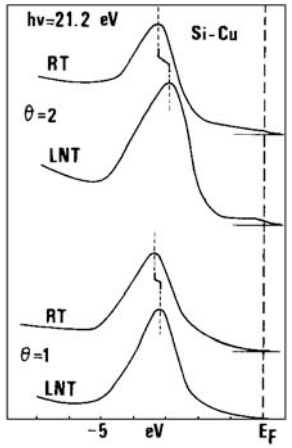
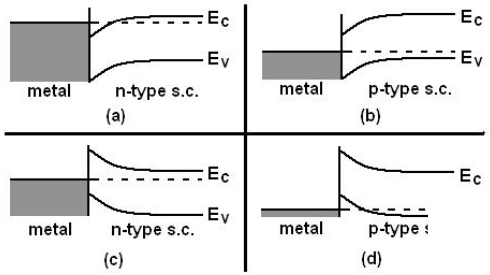
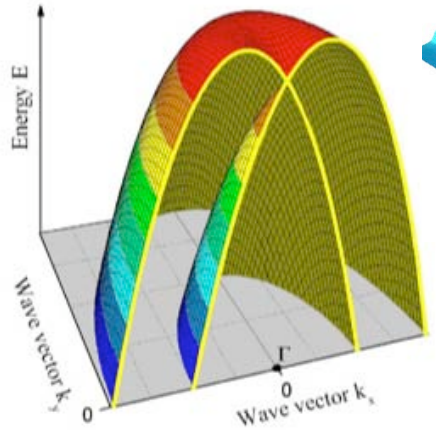
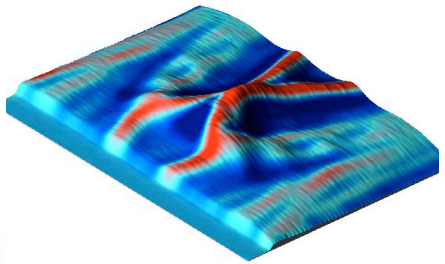
From the physics of interfaces to new physics with interfaces

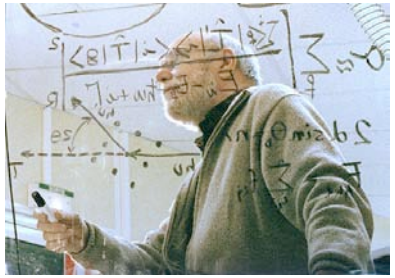








Marco Grioni
IPMC - EPFL



ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

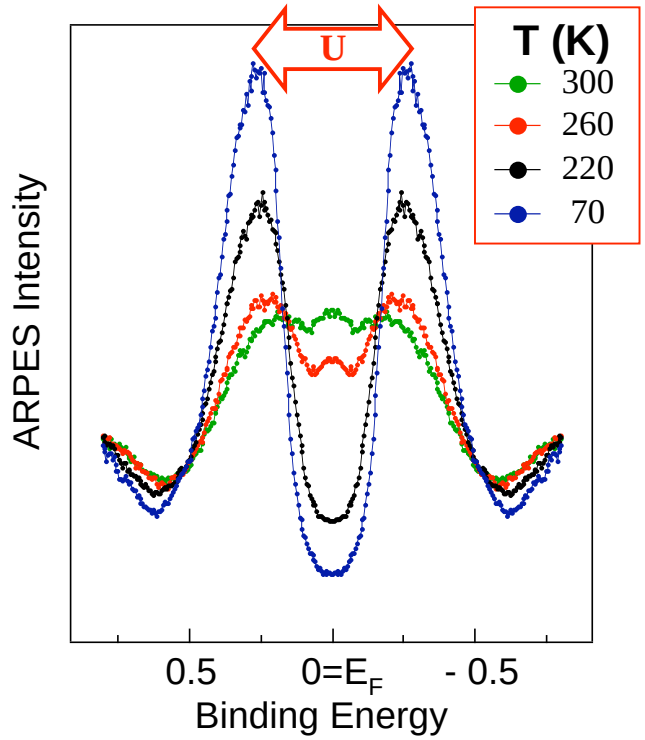
Coworkers and collaborators :

- E. Frantzeskakis, L. Moreschini, M. Papagno, D. Pacilé, S. Pons, EPFL
- Ch. Ast, K. Kern MPI-Stuttgart
- J. Henk, H. Mirosseini, MPI-Halle
  P. Bruno* (Grenoble)
- F. Reinert Würzburg

Electrons confined in two dimensions

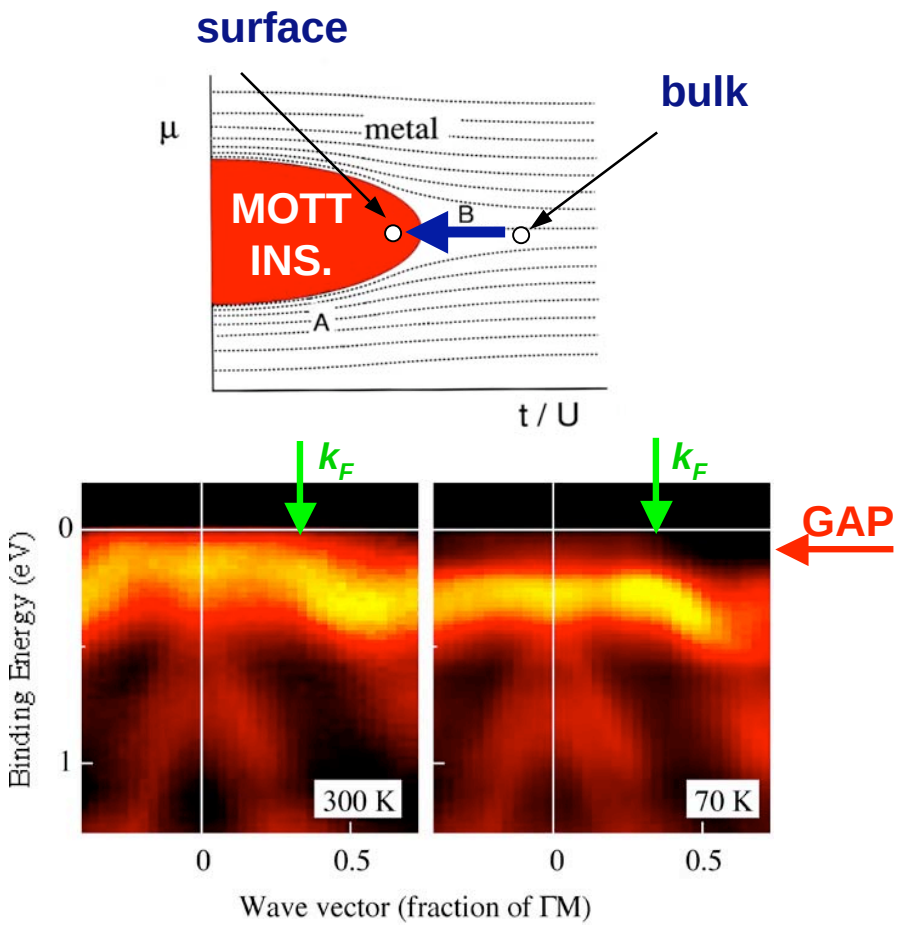
Different ground states may be stable at a surface/interface due to *stronger interactions*, *dimensionality*, *symmetry*

Symmetrized ARPES spectra at the Fermi surface



Perfetti et al., Phys. Rev. Lett. **90**, 166401 (2001).

A *surface* Mott transition: 1T-$TaSe_2$



A different kind of symmetry breaking

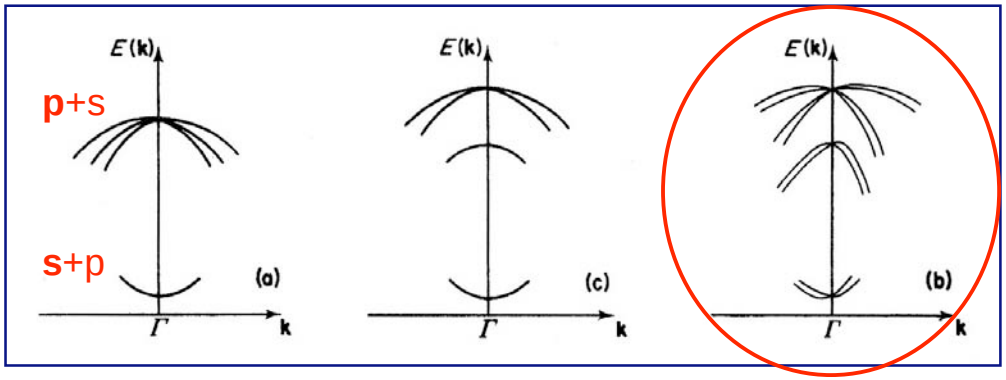
1. $E(k,\uparrow) = E(-k,\downarrow)$ ***time-reversal*** symmetry

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

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

at the surface of a solid, inversion symmetry is broken.
With SO interaction:

