# Topological Band and Correlated Insulators

## Part 2

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Caltech

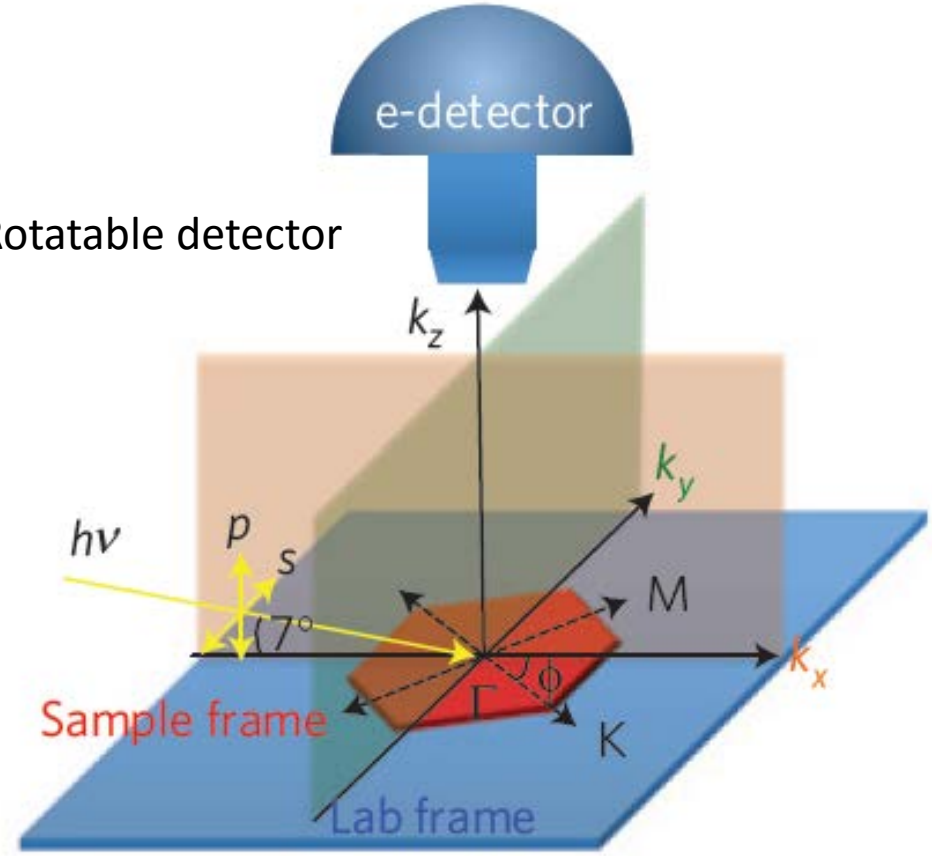
IQIM

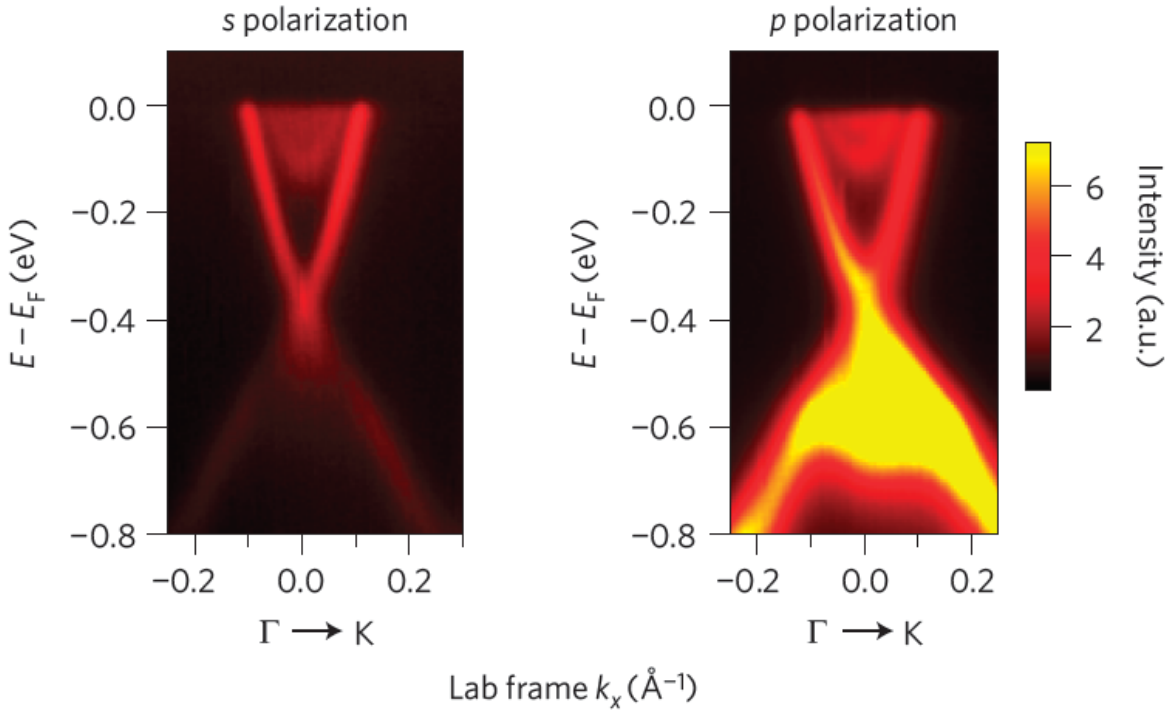
# Outline

- Orbital texture of topological surface states
- Correlated topological insulators
  - Heavy transition metal oxides
  - *f*-electron heavy fermion systems
- Superconducting topological insulators

# Orbital texture

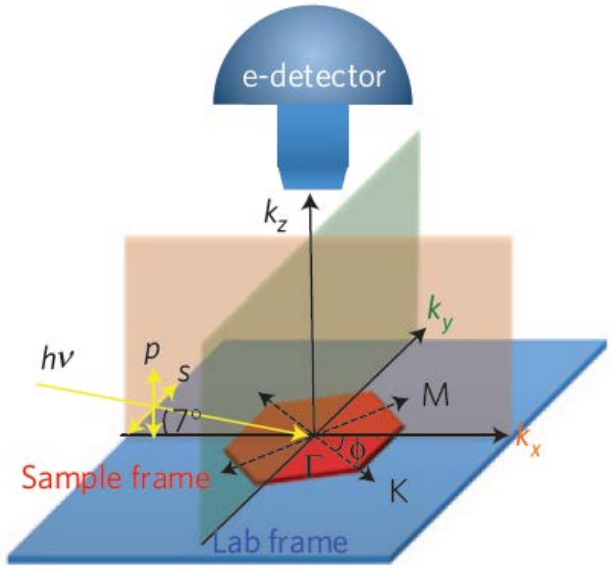
Rotatable detector

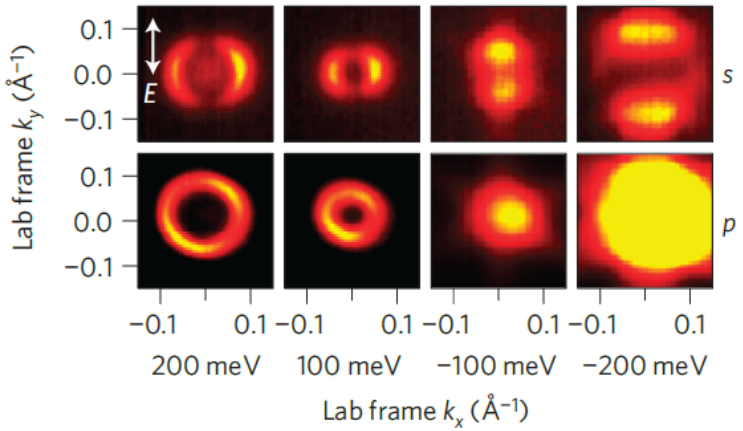


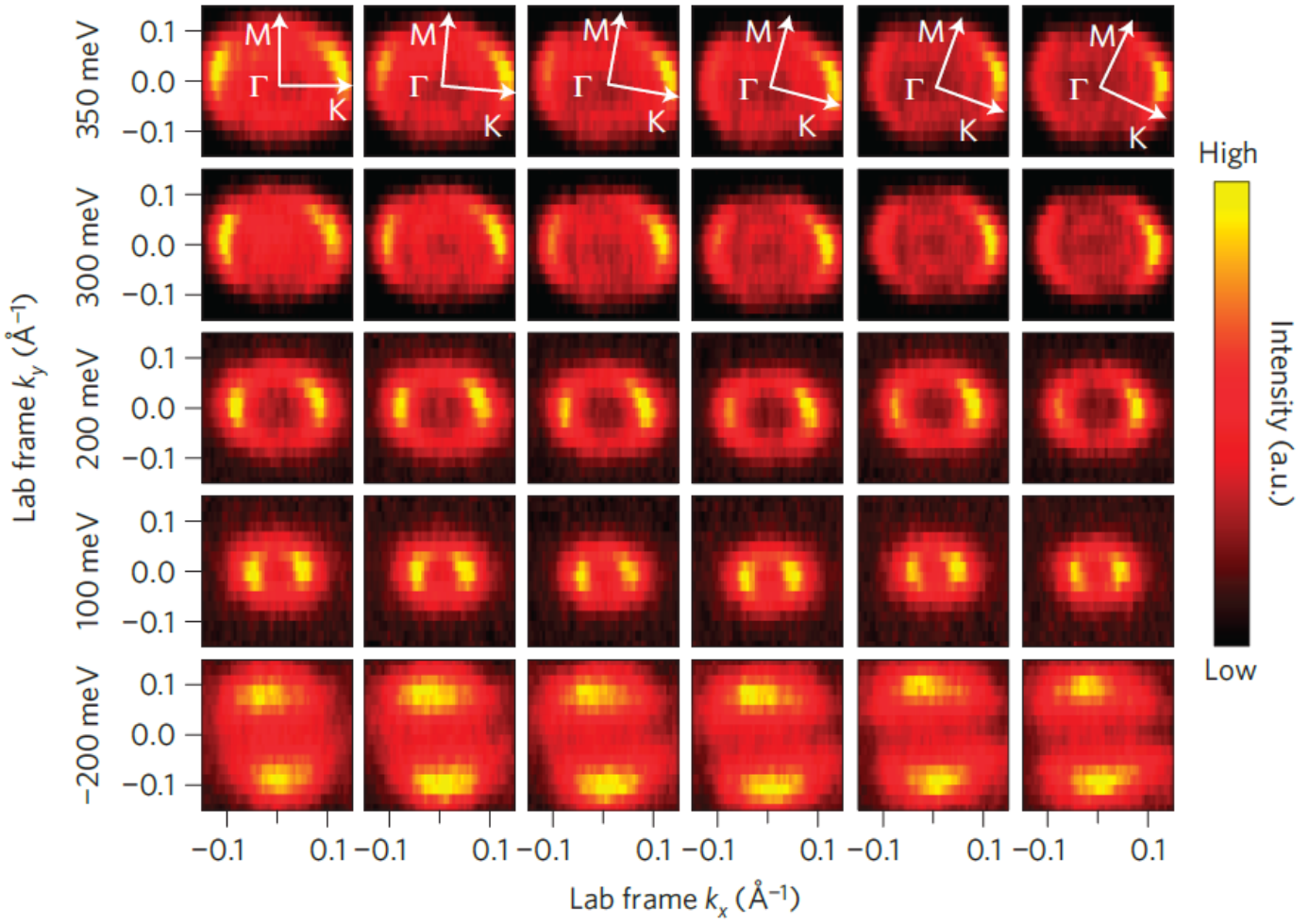




Cao et al., Nat. Phy. **9**, 499 (2013)

# Orbital texture

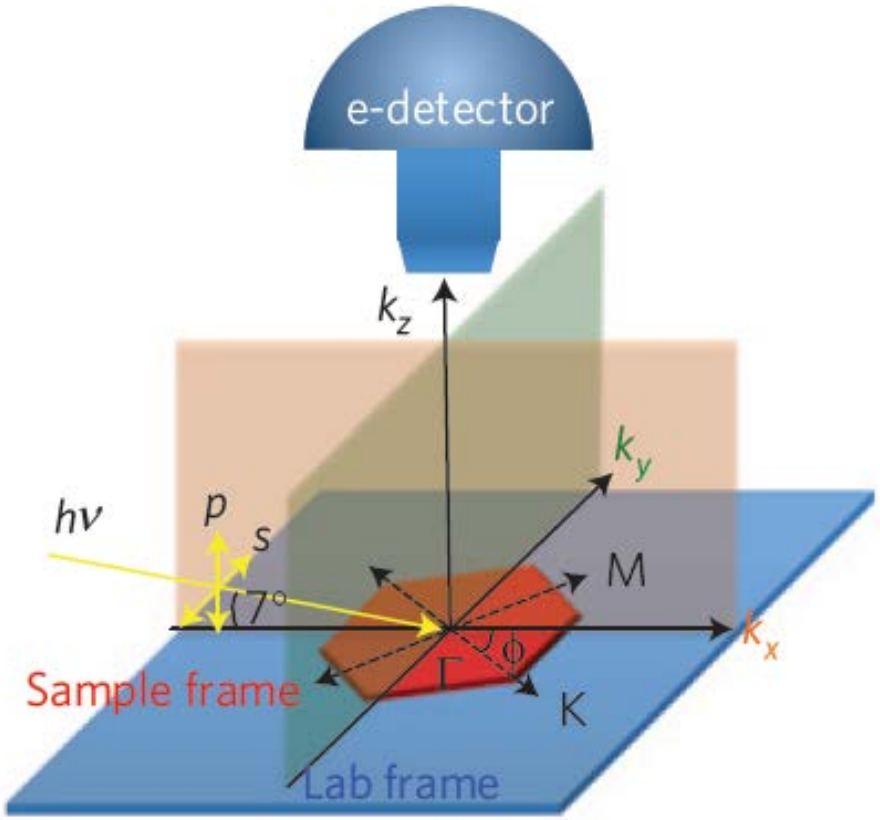


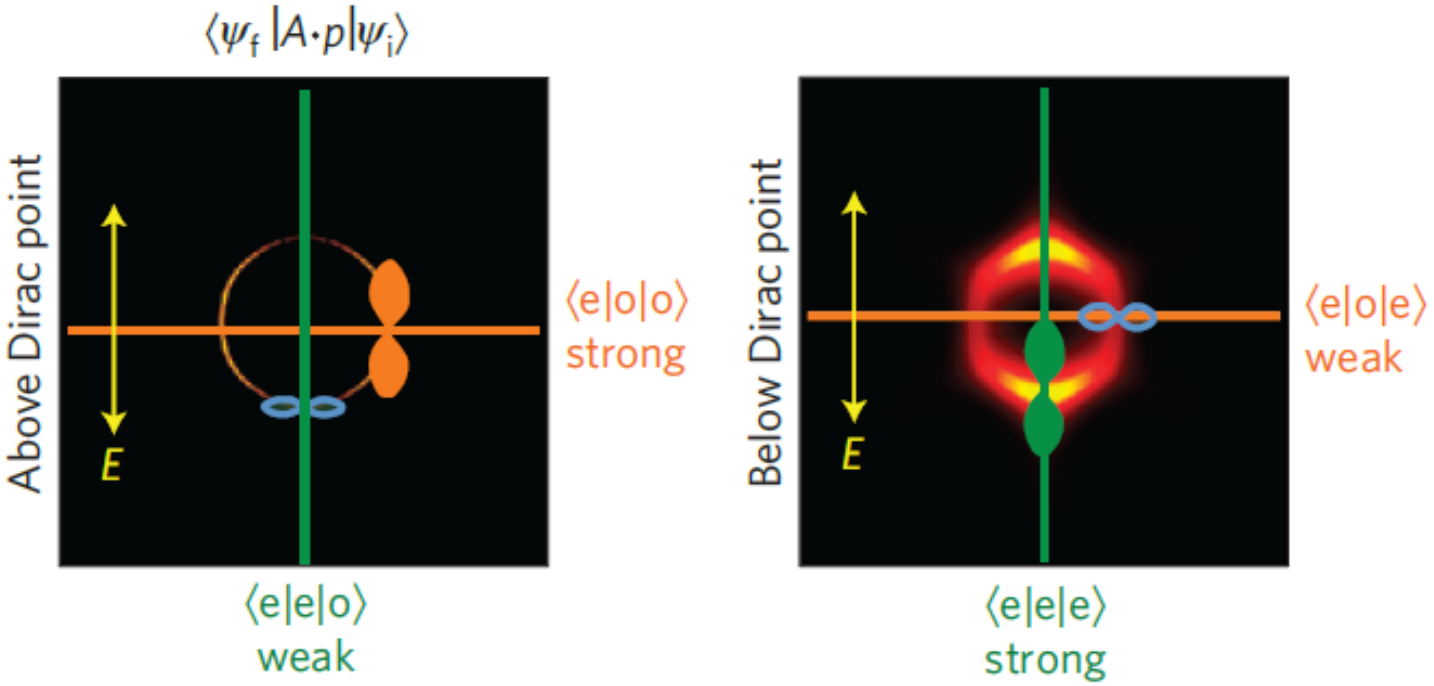




Cao et al., Nat. Phy. **9**, 499 (2013)

