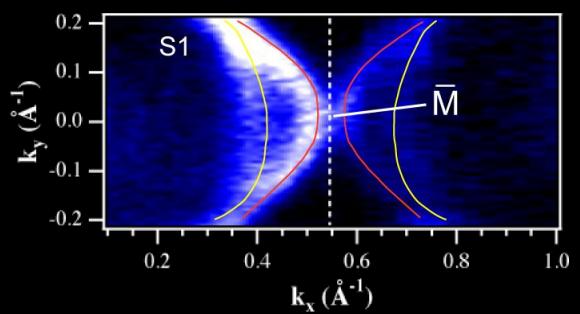
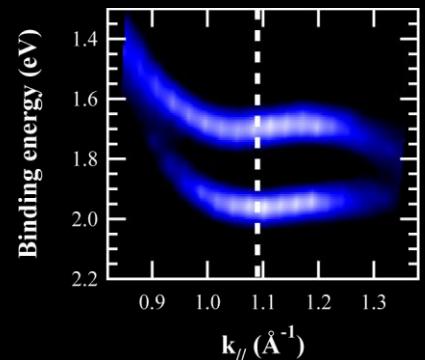
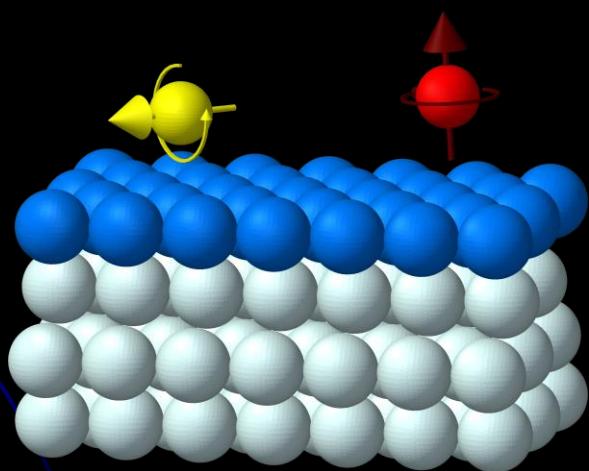


# 対称性に起因する特異なRashba効果

坂本一之

千葉大学大学院融合科学研究所



# 対称性に起因する特異なRashba効果

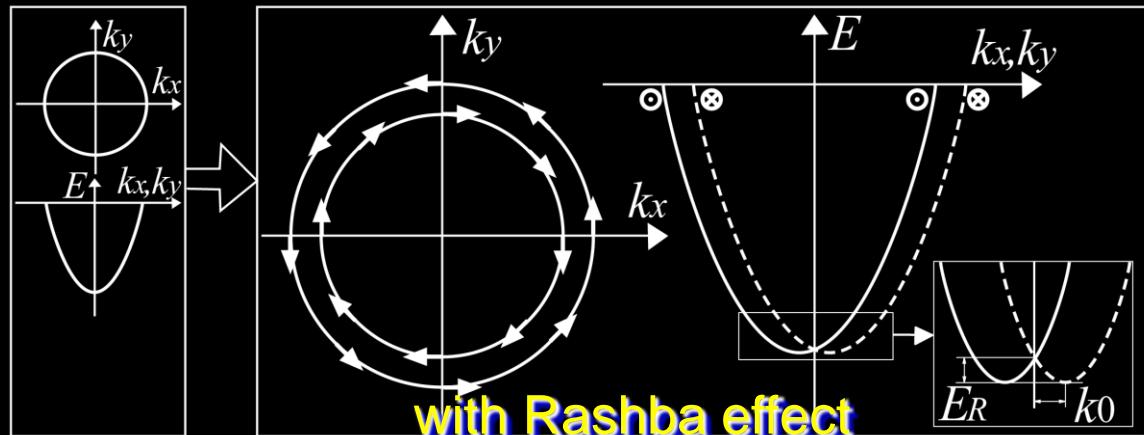
坂本一之

千葉大学大学院融合科学研究所

## Outline

1. Introduction
2. Results and discussion
  - TI/Si(111)-( $\sqrt{3}\times\sqrt{3}$ ), -(1x1)  
(PRL 102, 096805 (2009), PRB 74, 075335 (2006))
  - Bi/Si(111)-( $\sqrt{3}\times\sqrt{3}$ )  
(PRL 103, 156801 (2009))
3. Conclusion

# *Introduction; Rashba effect*



$$[E(k,\uparrow) = E(-k,\downarrow)]$$

time-reversal symmetry

$$H_{RB} = \alpha_R (|\varepsilon|) \sigma \cdot (\mathbf{k}_{\parallel} \times \hat{e}_z)$$

$\alpha_R$ ; Rashba parameter

$$\alpha_R = \hbar^2 k_0 / m^*$$

$\sigma$ ; Pauli spin matrices

$\varepsilon$ ; electric field determined by  
the potential gradient

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

# Introduction; Rashba effect



## Materials

Ag(111)

Au(111)

Bi(111)

Bi/Ag(111)



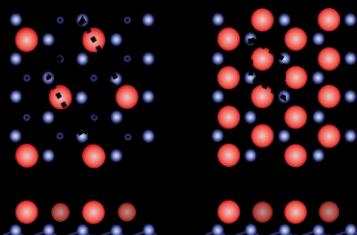
**Tl on a Si(111) surface**  
**Bi on a Si(111) surface**

# Introduction; Tl/Si(111)

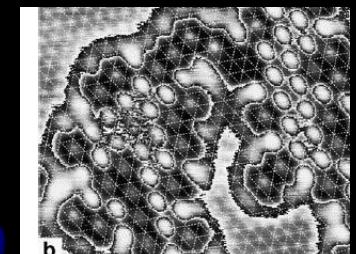
Group III metals (Al, Ga, and In) on Si(111);  
magic cluster arrays at modest temperature (PRL 81, 164 (1998))  
 $(\sqrt{3} \times \sqrt{3})$  reconstruction at higher temperature (PRL 81, 164 (1998))

Tl; peculiar behavior in the form of the so-called “inert pair effect”  
On a Si(111) surface; 1ML (1x1) phase **monovalent** atom  
1/3 ML ( $\sqrt{3} \times \sqrt{3}$ ) phase **trivalent**

