

Tailoring the electronic structure of a topological insulator via the surface structure



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Physics & Astronomy

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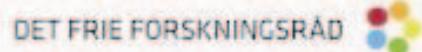
Malthe Stensgaard

Xie-Gang Zhu

Wendell Simoes da Silva

Søren Ulstrup

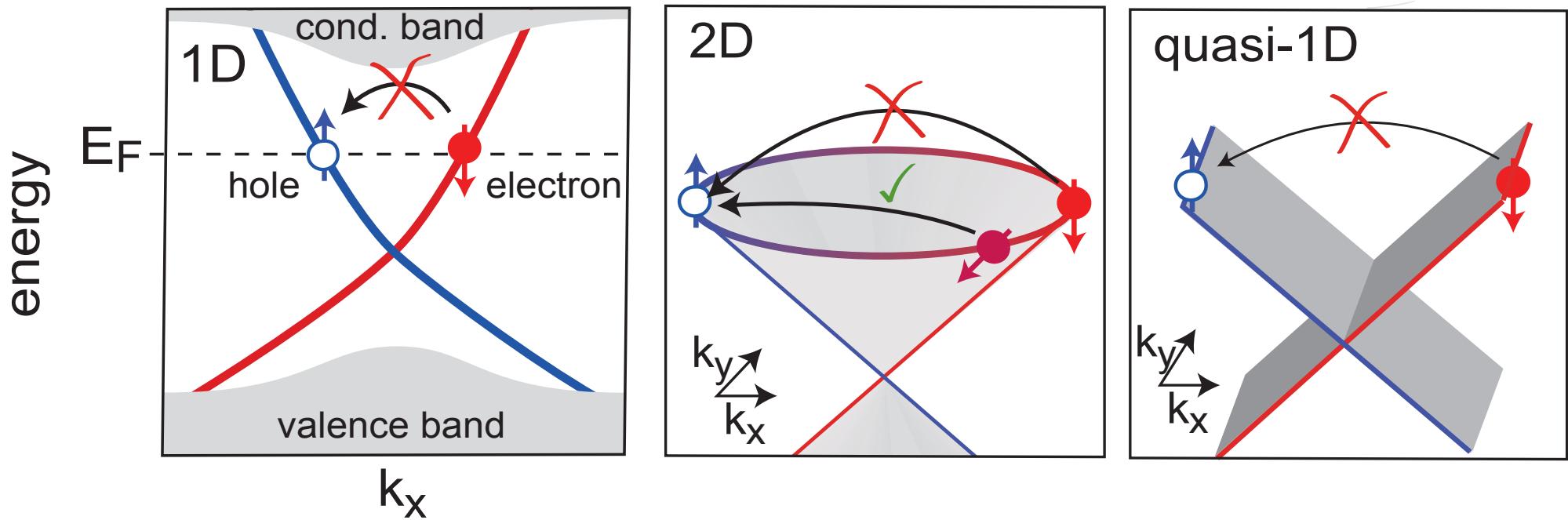
Maciej Dendzik



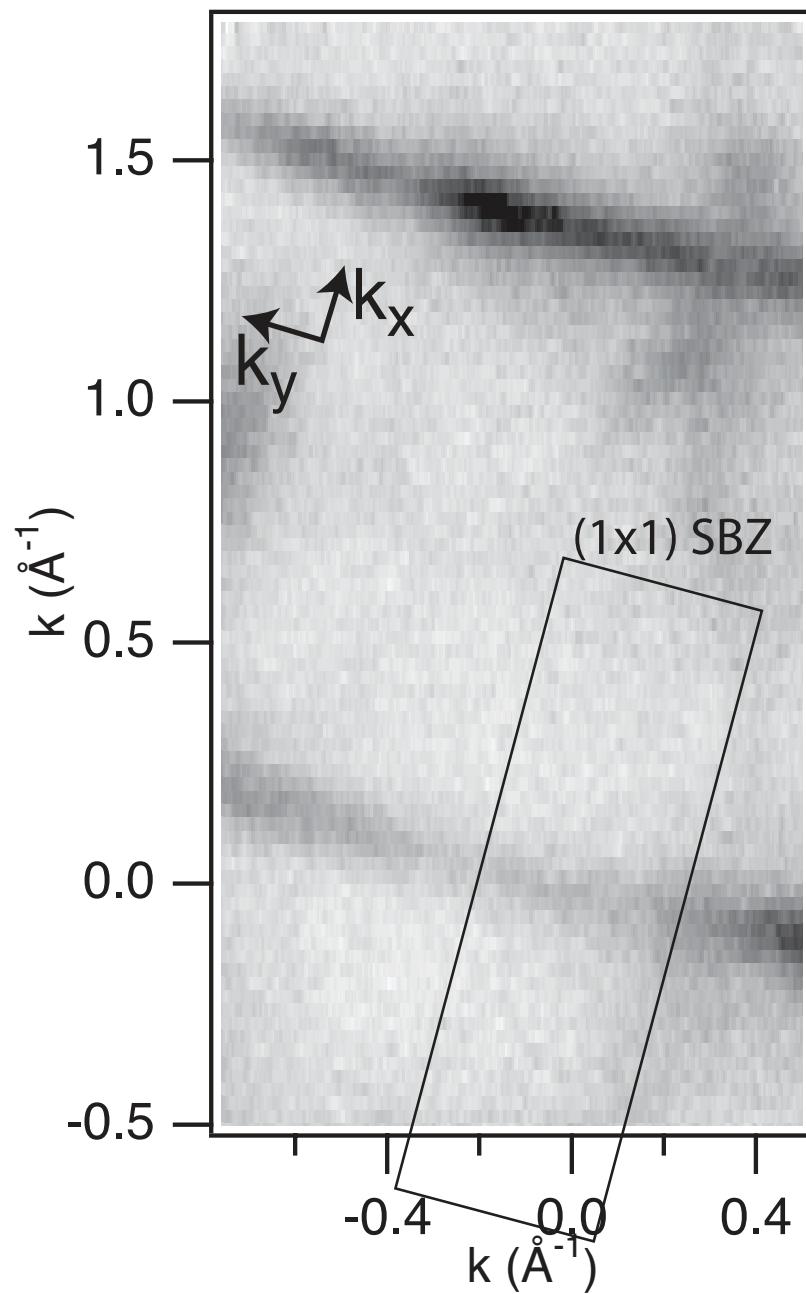
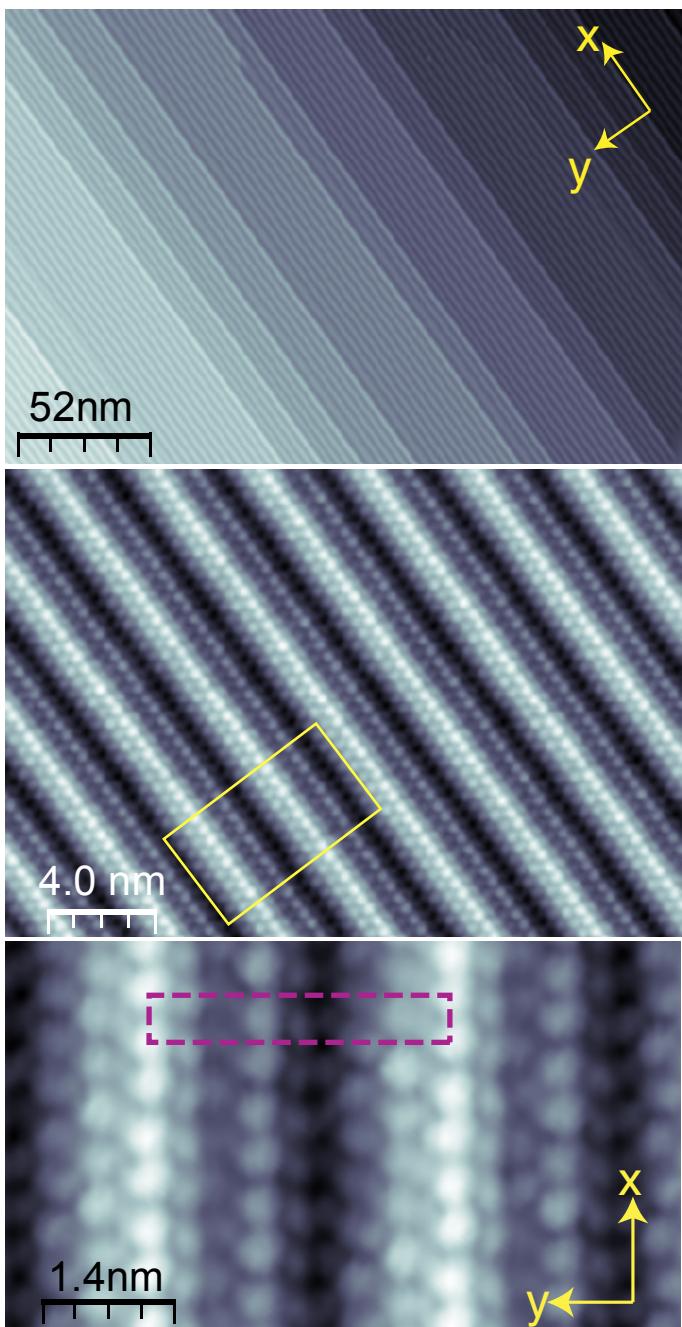
outline

- introduction and motivation
- $\text{Bi}_{1-x}\text{Sb}_x(110)$: experiment
- tight-binding calculations

the problem of scattering

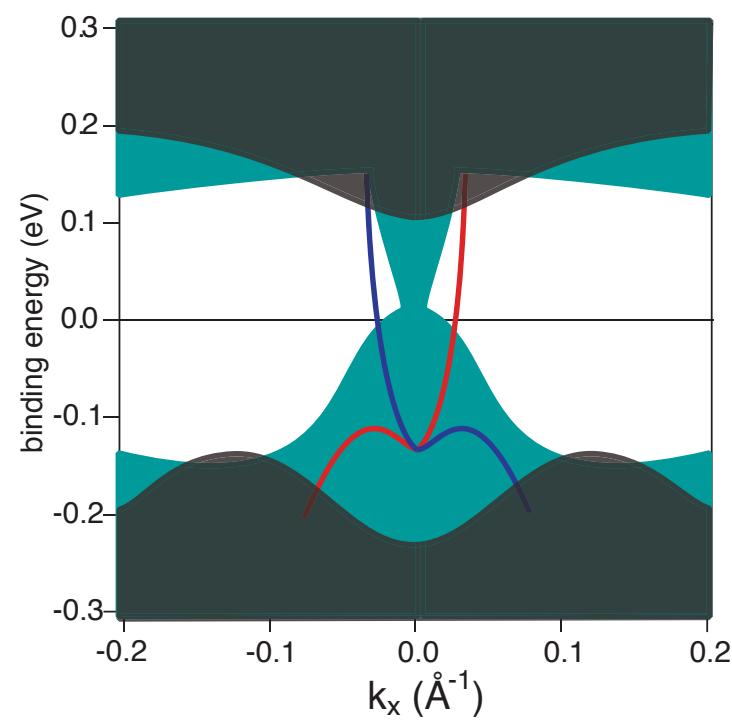
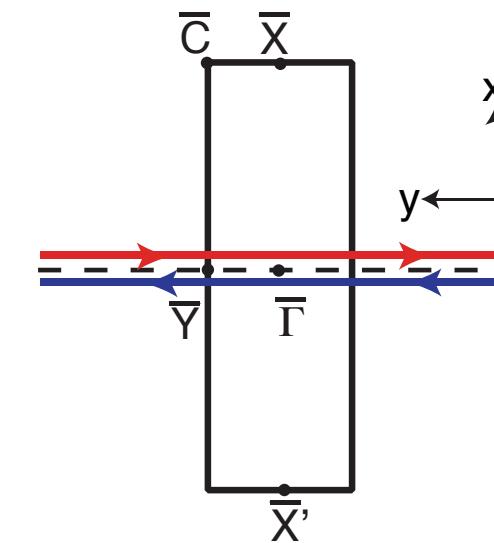
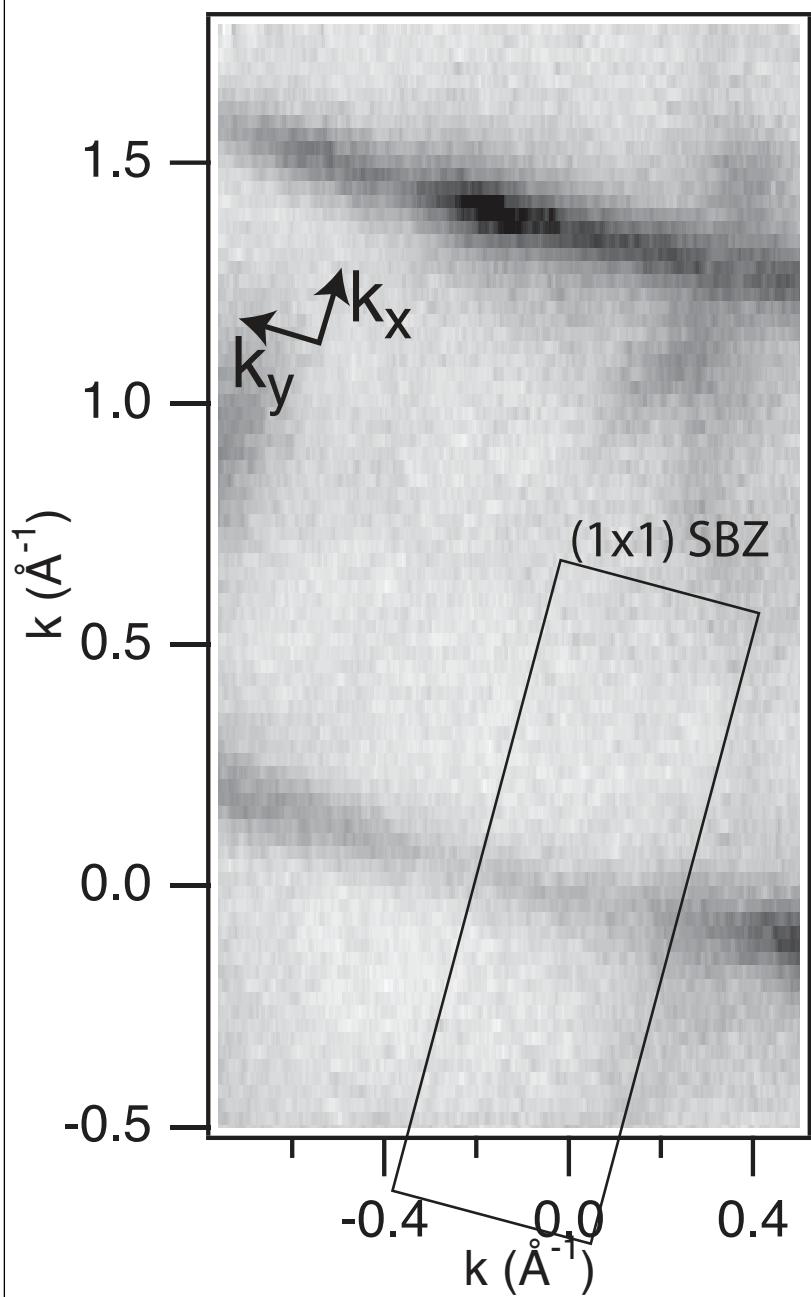


a highly one-dimensional surface: Bi(114)