$E(k,\uparrow) \neq E(k,\downarrow)$ **even without an external magnetic field**



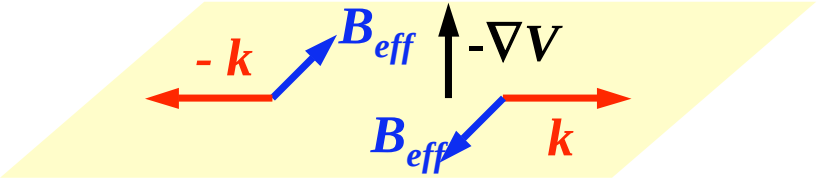
no SO **with SO** **SO - no inversion**

Heine: *Group Theory in Quantum Mechanics*

Free-electrons at a surface - the Rashba effect

2D free electrons moving in an E field

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

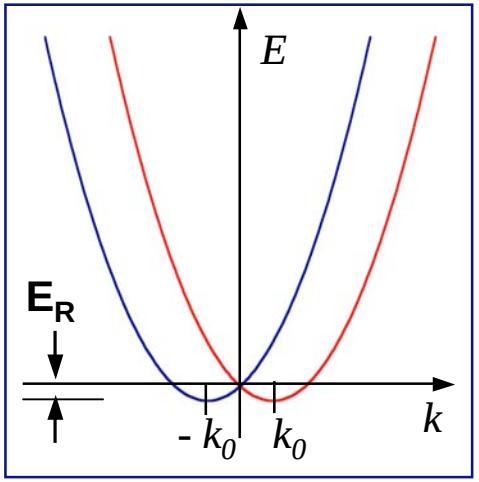


Zeeman coupling

"see" a magnetic field

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

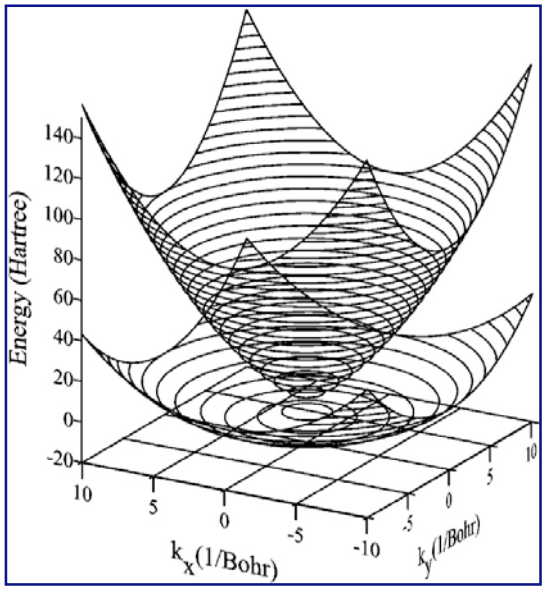
$$H_{SOC} \approx -\vec{\mu}_S \cdot \vec{B} = \alpha_R(\vec{e}_z \times \vec{p})\cdot\sigma$$



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

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

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



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

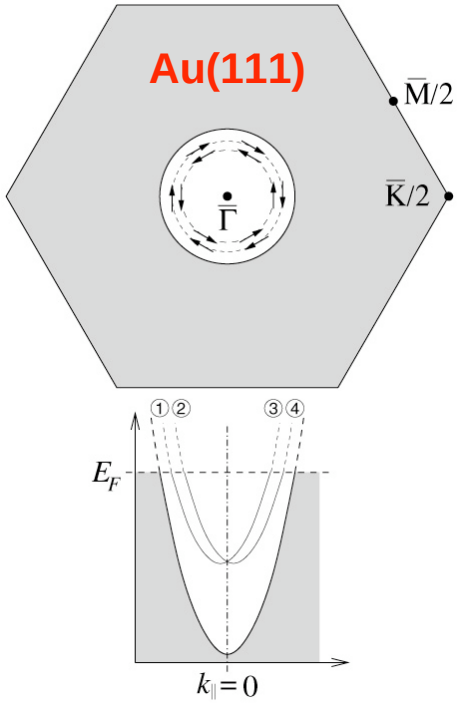
rotational invariance

Atomic SO → much larger splittings

Shockley states at the surface of noble metals :

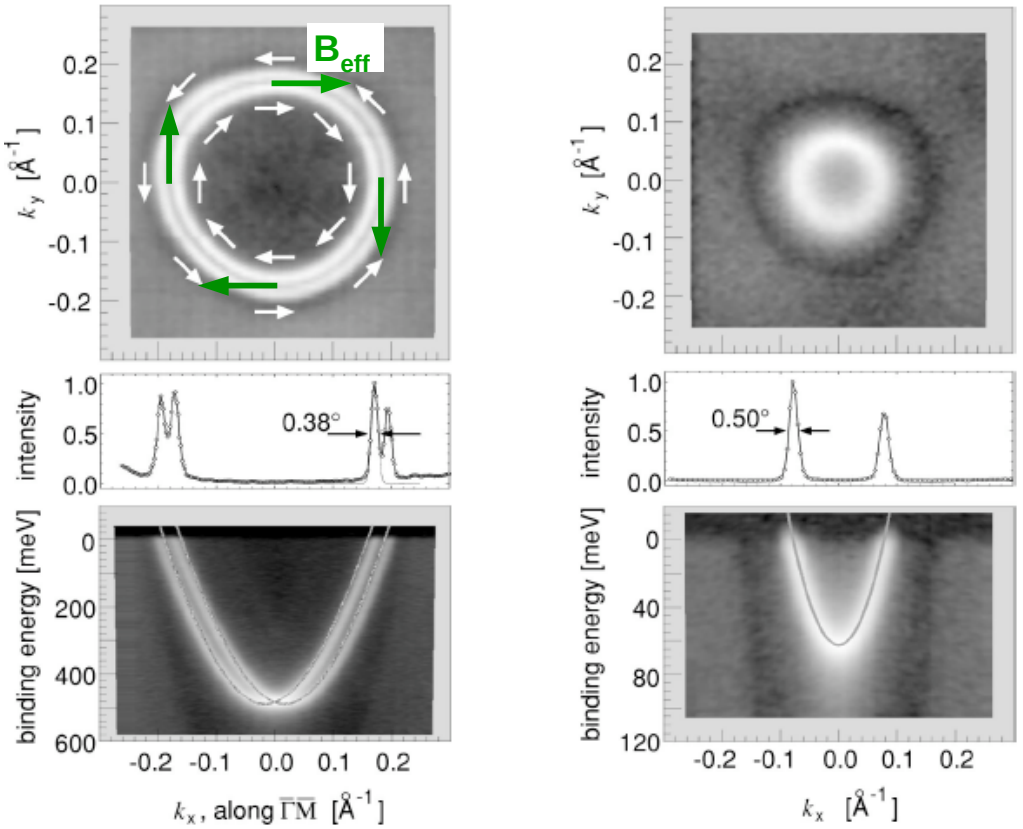
The circular Fermi surface
is split into two
spin-polarized branches

Spins turn in plane



LaShell (1996)

Au (111) **Reinert (2001)** **Ag (111)**

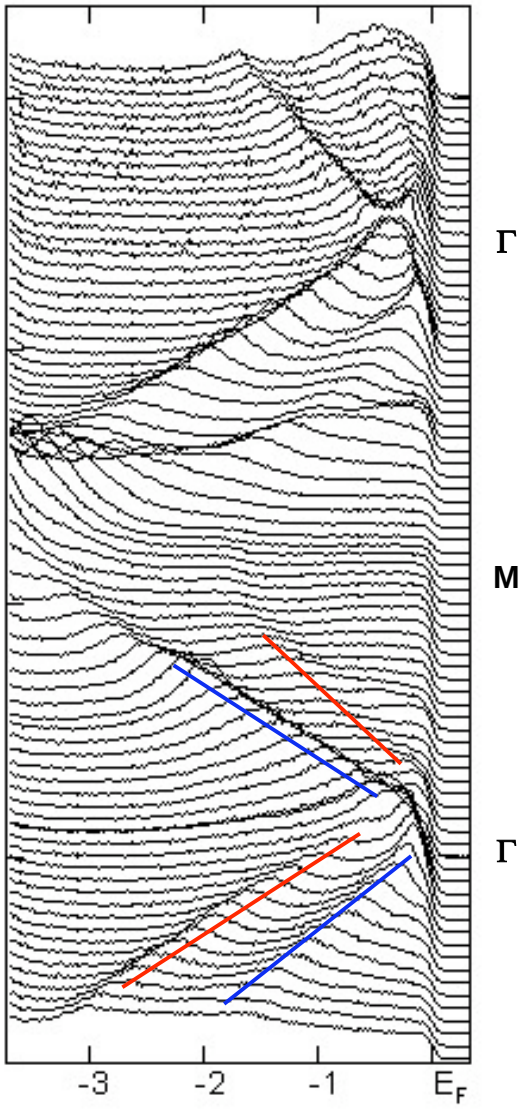


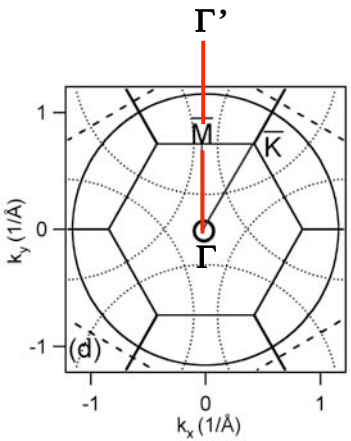
k_0 = 0.012 Å^{-1}; **E_R ~ 2 meV**; k_0 ~ 0.004 Å^{-1}; **E_R ~ 0.2 meV**

