Antiferromagnetic Topological Insulator
model analysis and material design

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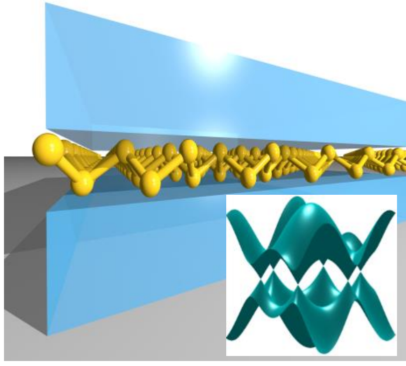
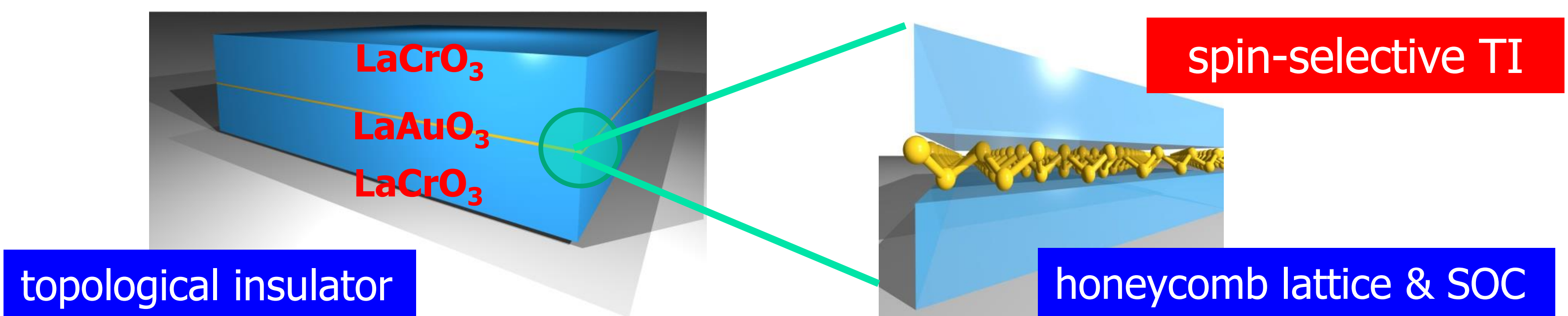


EQPCM2013, June 12, 2013 @ ISSP, U. of Tokyo, Kashiwa

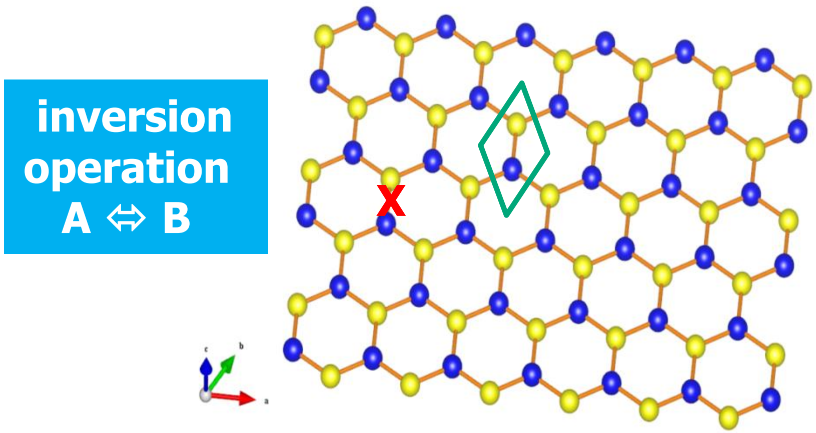
Introduction

- Quantum Hall effect: 2DEG under strong H by von Klitzing (1980)
  - integer Hall conductance: $\sigma_{xy} = \nu e^2 / h$
  - TKNN theory: topology
- Quantum spin Hall effect and topological insulator
  - Kane and Mele: graphene (2005)
  - SC Zhang et al.: HgTe thin film (2006, 2007)
- Topological insulator with broken time-reversal symmetry
  - FM TI: theory by IOP and experiment by IOP and Tsinghua U. (2010, 13)
  - Antiferromagnetic TI: non-zero charge and spin Chern numbers

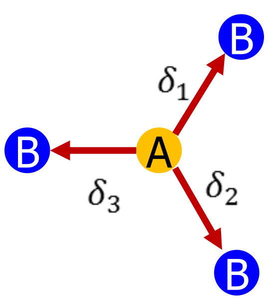


Electron on honeycomb lattice

- Honeycomb lattice:



- Tight-binding Hamiltonian:



$$\hat{H}_{\mathbf{k}} = \begin{pmatrix} 0 & \Delta_{\mathbf{k}} \\ \Delta^*_{\mathbf{k}} & 0 \end{pmatrix}$$

$$\Delta_{\mathbf{k}} = -t\sum_{i=1}^{3}\exp(i\mathbf{k}\cdot\delta_i)$$

$$E_{\pm} = \pm|\Delta_{\mathbf{k}}|$$

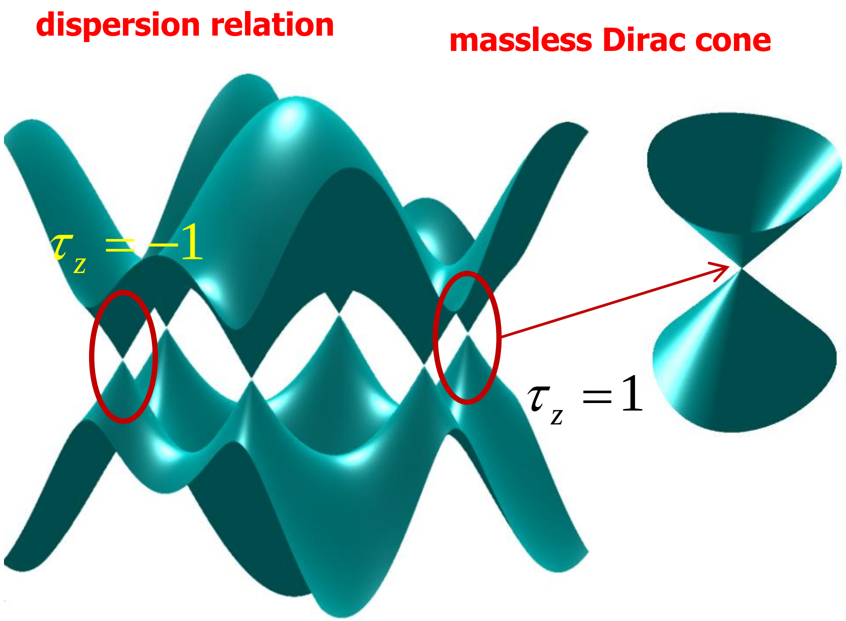
- sublattice ⇔ pseudo spin $\quad \psi = \begin{pmatrix} \phi_A \\ \phi_B \end{pmatrix}$

- Bravais vectors:

$$\vec{a}_1 = \sqrt{3}d\,(0,1) \text{ and } \vec{a}_2 = \sqrt{3}d\left(\sqrt{3}/2, 1/2\right)$$

- reciprocal vectors:

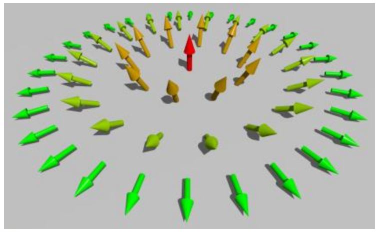
$$\vec{b}_1 = \frac{4\pi}{3d}\left(-1/2, \sqrt{3}/2\right) \text{ and } \vec{b}_2 = \frac{4\pi}{3d}(1,0)$$



