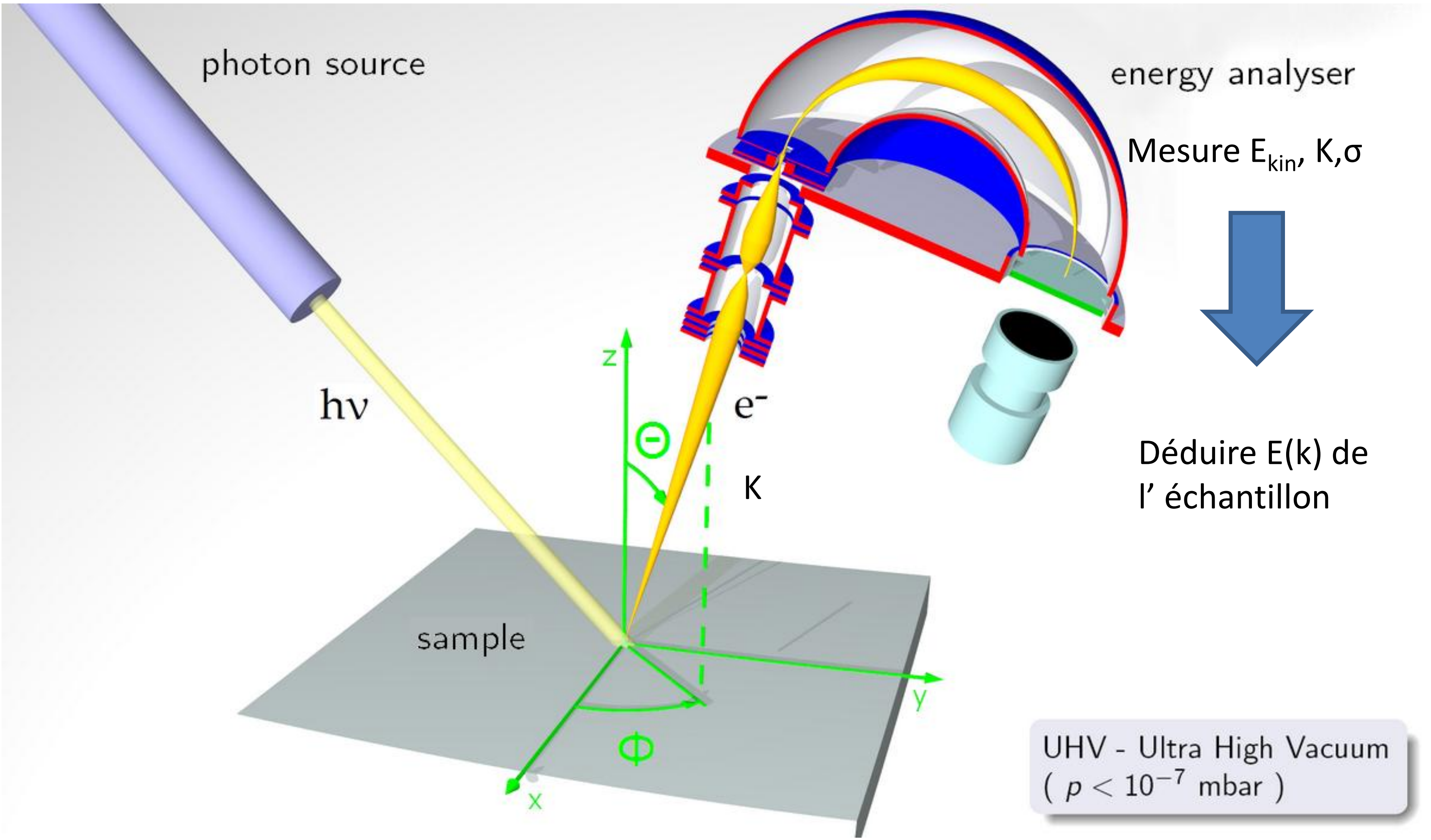
Etudes des états de surface ARPES et STM

Laurent Levy no 2

Principe de l'ARPES



Relation energie-quantite de mouvement

$$k_{//} = K_{//} = \frac{\sqrt{2mE_{kin}}}{\hbar}\sin\theta$$

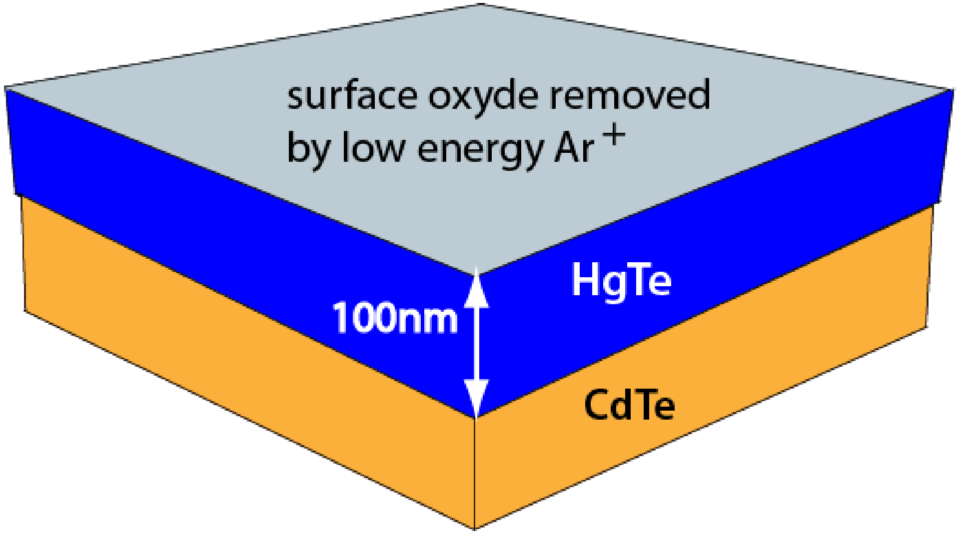
$$k_{\perp} = \frac{\sqrt{2m\left(E_{kin}\cos^2\theta + V_0\right)}}{\hbar}$$

« bonne surface »

$$h\nu = E_{kin} + \phi + E_B$$

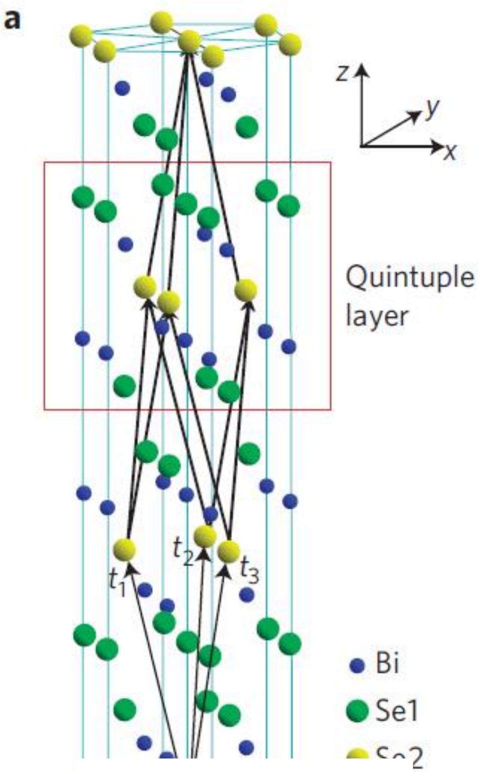
Ce qu'on cherche

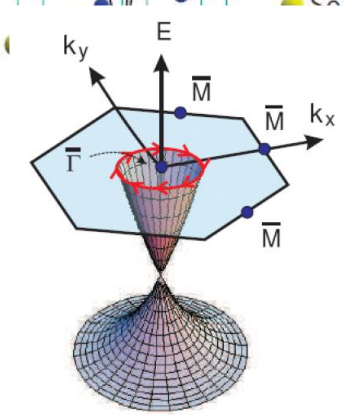
Material workfunction
HgTe 5.8 eV



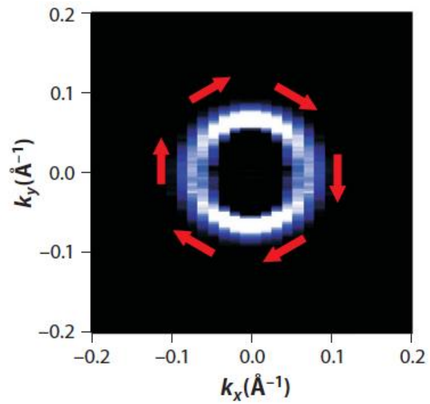
Pour les états de surface $k_{\perp}$=0

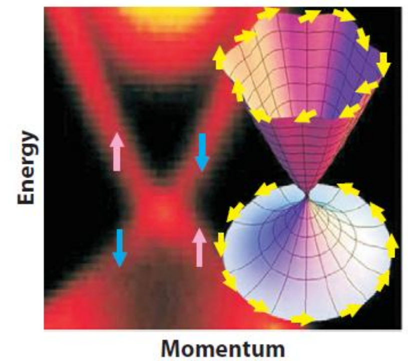
Single Dirac cone topological insulators with large gaps: Bi_2Se_3

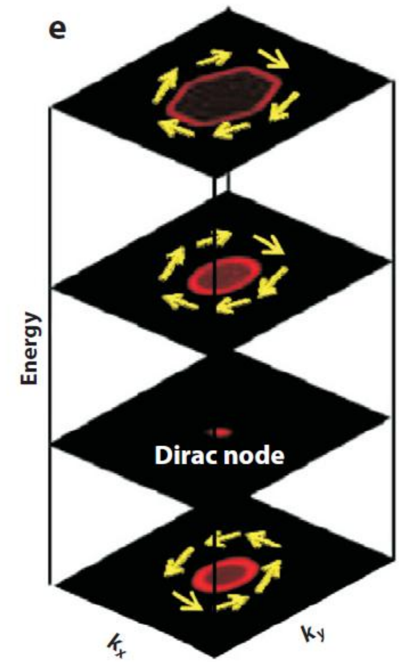


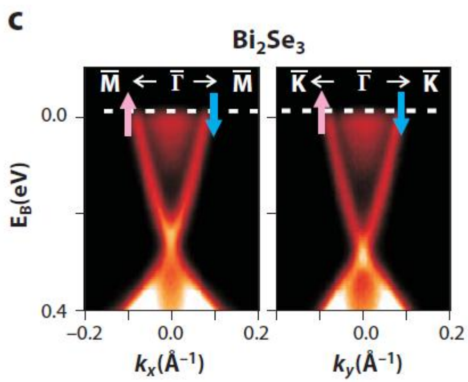


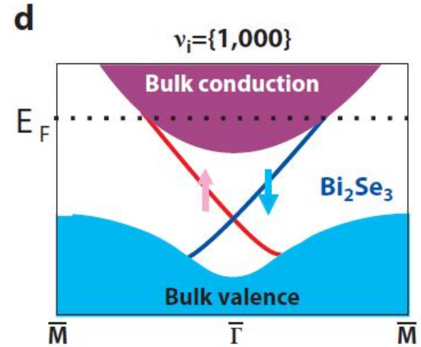
Spin resolved ARPES (Hasan)