# Orbital texture

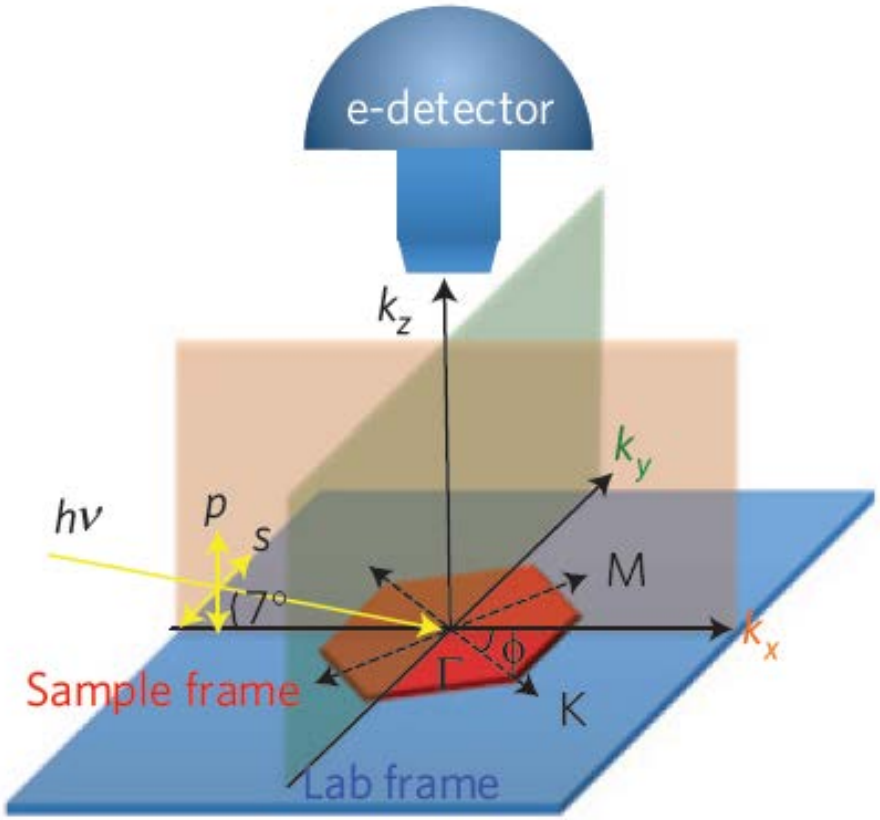


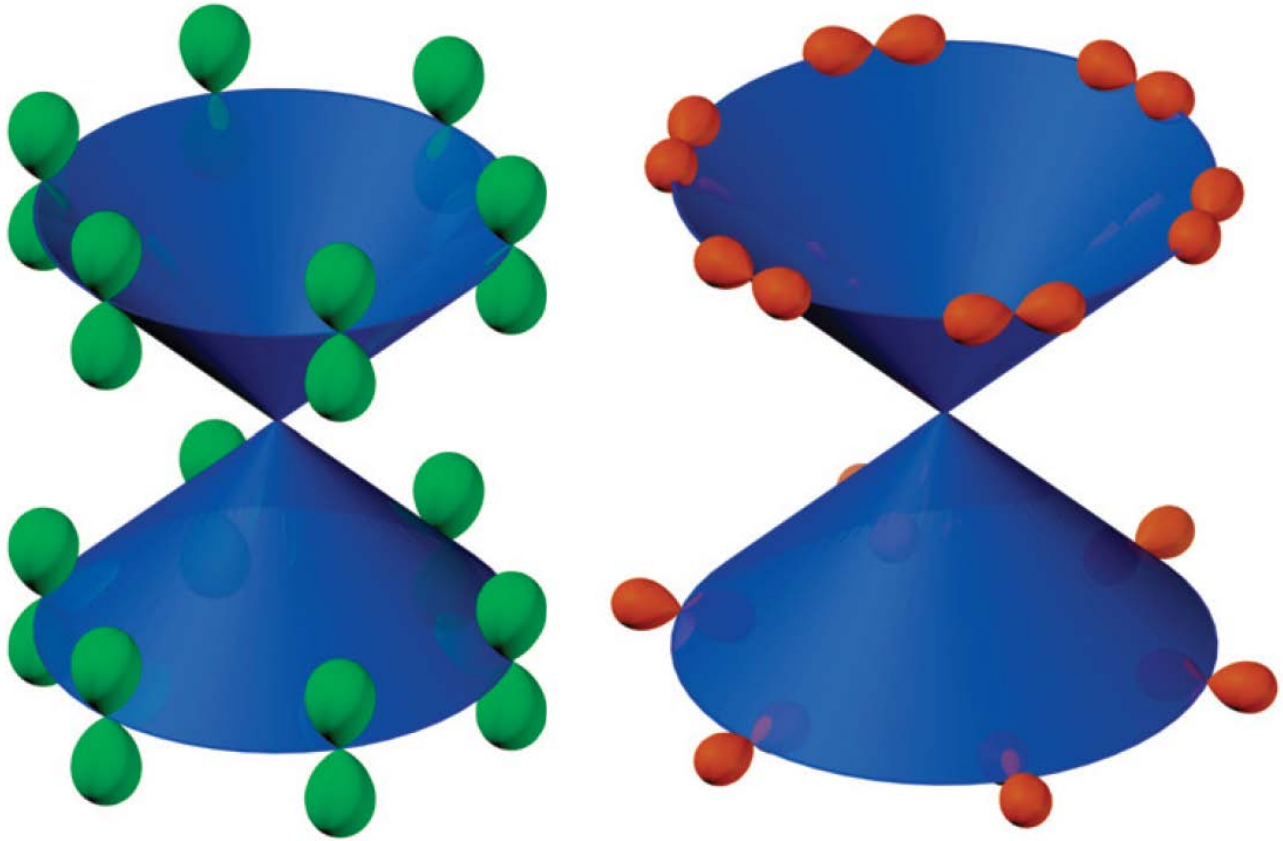

ARPES "matrix element"




Cao et al., Nat. Phy. **9**, 499 (2013)

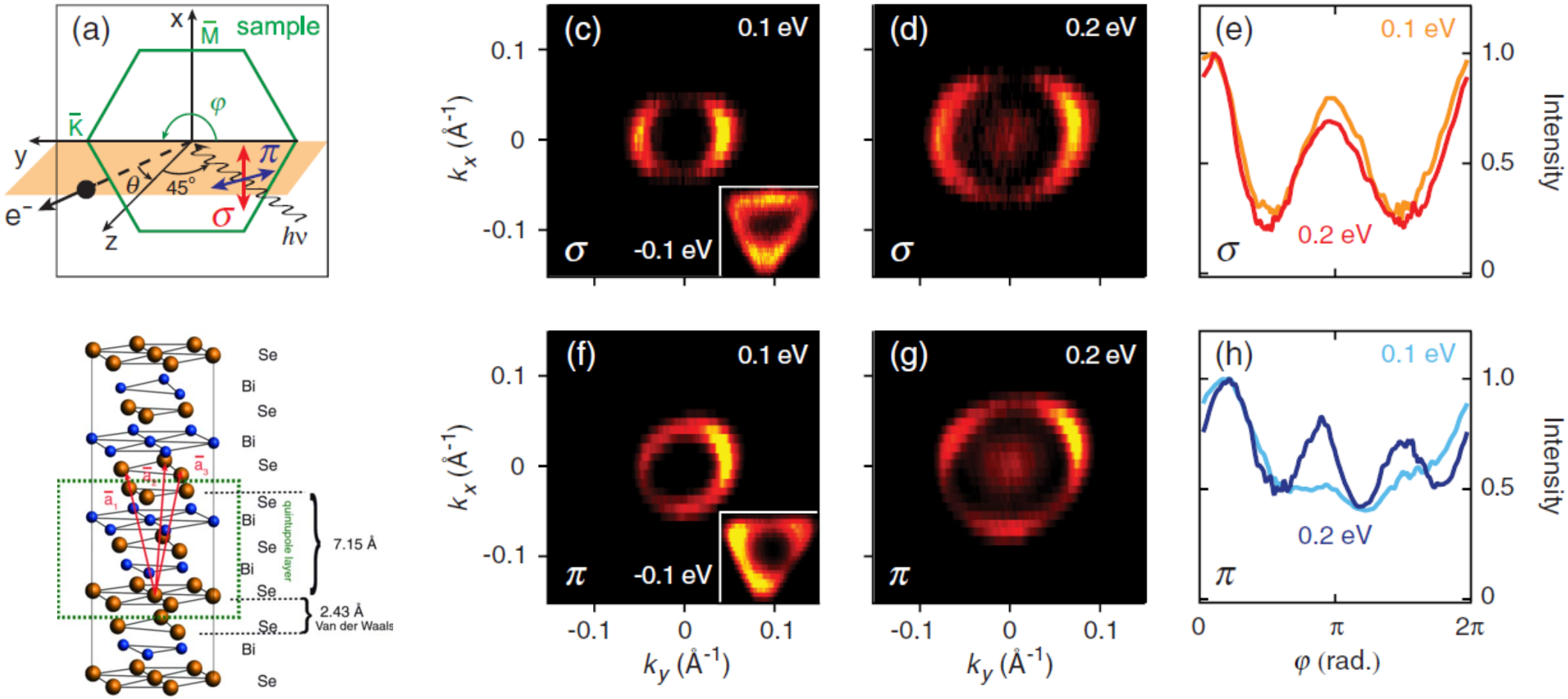
# Orbital texture



Cao et al., Nat. Phy. **9**, 499 (2013)

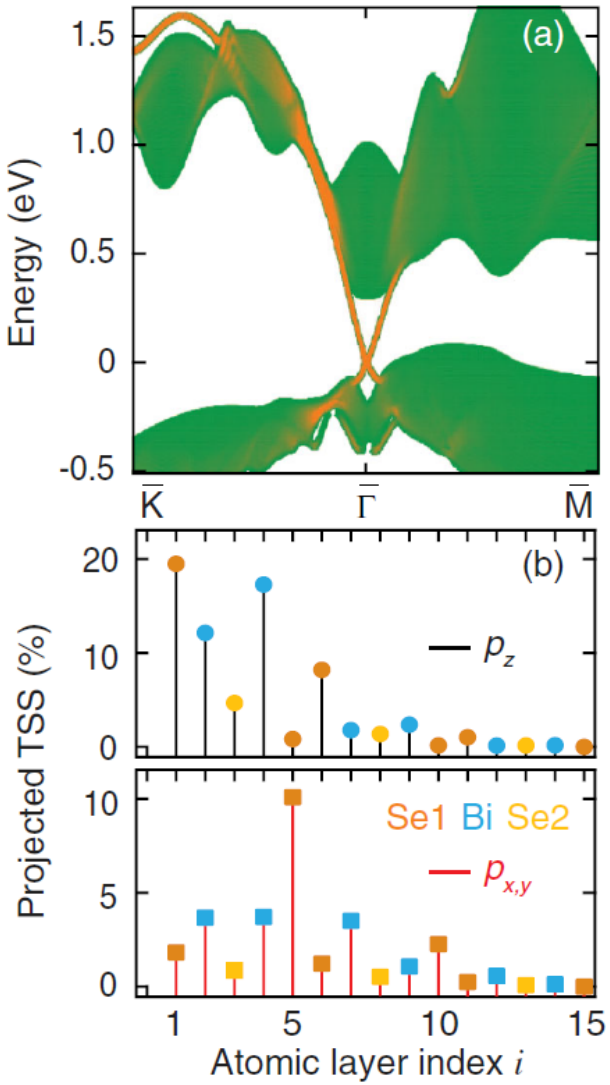
# Orbital texture

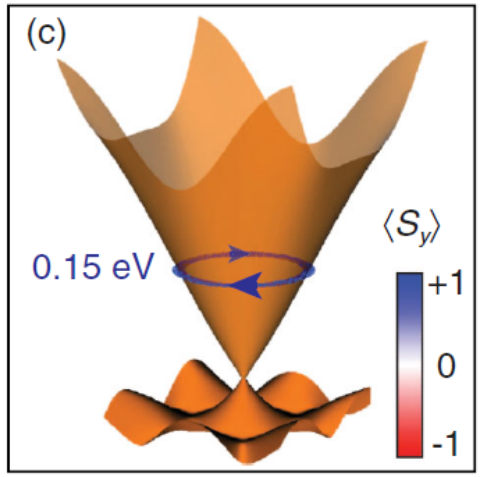


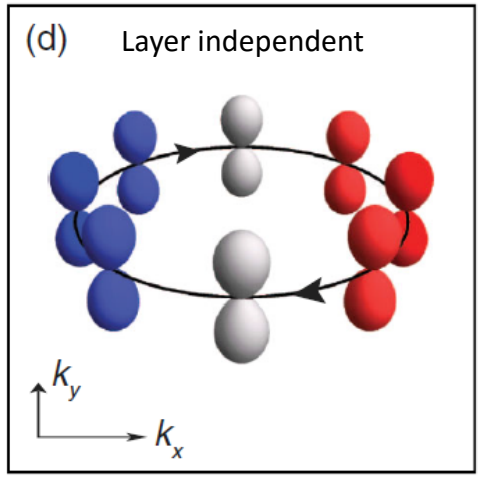

Zhu et al., Phys. Rev. Lett. **110**, 216401 (2013)

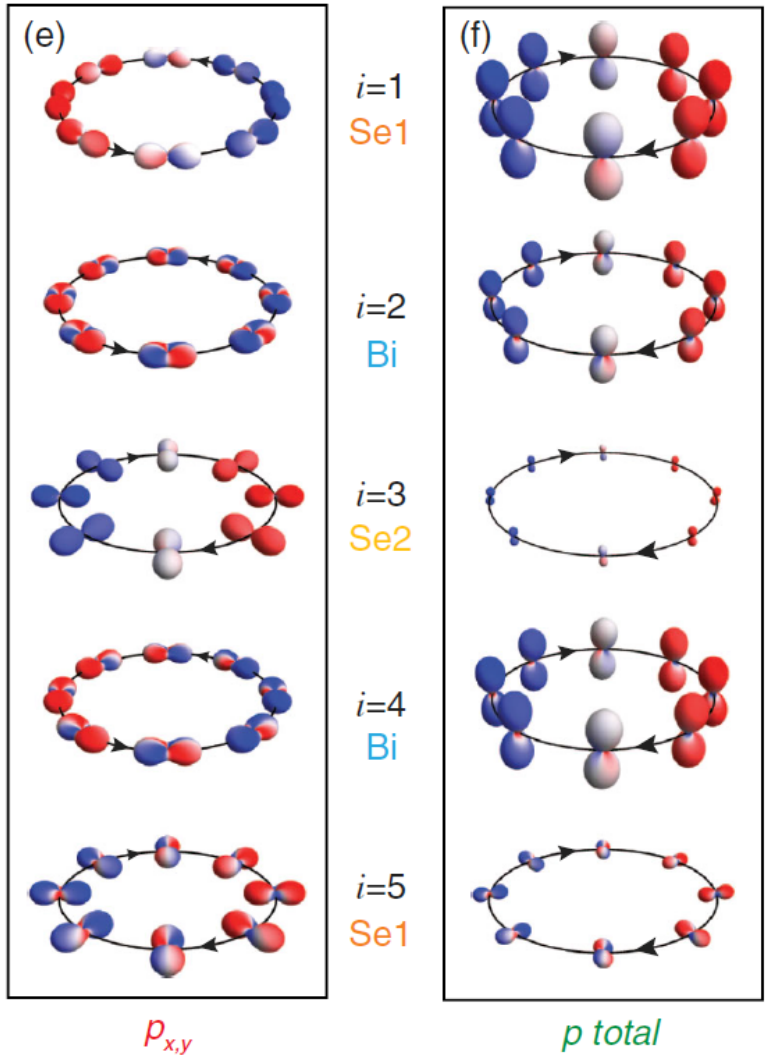
# Layer-dependent spin-orbital texture

DFT 250-layer slab




Zhu et al., Phys. Rev. Lett. **110**, 216401 (2013)

# Layer-dependent orbital texture manifested in ARPES

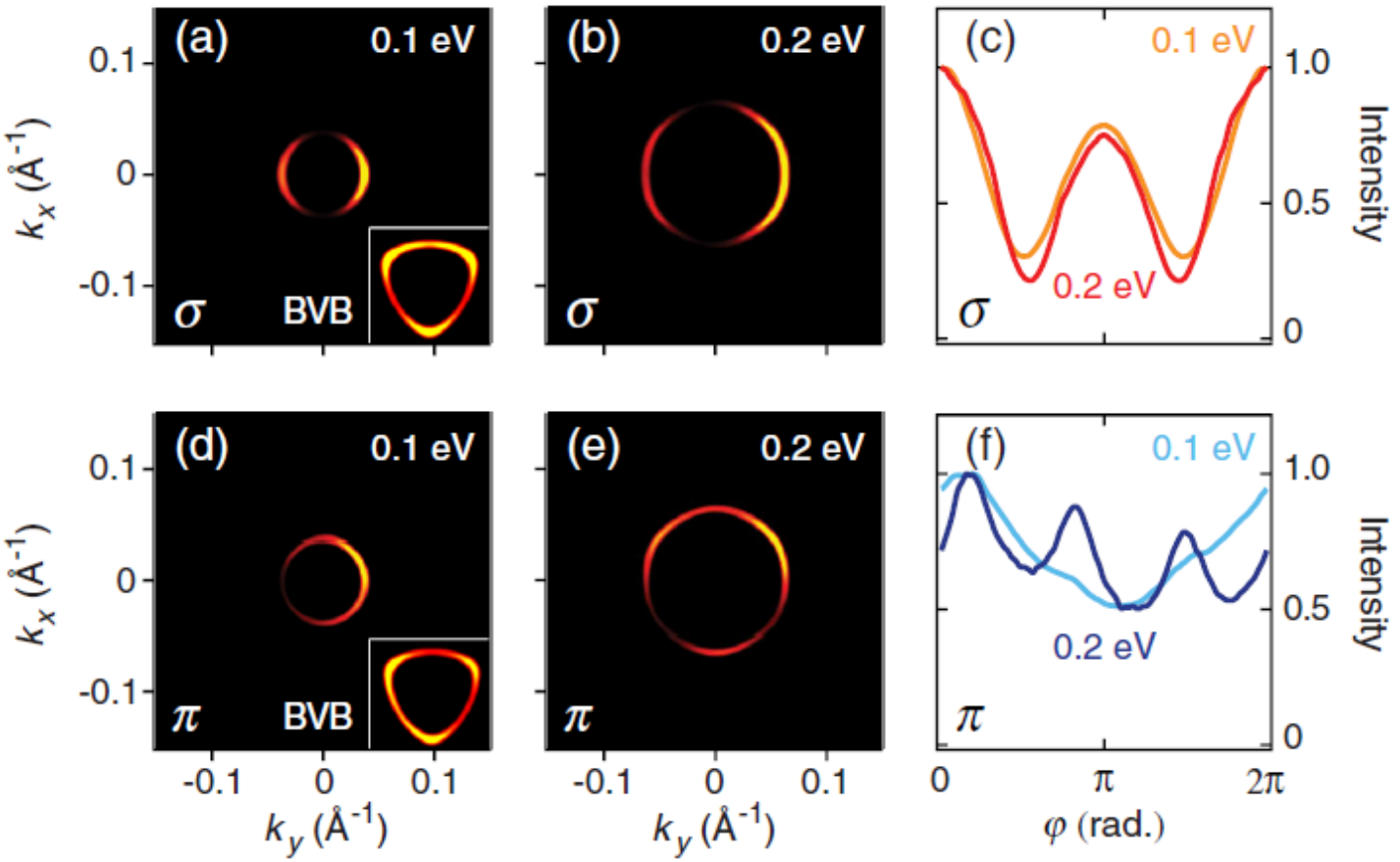
$$I \propto |\langle e^{i\mathbf{k}\cdot\mathbf{r}} | \mathbf{A}\cdot\mathbf{p} | \Psi_{\mathrm{TSS}} \rangle|^2$$

$$\Psi_{\mathrm{TSS}} = \sum_{i,\sigma} \alpha_i \psi^{\sigma}_{i,\mathbf{k}_\parallel}$$

layer spin

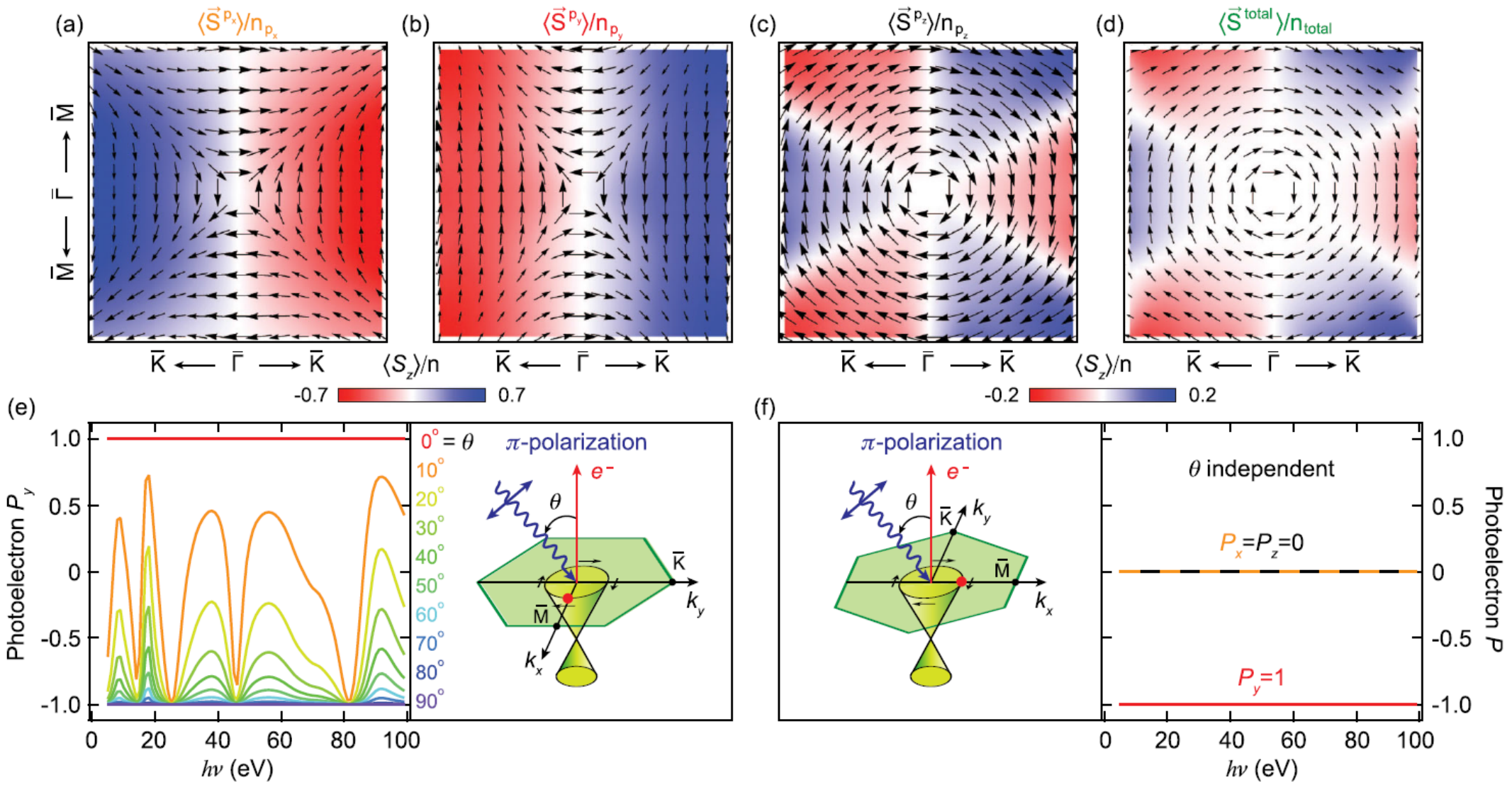
$$I \propto \sum_{\sigma} |\sum_i e^{-ik_z z_i} \langle e^{i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel} | \mathbf{A}\cdot\mathbf{p} | \alpha_i \psi^{\sigma}_{i,\mathbf{k}_\parallel} \rangle|^2$$

