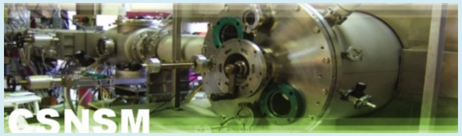
# Topological 2DEG at the 111 surface of KTaO3

M. G a b a y

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C. Bareille
F. Fortuna

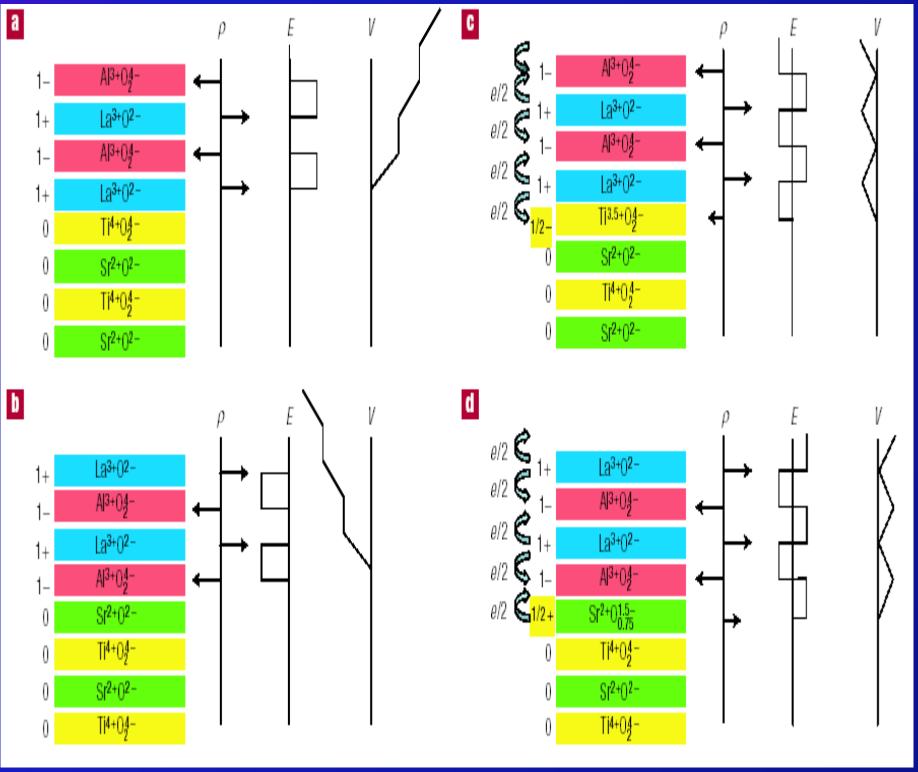

M. Rozenberg, O. Hijano Cubelos

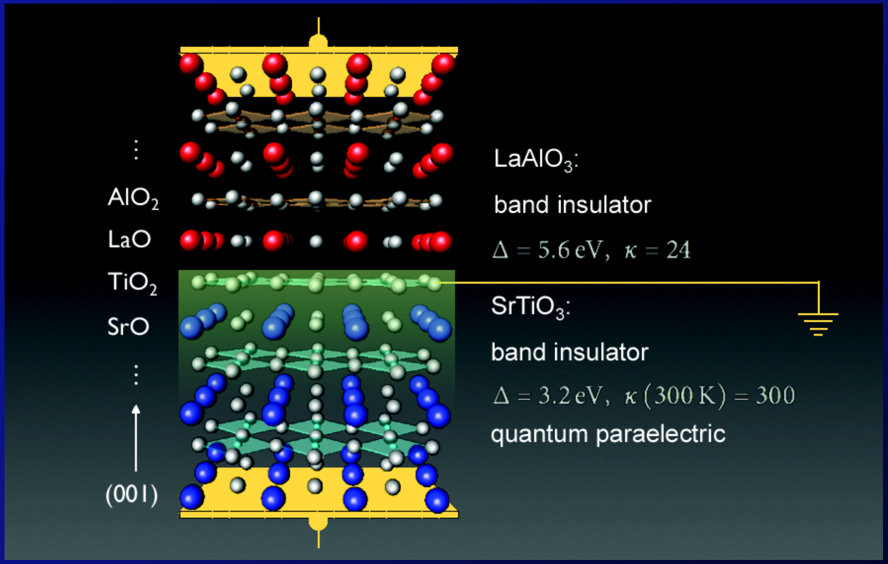
THALES

A. Barthélémy, M. Bibes,

# 2DEGS in perovskite oxides

❖ **Interface polar-non polar compounds**

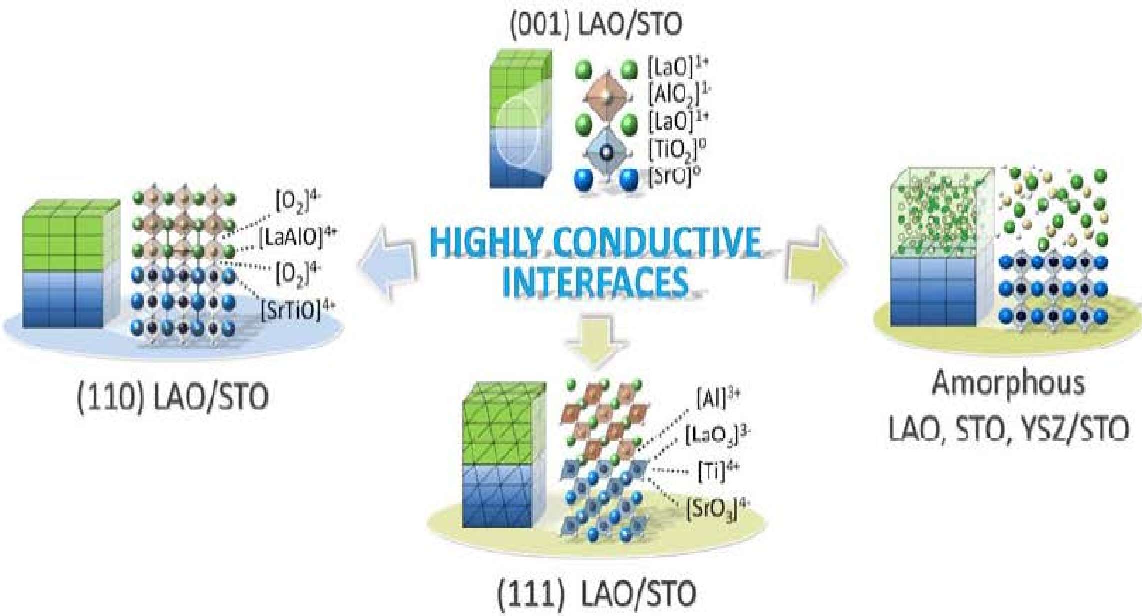


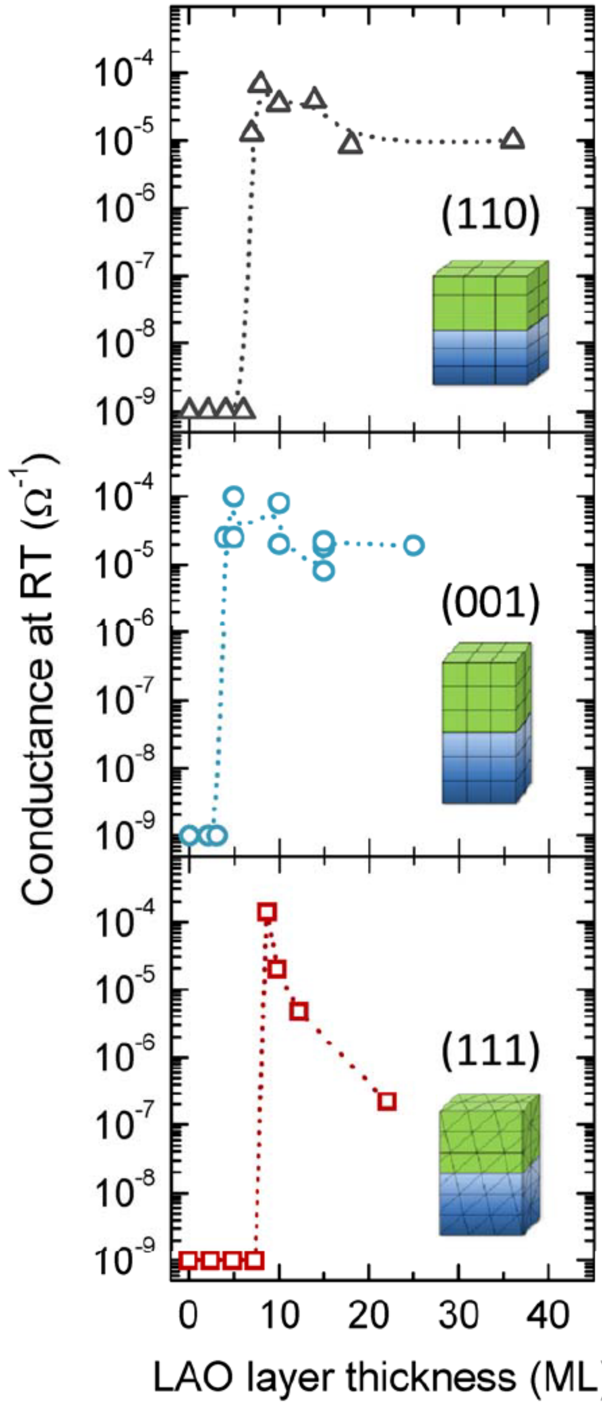




NAOYUKI NAKAGAWA[1,2], HAROLD Y. HWANG[1,2] AND DAVID A. MULLER

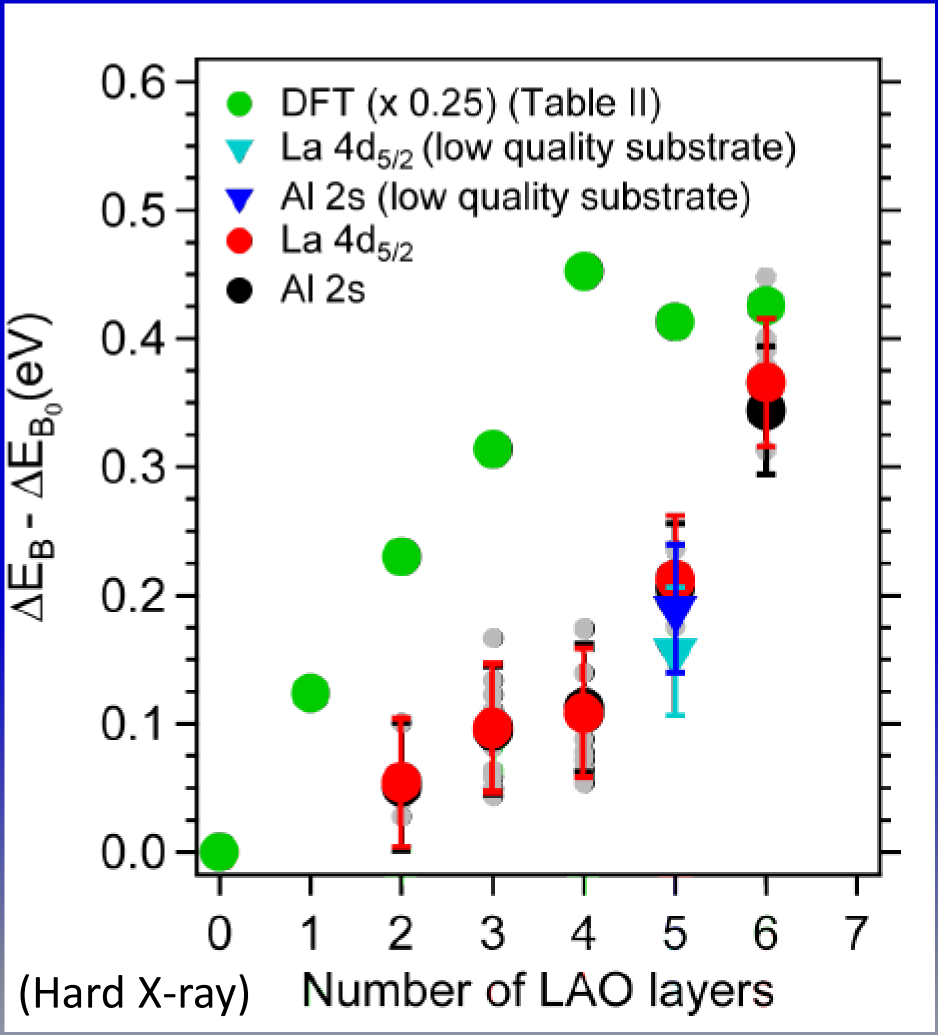
nature materials | VOL 5 | MARCH 2006

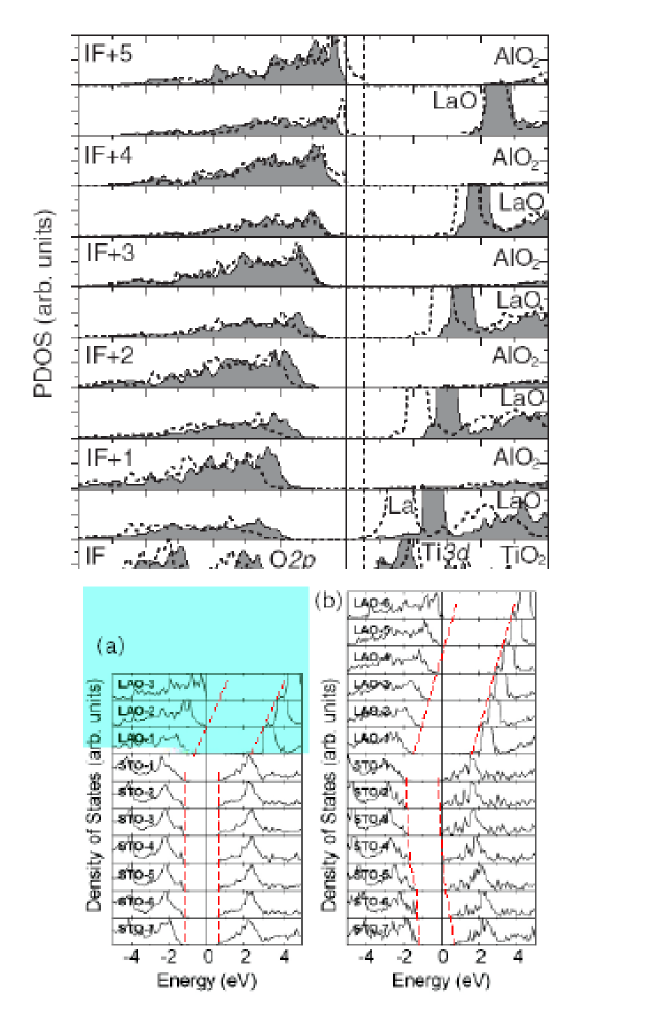