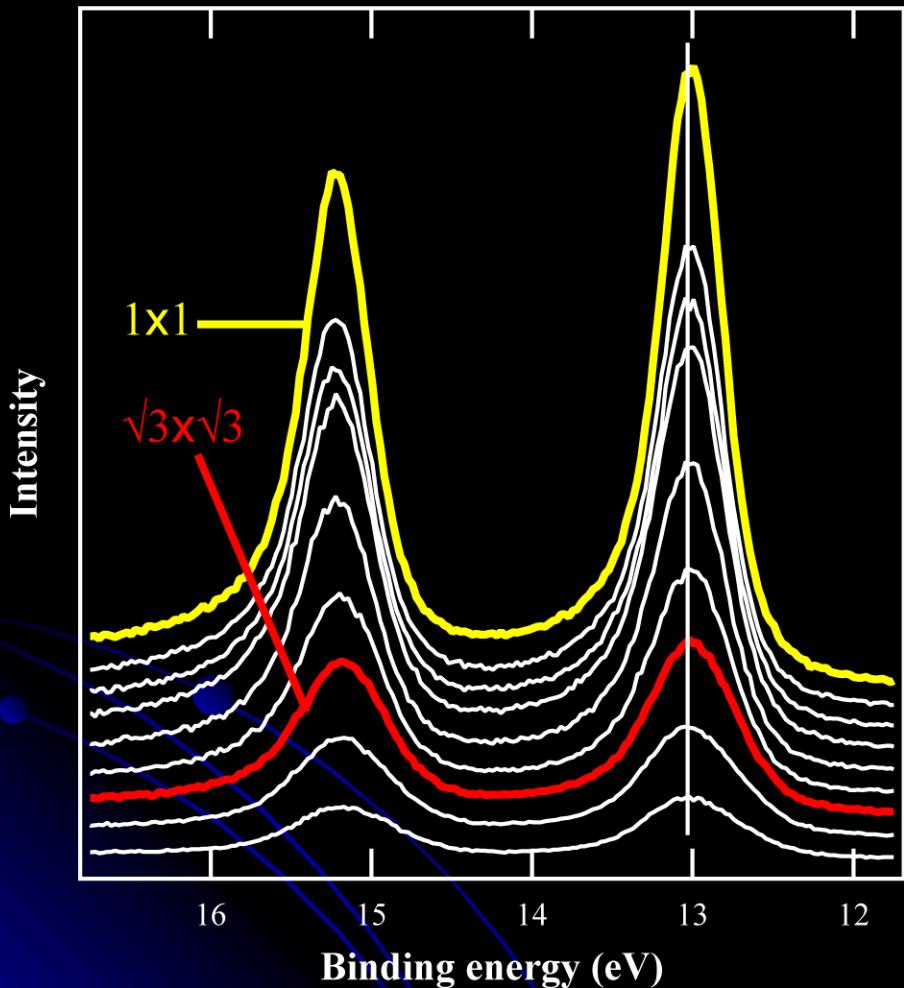
**variable valency** for Tl on a Si(111) ?  
(SS 543, L663 (2003), PRB 66, 233312 (2002))



SS 543, L663 (2003)



# Results; Tl 5d core-level



Coverage-dependent Tl 5d core-level spectra obtained with a photon energy of 50 eV.

$I_{(1\times 1)} : I_{(\sqrt{3}\times\sqrt{3})} = 3:1$   
 $(1\times 1)$  surface; **1ML**,  
 $(\sqrt{3}\times\sqrt{3})$  surface;  **$1/3$  ML**

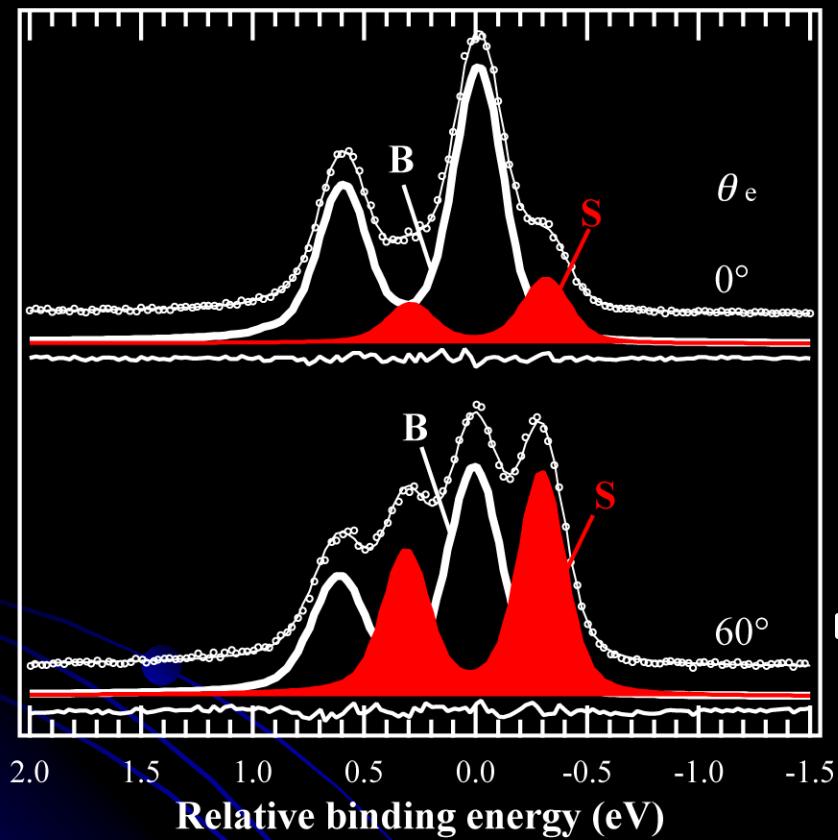
constant binding energy

difference in  $E_B$  of the  
5d core-level or the  $Tl^{1+}$   
and  $Tl^{3+}$  0.58 eV  
J. Phys. Soc. Jpn., 1532 (2004)

Identical valence state

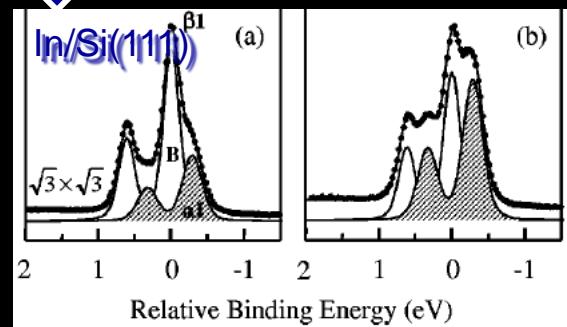
# Results; Ti/Si(111)-(1x1) Si 2p core-level

Intensity (arb. units)



Si 2p core-level spectra of the  
Ti/Si(111)-(1x1) surface measured  
with  $h\nu=135$  eV .