Based on DFT slab calculations



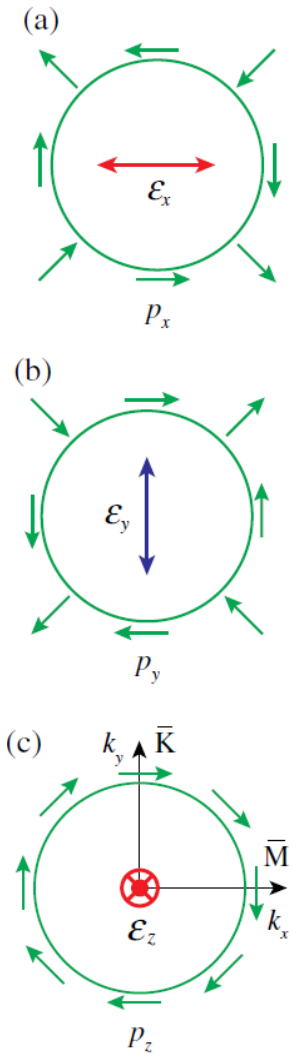

Zhu et al., Phys. Rev. Lett. **110**, 216401 (2013)

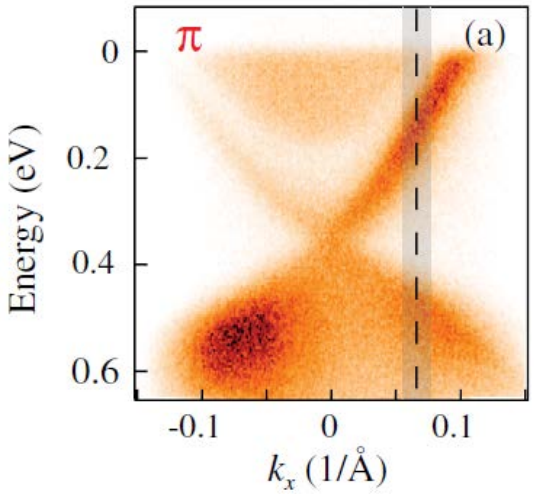
# Spin-orbital texture

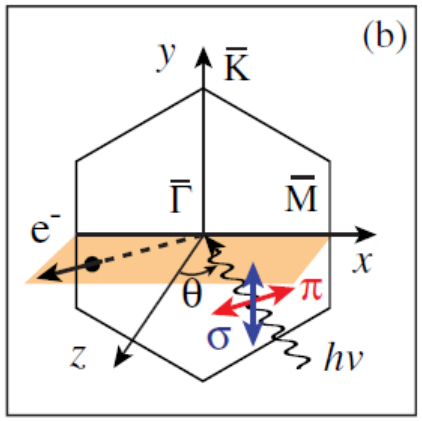



Zhu et al., Phys. Rev. Lett. **110**, 216401 (2013)

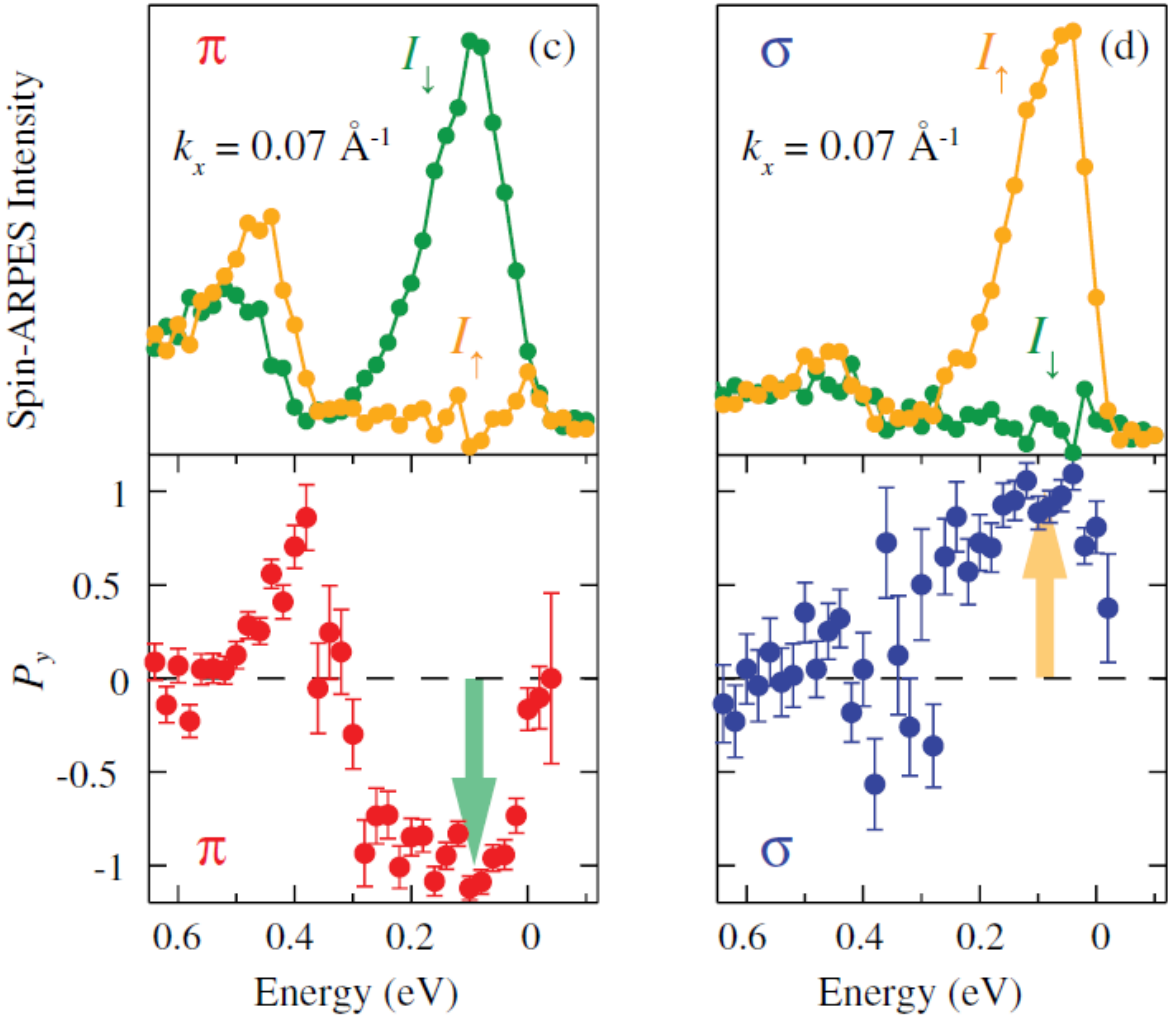
# Polarization control of photoelectron spin



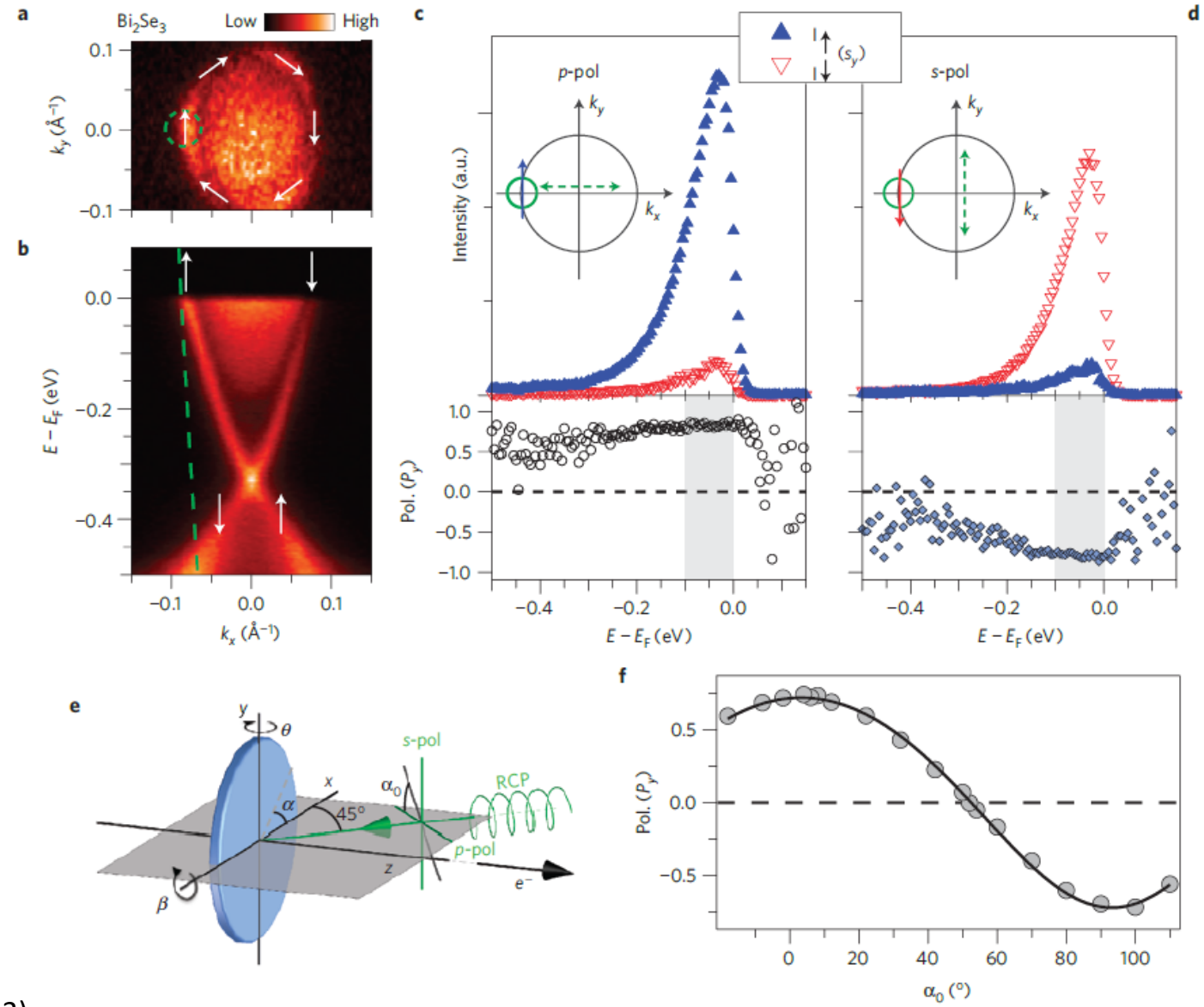




y-component of spin



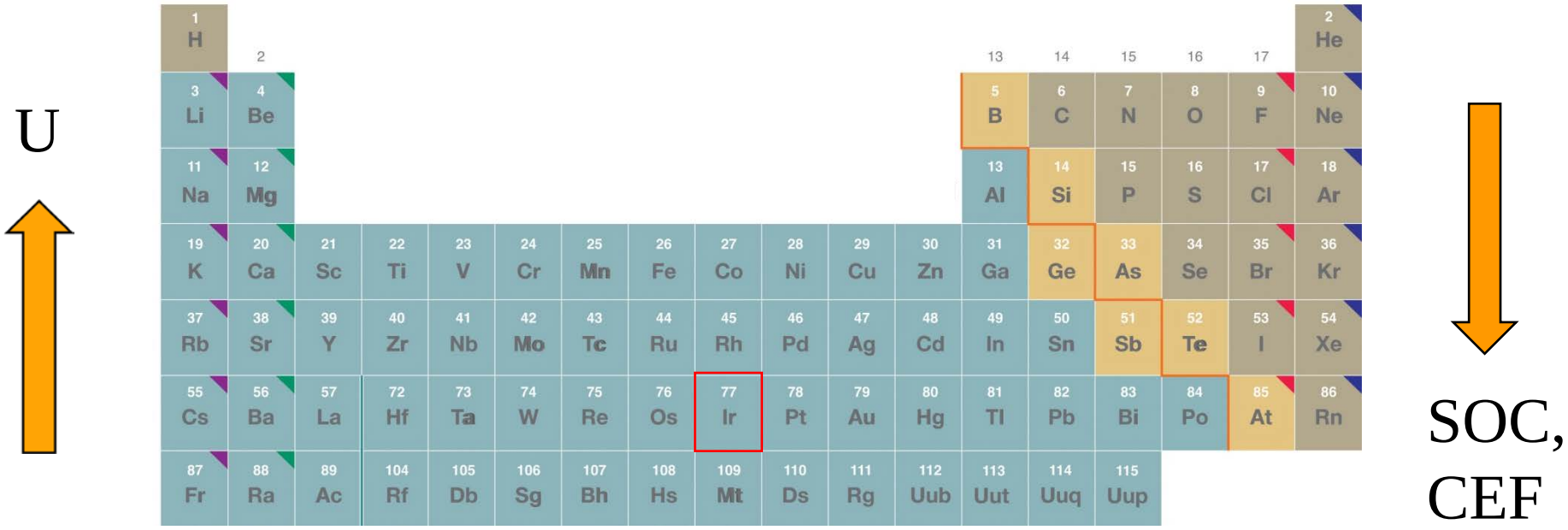

Zhu et al., Phys. Rev. Lett. **112**, 076802 (2014)

# Polarization control of photoelectron spin



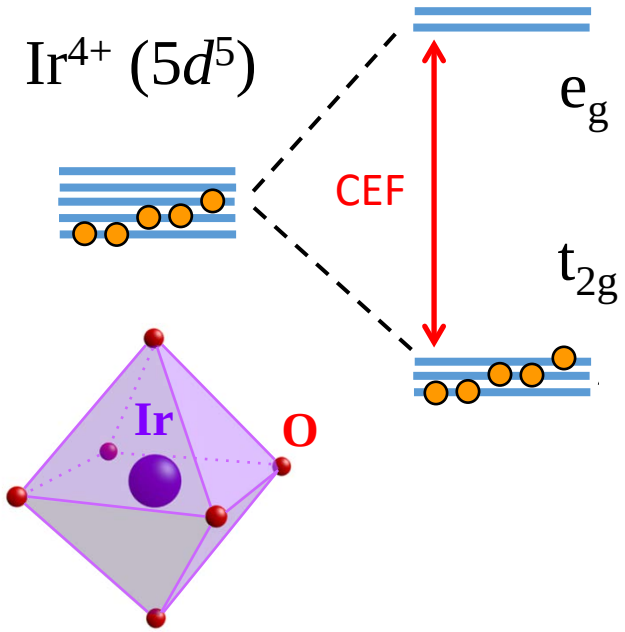

Jozwiak et al., Nat. Phy. **9**, 293 (2013)

# Correlated topological insulators – 5*d* transition metal oxides




- Interplay between electron correlations, crystal electric field and spin-orbit coupling and (U ~ SOC ~ CEF)
- Potential for exotic physics driven by strong SOC (~0.5eV)

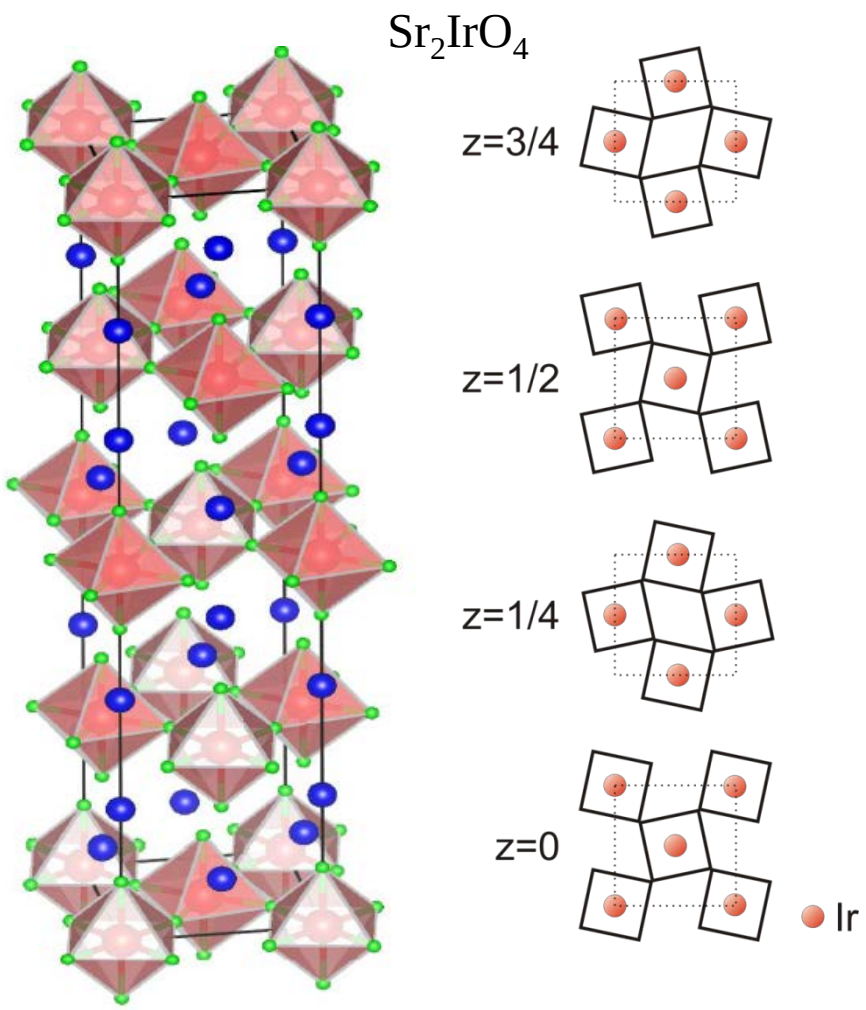
# $J_{eff}$ = ½ Mott insulators in 5*d* systems