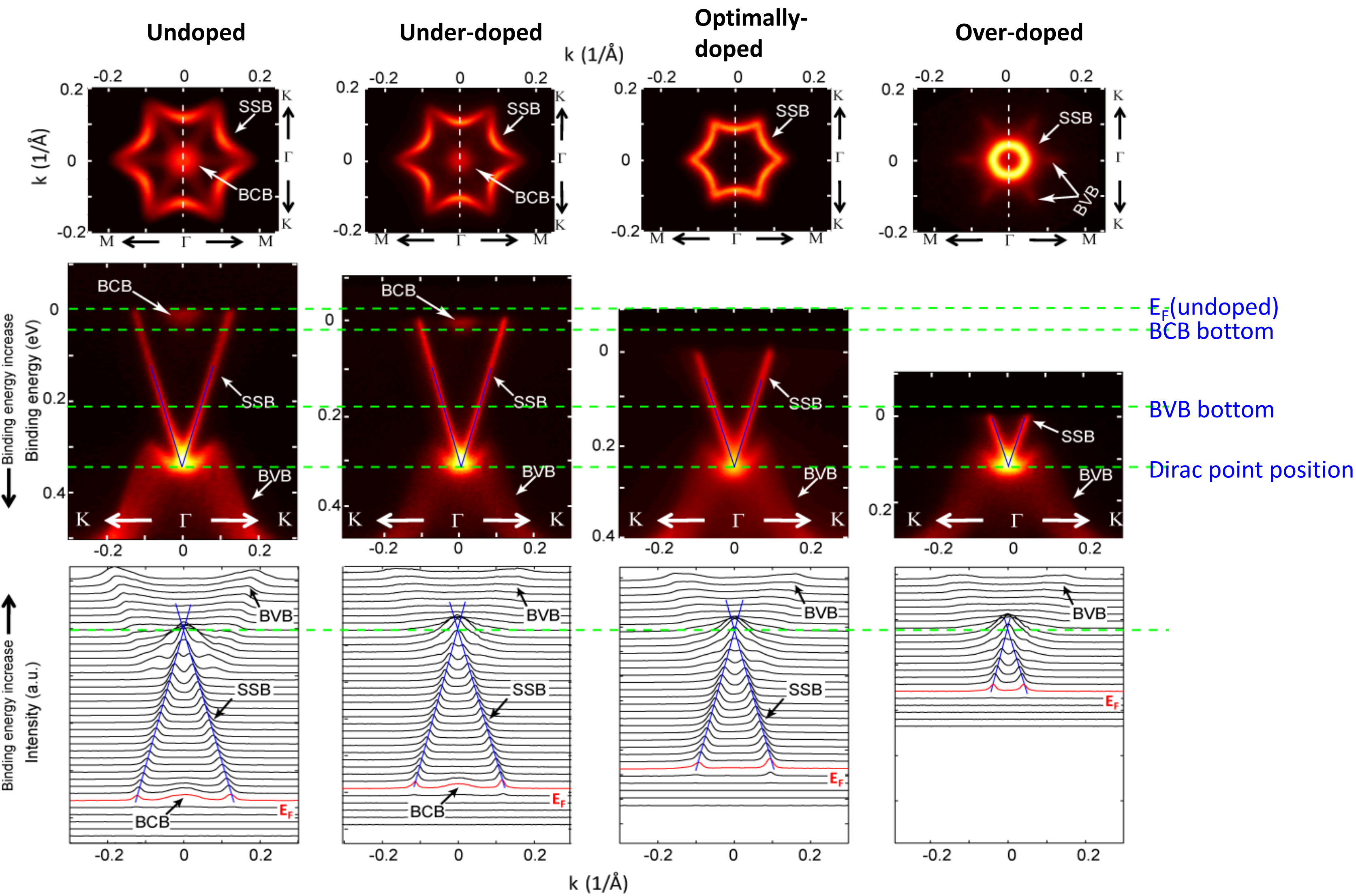








Bi_2Te_3-dopage étudié en ARPES



Spectre spin-orbital des états de surface en champ magnétique

$$H = H_o + H_s$$ Hamiltonien avec spin

$$H_o = \frac{\Pi^2}{2m_*} + v\left(\Pi_x \sigma_y - \Pi_y \sigma_x\right) \quad \vec{\Pi} = \vec{p} + e\vec{A} \quad \vec{A} = \begin{pmatrix} By \\ 0 \\ 0 \end{pmatrix}$$

Solutions de la forme

$$e^{ik_x x}\left|n\right\rangle$$

$$H_s = g\mu_B B\sigma_z \quad a = \frac{\ell_B}{\hbar\sqrt{2}}\left(\Pi_x - i\Pi_y\right)$$

$$\left[a, a^+\right] = 1$$

$$H = \hbar\omega_c\left(aa^+ + \frac{1}{2} - \frac{g}{2}\sigma_z\right) + i\sqrt{2}\eta\left(a\sigma^- - a^+\sigma^+\right) \quad |n\rangle_\pm = \begin{pmatrix} \cos\alpha_n |n\rangle \\ i\sin\alpha_n |n-1\rangle \end{pmatrix}$$

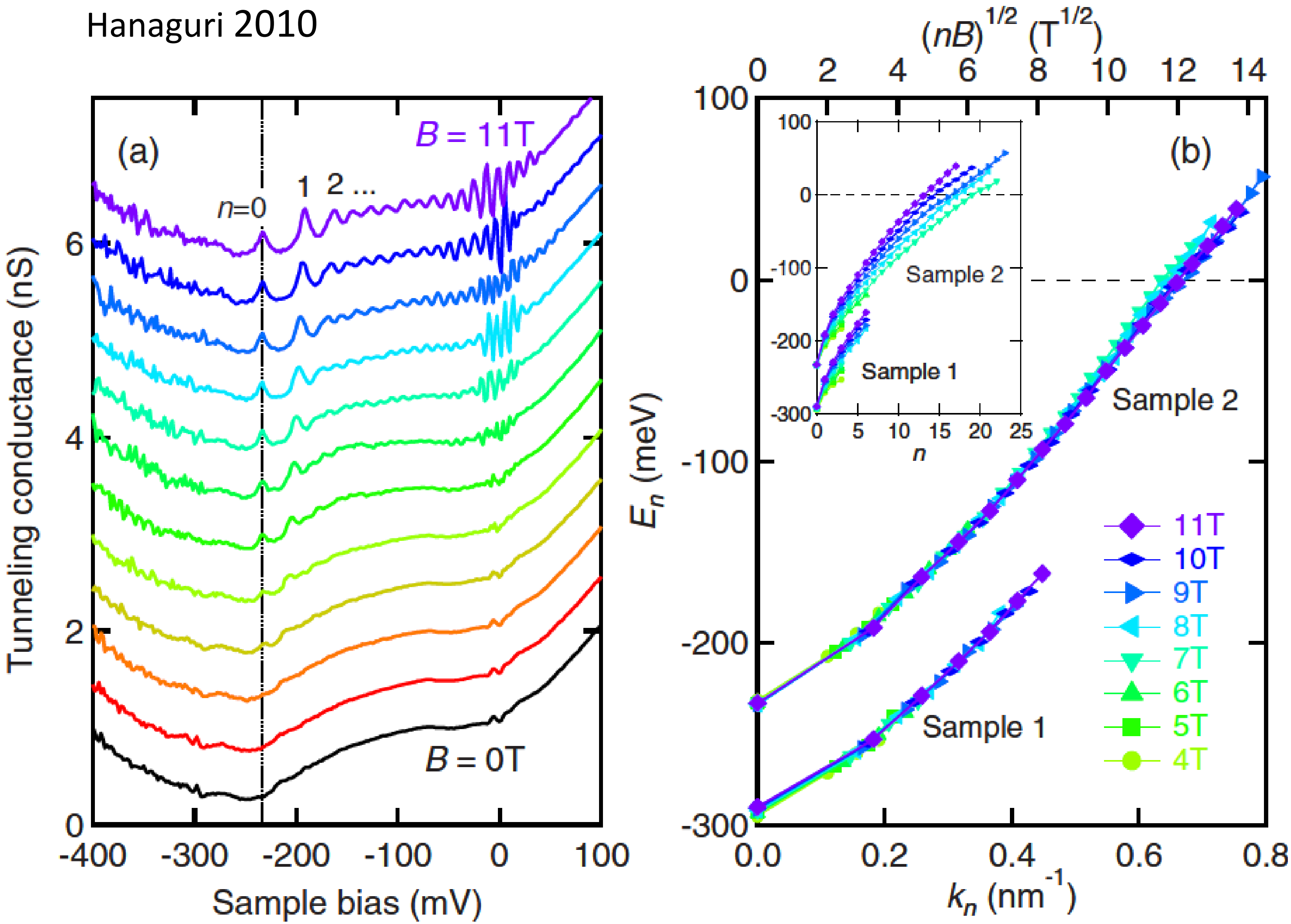
$$g = \frac{m_*}{2m_e} g_z \quad \eta = v m_* \frac{\ell_B}{\hbar}$$

$$\epsilon(n)_\pm = \hbar\omega_c n \pm \sqrt{\left(\frac{(1-g)\hbar\omega_c}{2}\right)^2 + 2nv_F^2 eB}$$

Mesure ?

Bi_2Se_3: UHV spectroscopie STM en champ

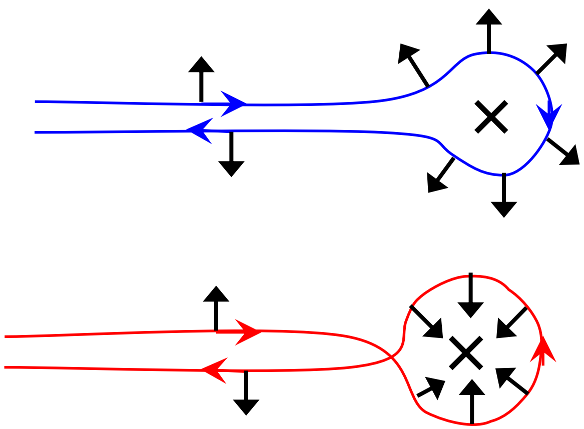
Hanaguri 2010



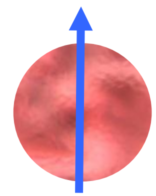
Isolant topologique et inversion par rapport au sens du temps

Suppression de la retrodiffusion

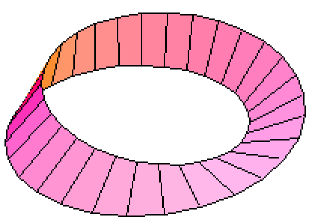
$$\left| e^{i(\phi+\pi/2)} \left| A_{\uparrow\downarrow} \right| + e^{i(\phi-\pi/2)} \left| A_{\uparrow\downarrow} \right| \right|^2 \equiv 0$$



Spin=1/2



ψ=>-ψ



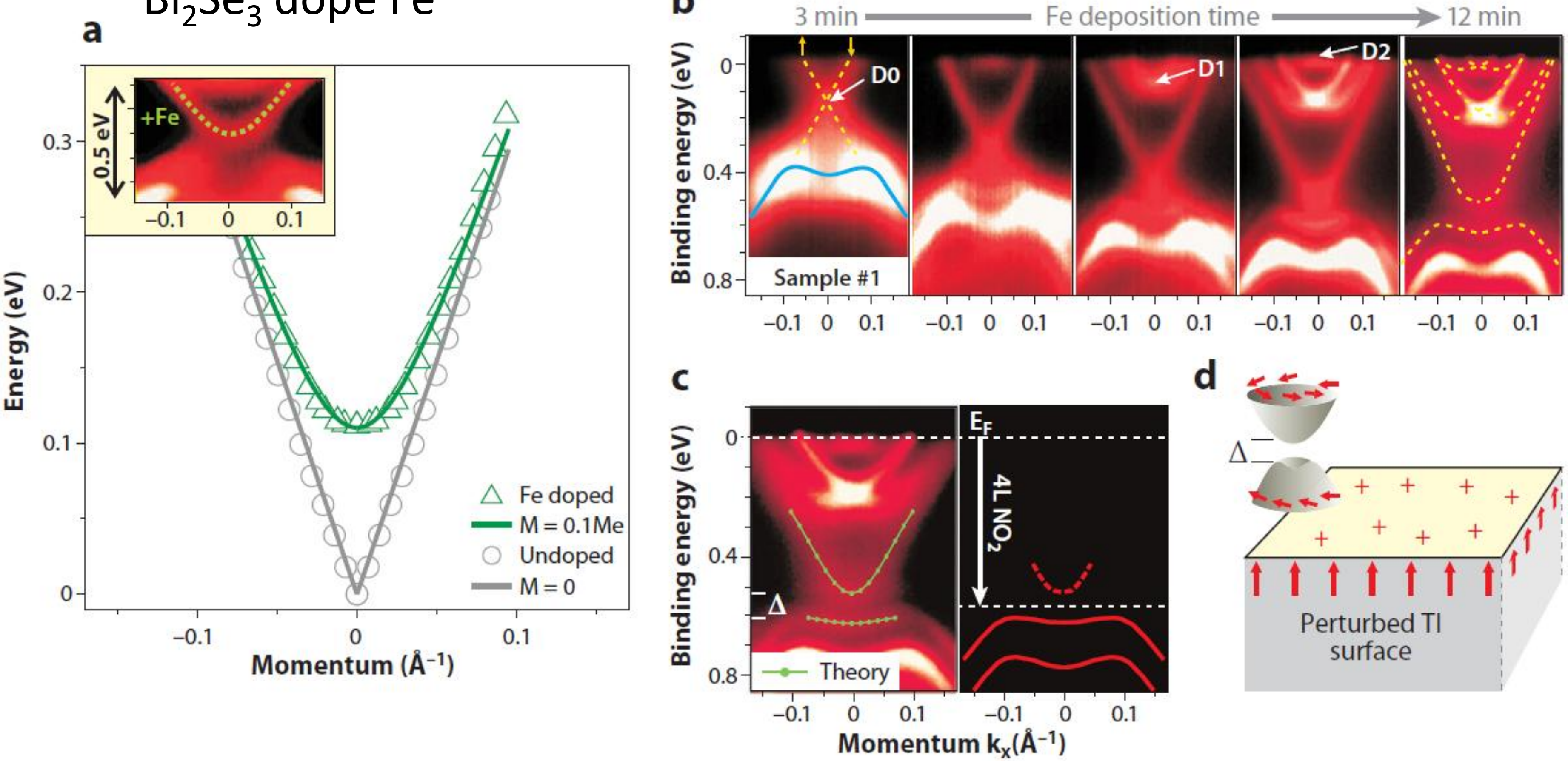
Impuretés magnétiques tuent t→-t

Expériences ?