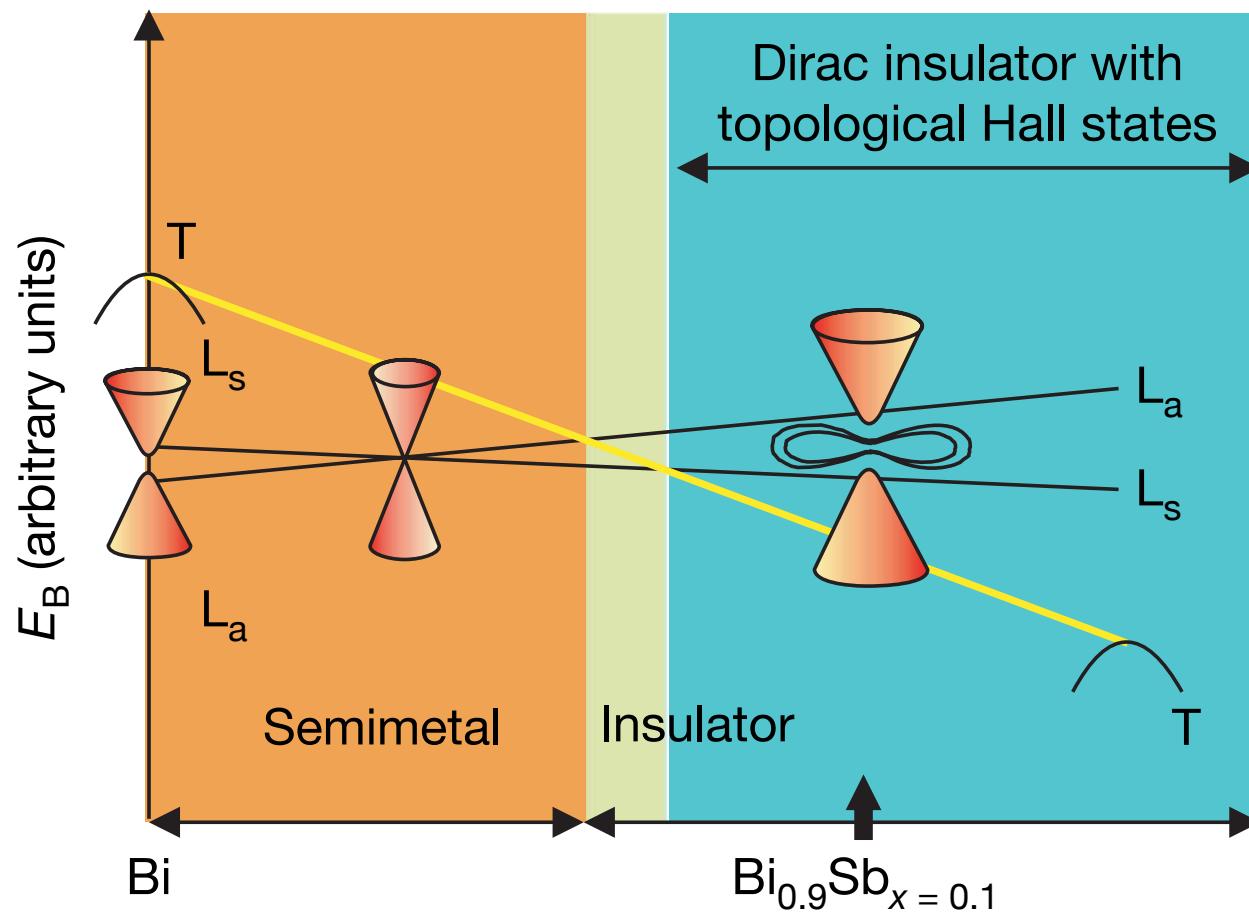


J. Wells et al., PRL 101, 096802 (2009).

electronic structure of Bi(114)

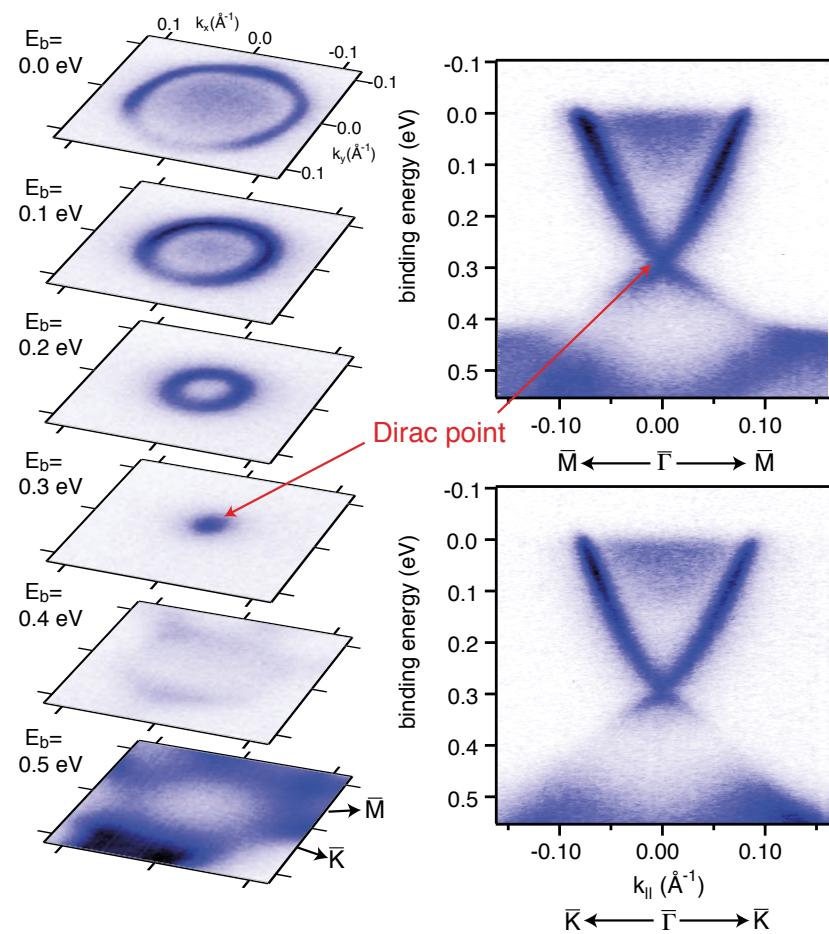


relation of Bi and $\text{Bi}_{1-x}\text{Sb}_x$

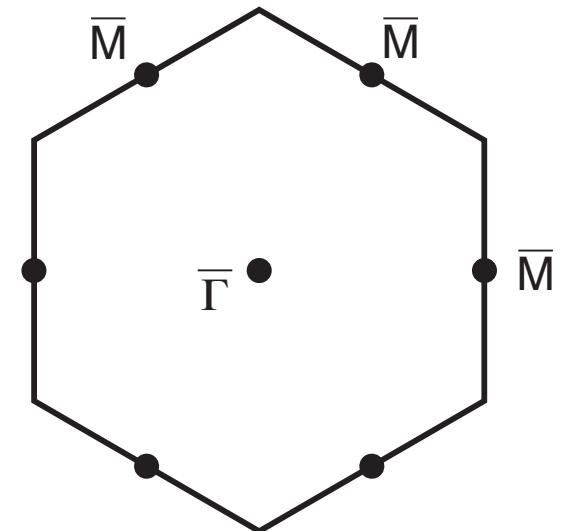
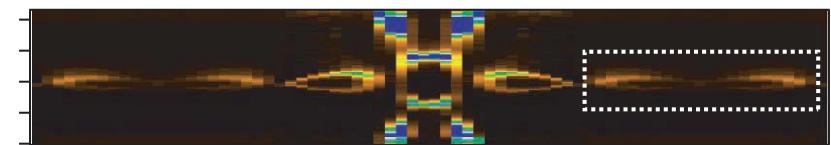


Liang Fu and C. L. Kane, Phys. Rev. B **76**, 045302 (2007)
Shuichi Murakami, New Journal of Physics **9**, 356 (2007)
image: D. Hsieh et al., Nature **460**, 1101 (2009)

$\text{Bi}_2\text{Se}_3(111)$ -class



$\text{Bi}_{1-x}\text{Sb}_x(111)$



H.-J. Noh et al., *Europhys. Lett.* **81**, 57006 (2008)

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

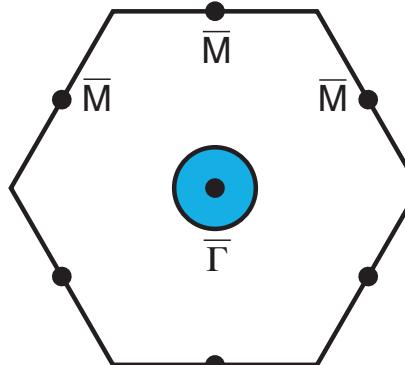
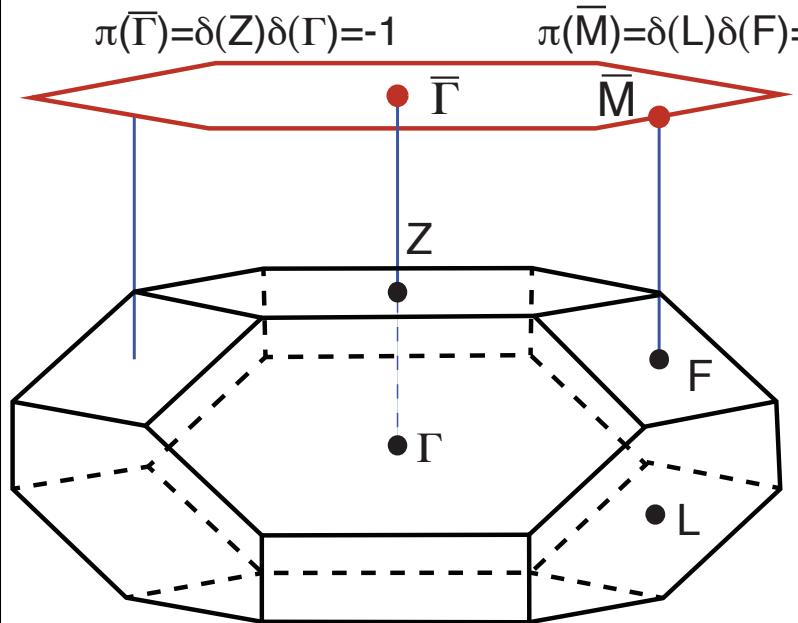
Y. Xia et al., *Nature Physics* **5**, 398 (2009)

D. Hsieh et al., *Nature* **460**, 1101 (2009)

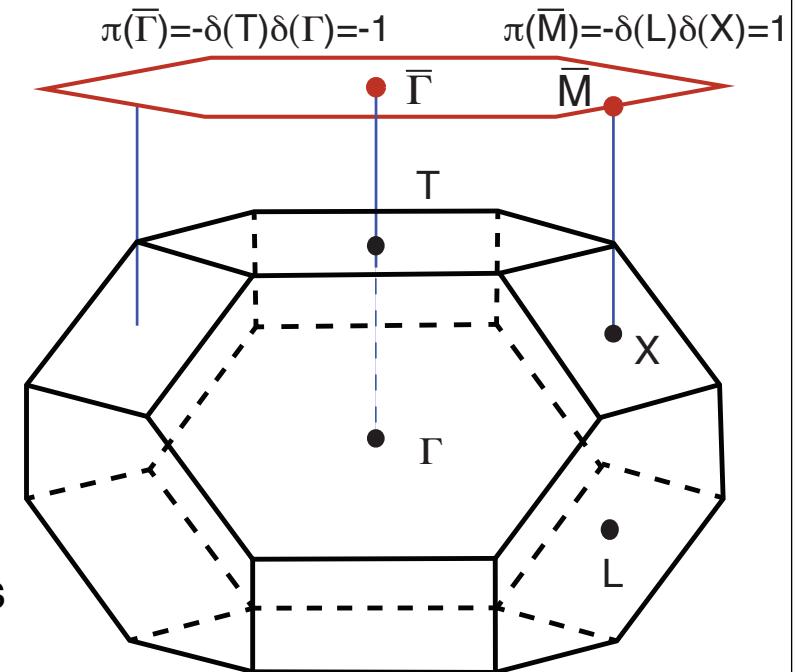
(picture from Bianchi et al. *Nat. Comm.* **1**, 128 (2010))

D. Hsieh et al., *Nature* **425**, 970 (2008)

Bi₂Se₃-class



Bi_{1-x}Sb_x



bulk parity invariants

$$\delta(\Gamma) = -1$$

$$\delta(Z) = 1$$

$$\delta(L) = 1$$

$$\delta(F) = 1$$

$$n_b = 14$$

$$\delta(\Gamma_i) = \prod_{n=1} \xi_{2n}(\Gamma_i)$$

$$\mathbb{Z}_2 \text{ invariant } (-1)^{\nu_0} = \prod_{n=1}^8 \delta_i$$

surface fermion parity

$$\pi(\lambda_a) = (-1)^{n_b} \delta(\Gamma_i) \delta(\Gamma_j)$$

$$\delta(\Gamma) = -1$$

$$\delta(T) = -1$$

$$\delta(X) = -1$$

$$x < 0.08$$

$$x > 0.08$$

$$\delta(L) = -1 \quad \delta(L) = 1$$

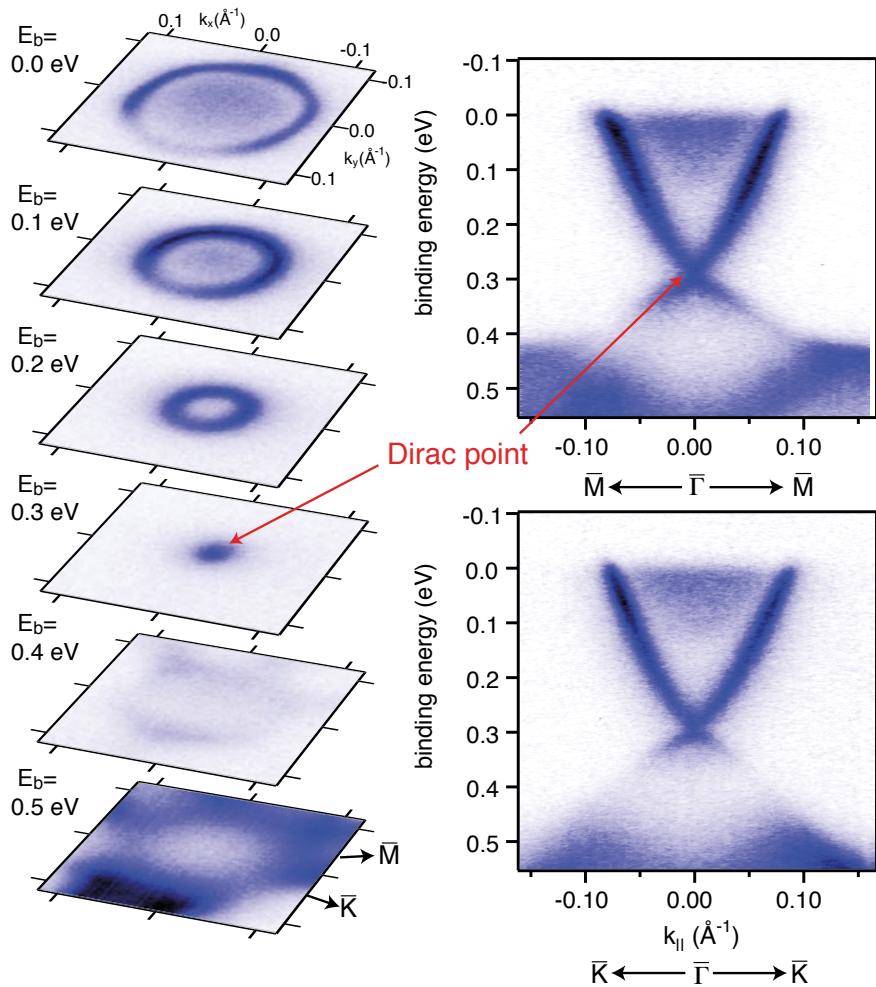
$$n_b = 5$$

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

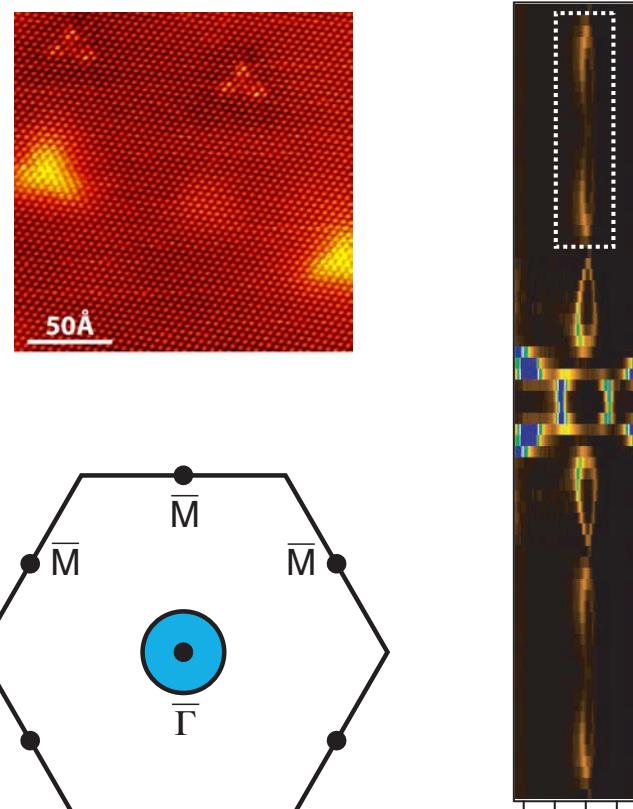
Liang Fu and C. L. Kane, Phys. Rev. B 76, 045302 (2007)

Jeffrey C. Y. Teo and Liang Fu and C. L. Kane, Phys. Rev. B 78 045426 (2008)

Bi₂Se₃-class



Bi_{1-x}Sb_x



H.-J. Noh et al., Europhys. Lett. **81**, 57006 (2008)

