SOI and symmetry: Lifting the Kramers' degeneracy

$$1.\ \boldsymbol{E}(\boldsymbol{k},\uparrow) = \boldsymbol{E}(-\boldsymbol{k},\downarrow)$$ ***time-reversal*** symmetry

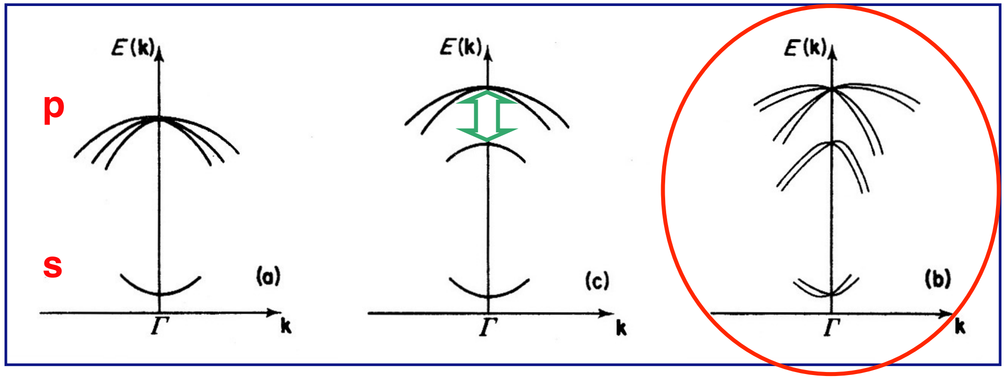
$$2.\ \boldsymbol{E}(\boldsymbol{k},\uparrow) = \boldsymbol{E}(-\boldsymbol{k},\uparrow)$$ ***inversion*** symmetry

$$1+2.\ \boldsymbol{E}(\boldsymbol{k},\uparrow) = \boldsymbol{E}(\boldsymbol{k},\downarrow)$$ **Kramers' degeneracy**

In the bulk of a non-CS solid or at the surface, inversion symmetry is broken

With SO interaction: $\boldsymbol{E}(\boldsymbol{k},\uparrow) \neq \boldsymbol{E}(\boldsymbol{k},\downarrow)$ **without external magnetic field**

Except at Γ and at a few other "special" (**TRI**) points



no SO **with SO** **SO - no inversion**

Rashba and *Dresselhaus* effects

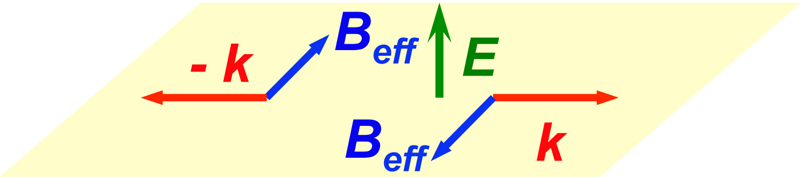
The Rashba effect in a 2DEG

Free electrons at the surface "see" an electric field

$$\vec{E} = -\nabla V = -\frac{dV}{dz}\vec{e}_z$$

and a magnetic field

$$\vec{B}_{eff} = \frac{1}{c^2}\vec{v}\times\vec{E} = \frac{\hbar}{m^* c^2}\vec{k}\times\vec{E}$$

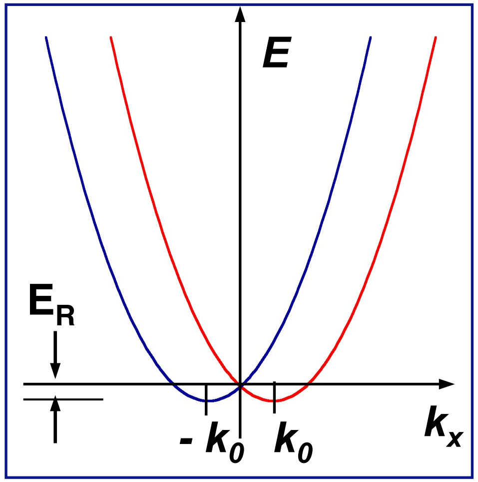


E. Rashba

Zeeman coupling

$$H_{SOC} \approx -\vec{\mu}_S \cdot \vec{B} = \alpha_R(\vec{e}_z \times \vec{p})\cdot\sigma$$

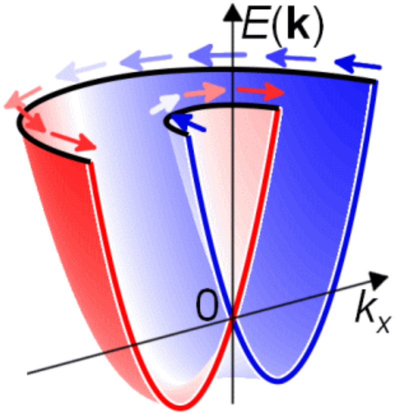
The quantization axis is linked to k



$$E = \frac{\hbar^2 k^2}{2m^*} \pm \alpha_R k$$

$$E_R = |E(\pm k_0)|$$

$$\alpha_R \approx E \qquad k_0 = \frac{m^*\alpha_R}{\hbar^2}$$



Spin polarization

The expected Rashba energy E_R is very small: $E_R \sim 10^{-6}$ eV!

Rashba vs. Zeeman

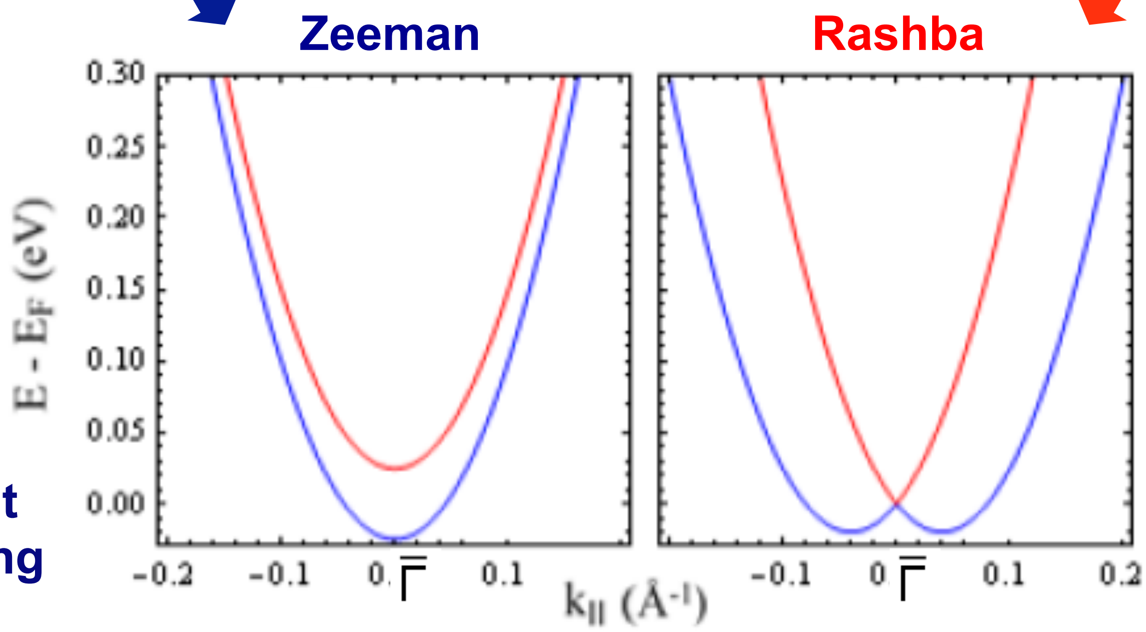
External in-plane **B**

$$\begin{pmatrix} \frac{\hbar^2(k_x+k_y)^2}{2m^*} & -iE_P \\ iE_P & \frac{\hbar^2(k_x+k_y)^2}{2m^*} \end{pmatrix}$$

$$E_P = -\boldsymbol{M}\cdot\boldsymbol{B}$$

“Effective” in-plane **B**

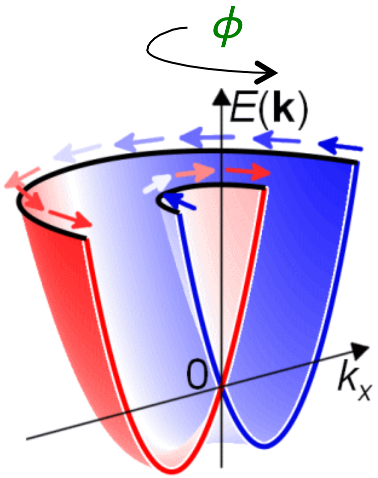
$$\begin{pmatrix} \frac{\hbar^2(k_x+k_y)^2}{2m^*} & \alpha_R(-ik_x-k_y) \\ \alpha_R(ik_x-k_y) & \frac{\hbar^2(k_x+k_y)^2}{2m^*} \end{pmatrix}$$



Constant E-splitting

k-linear E-splitting

The spin polarization



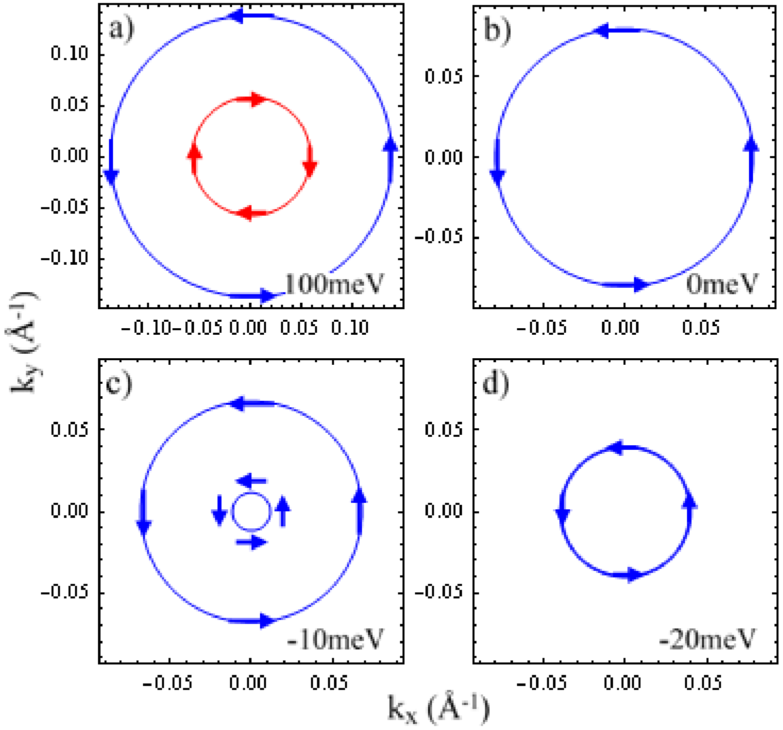
SO mixes UP and DOWN spins

$$|\psi_+(\vec{k})\rangle = \frac{e^{i(k_x x+k_y y)}}{2^{1/2}}\left(\,|\uparrow\rangle + e^{i\phi(k)}|\downarrow\rangle\right)$$

Upper branch

$$|\psi_-(\vec{k})\rangle = \frac{e^{i(k_x x+k_y y)}}{2^{1/2}}\left(\,|\uparrow\rangle - e^{i\phi(k)}|\downarrow\rangle\right)$$

Lower branch



$$\langle\sigma_x\rangle_\pm = \pm\,\cos\phi(k)\ ;$$

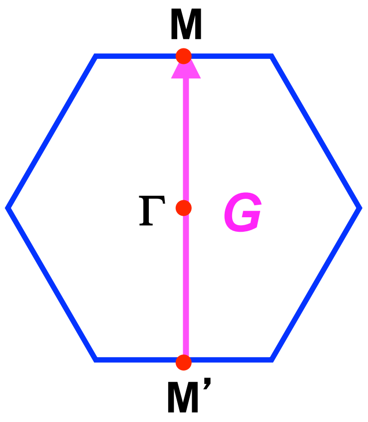
$$\langle\sigma_y\rangle_\pm = \pm\,\sin\phi(k)\ ;$$

$$\langle\sigma_z\rangle_\pm = 0$$

Spin polarization

Time Reversal Invariant points

Hexagonal symmetry



$$E(\vec{k},\uparrow)=E(-\vec{k},\downarrow)$$

TR symmetry

$$k=0 \quad \rightarrow \quad E(\Gamma,\uparrow)=E(\Gamma,\downarrow)$$

$$E(M,\uparrow)=E(M',\downarrow)$$

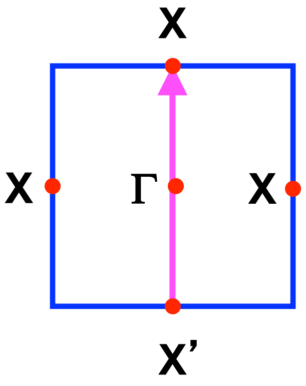
TR symmetry

$$E(M',\downarrow)=E(M'+\vec{G},\downarrow)=E(M,\downarrow)$$

Translational symmetry

$$E(M,\uparrow)=E(M,\downarrow)$$

Square symmetry



$$E(X,\uparrow)=E(X',\downarrow)$$

TR symmetry

$$E(X',\downarrow)=E(X'+\vec{G},\downarrow)=E(X,\downarrow)$$

Translational symmetry

$$E(X,\uparrow)=E(X,\downarrow)$$

Spin manipulation without magnetic fields

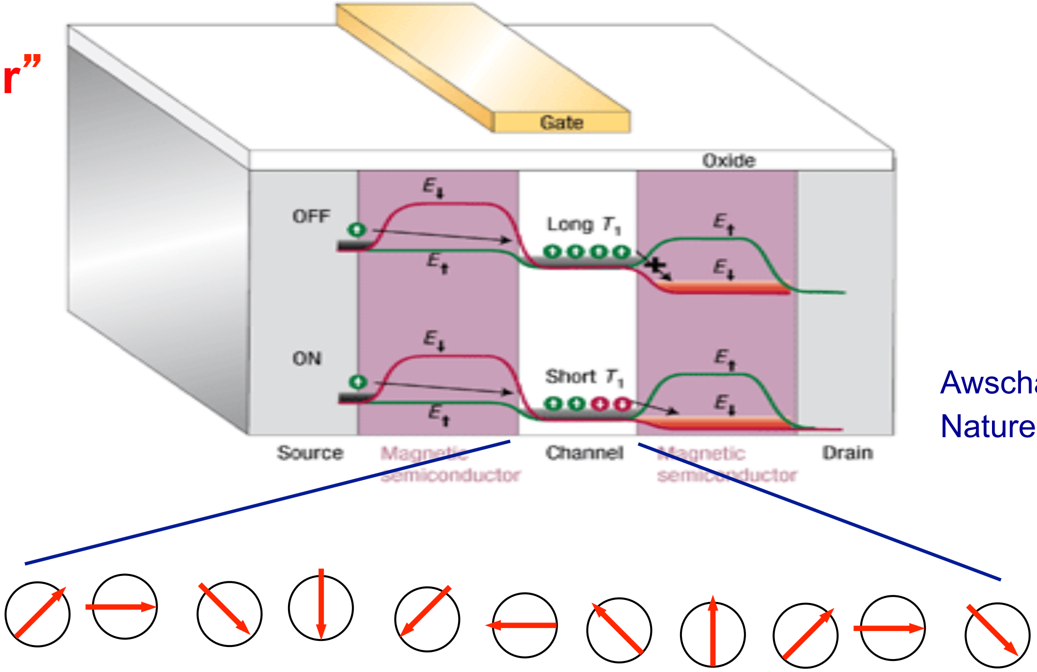
Polarized electrons are injected in a mixed |up > + |down> spin state.

The spin precesses along the channel: $\Delta\theta \approx L\alpha_R$

It can be modulated by V_G

The "spin transistor"

S. Datta and B. Das,
APL 56, 665 (1990).



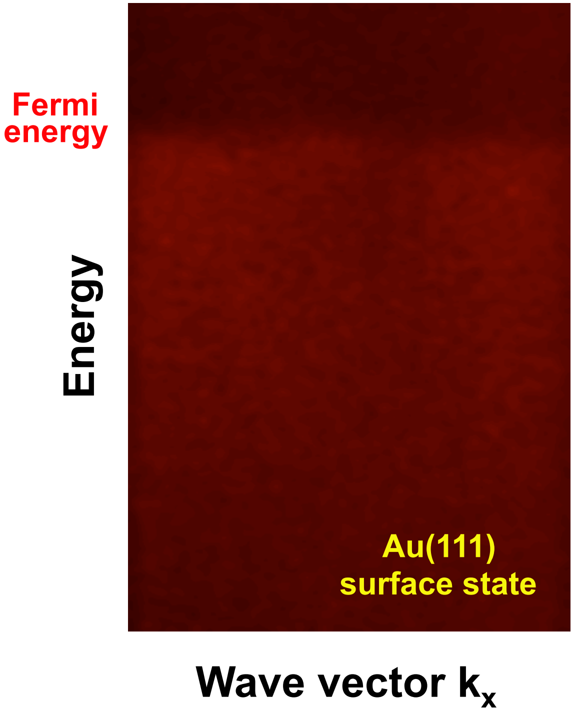
Awschalom and Flatté,
Nature Phys. 3, 153 (2007).

Rabi oscillations

For InGaAs/InAlAs heterojunctions: $L(\Delta\theta = \pi) \approx 0.5\ \mu m$

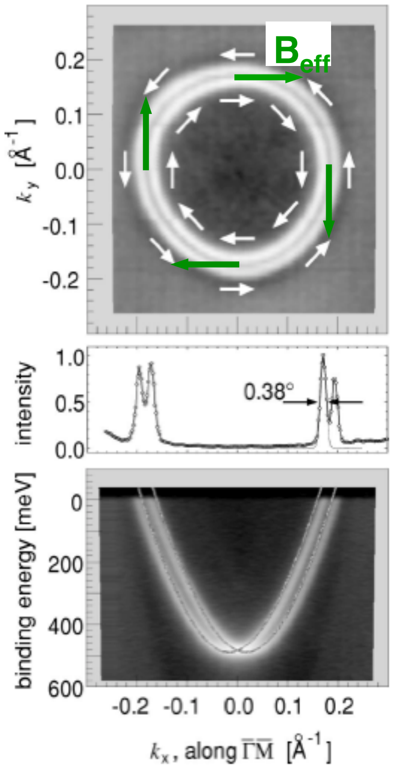
Shockley state at the Au(111) surface : ARPES

The circular Fermi surface is split into two spin-polarized branches



LaShell et al., PRL (1997).