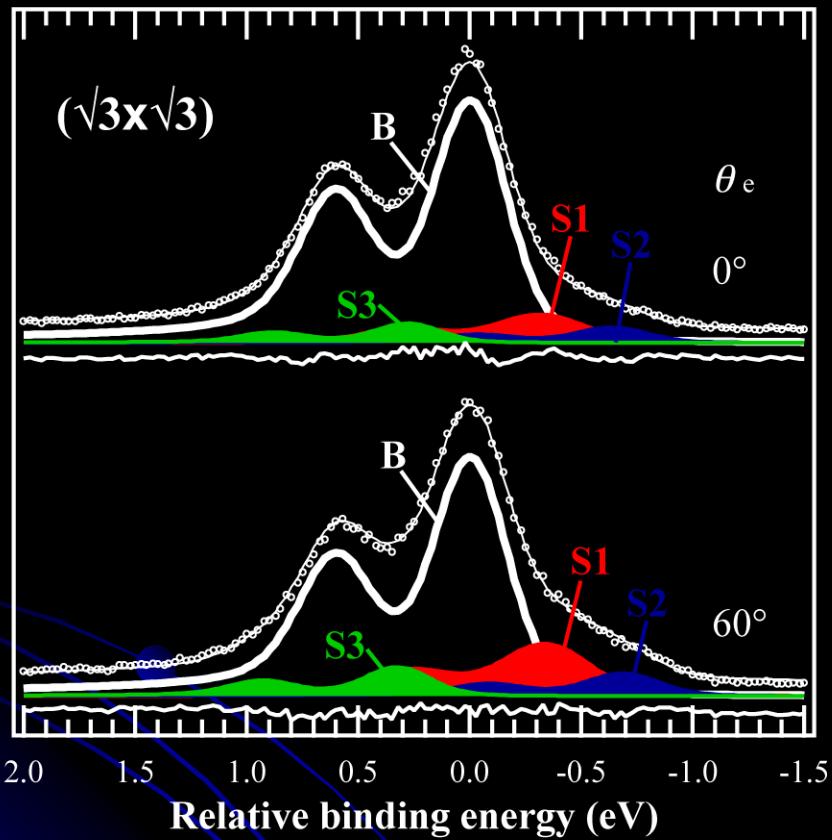
common unreconstructed  
(1x1) structure



PRB 67, 035414 (2003)

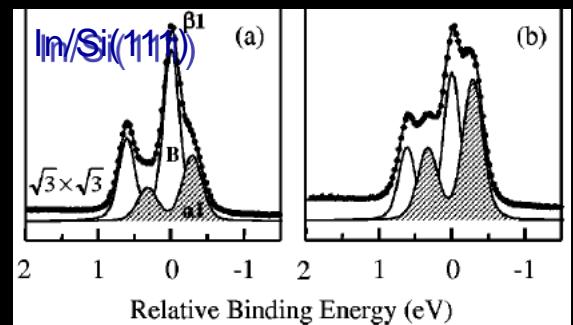
# Results; Ti/Si(111)-( $\sqrt{3} \times \sqrt{3}$ ) Si 2p core-level

Intensity (arb. units)



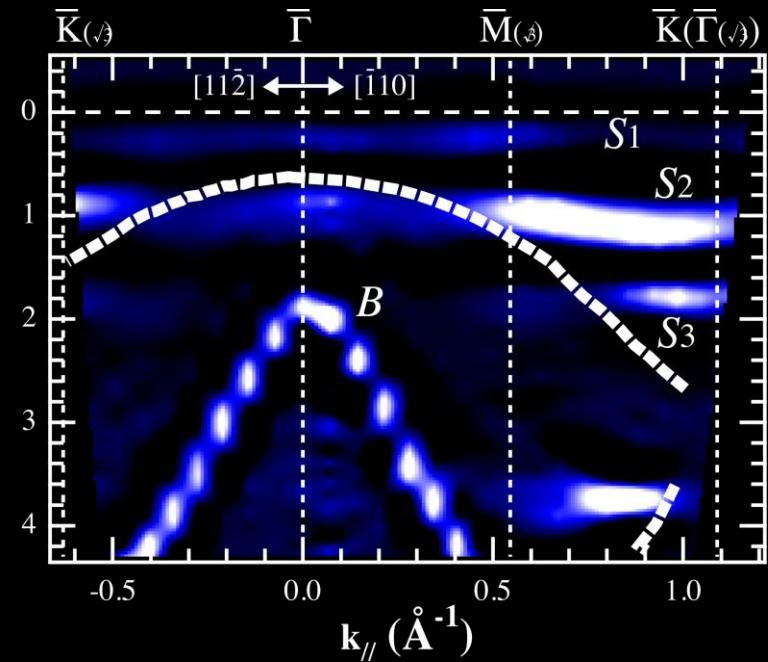
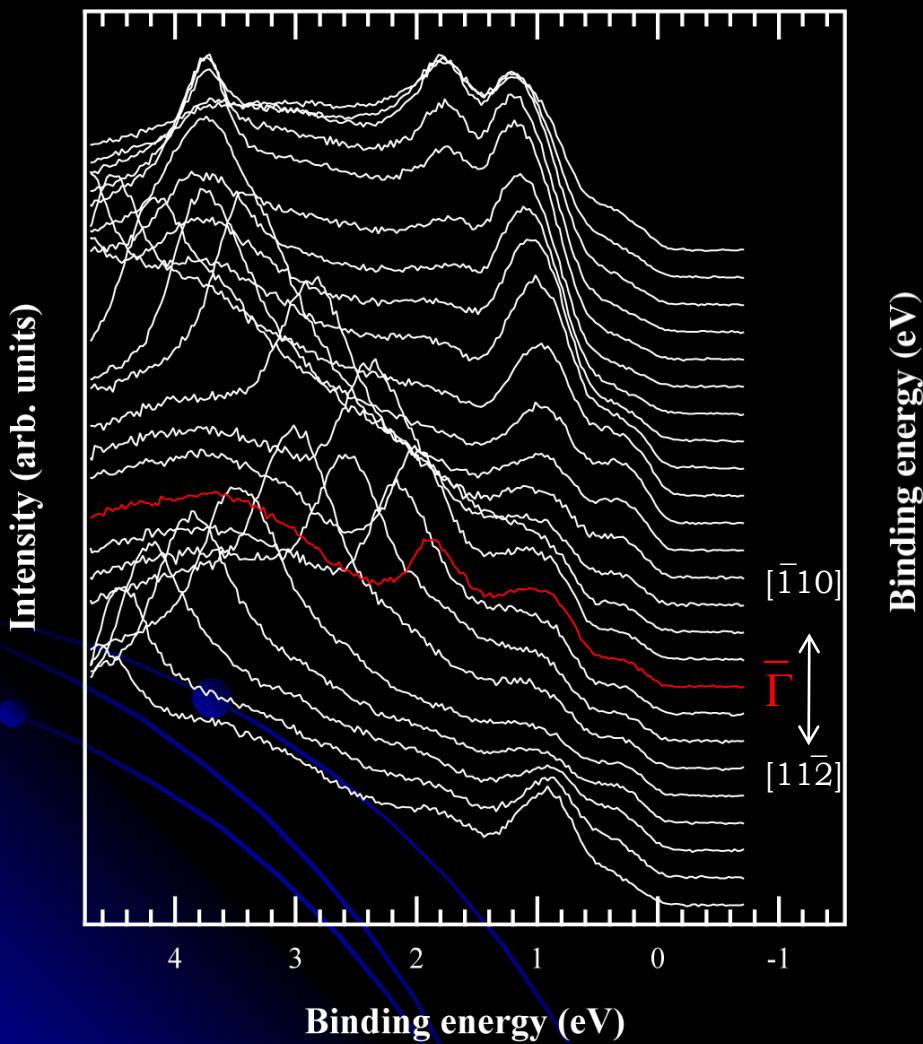
Si 2p core-level spectra of the  
Ti/Si(111)-( $\sqrt{3} \times \sqrt{3}$ ) surface  
measured with  $h\nu=135$  eV.