Valleys: $K, K' = \frac{4\pi}{3d}(\pm 1, 0)$

Topology of Dirac electron

meron: $\vec{B}/|\vec{B}|$

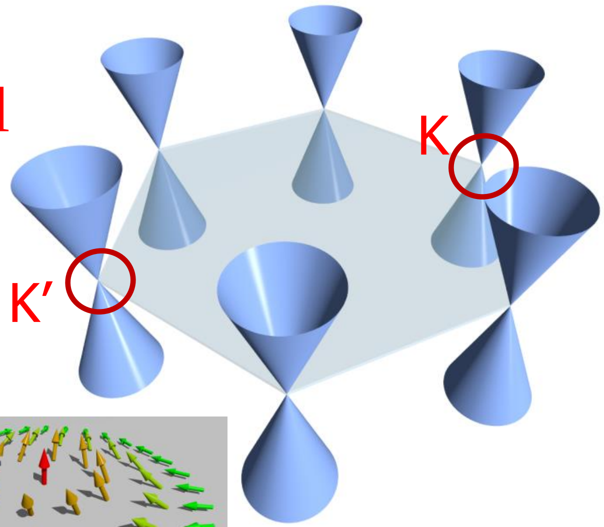


- Low-energy Hamiltonian: $\tau_z = \pm 1$: valley

$$H_{K,K'} = \begin{pmatrix} U & k_x - i\tau_z k_y \\ k_x + i\tau_z k_y & -U \end{pmatrix}$$

$$E = \pm\sqrt{U^2 + k^2}$$

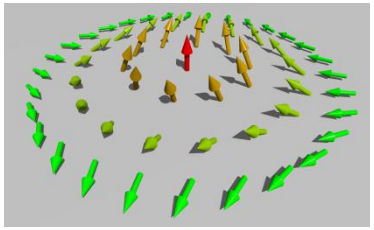
U: staggered potential



- Topology and Berry phase

$$H_{K,K'} = \vec{B}\cdot\vec{\sigma}; \quad \vec{B} = \left(k_x, \tau_z k_y, U\right)$$

Pauli matrix $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$



Chern number

$$C = \sum_{b.z.} c\left(U, \tau_z\right)$$

pseudo-spin-1/2 in a fictitious field B

Berry phase of w.f. ⇔ winding number of B

magnetic monopole in k space → $c\left(U,\tau_z\right) = \tau_z \mathrm{sgn}\left(U\right)/2$

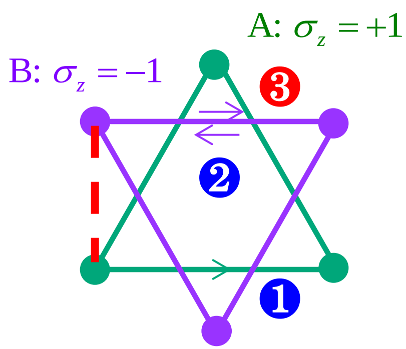
Spin-orbit coupling

- Spin-orbit coupling: $$H_{SO} = \frac{\hbar}{4m_0^2c^2}\left(\vec{\nabla}V \times \vec{p}\right)\cdot\vec{s}$$

- Next-nearest-neighbor hopping on honeycomb lattice
  - in-plane force $\vec{F}_{\parallel} \neq 0$ & in-plane hop: coupling to s_z
  - hopping in A sublattice ❶

    same as hopping in B sublattice ❷

    opposite to hopping in B sublattice ❸



$$H_{SO} = \lambda s_z \tau_z \sigma_z$$

intrinsic spin-orbit coupling

on the diagonal of Hamiltonian

- Rashba spin-orbit coupling: $\vec{F}_{\perp} \neq 0$
  - electric field
  - buckled plane

negligibly small

Topology on honeycomb

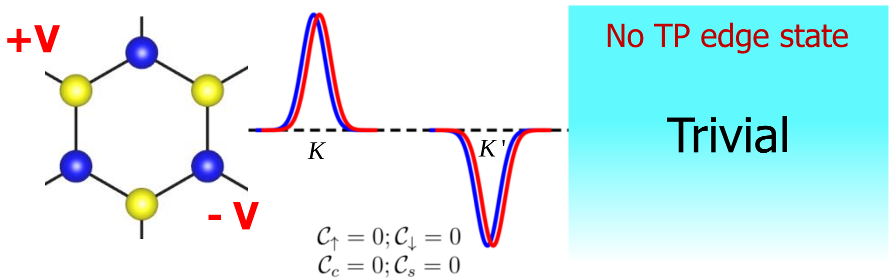
$$c(U,\tau_z)=\tau_z\mathrm{sgn}(U)/2$$

$$C_{\uparrow,\downarrow}=\sum_{b.z}c_{\uparrow,\downarrow}(U,\tau_z)$$

$$C_c=C_\uparrow+C_\downarrow;\ C_s=C_\uparrow-C_\downarrow$$

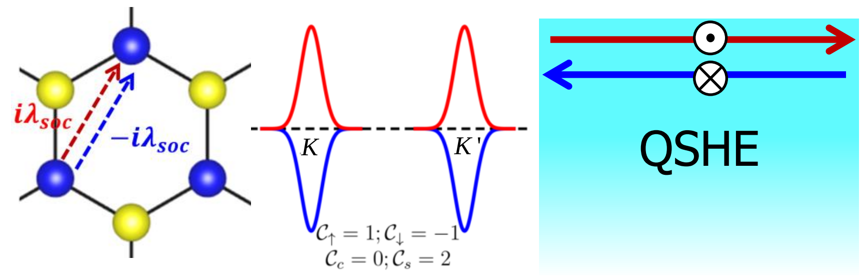
$$H=k_x\sigma_x+\tau_z k_y\sigma_y+V\sigma_z$$

Red: spin up
Blue: spin down



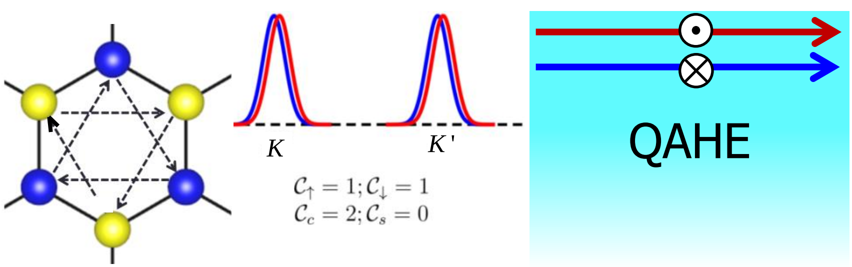
graphene + staggered electric potential

$$H=k_x\sigma_x+\tau_z k_y\sigma_y+\lambda s_z\tau_z\sigma_z$$



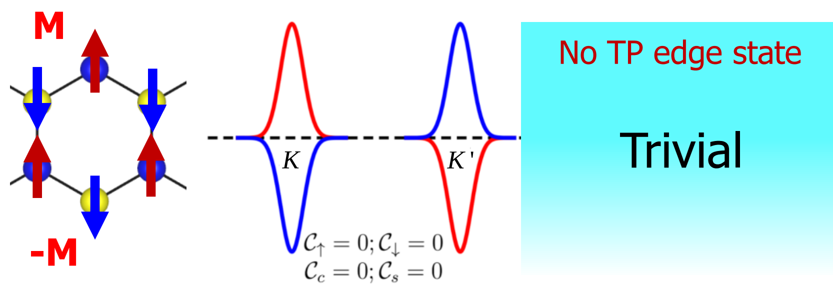
QSHE, Kane&Mele 2005
graphene + intrinsic spin-orbit coupling

$$H=k_x\sigma_x+\tau_z k_y\sigma_y+t\tau_z\sigma_z$$



QAHE, Haldane 1985, Yao etal 2010
graphene + chiral NNN hopping (spinless)

$$H=k_x\sigma_x+\tau_z k_y\sigma_y+Ms_z\sigma_z$$



graphene + antiferromagnetic field

Our new idea for a full band engineering

- Effective Hamiltonian

$$H = \sigma_x k_x + \tau_z \sigma_y k_y + \left(\lambda s_z \tau_z + M s_z + V\right)\sigma_z$$

