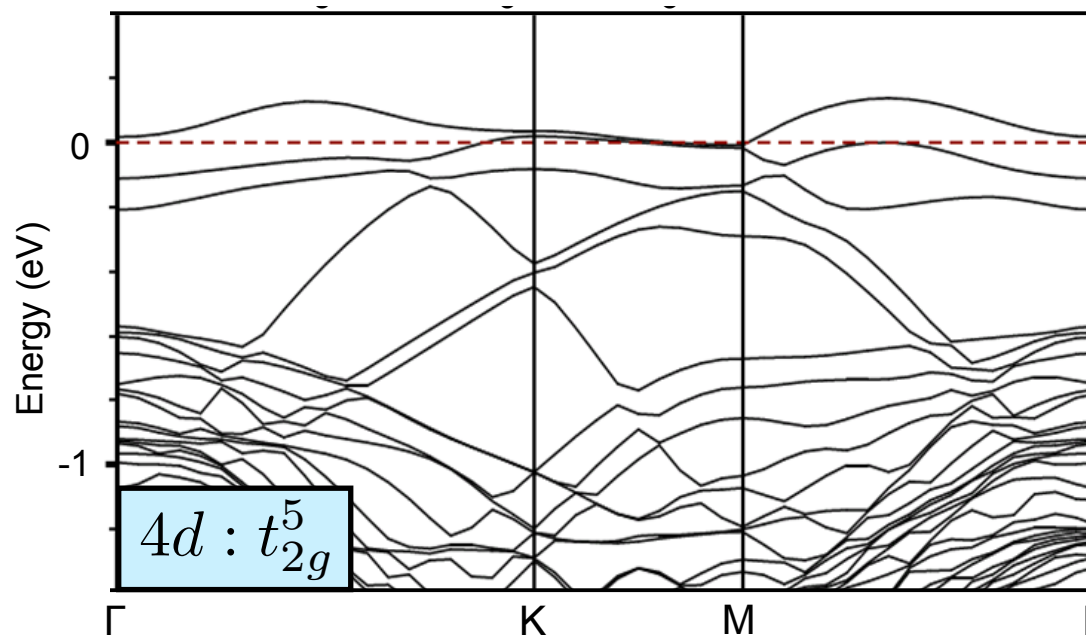
**LaAlO<sub>3</sub>/LaReO<sub>3</sub>/LaAlO<sub>3</sub>**



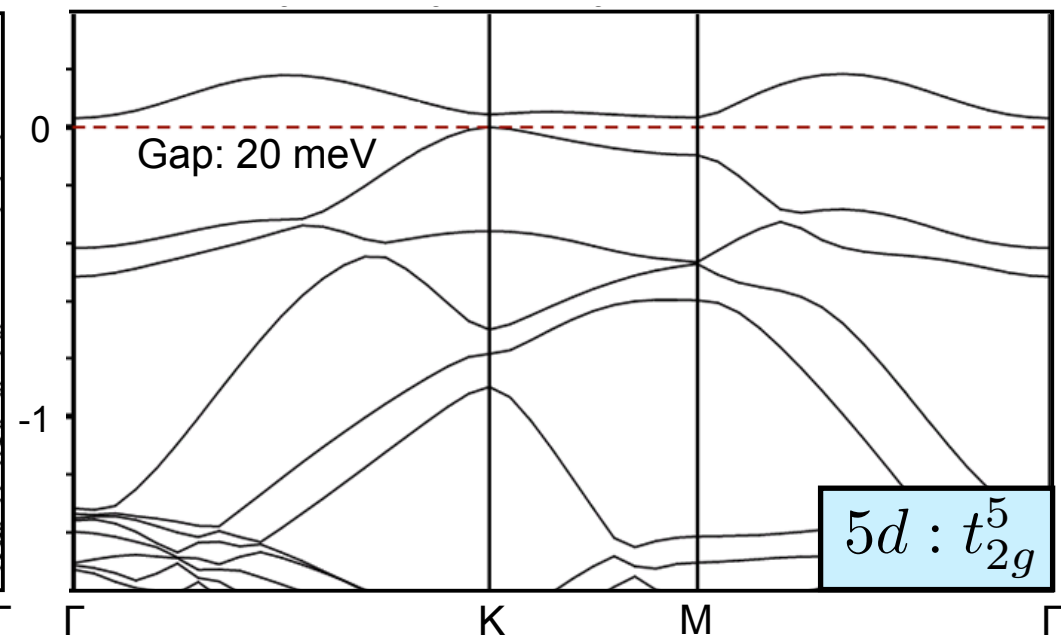
**LaAlO<sub>3</sub>/LaOsO<sub>3</sub>/LaAlO<sub>3</sub>**