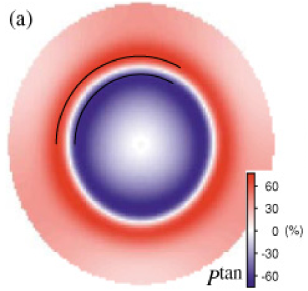
Reinert et al., PRB (2001).



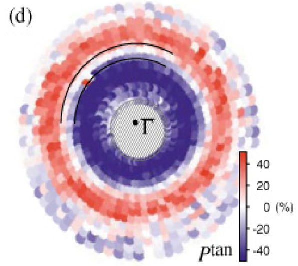
$k_0 = 0.012$ Å^{-1} **$E_R \sim 2$ meV**

LARGE !

Spin polarization



Theory



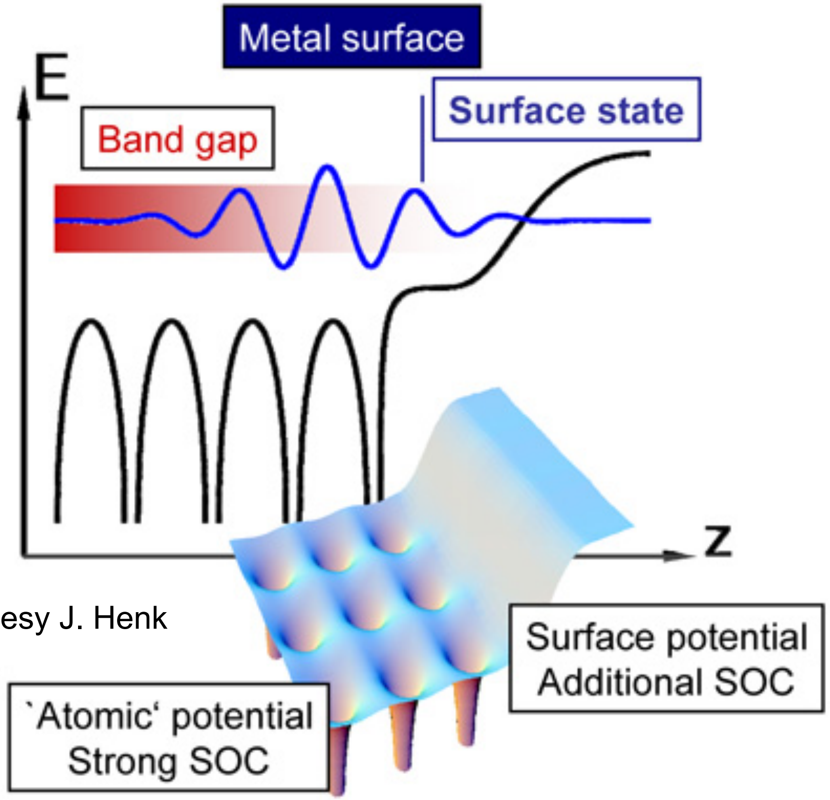
SP-ARPES

M. Hoesch et al., (2004)

Much stronger fields near the nuclei !

The E field is largest near the nuclei

The intra-atomic SO interaction MUST be important

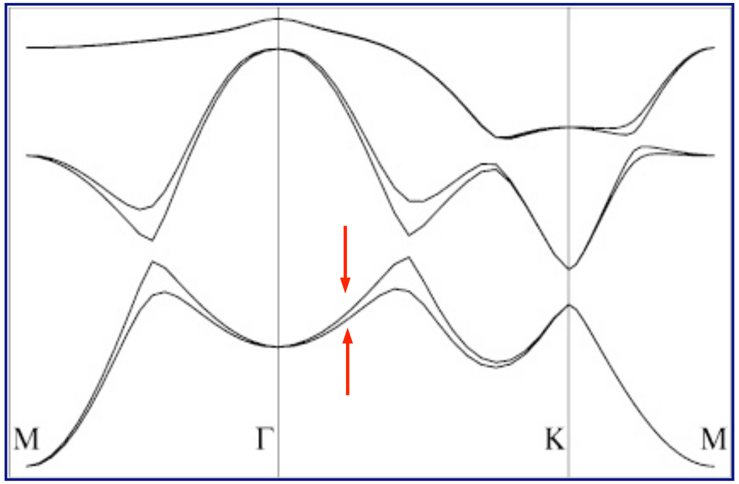


Courtesy J. Henk

atomic SO parameter

surface term

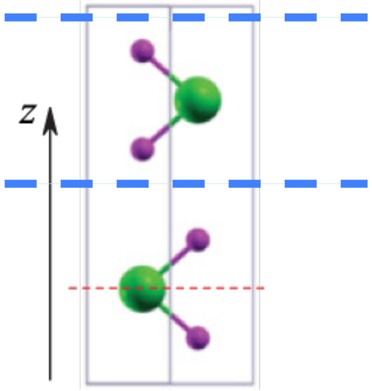
$$\alpha_R \approx \alpha_{AT} \cdot \left(\frac{dV}{dz}\right)$$



L. Petersen and P. Hedegård,
Surf. Sci. **459**, 49 (2000)

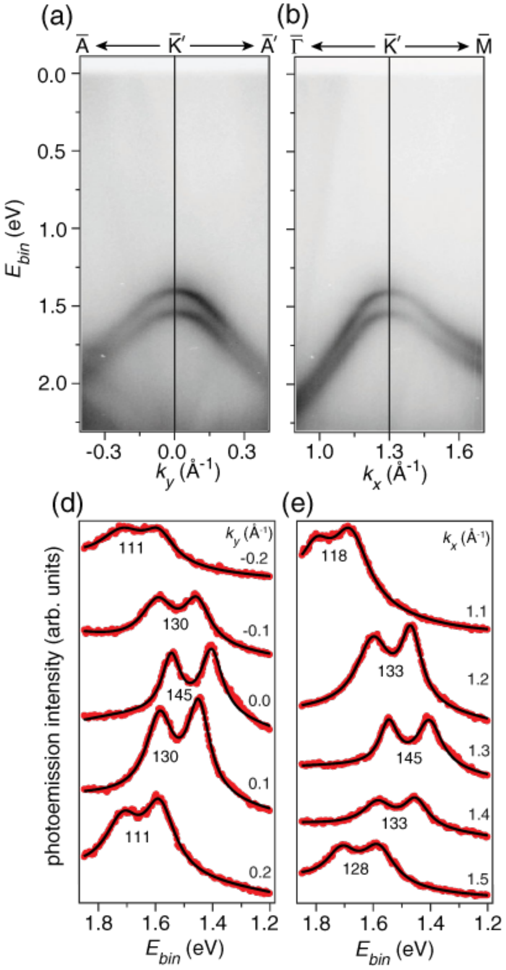
Much larger splittings are possible

Single-layer solids - ARPES



The SL lacks inversion symmetry

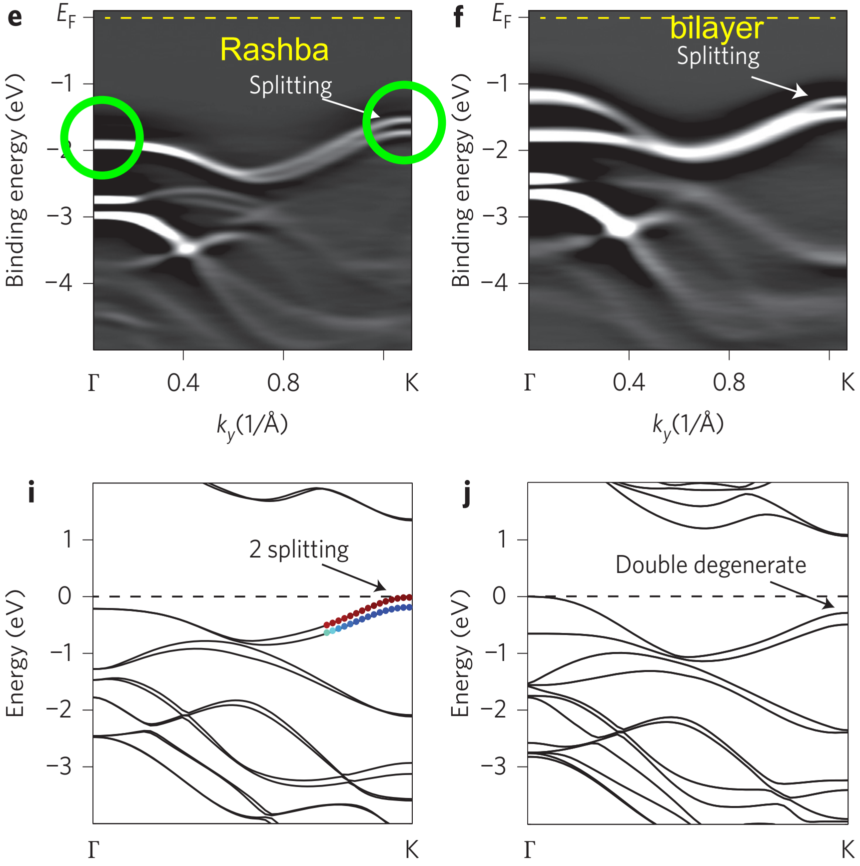
SL MoS_2



$MoSe_2$

SL

Bilayer

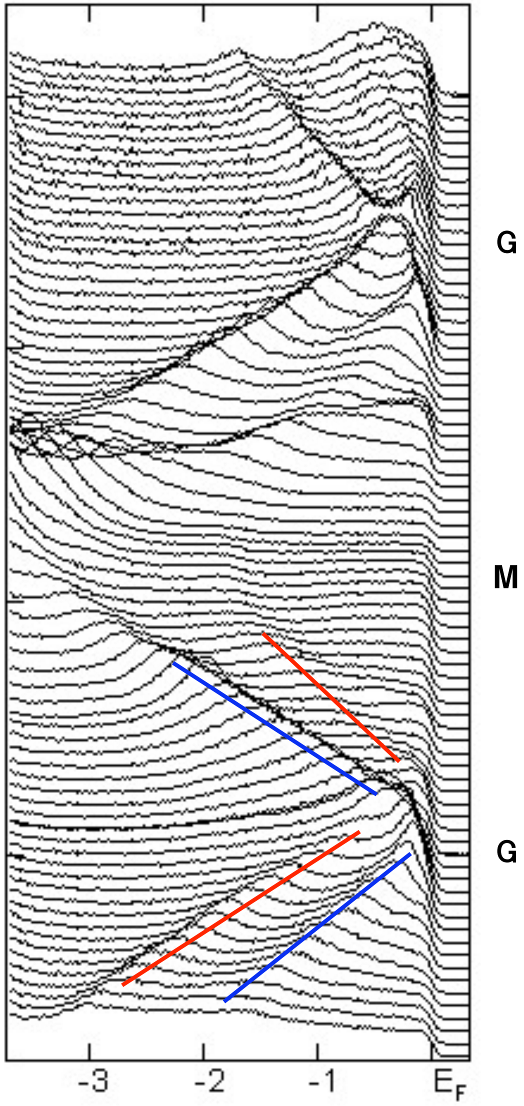


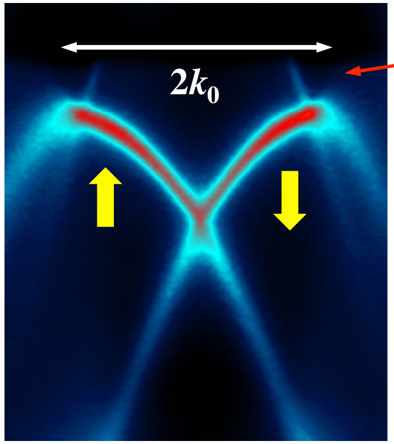
J.A. Miwa et al., PRL **114**, 046802 (2015)

Y. Zhang et al., Nat. Nanotech. **9**, 111 (2014)

Surface alloys with high-Z elements: Bi/Ag(111)

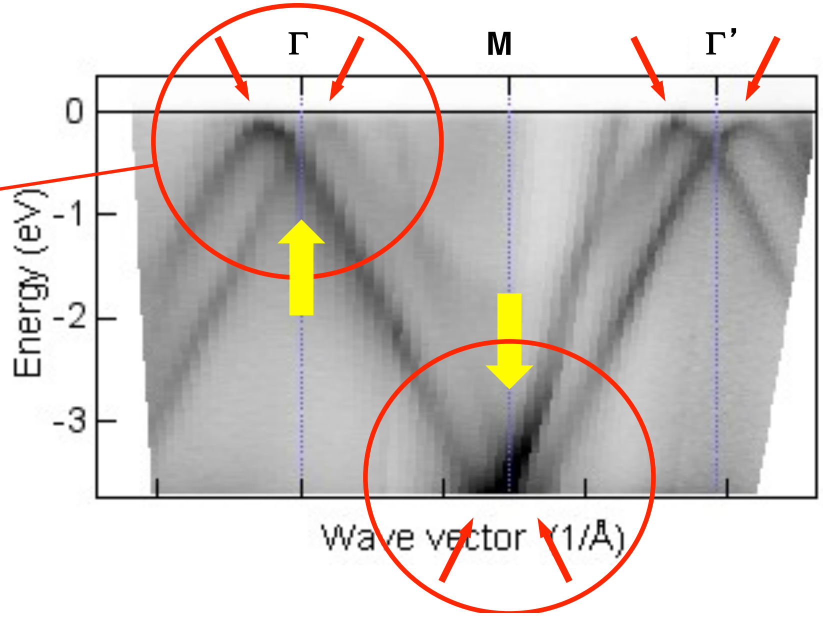
Ast et al., Phys. Rev. Lett. **98**, 186807 (2007)



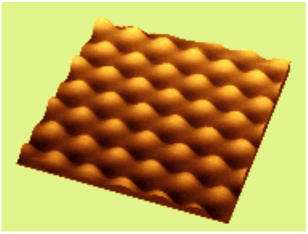


E_R = 200 meV

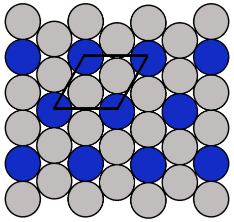
GIANT !

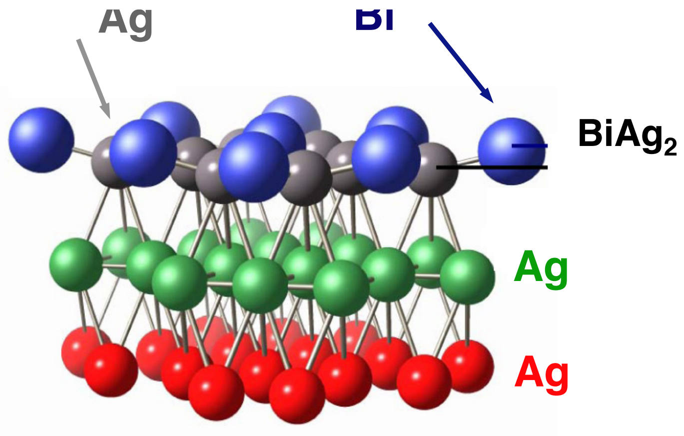


Surface bands degenerate at Γ and M (time-reversal invariant points)



STM

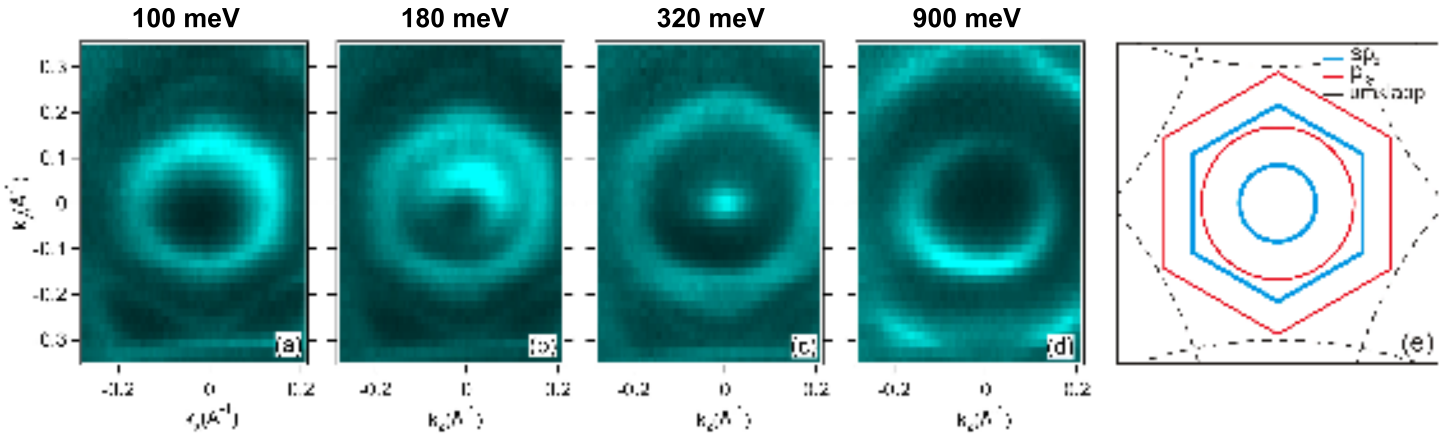


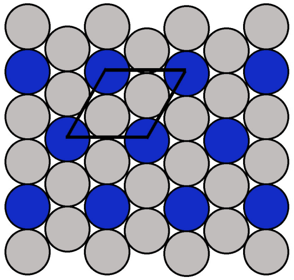


C.R. Ast et al., PRL **98**, 186807 (2007)