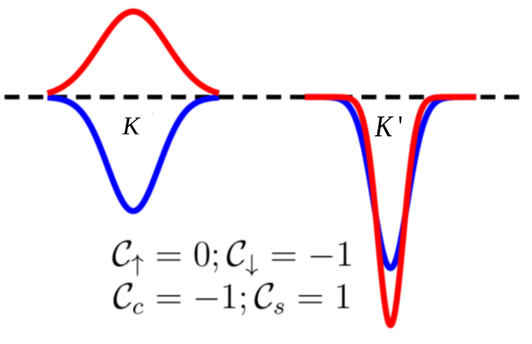
  - degrees of freedom: spin, sublattice, valley
  - control handles: SOC, AFM field, staggered electric potential

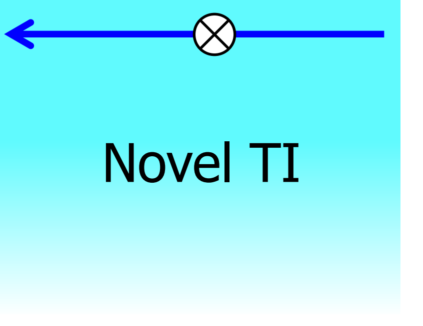
fields involved in different ways → *finer resolution*

- Novel topological insulator

$$U = \lambda s_z \tau_z + M s_z + V$$

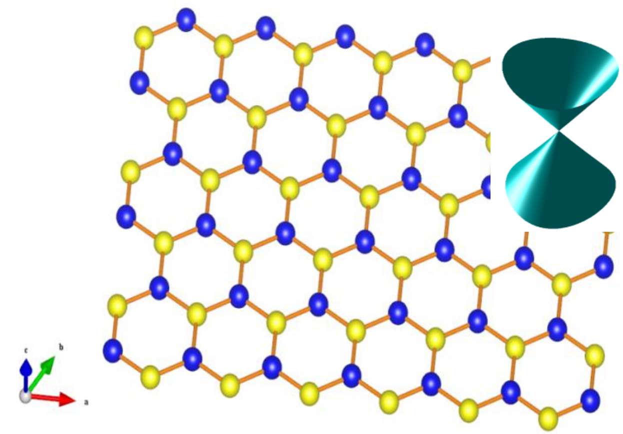
reverse effective potential at <u>single</u> valley & spin





Simultaneous nonzero charge and spin Chern numbers
⇔ spin-polarized charge current at edges, broken chiral symmetry

Half metal



- Semi metal: Red: spin up Blue: spin down

E=0

A sublattice B sublattice

- AFM exchange field M:

E=0

SDW

- Staggered electric potential V:

E=0

CDW

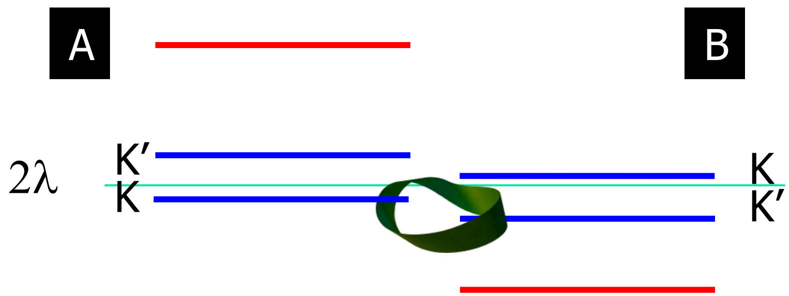
- AFM exchange field & staggered electric field :

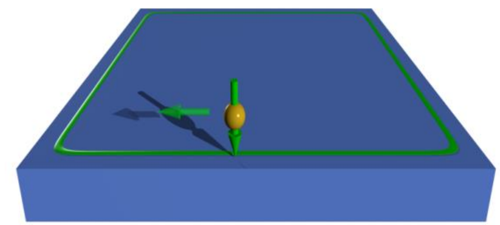
half metal

Cf F. -C. Zhang et al. (2013)

AFM topological insulator

- AFM exchange field & staggered electric potential & spin-orbit coupling (λ)





chiral edge current ~ Mobius ring

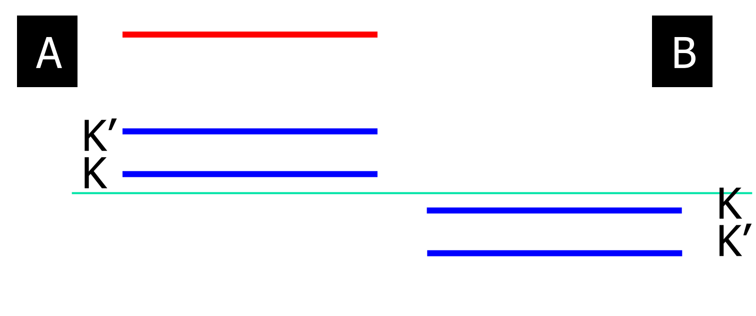
holography ~ bulk-edge correspondence

SOC

left- vs. right-side traffic in HK & mainland, China

- Trivial state

CDW′

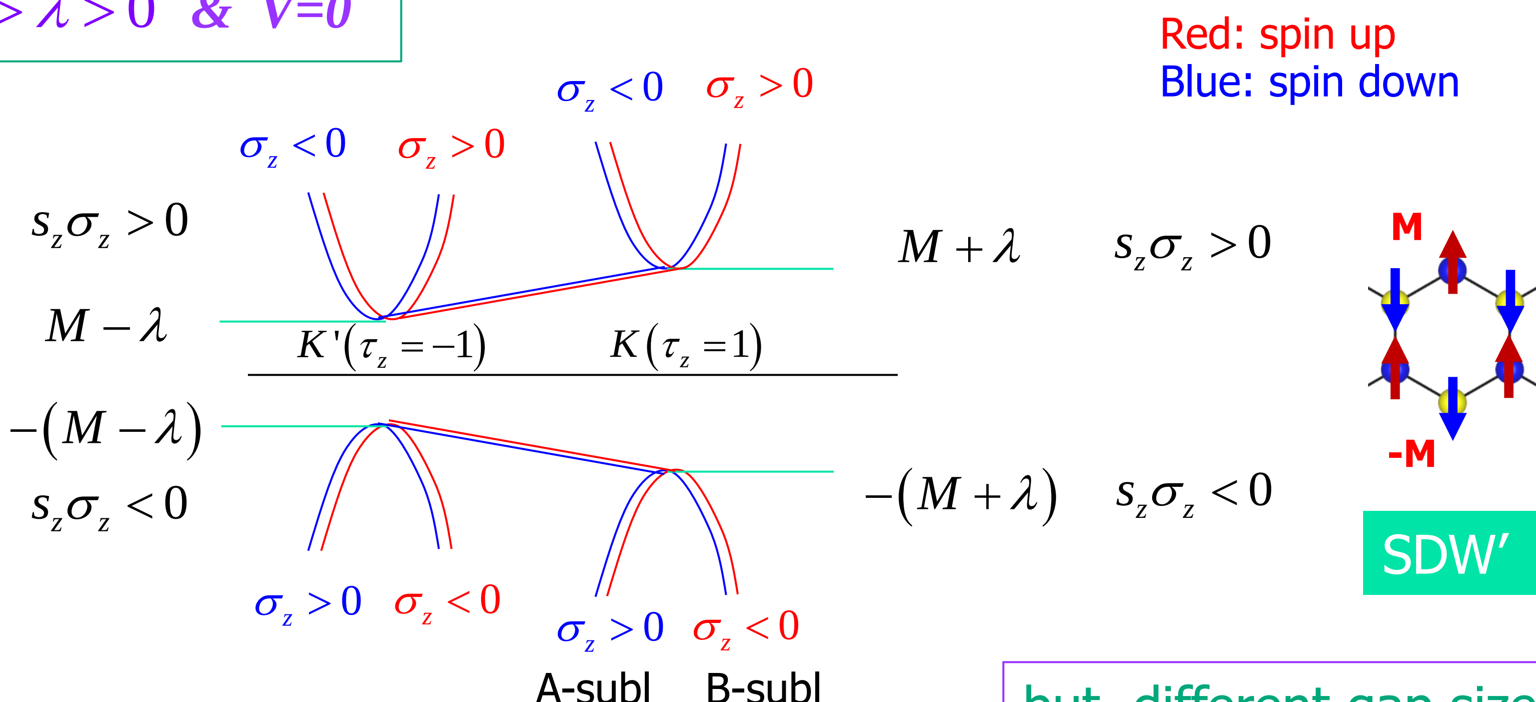


Band engineering: EM cross control

- Effective Hamiltonian

$$H = \sigma_x k_x + \tau_z \sigma_y k_y + \left(\lambda s_z \tau_z + M s_z + V\right)\sigma_z$$