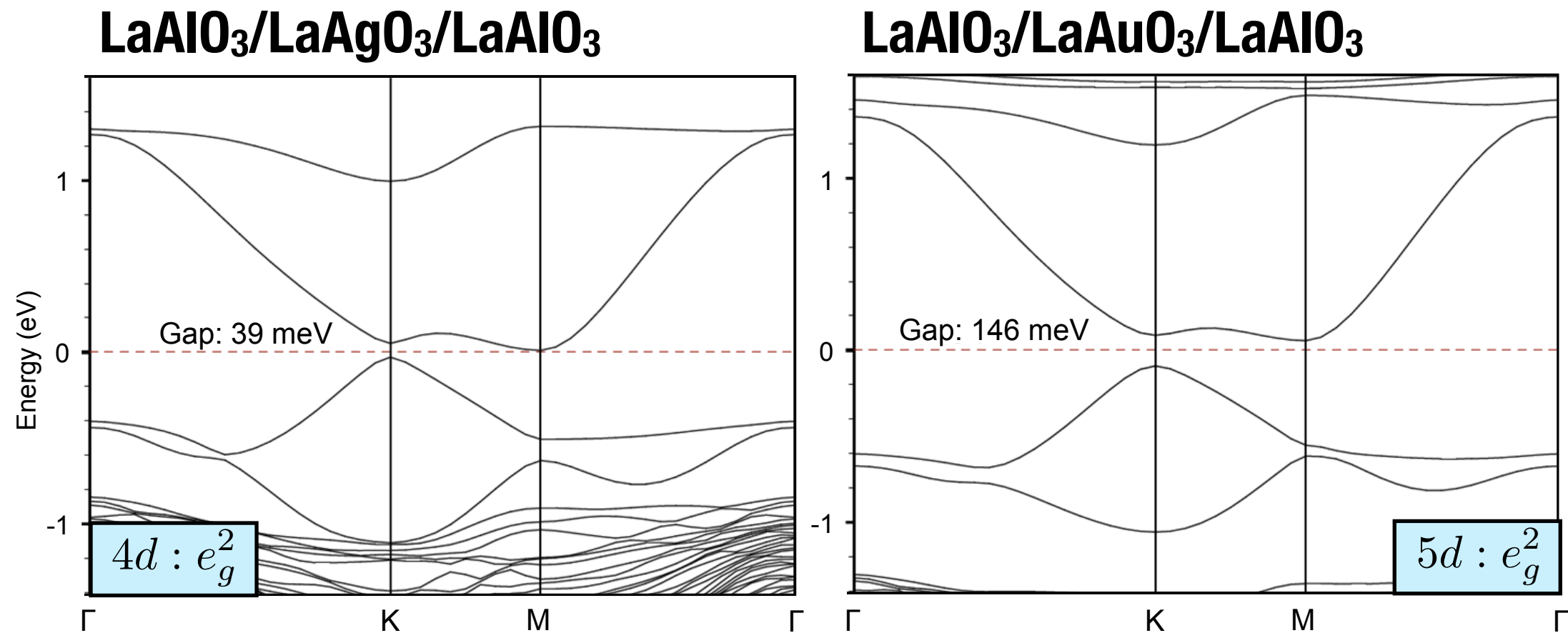
**SrTiO<sub>3</sub>/SrRhO<sub>3</sub>/SrTiO<sub>3</sub>**