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

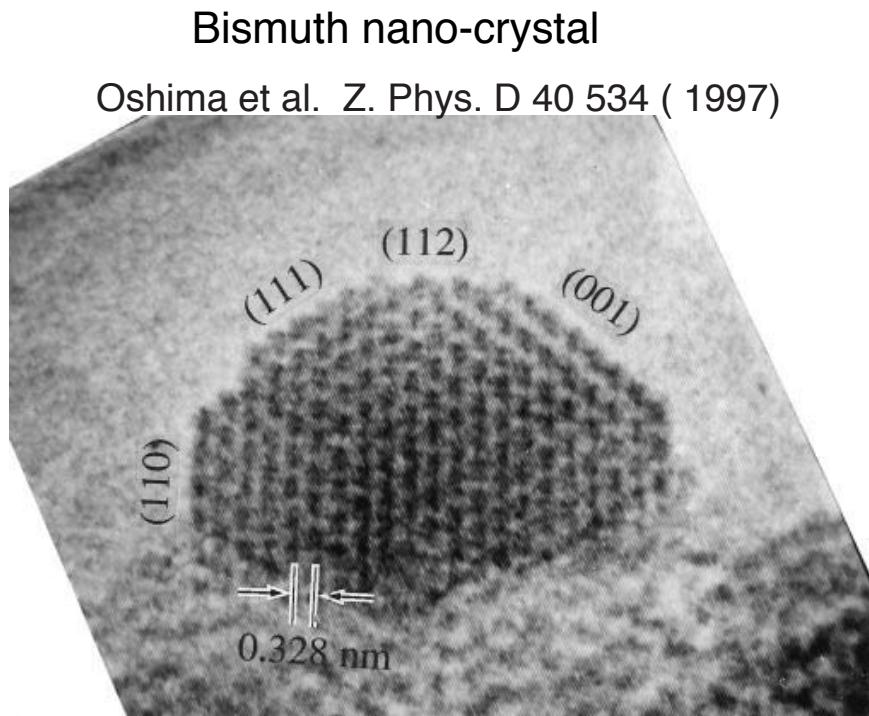
Y. Xia et al., Nature Physics **5**, 398 (2009)

D. Hsieh et al., Nature **460**, 1101 (2009)

(picture from Bianchi et al. Nat. Comm. **1**, 128 (2010))

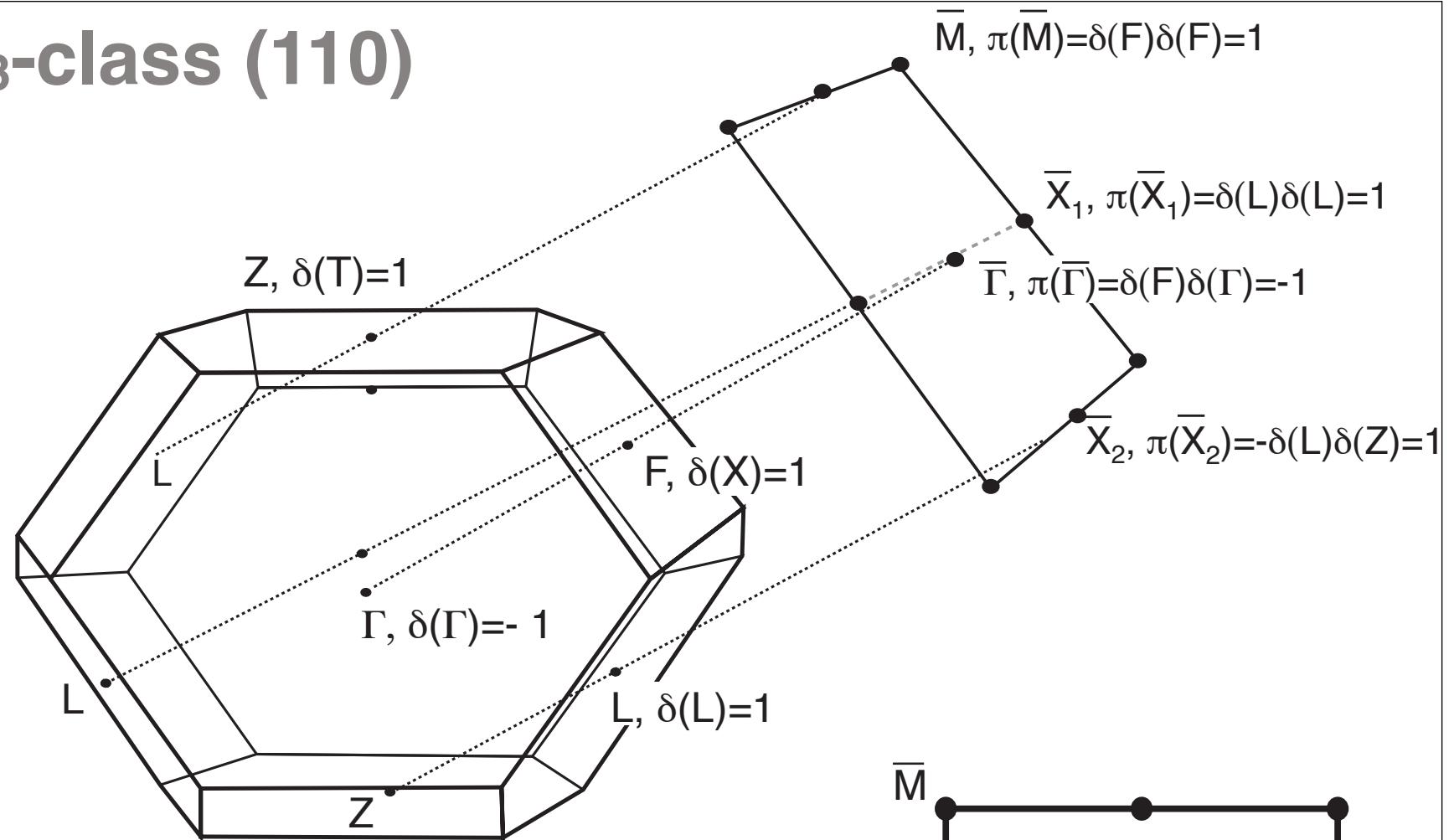
D. Hsieh et al., Nature **425**, 970 (2008)

What about non-(111) surfaces?



- smooth connectivity of states?
- topological predictions confirmed?
- use surface crystal lattice to tailor surface band structure.

Bi₂Se₃-class (110)



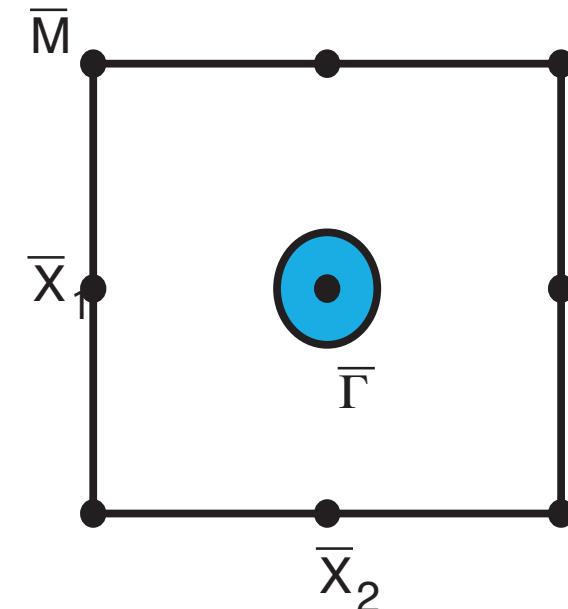
$$\delta(\Gamma) = -1$$

$$\delta(Z) = 1$$

$$\delta(L) = 1$$

$$\delta(F) = 1$$

$$\pi(\lambda_a) = (-1)^{14} \delta(\Gamma_i) \delta(\Gamma_j)$$



Bi_{1-x}Sb_x(110)

$$\delta(\Gamma) = -1$$

$$\delta(T) = -1$$

$$\delta(X) = -1$$

$$x < 0.08$$

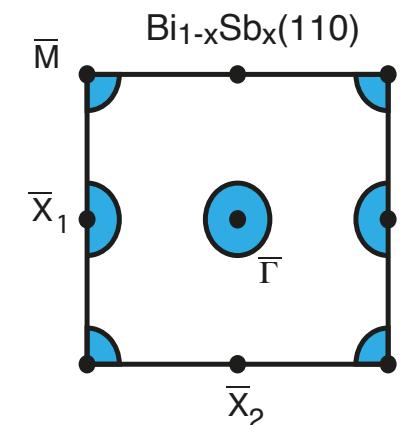
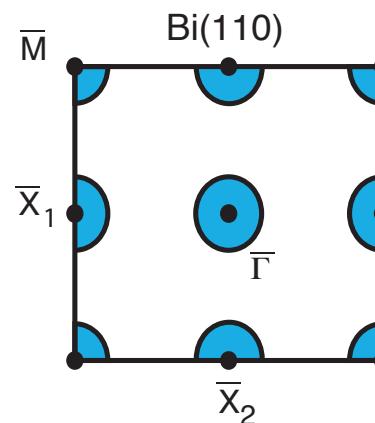
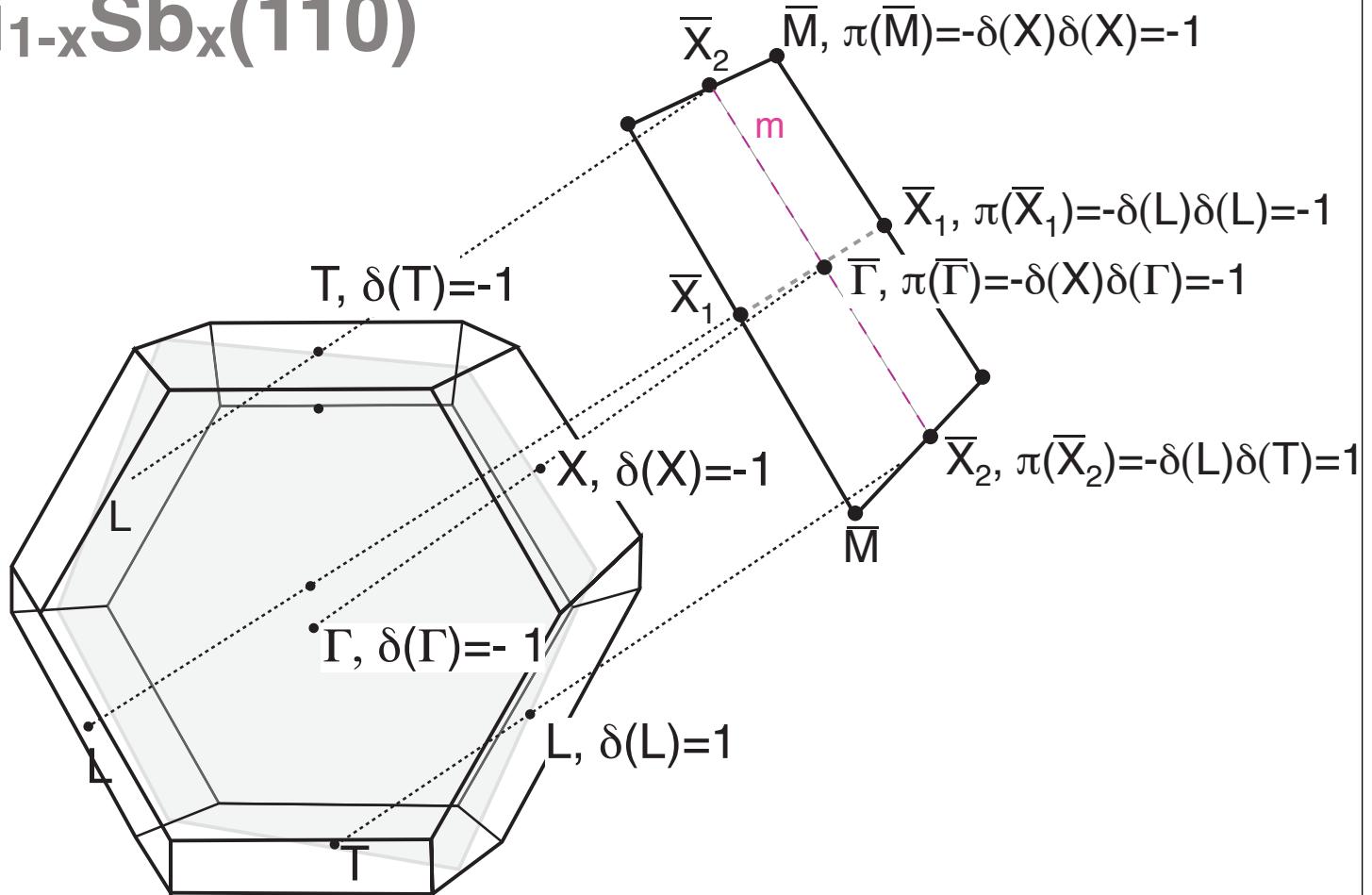
$$\delta(L) = -1$$

$$x > 0.08$$

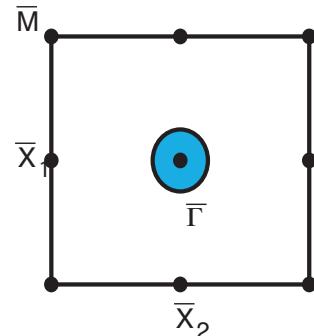
$$\delta(L) = 1$$

surface fermion parity

$$\pi(\lambda_a) = (-1)^5 \delta(\Gamma_i) \delta(\Gamma_j)$$



topology of non-(111) surfaces



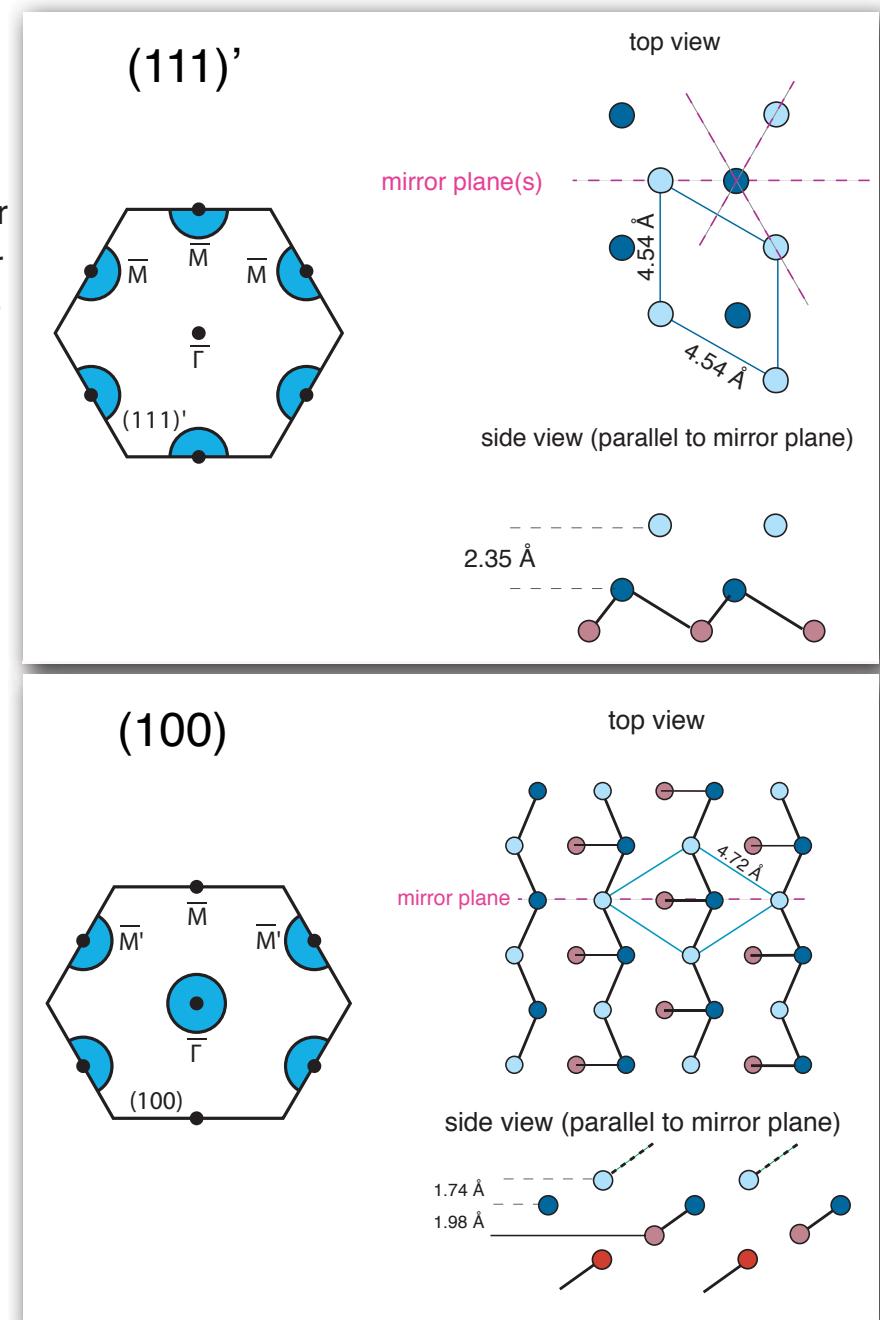
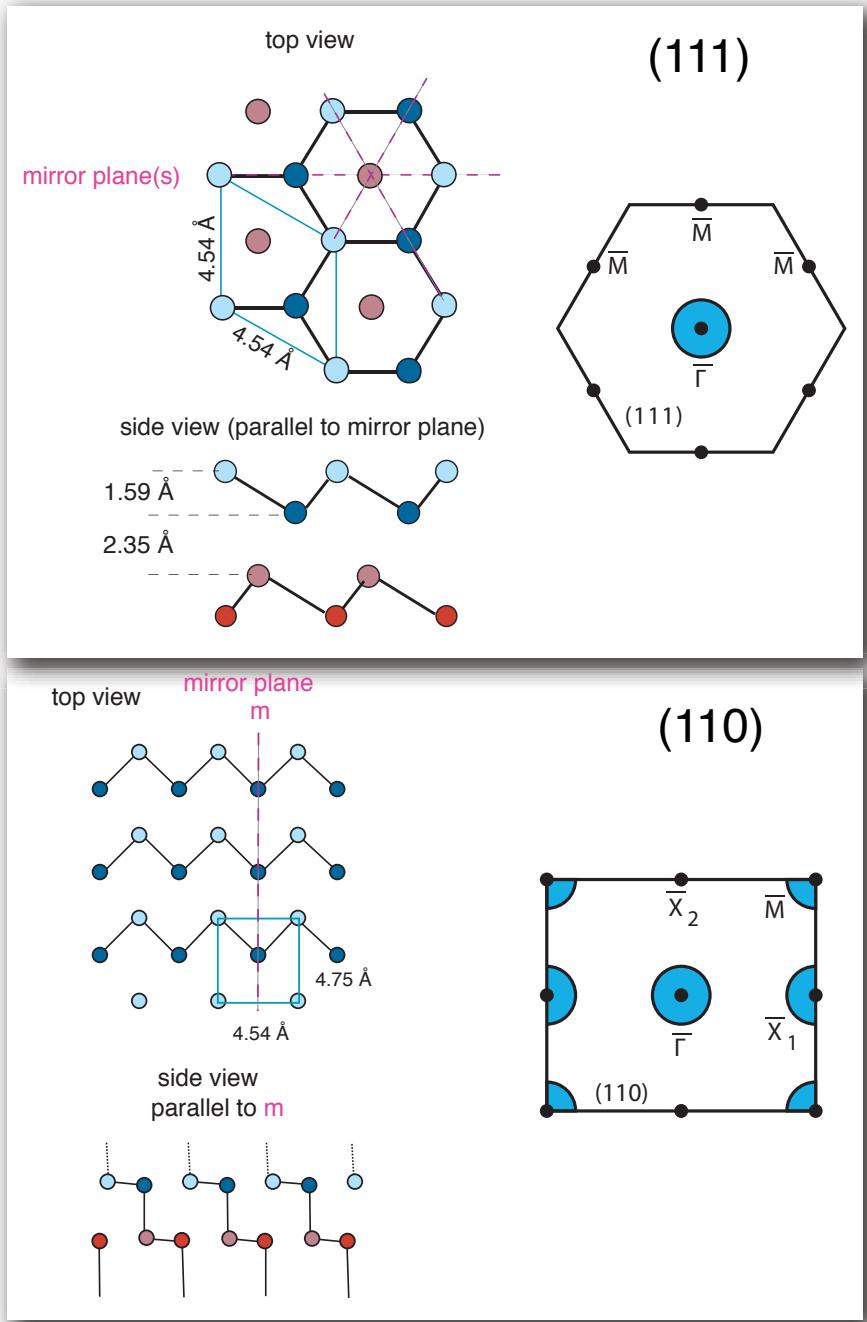
-type