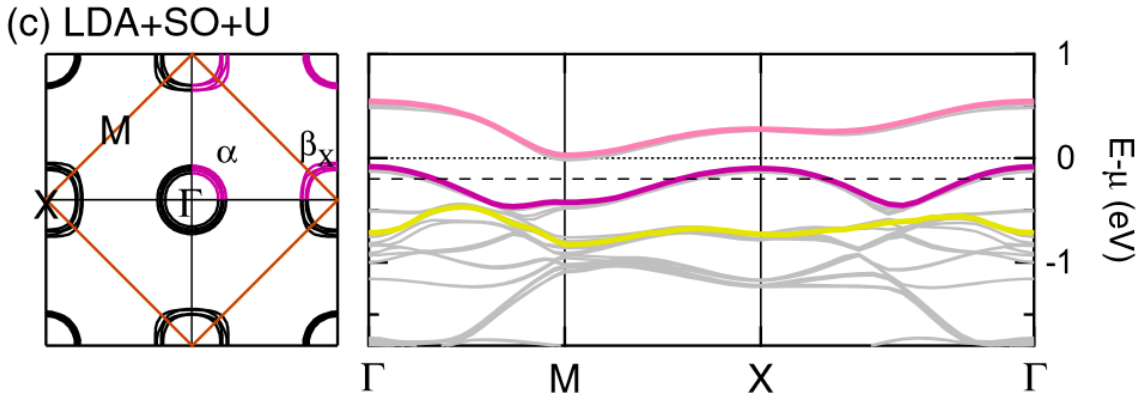

Kim *et al.*, PRL 101, 076402 (2008)

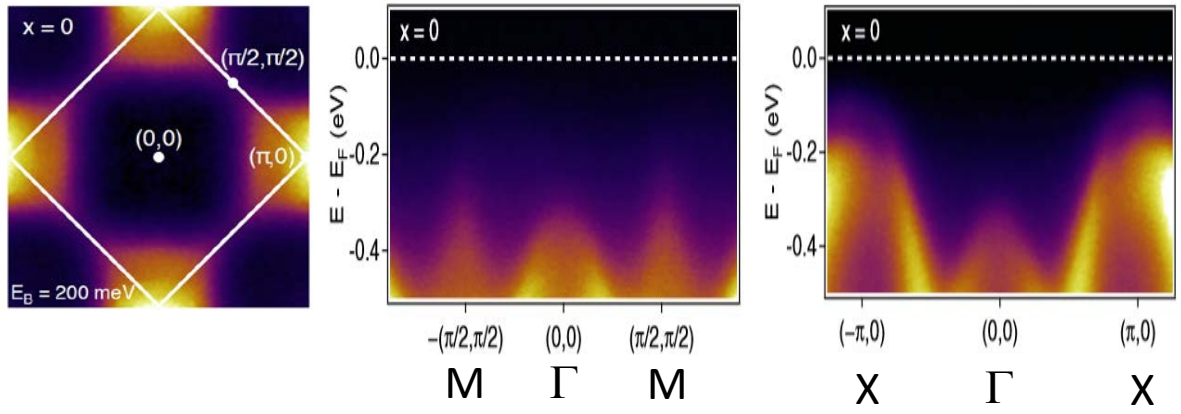
# The Ruddlesden-Popper series ($Sr_{n+1}Ir_nO_{3n+1}$)

n = 1 single layer (insulator)




Kim *et al.*, PRL 101, 076402 (2008)




de la Torre *et al.*, PRL 115, 176402 (2015)

# The Ruddlesden-Popper series ($Sr_{n+1}Ir_nO_{3n+1}$)

n = 2 bilayer (insulator)

$Sr_3Ir_2O_7$

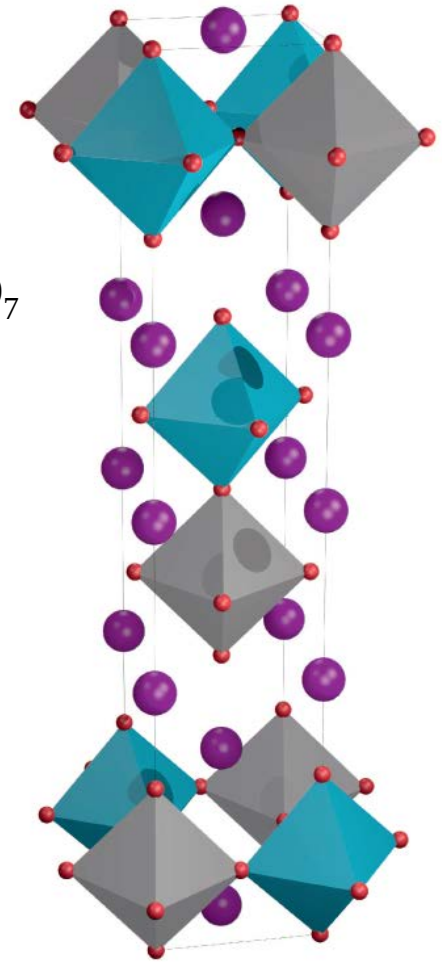
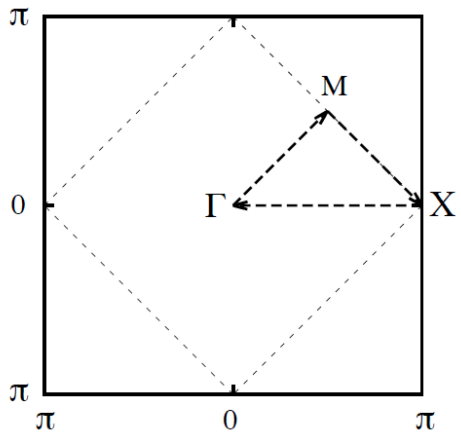
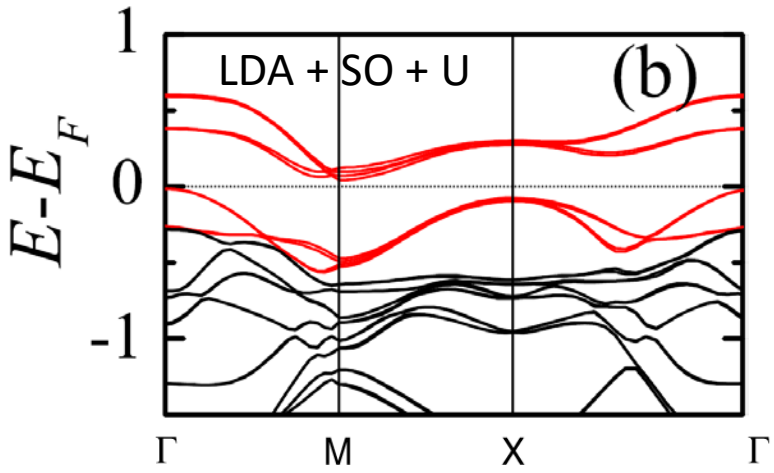
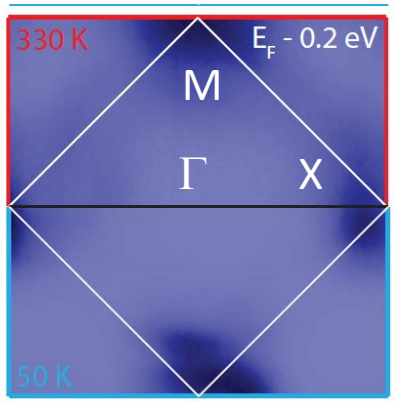


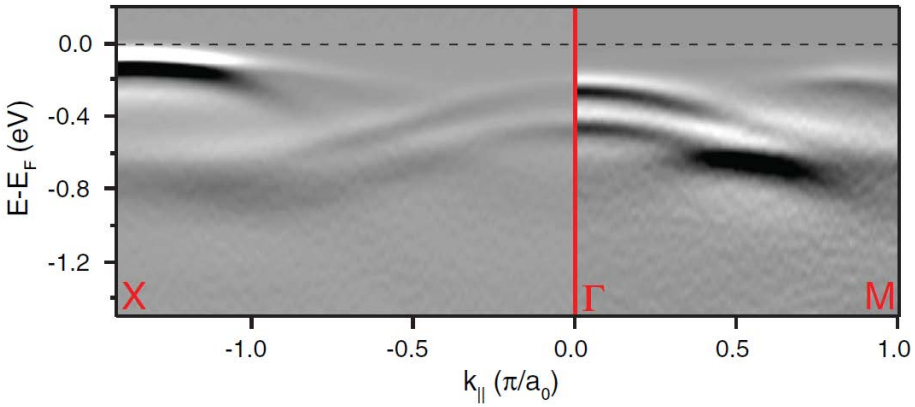
Image: Stefano Boseggia thesis

Moon *et al.*, PRL 101, 226402 (2008)




King *et al.*, PRB 87, 241106(R) (2013)

# The Ruddlesden-Popper series ($Sr_{n+1}Ir_nO_{3n+1}$)

n = ∞ infinite layer

$SrIrO_3$ : orthorhombic Pbnm

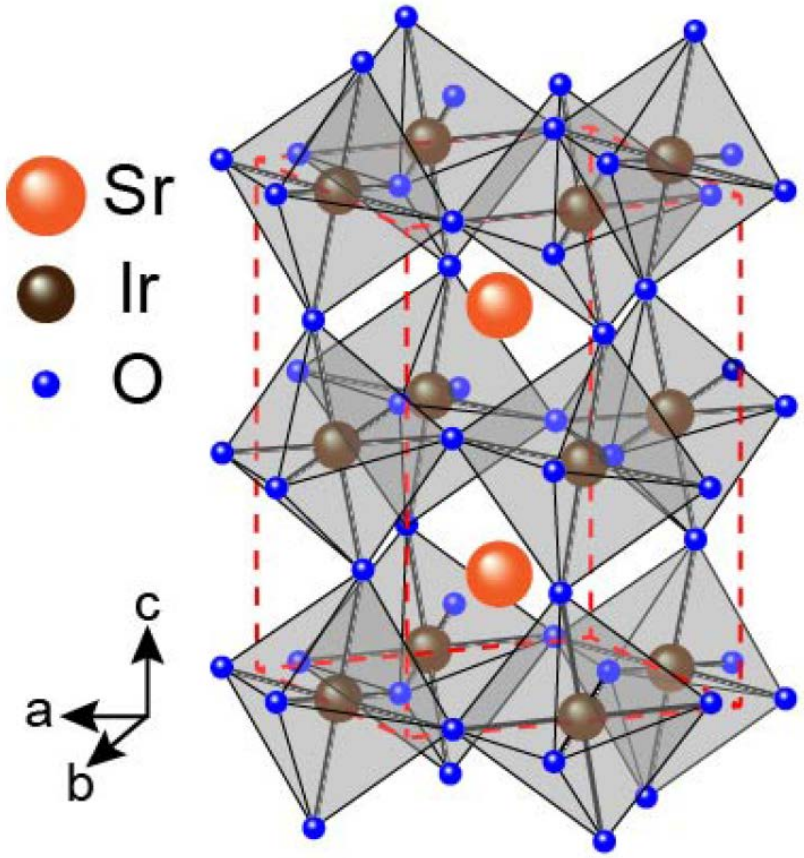
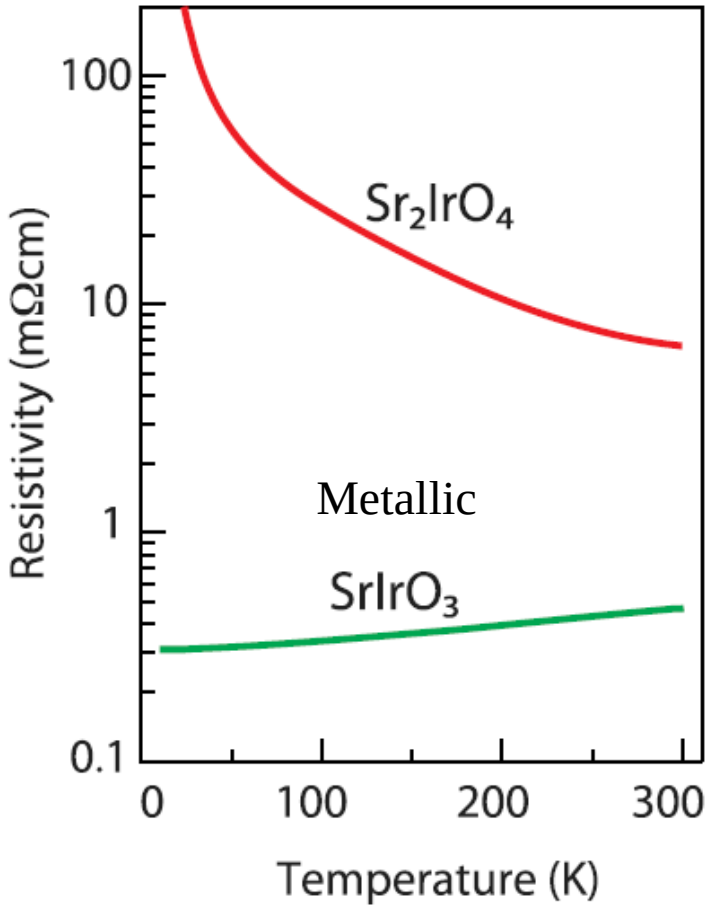
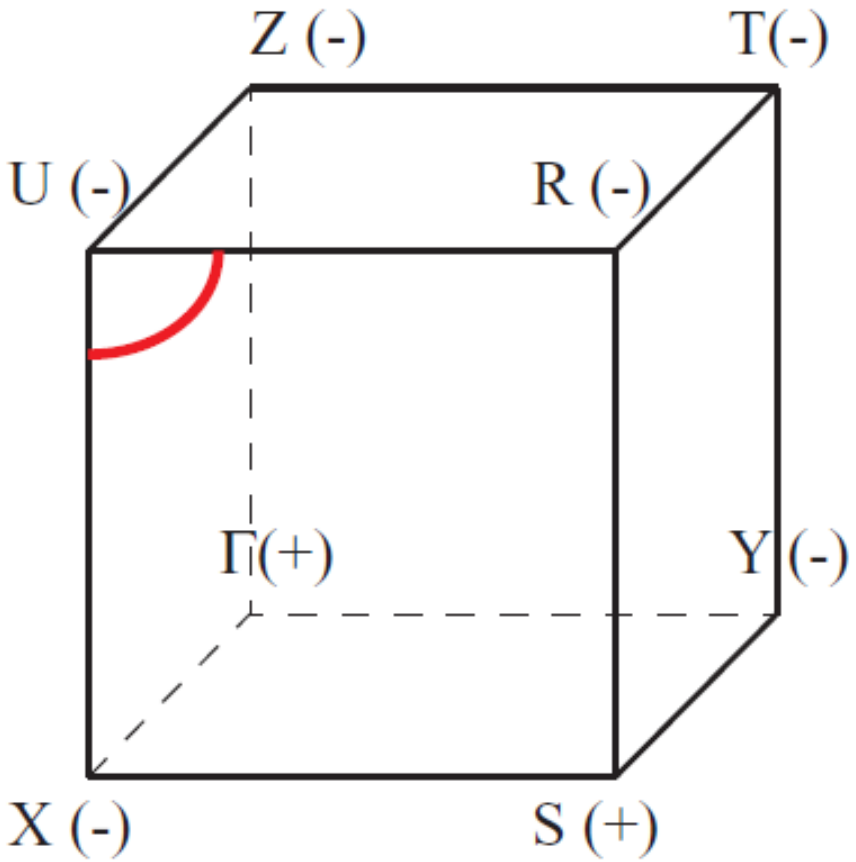



Image: Liu *et al.*, ArXiv:1501:00654 (2015)

Nie *et al.*, PRL 114, 016401 (2015)

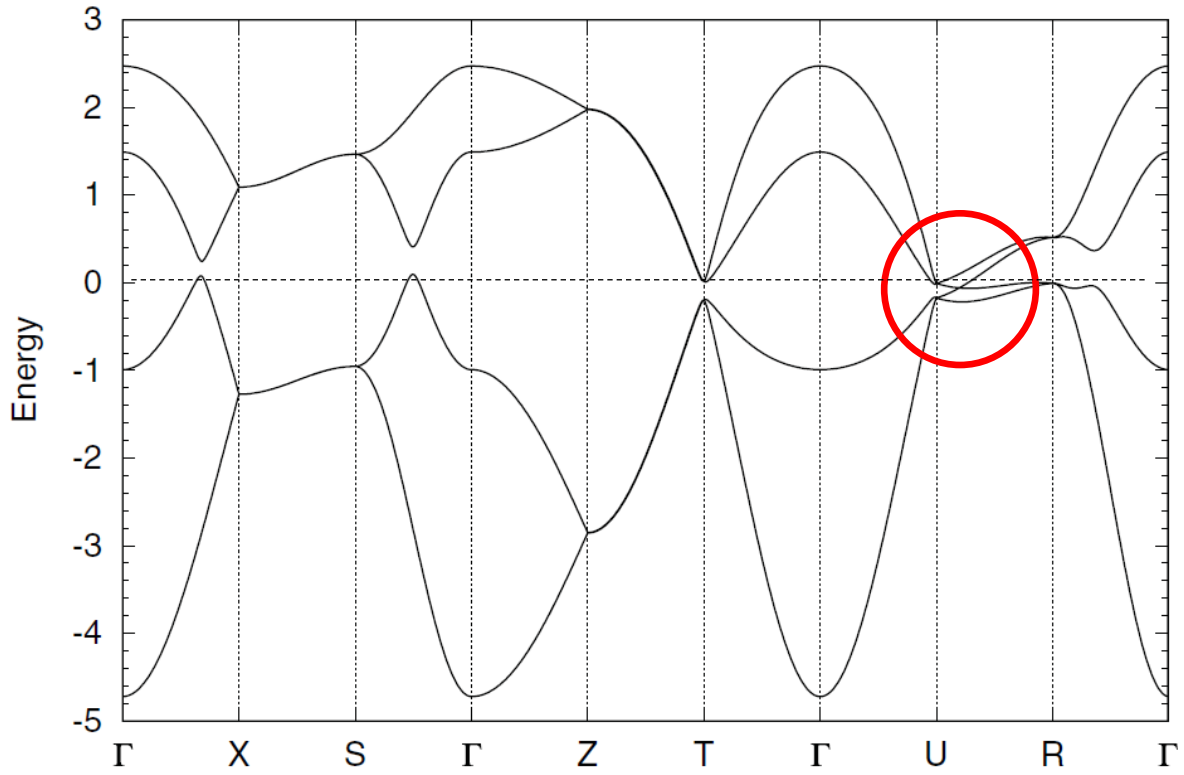


# Semi-metallic $SrIrO_3$ – band structure




Tight-binding model with only $J_{eff}$ = ½ states

Carter *et al.*, PRB 85, 115105 (2012)