Effet du dopage magnétique sur le spectre

Dopé initialement p avec Ca 0.25%

Bi_2Se_3 dopé Fe



Rupture t→-t
Hybridation etats de volume et de surface

Apparition de splitting de spin: effet Rashba

Propriété électromagnétiques des isolants topologiques

$$H = \int d^3r \left(\varepsilon \frac{E^2}{2} + \frac{B^2}{2\mu} \right)$$ Energie

$$S = \int d^3r dt \left(\varepsilon \frac{E^2}{2} - \frac{B^2}{2\mu} \right)$$ Action, intégrale du Lagrangien

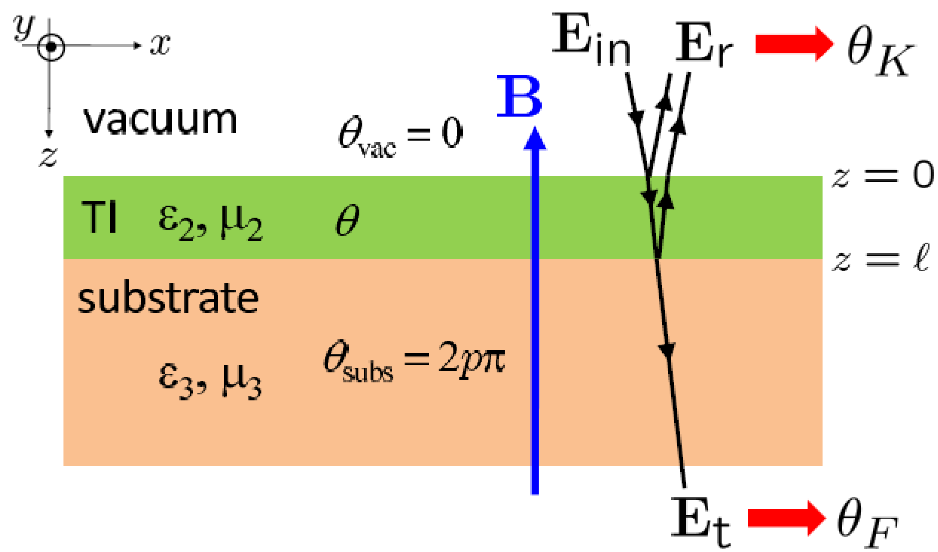
$$S_{top} = \left(\frac{\theta}{2\pi} \right) \left(\frac{\alpha}{2\pi} \right) \int dr dt \vec{E} \bullet \vec{B}$$ terme topologique

Constante de structure fine

Système invariants t→-t
Θ=0, isolants triviaux
Θ=π, isolants topologiques

Comment observer θ ?

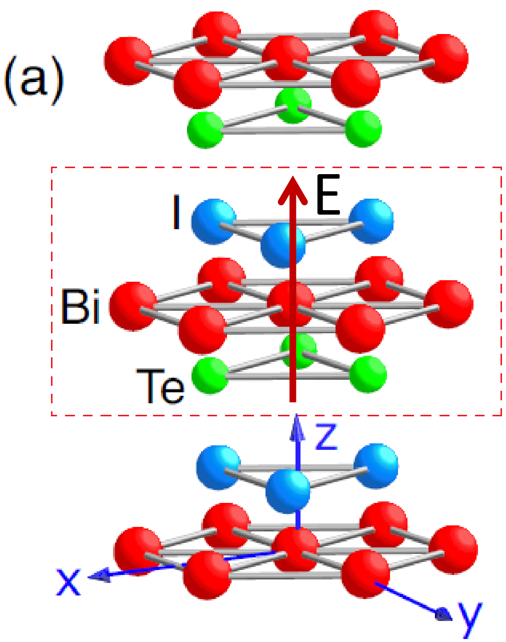
Dépôt de film magnétique Θ=π→0



Rotation Faraday et effet Kerr

Les effets sont soit petits (α=1/137)
soit nuls (compensation des 2 faces)

L'effet Rashba- BiTeI – système polaire



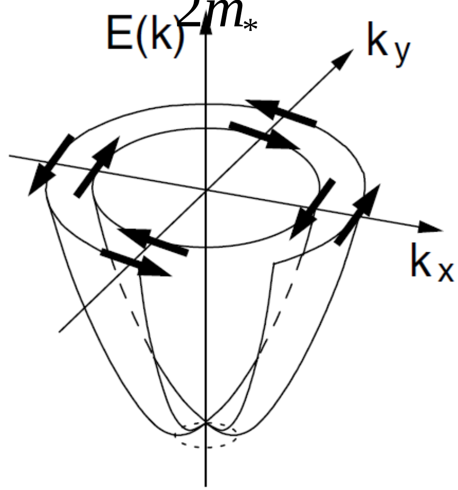
$$H = \frac{p^2}{2m_*} + \nu\vec{\sigma} \bullet \left(\vec{p} \times \vec{E}\right)$$

Champ magnétique effectif dans le référentiel propre de l'électron

$$\hbar \nu E\left(\sigma_x q_y - \sigma_y q_x\right)$$

$$= \hbar \nu E \begin{pmatrix} 0 & iq^+ \\ -iq^- & 0 \end{pmatrix}$$

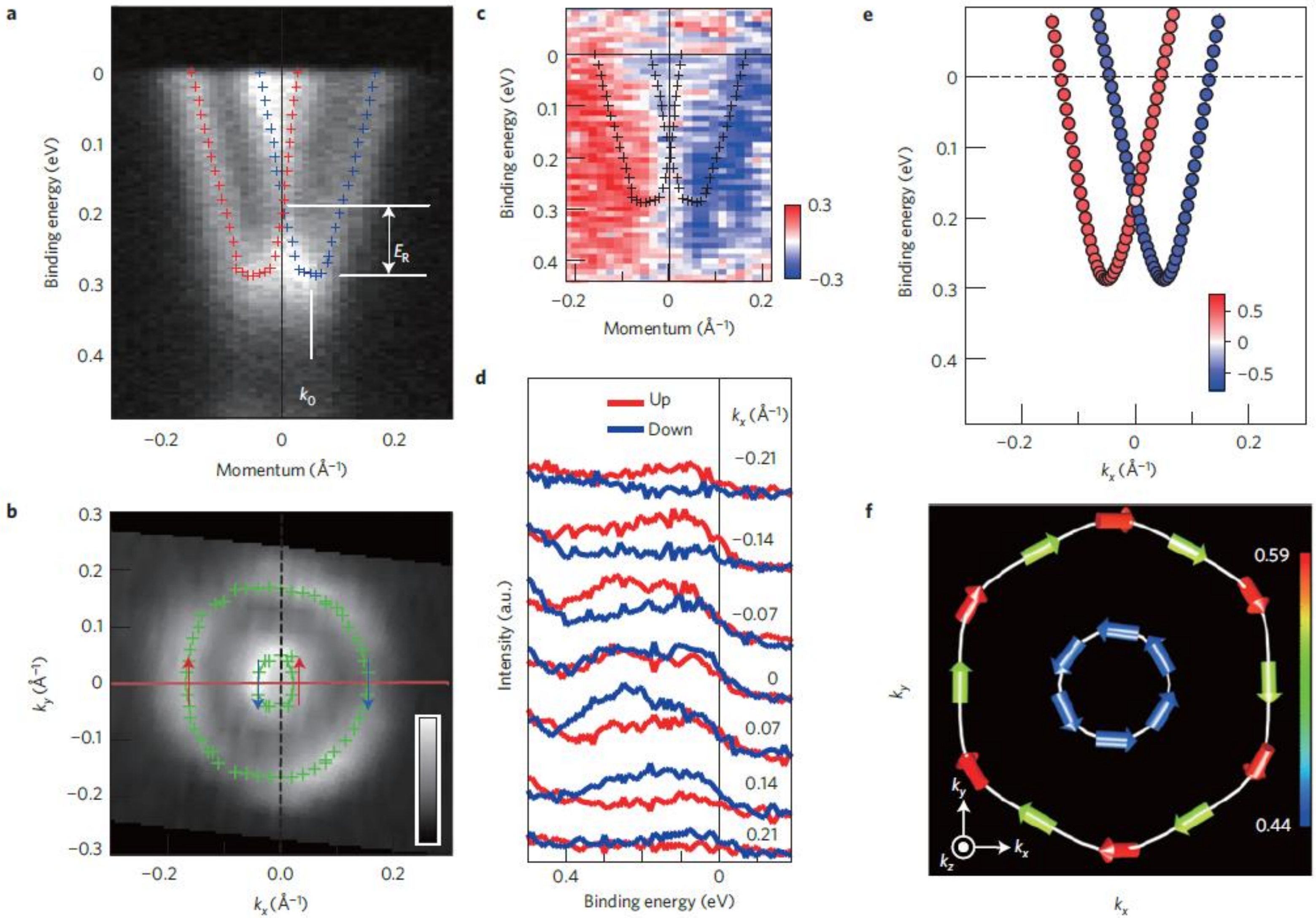
$$\varepsilon_\pm = \frac{(\hbar q)^2}{2m_*} \pm \hbar \nu E q_{//} = \frac{\hbar\left(q - q_0\right)^2}{2m_*} - \frac{\left(\hbar q_0\right)^2}{2m_*}$$



Quand on change de face
Le champ électrique change de signe

Attention: les paraboles sont remplies !

ARPES résolue en spin: spectre Rashba de BiTeI

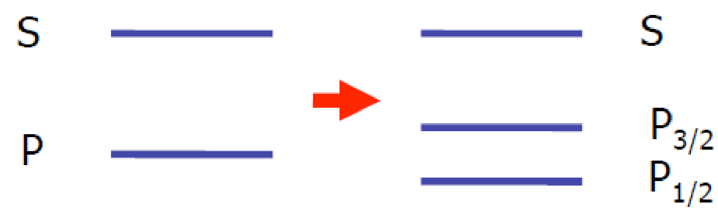


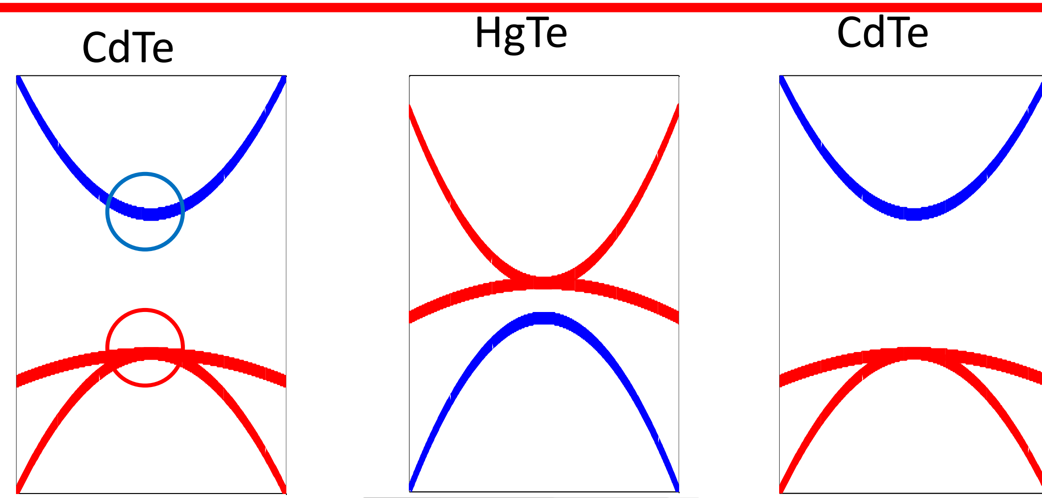
Ishizaka et al., Nat. Mat (2012)

Possibilité de fermer le gap isolant
sous pression hydrostatique (Nagaaosa)