G. Herranz et al. Scientific Reports 2, 758 (2012)




See also Ariando et al., Nature Communications 4, 1838 (2013)



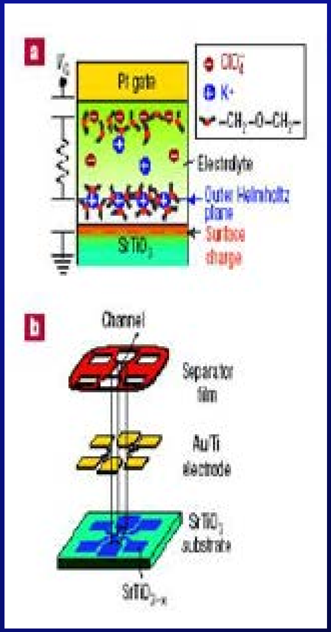

E. Slooten et al. PHYSICAL REVIEW B **87**, 085128 (2013)

Rossitza Pentcheva[1] and Warren E. Pickett
PRL **102**, 107602 (2009)

# 2DEGS in perovskite oxides

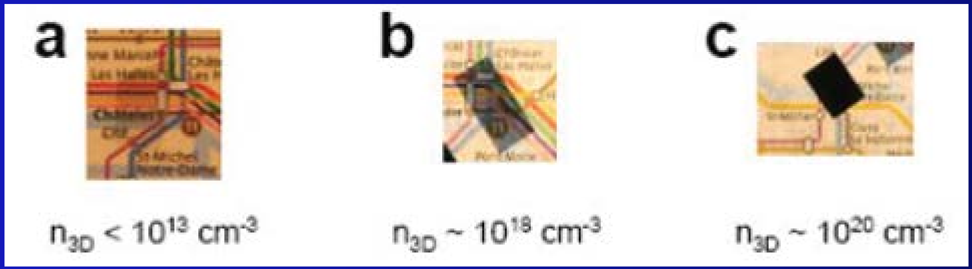
❖ Interface polar-non polar compounds

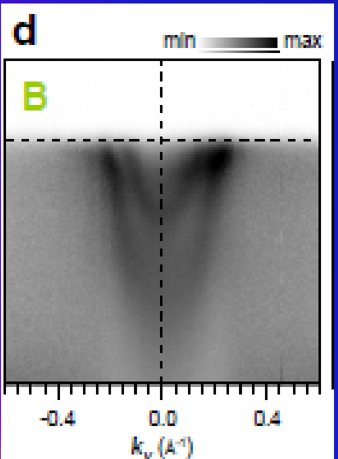
❖ Surface non polar material



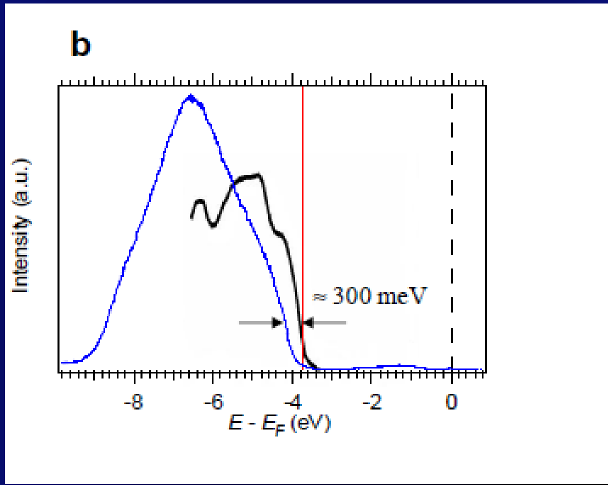
# 2DEGS in perovskite oxides

- ❖ Interface polar-non polar compounds
- ❖ Surface non polar material
- ❖ Or cleaved surface in high vacuum