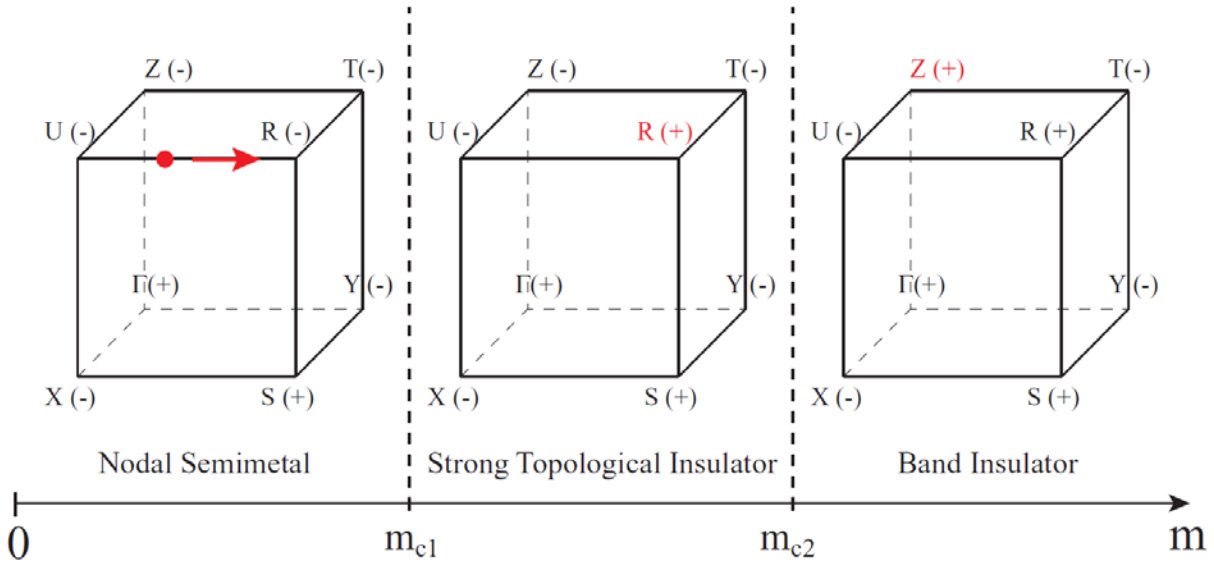


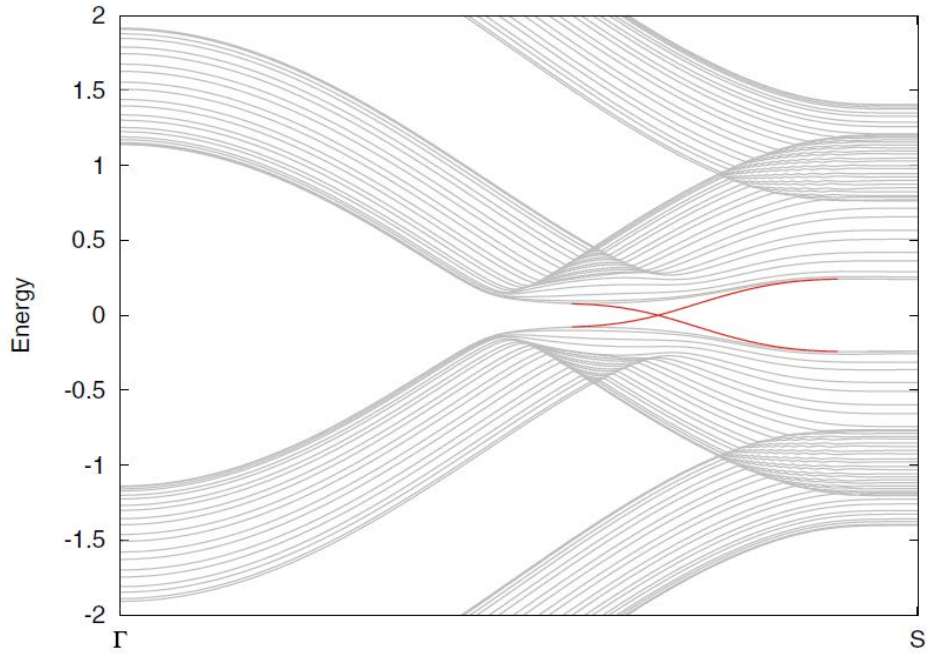

Node near U protected by *n*-glide symmetry

Liu *et al.*, ArXiv:1506:03559 (2015)

# Semi-metallic → semi-conducting transition in $SrIrO_3$

Add staggered sublayer potential or SOC term: $m\sigma_x$
($\sigma_x$ = layer index)



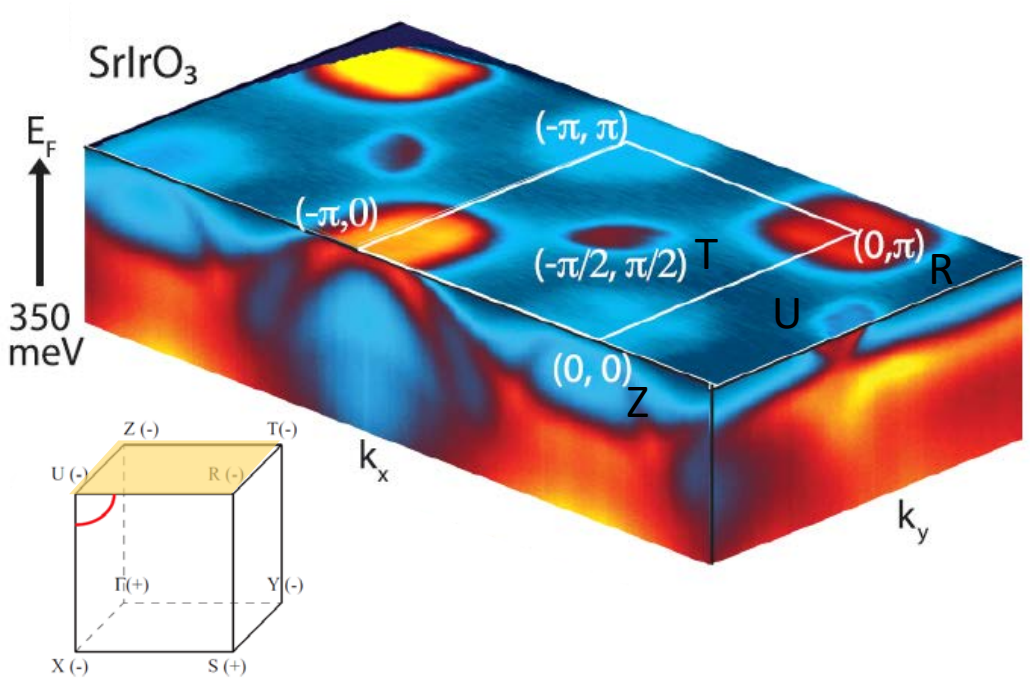



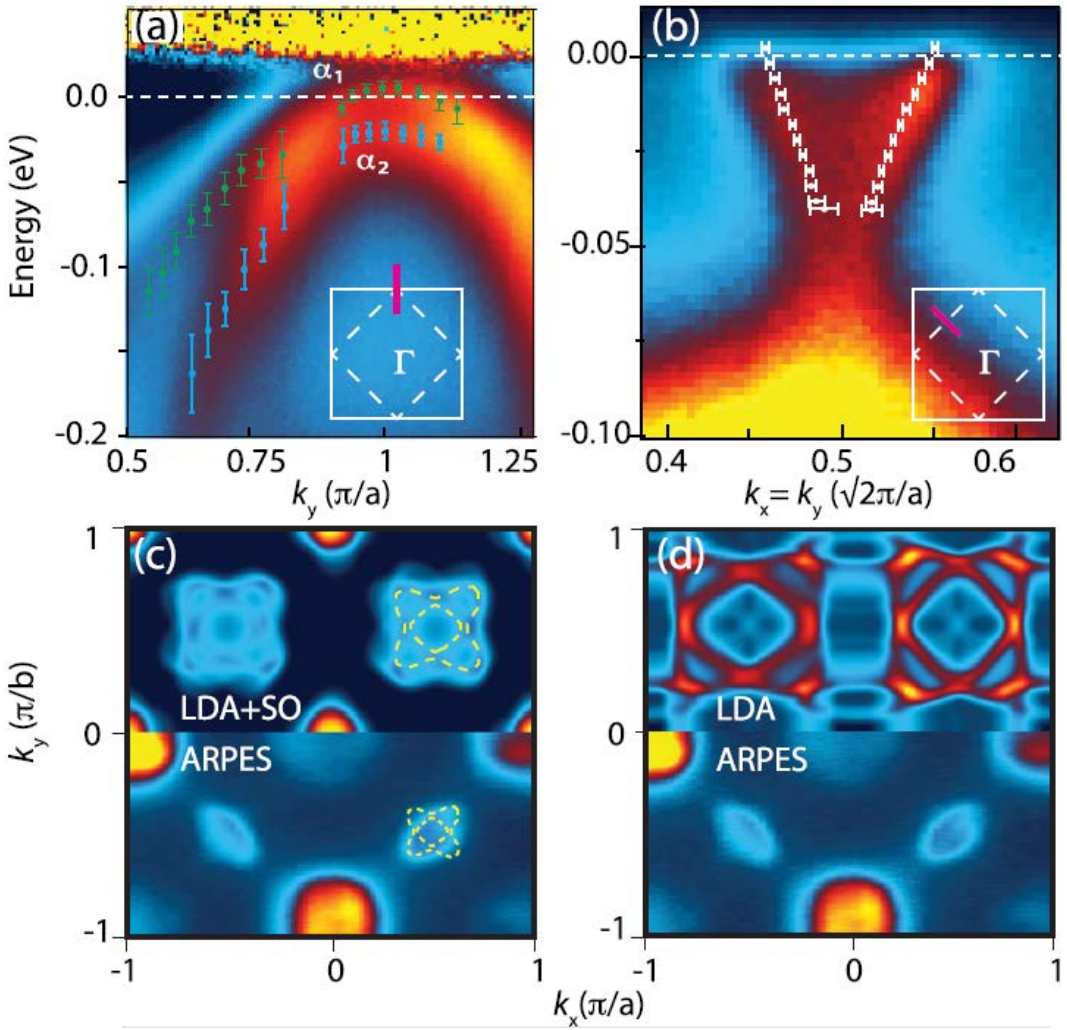

Carter *et al.*, PRB 85, 115105 (2012)

# $SrIrO_3$ thin film - ARPES

No bulk single crystals available yet
Pseudo-cubic structure difficult to cleave

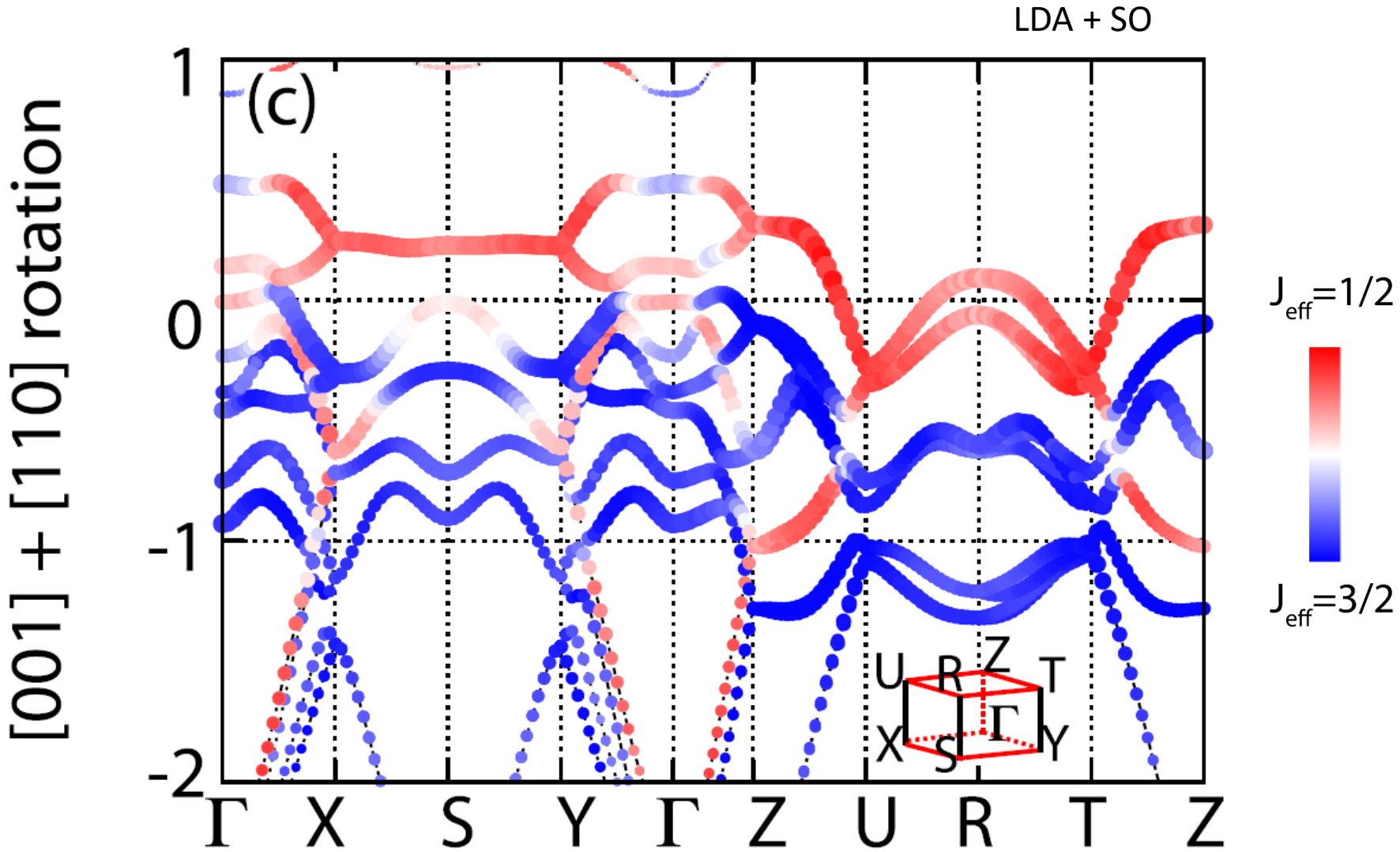
MBE grown $SrIrO_3$(001) on LSAT




Nie *et al.*, PRL 114, 016401 (2015)

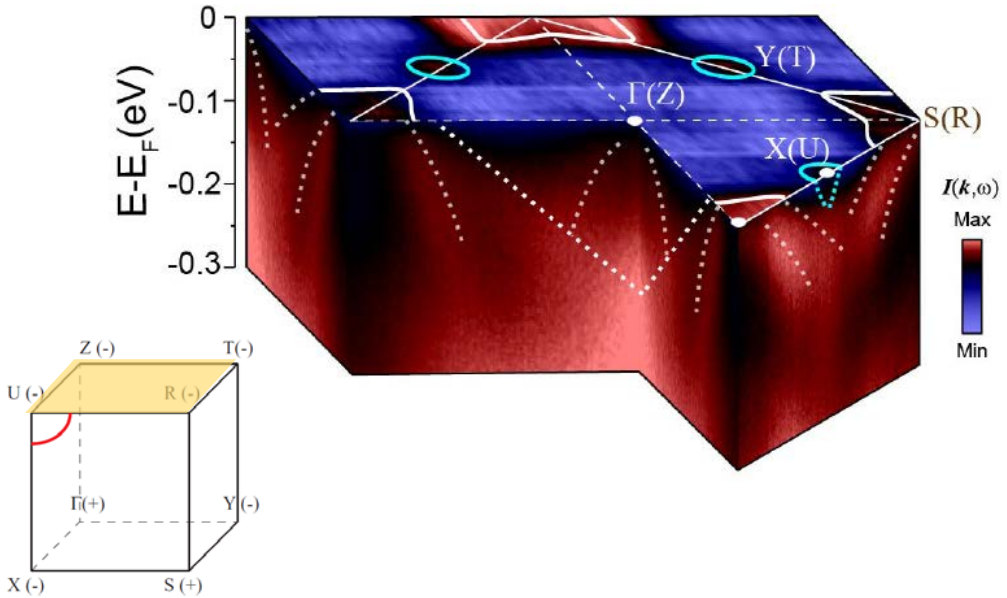
# LDA band structure of $SrIrO_3$

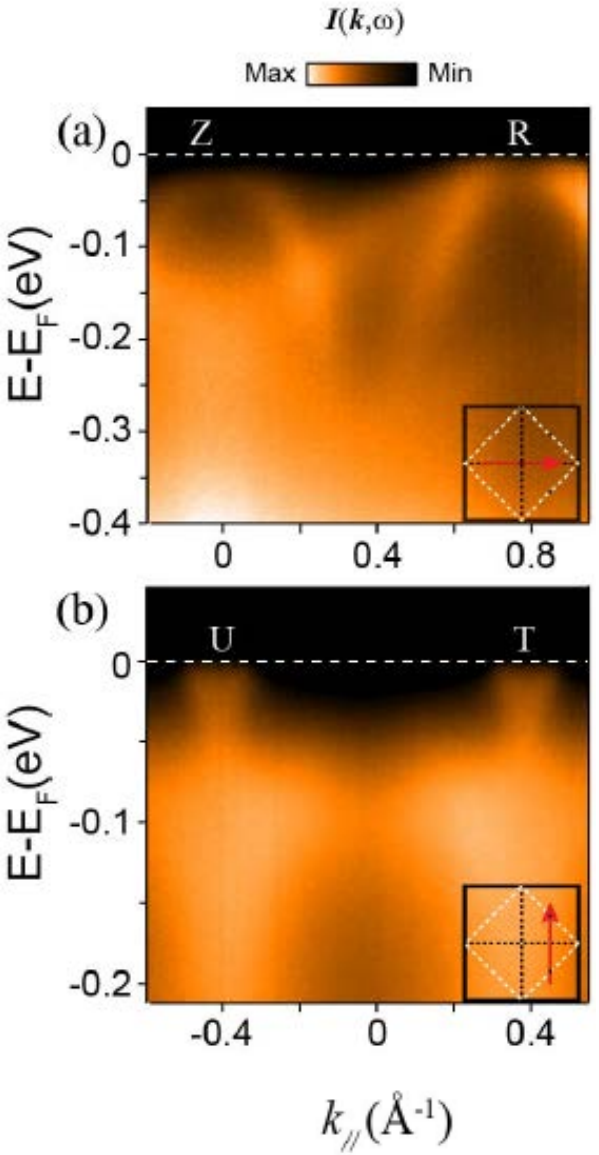



Nie *et al.*, PRL 114, 016401 (2015)

# $SrIrO_3$ thin film - ARPES

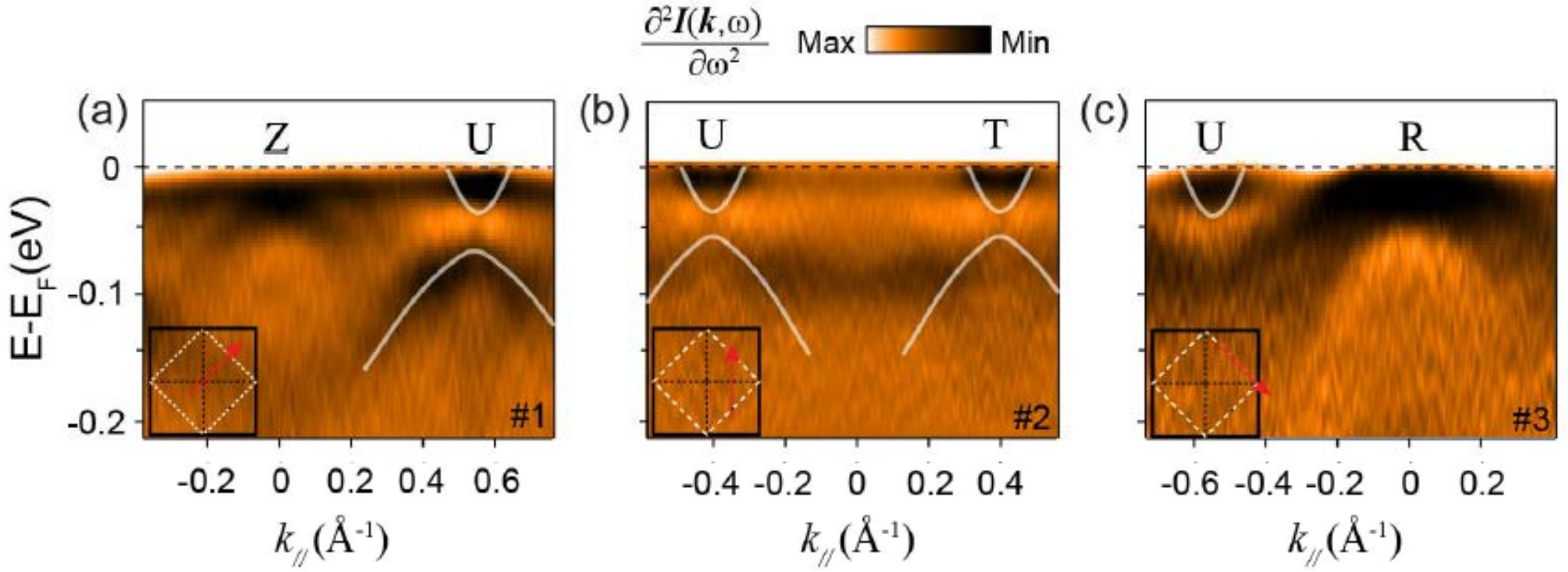
MBE grown $SrIrO_3$(001) on $SrTiO_3$(001)