Bi_2Se_3
 Bi_2Te_3
 $\text{Bi}_2\text{Te}_2\text{Se}$
...

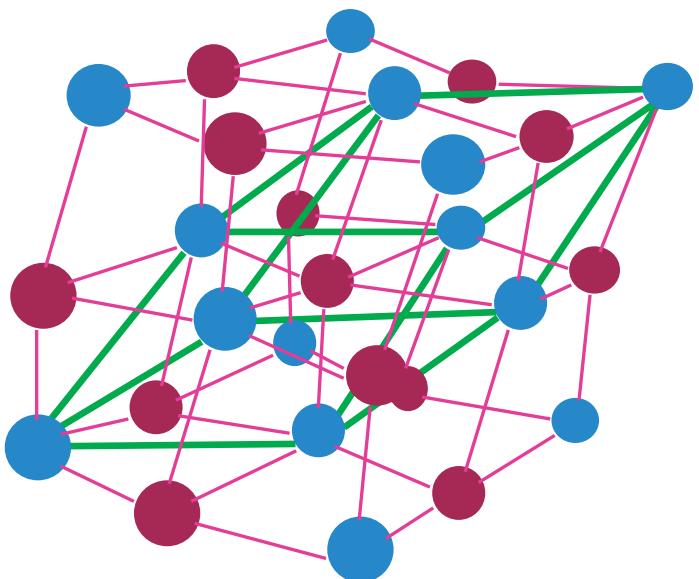
more interesting

$\text{Bi}_{1-x}\text{Sb}_x$
 PbBi_2Te_4
 SmB_6
(TCI)

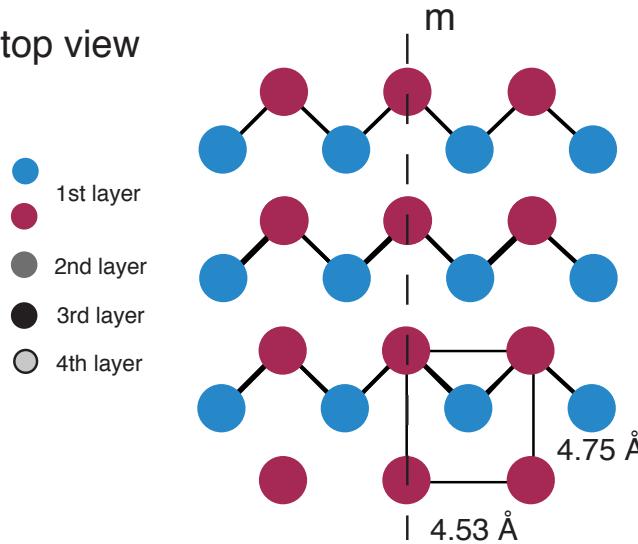
some possible modifications for $\text{Bi}_{1-x}\text{Sb}_x$



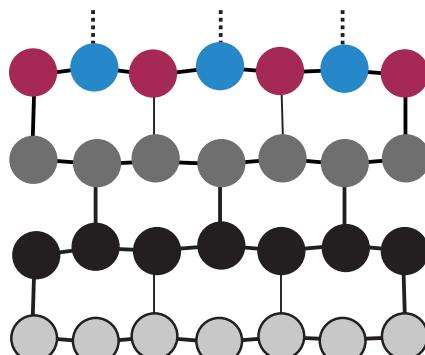
geometric structure of Bi(110)



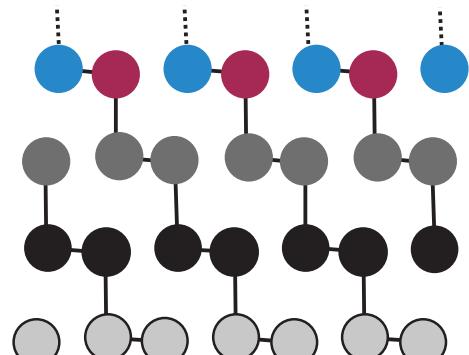
top view



side view
perpendicular to m



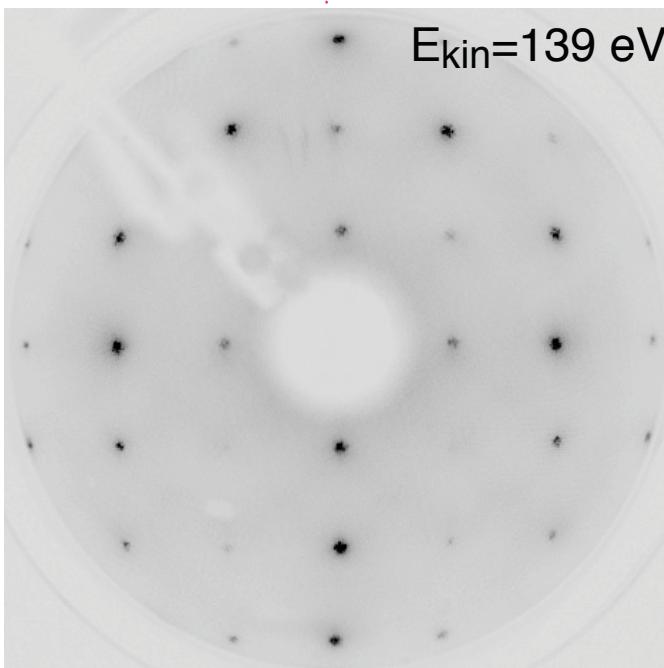
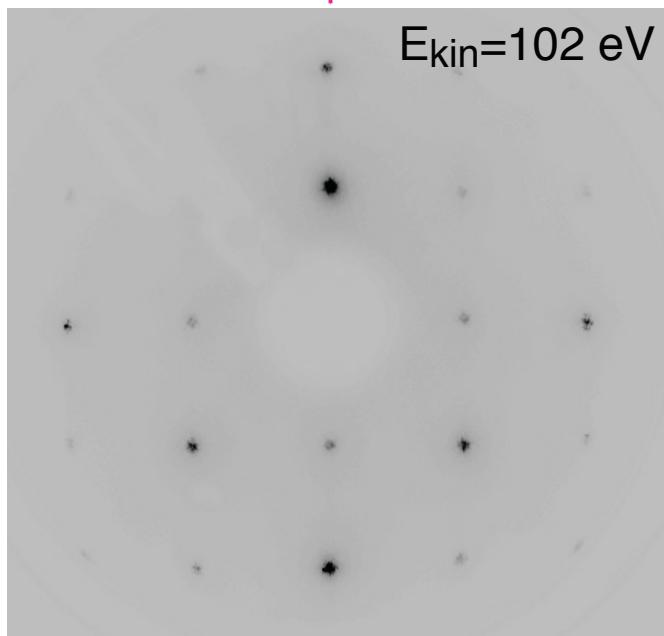
side view
parallel to m



- one dangling bond per unit cell
- only one mirror plane

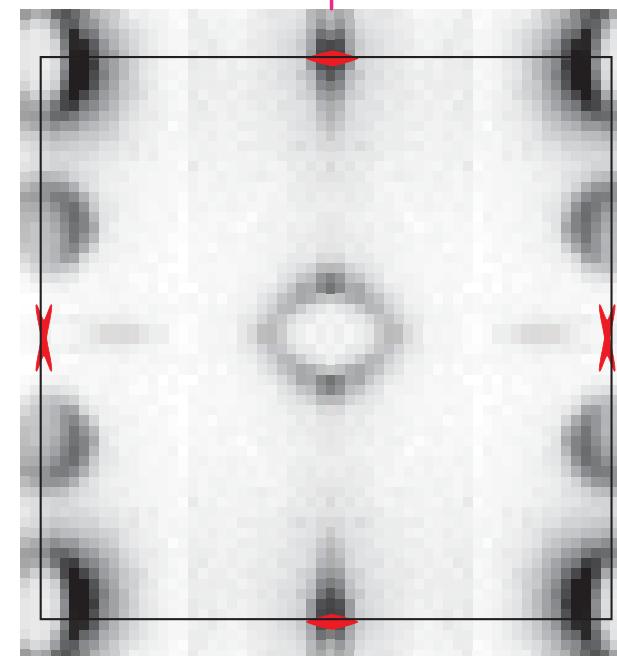
symmetry

mirror
line



Fermi contour

mirror
line



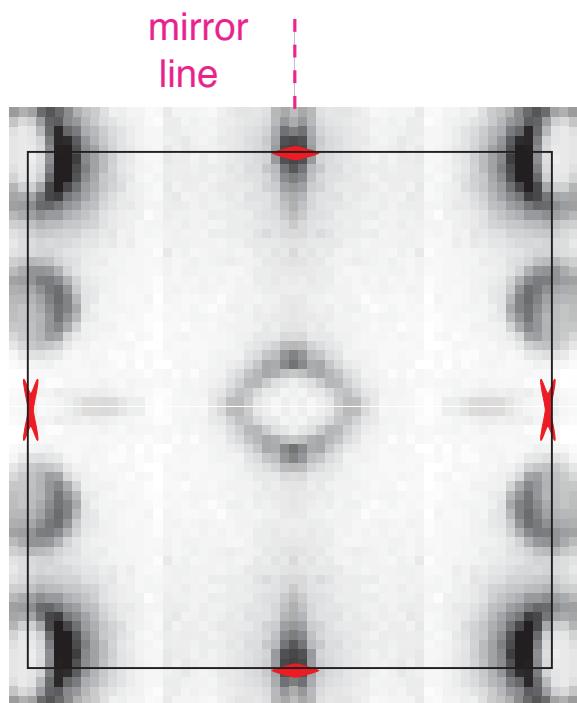
bulk Fermi surface projection in red

time-reversal symmetry:

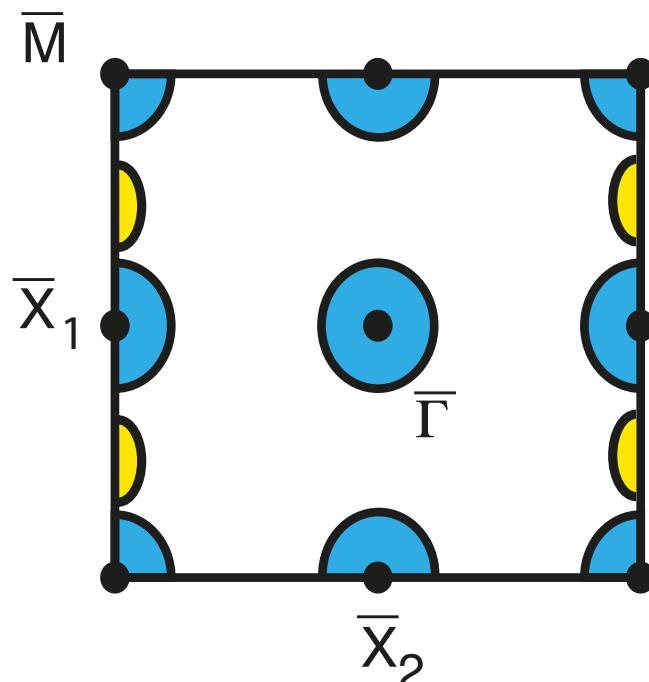
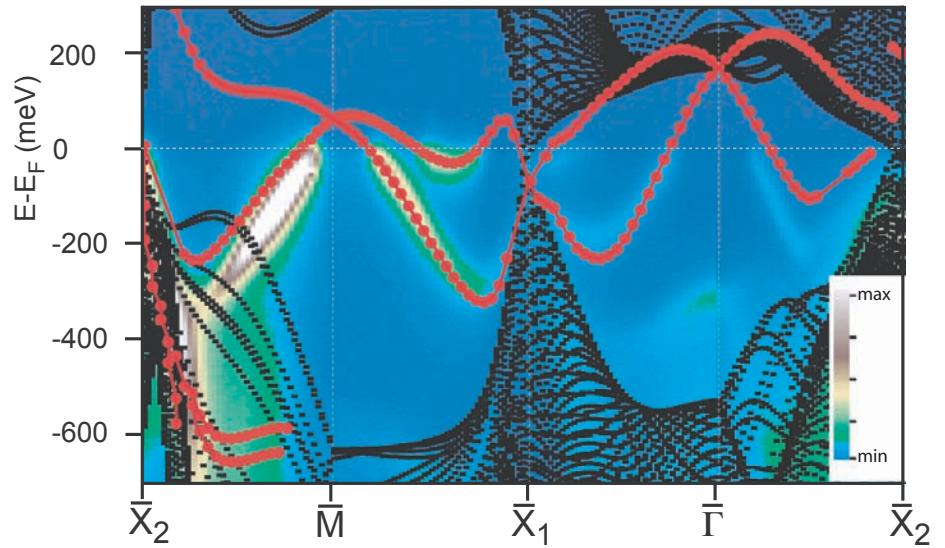
$$\epsilon \xrightarrow{\quad \uparrow \quad} \quad \epsilon \xrightarrow{\quad \downarrow \quad}$$