the two ( $\sqrt{3} \times \sqrt{3}$ ) surfaces have  
**different atomic structures**



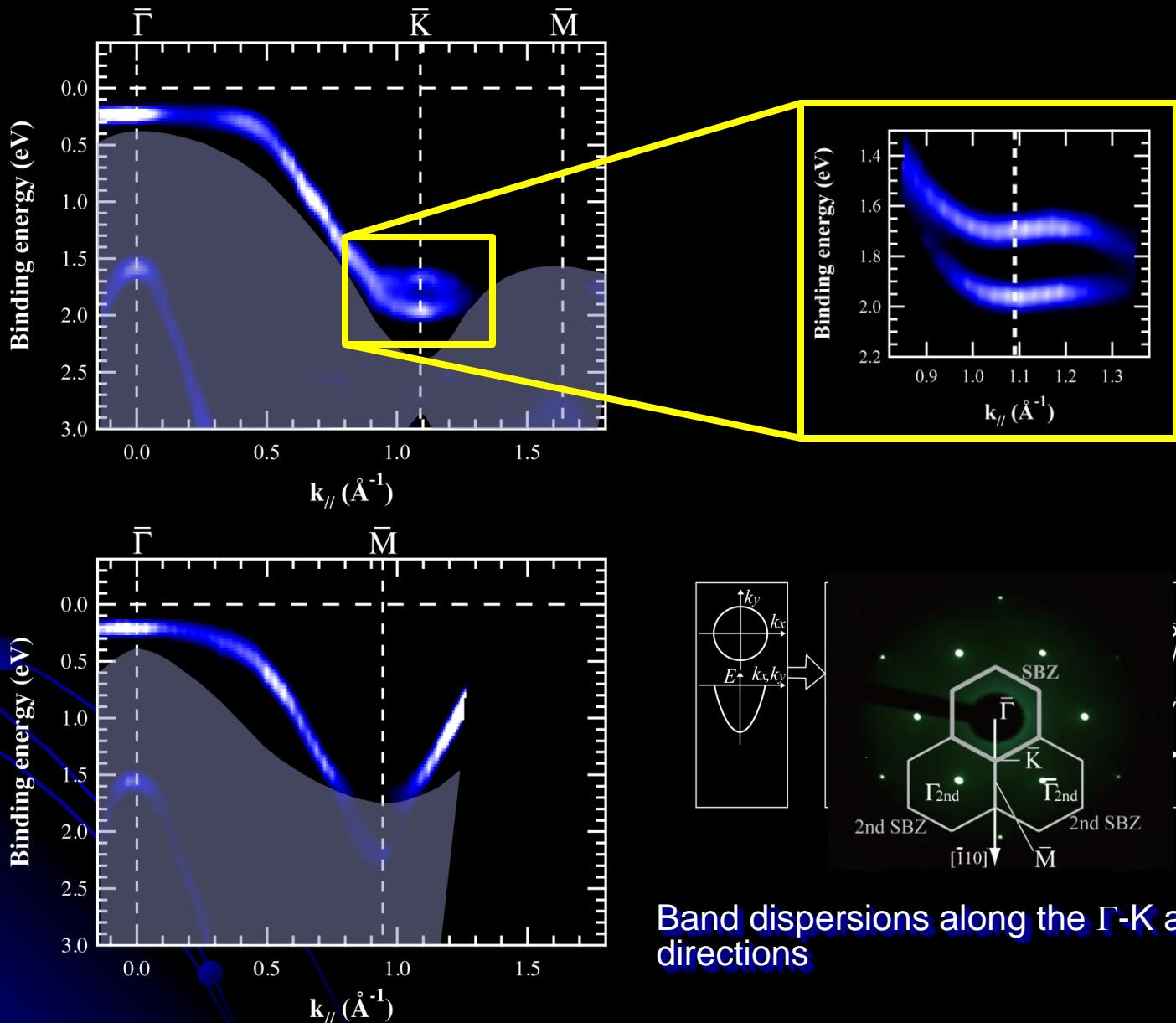
PRB 67, 035414 (2003)