**SrTiO<sub>3</sub>/SrIrO<sub>3</sub>/SrTiO<sub>3</sub>**



# $e_g$ Systems

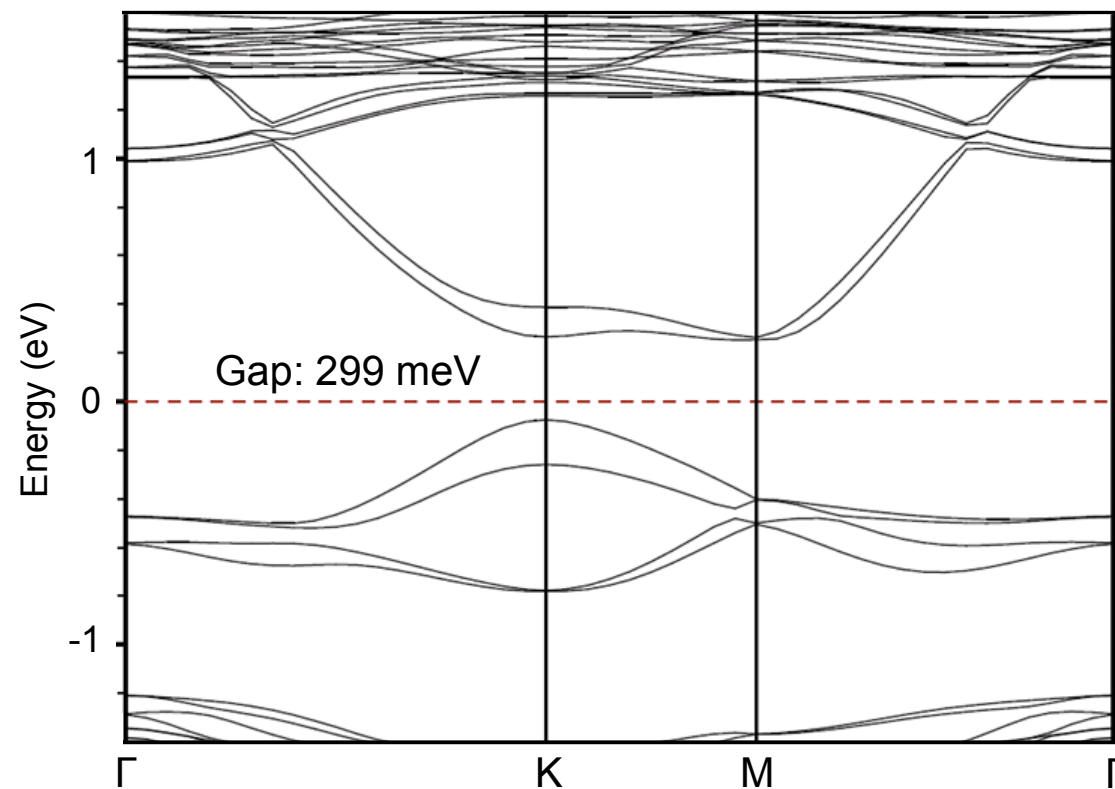


**LaAuO<sub>3</sub> bilayer has an energy gap  $\sim 2000$  K**



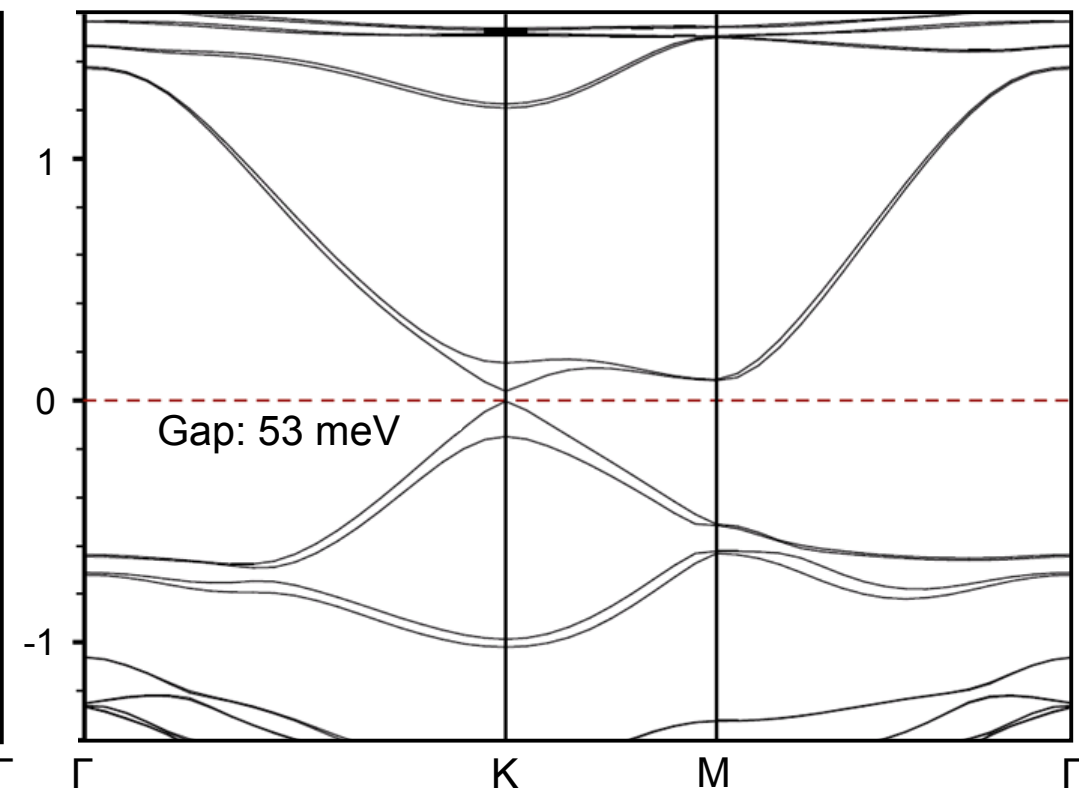
# Asymmetric Substrates

**LaAlO<sub>3</sub>/LaAuO<sub>3</sub>/LaScO<sub>3</sub>**



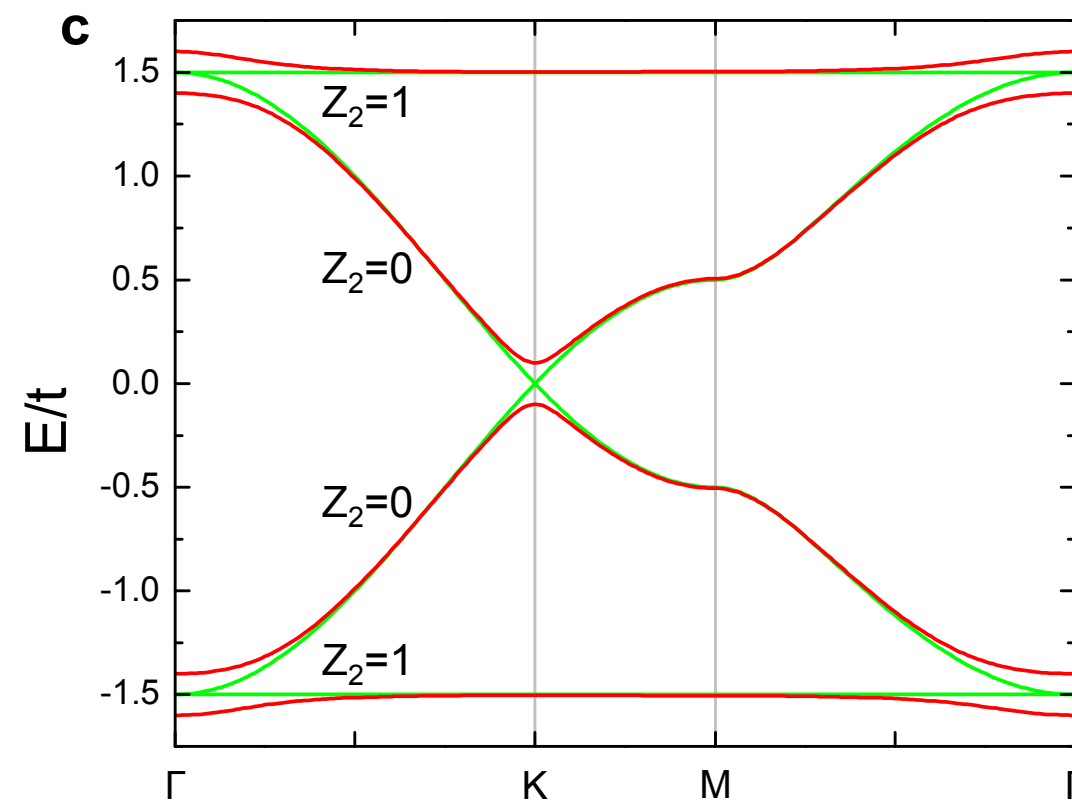
Trivial insulator

**LaAlO<sub>3</sub>/LaAuO<sub>3</sub>/YAlO<sub>3</sub>**



Topological insulator

# Physics inside Flat $Z_2$ Bands

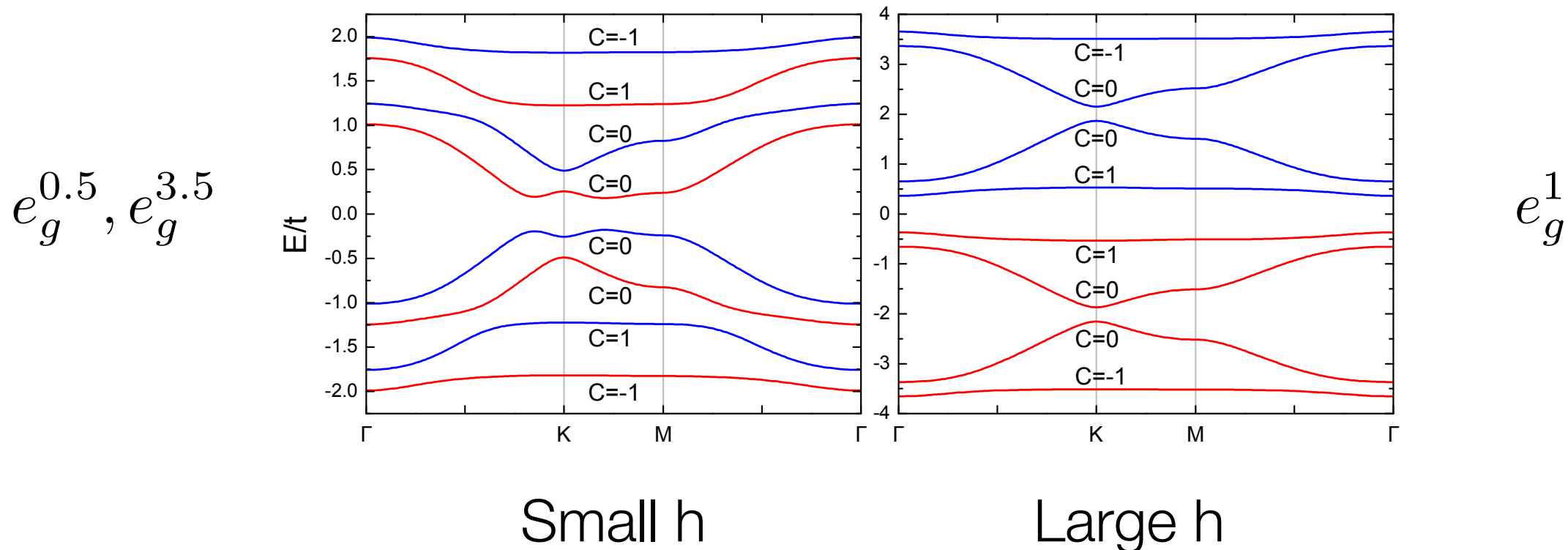


# Integer Quantum Hall Effect

## How to break time-reversal symmetry?

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