Liu *et al.*, ArXiv:1501:00654 (2015)

# $SrIrO_3$ thin film - ARPES

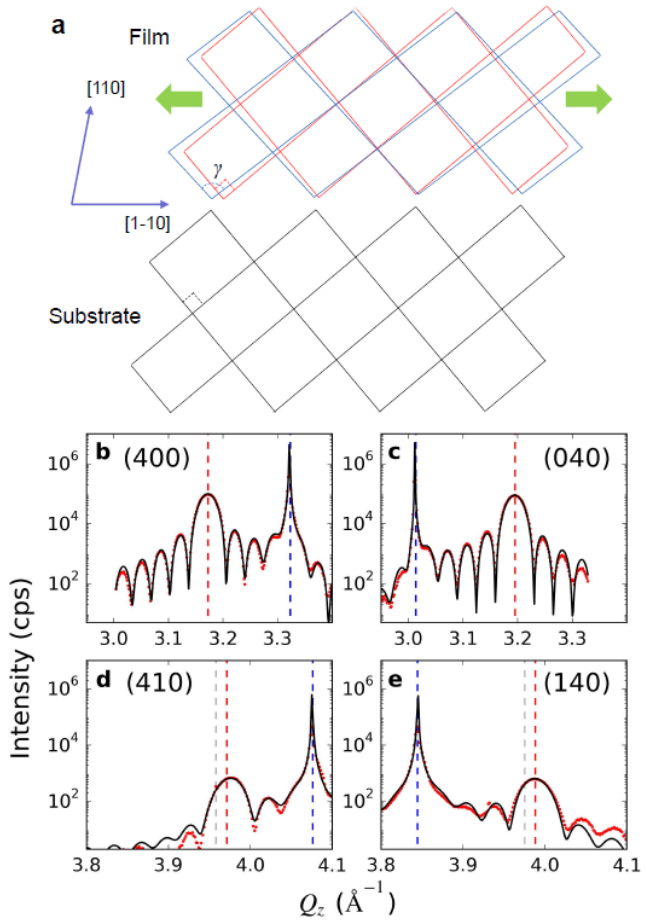



Liu *et al*., ArXiv:1501:00654 (2015)

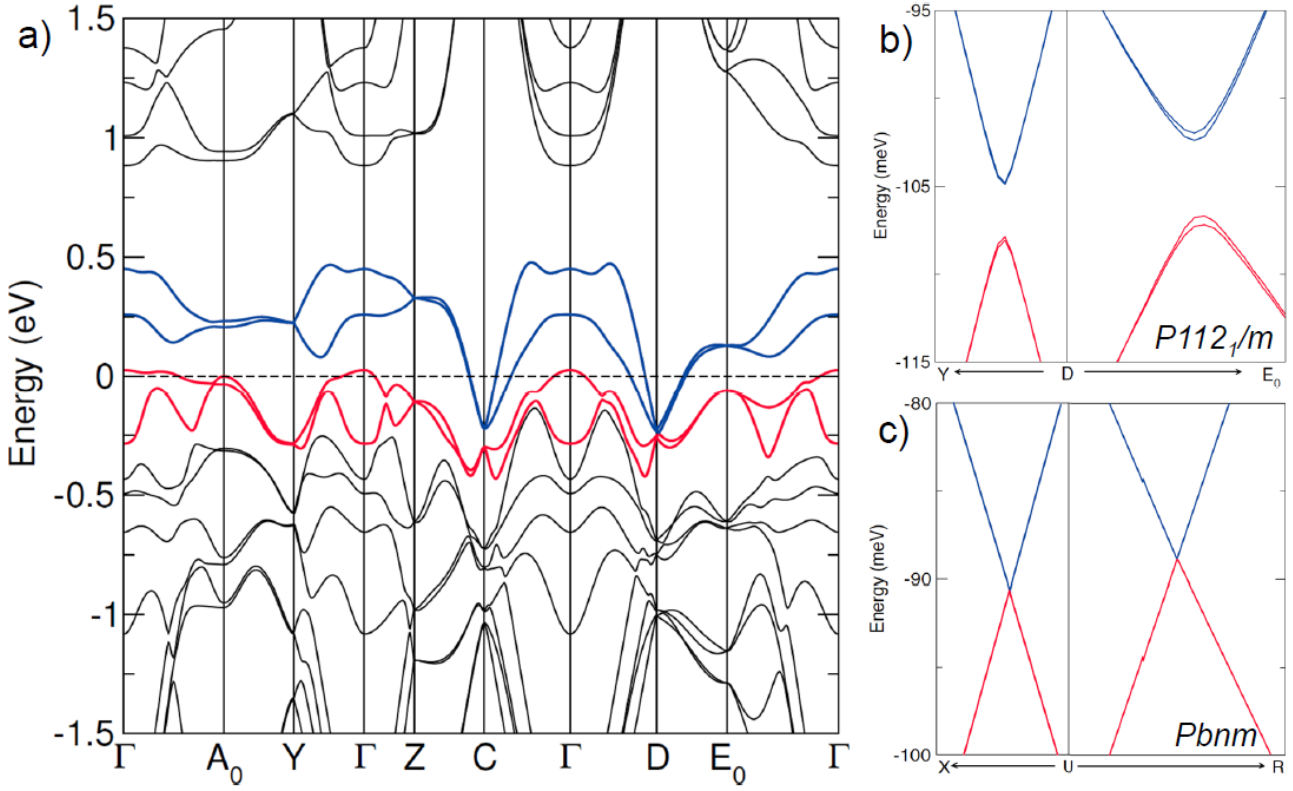
# $SrIrO_3$ thin film - ARPES

PLD grown $SrIrO_3$(001) on $GdScO_3$(110)

X-ray diffraction shows strain induced monoclinicity




Pbnm → $P112_1/m$ breaks *n*-glide symmetry

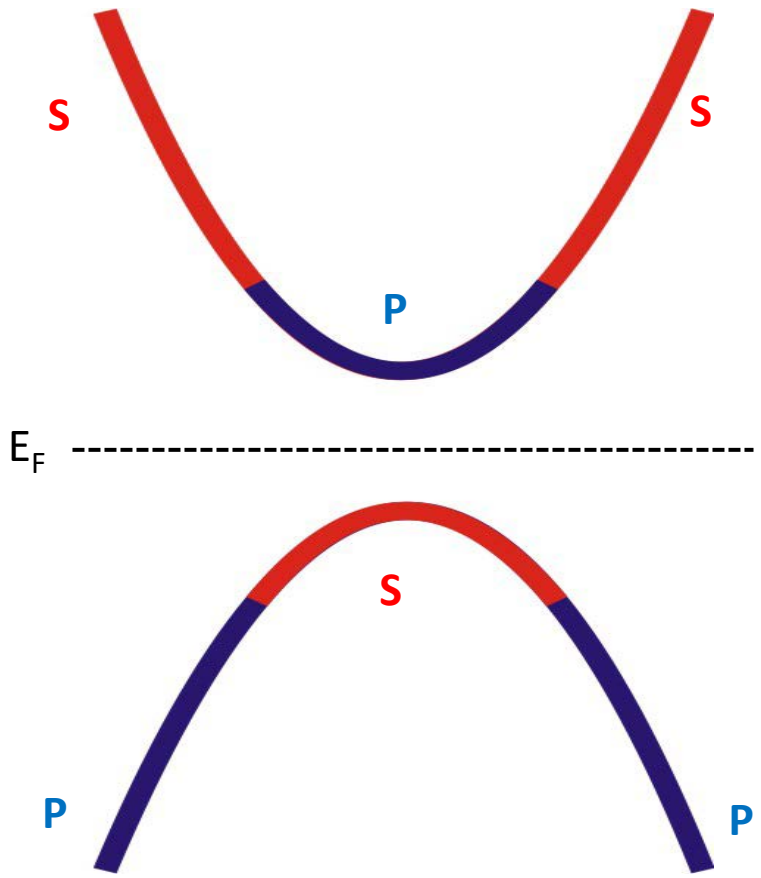



(U, X, R) → (D, Y, $E_0$)

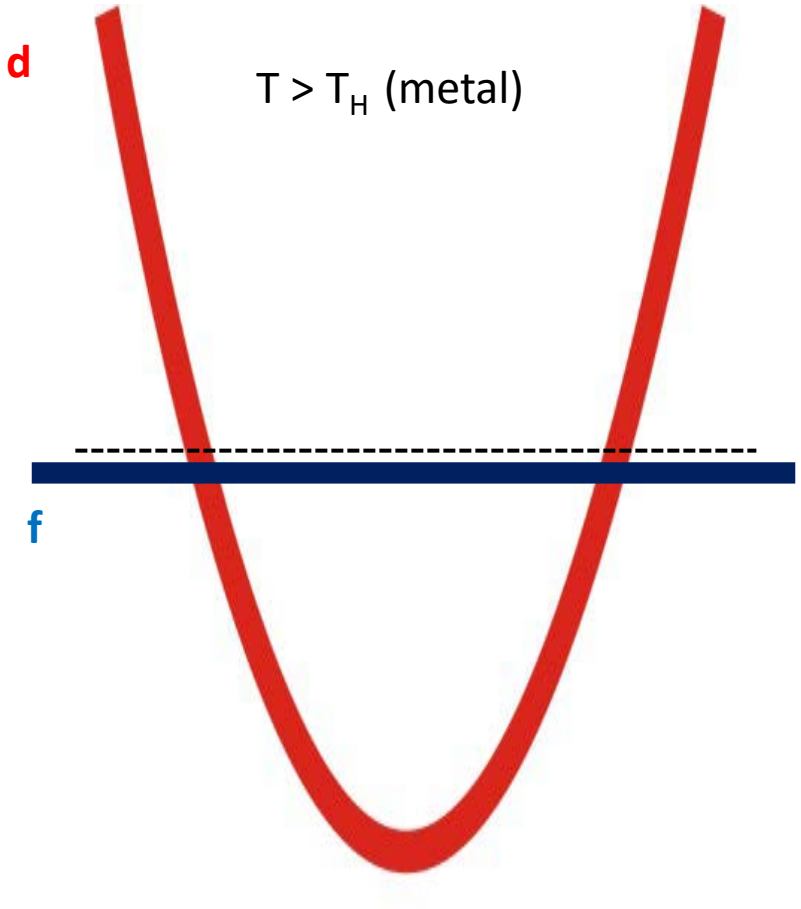
Liu *et al.*, ArXiv:1501:00654 (2015)

# Correlated topological insulators – heavy *f*-electron materials

SOC Band Insulator

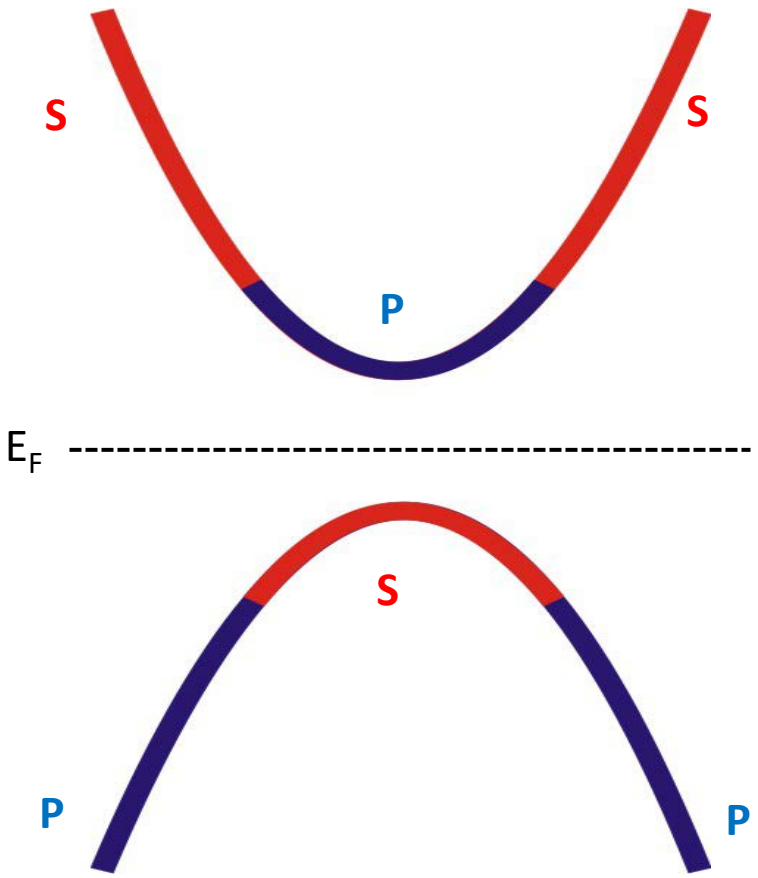



Correlated Kondo Insulator



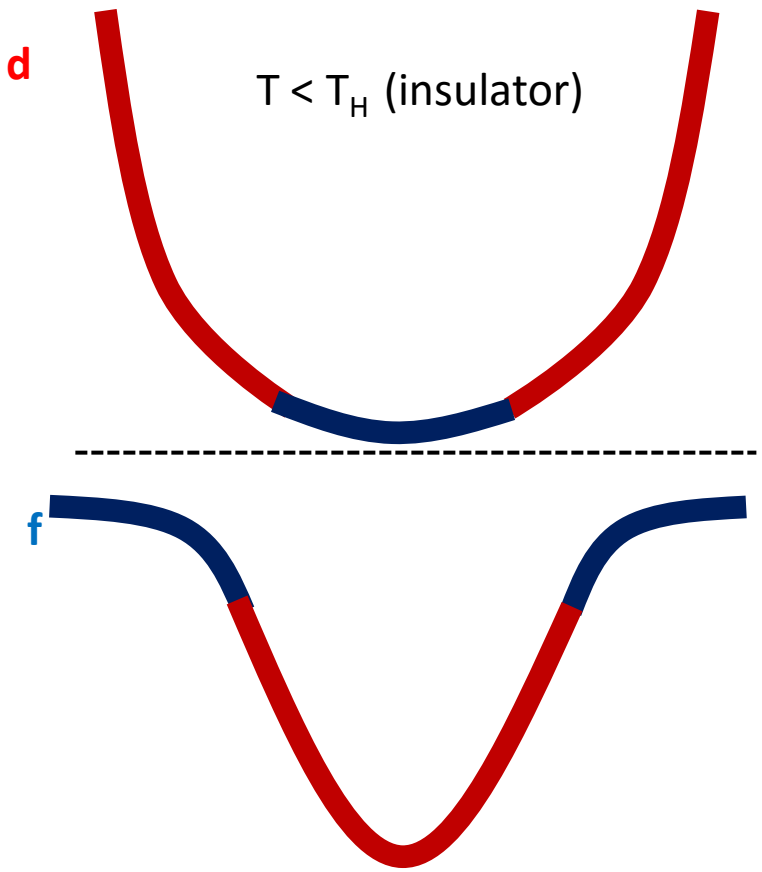
# Correlated topological insulators – heavy *f*-electron materials

SOC Band Insulator




$\Delta \sim 0.5$ eV , $T = \Delta/k_B \sim 5000$ K

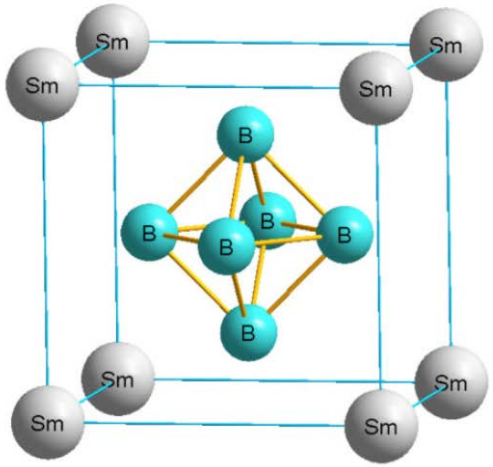
Correlated Kondo Insulator




$\Delta \sim 10$ meV , $T \sim 100$ K

# $SmB_6$

Lu et al., PRL **110**, 096401 (2013)



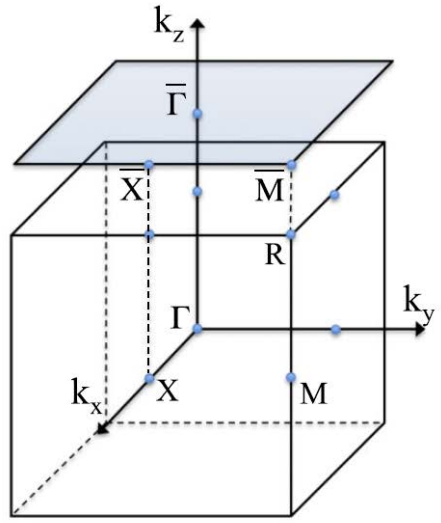
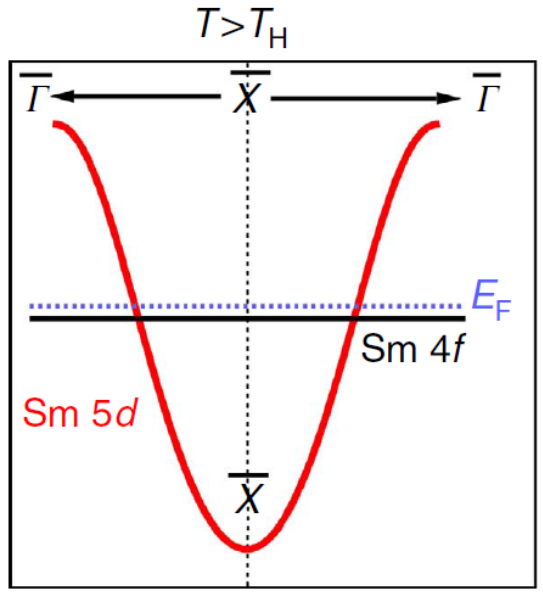
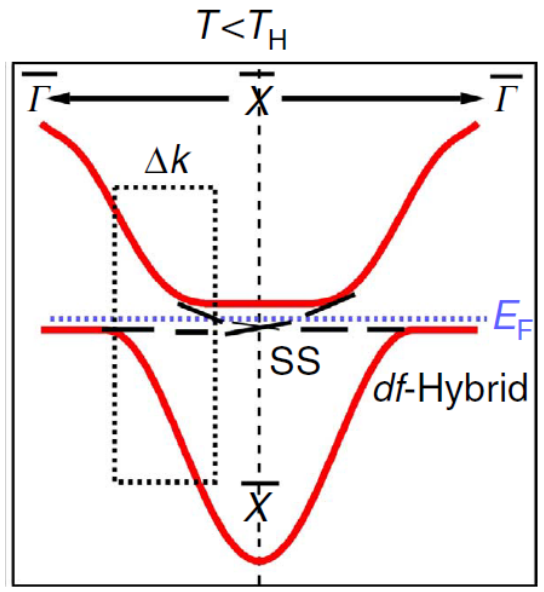




TABLE I. The products of parity eigenvalues of the occupied states for TRIM points, Γ, $X$, $R$, and $M$ in the BZ.