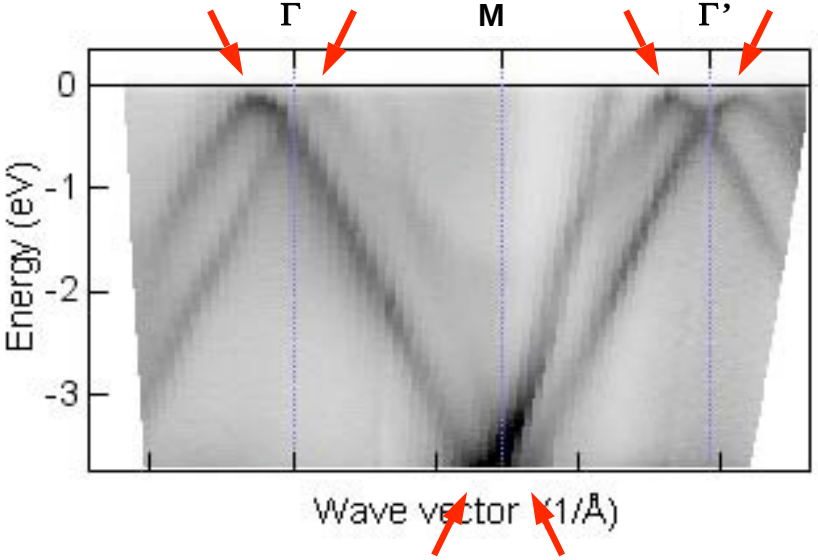
ΔE_{SO}= 470 meV ΔE_{SO}= 110 meV

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

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

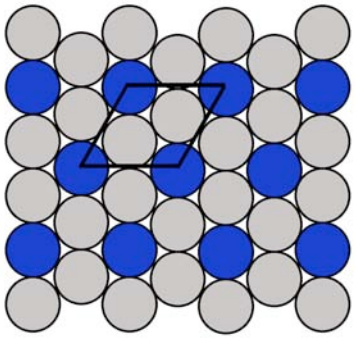


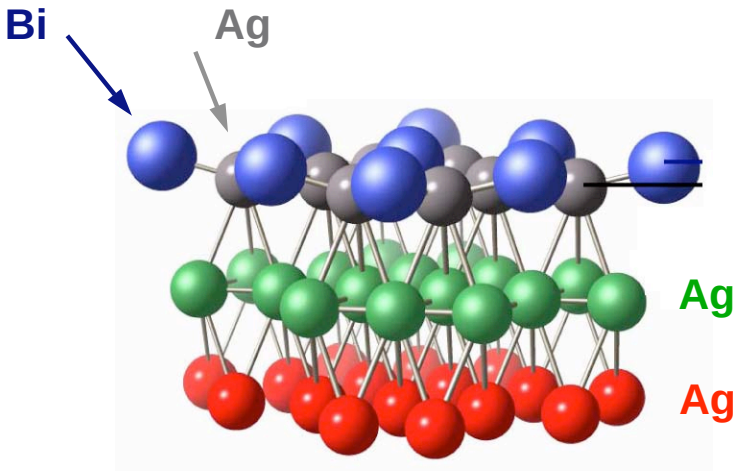




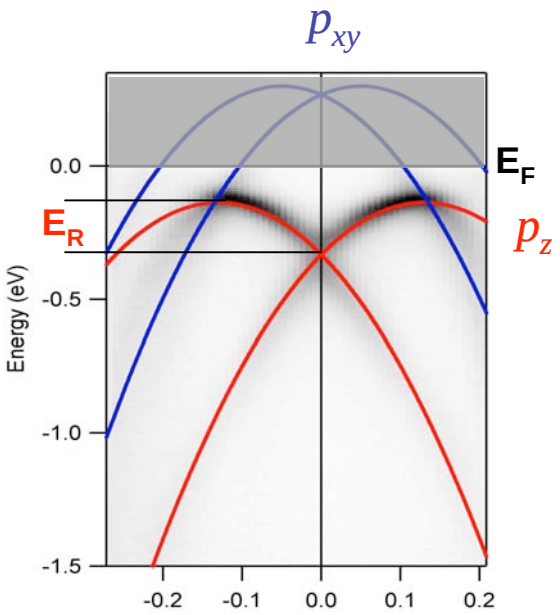
Surface bands degenerate at Γ points and halfway in between

$BiAg_2$





Giant spin-orbit splitting (?)



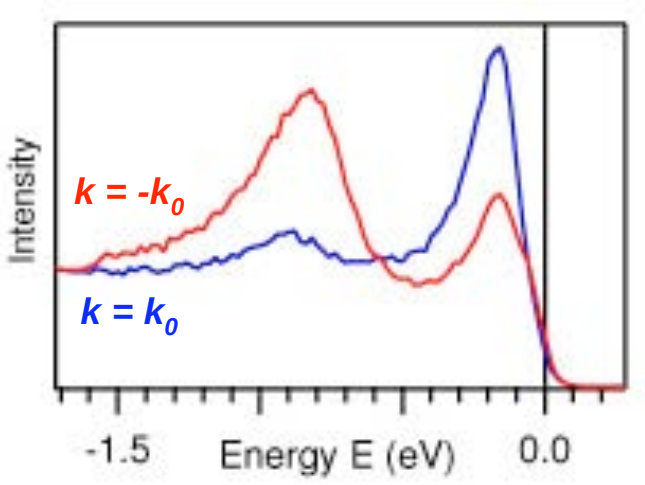
k_0 = 0.13 Å^{-1}; α_R ~ 3 eV Å;
E_R = 200 meV

Au(111): k_0 = 0.012 Å^{-1}; α_R = 0.33 eV Å;
E_R ~ 2 meV

Bi(111): k_0 = 0.05 Å^{-1}; α_R = 0.56 eV Å;
E_R = 14 meV

Two sets of split surface bands

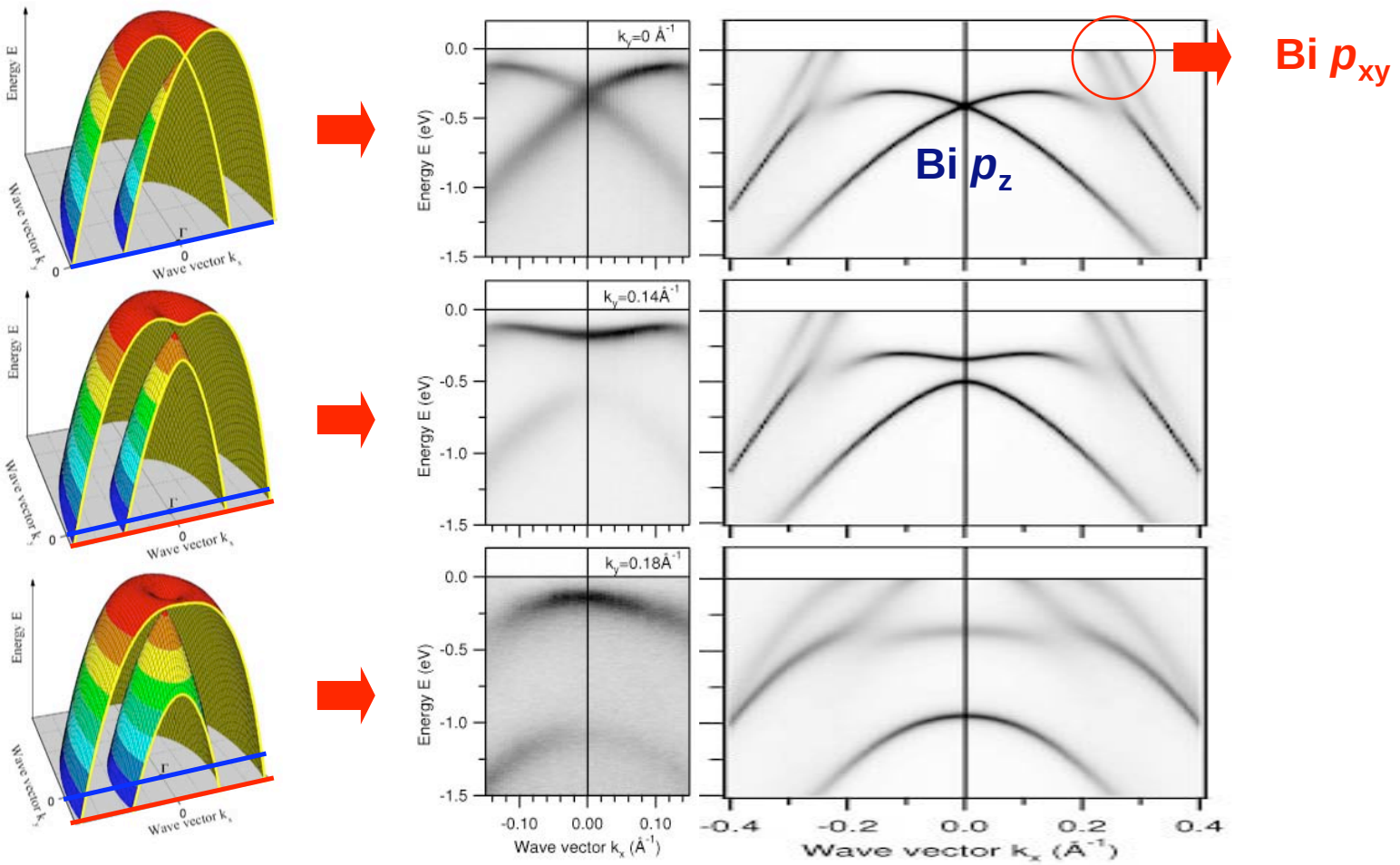
Is it SO splitting ? Why so large?