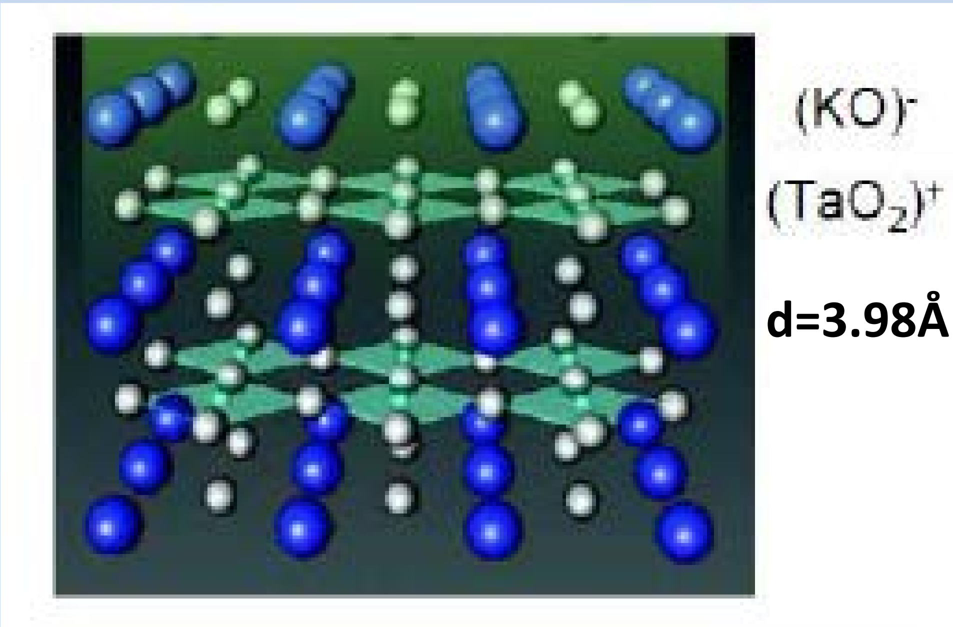


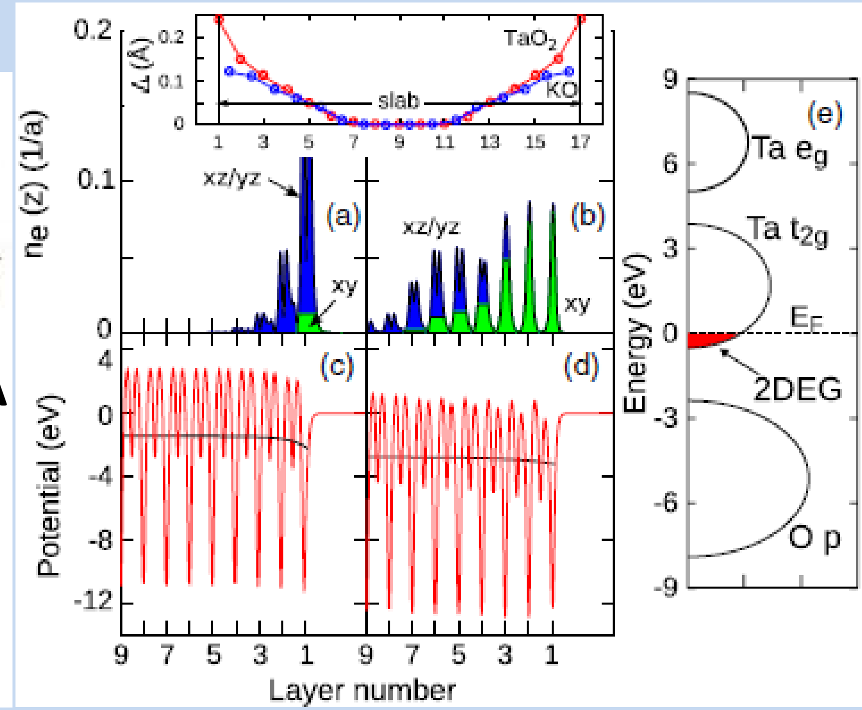




A. Santander-Syro et al. Nature 469, 189-193 (2011)



# This mechanism also works for other transition-metal oxides!

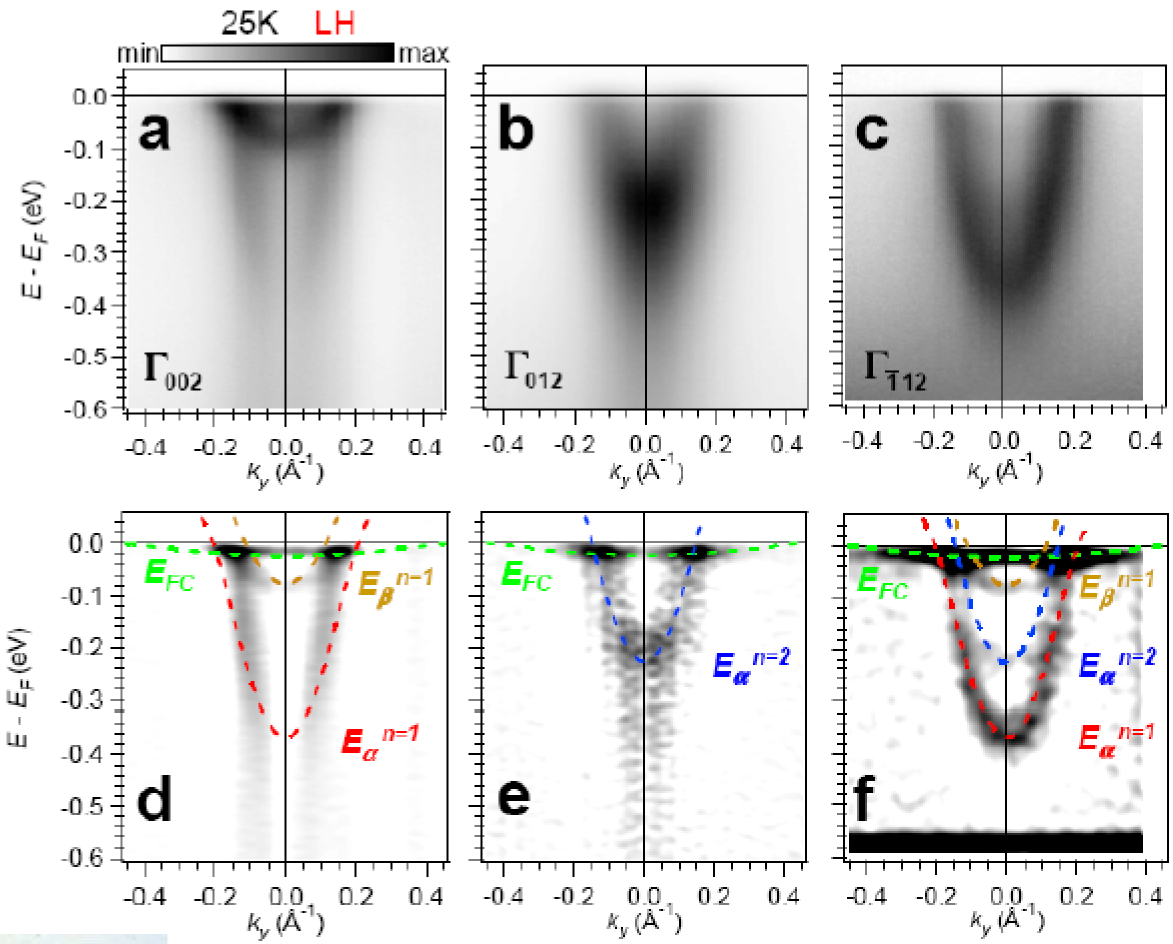



Shanavas, Satpathy PRL **112**, 086802 (2014)