Bi(110) surface states and topology

Fermi surface: experiment

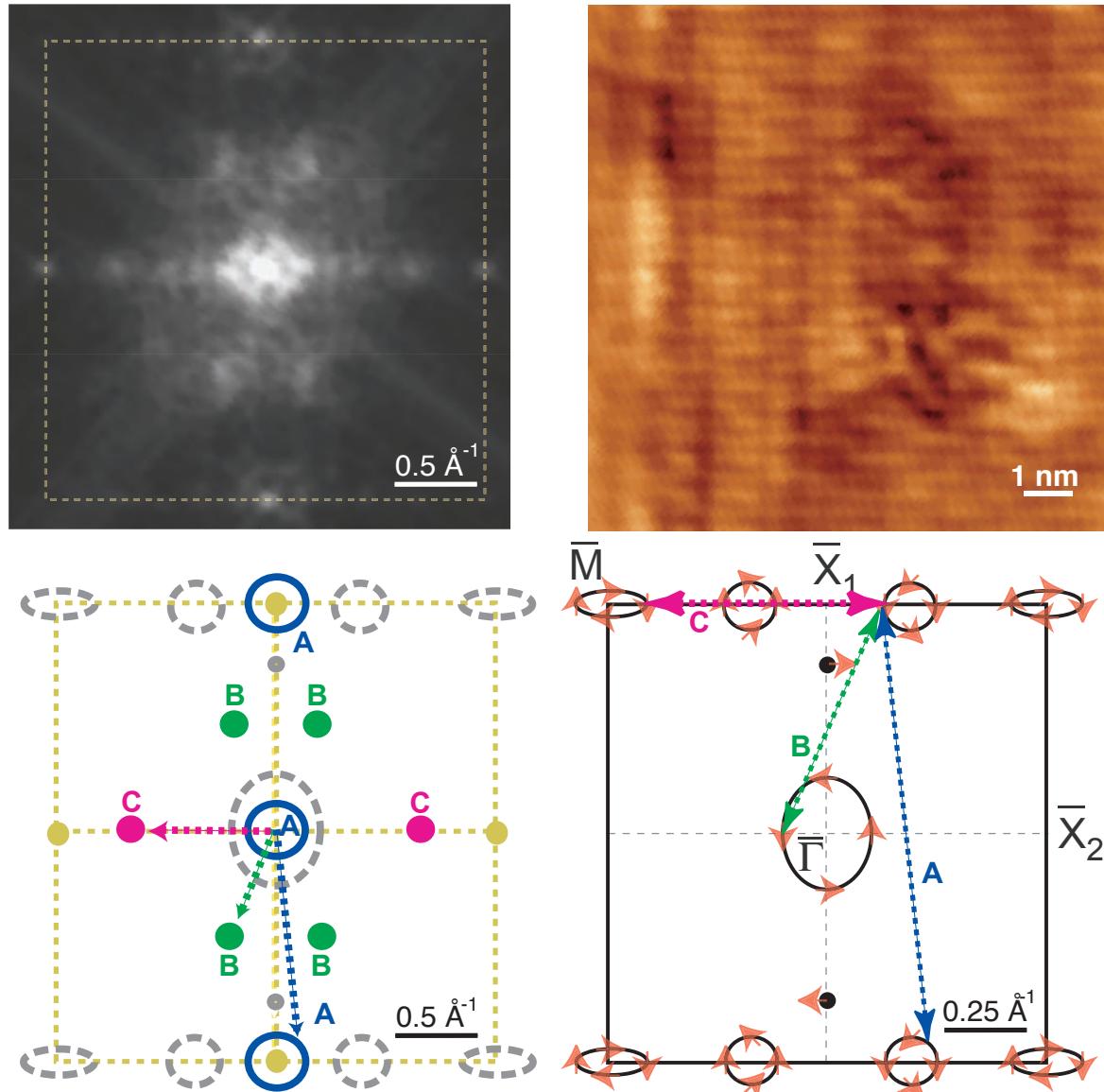


bulk Fermi surface projection in red



topological predictions in blue
additionally observed (trivial) features in yellow

forbidden backscattering



outline

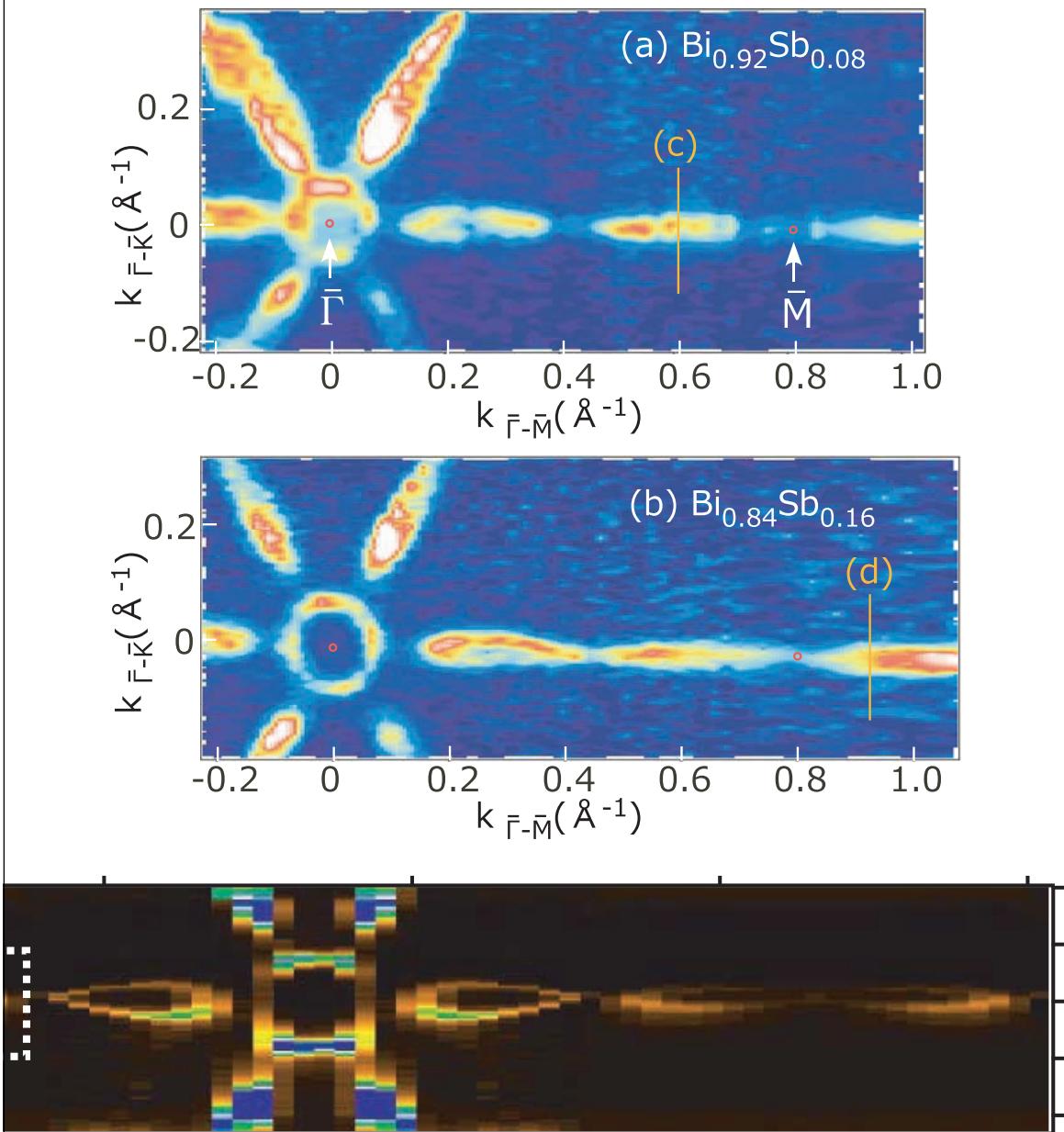
- introduction and motivation
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preparing non-(111) surfaces

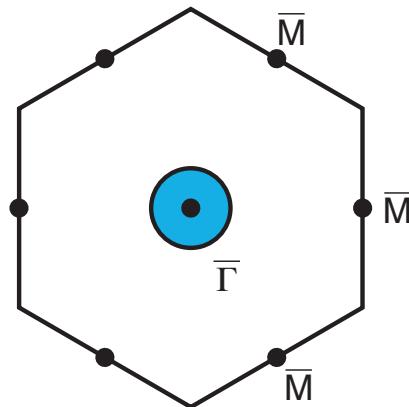
- cleaving? **✗**
- cutting / polishing / in situ sputtering? **(✗)**
- epitaxial growth **(✓)**



Epitaxial Bi_{1-x}Sb_x(111) on Si(111)



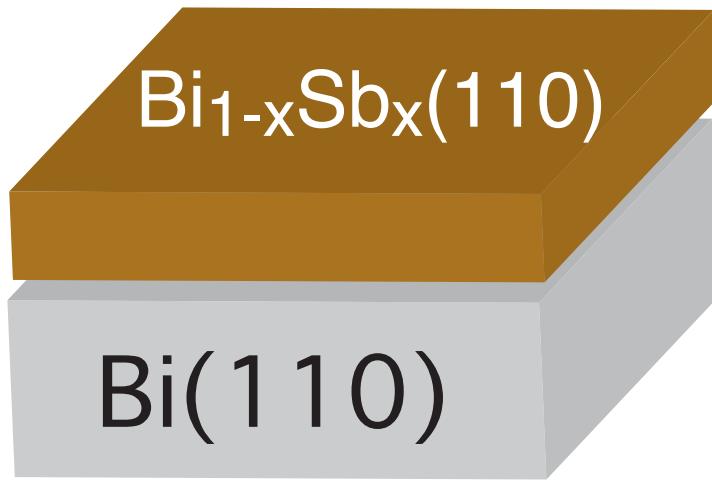
epitaxial BiSb(111): T. Hirahara et al.,
Phys. Rev. B **81**, 165422 (2010)



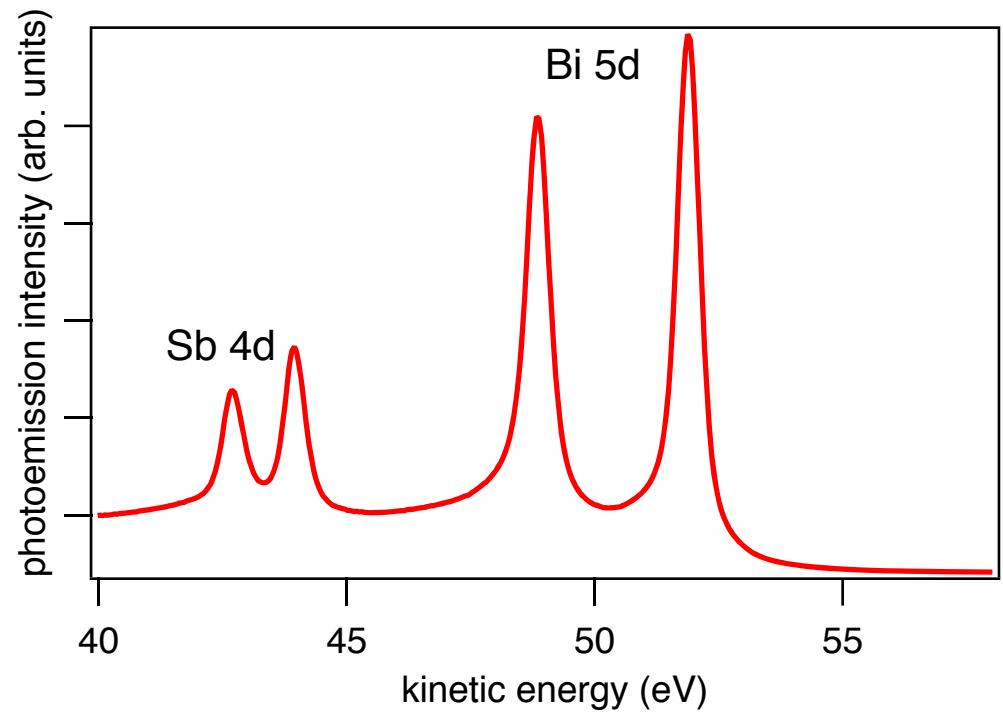
bulk BiSb(111): D. Hsieh et al.,
Nature **460**, 1101 (2009)

lattice mismatch
 $a = 0.45469 - 0.02398x$ for
 $x=0.1$ this is 0.5%
 $c = 1.186294 - 0.058632 [1 + 1.26 (x^{-1} - 1)]^{-1}$ for $x=0.1$
this is 0.4%

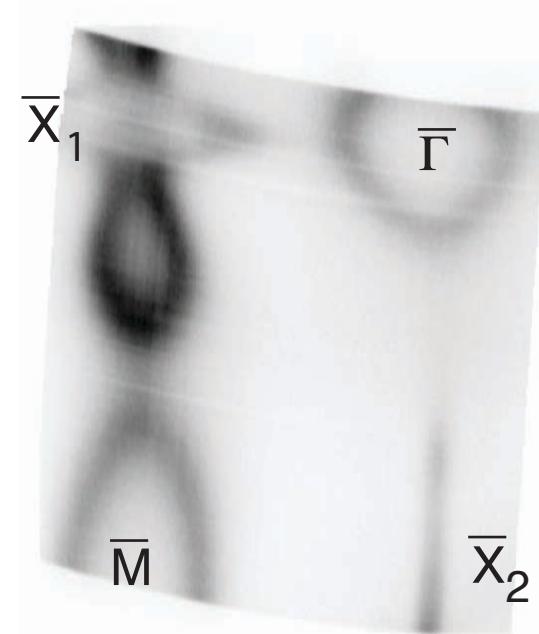
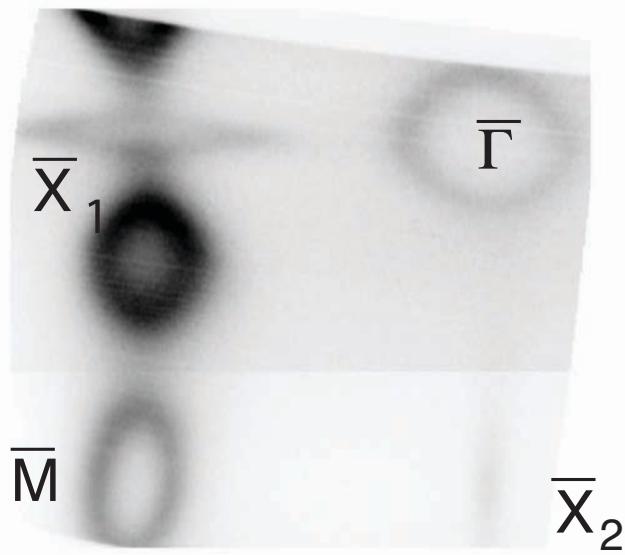
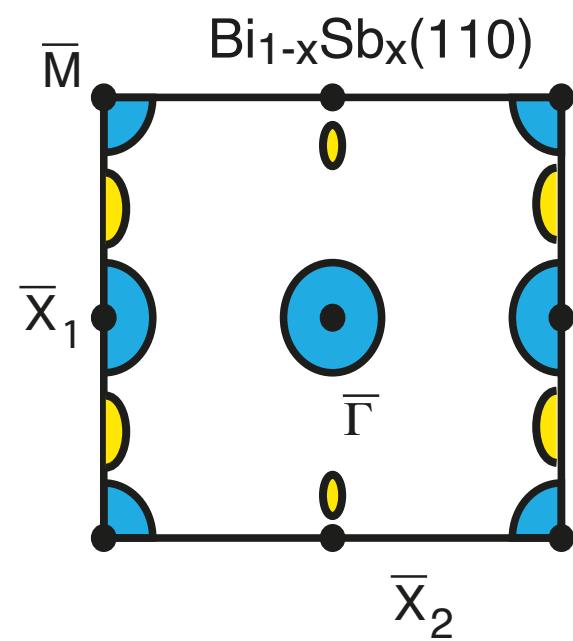
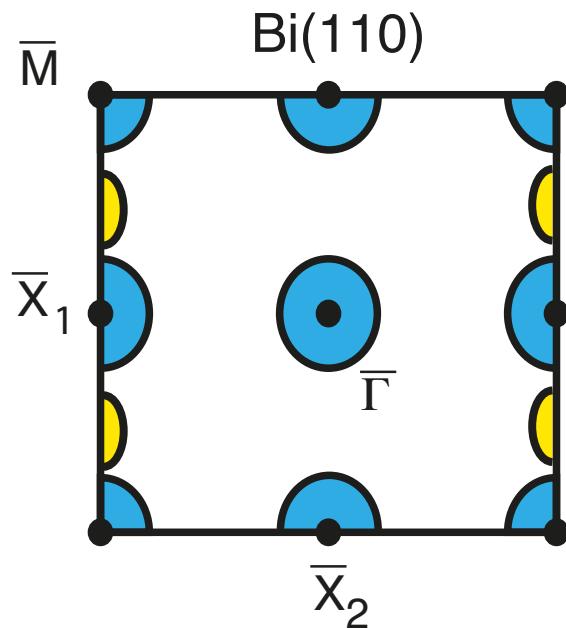
Epitaxial $\text{Bi}_{1-x}\text{Sb}_x(110)$