$M > \lambda > 0$ **&** $V=0$

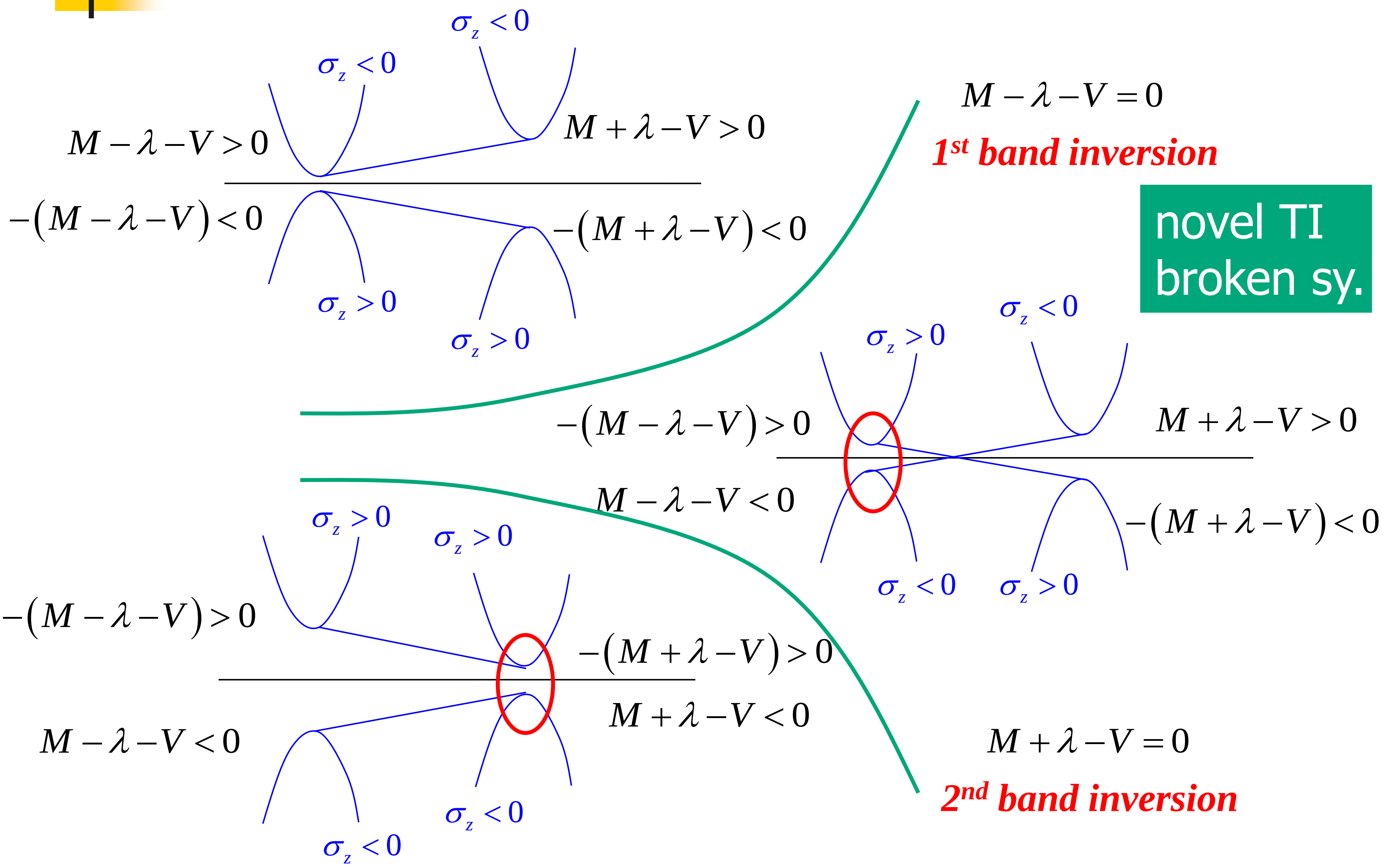


but, different gap sizes !

- Degeneracy from symmetry at V=0

Time-reversal ($\mathcal{T}$) & inversion ($\mathcal{P}$) cf. ***both symmetries broken individually***