In-plane symmetry breaking and anisotropy

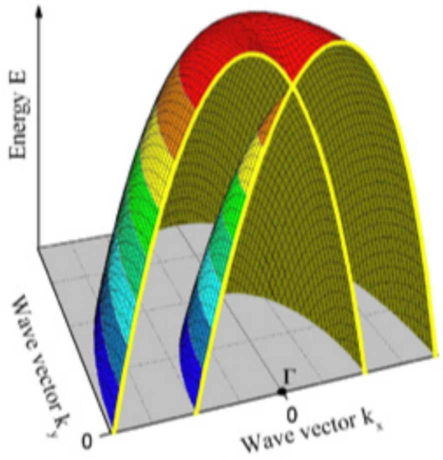
ARPES constant energy cuts in k-space



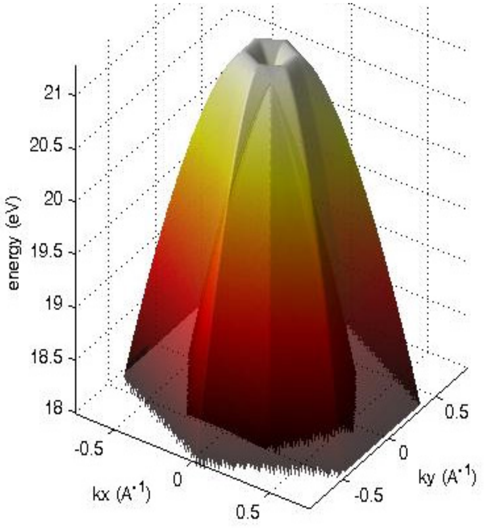


Unlike the case of Au(111) the spin-split FS is clearly influenced by the crystal potential

in-plane gradient

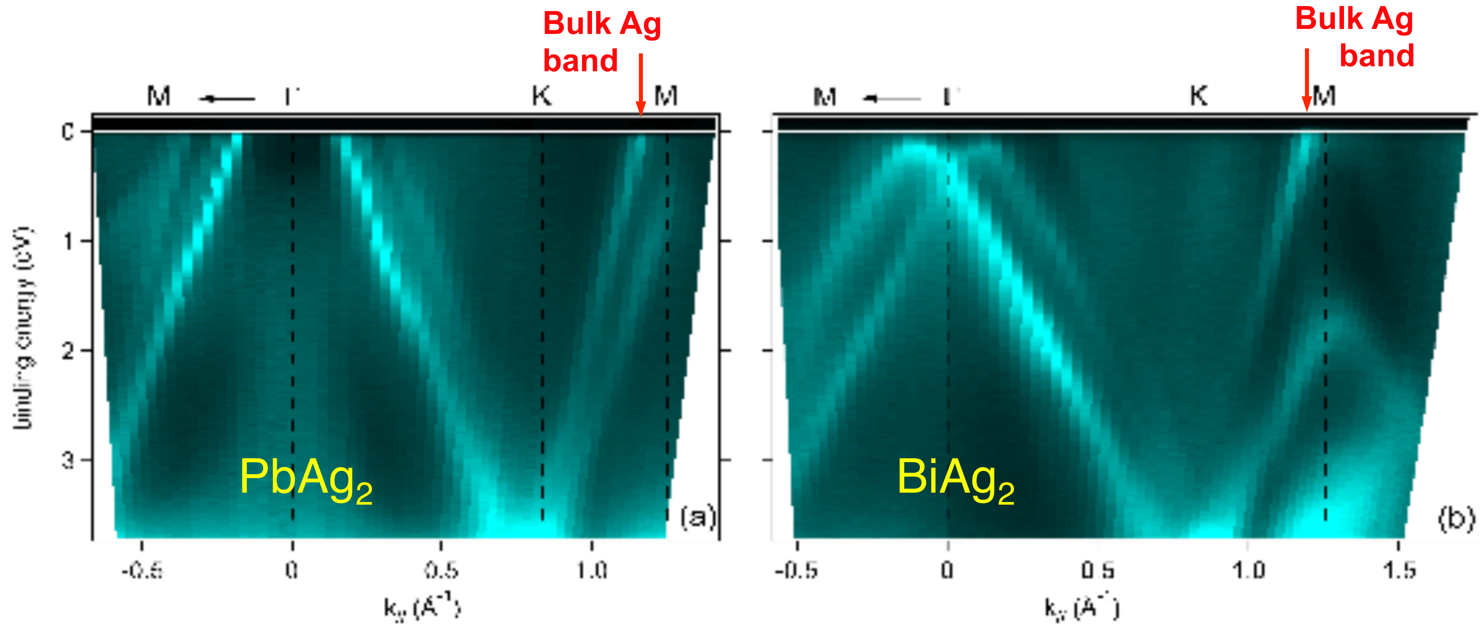


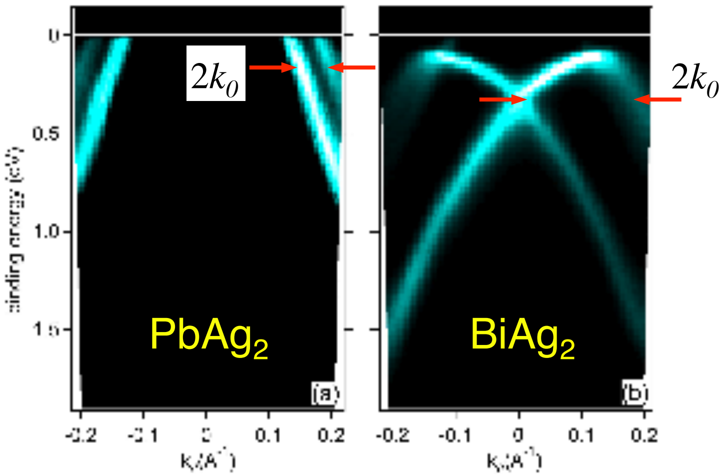
Simple (Au(111))



More realistic

Turning the band-filling knob: Pb-Ag(111)





Same structure: BiAg$_2$ surface alloy

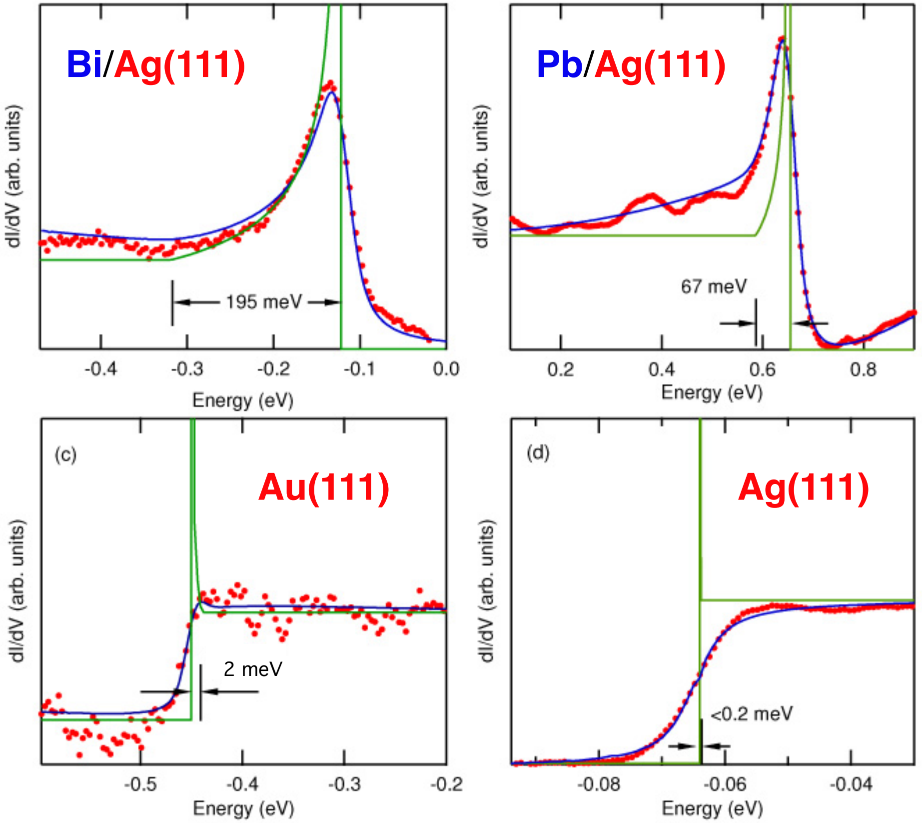
Rigid band shift to accommodate the extra electron

The **splitting** of the bands increases by a **factor 4** between PbAg$_2$ and BiAg$_2$
(the atomic SO parameter is 40% larger)

Spin splitting and the density of states

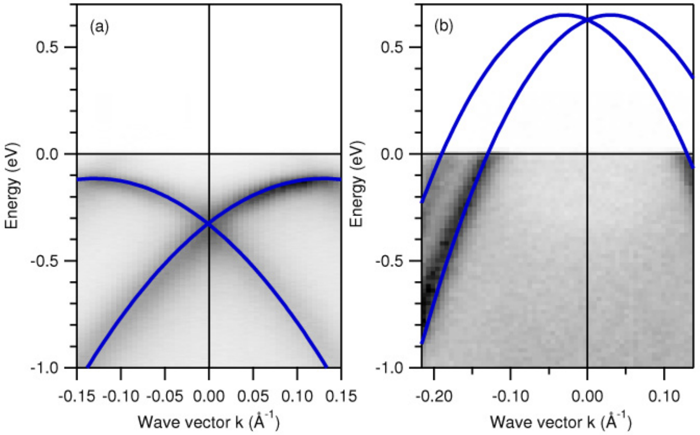
Signatures of spin-split states in tunneling spectra

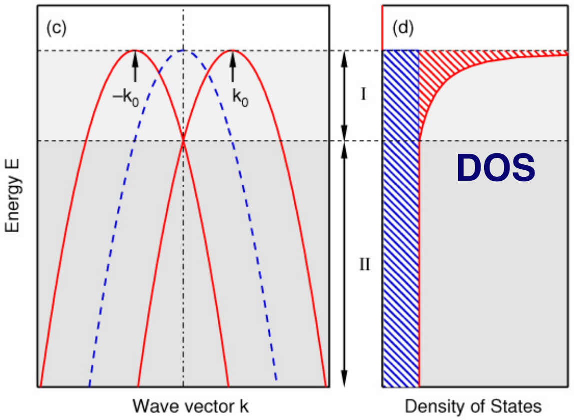
STS: MPI Stuttgart



Ast et al., Phys. Rev. B. **75**, 201401(R) (2007)

Bi/Ag(111) **Pb/Ag(111)**

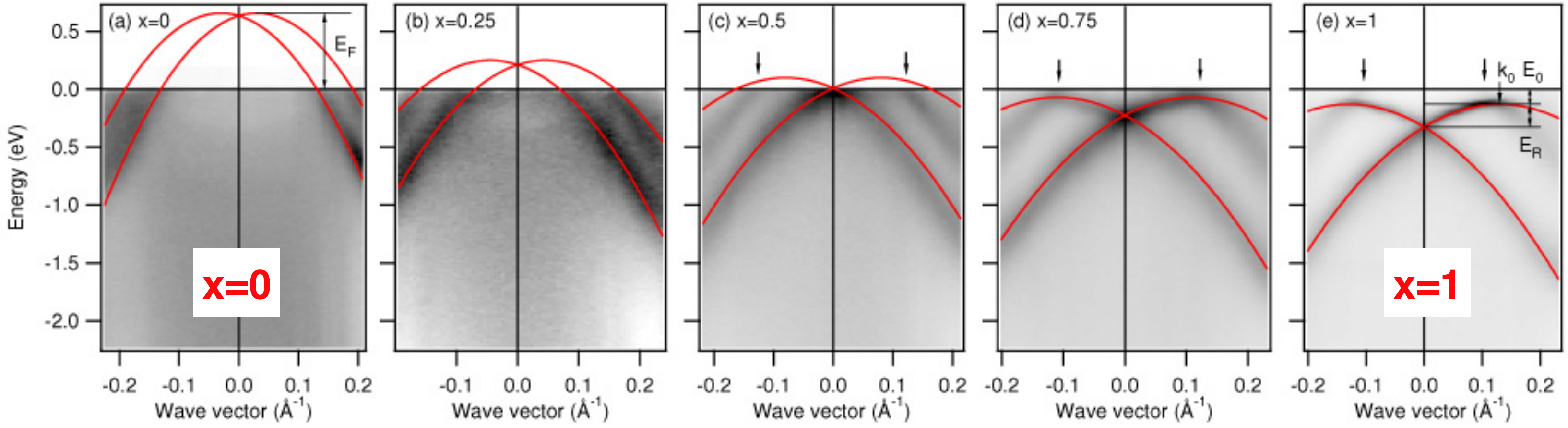




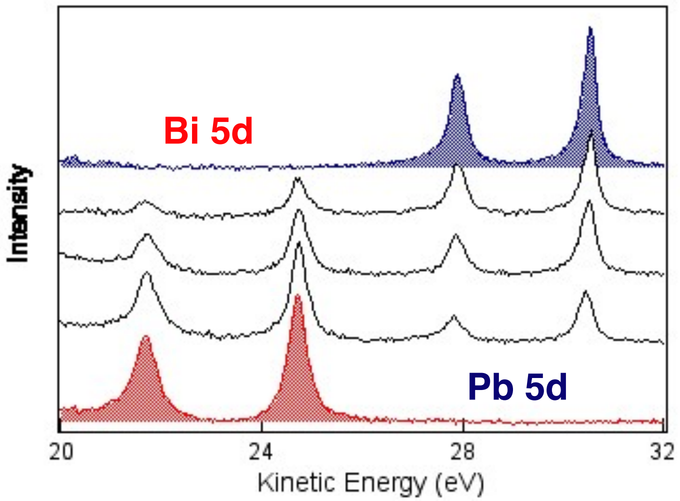
“1D-like divergence”

Chemical tuning of E_F and of the SO splitting

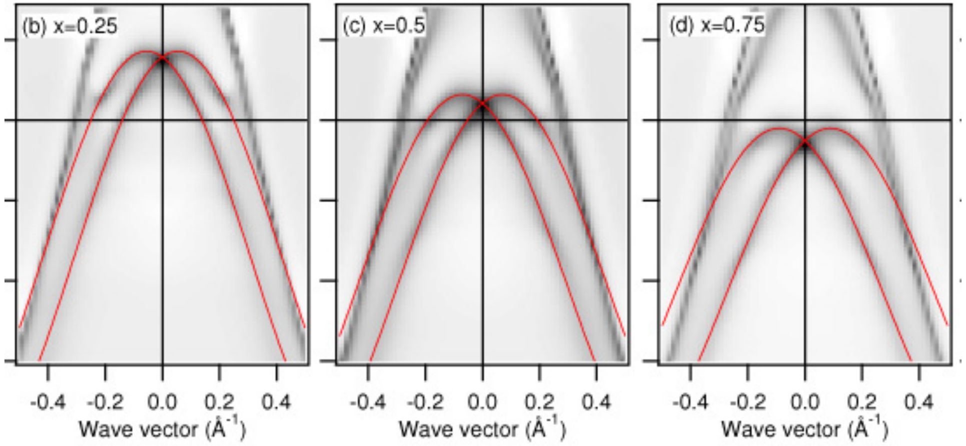
$(Bi_xPb_{1-x})Ag_2$ ordered alloys



Internal calibration from core levels



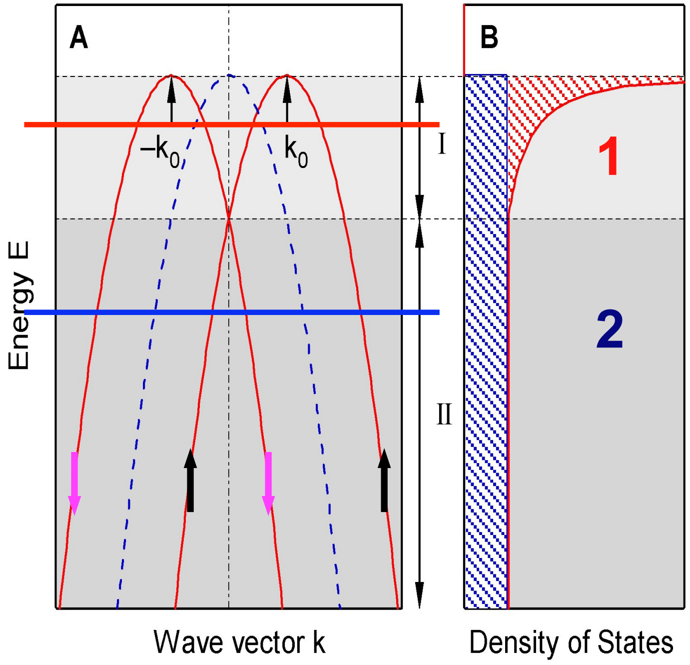
THEORY (J. Henk)



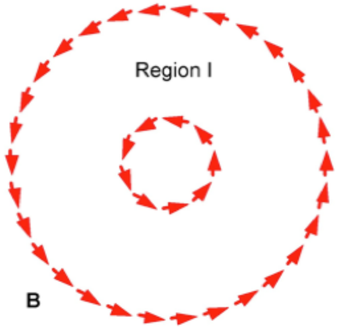
Adjusting the spin pattern by interface engineering

The spin pattern varies along the split band

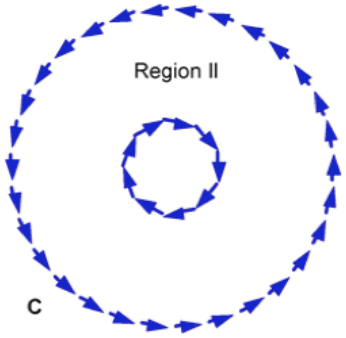
Two different situations are realized by tuning E_F through the band as a function of stoichiometry