| Γ | $3X$ | $R$ | $3M$ |
|---|---|---|---|
| + | − | + | + |

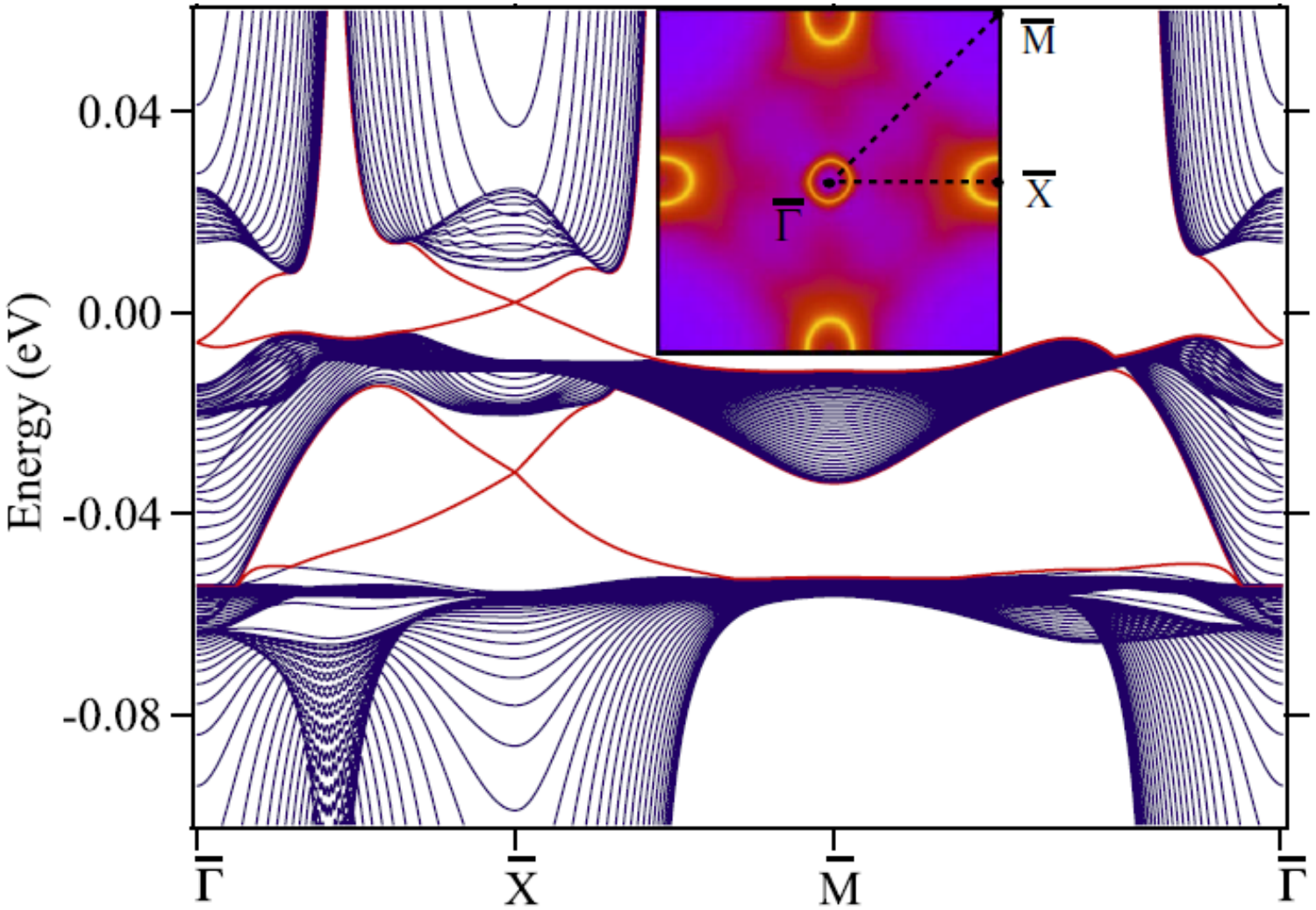
M. Dzero *et al.*, PRL **104**, 106408 (2010).
M. Dzero *et al.*, PRB **85**, 045130 (2012).
H. Miyazaki *et al.*, PRB **86**, 075105 (2012).
T. Takimoto *et al.*, J. Phys. Soc. Jpn. **80**, 123710 (2011).



# $SmB_6$: A candidate 3D topological Kondo insulator

LDA + Gutzwiller calculation

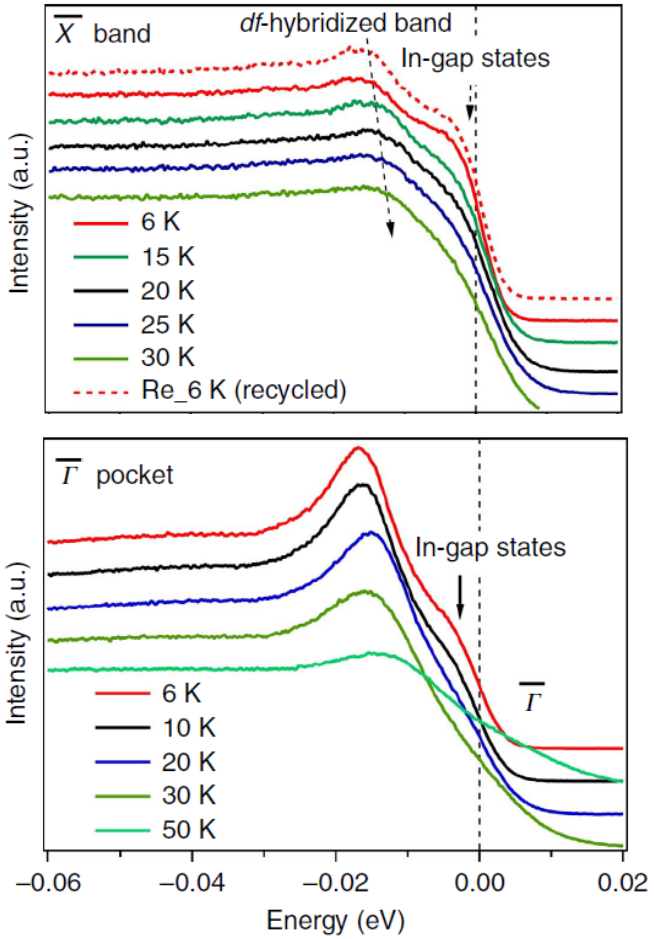


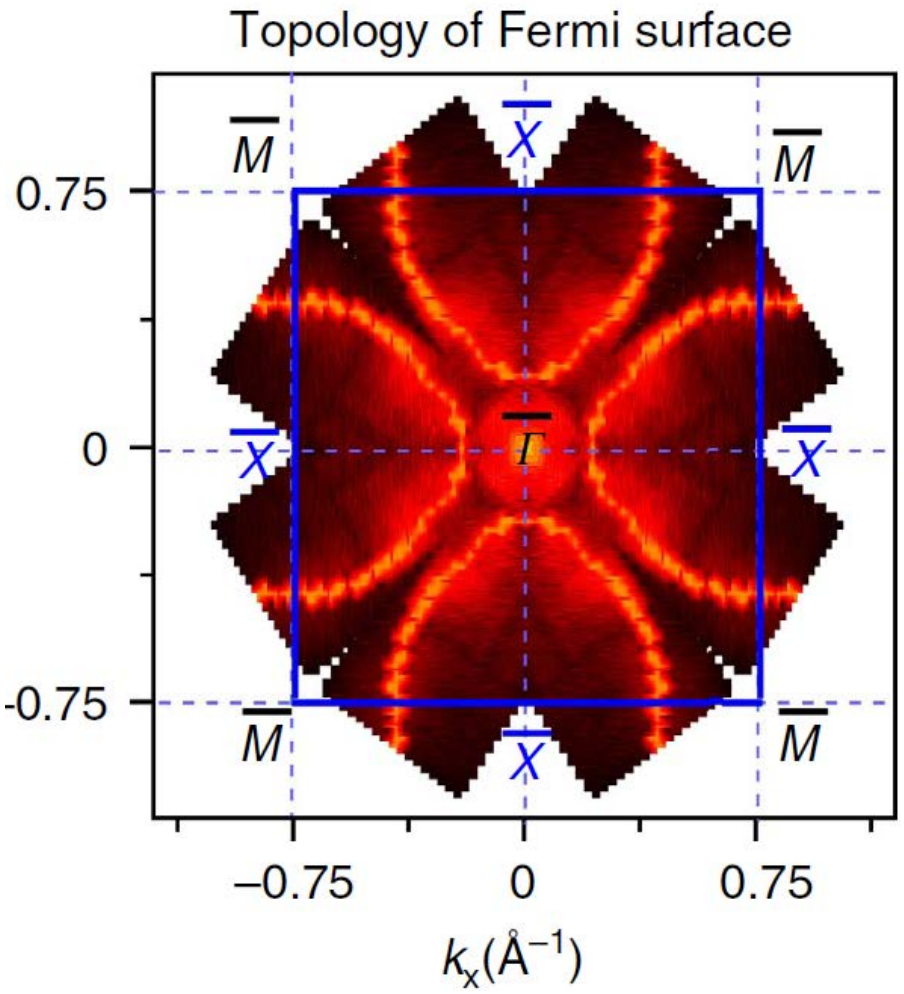

Lu et al., PRL **110**, 096401 (2013)

# $SmB_6$: A candidate 3D topological Kondo insulator

$\Delta E$ = 5 meV, T = 7 K

Neupane et al., Nat. Comm. **4**, 2991 (2013)



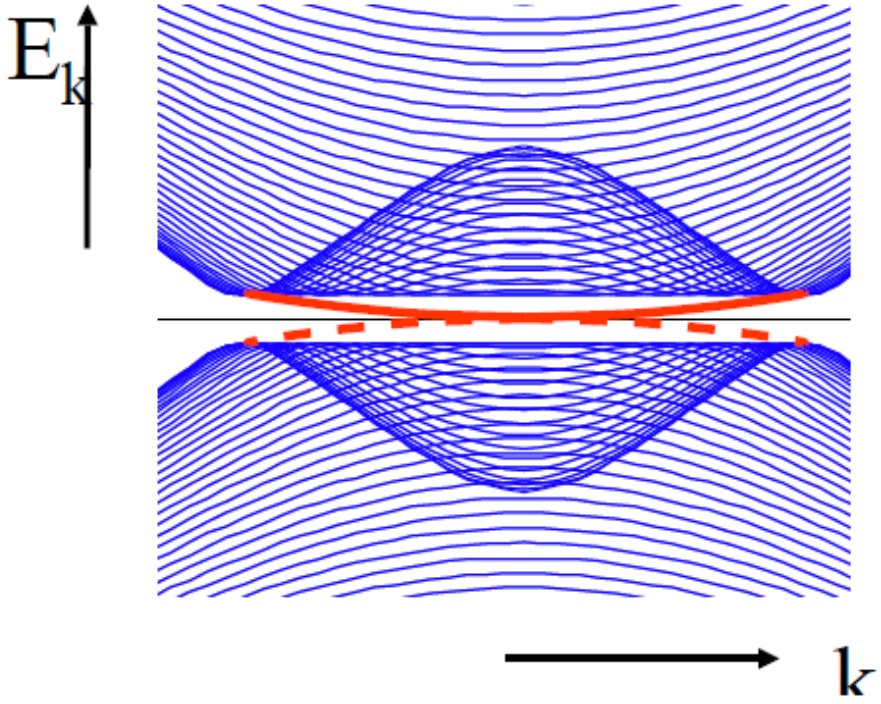

Jiang et al., Nat. Comm. **4**, 3010 (2013)

Frantzeskakis et al., Phys. Rev. X **3**, 041024 (2013)

Xu et al., PRB **88**, 121102(R) (2013)

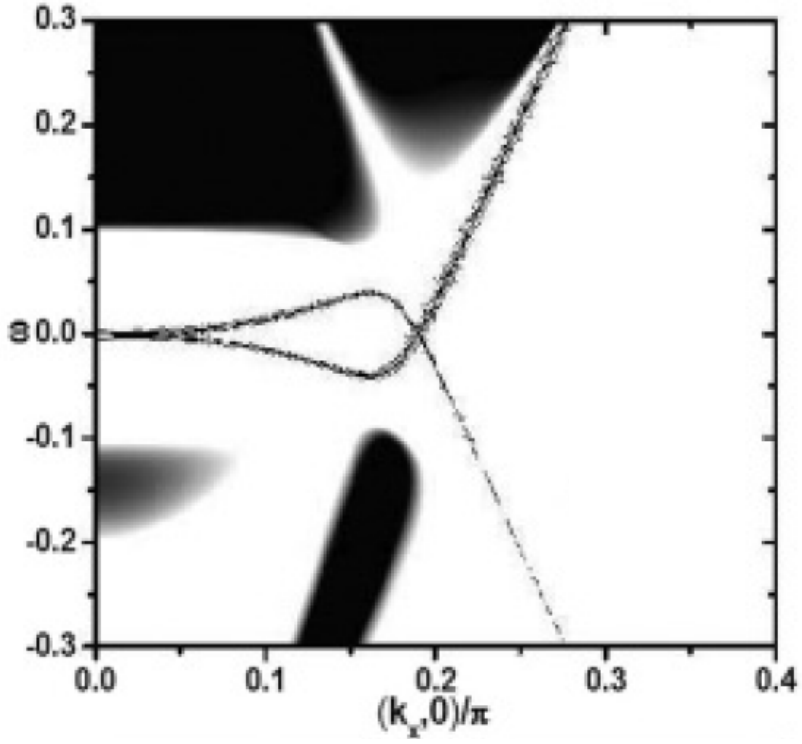
# Superconducting topological insulators - $Cu_xBi_2Se_3$

Fu & Berg, PRL **105**, 097001 (2010).




Calculated electronic structure

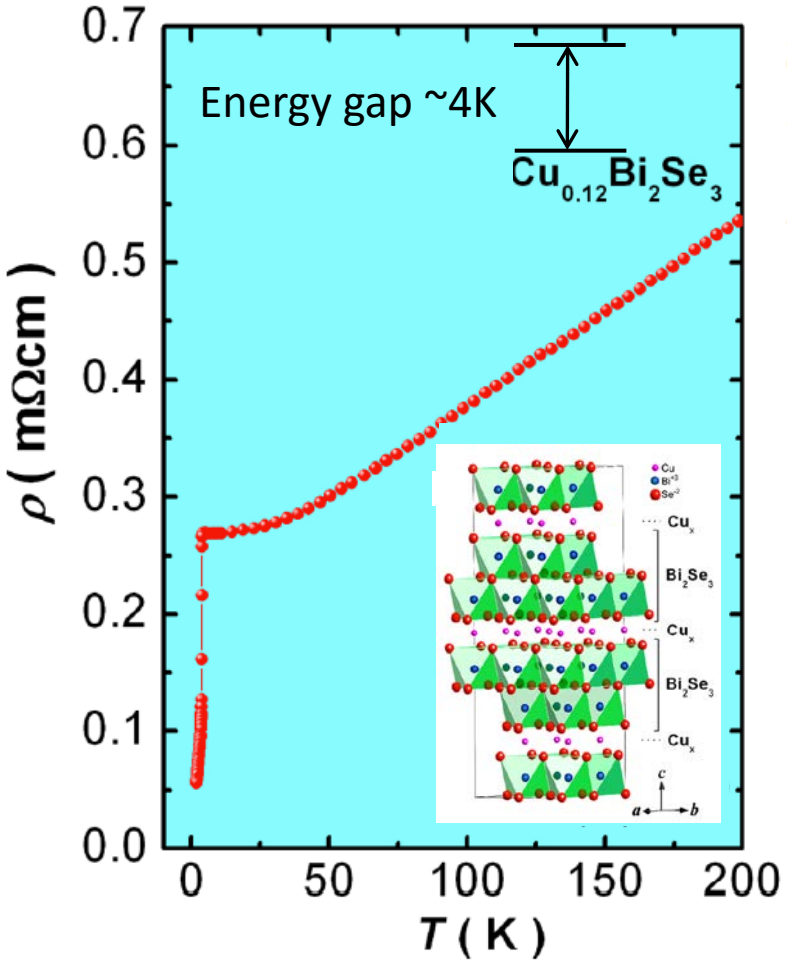
Hao & Ng, PRB **83**, 134516 (2011).



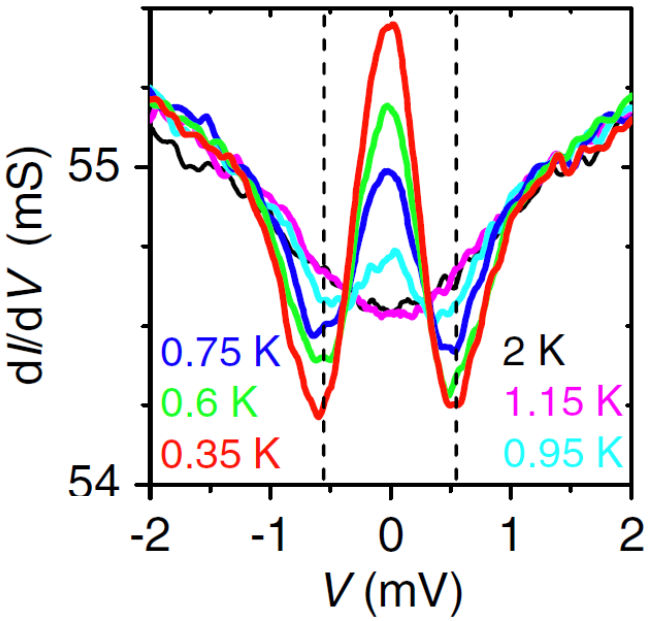

Calculated ARPES intensity

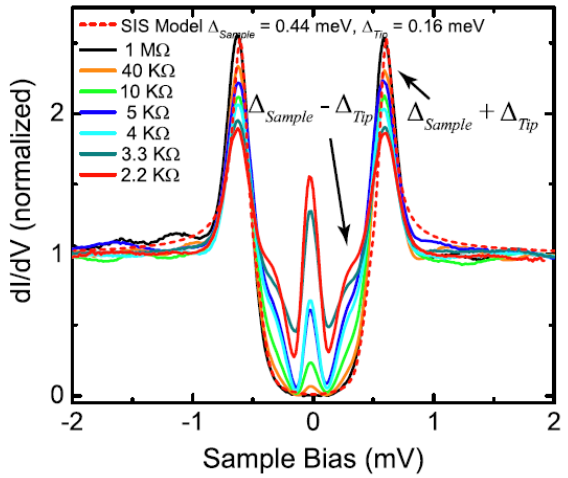
# $Cu_xBi_2Se_3$

Hor et al., PRL **107**, 217001 (2011).



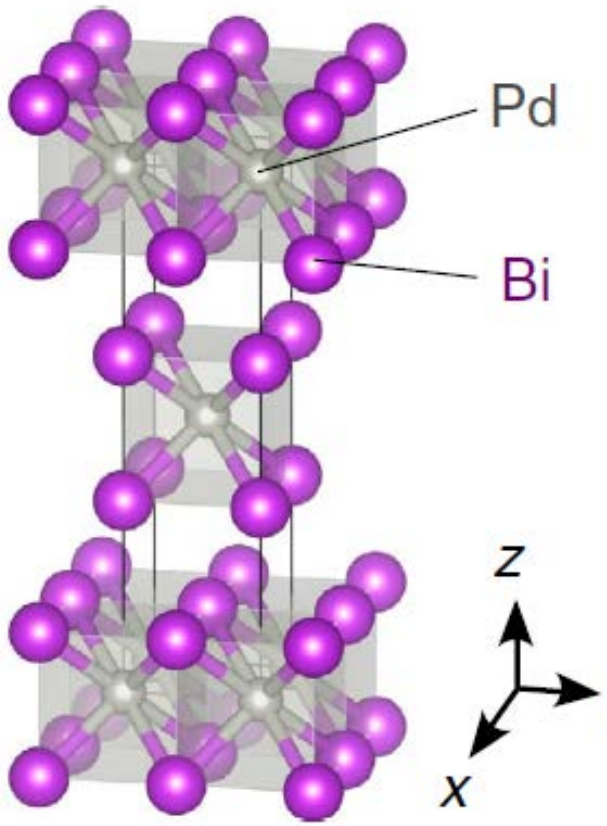

Sasaki et al., PRL **107**, 217001 (2011).