- KTO 001 is polar!
- Ta is a 5d transition metal element
- Large direct band gap (~4.2 eV)
- Large bulk spin-orbit $\Delta_{so}$~0.47 eV
- $\Delta_{so}$ is comparable to $E_F$ of the 2DEG and larger than the sub-band energy separation

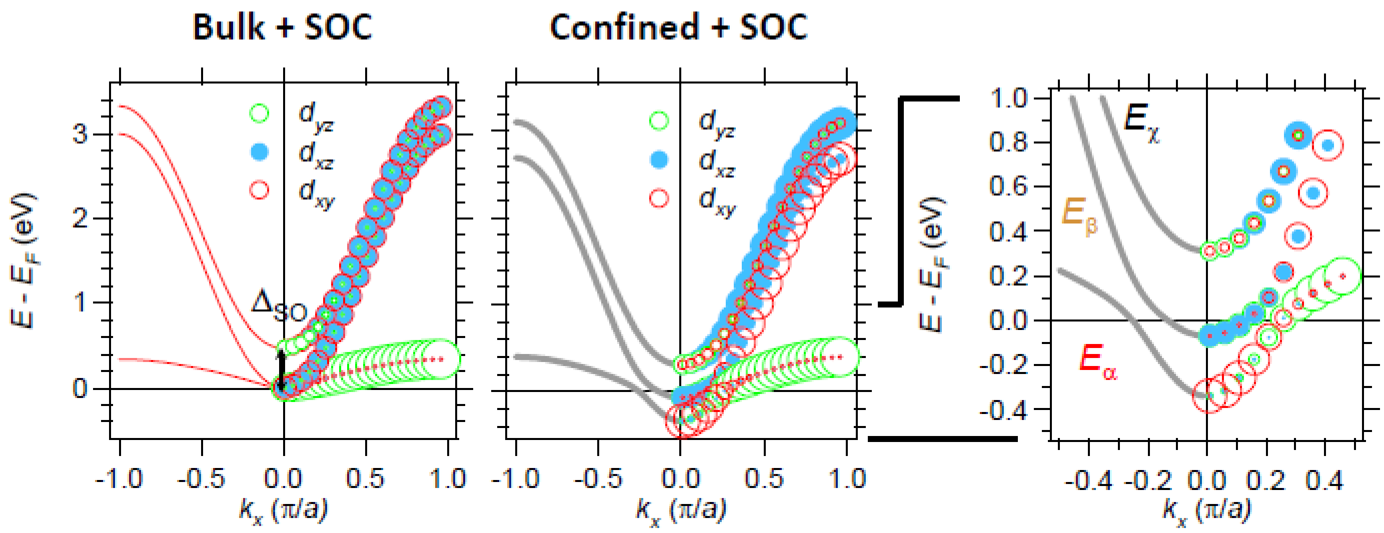
# 2DEG subbands at the surface of $KTaO_3$ 001




Santander-Syro et al. Phys. Rev. B 86, 121107(R) (2012)
King et al. Phys. Rev. Lett. 108, 117602 (2012)

$n_{2D}$~0.2 e/u.c   L ~ 3 u.c  (comparable to STO)
F~250MV/m

# KTaO$_3$ bulk vs 2D-confined:
# **The game of energy scales**




**$\Delta_{SO}$ ~ $E_F$ ~ energy separation between subbands**

Beyond subband orbital ordering:

**→ Orbital symmetry changes (reconstructs) in the 2DEG**

# KTO along (001) direction

**Santander-Syro et al. Phys. Rev. B 86, 121107(R) (2012)**

- Hypothetical BULK structure without SOI (from LDA) :

Light mass $m_l \sim 0.25 m_e$ ; Heavy mass $m_h \sim 5.3 m_e$

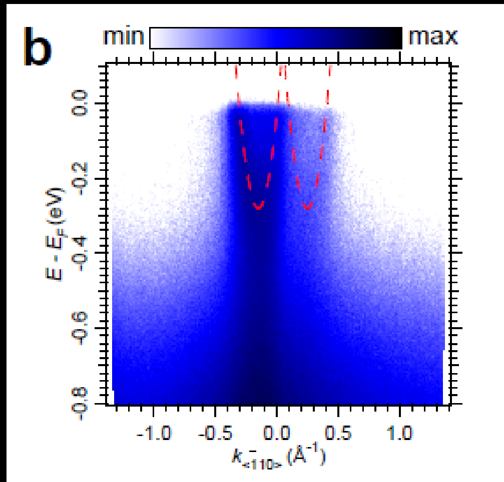
- BULK structure with SOI (k.p):

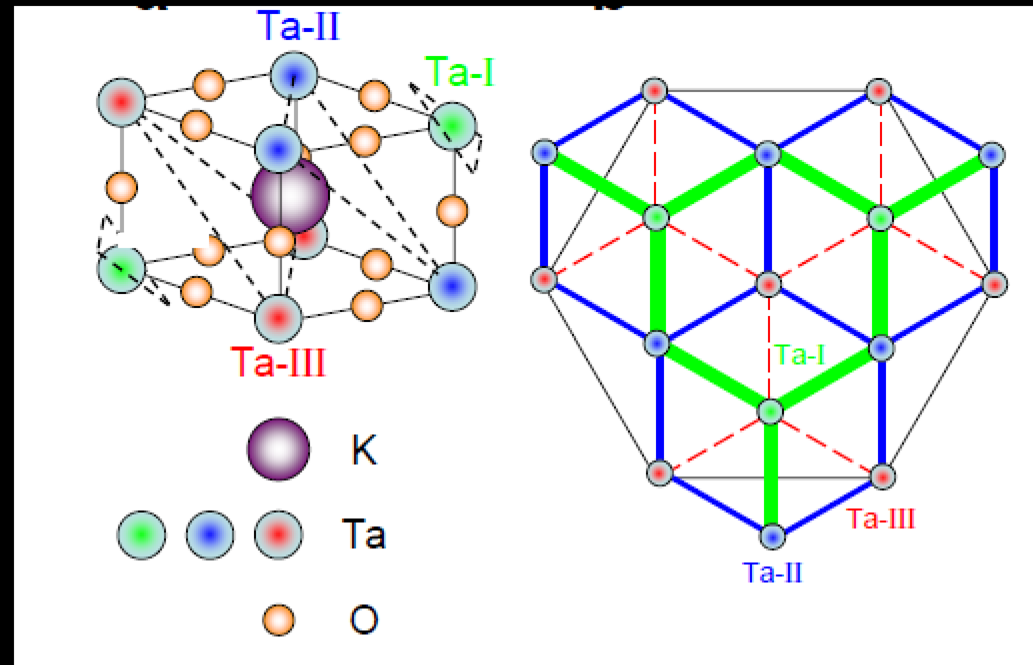
Light mass $m_l \sim 0.25 m_e$ ; Heavy mass $m_h \sim 0.66 m_e$ ; SO mass ; $m_{SO} \sim 0.35 m_e$
for $m_h$, cf SdH measurements S. Harashima et al. PRB 88, 085102 (2013).

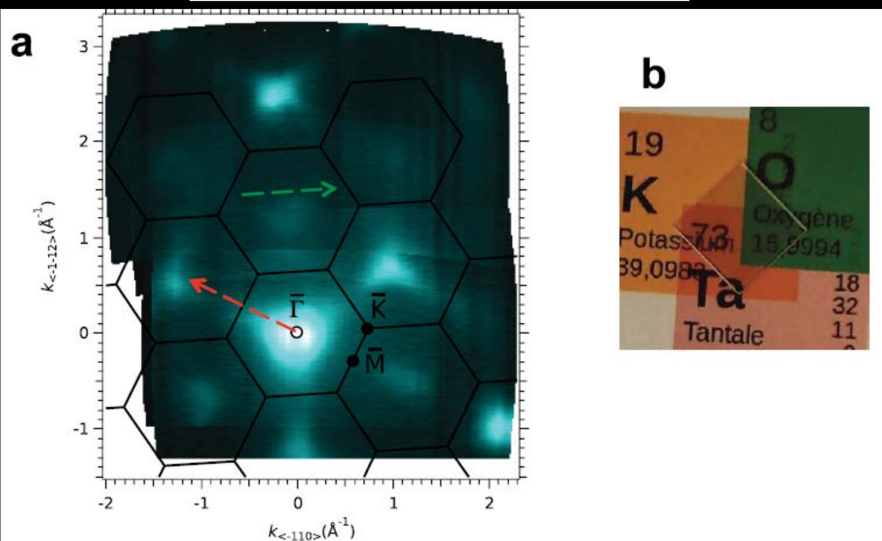
- CONFINED structure with SOI

Light mass $m_\alpha \sim 0.25 m_e$ ; Heavy mass $m_\beta \sim 0.5 m_e$ ; SO mass ; $m_\gamma \sim 0.41 m_e$ (k.p)
Light mass $m_\alpha \sim 0.28 m_e$ ; Heavy mass $m_\beta \sim 0.7 m_e$ (ARPES)
$m \sim 0.9 \pm 0.08 m_e$ (SdH) (□ $m_\beta$ higher mobility near $E_F$ ?)
$k_{F\beta} \sim 0.12$□$^{-1} \Rightarrow \Delta_{rashba} \sim 10$ meV (cf Shanavas et al. PRL 112, 086802 (2014))