Electric field tuning

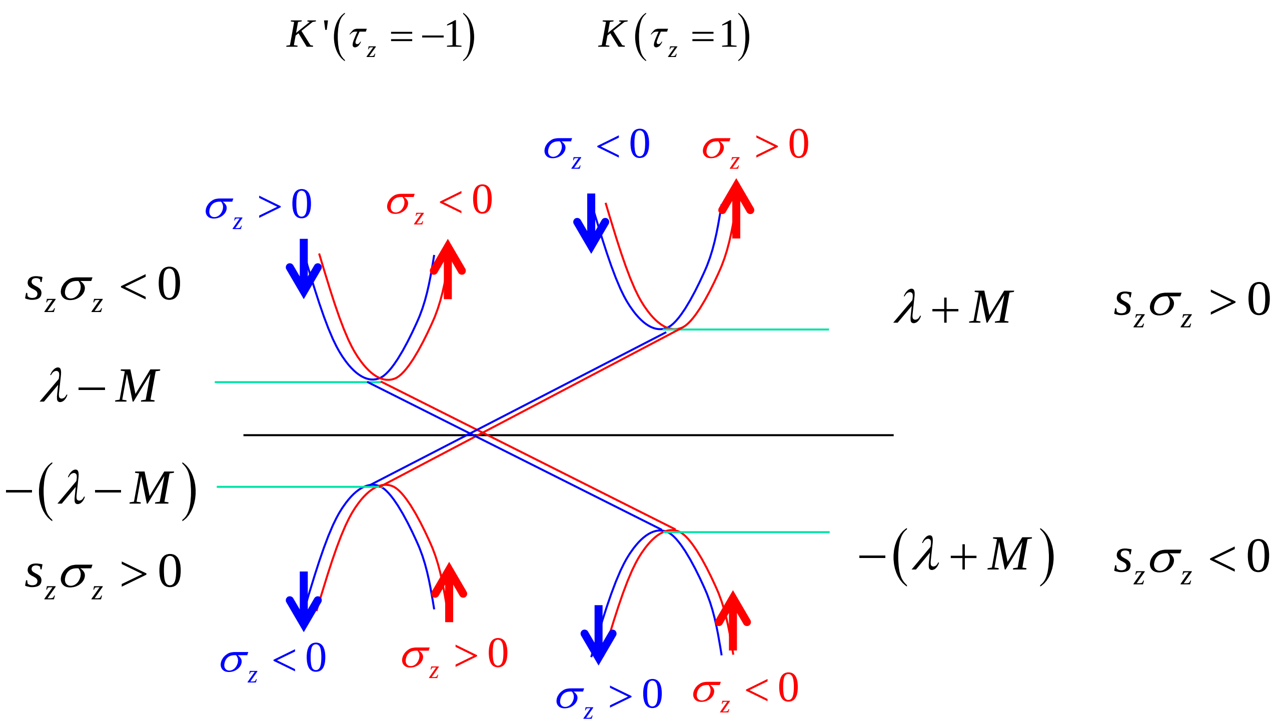


Band engineering

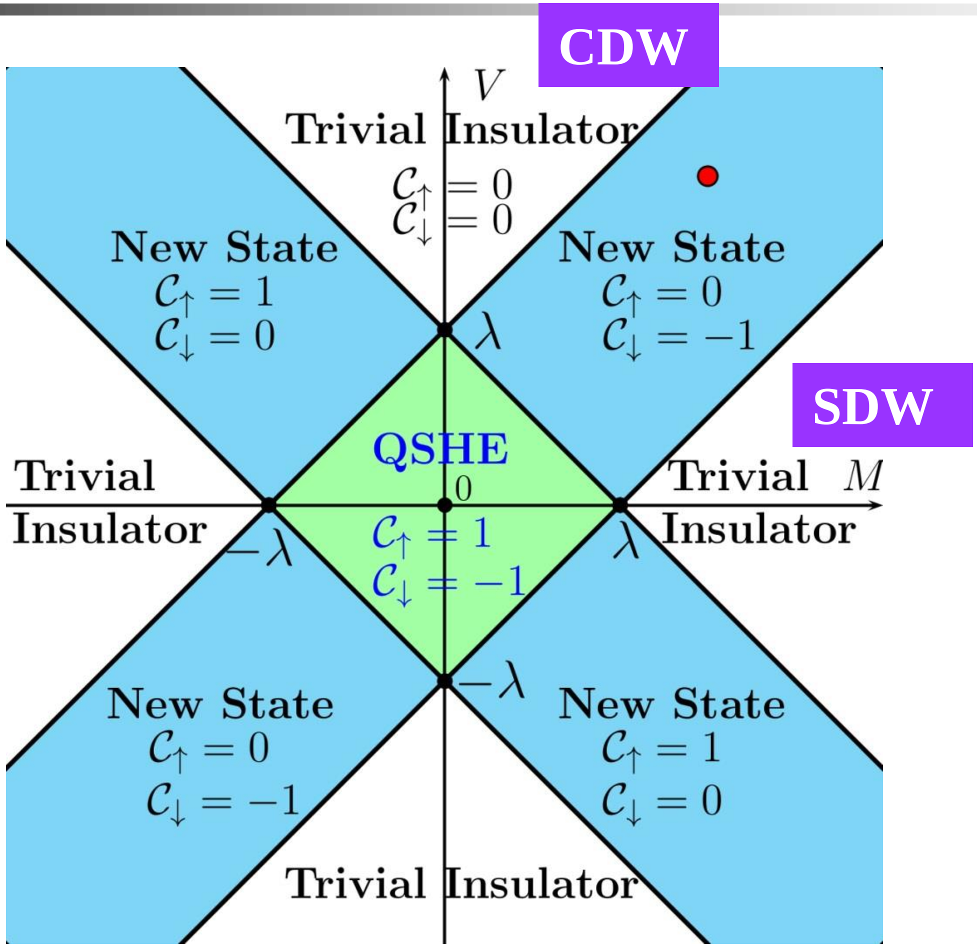
- Effective Hamiltonian

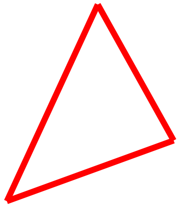
$$H = \sigma_x k_x + \tau_z \sigma_y k_y + \left(\lambda s_z \tau_z + M s_z + V \right) \sigma_z$$

$\lambda > M > 0$ ➔ ***V=0 @ QSHE***



Phase diagram

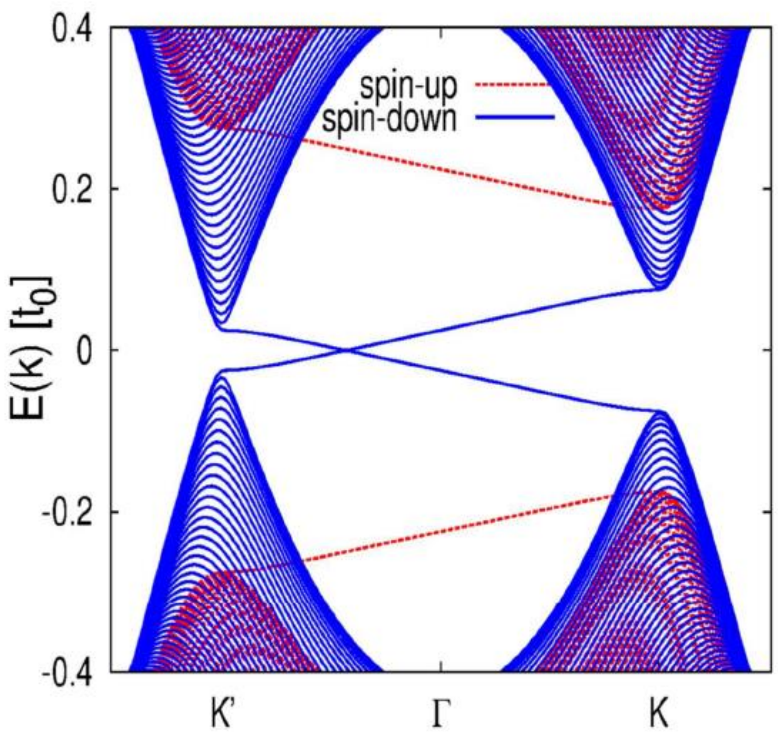




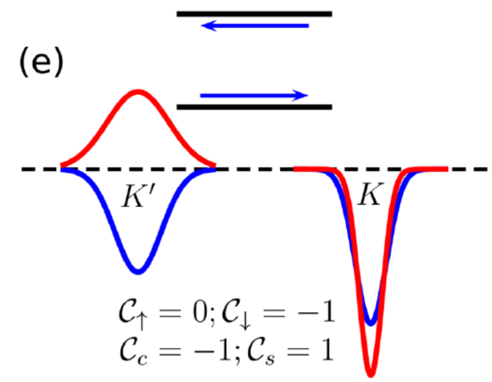
triangle of λ, M & V

interplay induces a new topological state

Edge state of finite sample



ribbon of width N=100



Bulk-edge correspondence
[holography]

↕

spin-polarized edge current

⇩

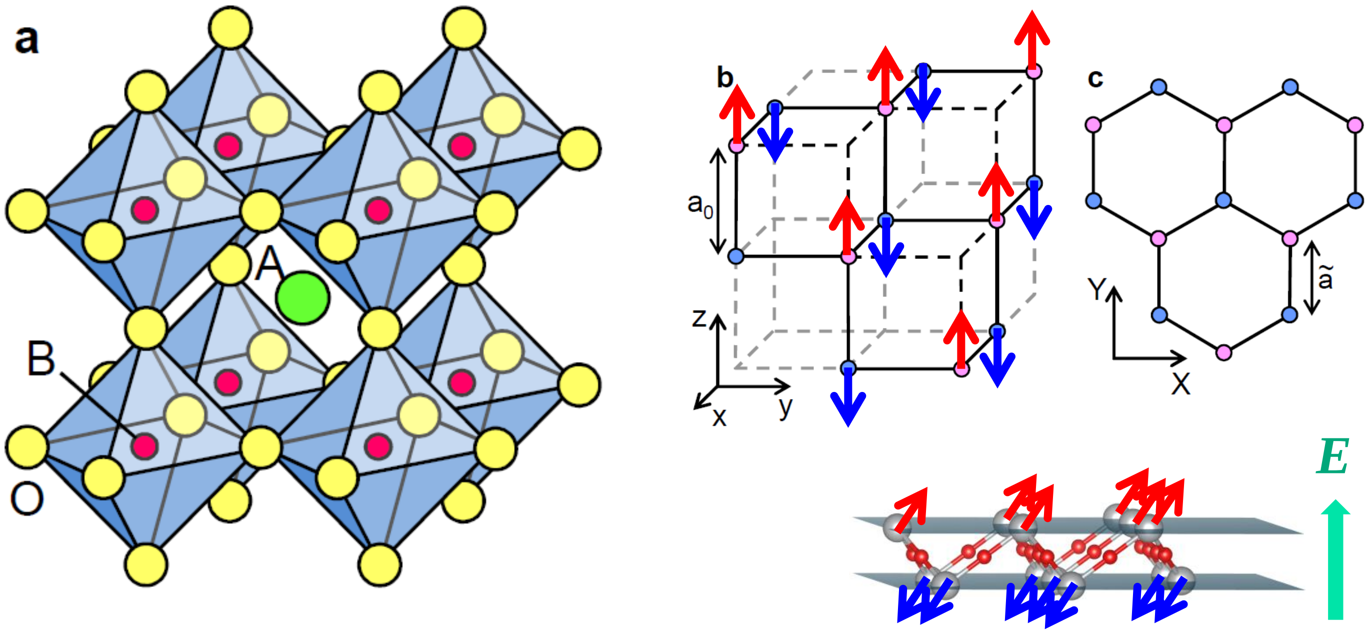
\# of occupied states:
spin up = spin down ⟷ $m_s = 0$ ⇨ HMAFM