Dichroism in the angular distribution

Theory comes to the rescue

ARPES

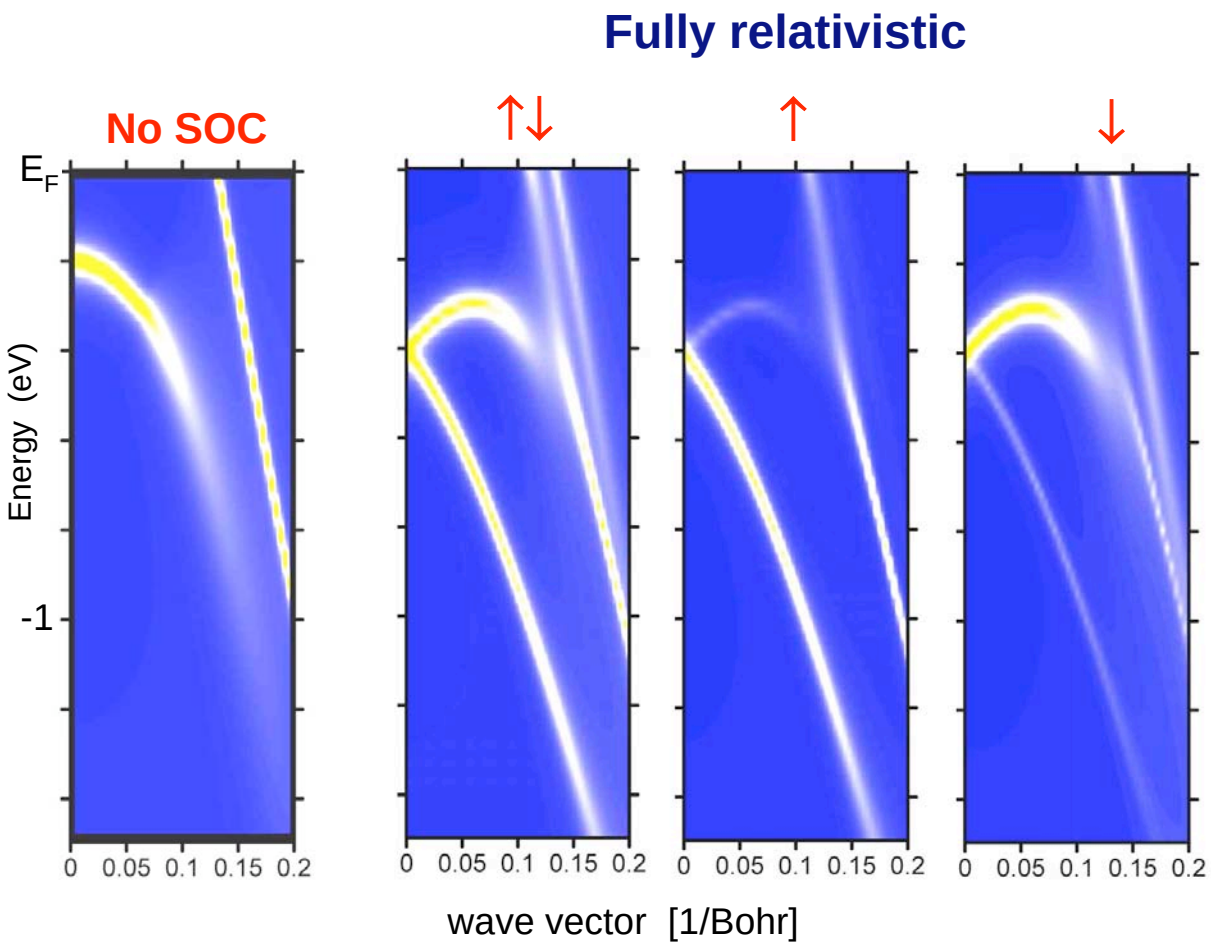


Simpl(*istic*) model

Fully relativistic calculation

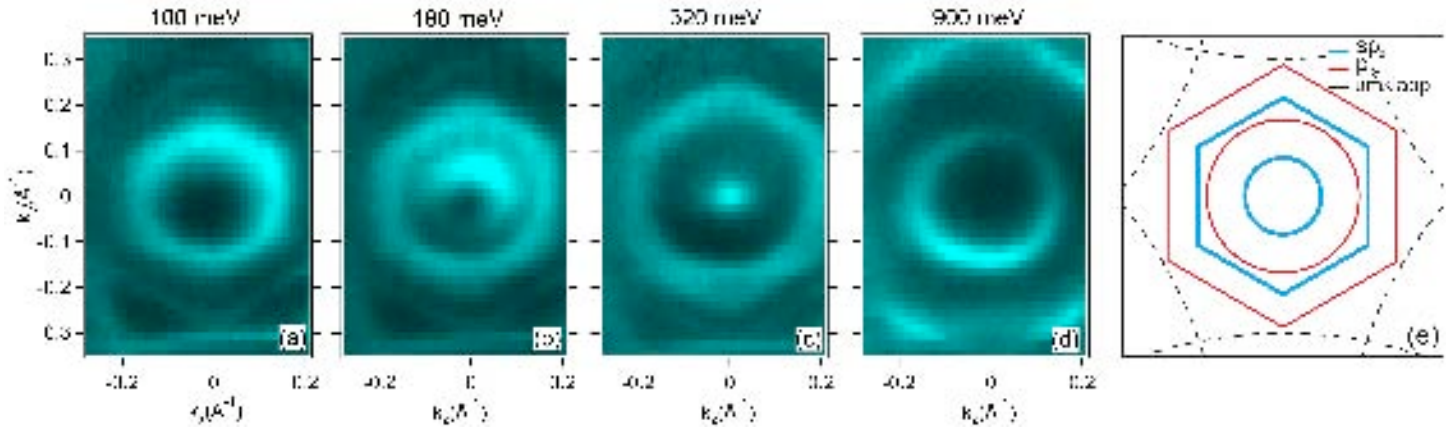
J. Henk, P. Bruno

The bands are spin-polarized

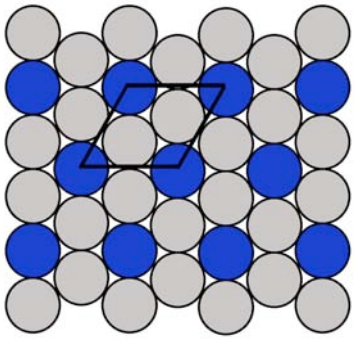


The hybrid states are tightly confined within the top layer

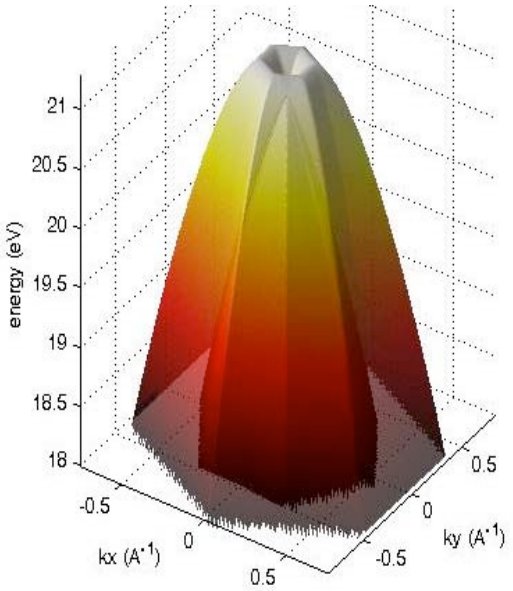
In-plane symmetry breaking and anisotropy



ARPES constant energy cuts

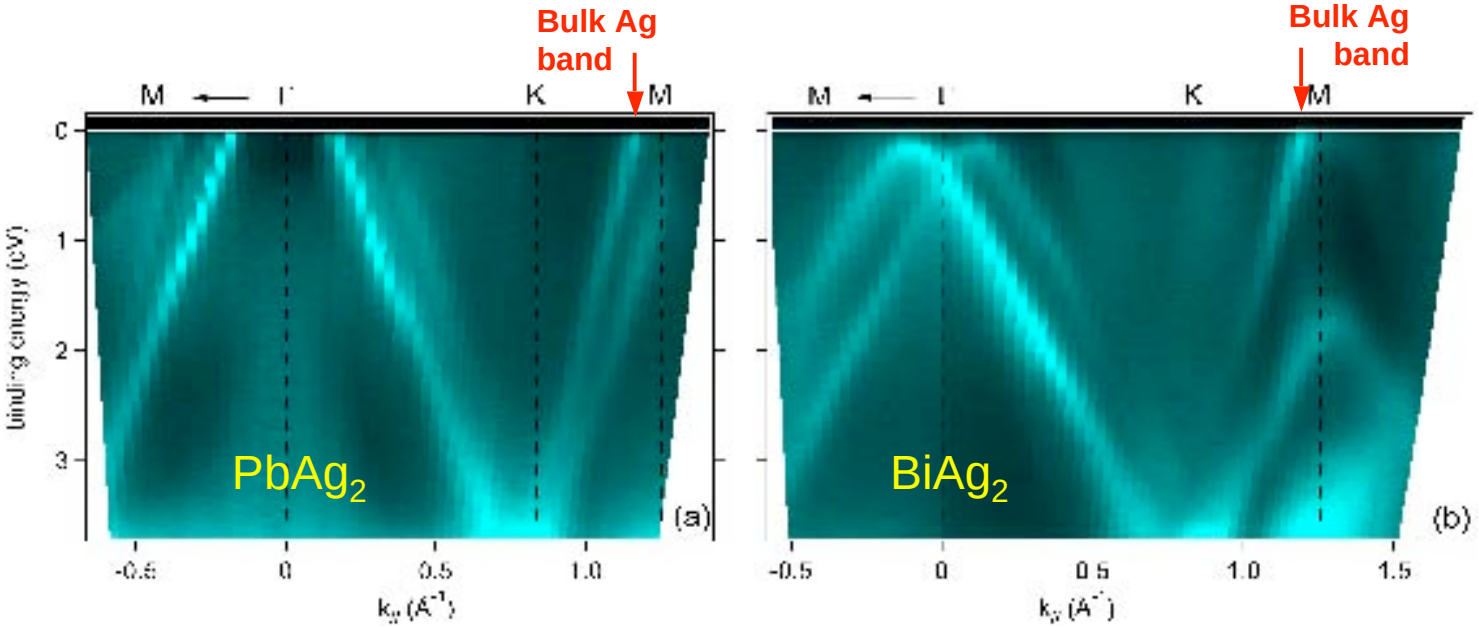


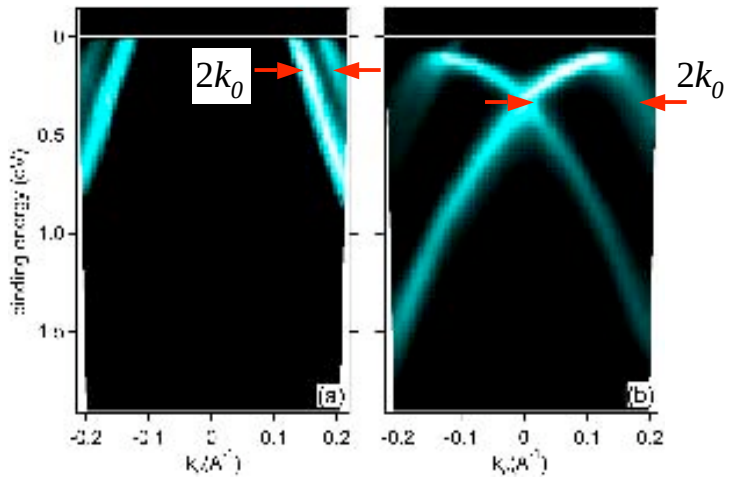
Unlike the case of Au(111), the spin-split FS is clearly influenced by the crystal potential