# Investigating the (111) surface of KTO



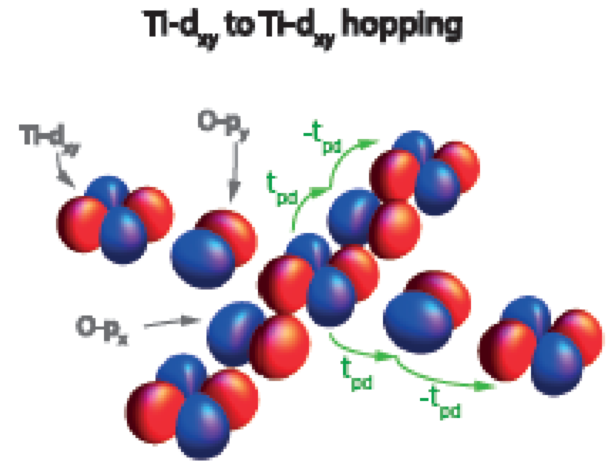



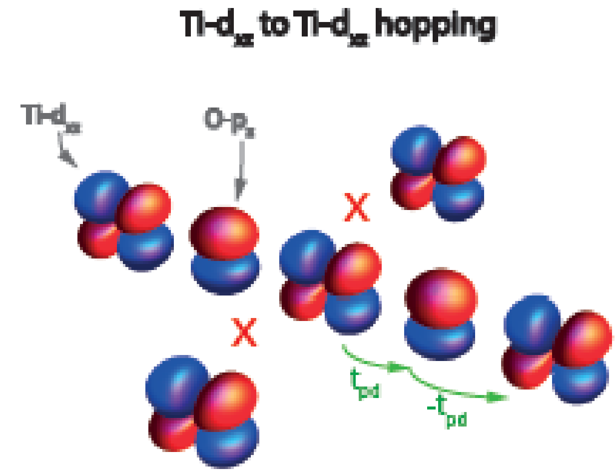

**5+ 5- charges in alternate layers**

*A. Santander-Syro et al.*
*Scientific Reports 4, 3586 (2014)*

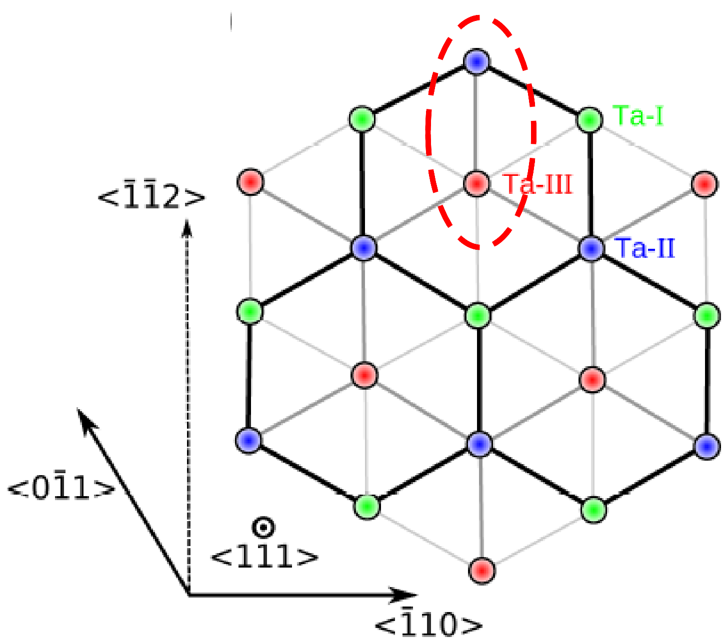
**F~ 170 MV/m L~1-2nm $n_{2D}$~$10^{14}$$cm^{-2}$**

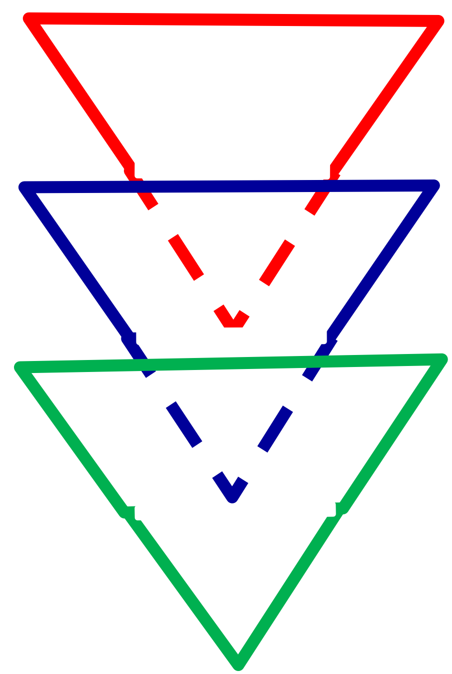
# 2-layer case (BN - Graphene)