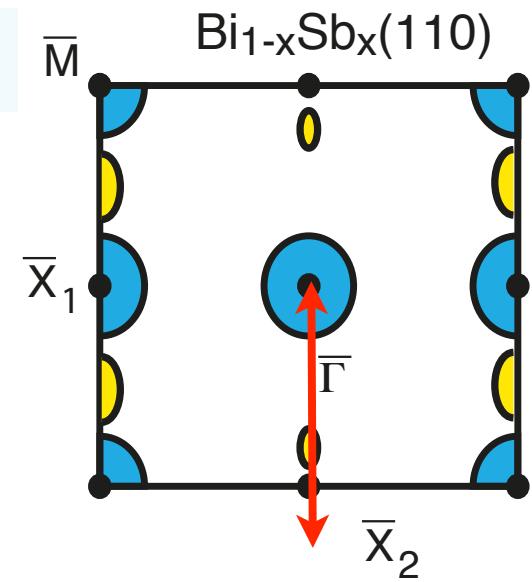
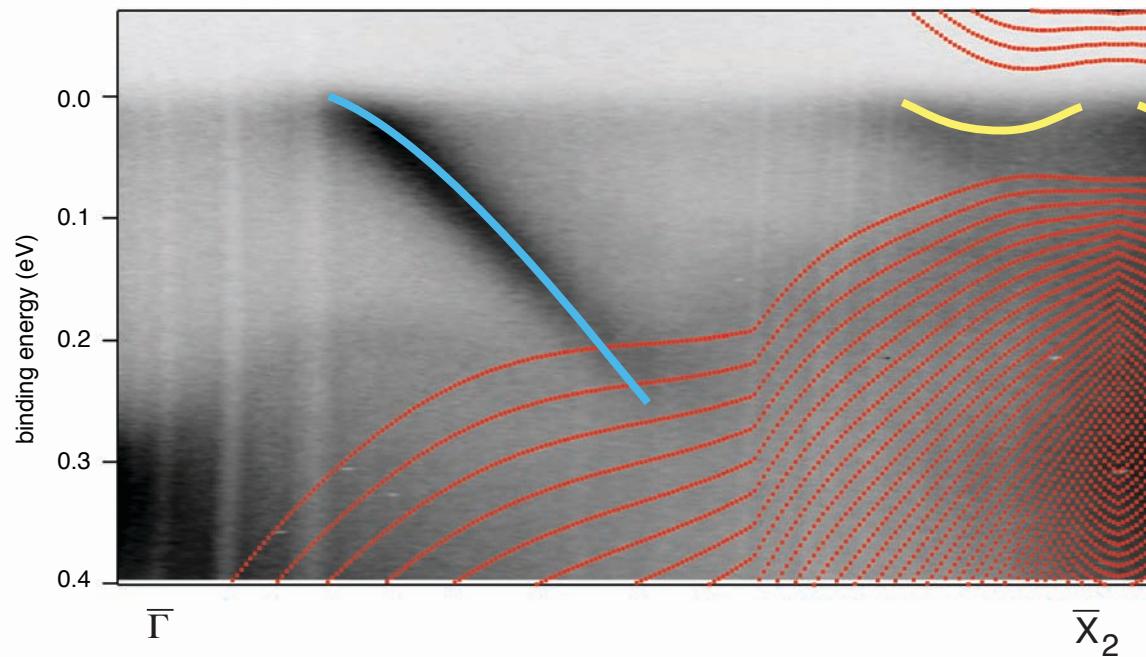
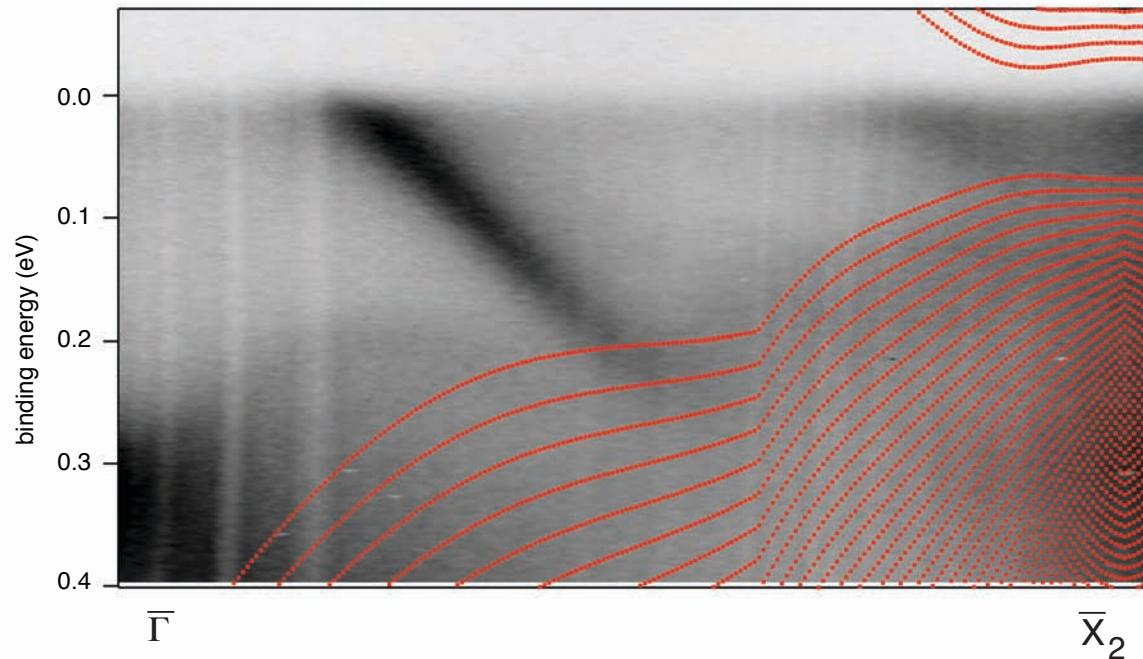
$x \approx 0.14$
lattice mismatch $\approx 0.5\%$
thickness ≈ 25 bilayers



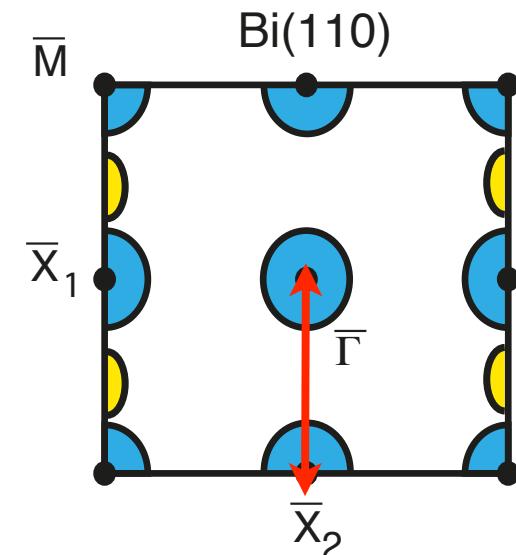
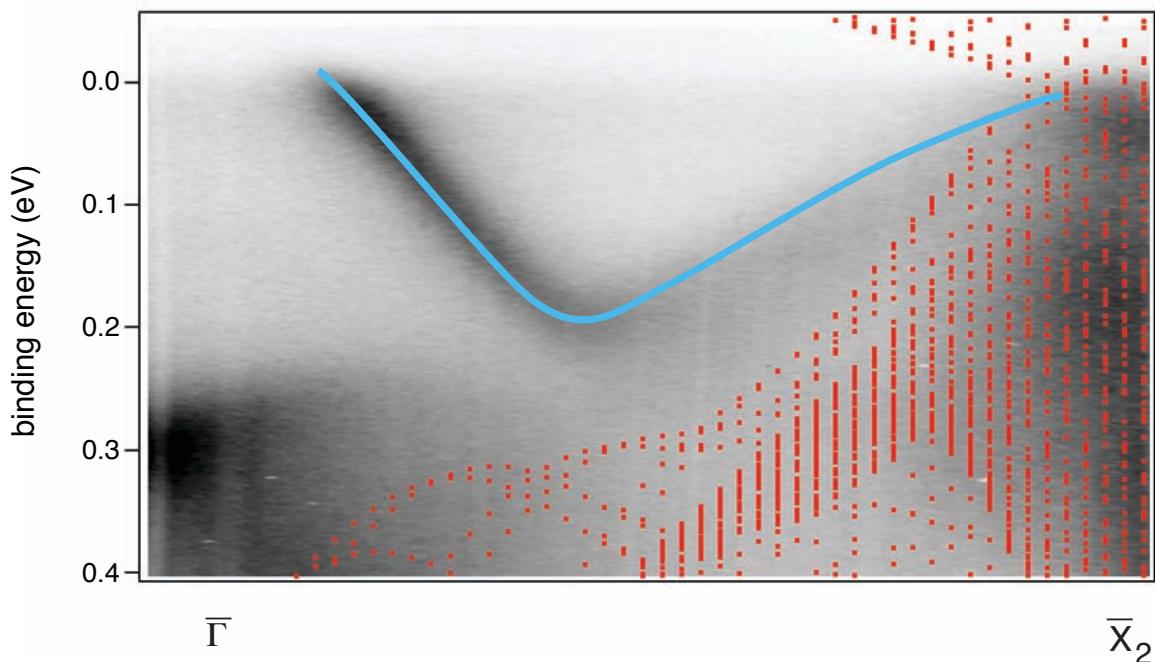
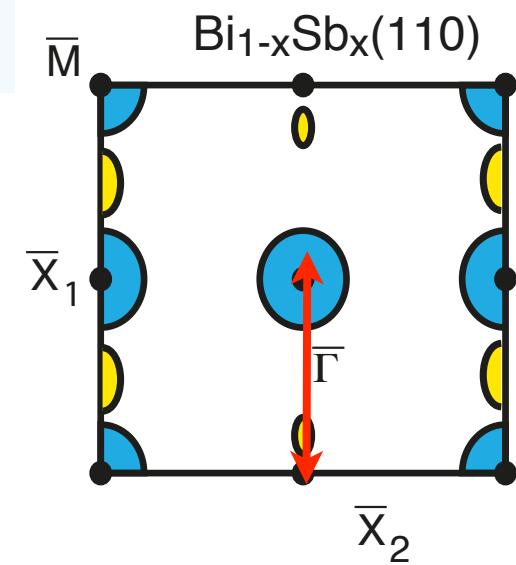
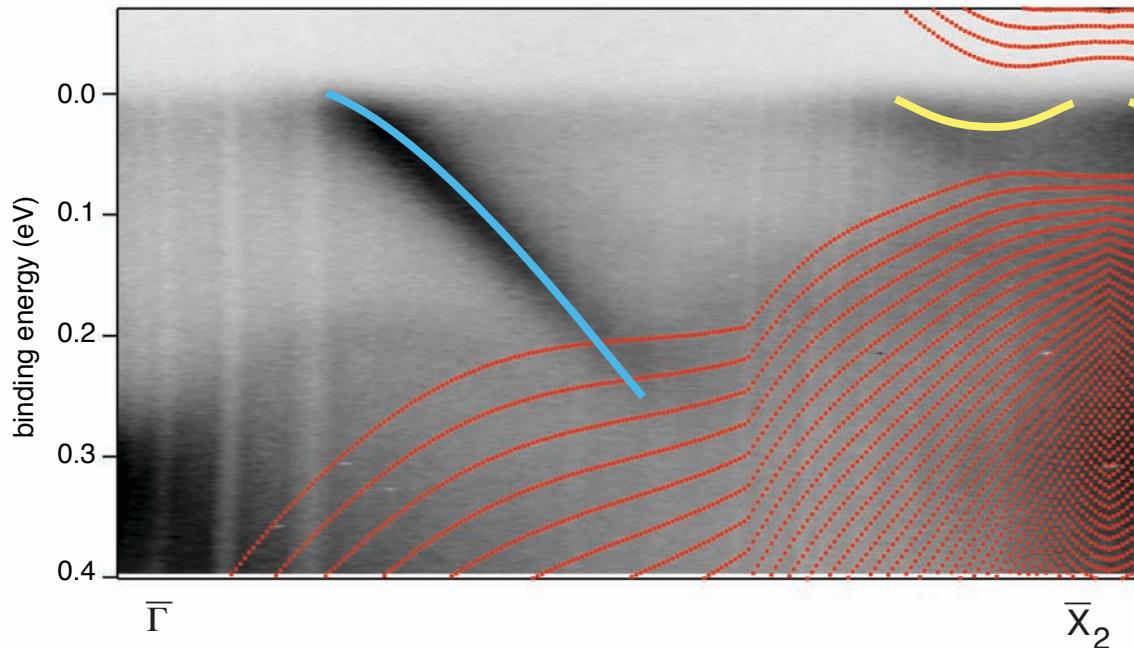
Electronic structure overview



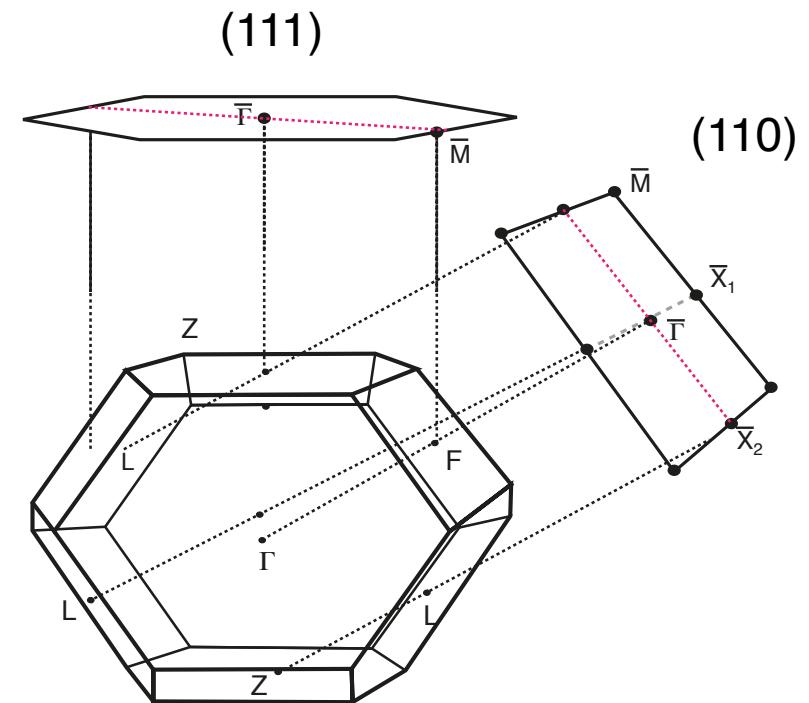
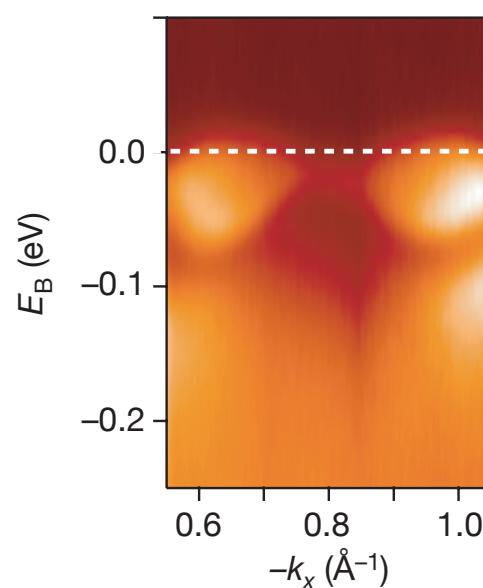
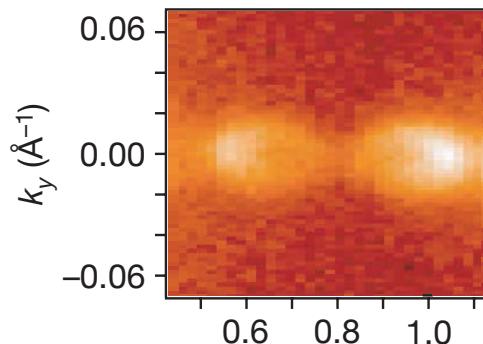
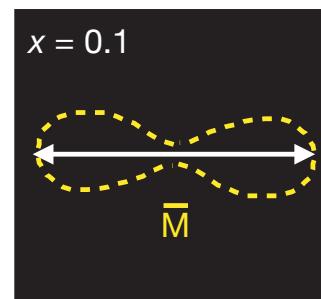
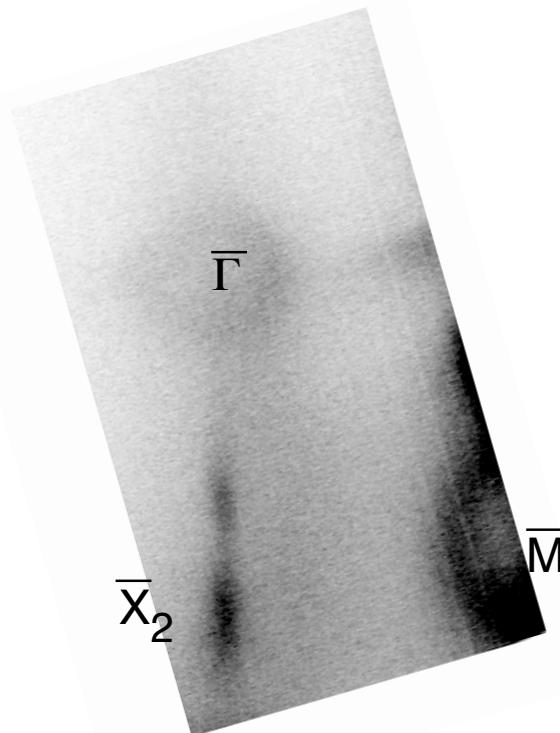
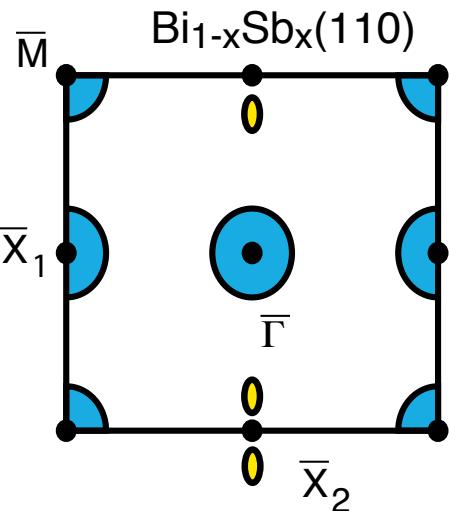
situation close to \bar{X}_2