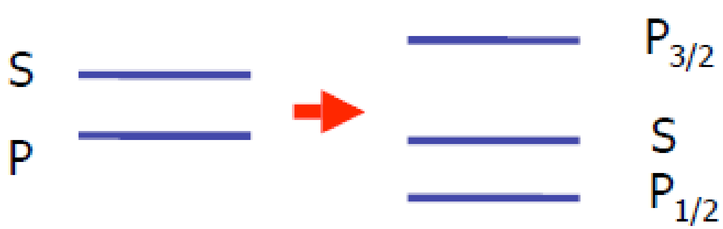
Autres familles d'isolants topologiques: HgTe, InAs/GaSb

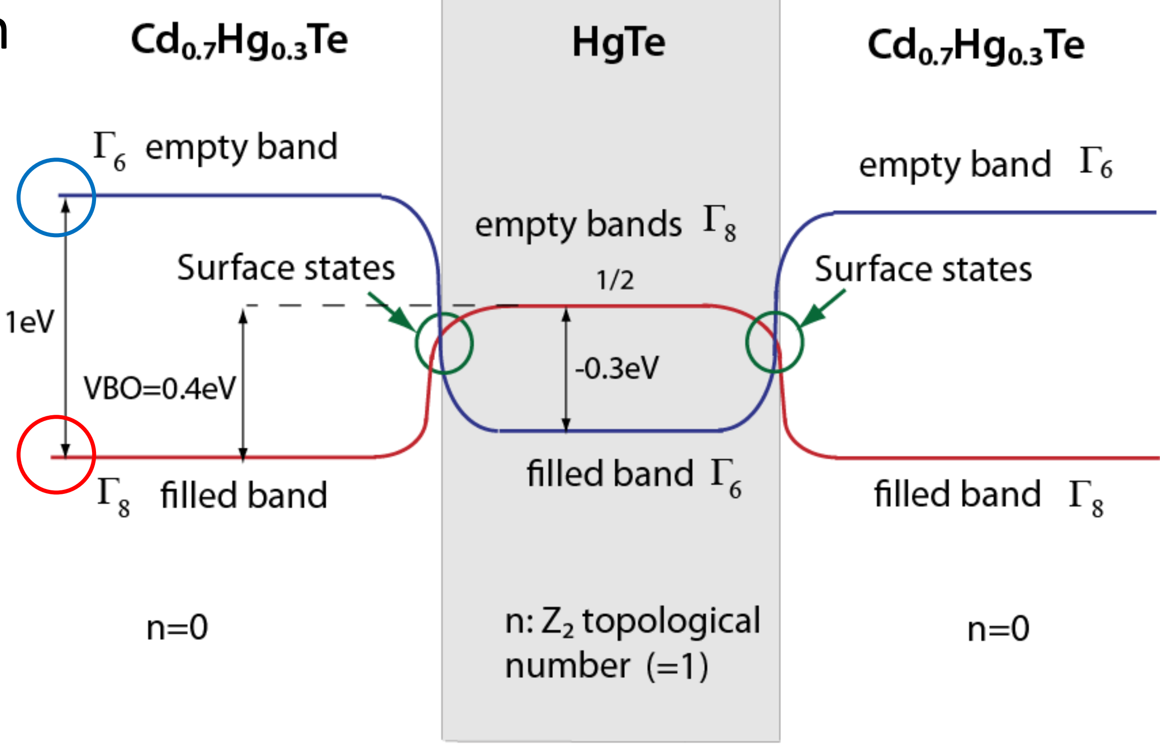
Structure de bande des HgTe-CdTe





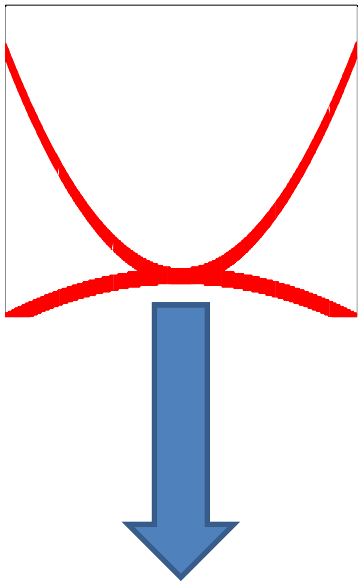
- Fort spin orbit$\Rightarrow$ inversion de bande

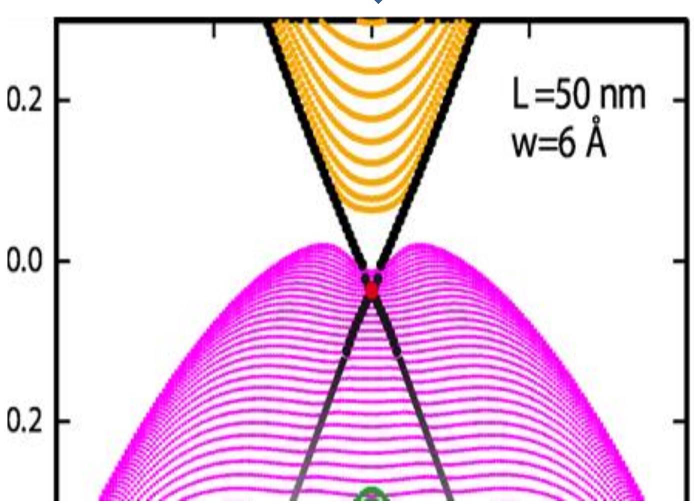


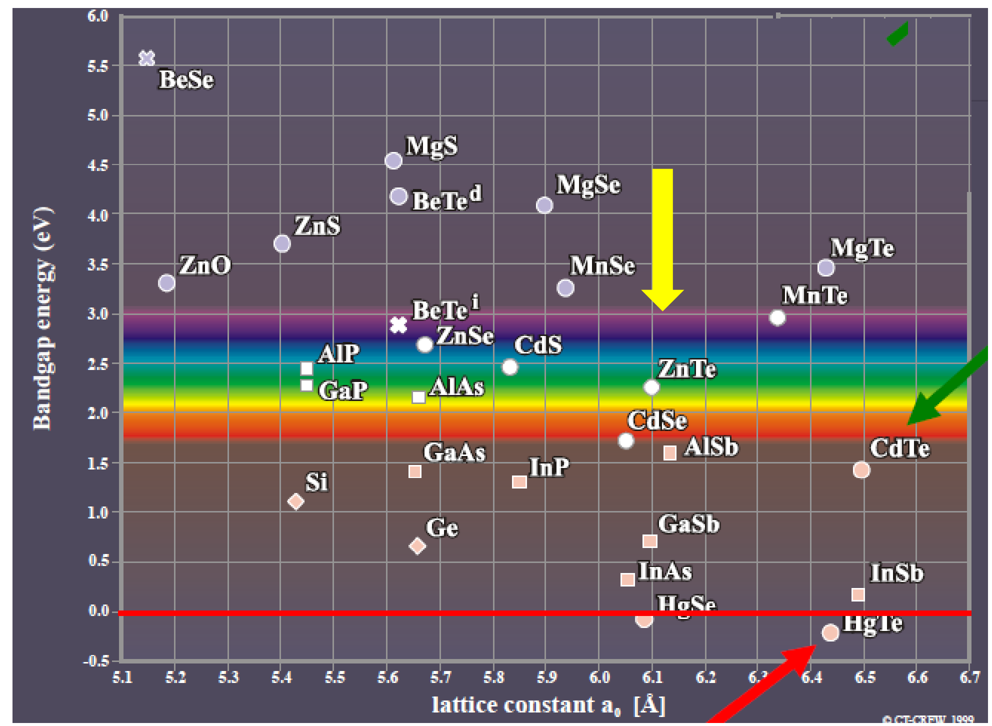


Ouverture de gap par contrainte

Semi-metal→Isolants topologiques





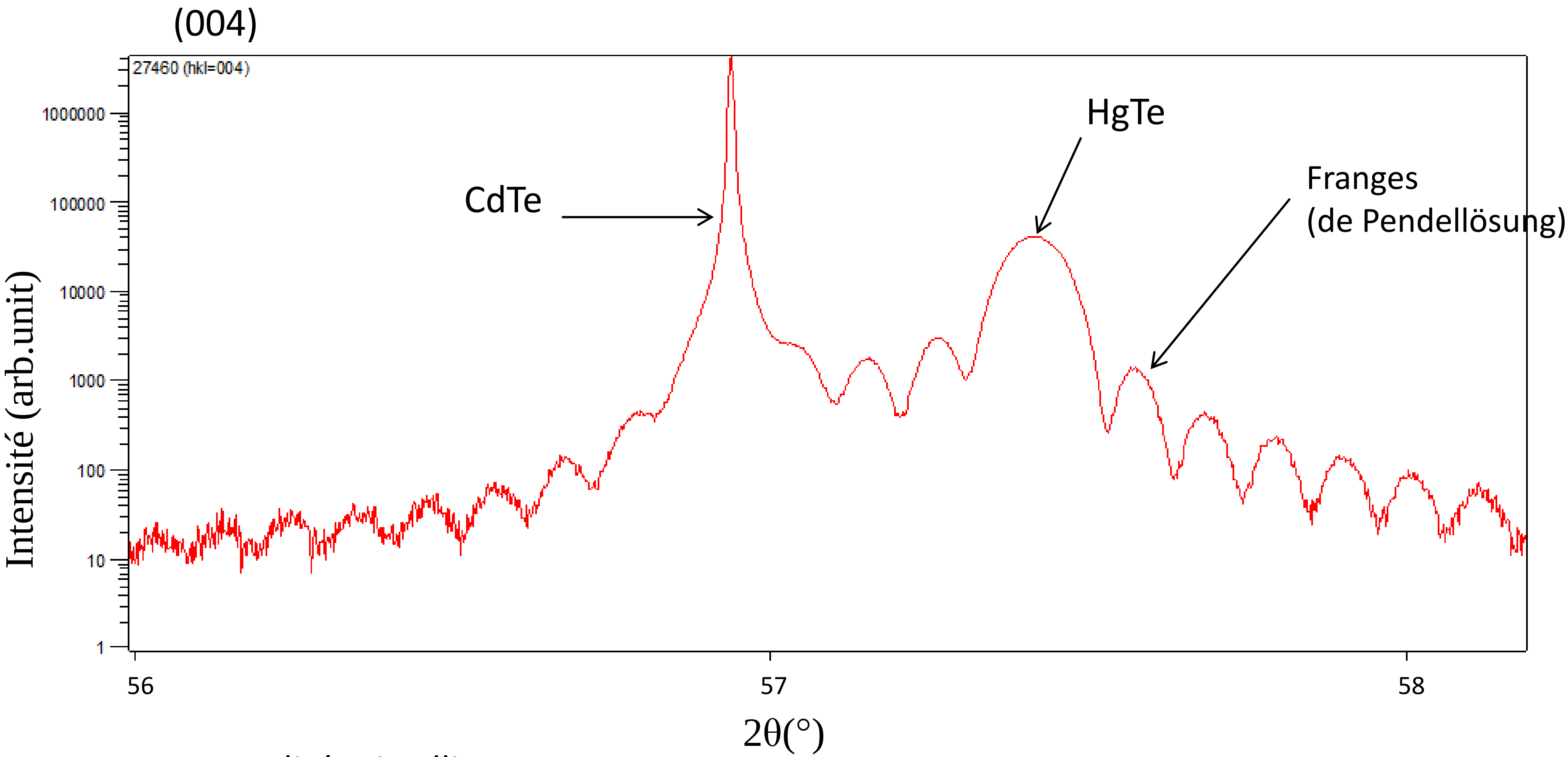


$$\text{HgTe}, \Delta_{so} = 0.99\text{eV}$$ Strong SO

$$\text{CdTe}, \Delta_{so} = 0.92\text{eV}$$

Contrainte et structure HOMOGENE

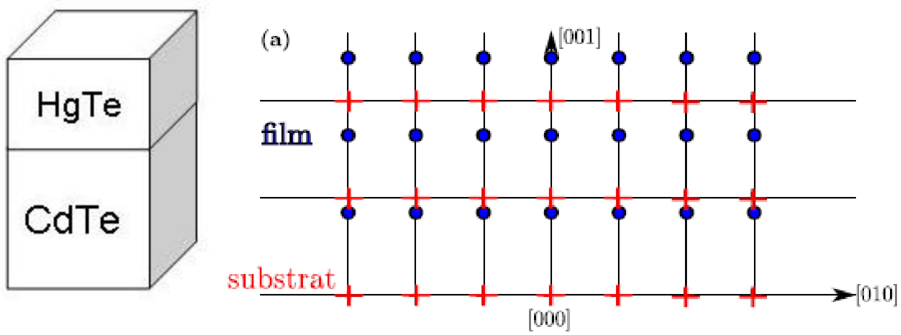
Ech : 27460 -> **buffer CdTe** + couche HgTe (100 nm)