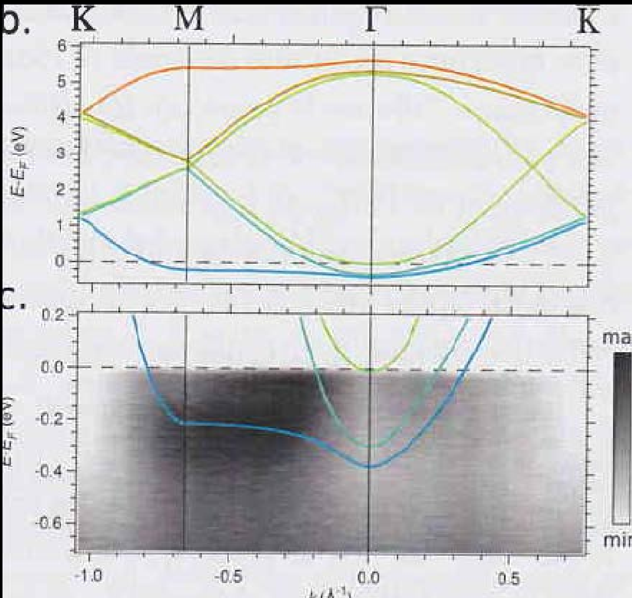



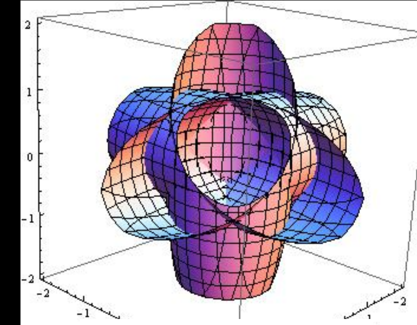

## Unit cell in real space



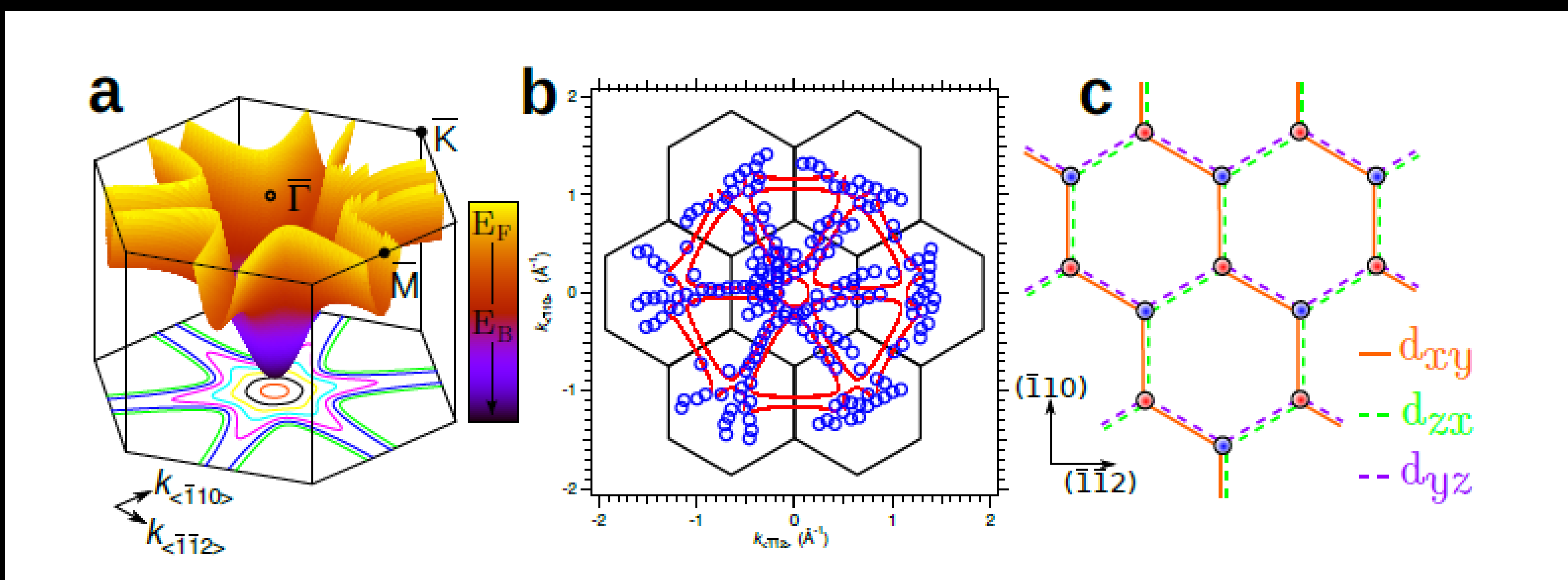



# Band-structure vs experiment for (111) surface of KTO



Bulk (111) FS
No SOI

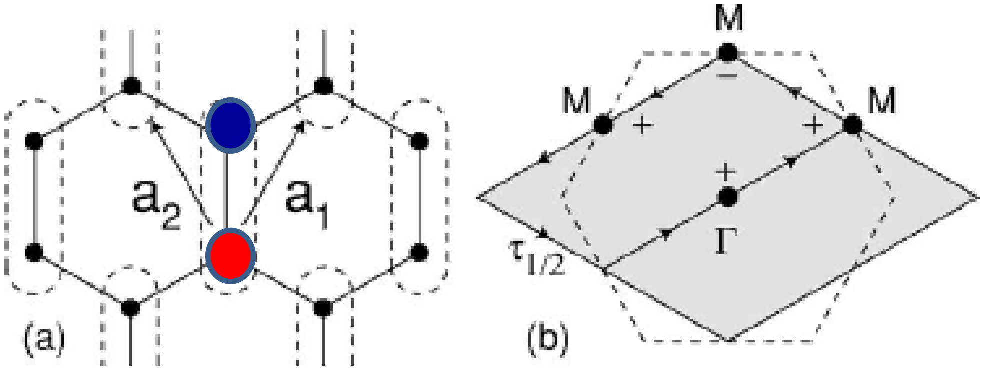


# A pinch of topology

## 2-layer case (Graphene-like)

**If TRI and parity ⇒ $Z_2$ index.**

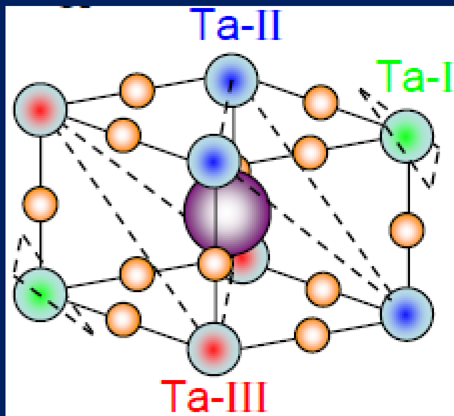
**V=0**




**Unit cell in real space**

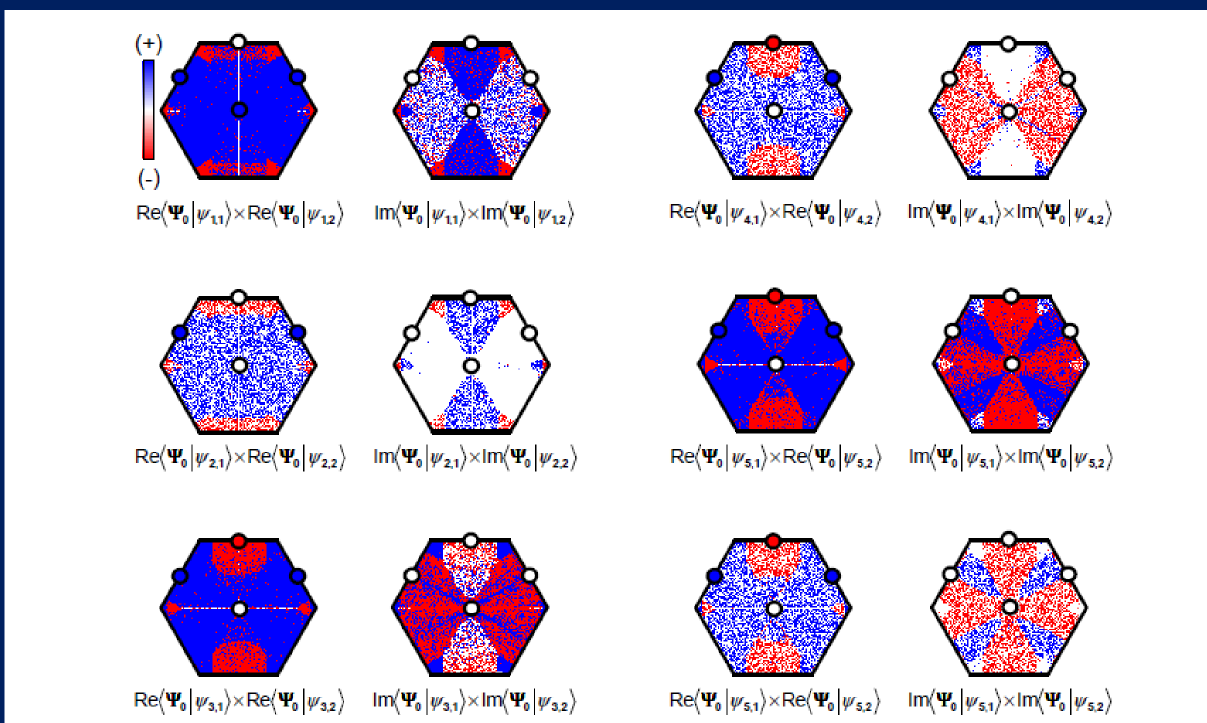
**TRIM points in the BZ**

(cf L.Fu & C.L. Kane, PRB 76,045302 (2007))