More realistic

Pb + 1*e*/ = Bi; rigid-band model





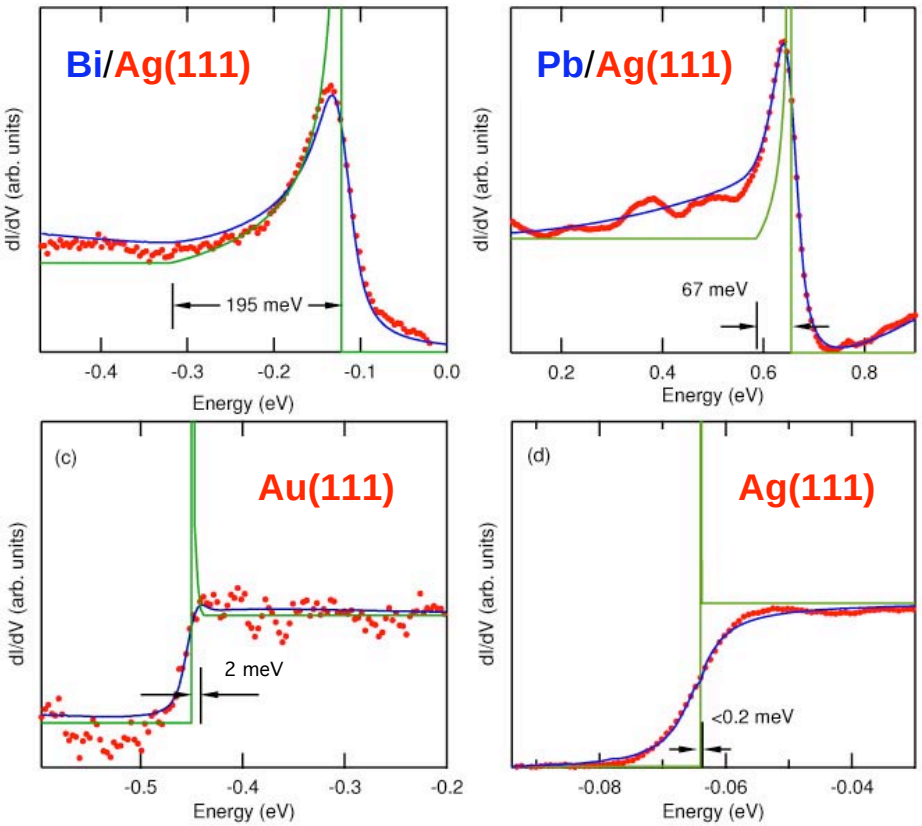
Same structure: $BiAg_2$ surface alloy

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

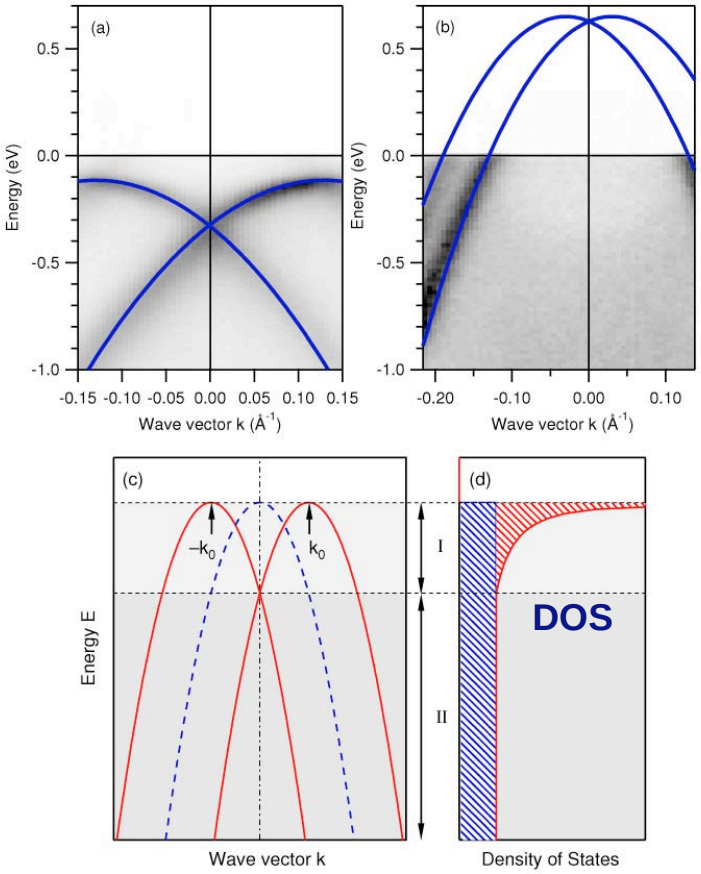
Signatures of spin-split states in tunneling spectra



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

STS: MPI Stuttgart

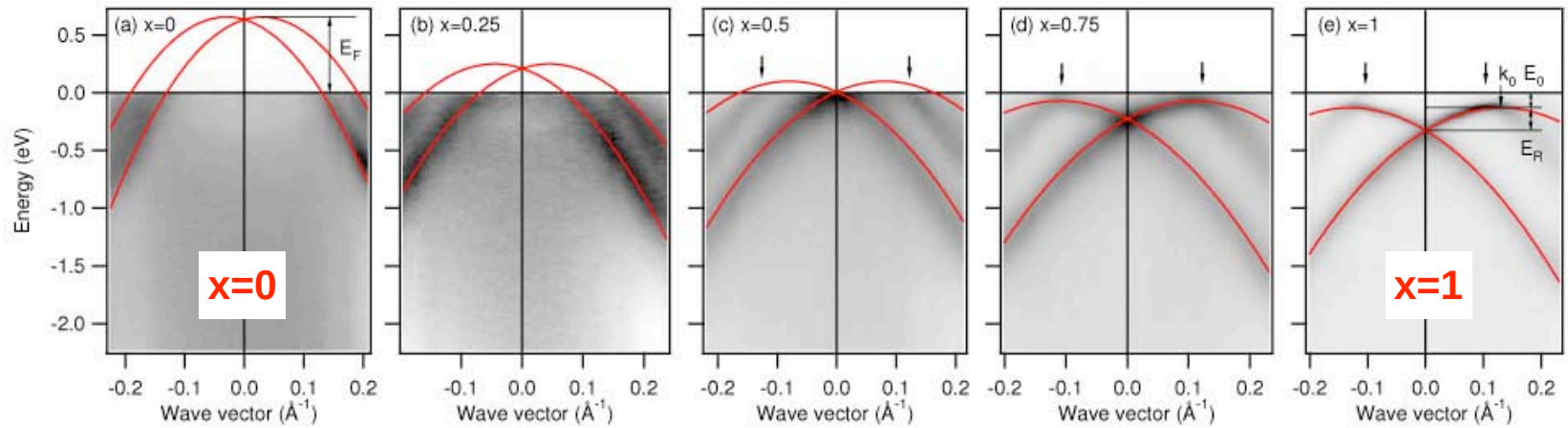
Bi/Ag(111) **Pb/Ag(111)**

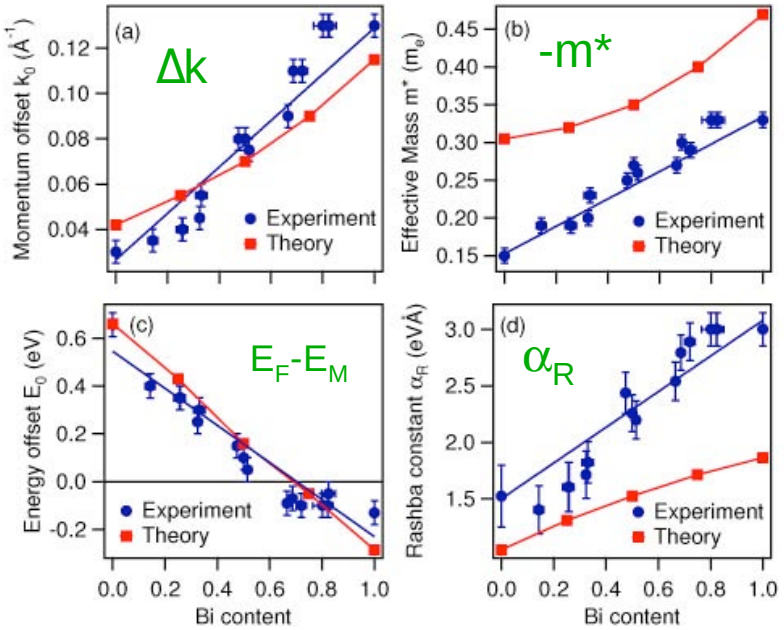


"1D-like divergence"

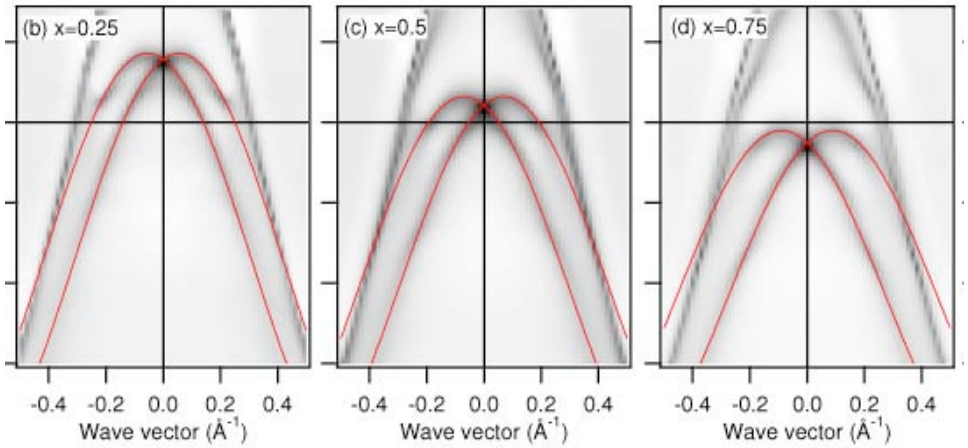
Chemical tuning of E_F and of the SO splitting