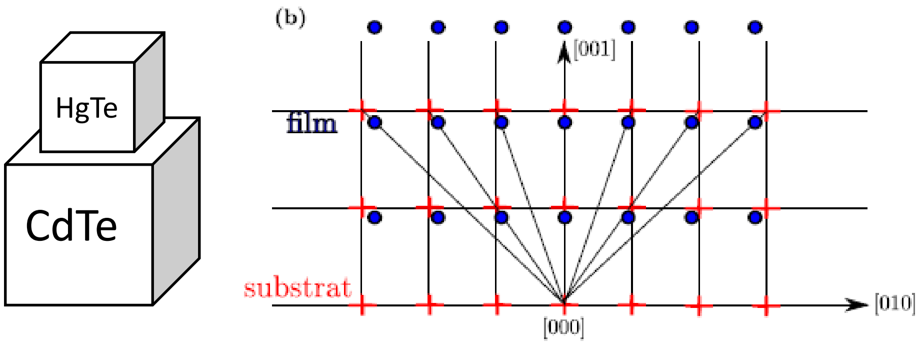
- Bonne qualité cristalline
- Contrainte uniaxiale -> estimée à 0,6%

Cartographie des contraintes dans l'espace réciproque

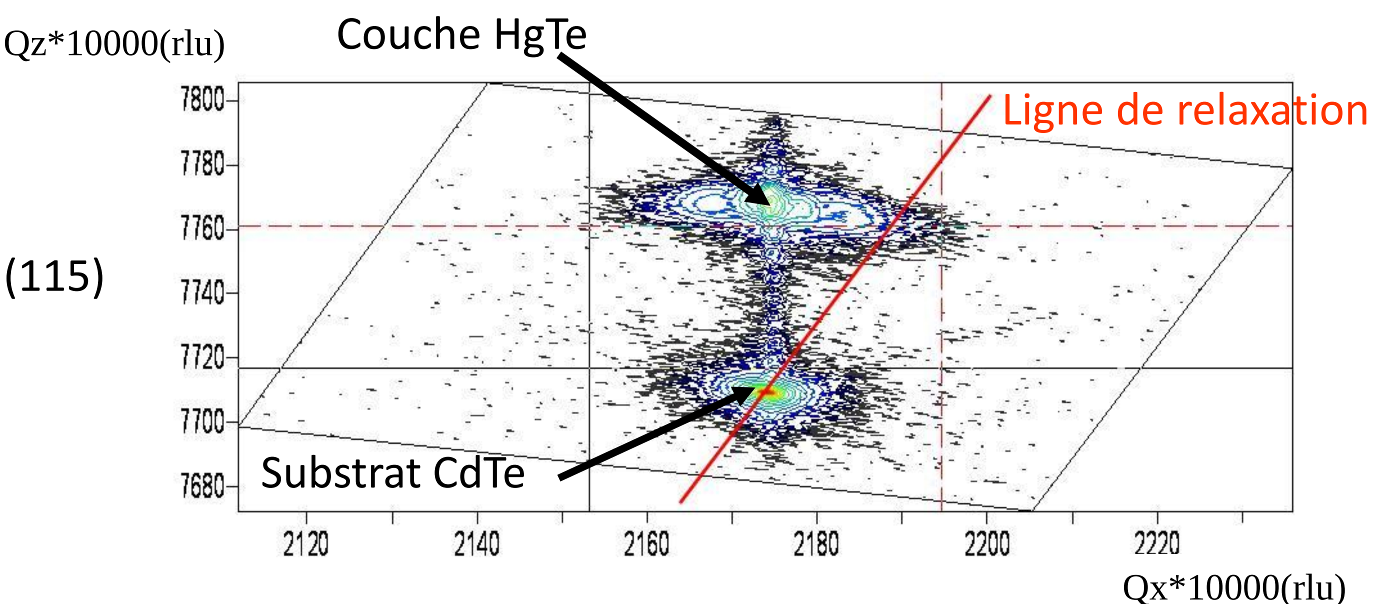
Cas contrainte homogène



Cas relaxation totale



(115)

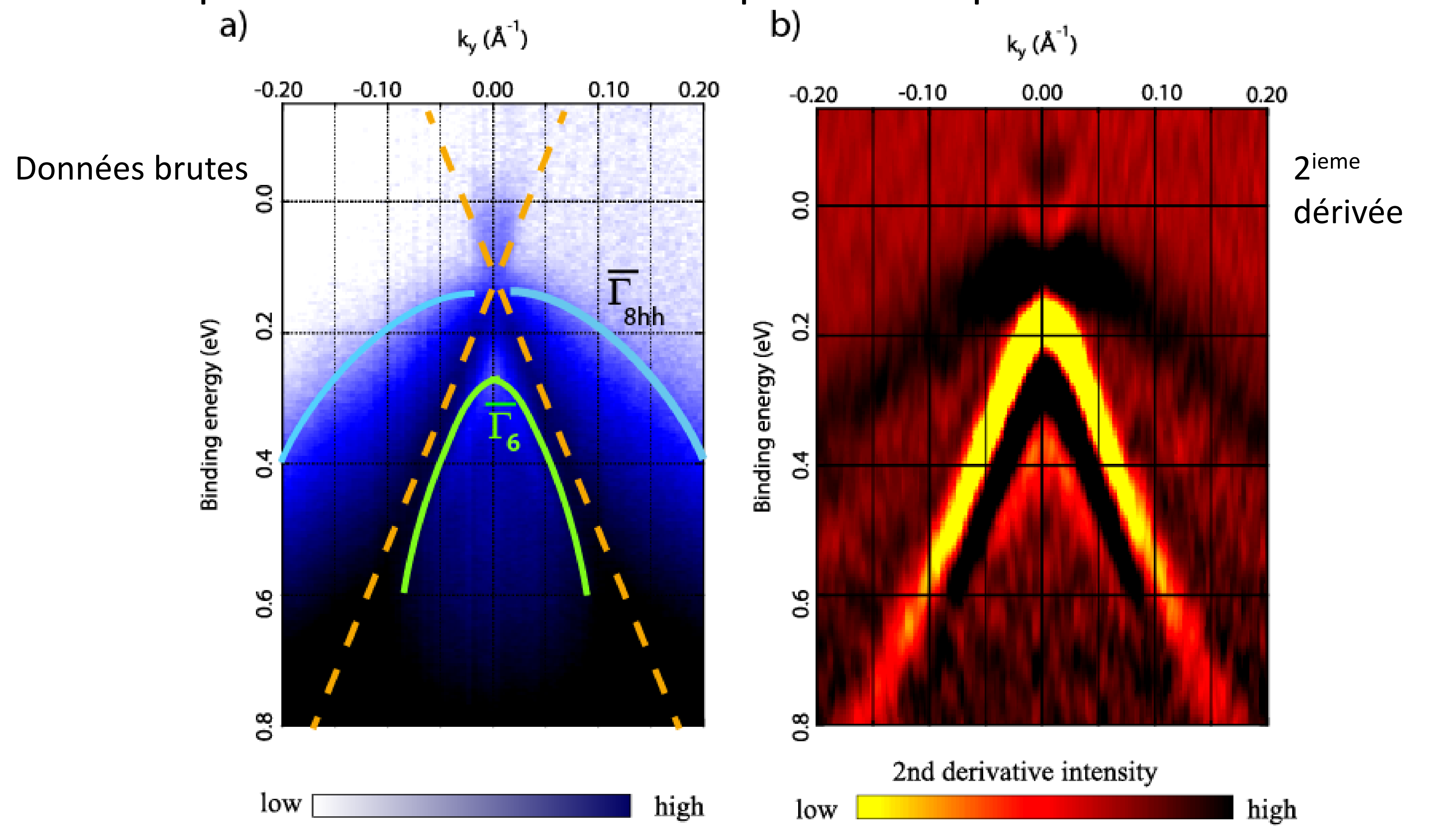


- ✓ Couche avec contrainte homogène

Ech : 27441 : épaisseur 150 nm

Spectre ARPES (polarisation-lineaire)

Spectre des etats de surface peu affecte par les etats de volume

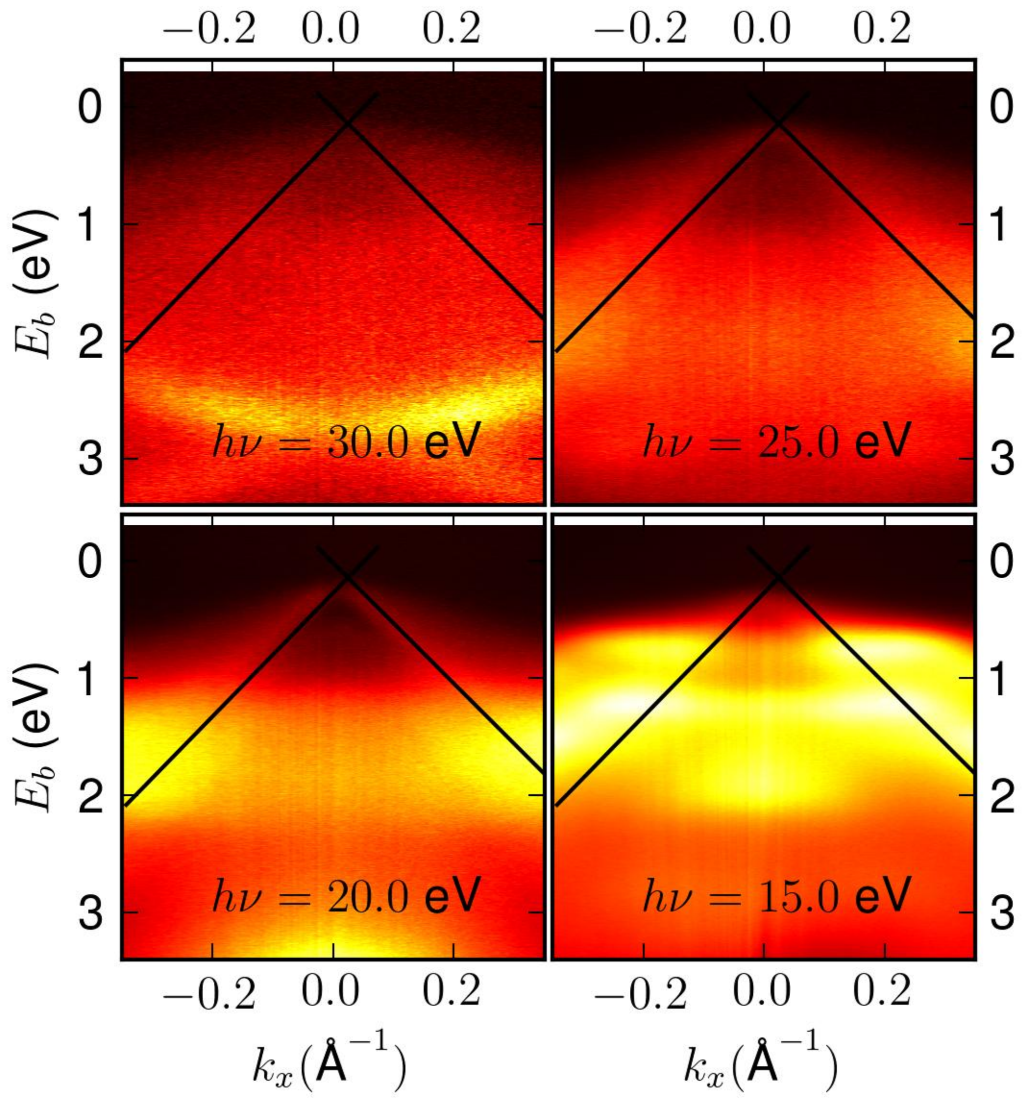


Point de Dirac≈ max de la bande Γ_{8hh} : degenerescence accidentelle!!!!!