# Results; Ti/Si(111)-( $\sqrt{3}\times\sqrt{3}$ ) ARPES

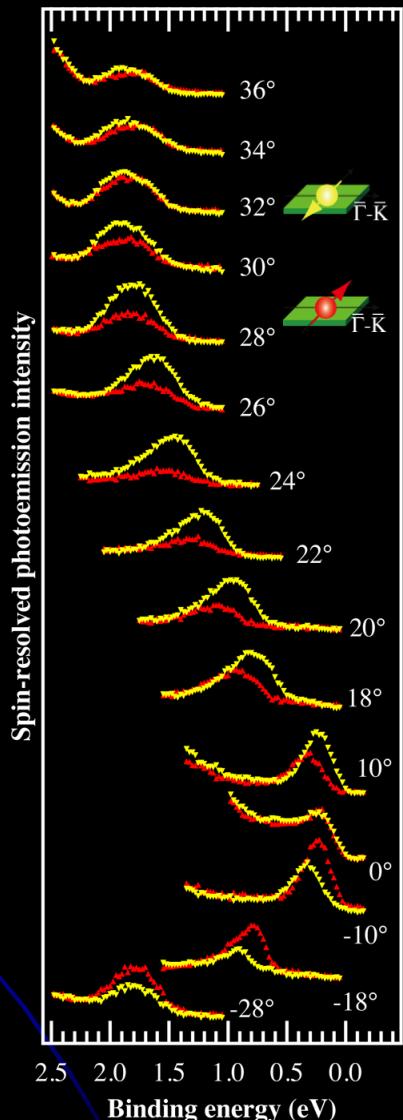


ARPES spectra measured using  $h\nu=21.2$  eV

# Results; Ti/Si(111)-(1x1) valence band

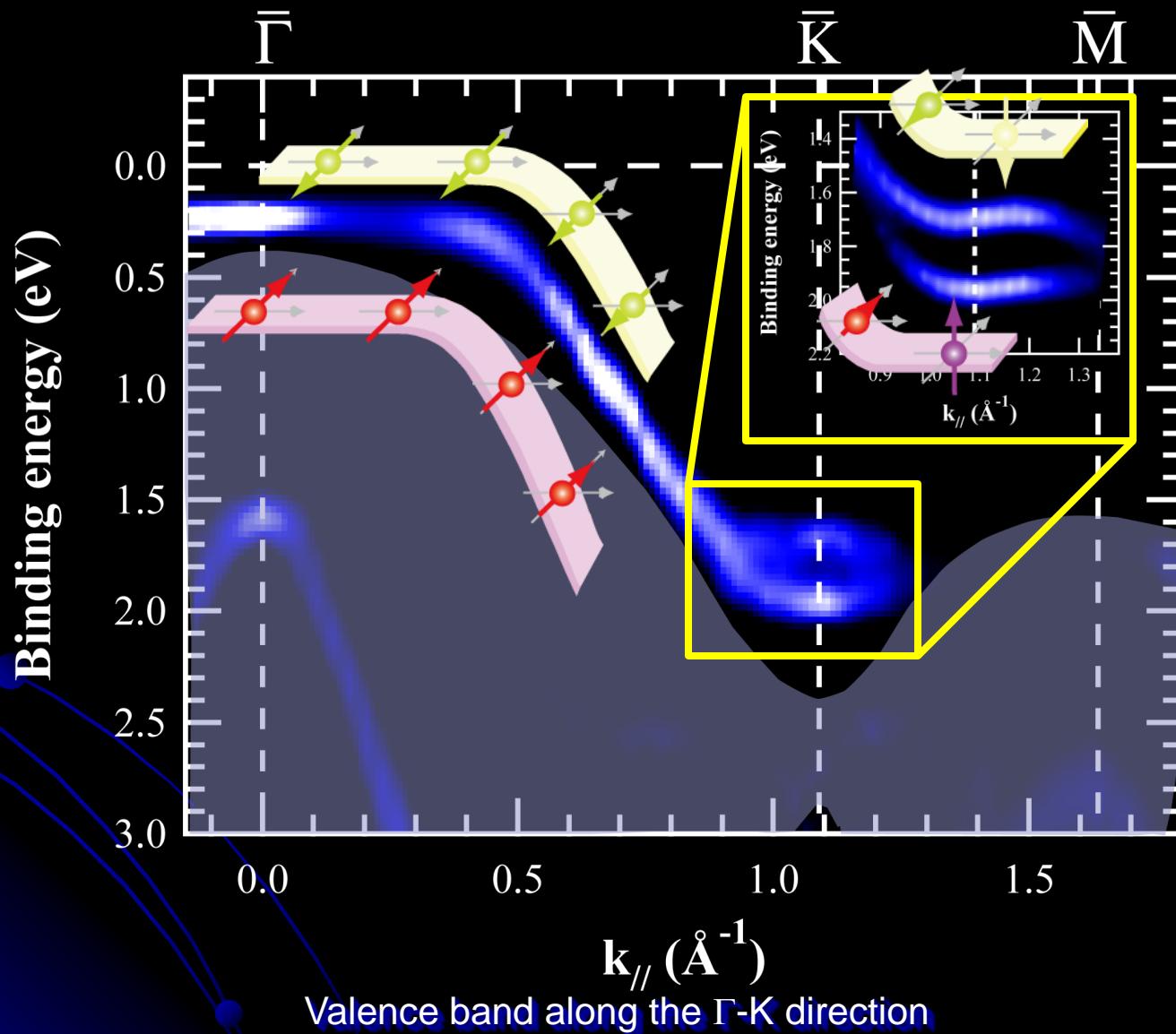


# Results; Ti/Si(111)-(1x1) SR-ARPES



SR-ARPES spectra measured along the  $\Gamma$ -K direction

# Results; Tl/Si(111)-(1x1) spin states



# *Discussion; extended RB effect*

$$\varphi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \exp(i\mathbf{k} \cdot \mathbf{r}) u_{n\mathbf{k}}(\mathbf{r})$$

Effective SOI Hamiltonian of the “extended RB effect”

$$H_{SOI}(\mathbf{k}) = \boldsymbol{\sigma} \cdot (\boldsymbol{\alpha}_n(\mathbf{k}) \times \mathbf{k}) + \underline{\boldsymbol{\sigma} \cdot \mathbf{B}_n(\mathbf{k})}$$