Ground state eigenstate $\Psi_0=\sum_{i=1,6;j=1,2} a_{ij}\psi_{ij}$

- j=1,2 → III, II
- $\psi_{i=1,6}$ → dyz↑, dxz↑, dxy↑, dyz↓, dxz↓, dxy↓

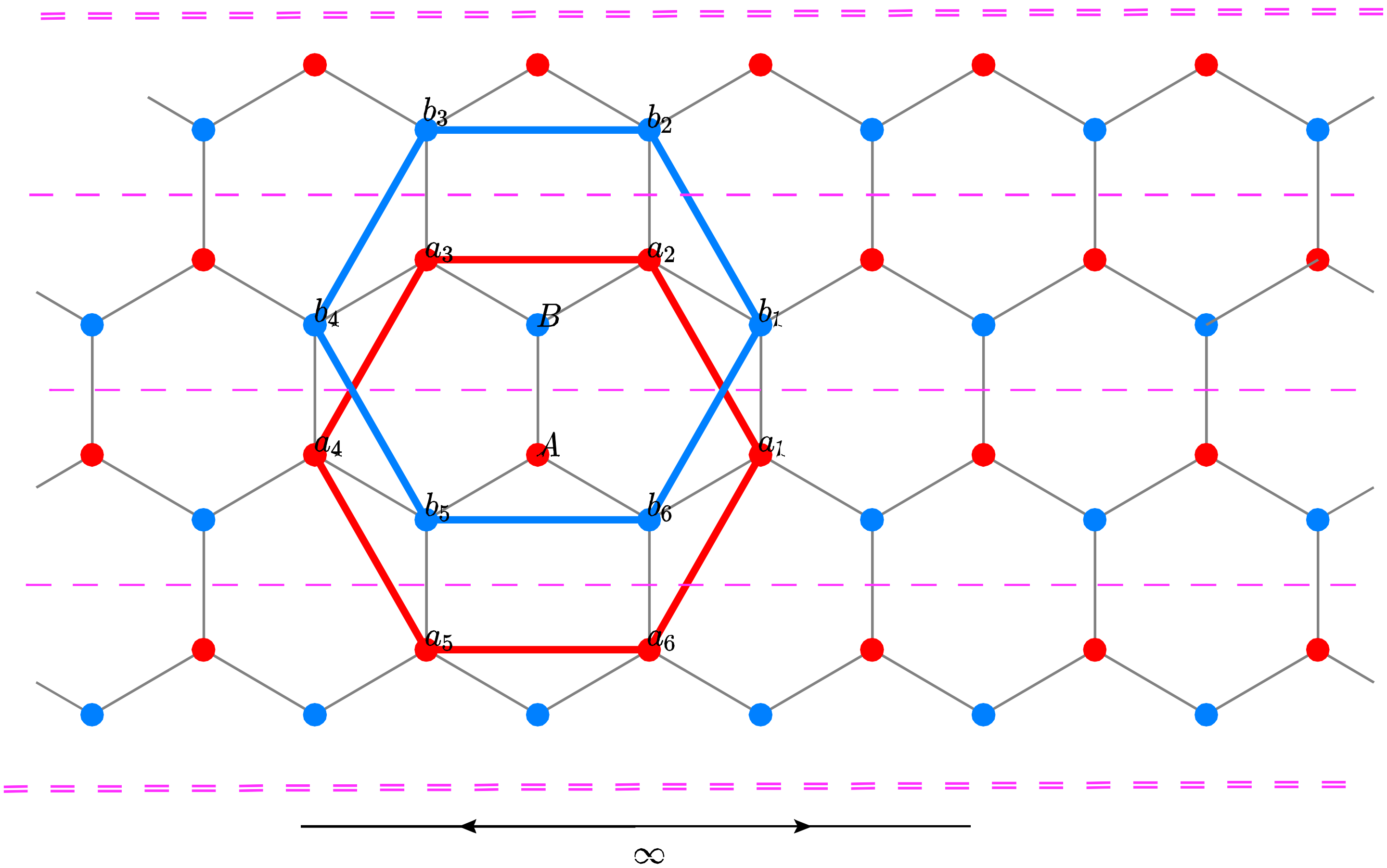



$a_{i,1} \times a_{i,2}$

↑ layer index ↑

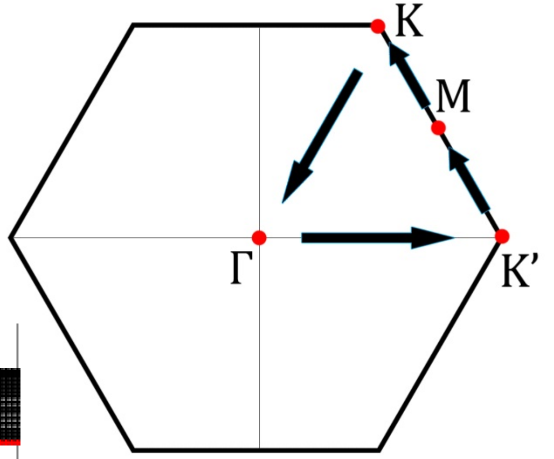
# Strips

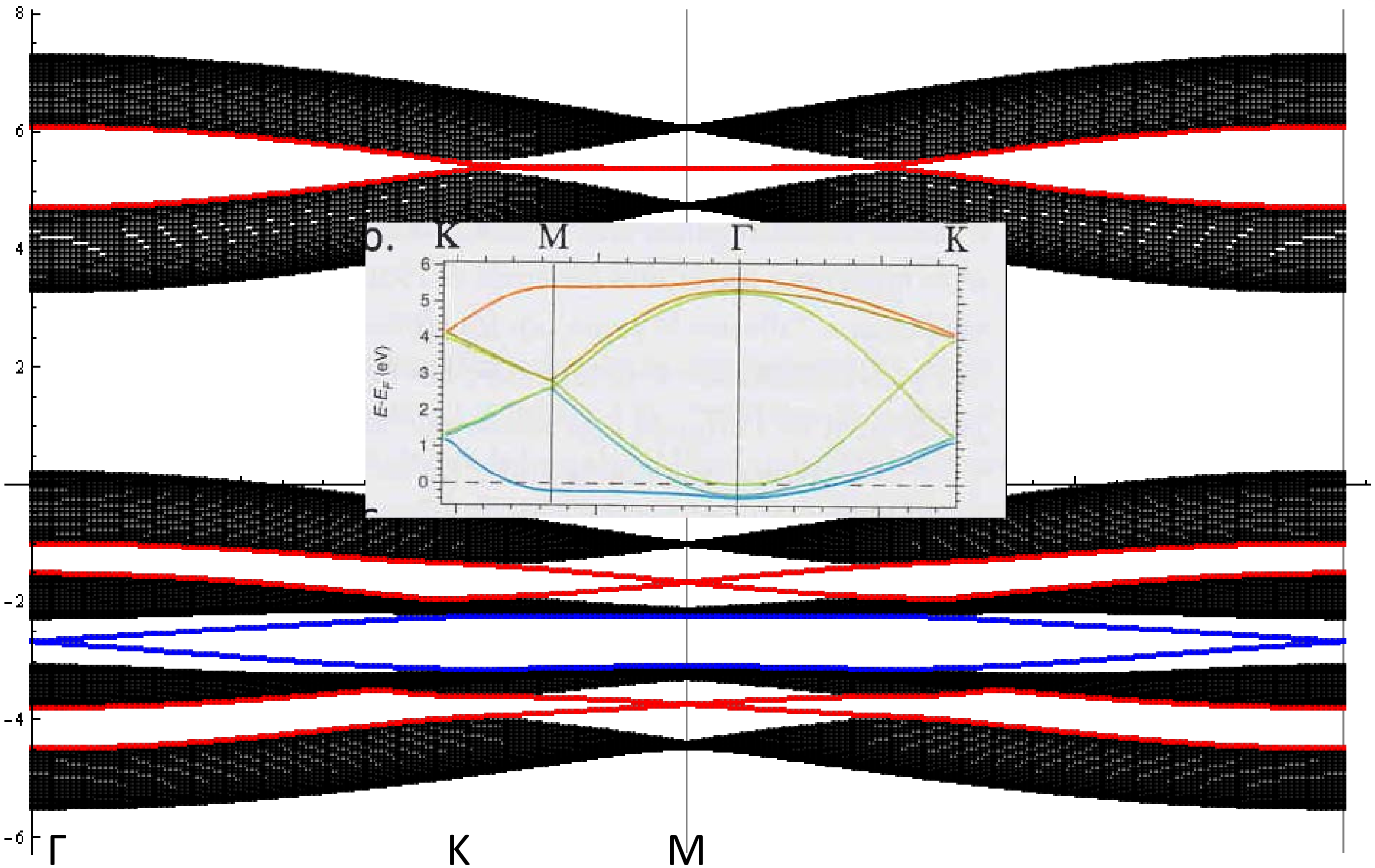
- Finite size geometry
- Example for 4 strips



# Idea: look for the edge states (I)

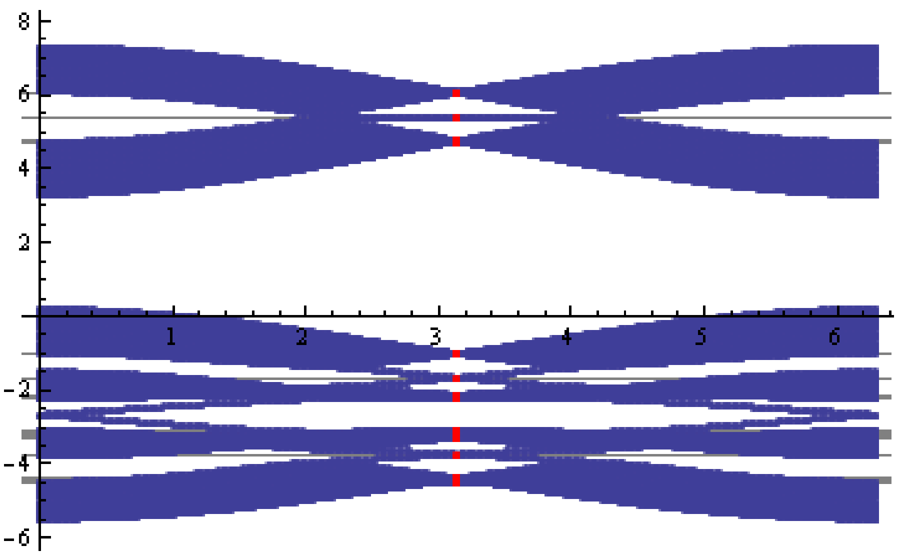
- Edge states are topological
- Found several edge states