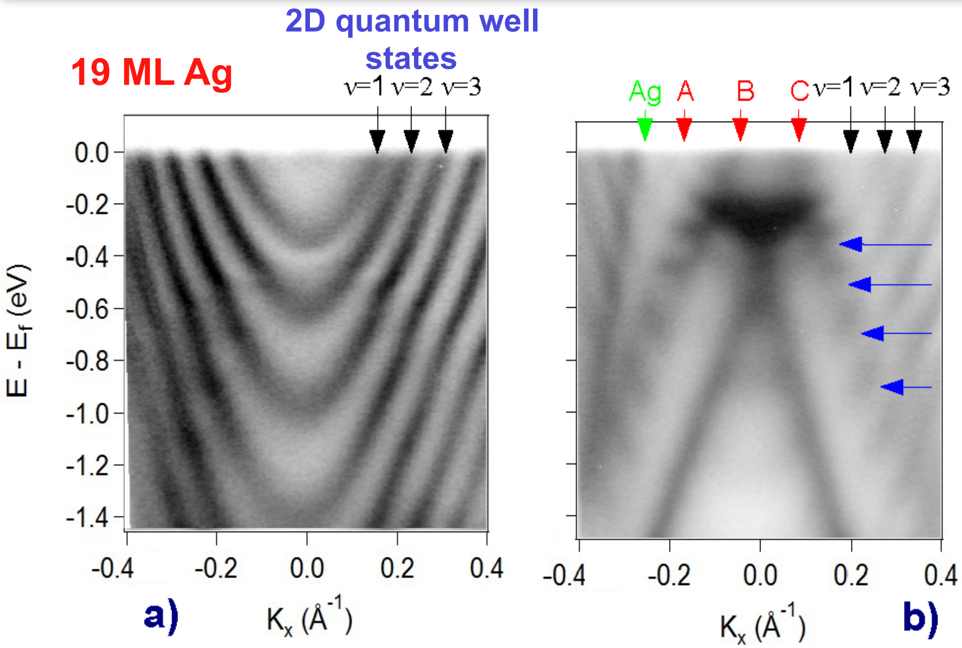
(1) chiral

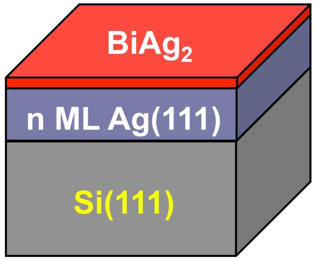


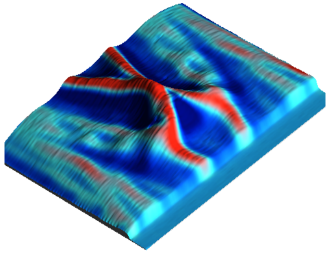
(2) non-chiral



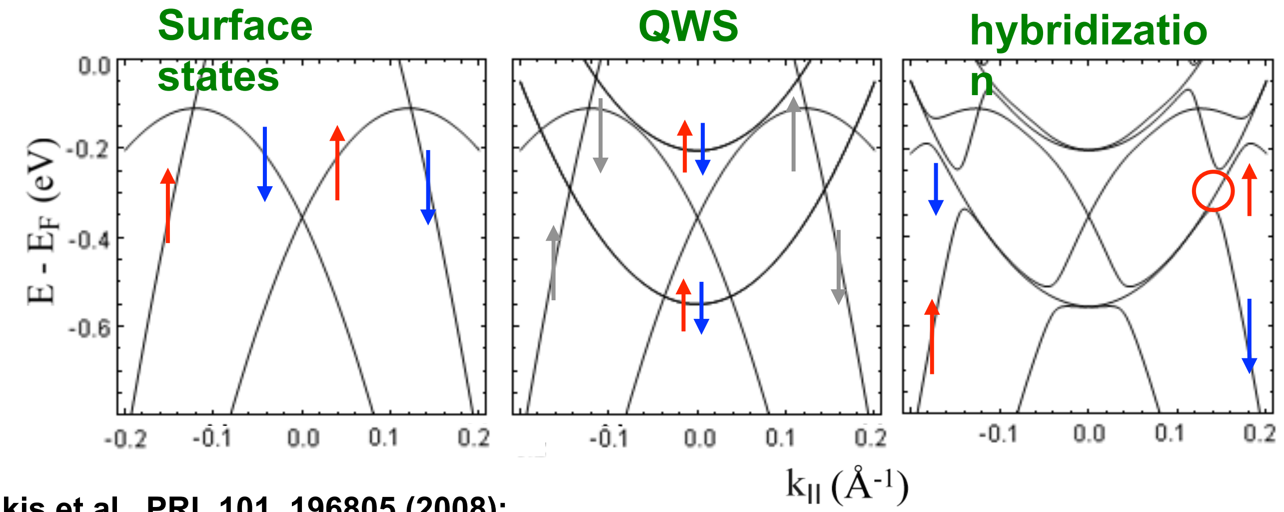
Thin Ag layer : quantum well states







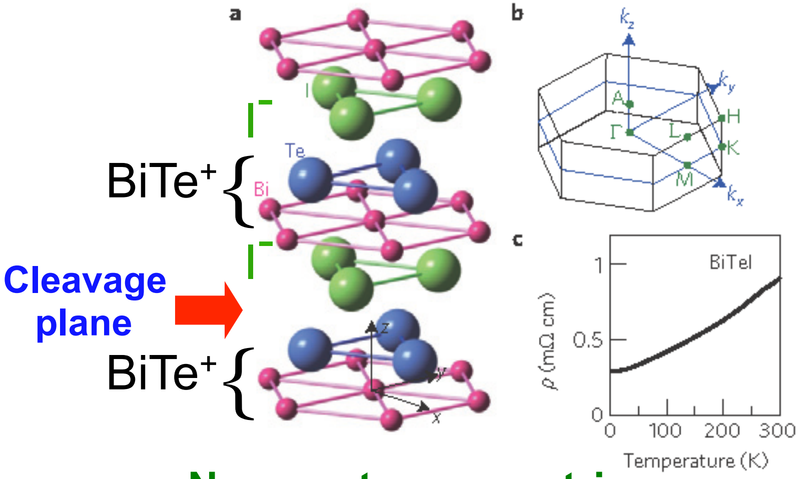
- The QWS are also spin-polarized (negligible splitting)
- Only states of same spin can hybridize
- Fully polarized states in hybridization gaps



E. Frantzeskakis et al., PRL 101, 196805 (2008);

K. He et al., PRL 101, 107604 (2008).

BiTeI: Rashba *and* Dresselhaus



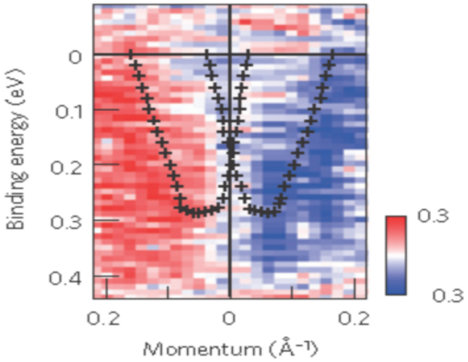
BiTe⁺{

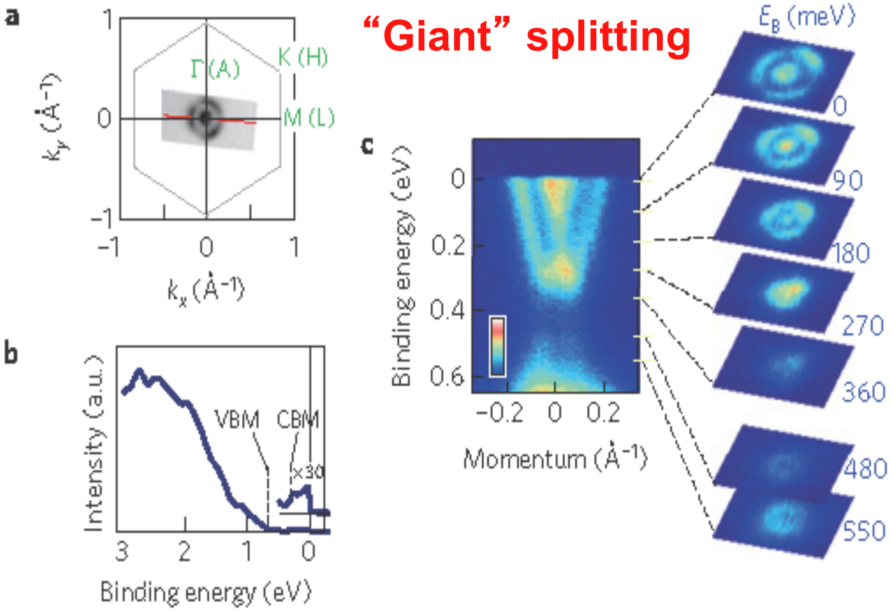
Cleavage plane

BiTe⁺{

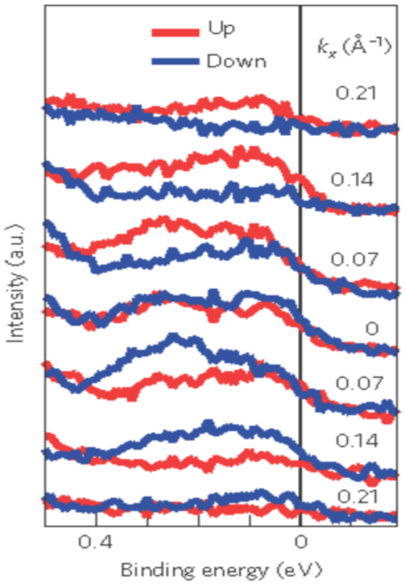
Non-centrosymmetric

SP-ARPES





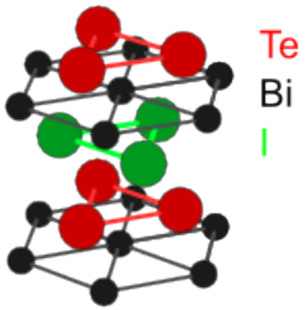
"Giant" splitting



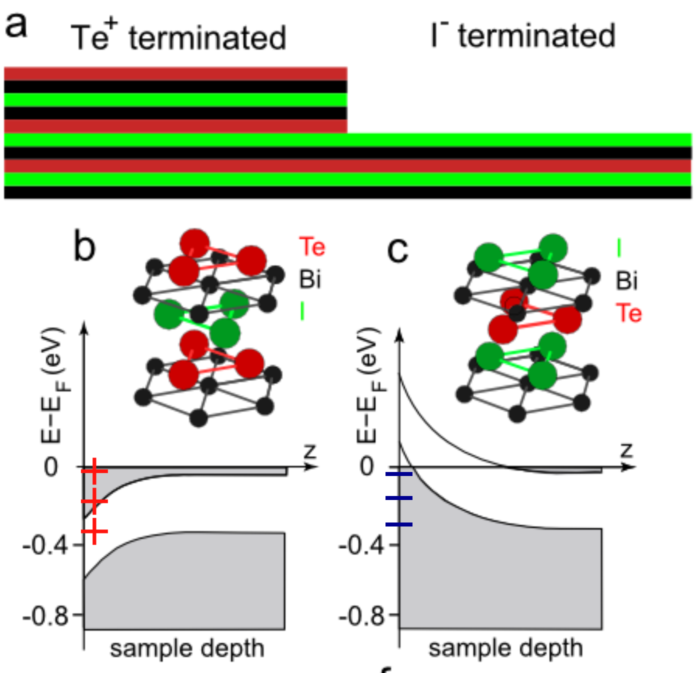
Rashba spin pattern

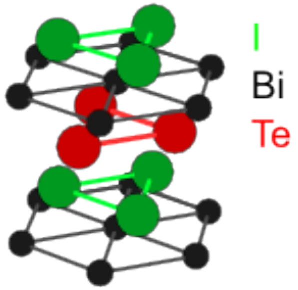
K. Ishizaka et al.,Nature Mat. **10**, 521 (2011)