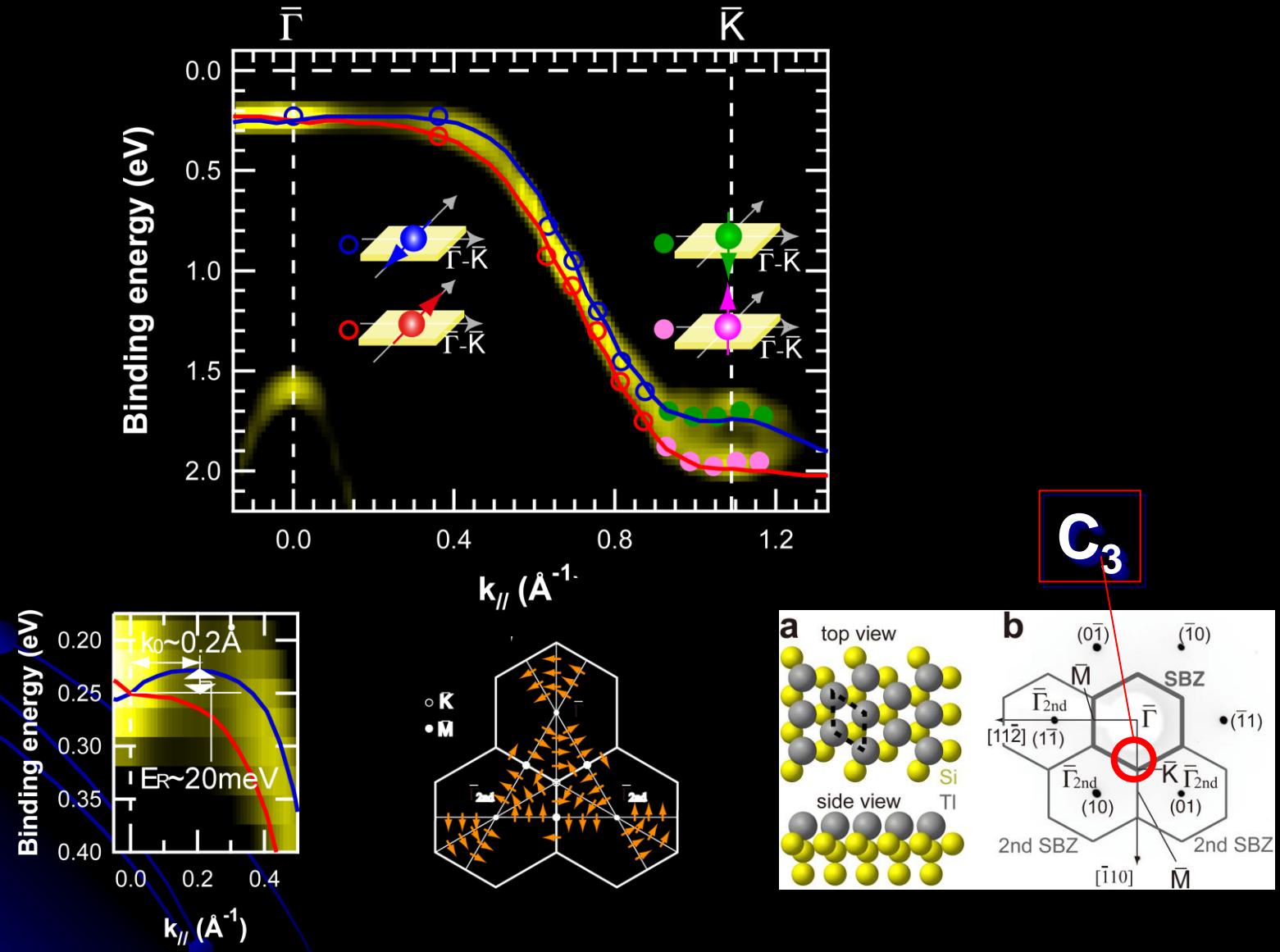


$$H_{RB} = \alpha_R(|\varepsilon|) \boldsymbol{\sigma} \cdot (\mathbf{k}_{\parallel} \times \hat{\mathbf{e}}_z)$$

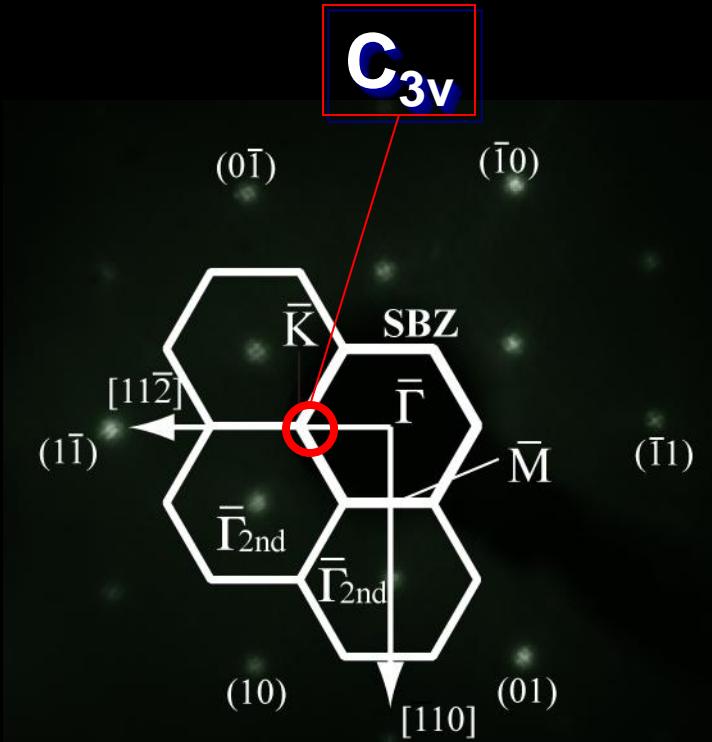
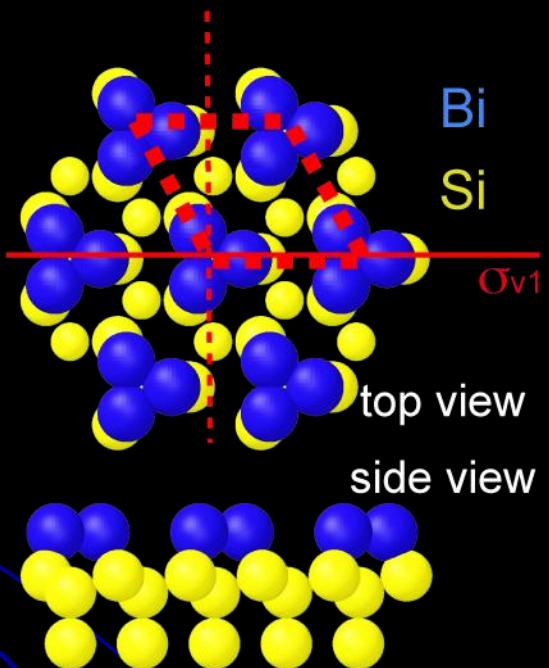
$$\vec{\alpha}_n(\vec{k}) = \frac{\hbar^2 N}{4m_e^2 c^2 \Omega} \int_{cell} d\vec{r} \left| u_{n\vec{k}}(\vec{r}) \right|^2 \nabla V(\vec{r})$$

$$\vec{B}_n(\vec{k}) = \frac{\hbar^2 N}{4m_e^2 c^2 \Omega} \int_{cell} d\vec{r} \frac{1}{r} \frac{dV(\vec{r})}{dr} u_{n\vec{k}}^*(\vec{r})(\vec{l}) u_{n\vec{k}}(\vec{r})$$