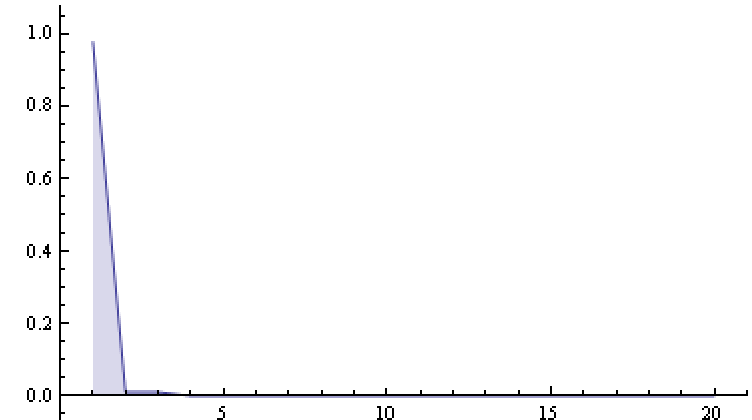



# Idea: look for the edge states (II)

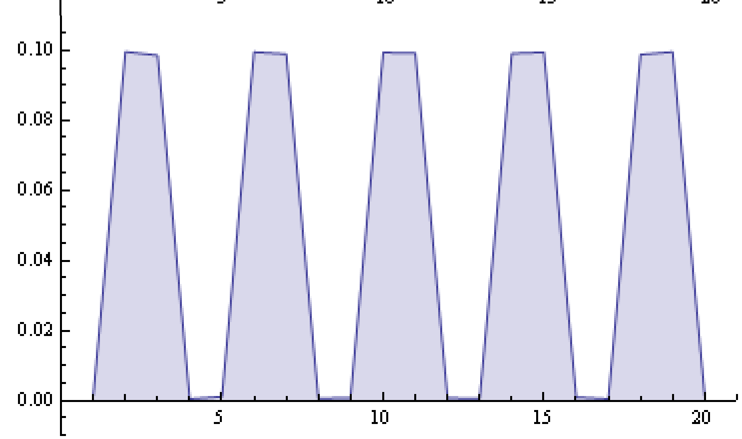
- Edge states are completely localized at the M point
- They delocalize when we move away from the M point




**Stable if V<< t**



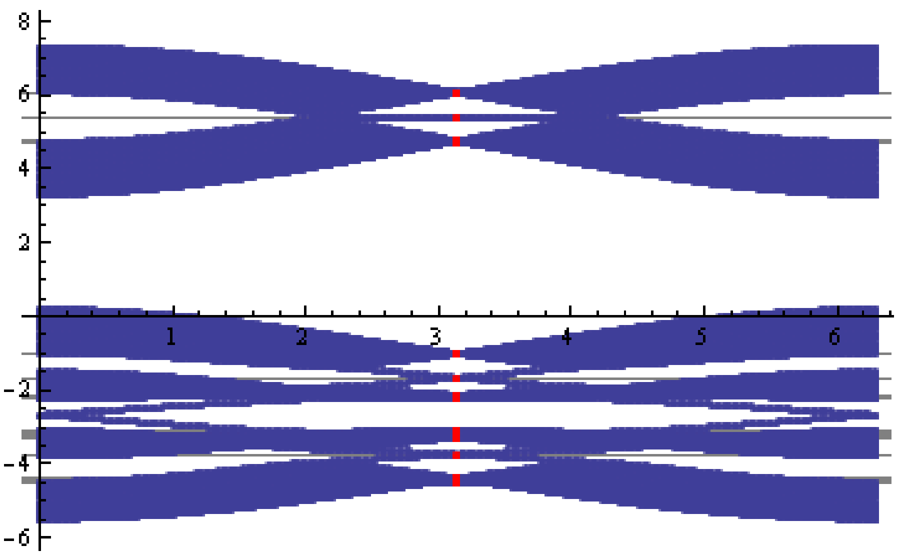

**Edge**
state



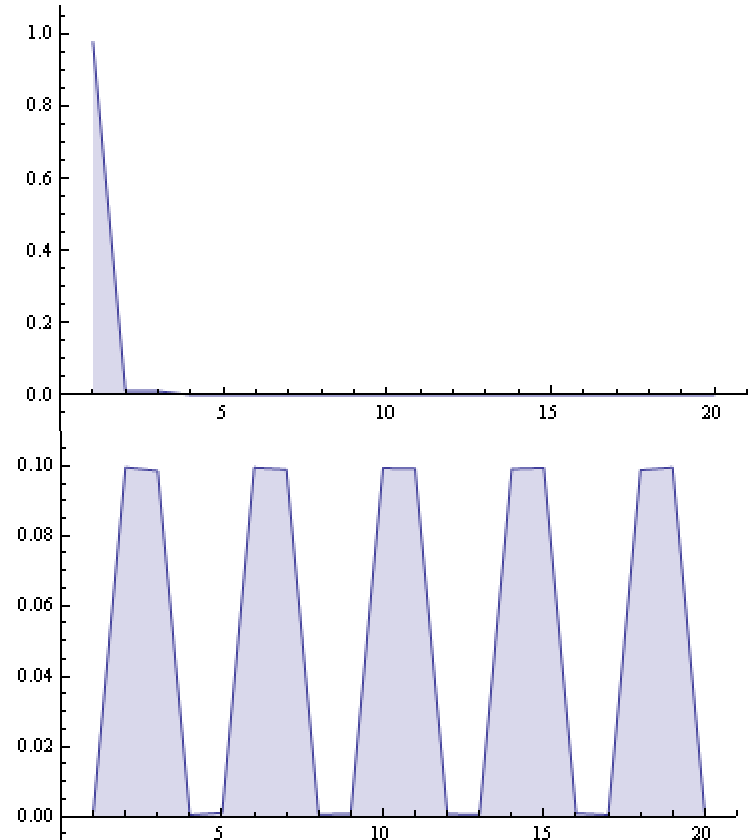

**« Bulk »**
state

# Idea: look for the edge states (III)

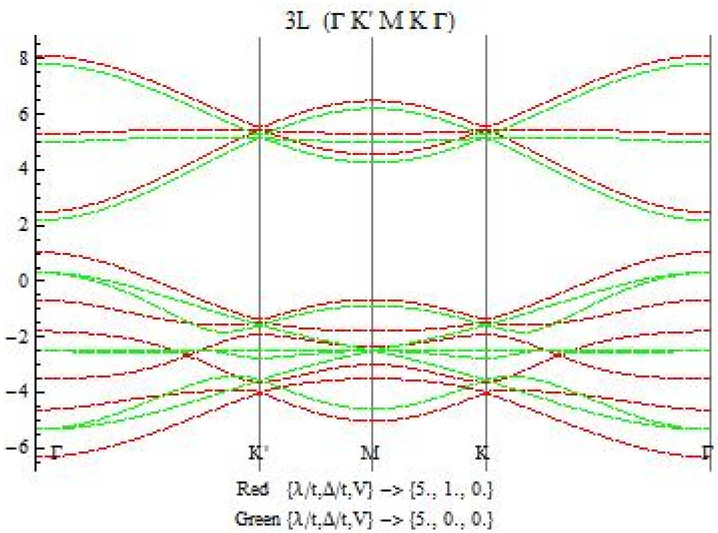
- Edge states are completely localized at the M point
- They delocalize when we move away from the M point

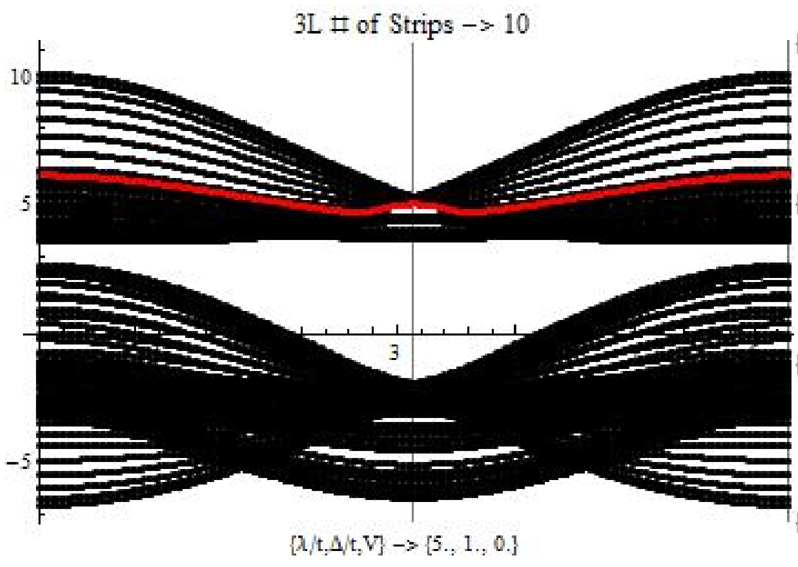



**Stable if V<< t**



# 3-layer case (T3 – Dice)




**Total**, **1 st layer**, **2 nd layer**, **3 rd layer**