More intriguing: two surface terminations



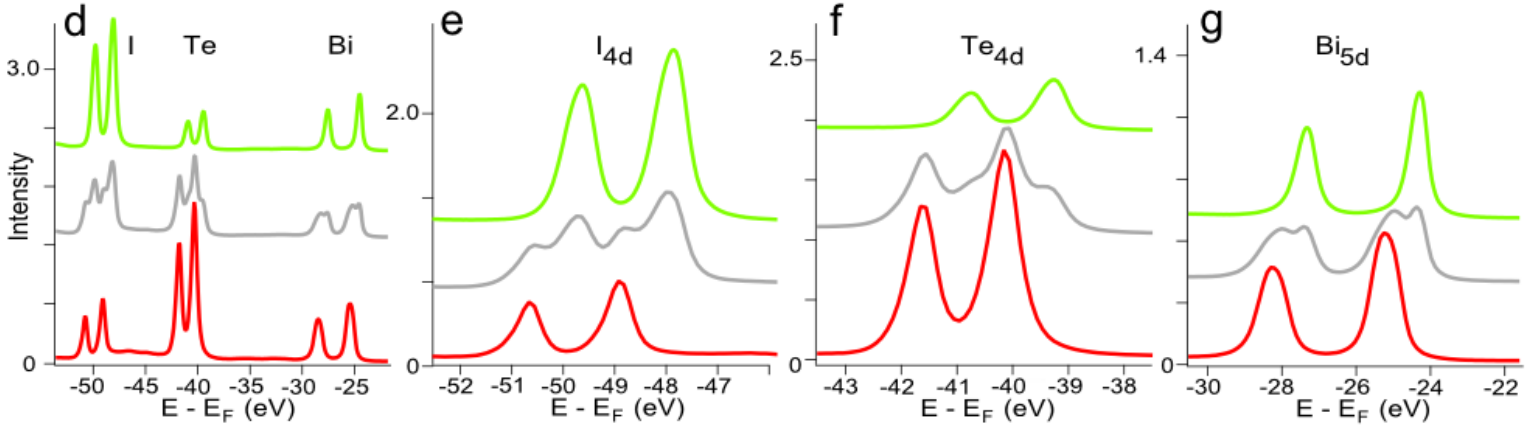
Stacking fault





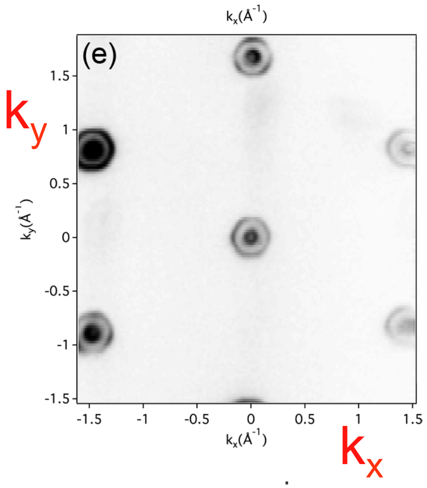
Accumulation layer

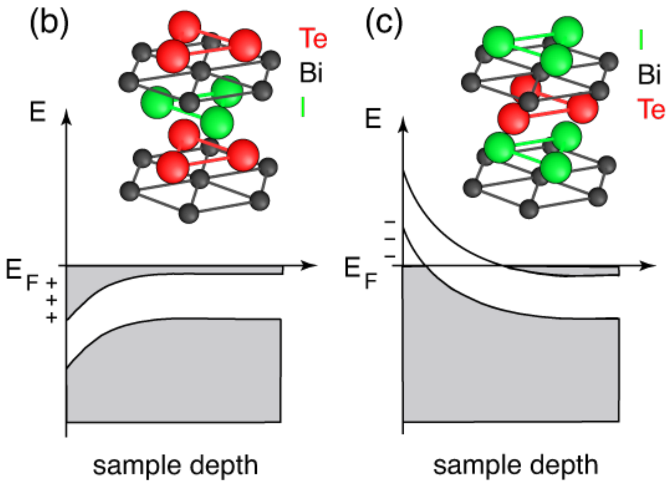
Depletion layer

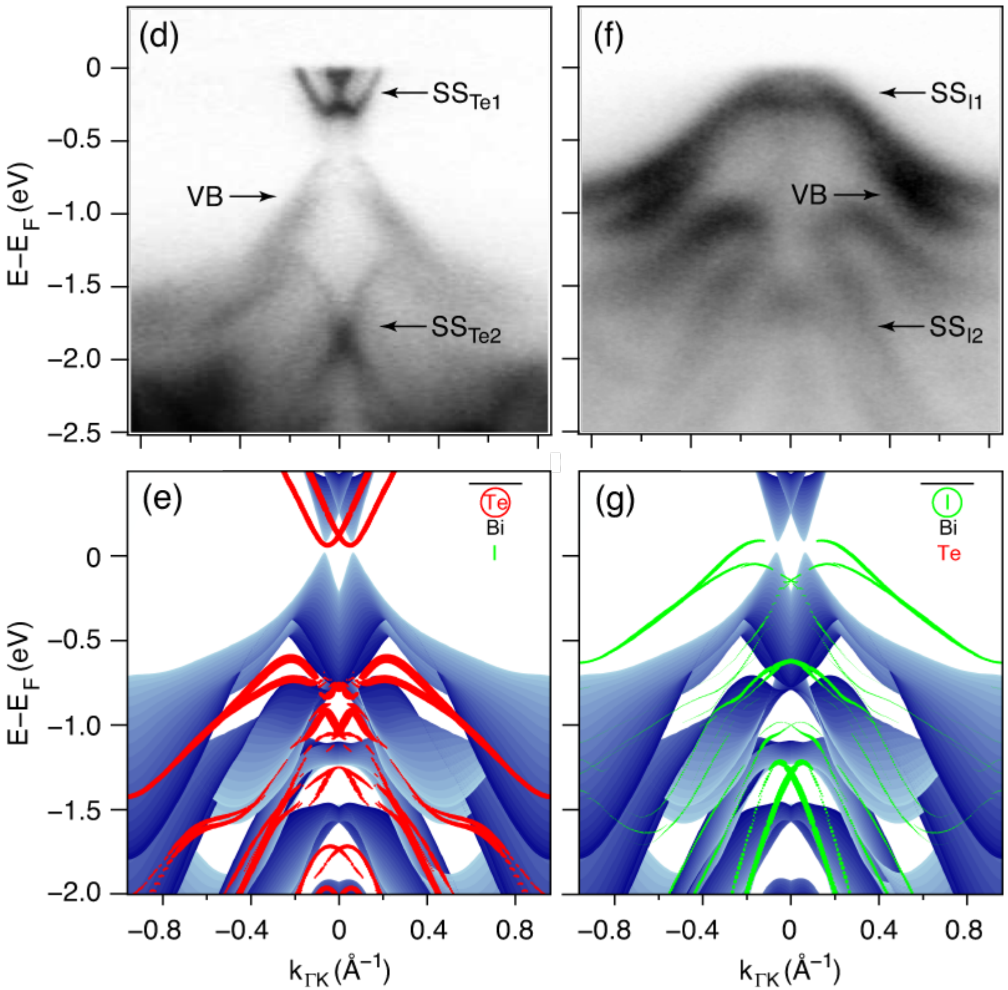


CORE LEVELS

Ambipolar Rashba effect



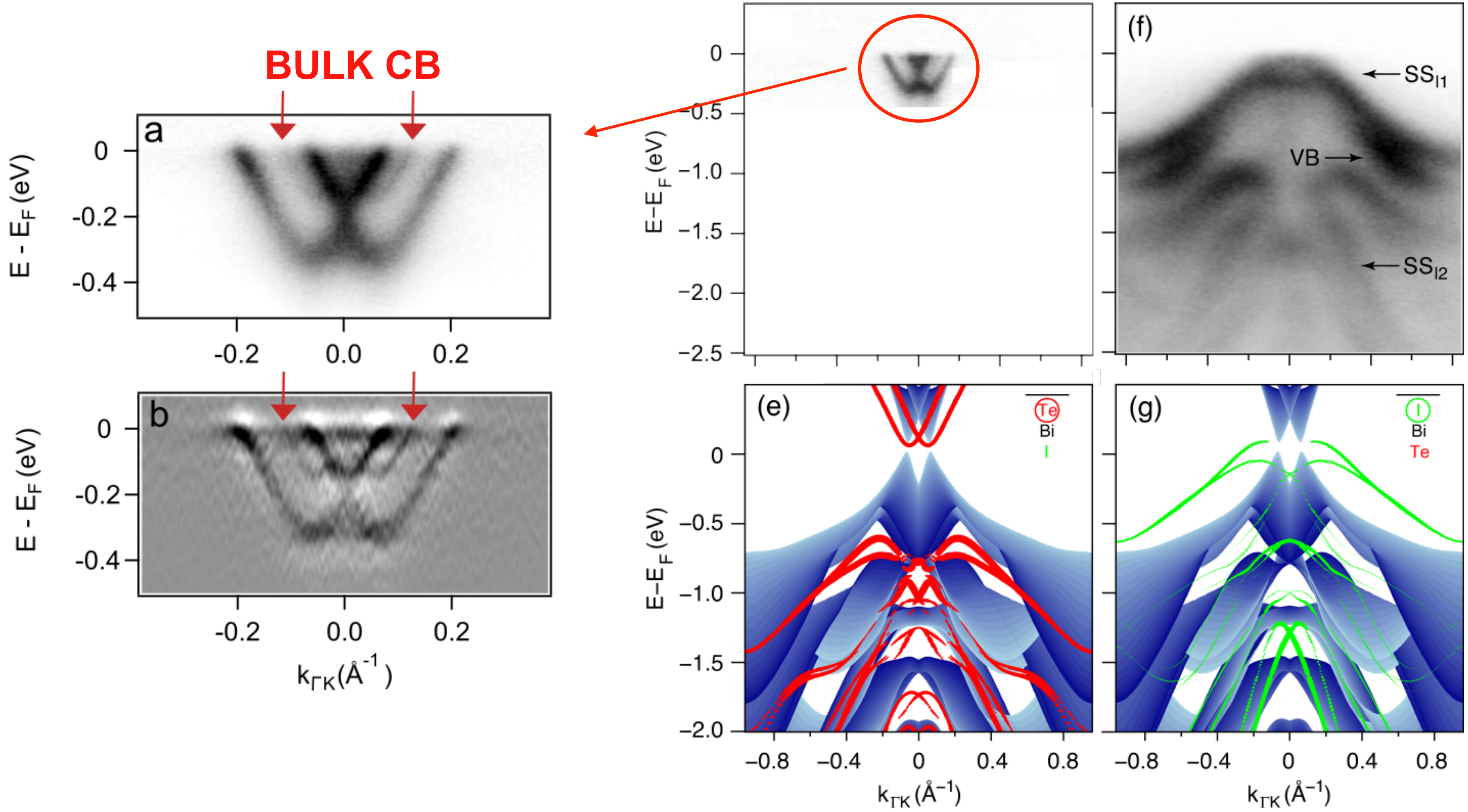




DFT + GGA (no band bending)

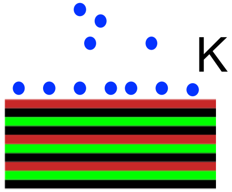
A. Crepaldi et al., PRL **109**, 096803 (2012)

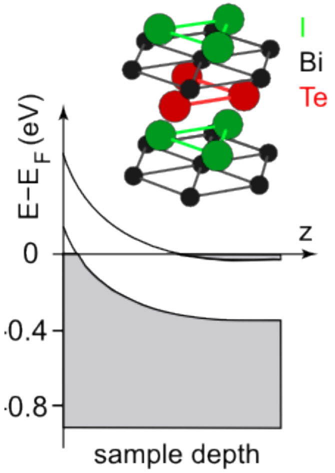
Surface AND bulk states



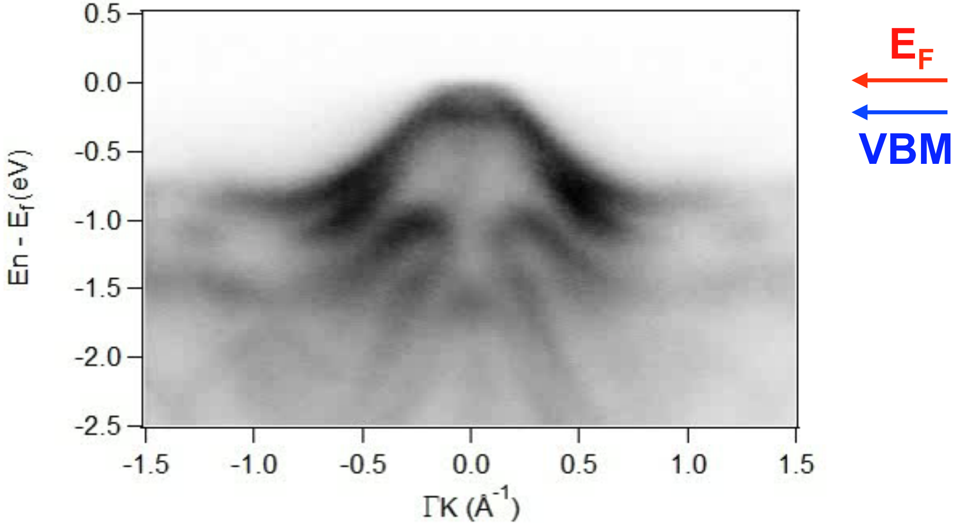
BULK CB

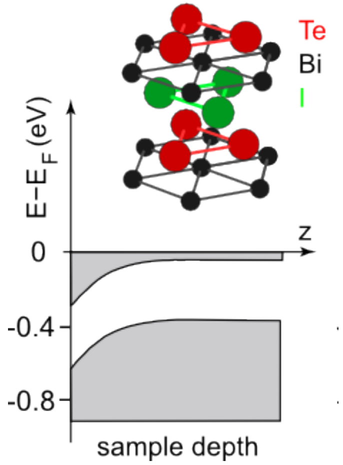
Tuning the band bending by surface doping

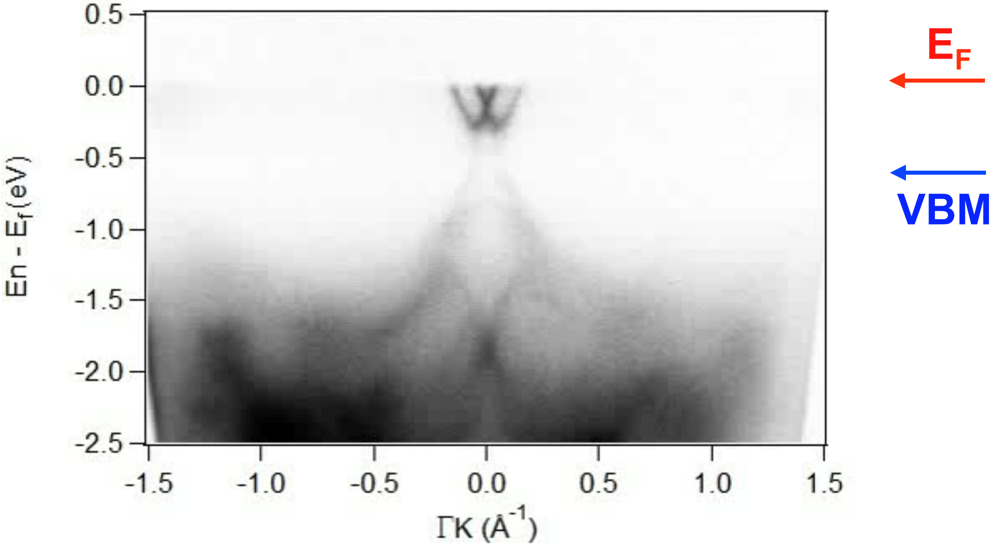




K doping

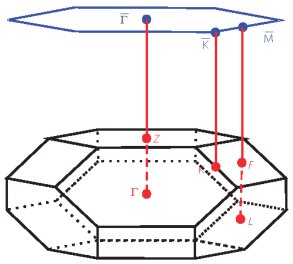


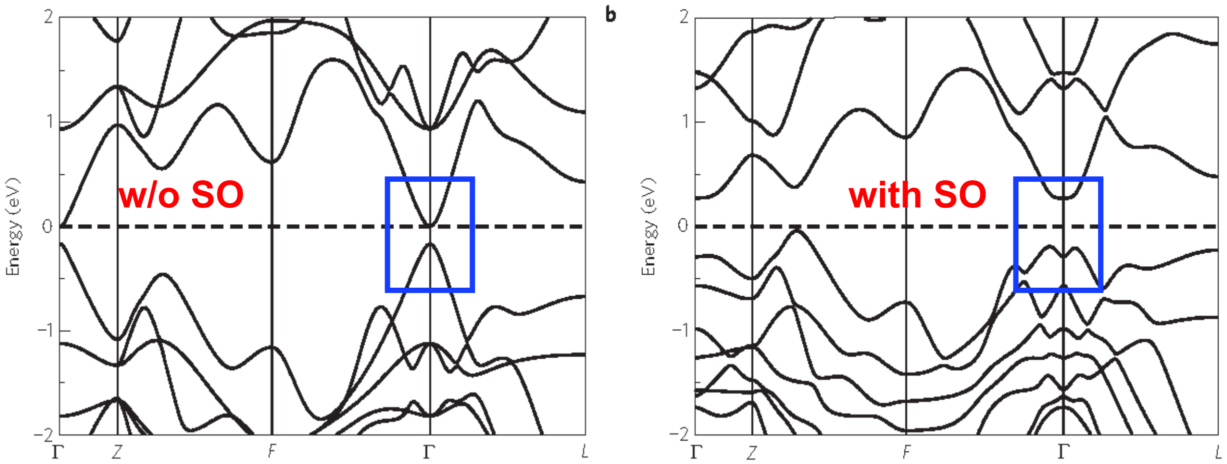




The SO interaction switches bands around the gap

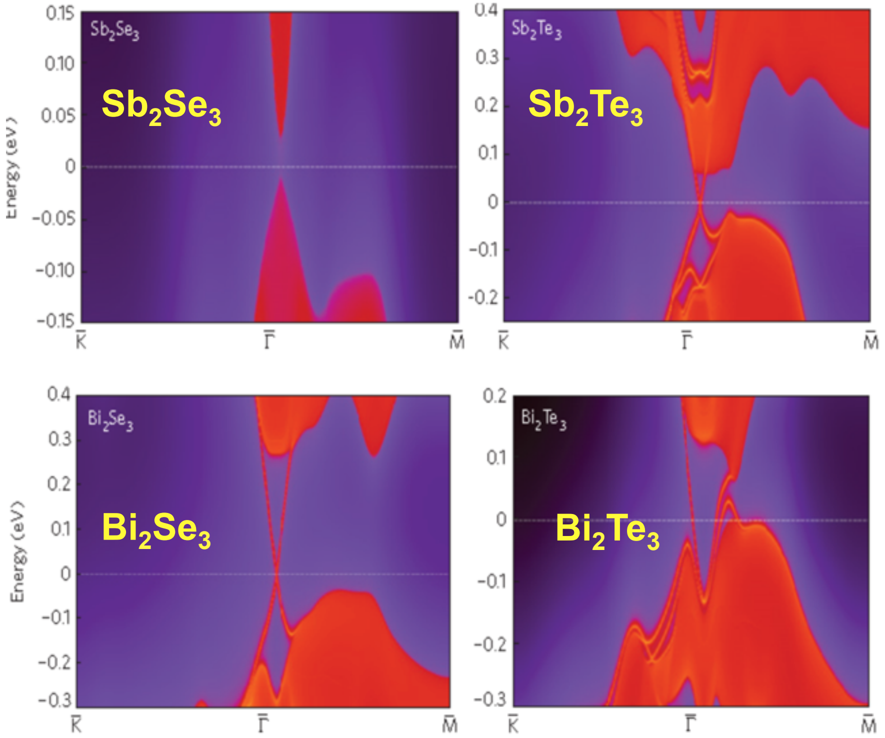
Bi_2Se_3





Sb_2Se_3	+ − + − + − + − + − + − − −; +	(+)
Sb_2Te_3	+ − + − + + − + − + − − − +; −	(−)
Bi_2Se_3	+ − + − + − + − + − + − − +; −	(−)
Bi_2Te_3	+ − + − + − + + − + − − − +; −	(−)

parity switching



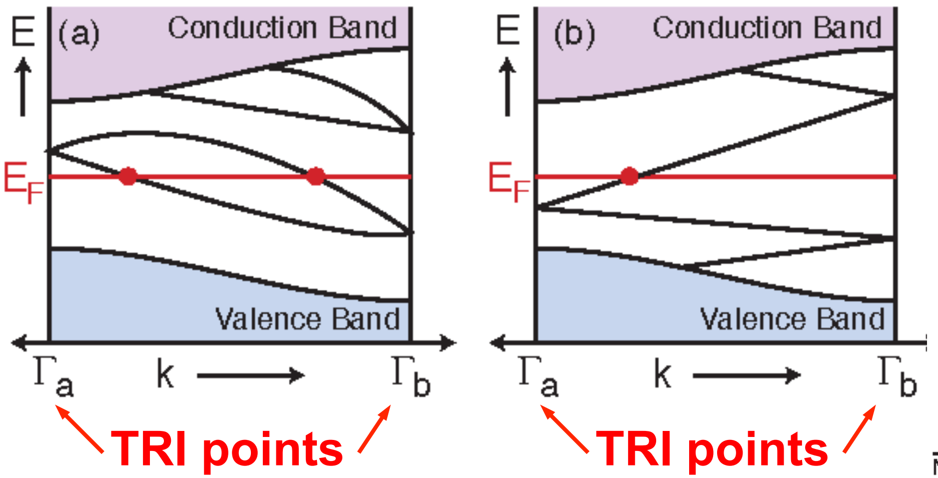
H. Zhang et al., Nature Phys. **5**, 438 (2009)

“Edge states” in 3D insulators

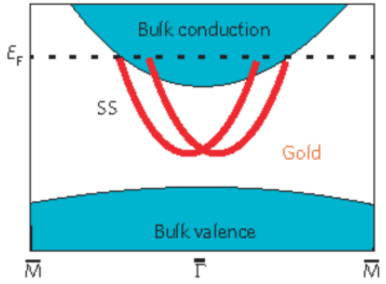
“Trivial” and topological insulators differ in a topologically invariant quantity (related to the symmetry properties of the wavefunctions)

Surface states:partner switching

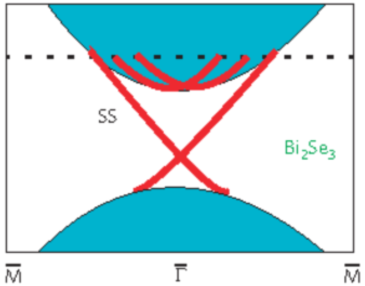
Trivial **Non-trivial**



TRI points **TRI points**



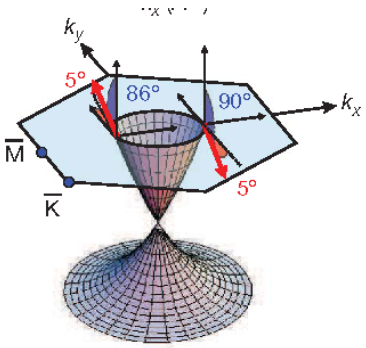
Au(111) - trivial



Bi_2Se_3

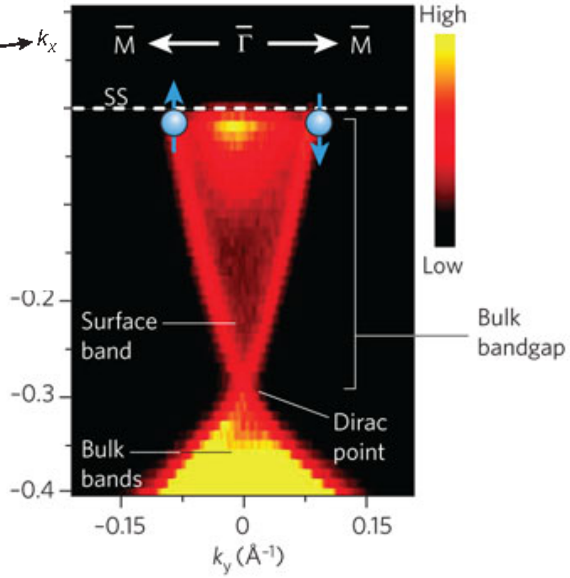
“Something” must happen at the Interface between a non-trivial and a trivial (e.g. the vacuum) insulator