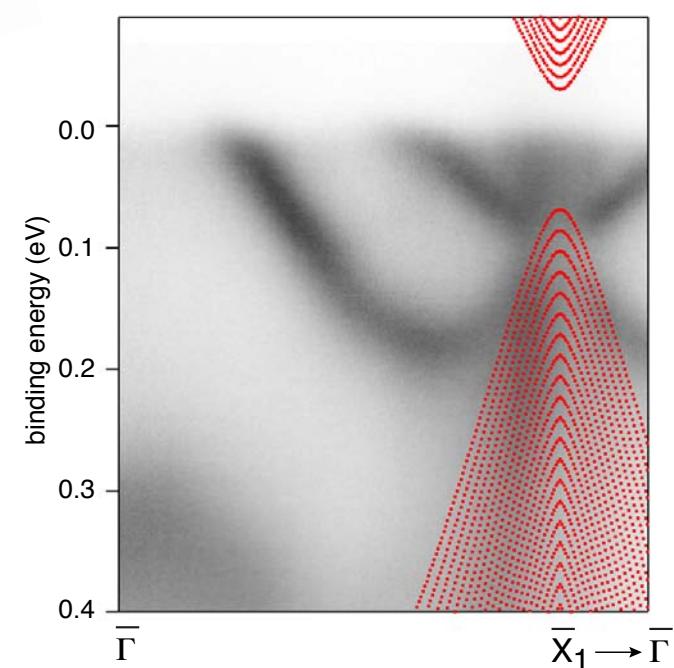
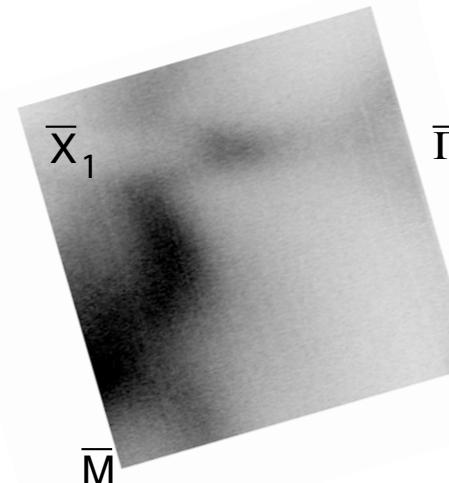
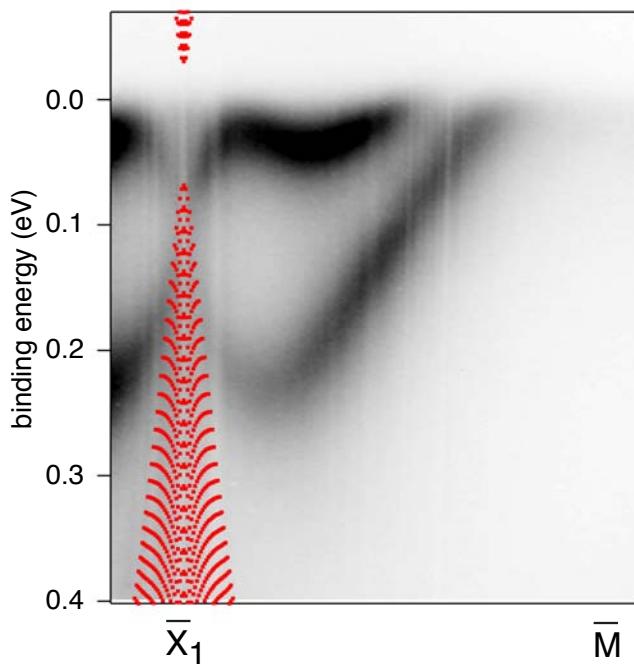
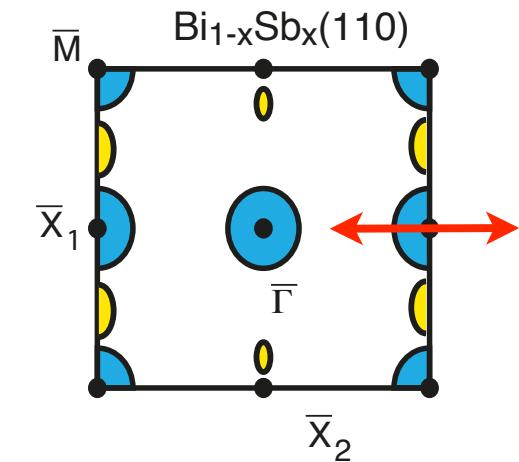
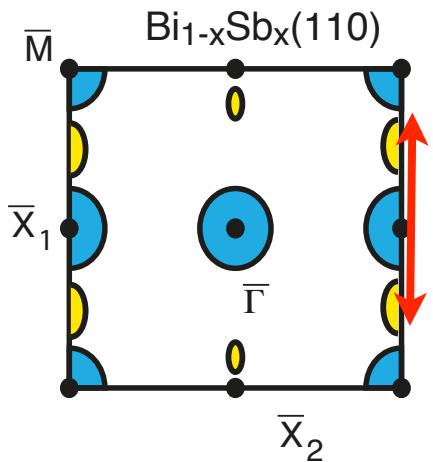
topological change



comparison to Bi_{1-x}Sb_x(111)



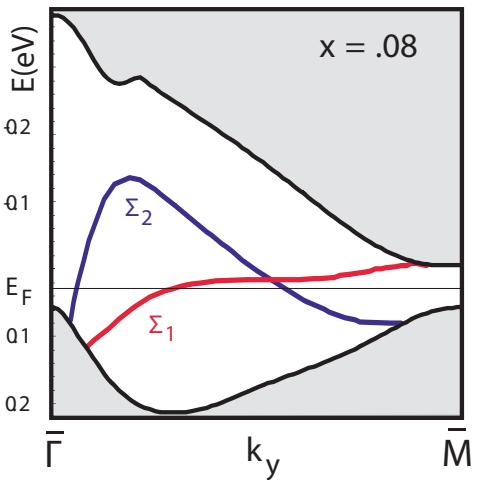
situation close to \bar{X}_1



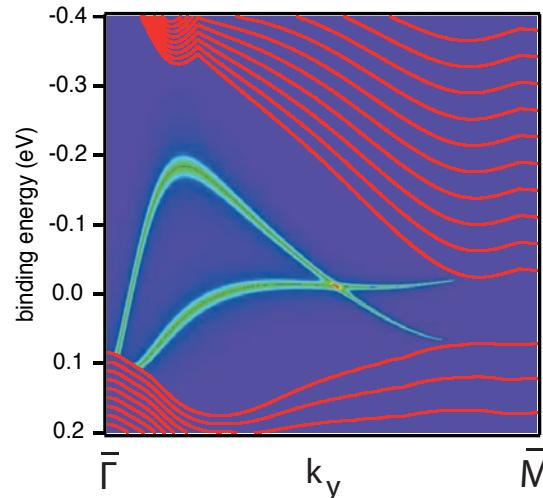
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- tight-binding calculations

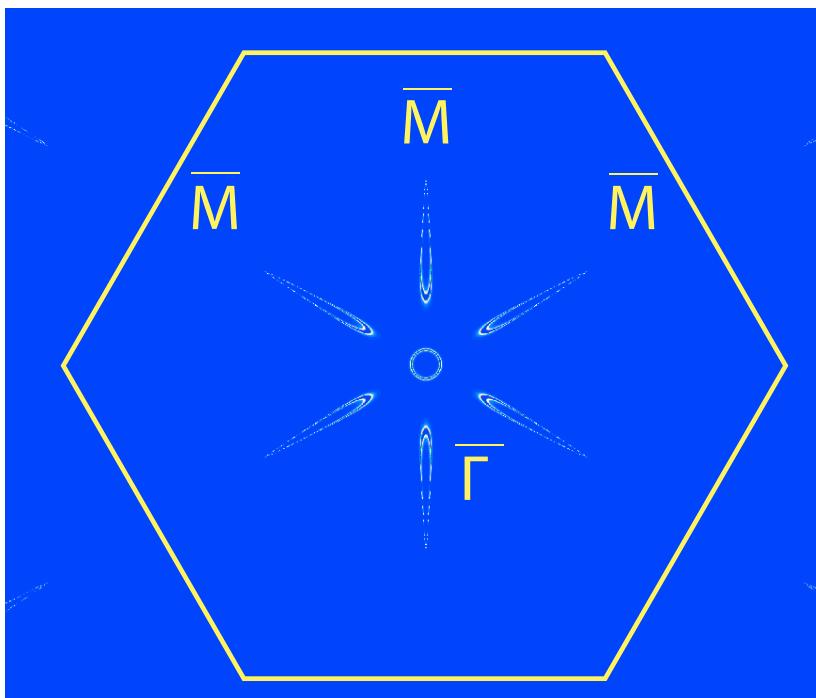
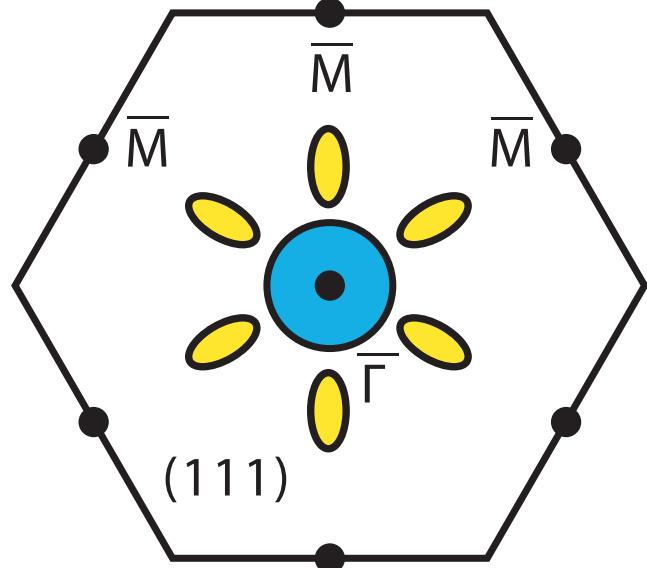
calculations Bi_{1-x}Sb_x(111)



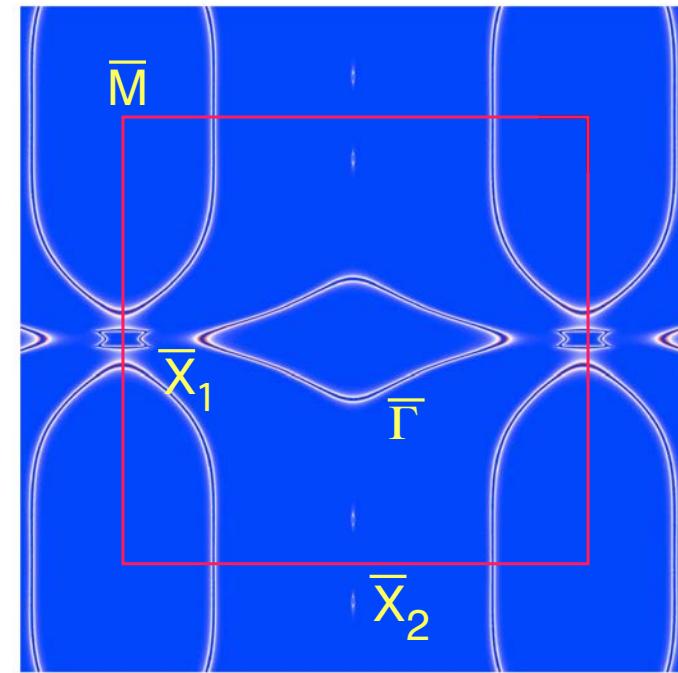
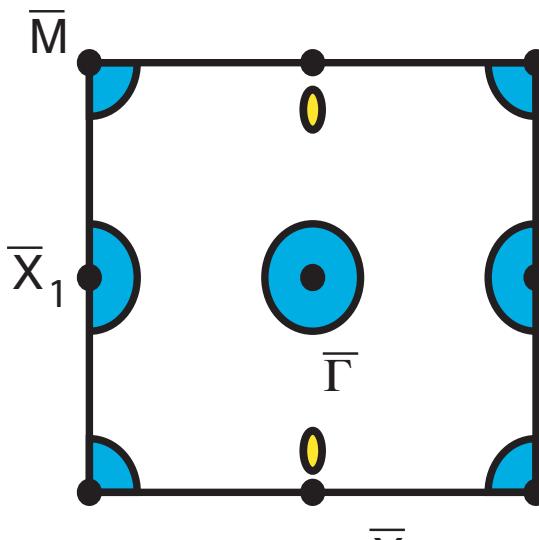
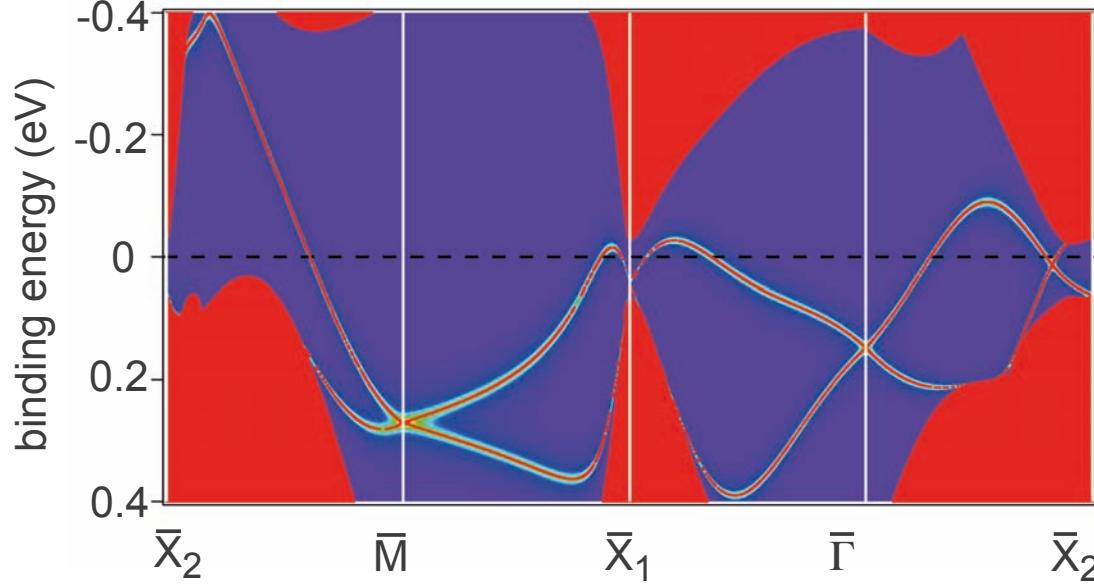
Jeffrey C. Y. Teo, Liang Fu and C. L. Kane,
Phys. Rev. B **78** 045426 (2008)



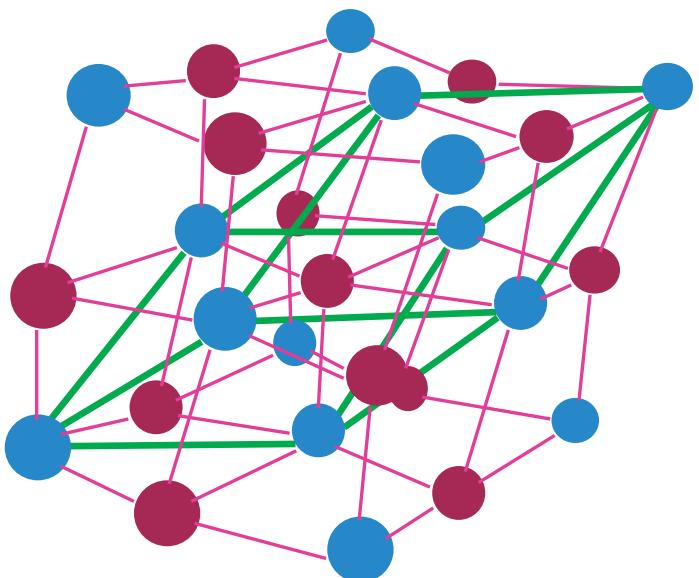
TB calculation method:
Liu, Allan, Phys. Rev. B **52**, 1566 (1995)
Teo, Fu, Kane, Phys. Rev. B **78** 045426 (2008)
Mele, Joannopoulos, Phys. Rev. B **17**, 1816 (1978)