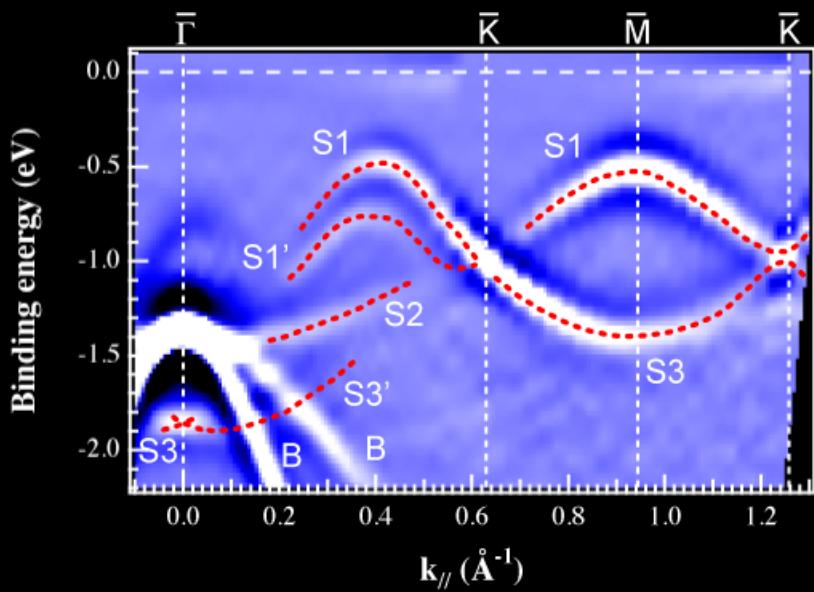
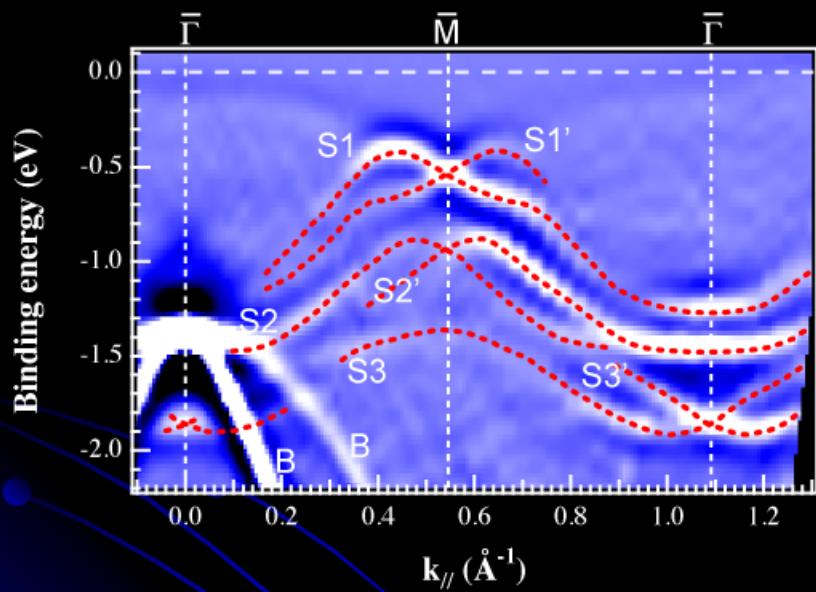
# *Discussion; origin of the standing spin*



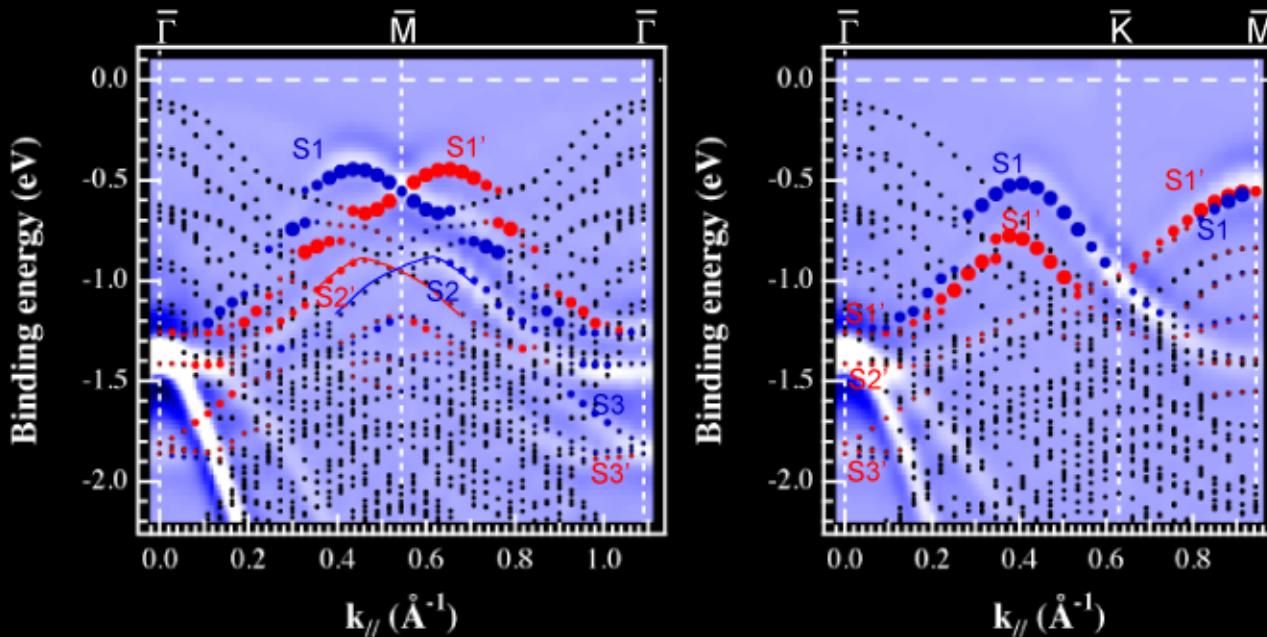
# Introduction; Bi/Si(111)-( $\sqrt{3}\times\sqrt{3}$ )