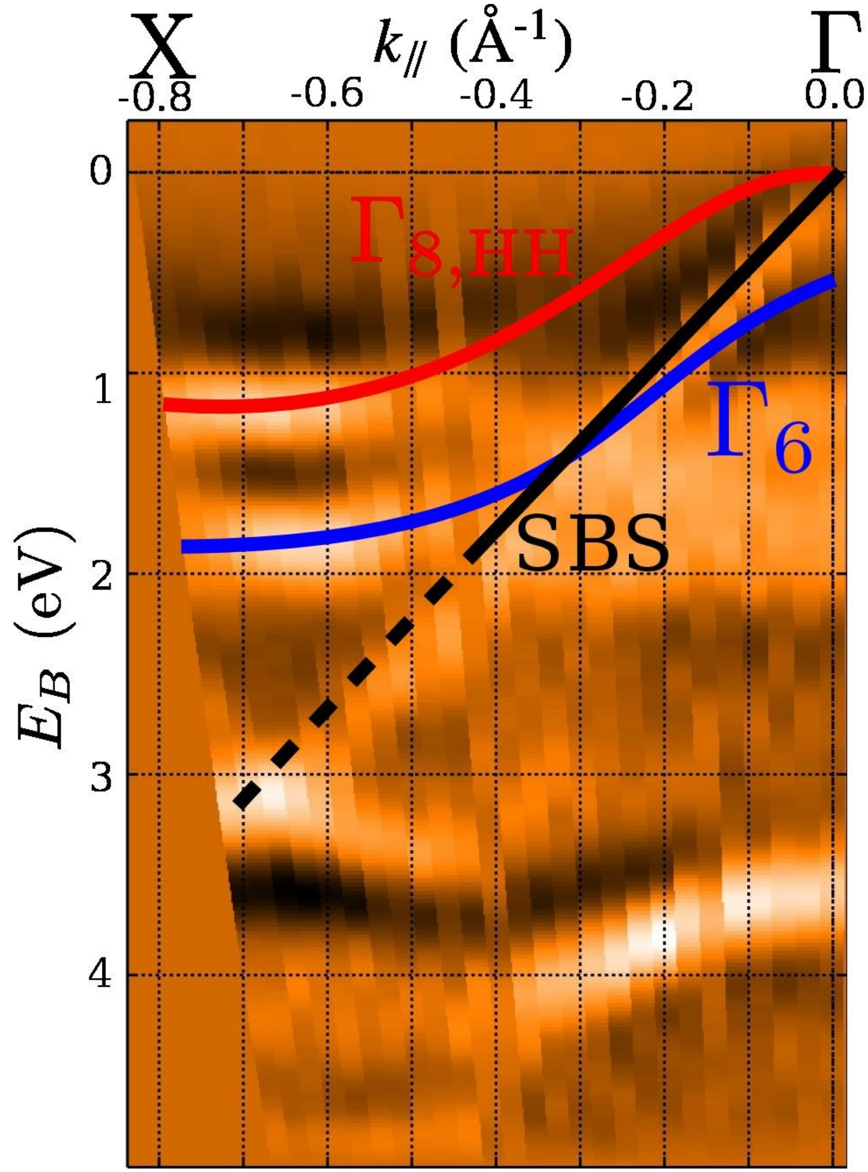
vitesse de bande v_F=510^5 m/sec

Dépendance avec l’énergie des photons

Bands independent of incident photon energy:
→surface state



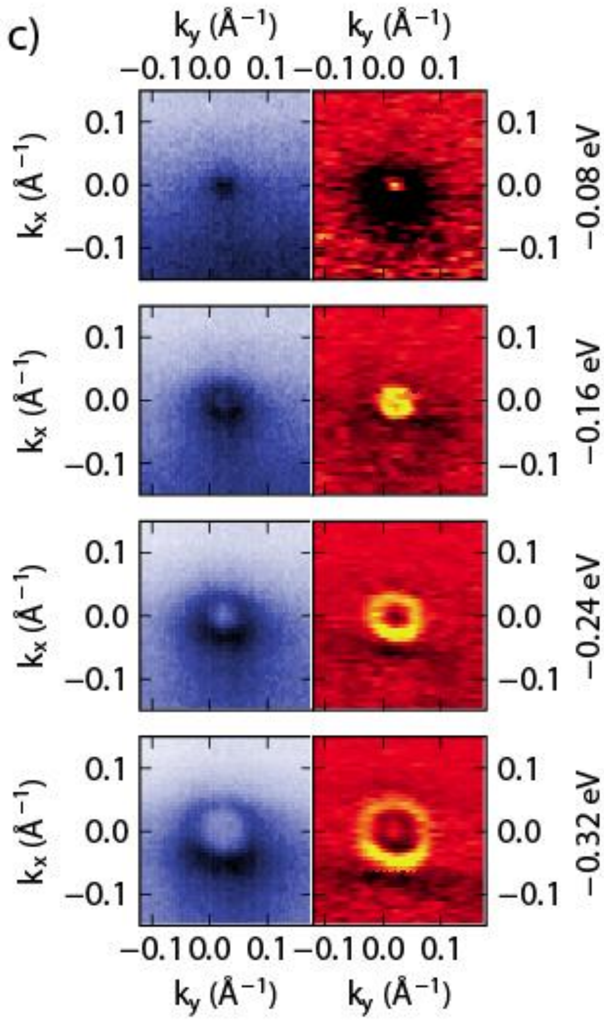
Scan large :les états de surface persistent!



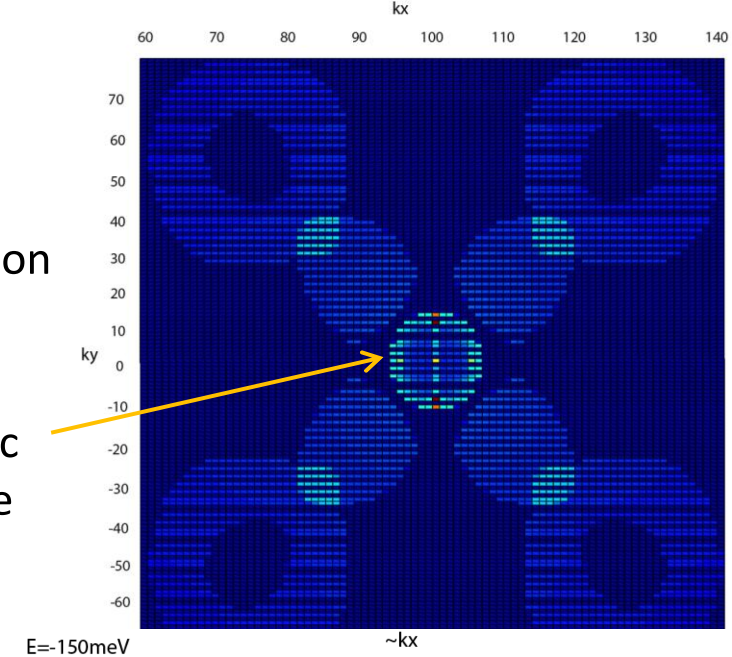
Topological argument:
SS are expected between inverted bands (Γ_6 Γ_{8lh})
More robust !!!!

Coupes a energie constante

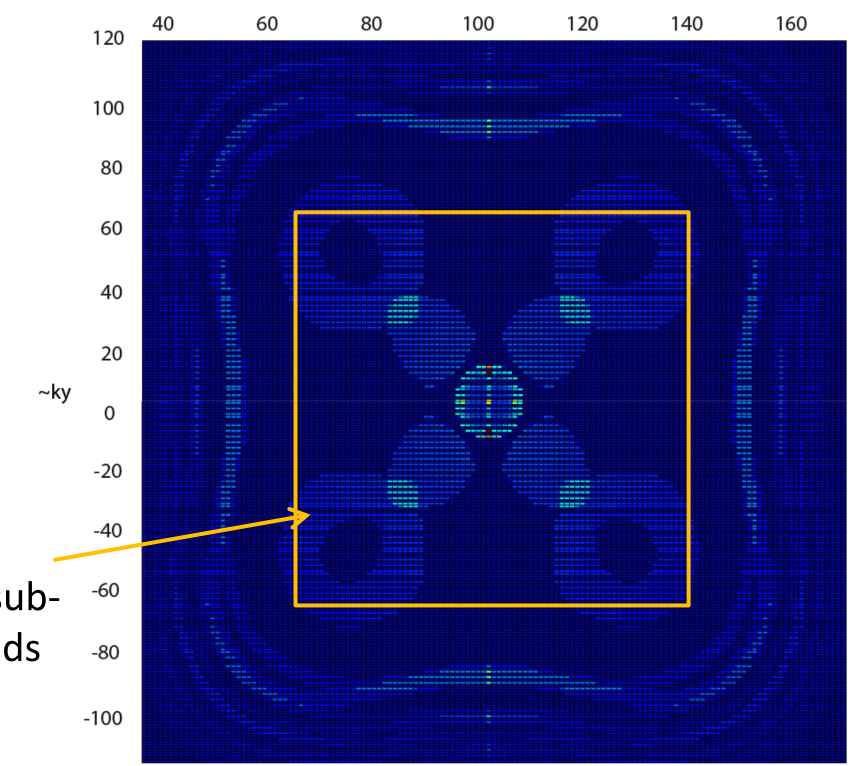
Circular section of the Dirac cone



Simulation



Dirac cone



Γ_8 sub-bands

Les structures de bandes REELLES des Zinc-Blende: le modèle de Kane

Etape 0: base d'états propres spin-orbite (Δ=1eV)

$\left|S, J=\frac{1}{2}, m_j\right\rangle$ $u_1(r) = |\Gamma_6, +1/2\rangle; u_2(r) = |\Gamma_6, -1/2\rangle$

$\left|P, J=\frac{3}{2}, m_j\right\rangle$ $u_3(r) = |\Gamma_8, +3/2\rangle; u_4(r) = |\Gamma_8, +1/2\rangle; u_5(r) = |\Gamma_8, -1/2\rangle; u_6(r) = |\Gamma_8, -3/2\rangle$

$\left|P, J=\frac{1}{2}, m_j\right\rangle$ $u_7(r) = |\Gamma_7, +1/2\rangle; u_8(r) = |\Gamma_7, -1/2\rangle$

$$H = \begin{pmatrix} T & 0 & 0 & 0 & ...0... & ....0... & ..0.. & 0 \\ 0 & T & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & U+V & 0, & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U-V & 0 & 0 & 0 & 0 \\ 0 & 0 & .....0.... & ...0.... & U-V & 0 & 0 & ..0.. \\ 0 & 0 & 0 & 0 & 0 & U+V & 0 & 0 \\ 0 & 0 & 0 & 0, & 0 & 0 & \Delta & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta \end{pmatrix}$$

$$T = E_c(z) + \frac{\hbar^2}{2m_0}\left(k_\parallel^2 + k_z^2\right)$$

$$U = E_v(z) - \frac{\hbar^2}{2m_0}\gamma_1\left(k_\parallel^2 + k_z^2\right)$$

$$V = -\frac{\hbar^2}{2m_0}\gamma_2\left(k_\parallel^2 - 2k_z^2\right)$$

MAIS EK=P²/2m N'EST PAS DIAGONAL DANS LA BASE SPIN-ORBITE

Energie cinétique non-diagonale dans la base SO

$$\left|L=1, S=\frac{1}{2}; J=\frac{3}{2}, m_J=\frac{1}{2}\right\rangle = \langle\ |\ \rangle \left|1,1;\frac{1}{2},-\frac{1}{2}\right\rangle + \langle\ |\ \rangle \left|1,0;\frac{1}{2},\frac{1}{2}\right\rangle$$

Addition des moments cinétiques

Approximation dite « k.P »: expansion autour des points de symétrie Γ (k=0)
Méthode de la fonction enveloppe (voir le livre de Bastard)

Γ_6 : $\frac{1}{2}$, $-\frac{1}{2}$ $\qquad$ Γ_8 : $\frac{3}{2}$, $\frac{1}{2}$, $-\frac{1}{2}$, $-\frac{3}{2}$

$$\begin{pmatrix}
T & 0 & -\sqrt{\frac{1}{2}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \sqrt{\frac{1}{6}}Pk_- & 0 \\
0 & T & 0 & -\sqrt{\frac{1}{6}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & -\sqrt{\frac{1}{2}}Pk_- \\
-\sqrt{\frac{1}{2}}Pk_- & 0 & U+V & \approx 0 & \approx 0 & 0 \\
\sqrt{\frac{2}{3}}Pk_z & \sqrt{\frac{1}{6}}Pk_- & \approx 0 & U-V & \approx 0 & 0 \\
\sqrt{\frac{1}{6}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \approx 0 & \approx 0 & U-V & \approx 0 \\
0 & \sqrt{\frac{1}{2}}Pk_+ & 0 & 0 & \approx 0 & U+V
\end{pmatrix}$$