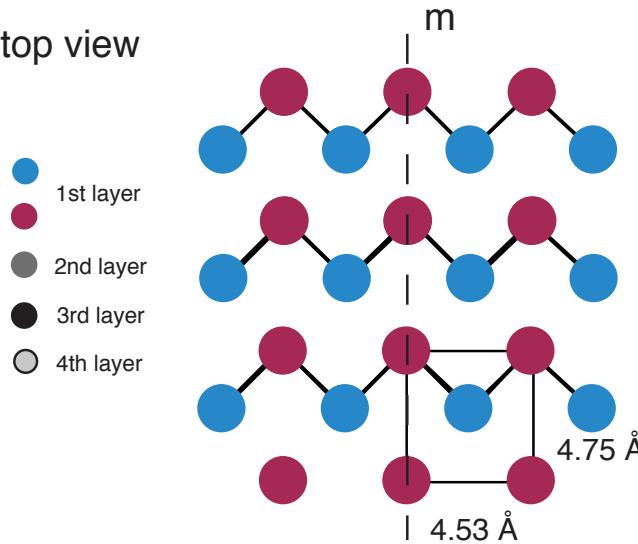
TB calculation Bi_{1-x}Sb_x(110)



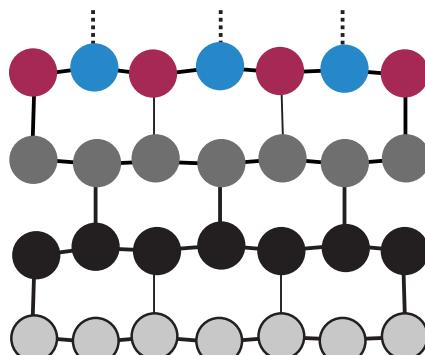
geometric structure of Bi(110)



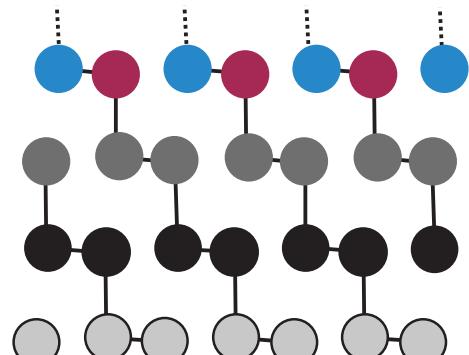
top view



side view
perpendicular to m

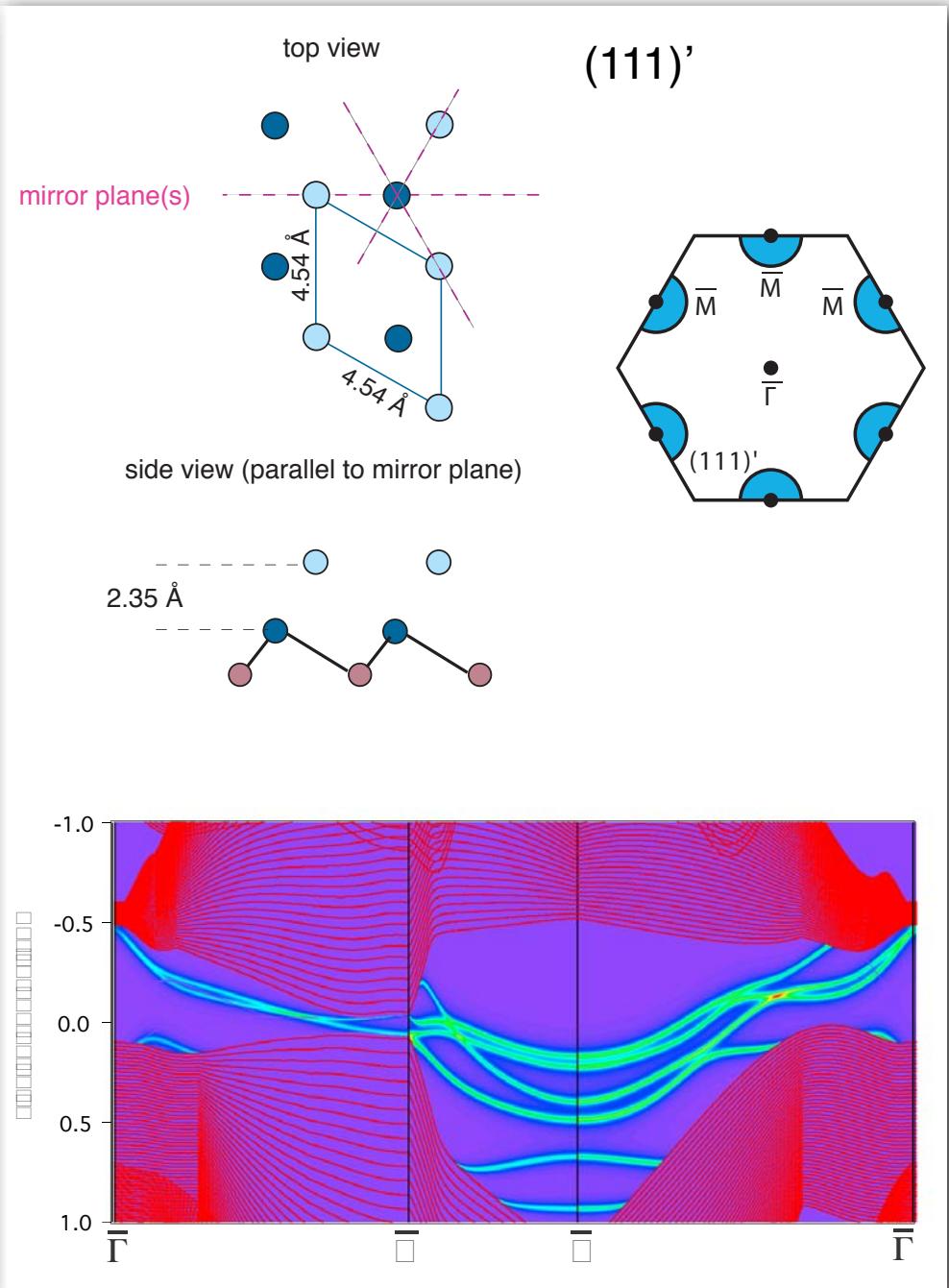
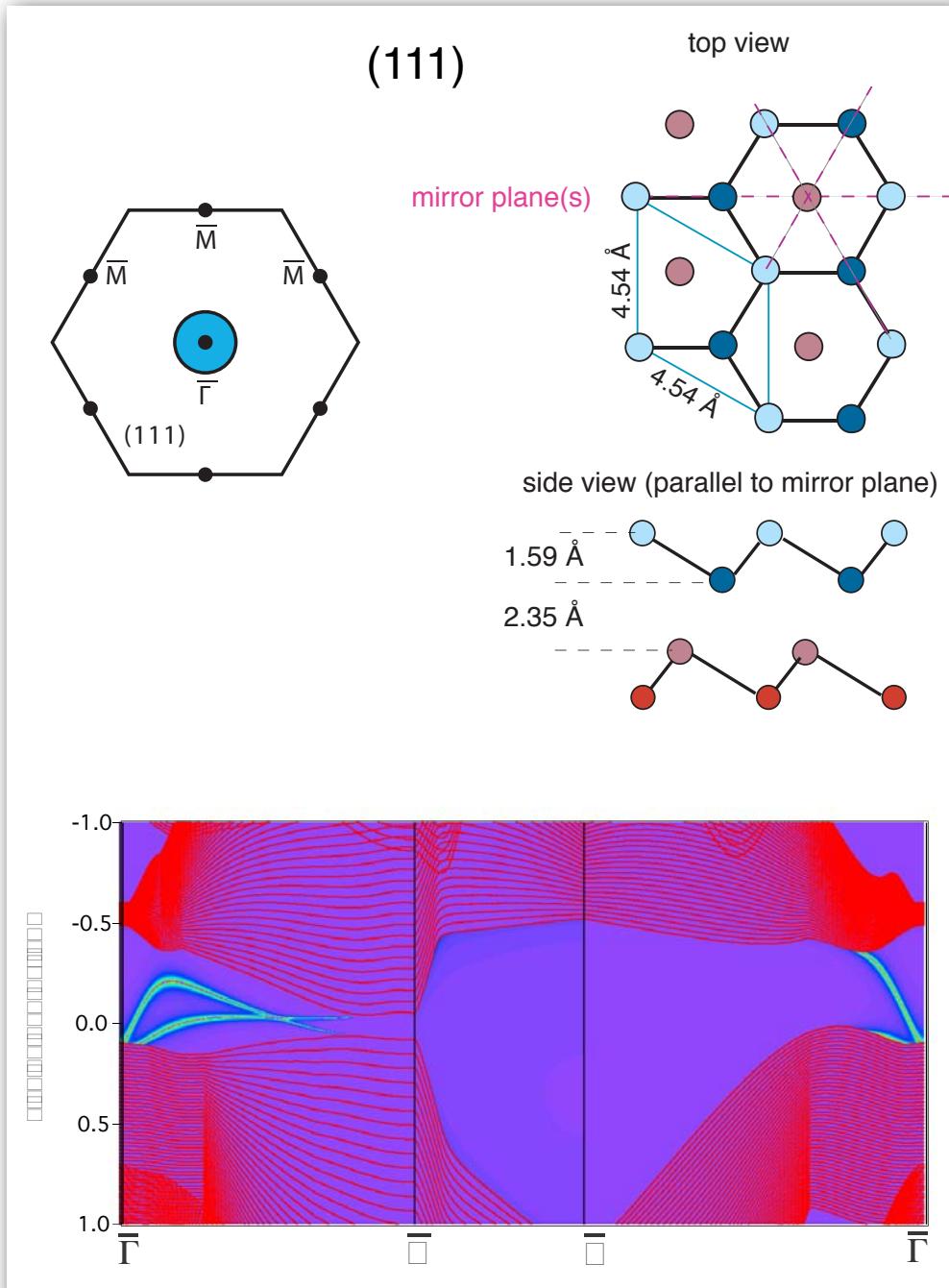


side view
parallel to m



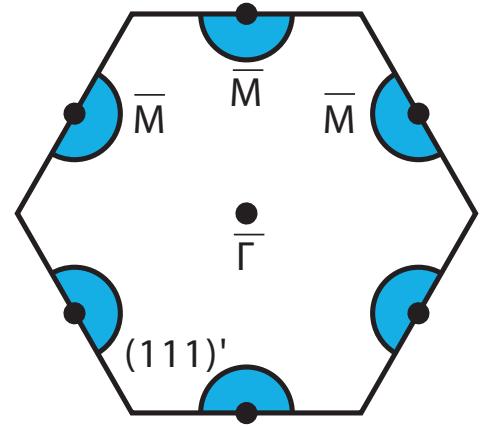
- one dangling bond per unit cell
- only one mirror plane

$\text{Bi}_{1-x}\text{Sb}_x(111)'$

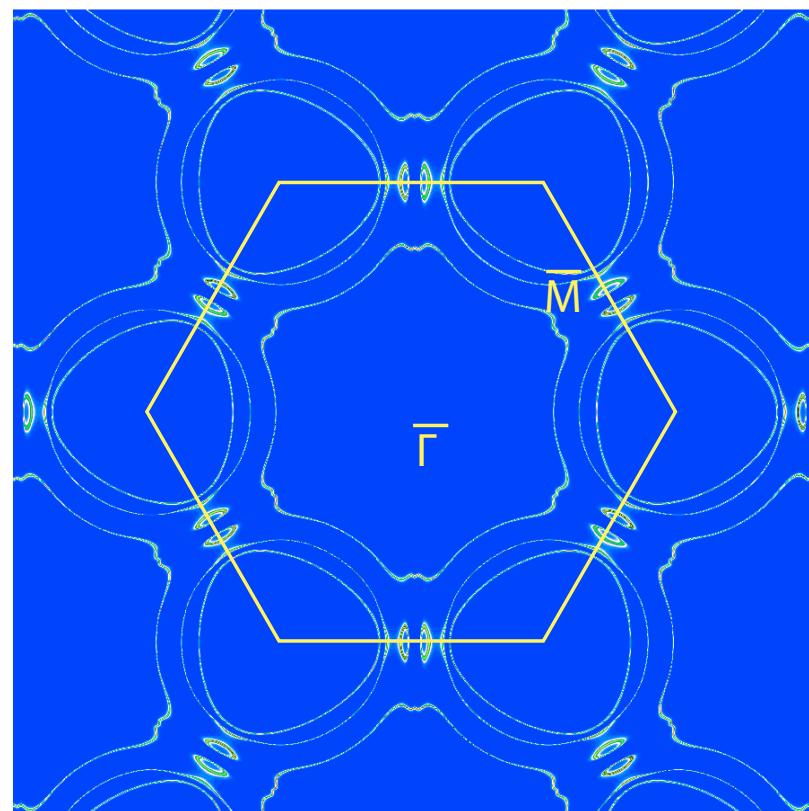
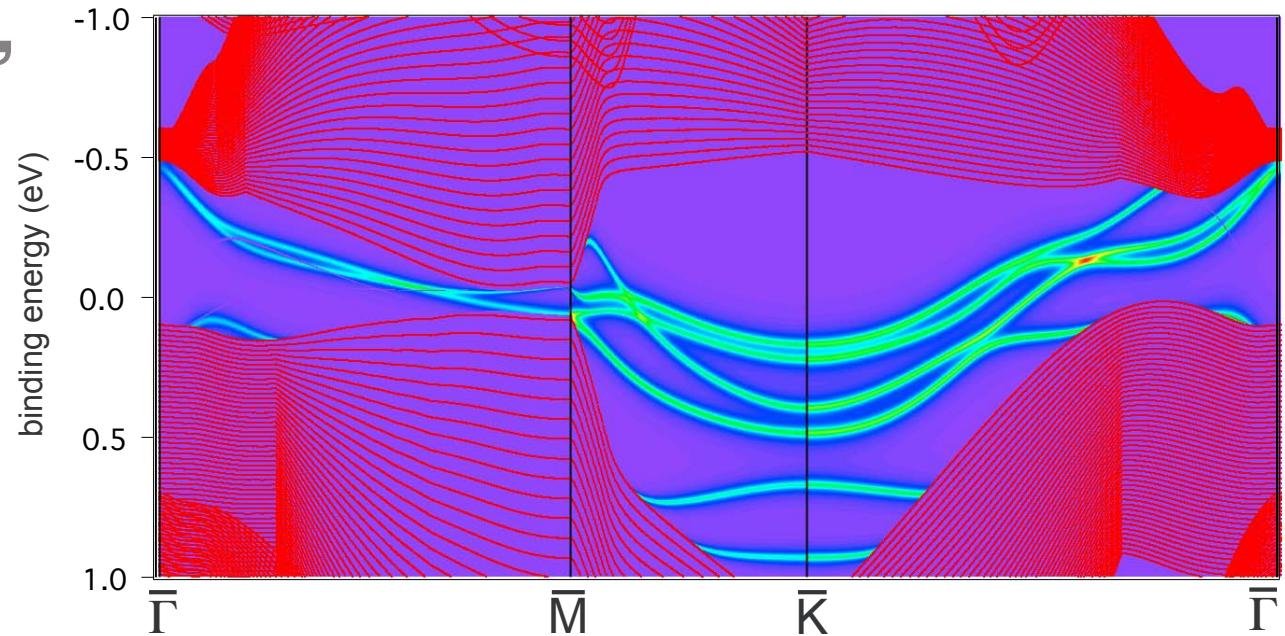
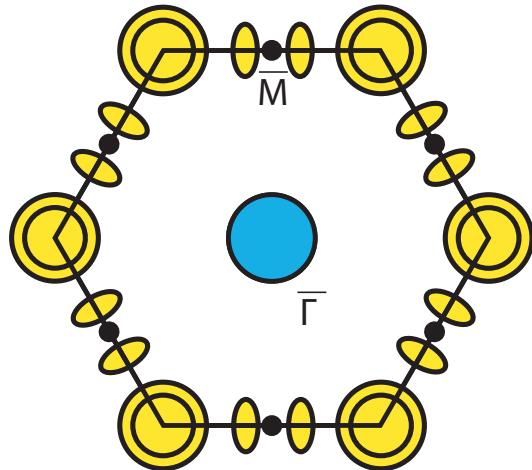


$\text{Bi}_{1-x}\text{Sb}_x(111)'$

(111)'-prediction



tight-binding result



conclusions

- Using epitaxial growth, it is possible to tailor the TI surface state topology via the surface orientation.
- $\text{Bi}_{1-x}\text{Sb}_x(110)$ is an example of a TI surface with odd number of Dirac points.
- Experimental surface electronic structure fits with topological predictions.
- Tight-binding calculations: topology guarantees overall metallic surface states but not any specific state.
- Topologically protected surface states can also exists on topologically trivial semimetals.