Metallic states appear at the surface

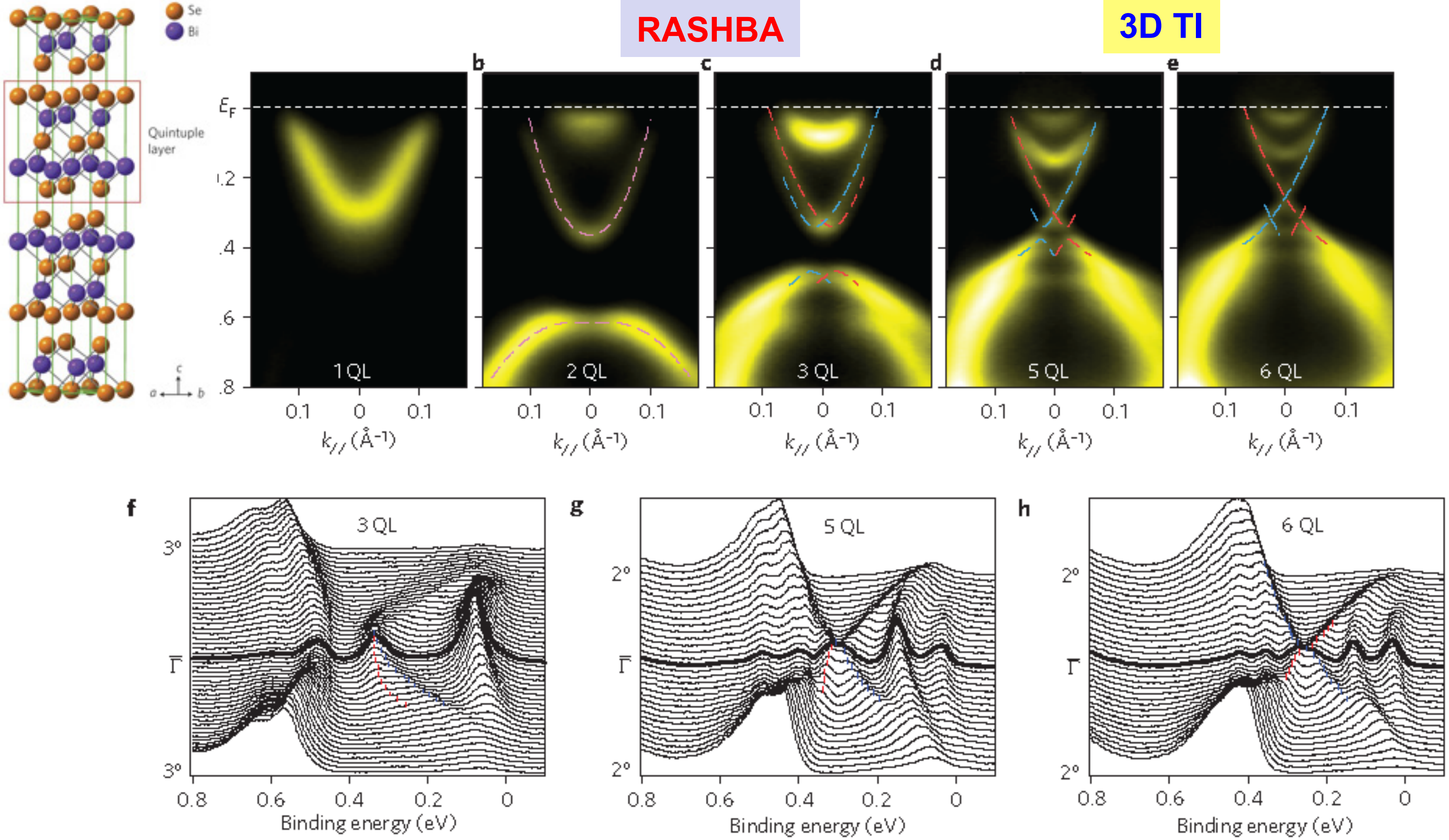


A single Dirac cone

Bi_2Se_3



Bi_2Se_3 thin films: from Rashba to TI layer-by-layer

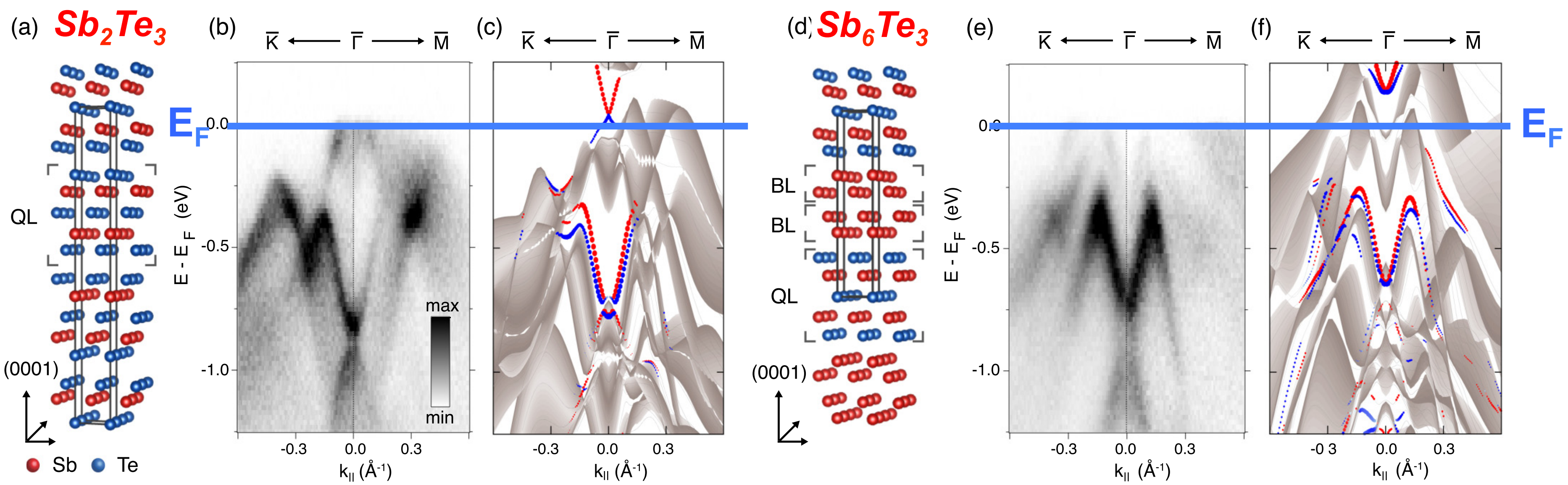


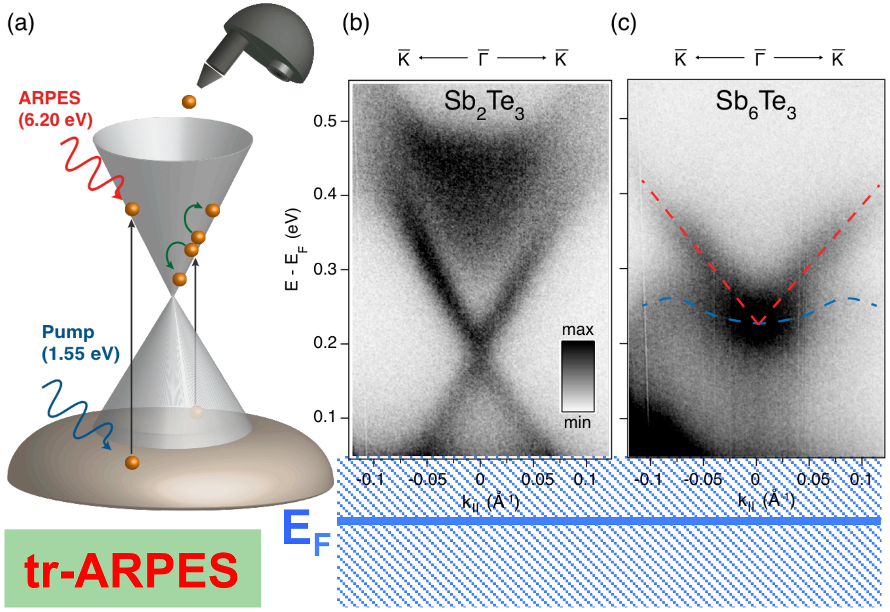
RASHBA

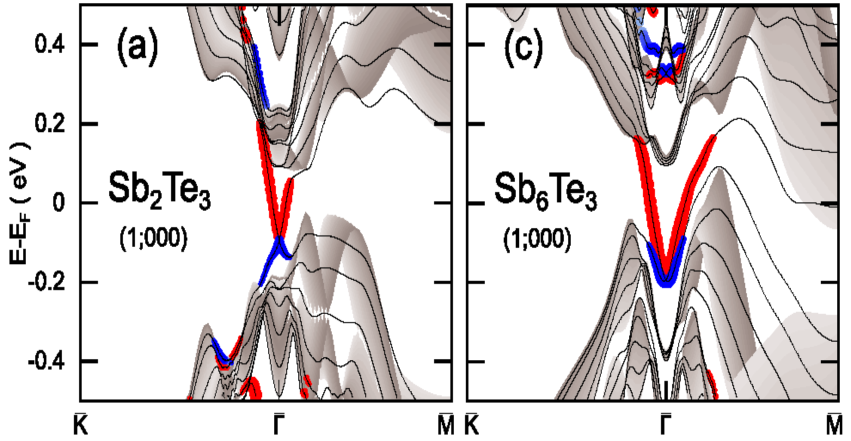
3D TI

Yi Zhang et al., Nature Phys. **6**, 584 (2010)

Pumping electrons into the empty states: tr-ARPES

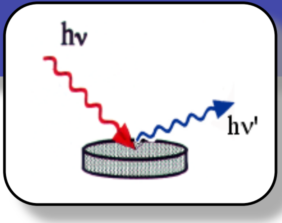




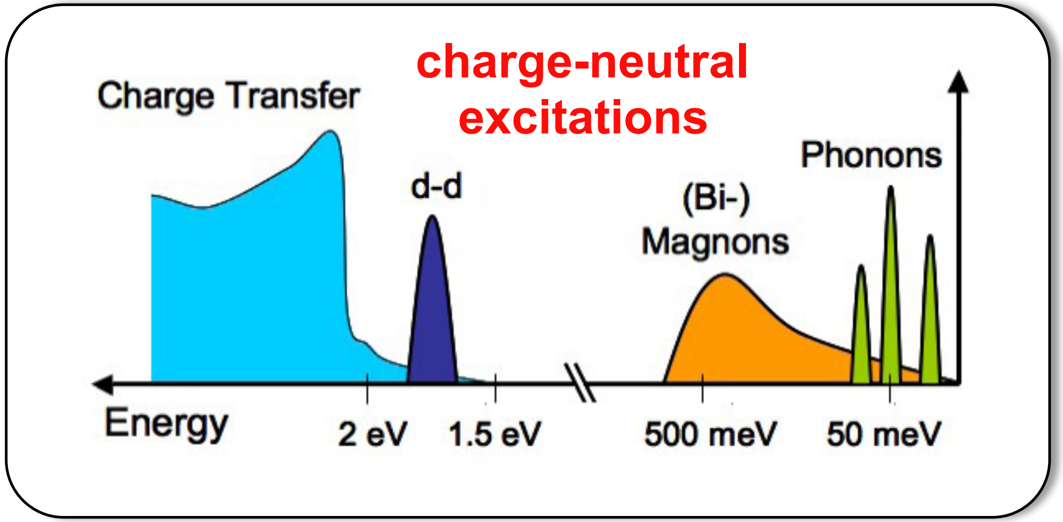


Johannsen et al., PRB **91**, 211001 (2015)

RIXS: optics...with a twist



RIXS probes multiple energy scales



Chemical selectivity from core hole, but the final state has no core hole → high resolution

q dependence

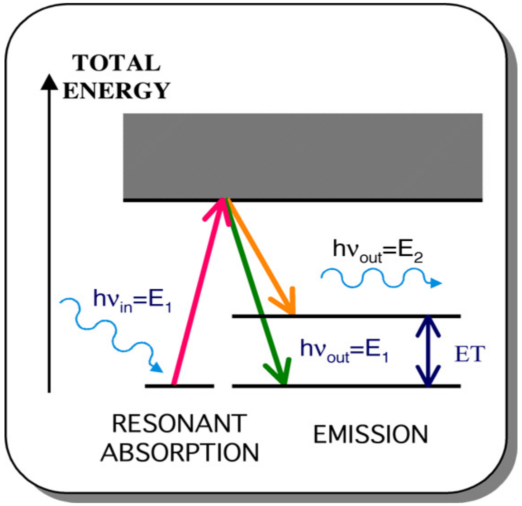
Photon in - photon out: OK for insulators; external fields

Sensitive to spin excitations

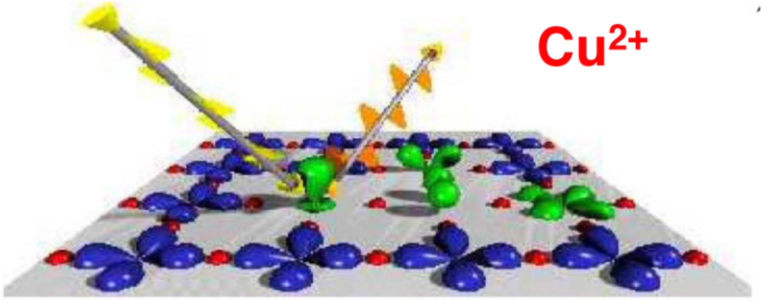
Ament et al., (2011)

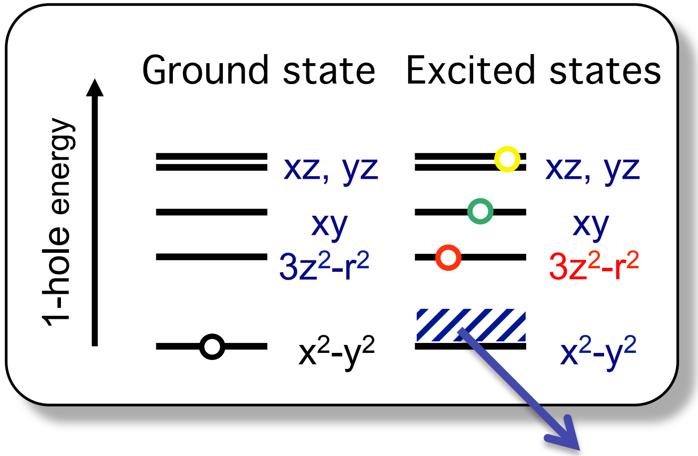
RIXS: Raman with x-rays

$L_{2,3}$ edges 2p → 3d ; directly probes the *d* states

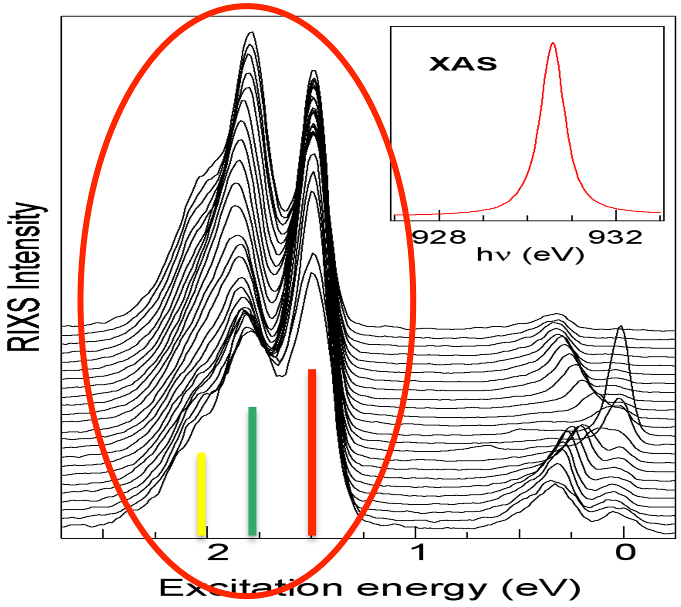


$3d^9 \rightarrow 2p^5 3d^{10} \rightarrow (3d^9)^*$





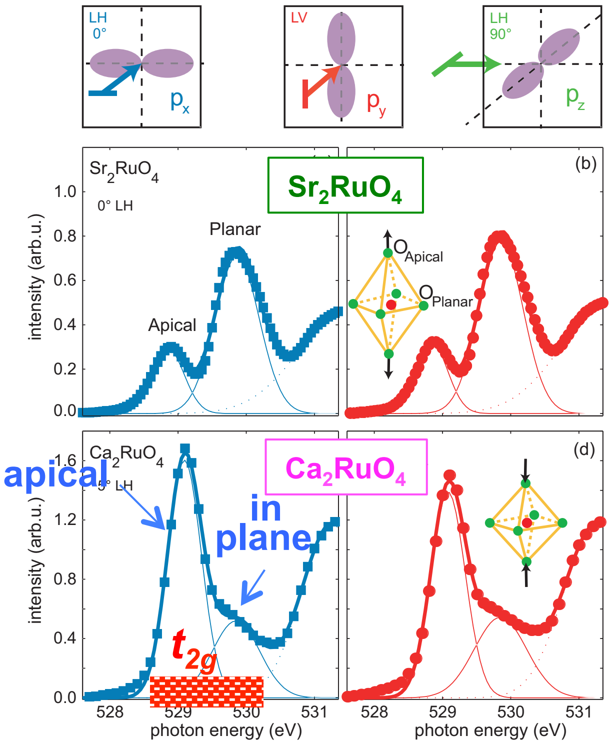
Collective excitations

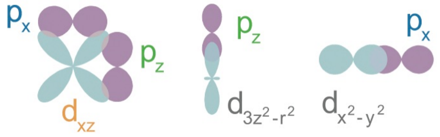


Ruthenates...again – RIXS probes inter-t_{2g} excitations

Fatuzzo et al., PRB (2015)