XH: Adv. Mater. (2012) Research News

Perovskite material ABO_3

- A family of honeycomb lattices:

D. Xiao et al. Nature Comm. Vol. 2, 596 (2011)



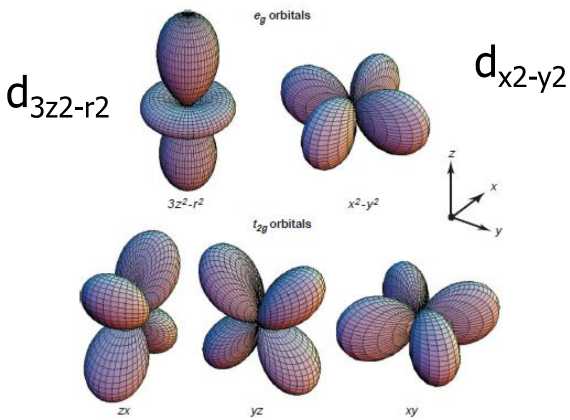
[111] direction: stacking of buckled honeycomb lattices

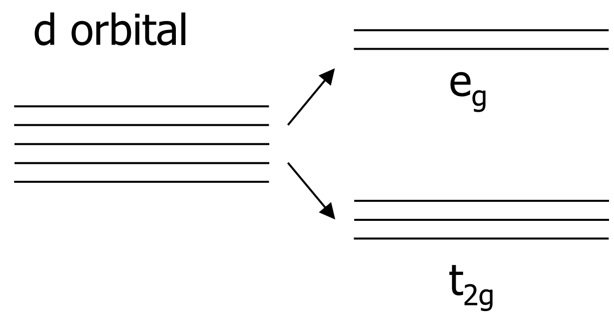
- Our platform for material design:

Mott insulator with G-type antiferromagnetic order: $LaCrO_3$

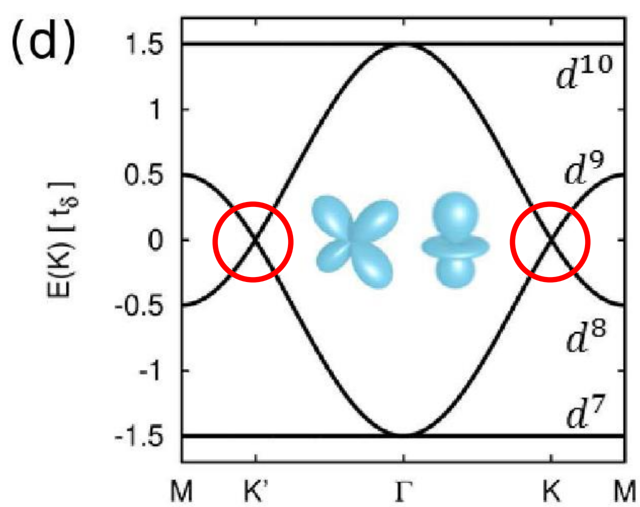
a uniform electric field along [111] direction → staggered electric potential

d^8 electrons and Dirac cones





non-interacting four-band model



$$d^8 = t_{2g}^6 e_g^2$$

Ag^{+3}

Au^{+3}

Molecule Beam Epitaxy: Layer by Layer

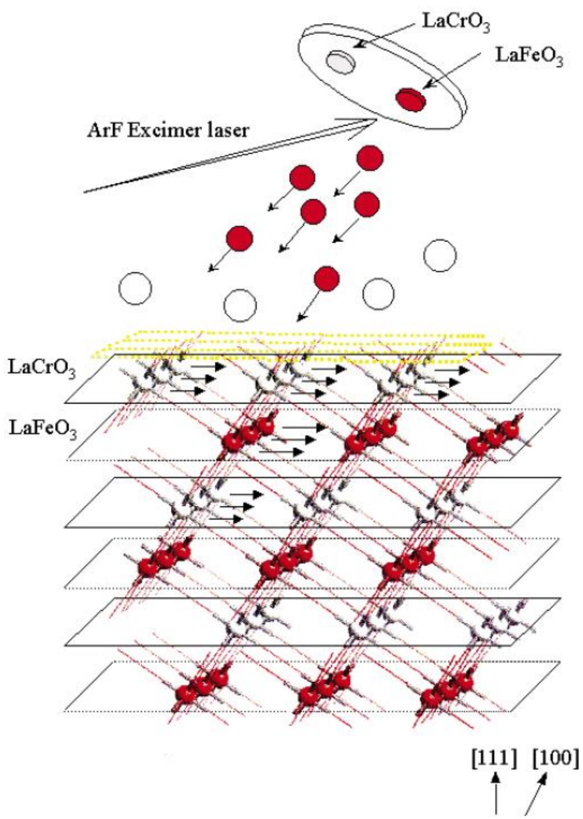
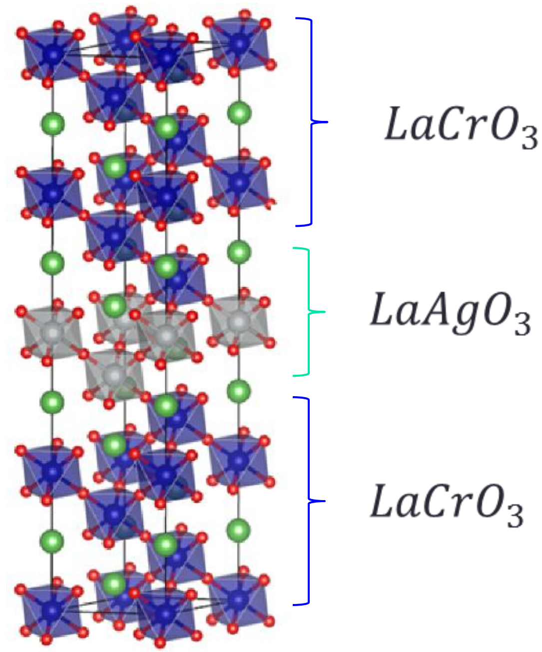