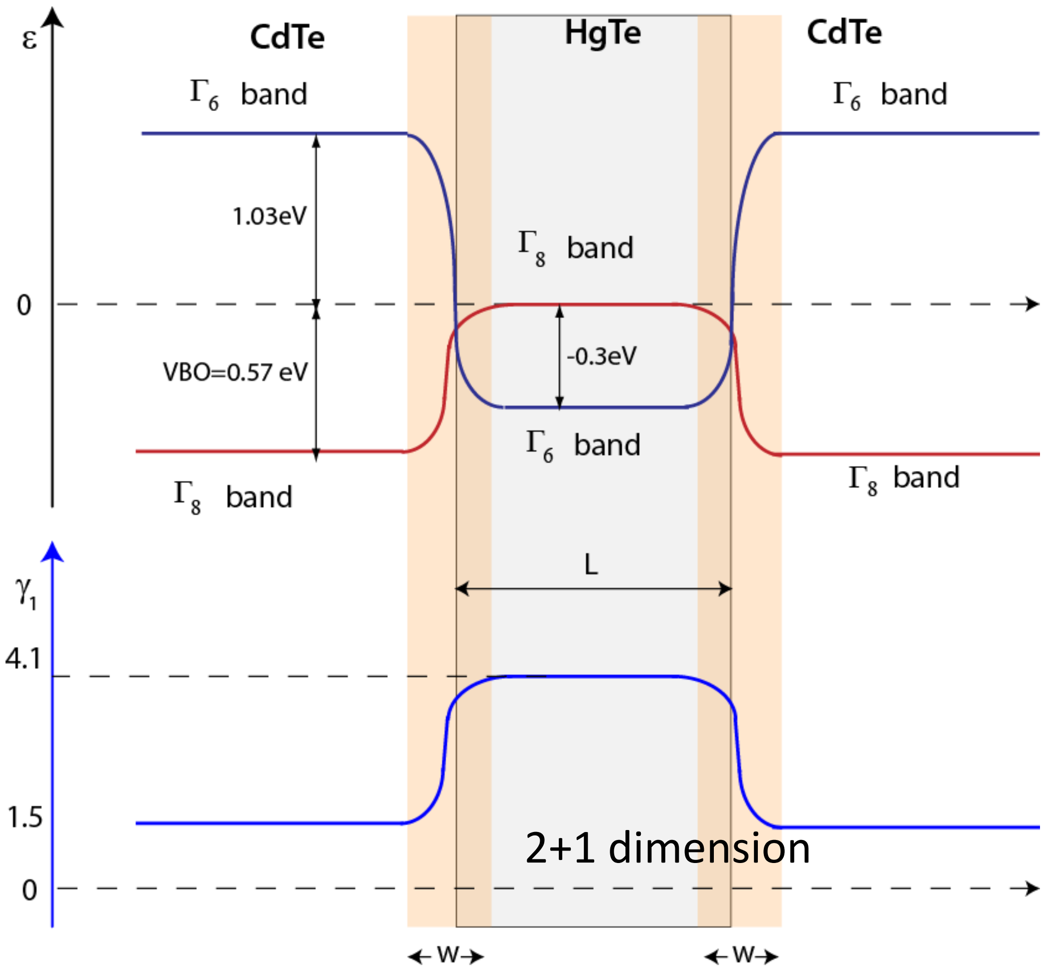
Système inhomogène

$$k_z \rightarrow \frac{1}{i}\frac{\partial}{\partial z}$$

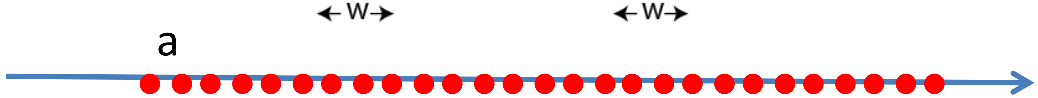
P est très grand ($P^2/2m$=19eV)

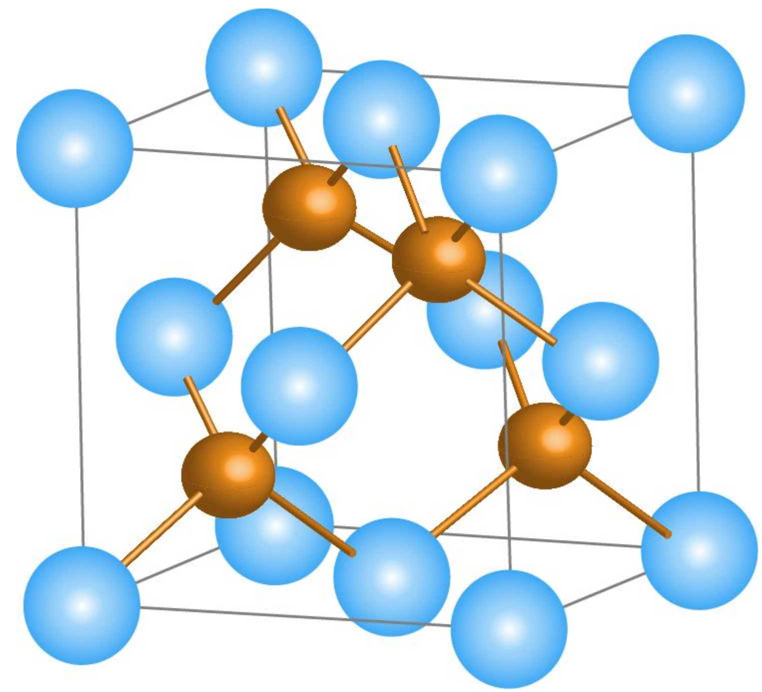
Valide k <0.1
Ajouter des termes qui décrivent l'effet de bandes lointaines

Structure de bandes des systèmes inhomogènes



2+1 dimension





Zinc-Blende materials
GaAs, InAs, GaSb CdTe, ZnTe

8-band Kane model
H(k||, ∂/∂z)

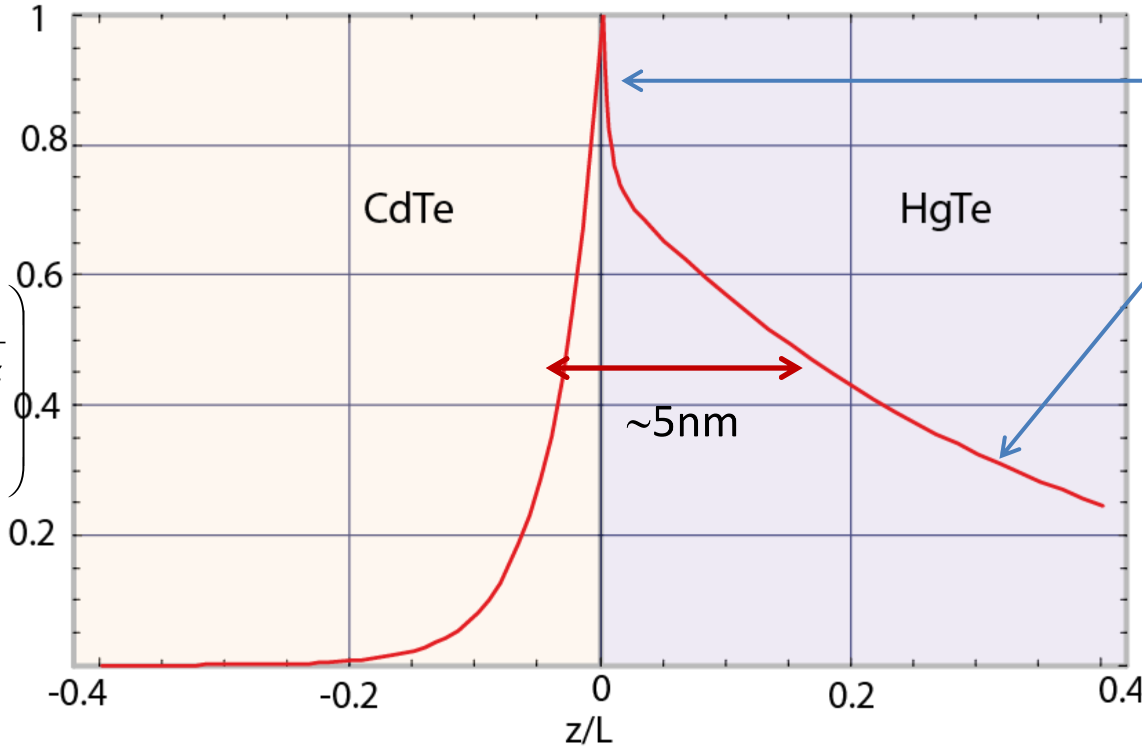
Good quantum number

Etats de surface au point de Dirac

k=0

$$\begin{pmatrix} \Gamma_6 & \Gamma_8 \\ T & -i\sqrt{\frac{2}{3}}P\frac{\partial}{\partial z} \\ i\sqrt{\frac{2}{3}}P\frac{\partial}{\partial z} & U-V \end{pmatrix}$$

+BC
=eigenstates
SS at Dirac point



E_D depends on BC

$$\psi(z=0)=0 \Rightarrow E_D = \frac{\gamma}{\gamma+1}E_g \approx -0.25eV$$ below Γ_{8hh}

Band velocity
(wo Γ_{8hh} hybridzation)

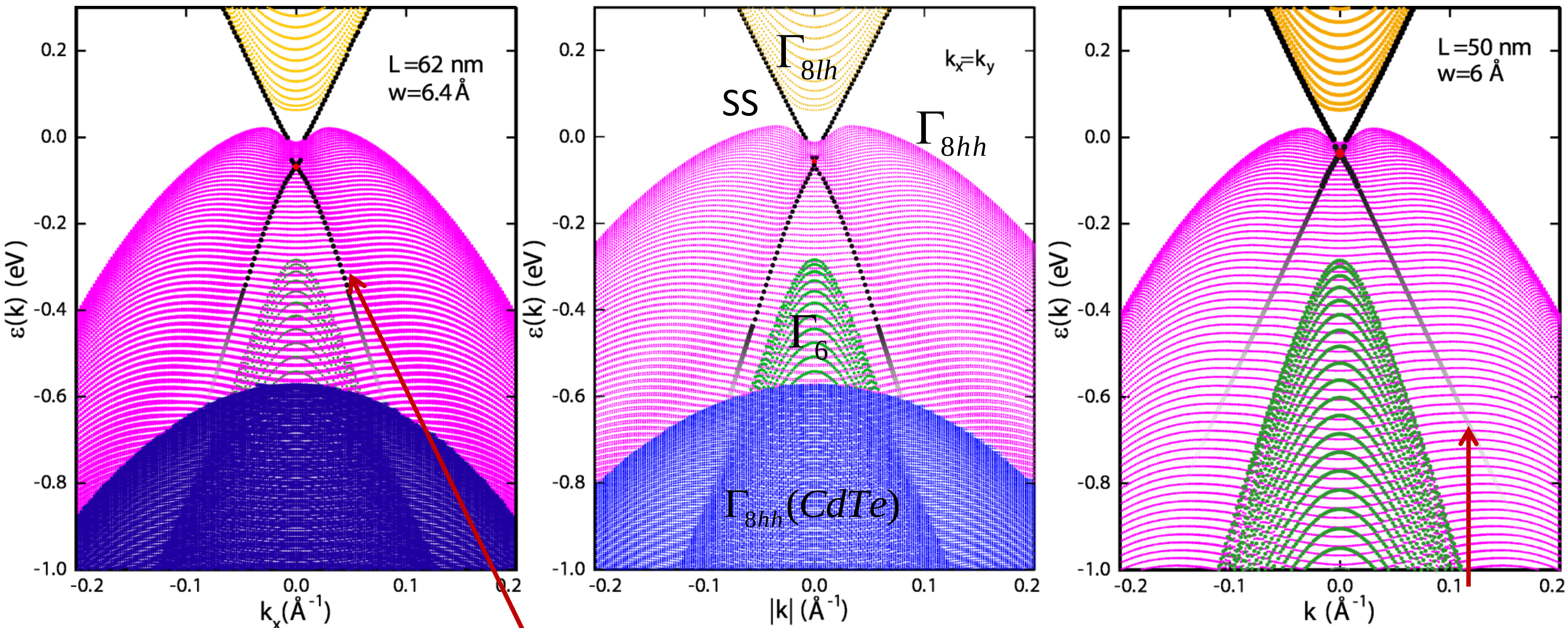
$$\hbar v_F = \sqrt{\frac{\gamma^2-1}{\gamma^2+1}}\sqrt{\frac{1}{6}}P$$

Jouffrey-Delplace-Carpentier

Etude numérique-a

Close to the experiment !