O 1s XAS



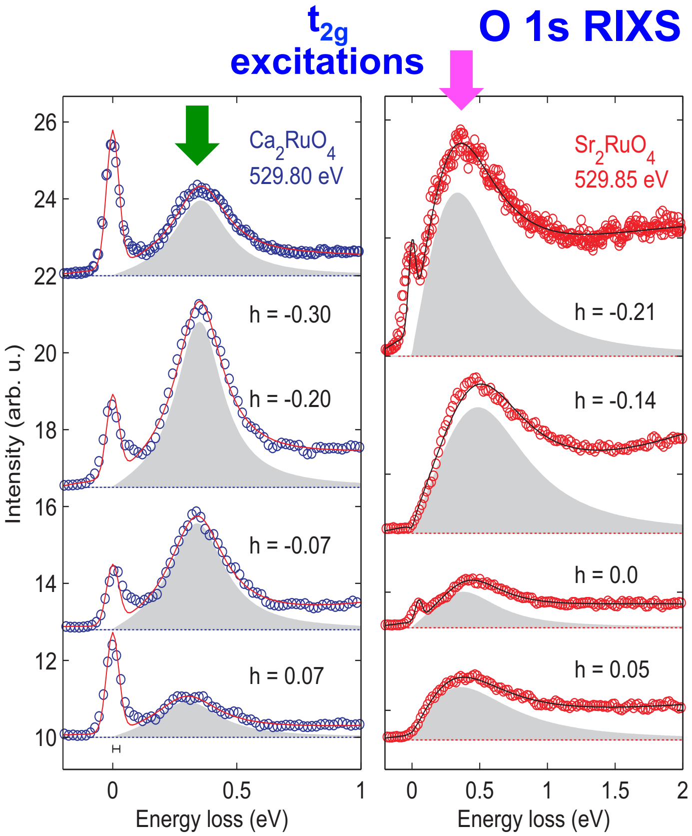


in-plane:

p_x → xy ; p_y → xy ; p_z → xz, yz

Apical:

p_x → xz ; p_y → yz

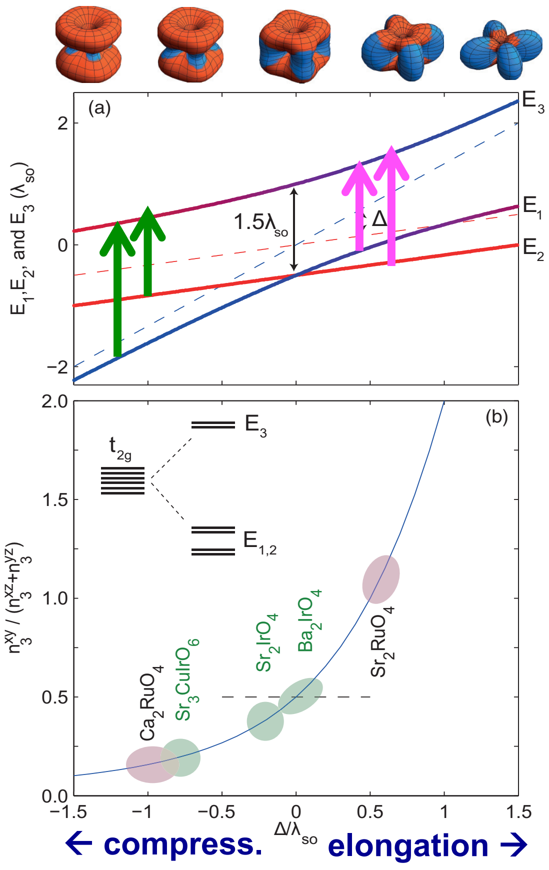


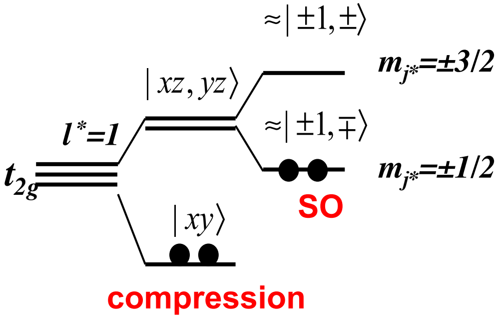
XAS → $n^{xy}/(n^{xz}+n^{yz})$

Model → Δ/λ_{SO}

RIXS → Δ; λ_{SO}

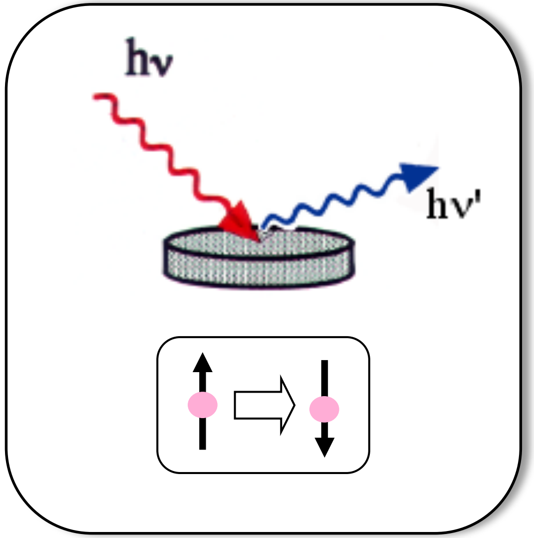
λ_{SO}=200 meV (both)





Low-energy excitations: spin flips

Photons do not couple directly to spins, but…



$3d^9 \rightarrow 2p^5 3d^{10} \rightarrow (3d^9)^*$

↓

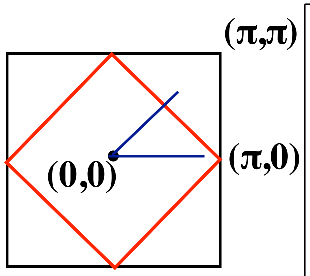
$\Delta E_{SO}(2p) \sim 20$ eV

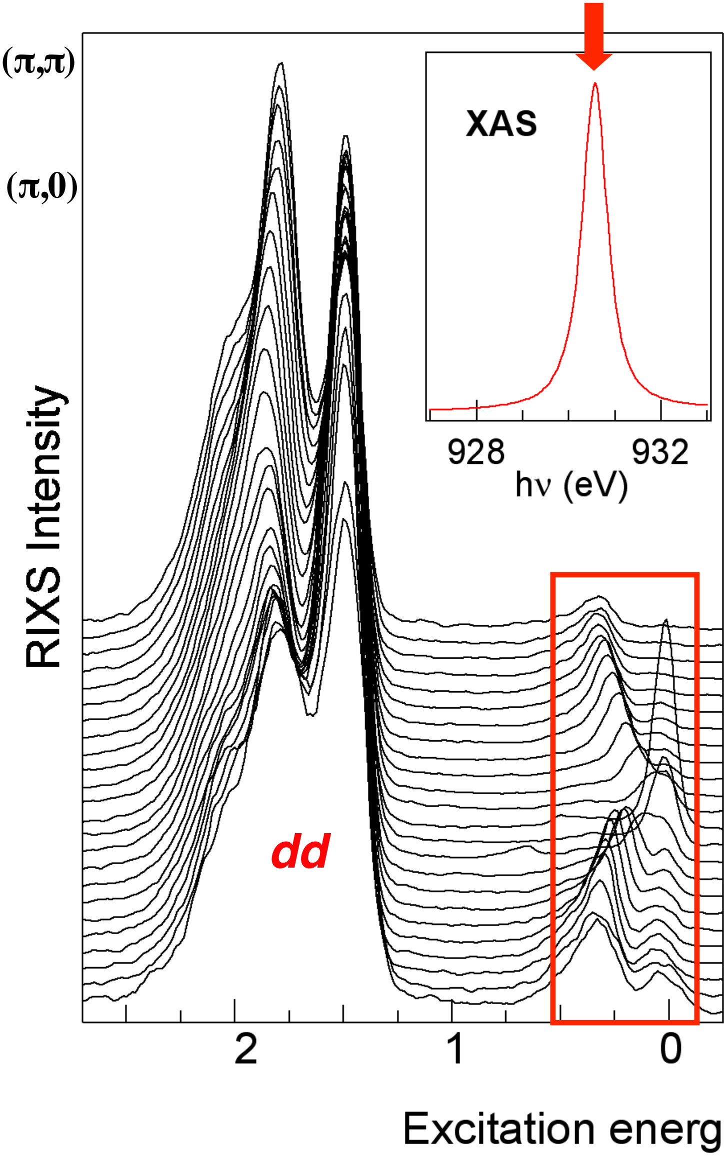
- F.M.F. De Groot et al., PRB 57, 14 548 (1998)
- LJP Ament et al., PRL 103, 117003 (2009)
- MW Haverkort, PRL 105, 167404 (2010)
- T. Nagao and J. Igarashi, PRB 85, 224436 (2012)

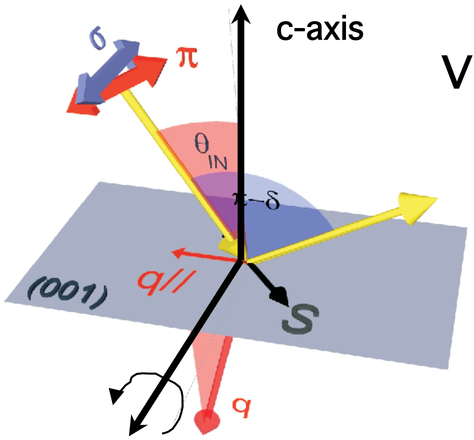
Spin-orbit is large in the intermediate state.
S is not a good quantum number
$\Delta S_z \neq 0$ transitions are possible !

→ **One flipped spin NOT an eigenstate for the solid: dispersion**

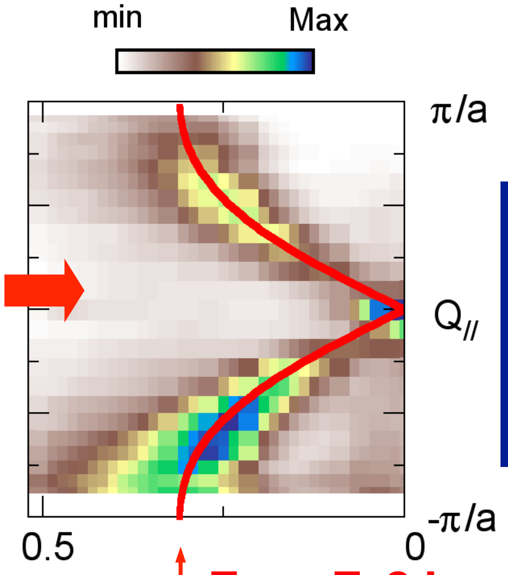
Magnons in a 2D S=1/2 Heisenberg AF: Sr$_2$CuO$_2$O$_2$







Variable in-plane projection $q_{||}$



(100) direction

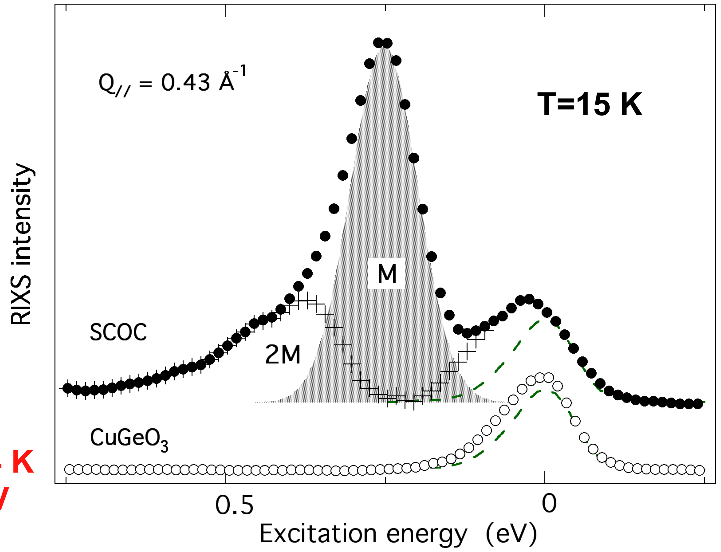
Magnon dispersion

Heisenberg model
J=140 meV

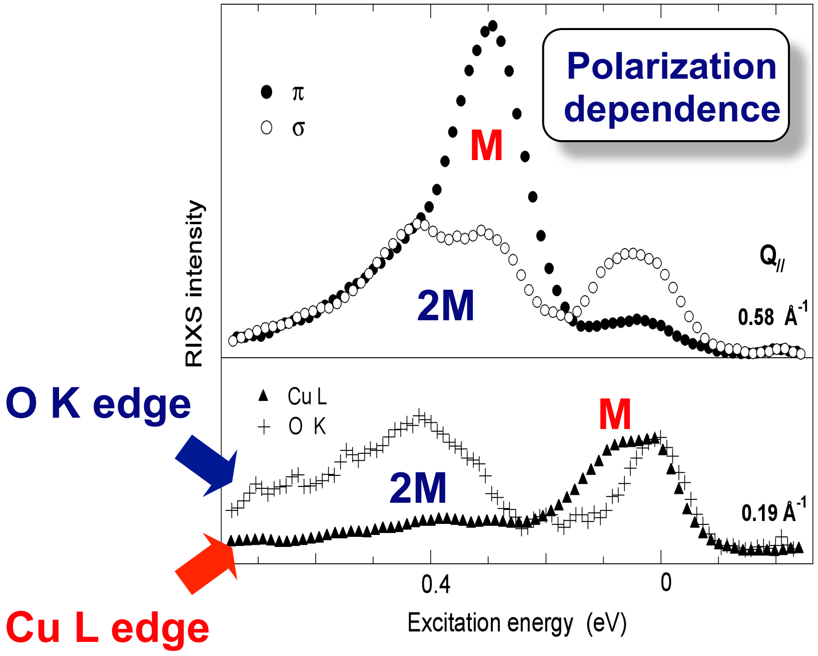
$E_{max}=Z_C 2J$

$Z_C=1.18$

Line shape analysis of the magnetic excitations

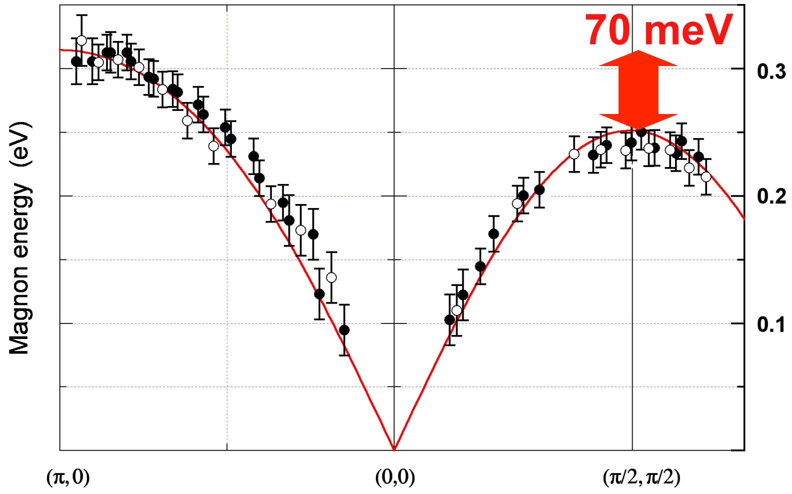


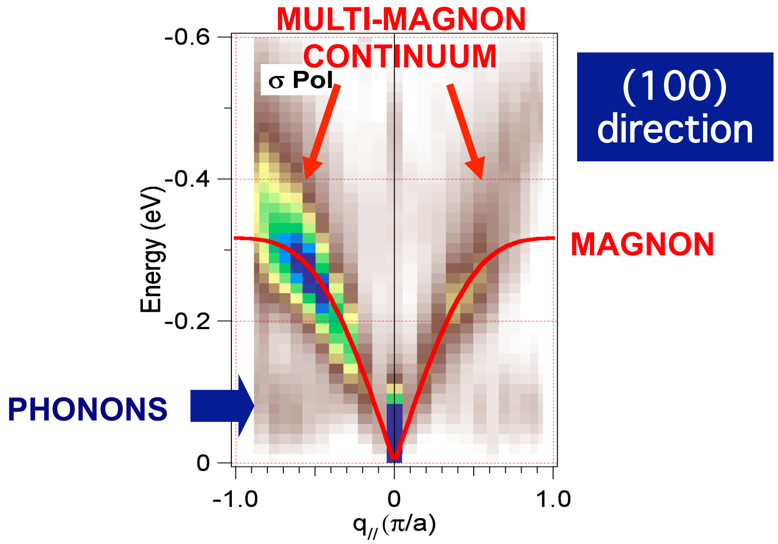
CuGeO$_3$
T_{SDW}=14 K
J=5 meV



O K edge

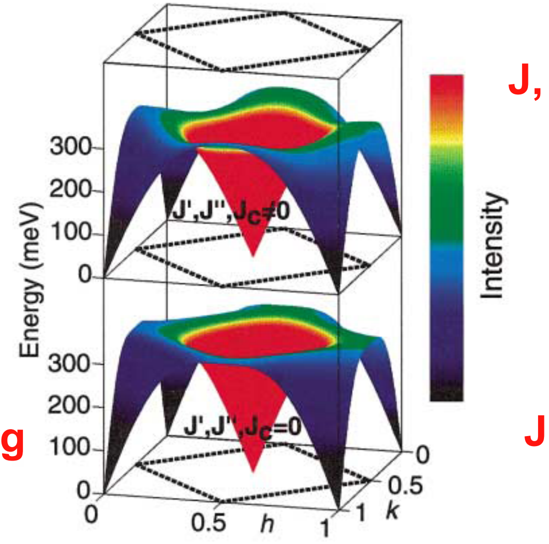
Cu L edge





Large dispersion along AFM BZ boundary

MBZ boundary dispersion: why is it interesting ?

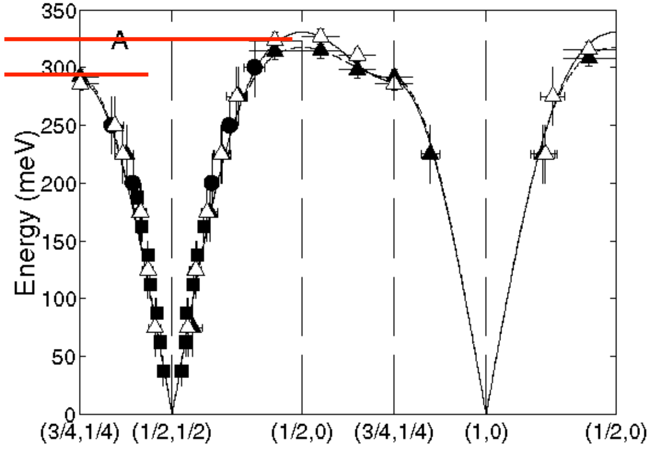


J, J', J'', J_c

J

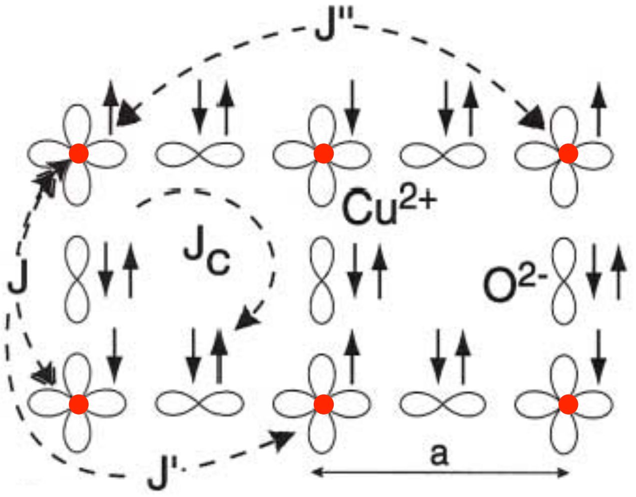
Heisenberg model

La_2CuO_4 - neutrons



20 meV

Dispersion along MBZ boundary is due to exchange interactions beyond NN



Notice: sub-mm samples !