# Results; Bi/Si(111)-( $\sqrt{3}\times\sqrt{3}$ ) ARPES

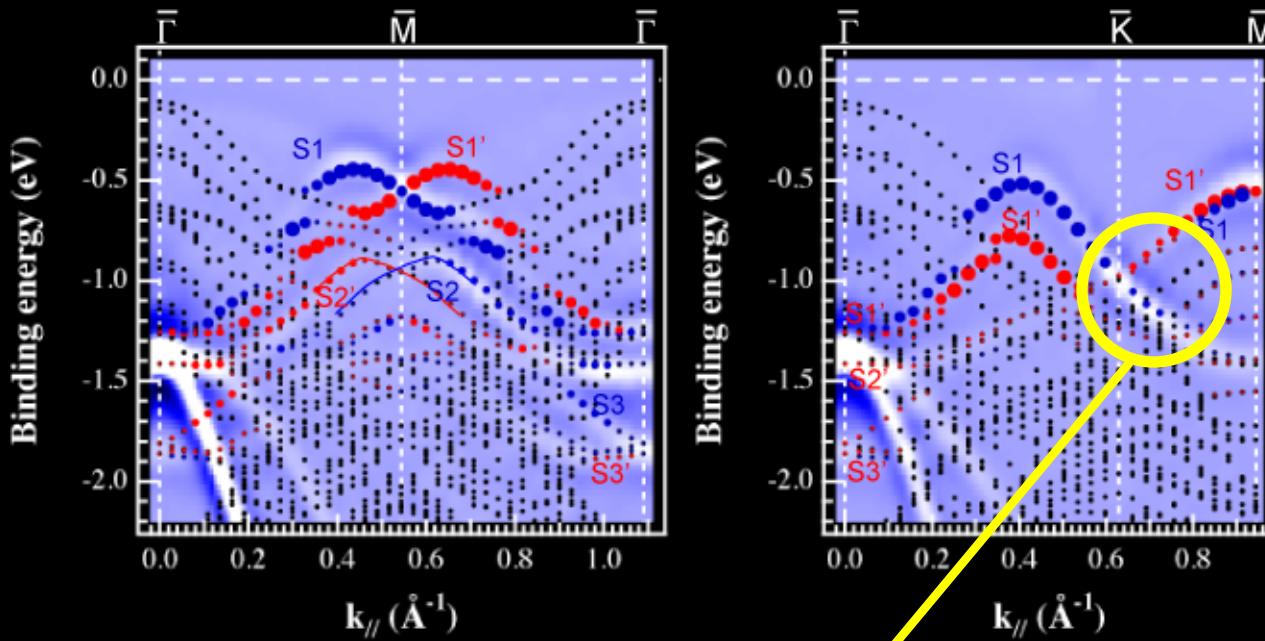


# Results; Bi/Si(111)-( $\sqrt{3}\times\sqrt{3}$ ) ARPES



Materials	$E_R$ (meV)	$k_O$ ( $\text{\AA}^{-1}$ )	
<b>S1</b>	<b>120</b>	<b>0.105</b>	I. Gierz <i>et al.</i> , PRL 103, 046803 (2009)
<b>S2</b>	<b>70</b>	<b>0.08</b>	
<b>S3</b>	<b>70</b>	<b>0.08</b>	
Bi/Ag(111)	200	0.13	C. Ast <i>et al.</i> , PRL 98, 186807 (2007)

# Results; Bi/Si(111)-( $\sqrt{3}\times\sqrt{3}$ ) ARPES



**Materials** Observation of a Rashba splitting though  
 $E_R$  (meV)  $k_R$  ( $\text{\AA}^{-1}$ ) there is no time reversal

**S1** **120** **0.105** I. Gierz *et al.*, PRL 103,  
 Peculiar Rashba splitting that originates from the  $C_{3v}$  symmetry  $\delta^{46}$  (2009)

**S2** **70** **0.08**

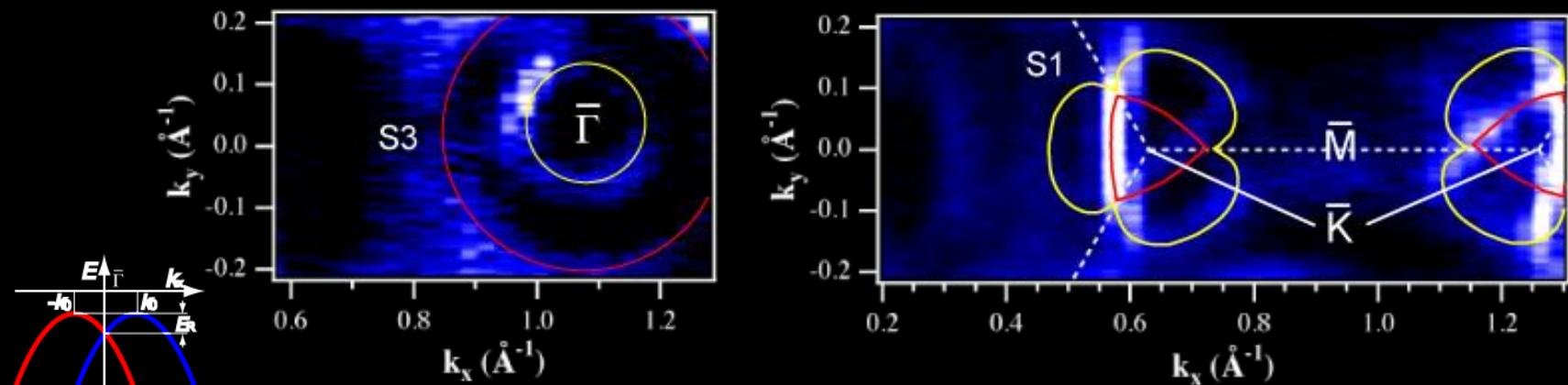
**S3** **70** **0.08**

Bi/Ag(111) **200** **0.13**

I. Gierz *et al.*, PRL 103,  
 046803 (2009)

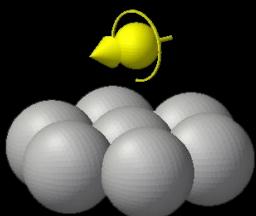
C. Ast *et al.*, PRL 98,  
 186807 (2007)

# Results; Bi/Si(111)-( $\sqrt{3}\times\sqrt{3}$ ) ARPES

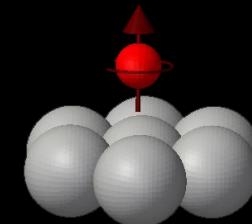


# Conclusion

Observation of **peculiar Rashba spins**



Tl/Si(111)-(1x1)  
Spin **standing perpendicular**



Bi/Si(111)-( $\sqrt{3} \times \sqrt{3}$ )

Rashba spin at a point **without time-reversal symmetry**  
**Non-vortical Rashba** spin structure



knowledge on the 2D symmetry is indispensable  
to understand the Rashba effect properly

# Acknowledgments

## Experiment team

Chiba University, Japan,

A. Imai, H. Kakuta, T. Kuzumaki, N. Ueno

Hiroshima University, Japan

A. Kimura, K. Miyamoto, H. Namatame, M. Taniguchi

Tohoku University, Japan

K. Sugawara, T. Sato, T. Takahashi

Linkoping University, Sweden

P.E.J. Eriksson, R.I.G. Uhrberg

TASC National Lab., Italy

E. Annese, J. Fujii

Financial supports  
JSPS Grant-in-Aid for  
Scientific Research (A)  
20244045 and (B)  
20340092, and the G-COE  
program of MEXT (G-03)

## Theory team

Kanazawa University, Japan

T. Oda, M. Tsujikawa

Hiroshima University, Japan

A. Kodama, T. Shishidou, T. Oguchi