CdTe/HgTe/CdTe   CdTe/HgTe/CdTe   Vac/HgTe/Vac



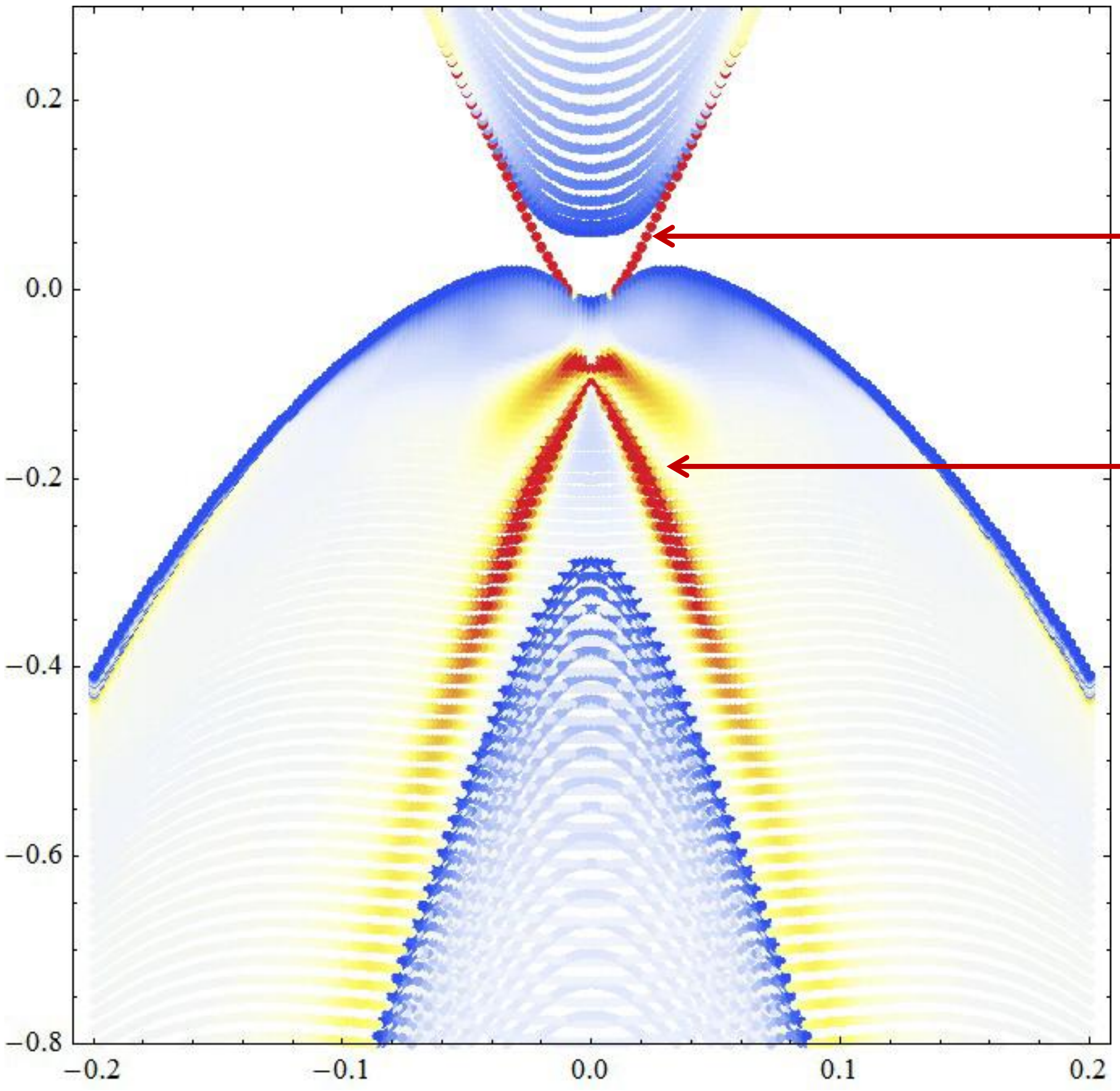
Γ-X1   Γ-K

Broadening
Of SS with
bulk hybridation
for k>0.1

Pente 5.5 10^5 m/sec
vF≡P/√6

En accord avec les expériences

Densité projetée sur la surface (5nm)



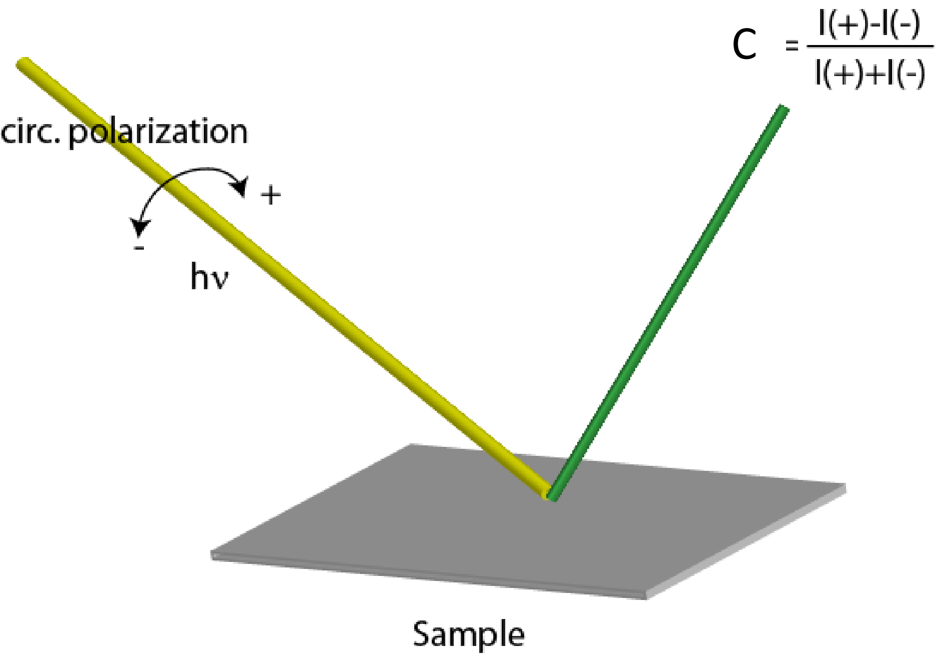
(CdTe/HgTe/CdTe

SS (gap-branch)

SS (volume-branch)

Differ by their spin

Dichroïsme circulaire en ARPES



$$C = -|a|^2 \langle S_z \rangle \cos\phi + 4ab \langle S_x \rangle \sin\phi$$

depend on the crystal symmetries at the surface

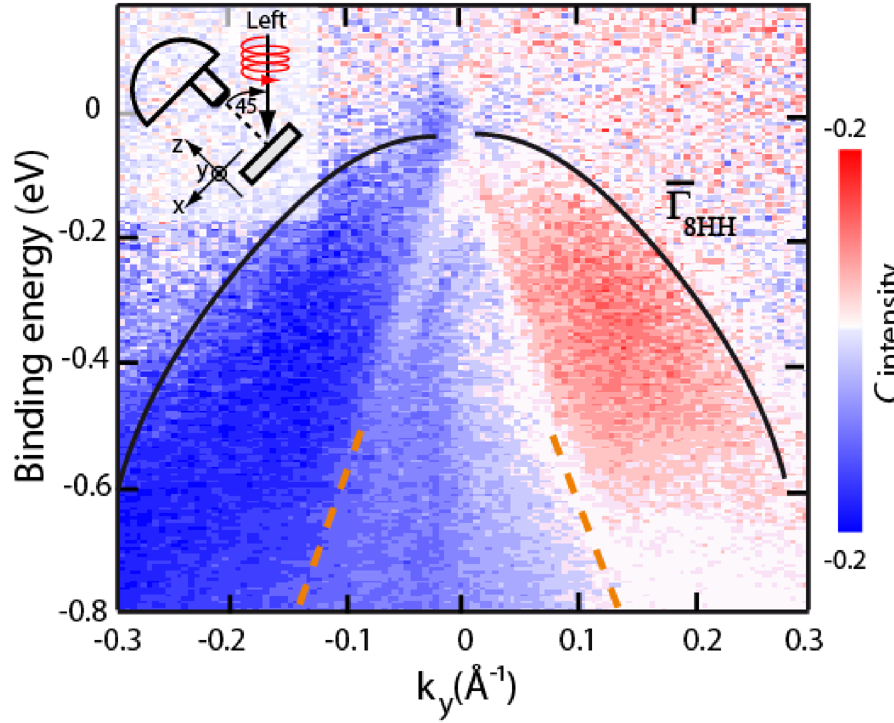
$$b << a$$

$$C \propto \langle S_z \rangle$$

Dichroïsme circulaire

$$C = -|a|^2 \langle S_z \rangle \cos\phi + 4ab \langle S_x \rangle \sin\phi$$

depend on the crystal symmetries at the surface



HgTe: $T_d \rightarrow C_{2v}$ (strain + surface)

$$\langle \Phi_f | P_x + iP_y | \Phi_i \rangle = ia$$

$$\langle \Phi_f | P_z | \Phi_i \rangle = ib$$

$$\vec{P} = \frac{e}{m}\vec{p} - \frac{\hbar e}{4m^2c^2}\vec{E} \times \vec{S}$$

$$b << a$$

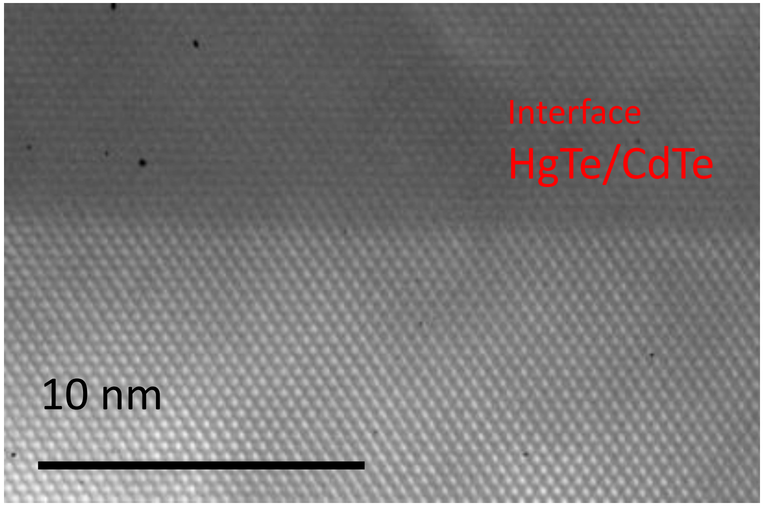
$$C \propto \langle S_z \rangle$$

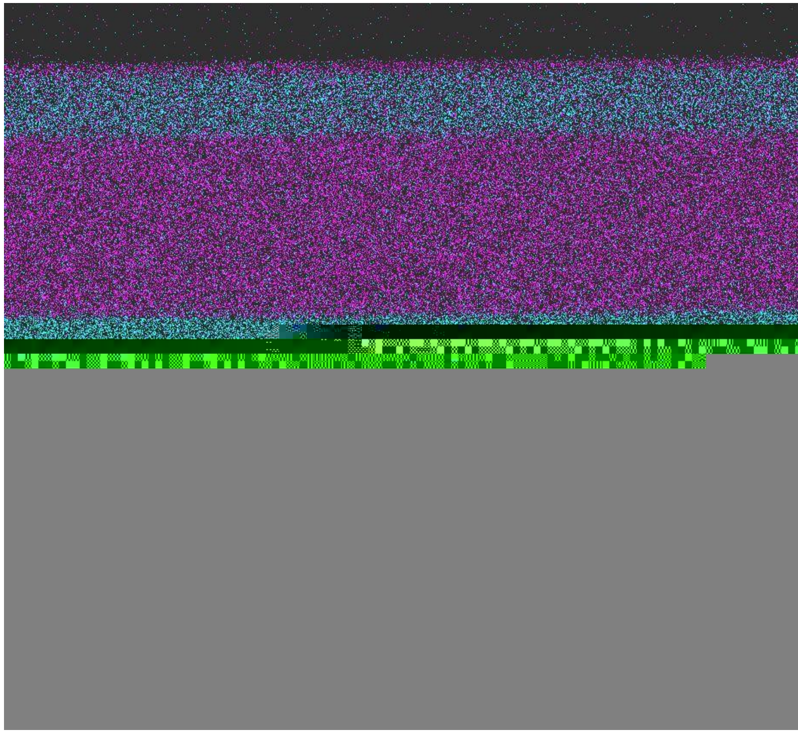
No dichroism from the surface state

20% dichroism from Γ_{8hh}

Dichroisme de la bande Γ_{8hh}

- Rashba: SO with surface E_z electric field ⟵ Surface electric field
- Dresselhaus (BIA) but also SIA ⟵ (Hg vs Te termination)





Petit résumé

- L’observation des états de surface 3D demontrent réalité aux isolants topologiques
- Spécificité d’HgTe: le point de Dirac point est au sommet de la bande de valence
- SS peu affecte par les bandes de volume, stable la ou la protection topologique n’est plus effective
- Le dichroïsme circulaire révèle une polarisation $\langle S_z \rangle$ des bandes Γ_{8hh} de volume alors que les SS n’ont pas de polarisation dans cette direction