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





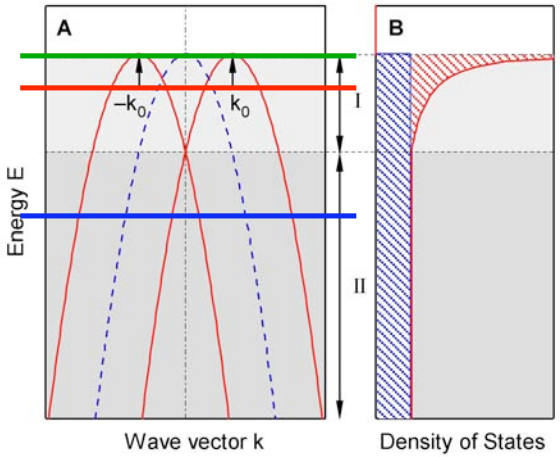
THEORY

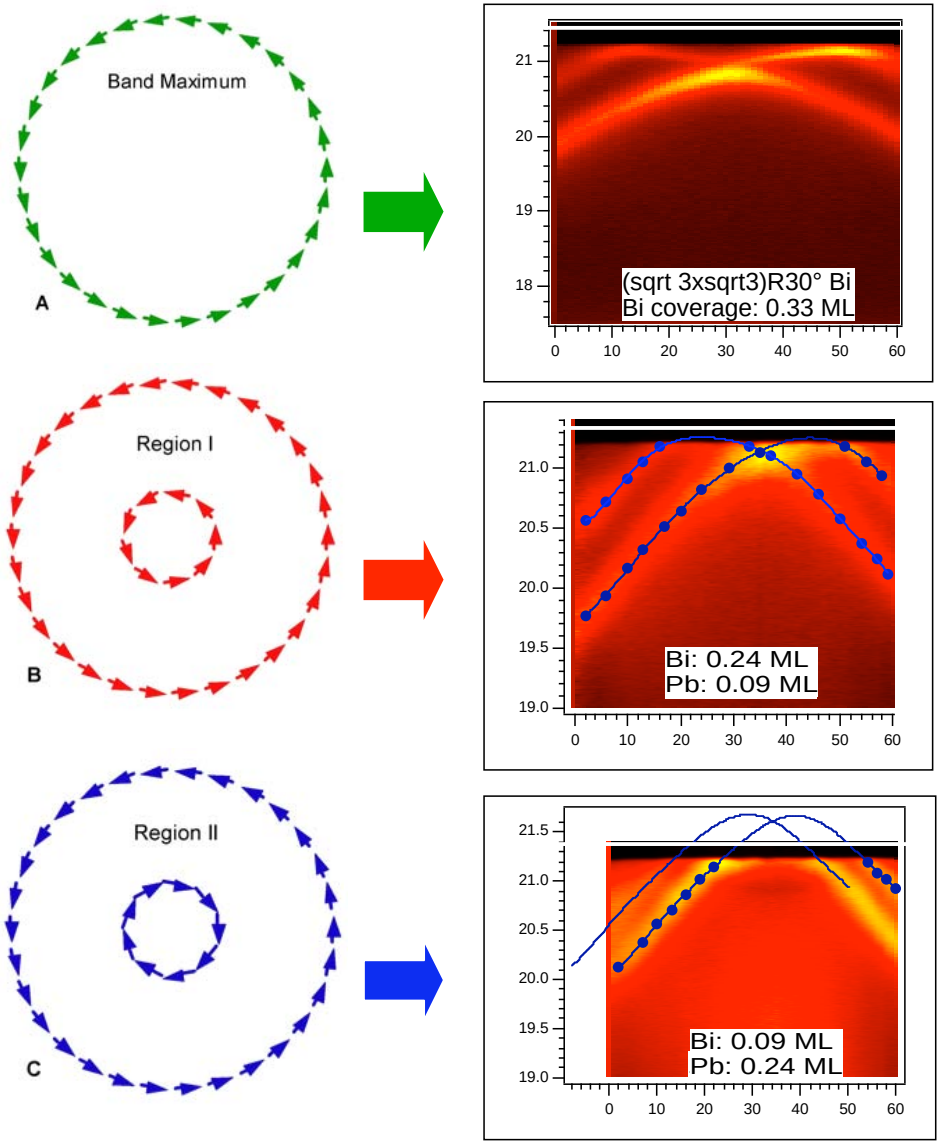


Adjusting the spin pattern by interface engineering

The spin pattern depends on the energy

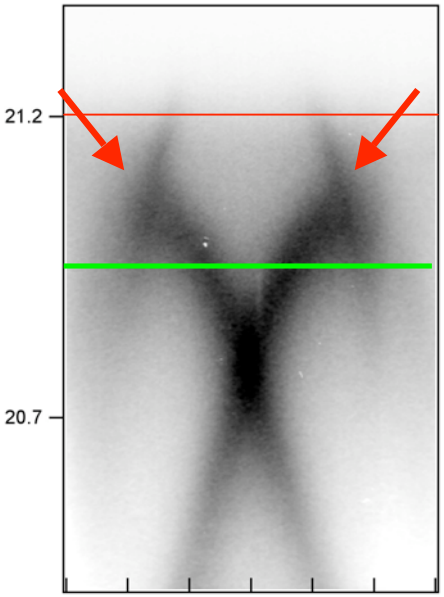
Three different situations are realized by tuning E_F through the band as a function of stoichiometry

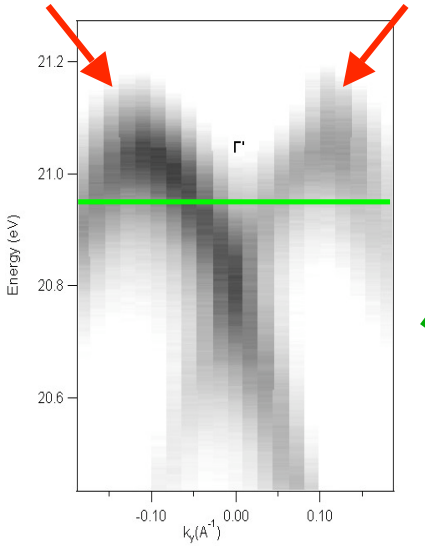


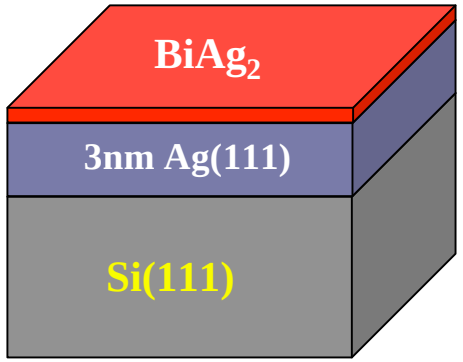


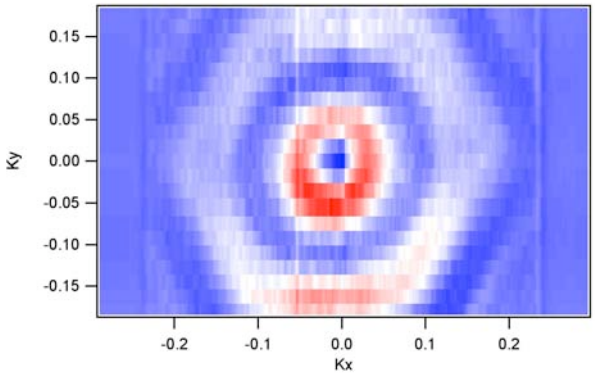
Giant SOS on a semiconductor substrate

The same SO split bands on a "thick" Ag crystalline interlayer







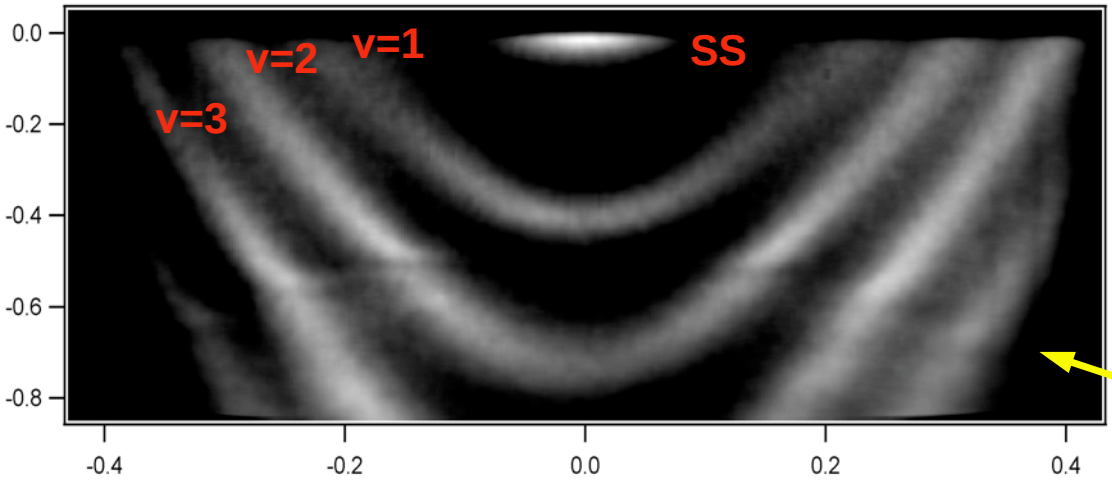


Constant Energy contours

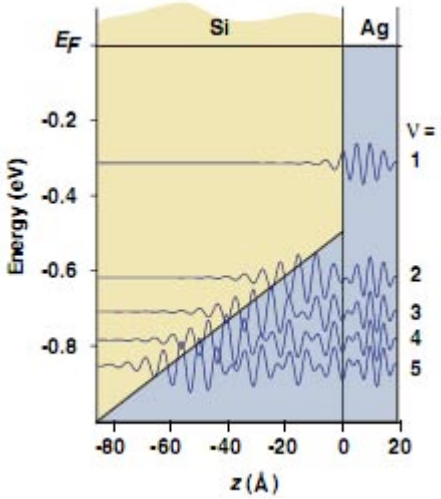
In perspective: the possibility of manipulating the electron spin without a magnetic field (spin transistor …)