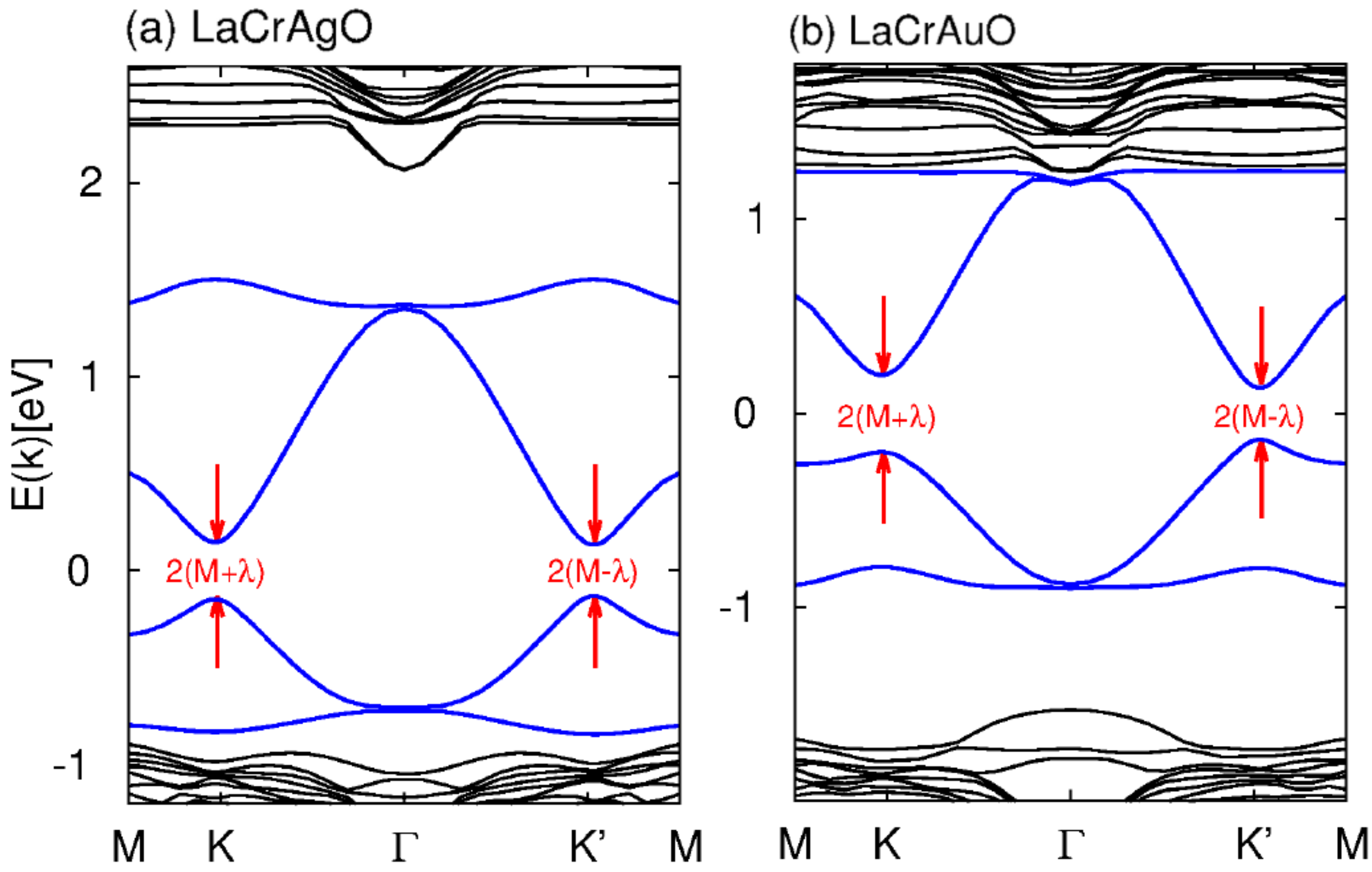
Fig. 1. A schematic diagram for the construction of the $LaCrO_3$-$LaFeO_3$ superlattice along the [111] direction by laser molecular beam epitaxy. The CrO layer and FeO layer are stacked alternately. For clarity the atoms of oxygen and lanthanum have been omitted.

Ref. Ueda, Tabata, Kawai Science vol.280, 1064 (1998)



replacing one buckled plane by $La_2Ag_2O_6$
→ Dirac electrons with sizable SOC

First principles calculation: V=0



blue states from Ag or Au exhibit double degeneracy: T x I symmetry

First principles calculations

TABLE I: Parameters for AFM order and SOC fit from GGA+U+SOC calculation. For KNiInF and KNiTlF the electronic configurations of In^{2+} and Tl^{2+} are $5s^1$ and $6s^1$.

field [meV]	LaCrAgO	LaCrAuO	LaFeAgO	LaFeAuO
M	141	166	541	467
λ	7.30	32.91	7.31	33.52
KNiPdF	KNiPtF	KNiInF*	KNiTlF*	
625	504	290	235	
11.38	33.40	5.05	18.58	

$\lambda = 30\text{meV}$

gap~2λ

large SOC ← heavy element

buckled honeycomb lattice ⇔ orbit mixing

Typical electric field of 0.1V/A → novel topological state

Topological states with AFM

- TI with simultaneous nonzero charge and spin Chern numbers

  Ezawa: PRL (2013); circularly polarized light on silicene

  PRB (2013); FM/silicene/FM sandwich

- Coupling between antiferromagnetic order and valley

  Li, Cao, Niu, Shi and Feng: PNAS vol.110, 3738 (2013)

- QAHE in ferromagnetic TI Cr-$(BiSb)_2Te_3$

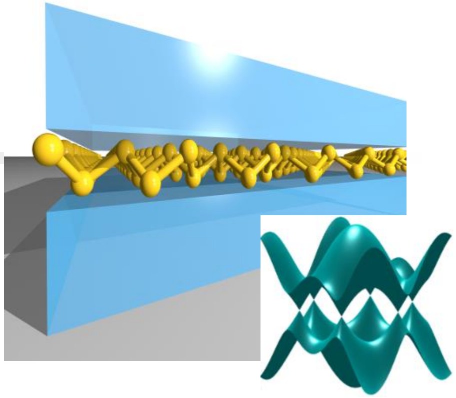
  IOP & Tsinghua group: Science (2010, 2013)

  charge Chern number =1; spin Chern number = 0 ⇔ skyrmion

  FM order of Cr + bonding of top and bottom surfaces ➔ "AFM"

Ours: charge Chern number =1; spin Chern number = 1

Summary



take home message: new topological insulator

degrees of freedom: spin, sublattice & valley

control field: SOC, AFM field, staggered electric potential

AFM TI: spin-polarized charge edge-current

Q: Chern insulator ?

A: simultaneous non-zero charge and spin Chern numbers

Q.-F. Liang, L.-H. Wu, and XH: to appear in NJP (arXiv.1301.4113)


Chromium
Cr: colorful used for decoration
Qin dynasty 2000 years ago
2013/04/25
@ Guggenheim Museum Bilbao

Rashba SOC

- Hamiltonian including Rashba-type SOC: 4x4

$$H(\boldsymbol{k}) = \begin{pmatrix} H_0^{\uparrow} & H_R \\ H_R^{\dagger} & H_0^{\downarrow}|_{\lambda_{so}\to-\lambda_{so}} \end{pmatrix}_{[a_\uparrow, b_\uparrow, a_\downarrow, b_\downarrow]}$$ with eigenstates $|\Psi_1\rangle = \begin{pmatrix} \varphi_a^{\uparrow} \\ \varphi_b^{\uparrow} \\ \varphi_a^{\downarrow} \\ \varphi_b^{\downarrow} \end{pmatrix}$ $|\Psi_2\rangle = \begin{pmatrix} \phi_a^{\uparrow} \\ \phi_b^{\uparrow} \\ \phi_a^{\downarrow} \\ \phi_b^{\downarrow} \end{pmatrix}$

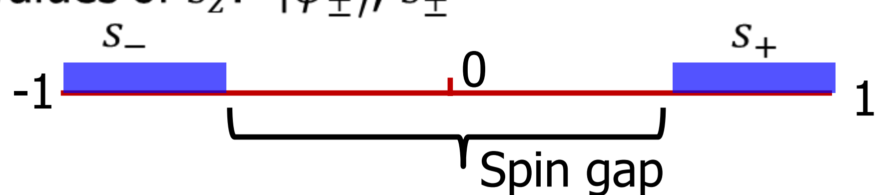
- Definition of C_s with two valence eigenstates $|\Psi_1\rangle$ and $|\Psi_2\rangle$

1. Projection of s_z over space spanned $|\Psi_1\rangle$ and $|\Psi_2\rangle$

$$\tilde{s}_z = \begin{pmatrix} \langle\psi_1|s_z|\psi_1\rangle & \langle\psi_1|s_z|\psi_2\rangle \\ \langle\psi_2|s_z|\psi_1\rangle & \langle\psi_2|s_z|\psi_2\rangle \end{pmatrix}$$ with $s_z = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}$

2. Eigenstates and eigenvalues of $\tilde{s}_z$: $|\psi_\pm\rangle$, $s_\pm$

Spectrum of $s_\pm$:



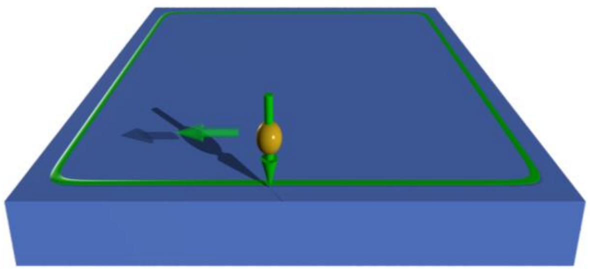
3. Spin-Chern number from $|\psi_\pm\rangle$

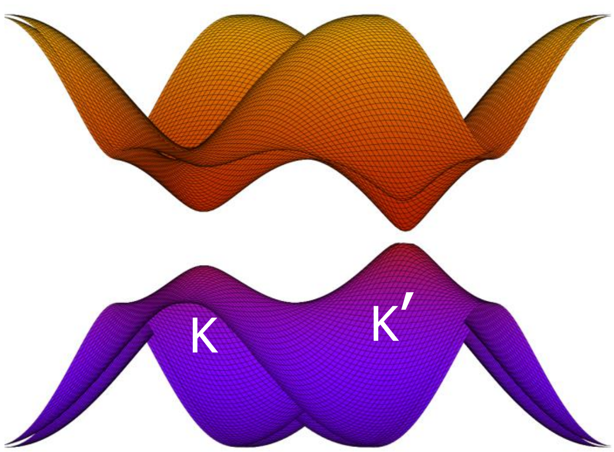
$$C_s = C_+ - C_- \quad \text{with} \quad C_\pm = \frac{1}{2\pi i}\int_{BZ} d^2\mathbf{k}\nabla_{\mathbf{k}} \times \langle\psi_\pm(\mathbf{k})|\partial_{\mathbf{k}}|\psi_\pm(\mathbf{k})\rangle$$

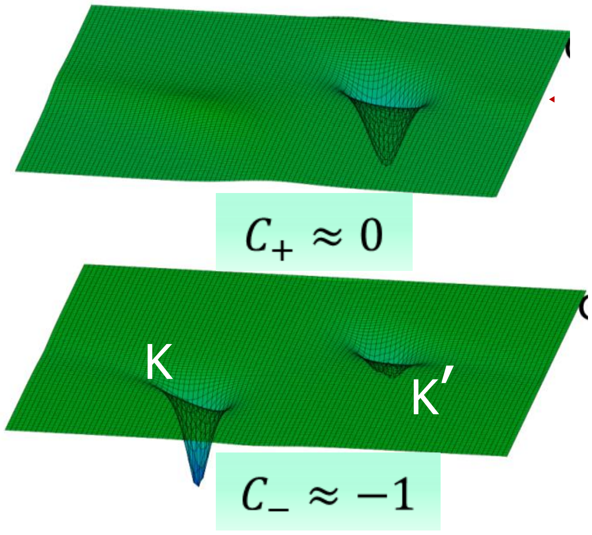
Rashba SOC

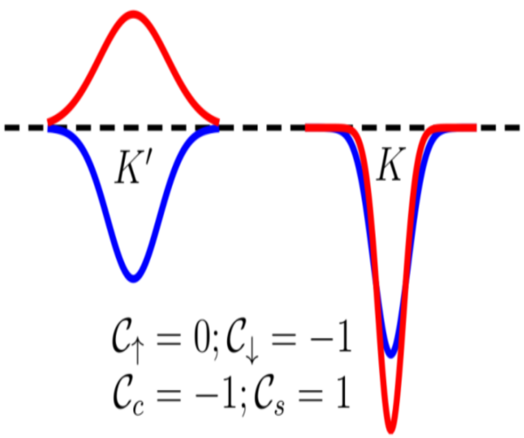
Rashba SOC: $\lambda_R = 0.2t_0$

same order as intrinsic SOC

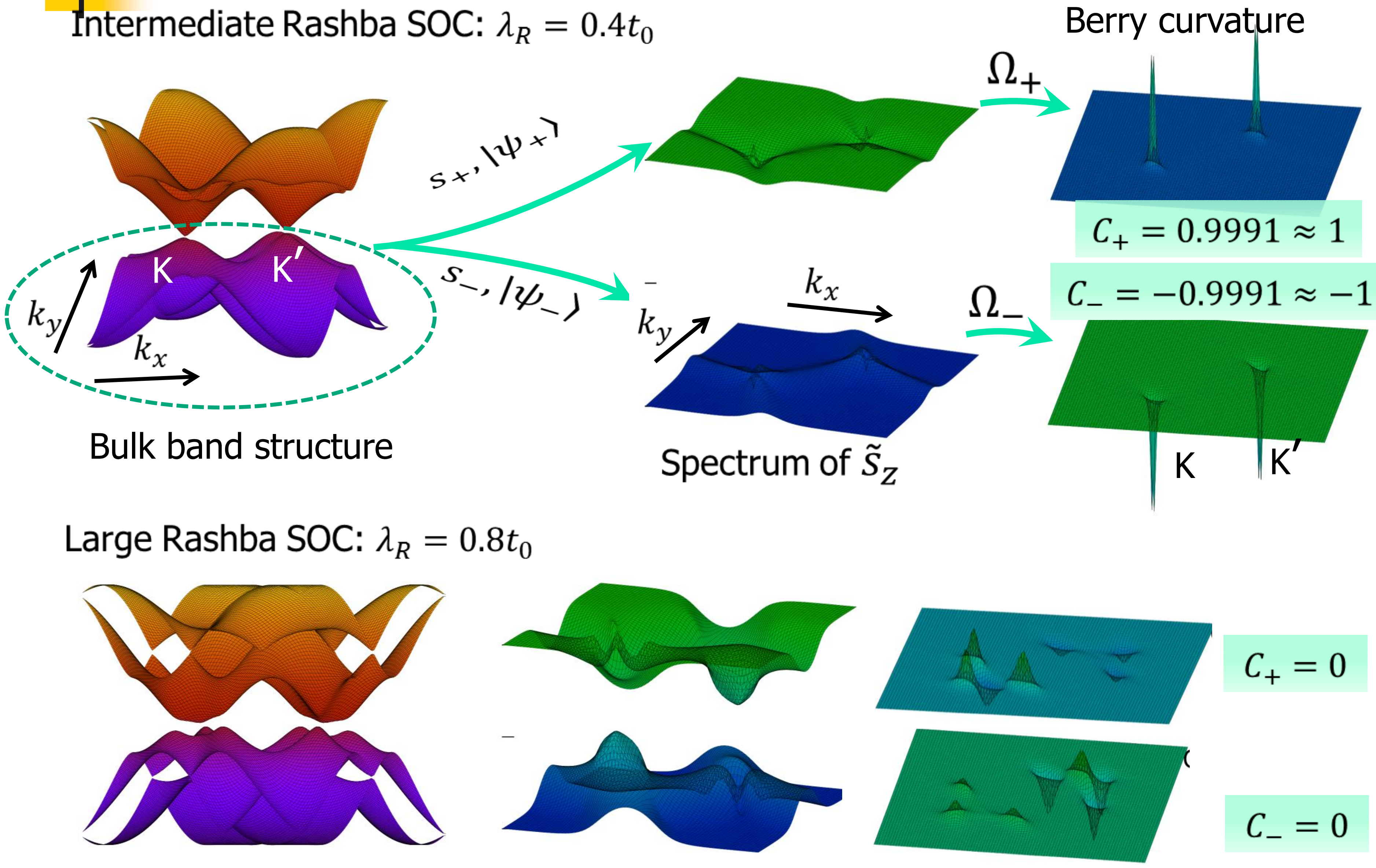








Rashba SOC



Intermediate Rashba SOC: $\lambda_R = 0.4t_0$
Berry curvature
Ω_+
$s_+, |\psi_+\rangle$
$C_+ = 0.9991 \approx 1$
K
K′
k_y
k_x
$s_-, |\psi_-\rangle$
k_x
k_y
Ω_-
$C_- = -0.9991 \approx -1$
Bulk band structure
Spectrum of $\tilde{s}_z$
K
K′
Large Rashba SOC: $\lambda_R = 0.8t_0$
$C_+ = 0$
$C_- = 0$