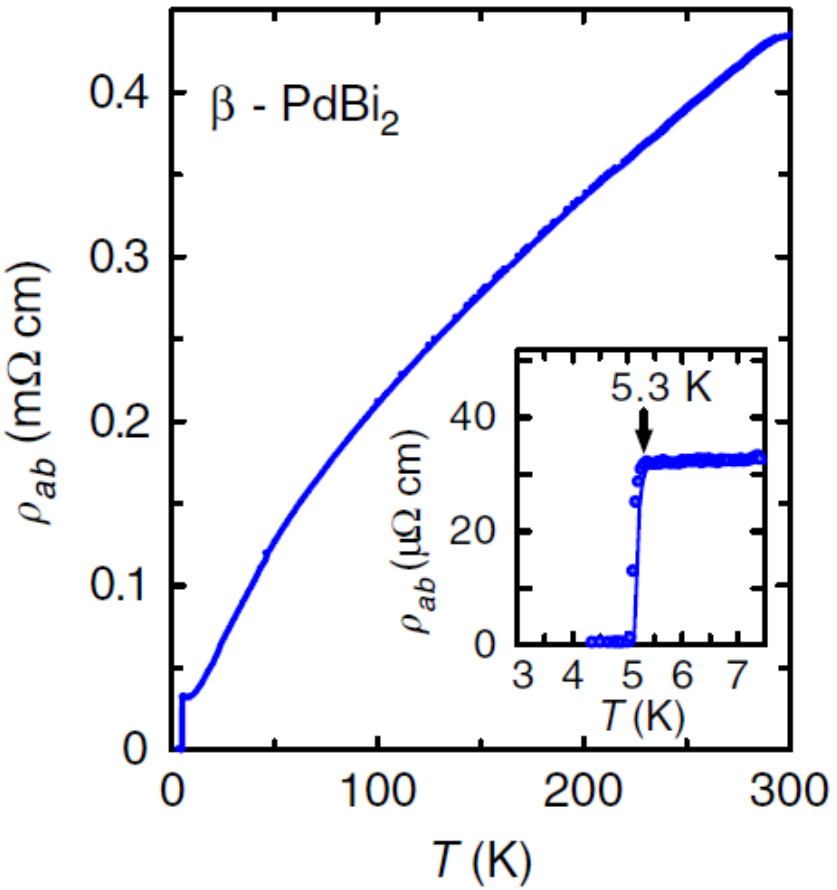




Levy et al., PRL **110**, 117001 (2013).

# β-$PdBi_2$

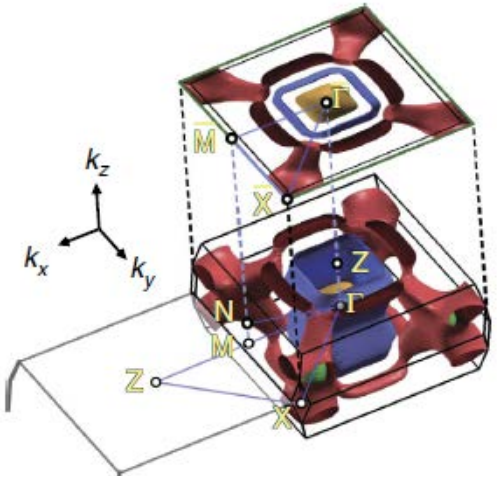


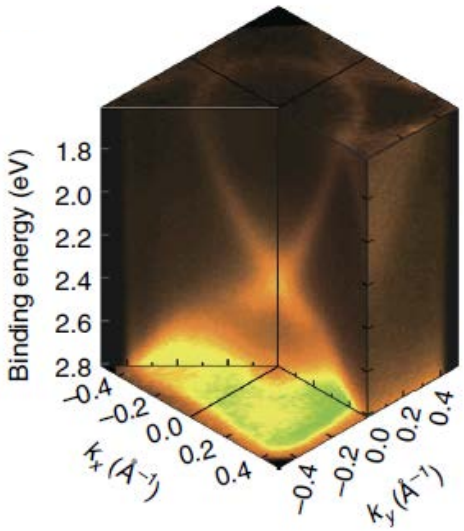

van der Waals bonded between $PdBi_2$ layers



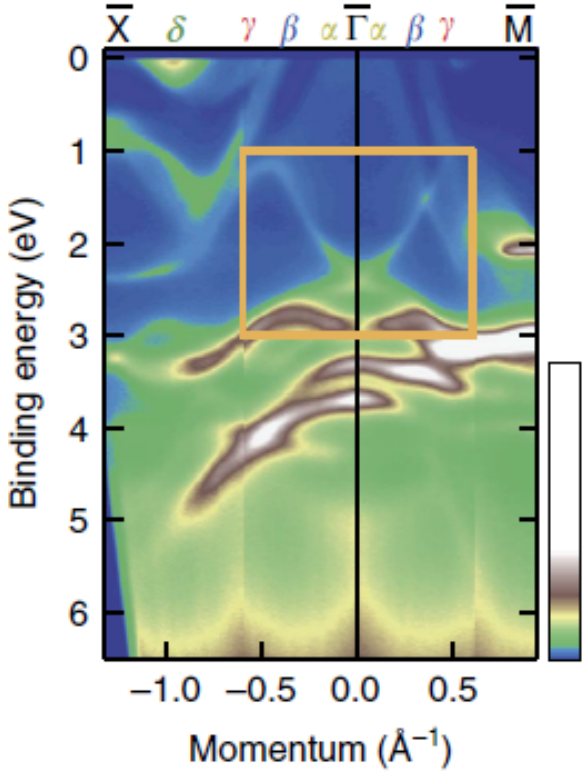

Sakano et al., Nat. Comm. **6**, 8595 (2015)

# β-$PdBi_2$

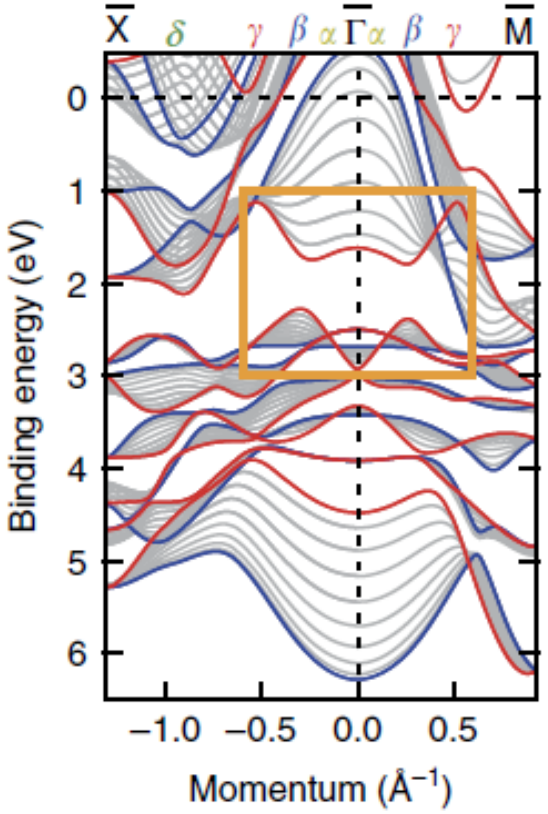


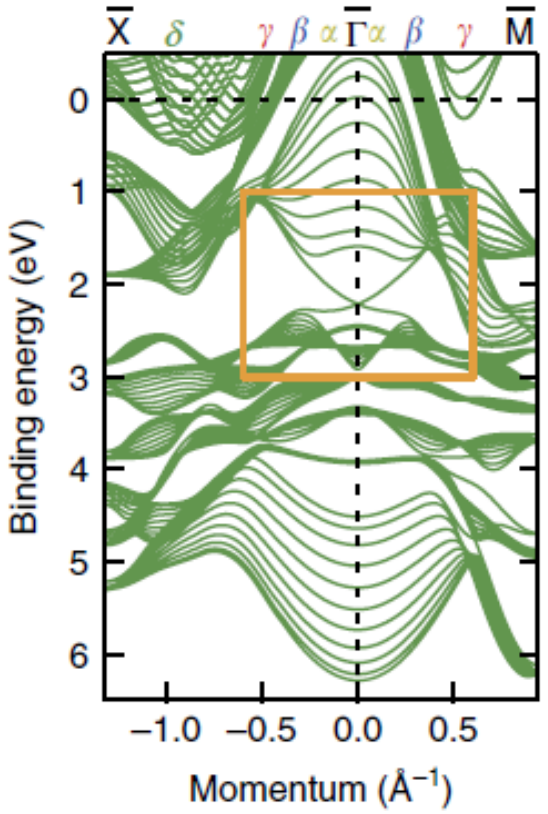

ARPES




LDA projected bulk

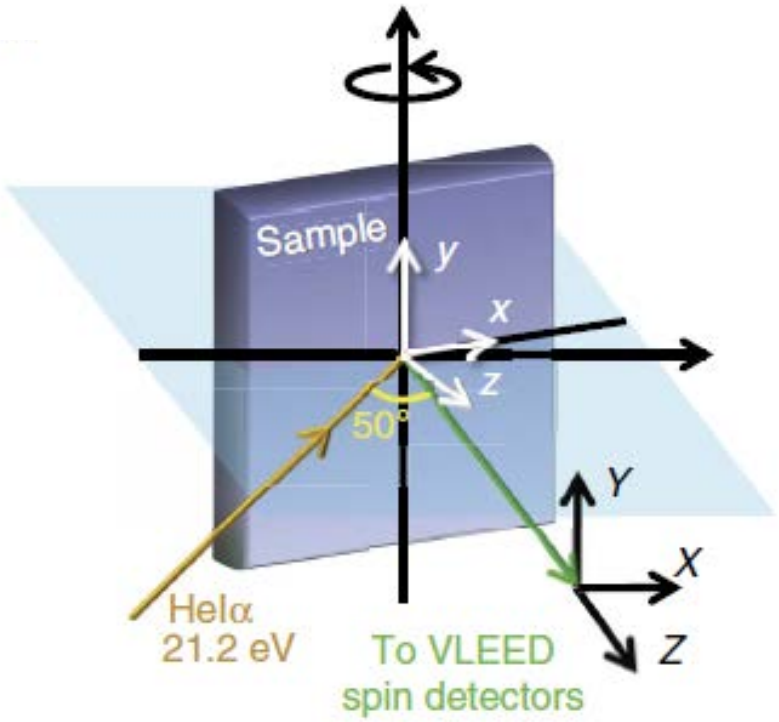


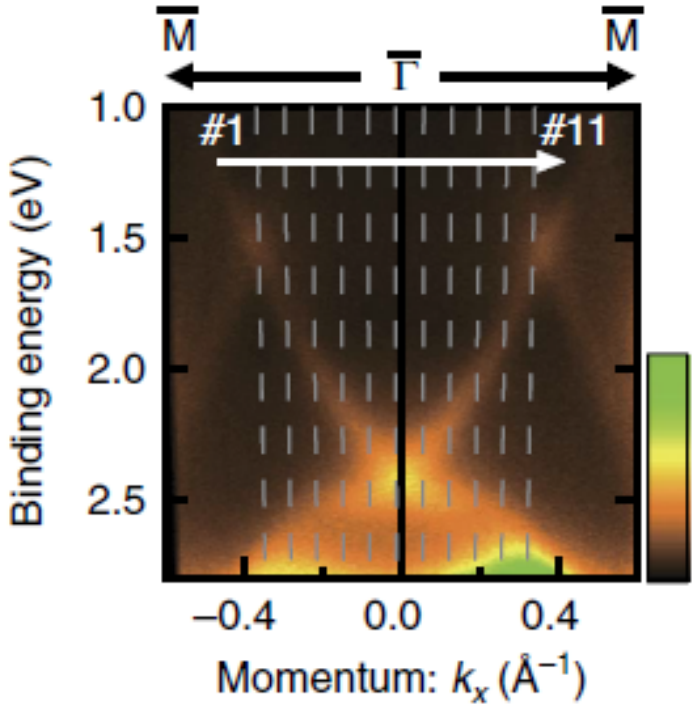

11-layer slab calculation

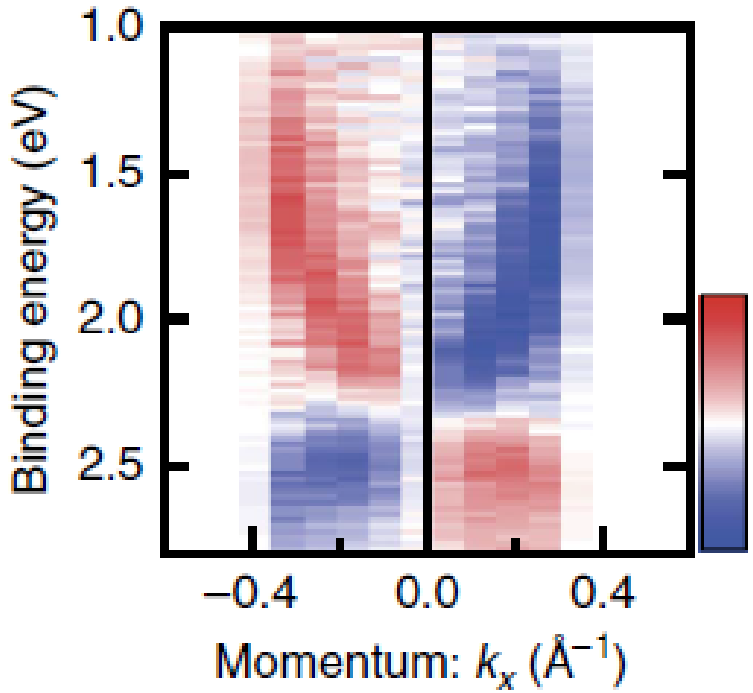



Sakano et al., Nat. Comm. **6**, 8595 (2015)

# β-$PdBi_2$



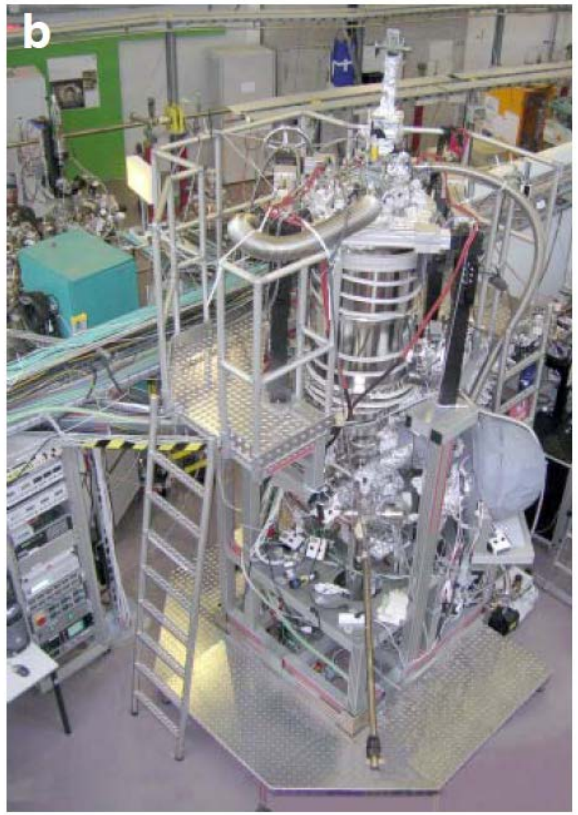



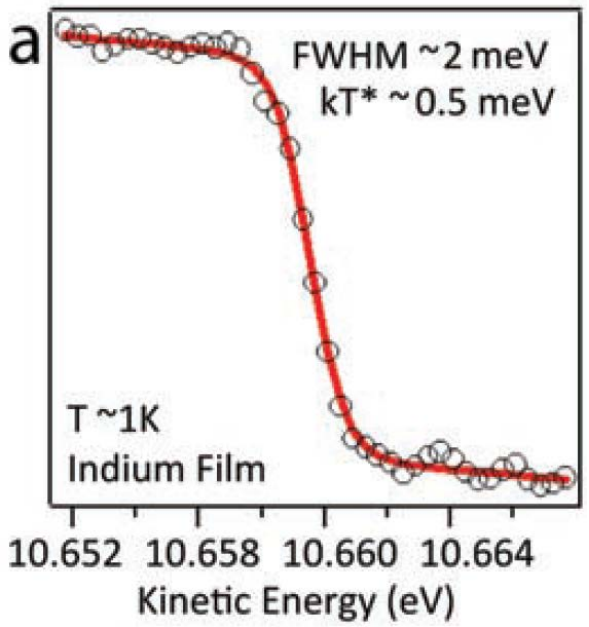




Sakano et al., Nat. Comm. **6**, 8595 (2015)

# Towards ultra-low temperature + high-resolution ARPES

Ultralow temperature ($1^3$ beamline @ BESSY II)

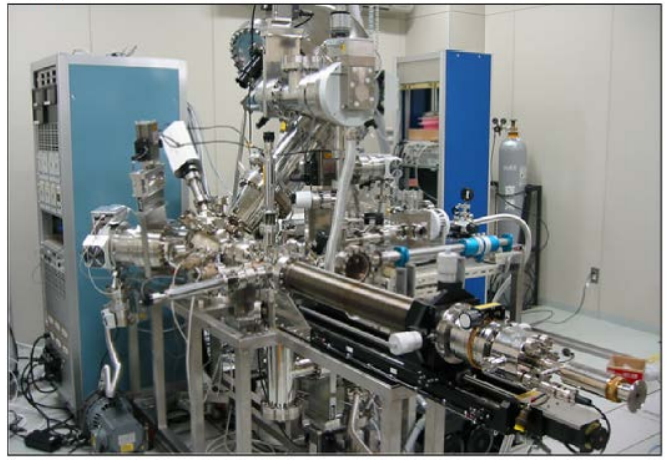


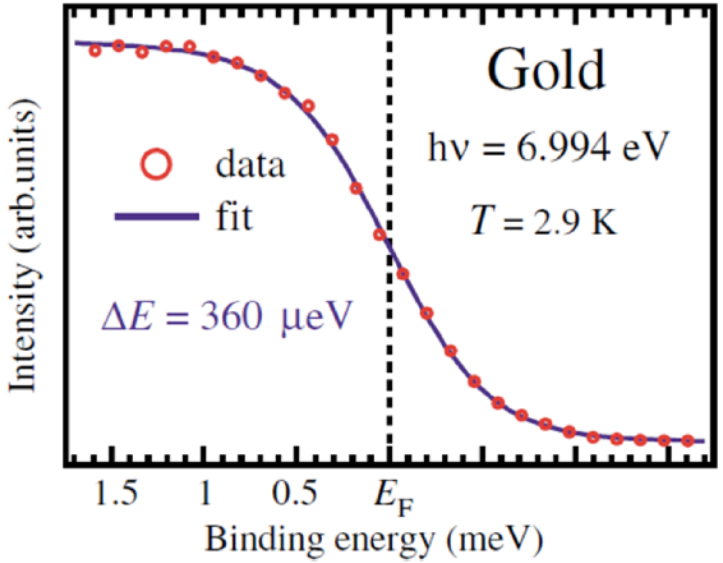




$\sqrt{1^2\ \text{meV} + 1^2\ \text{K} + 1^2\ \text{meV}} \rightarrow$ FWHM 1.46 meV, kT* ~ 0.36 meV

Ultrahigh resolution (Shin Lab; ISSP Tokyo)

Shimojima et al.,JPSJ **84**, 072001 (2015)





# Conclusions