$\Theta_{\uparrow} - \Theta_{\downarrow} = \pi \rightarrow L = (\pi/2k_0)$

Thin Ag layer : quantum well states

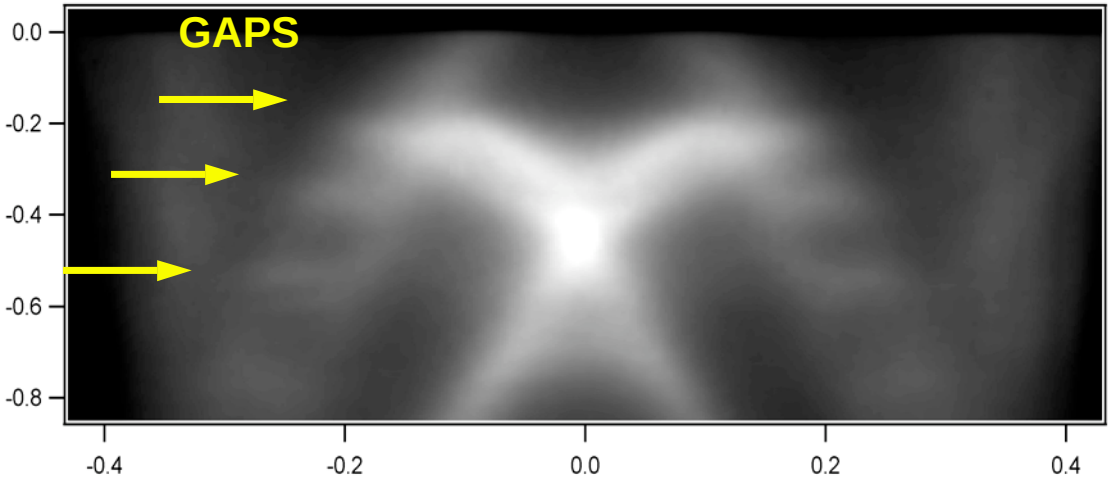


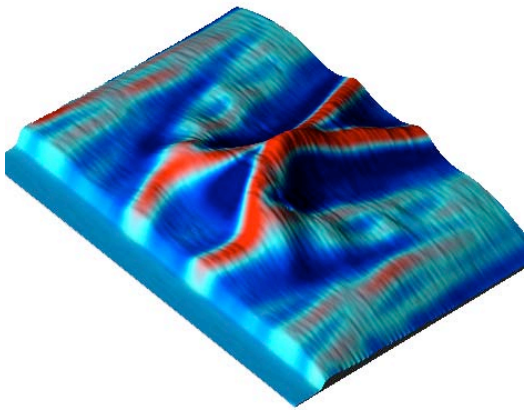
Si BAND EDGE



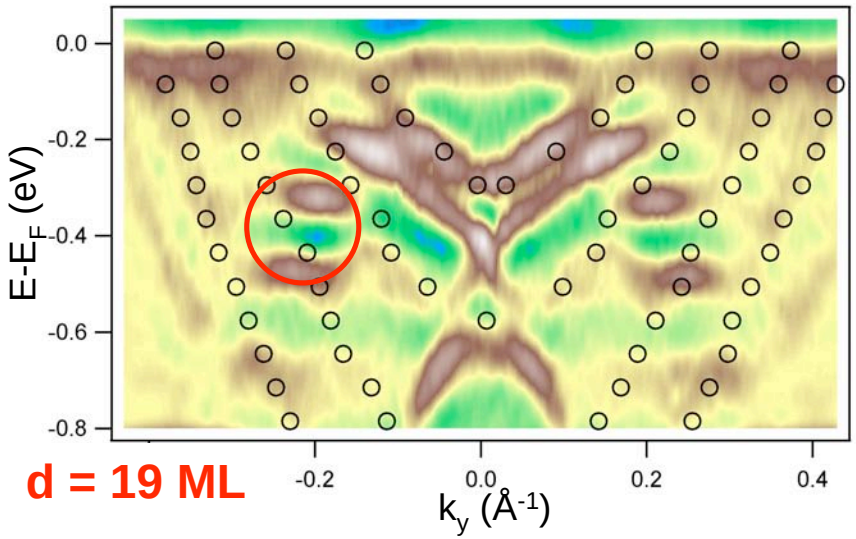
Speer, *Science* (2006)

17 ML + $BiAg_2$

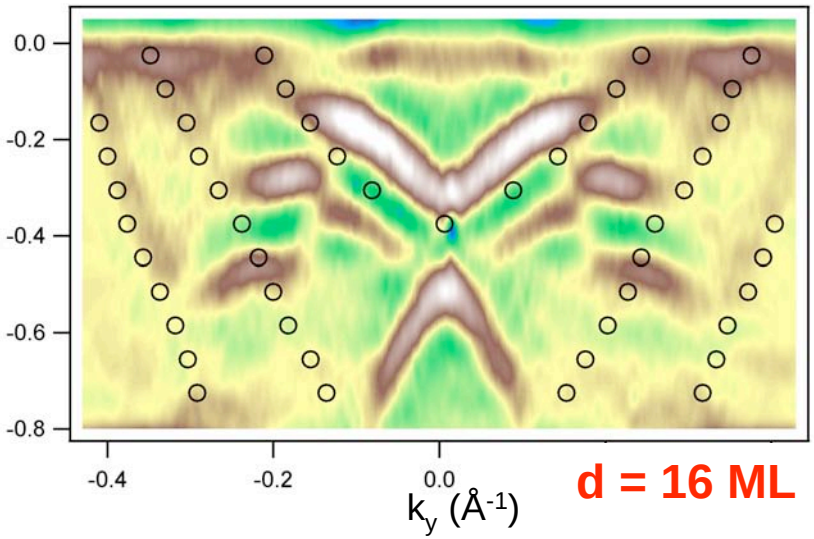




Tuning the gap structure by the Ag layer thickness

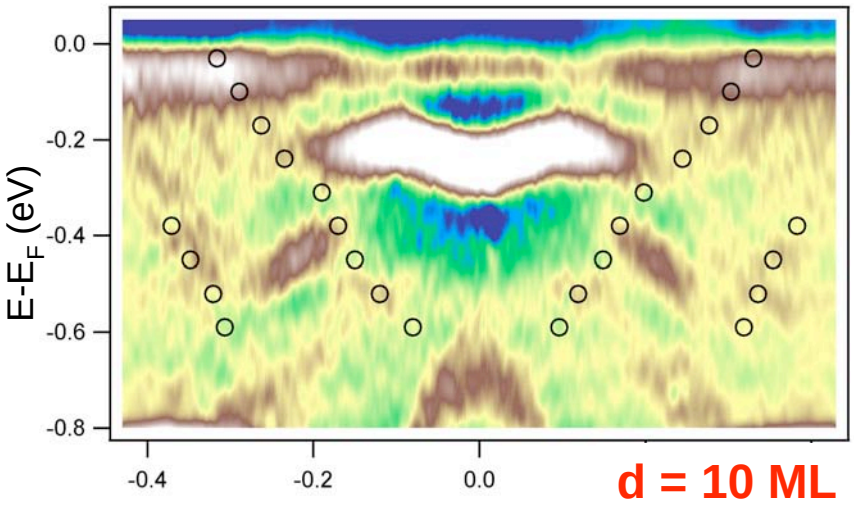


d = 19 ML



d = 16 ML

The QWS shift in energy and hybridize with the alloy SO-split states

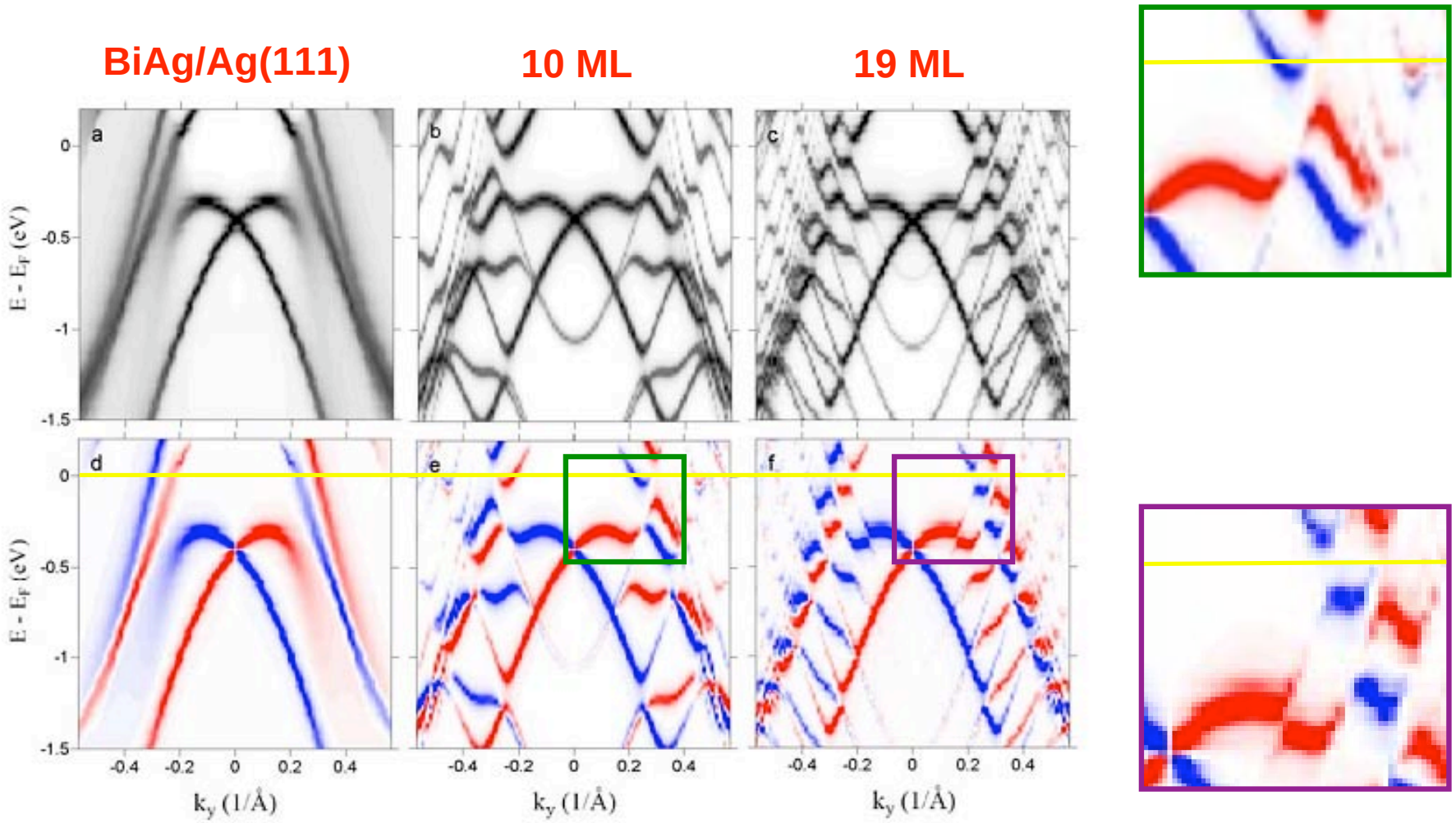


d = 10 ML

Frantzeskakis et al., Phys. Rev. Lett. **101**, 196805 (2008).