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



# Fractional Quantum Hall Effect

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

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

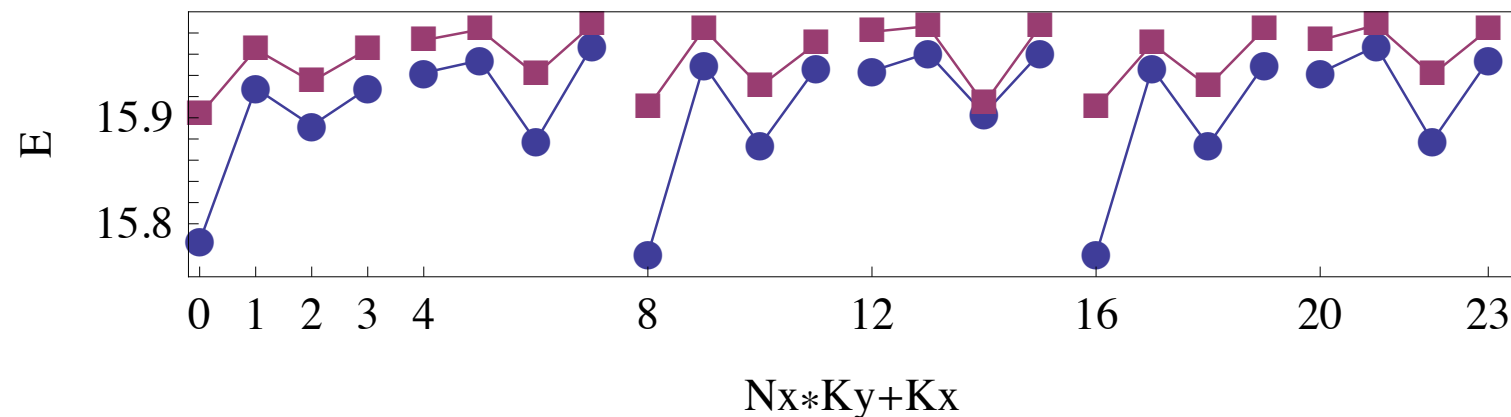
U: Onsite intra-orbital repulsion  
U': On-site inter-orbital repulsion  
V: Nearest-neighbor repulsion

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

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

# Fractional Quantum Hall Effect

- ▶ 3-fold degenerate GS



- ▶ Chern number

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

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

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

# What is Next?

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- ▶ 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**

**LaAuO<sub>3</sub>**



# Summary

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- ▶ Heterostructures of transition metal oxides provide an exciting platform for topological electronics
- ▶ Lots of perovskite (1 1 1)-bilayers are possible candidates for topological insulators. In particular,  $\text{LaAuO}_3$  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**