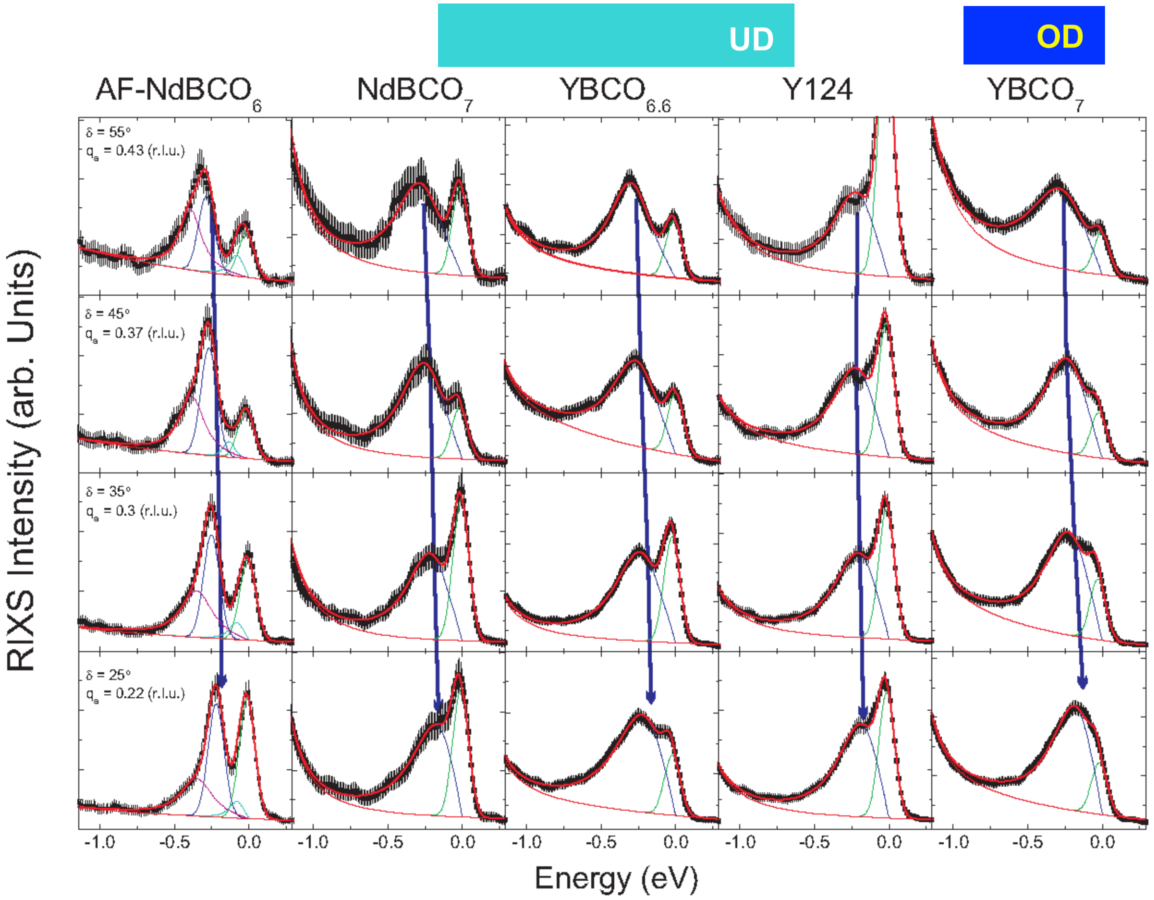
R. Coldea et al., PRL 86, 5377 (2001); N.S. Headings et al., PRL 105, 247001 (2010)

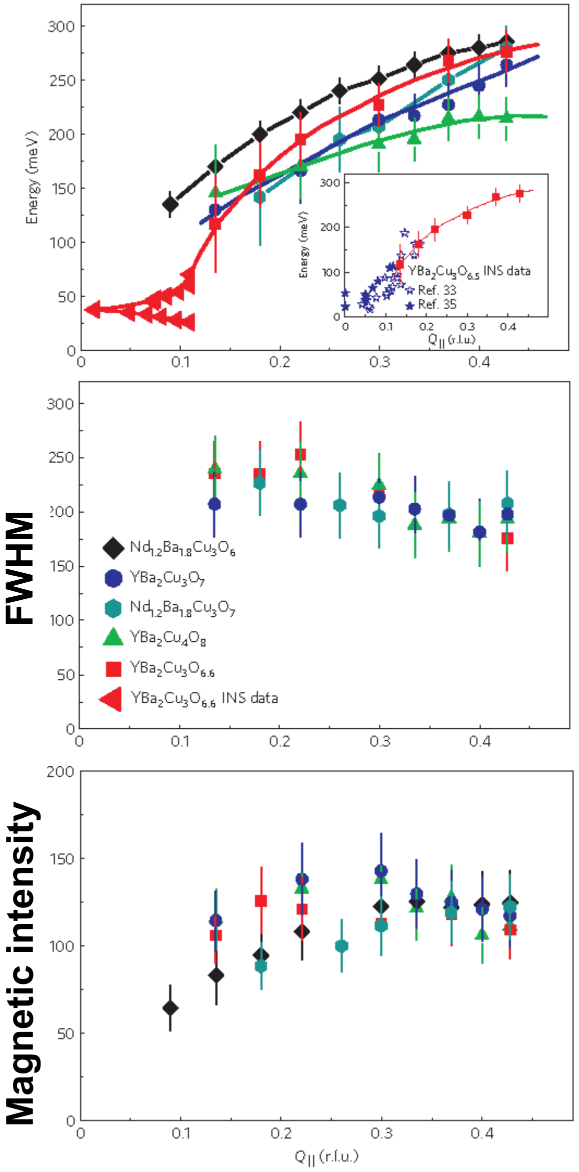
Paramagnons in the doped cuprates

Intense paramagnon excitations in a large family of high-temperature superconductors

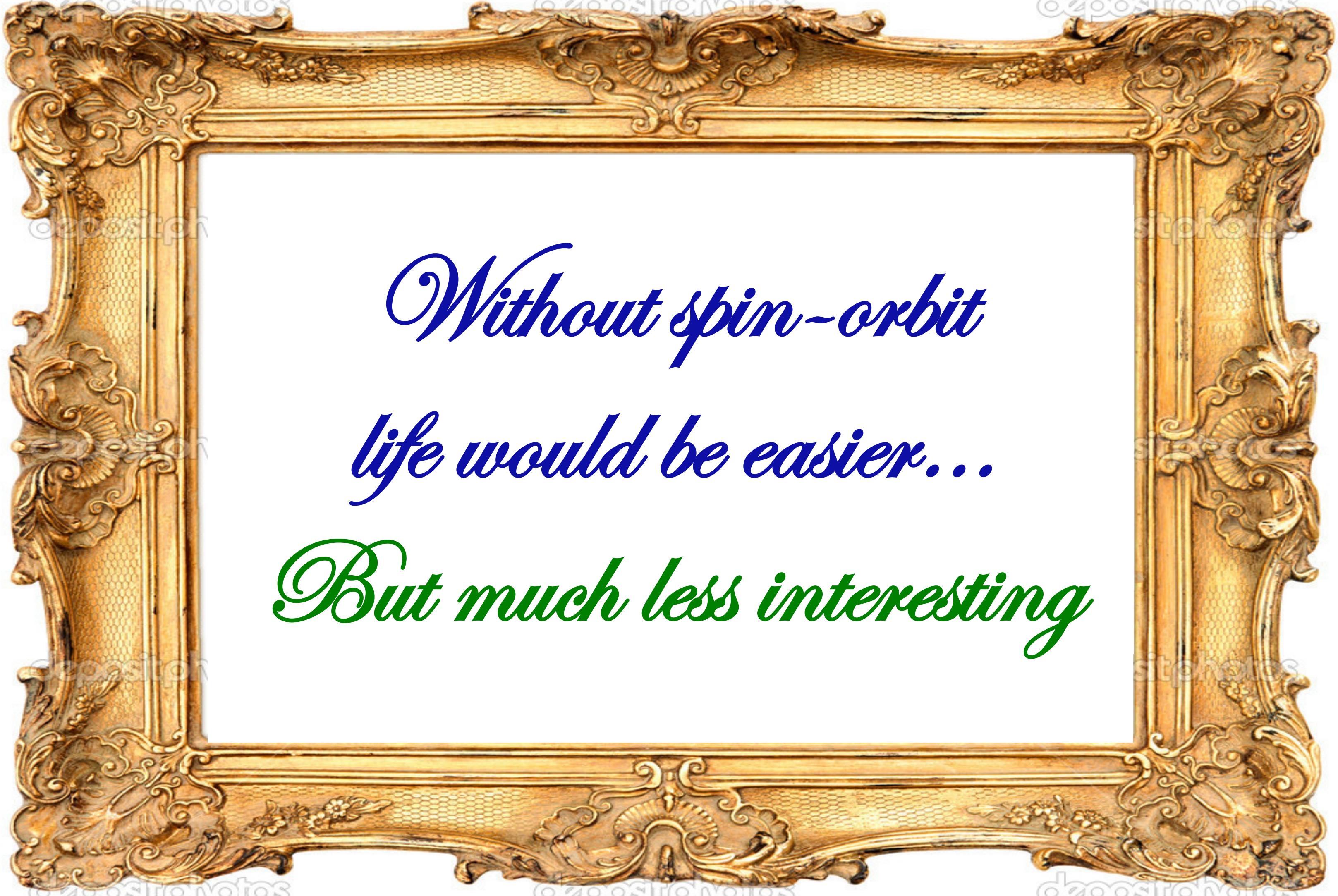
M. Le Tacon[1]*, G. Ghiringhelli[2], J. Chaloupka[1], M. Moretti Sala[2], V. Hinkov[1,3], M. W. Haverkort[1], M. Minola[2], M. Bakr[1], K. J. Zhou[4], S. Blanco-Canosa[1], C. Monney[4], Y. T. Song[1], G. L. Sun[1], C. T. Lin[1], G. M. De Luca[5], M. Salluzzo[5], G. Khaliullin[1], T. Schmitt[4], L. Braicovich[2] and B. Keimer[1]*

NATURE PHYSICS | VOL 7 | SEPTEMBER 2011





Conclusion



Without spin-orbit

life would be easier…

But much less interesting

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U. Fano, Phys. Rev. **178**, 131 (1969).

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B.T. Thole and G. van der Laan, Phys. Rev. Lett. **67**, 3306; Phys. Rev. B **44**, 12424 (1991)

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C. De Nadai et al., Phys. Rev. B **70**, 134409(2004)

C.N. Veenstra et al., Phys. Rev. Lett. **112**, 127002 (2014)

S. Moser et al., N. J. Phys. **16**, 013008 (2014)

Y. A. Bychkov and E. I. Rashba, JETP Lett. **39**, 78 (1984)

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C.R. Ast et al., Phys. Rev. Lett. **98**, 186807 (2007)

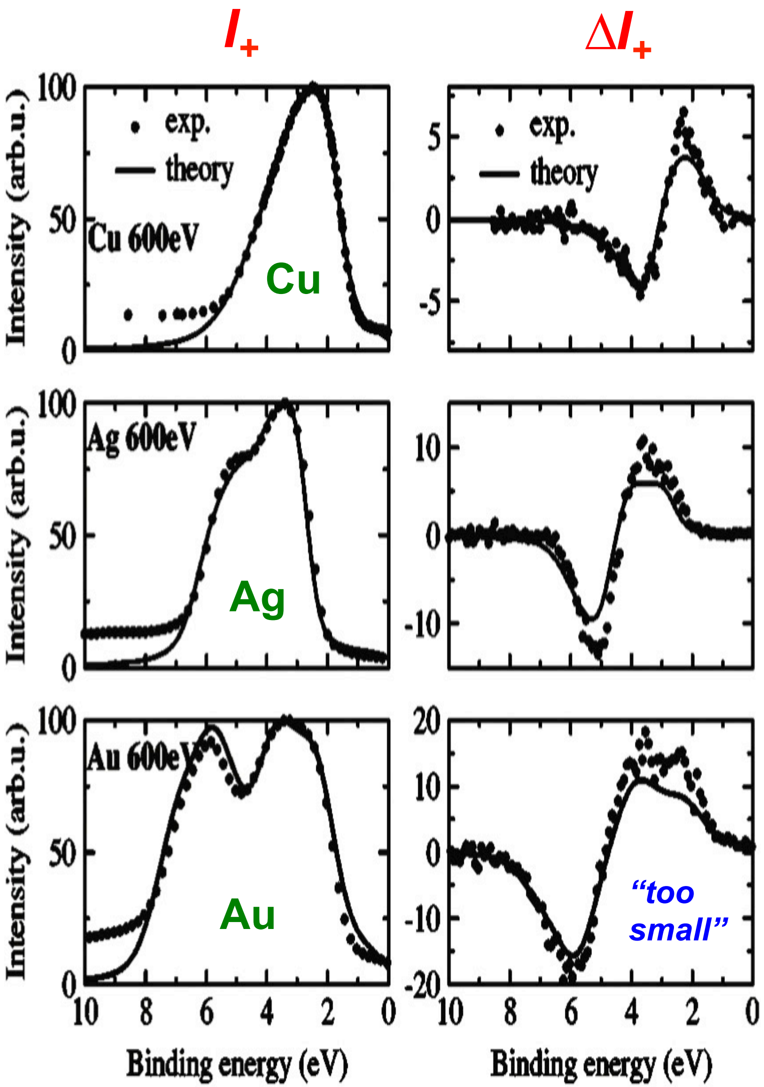
L.J.P. Ament et al., Rev. Mod. Phys. **83**, 705 (2011)

F.M.F. De Groot et al., Phys. Rev. B **57**, 14 548 (1998)

M. Guarise et al., Phys. Rev. Lett. **105**, 157006 (2010)

M. Le Tacon et al., Nat. Phys. **7**, 725 (2011)

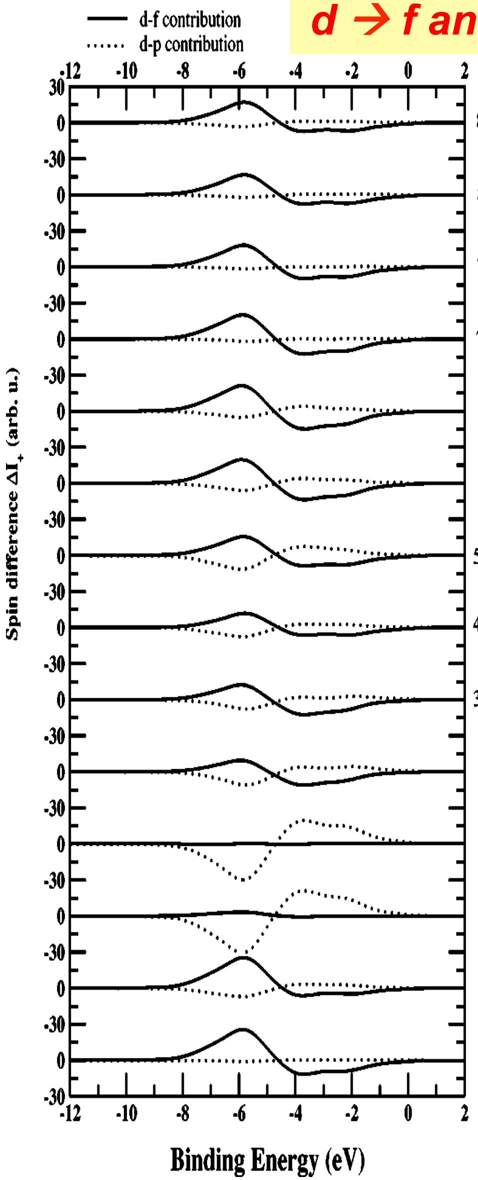
Spin-orbit spectrum: *caveats*



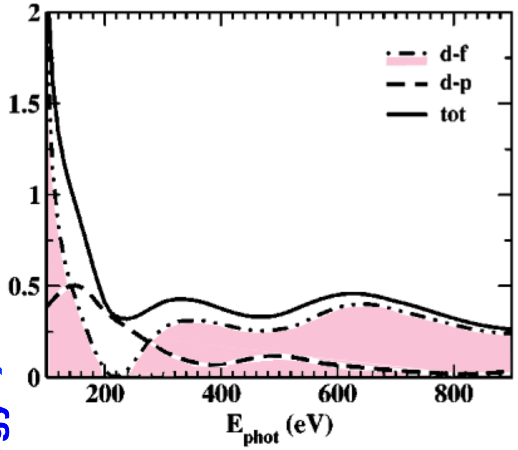
"too small"

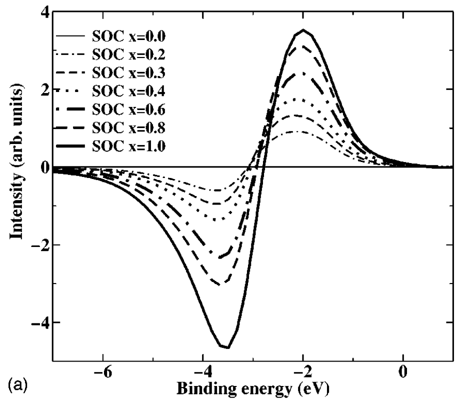
C. De Nadai (2004)

d → f and d → p : opposite signs



Photon energy →





The choice of photon energy is crucial