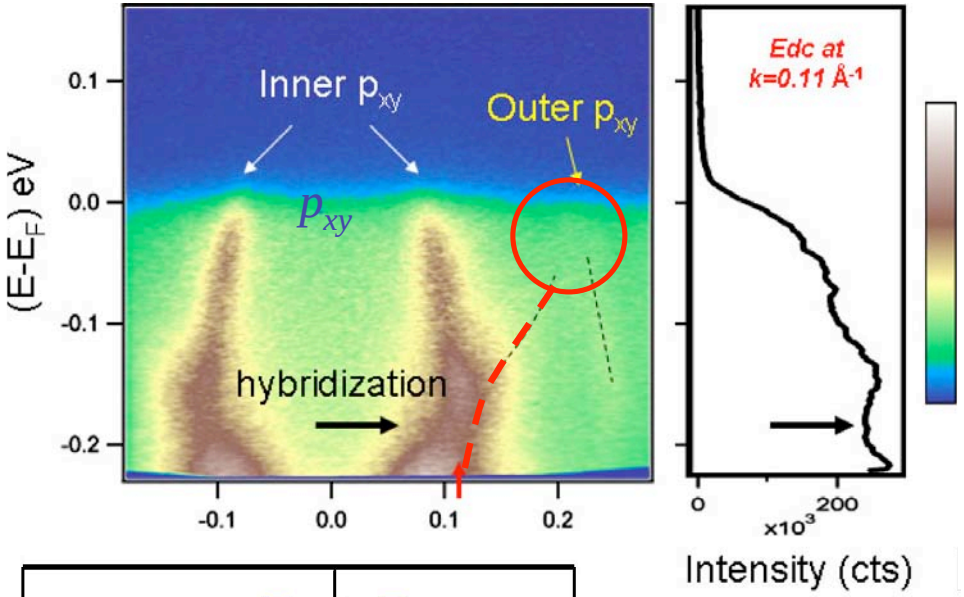
Tunable gaps with large polarization

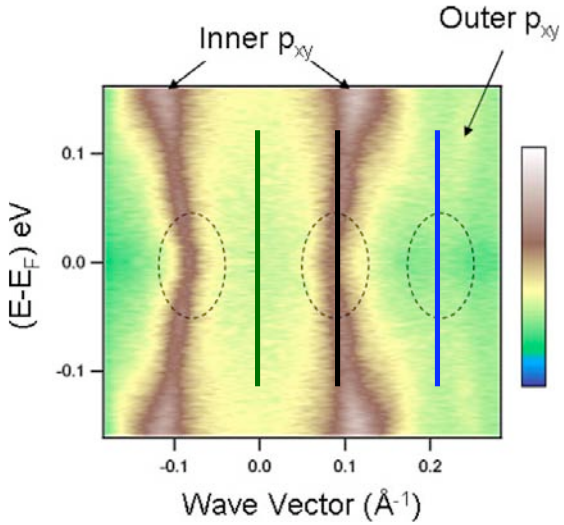
Relativistic calculation

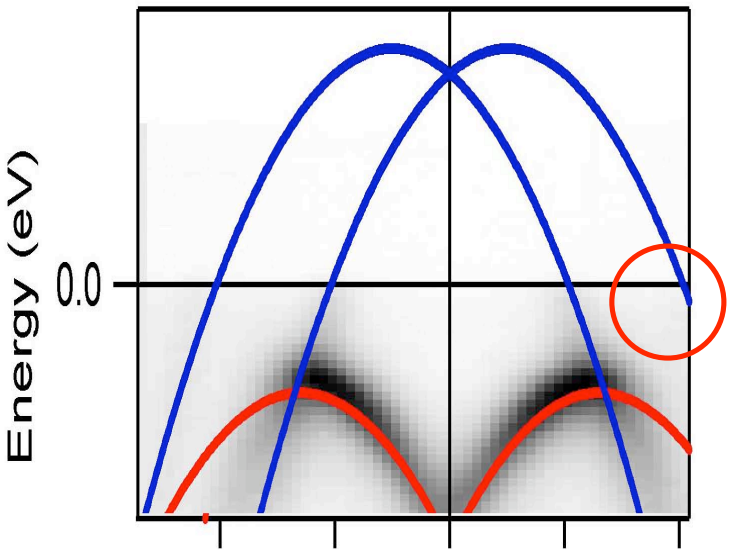


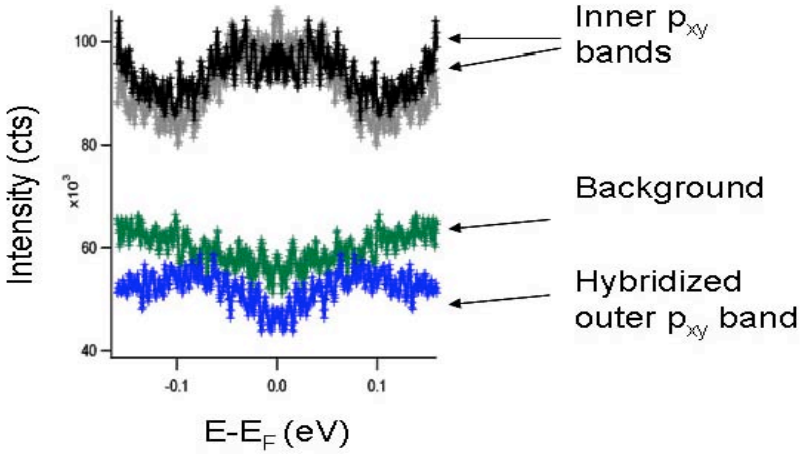
Tunable gaps with large polarization

Signature of a gap at E_F at the intersection of a QWS with a SO-split band



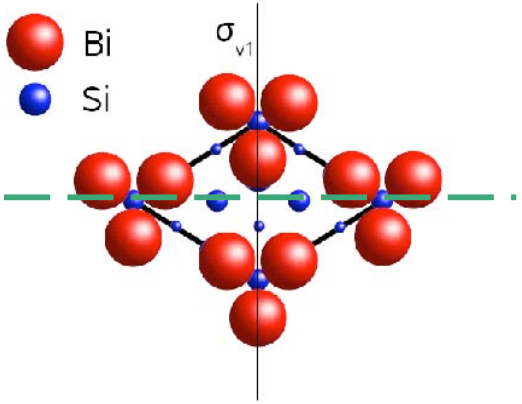




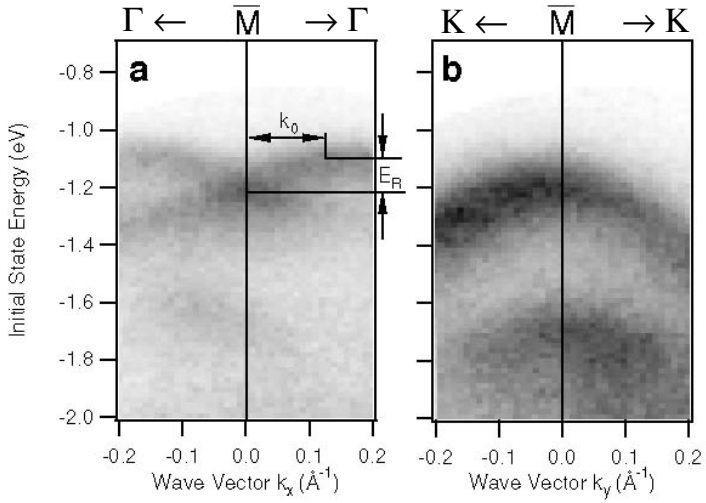


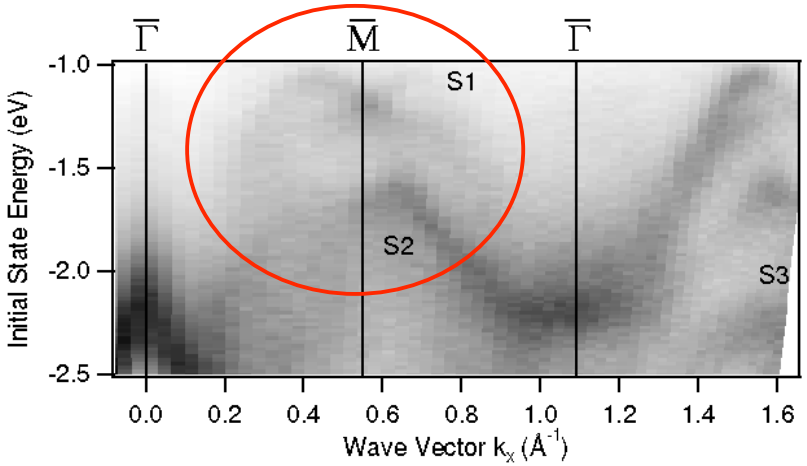
Coming round full circle: Bi-Si(111)

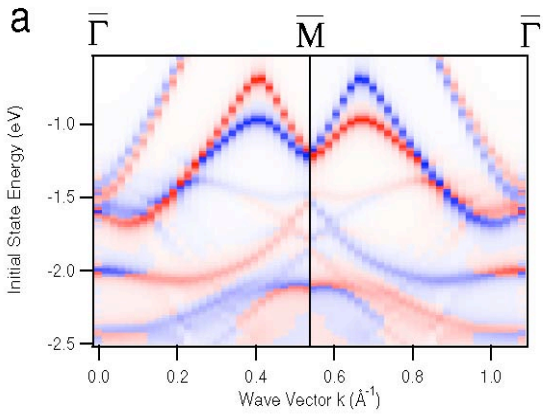
1ML Bi-Si(111) trimer phase



Broken reflection symmetry *in-plane*







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