Theory of Rashba splitting in quantum-well states

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Collaborator
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Theory : T. Ozaki

- R. Noguchi, K. Kuroda, M. Kawamura, K. Yaji, A. Harasawa, T. Iimori, S. Shin, F. Komori, T. Ozaki, T. Kondo, PRB **104**, L180409 (2021).
- M. Kawamura, T. Ozaki, In preparation.

OpenMX developer's meeting
2023/11/10

Outline

- Introduction
  - Rashba effect and its application
  - Large Rashba-parameter materials
- Quantum well state in Ag few MLs on Au(111)
  - Computational result
  - Discussion
- Theory of Rashba splitting
  - Spin-orbit interaction and intrinsic magnetic field
  - Tight-binding model and solution
- Application of model to QWS of Ag/Au(111)
- Summary

Intro

Rashba effect

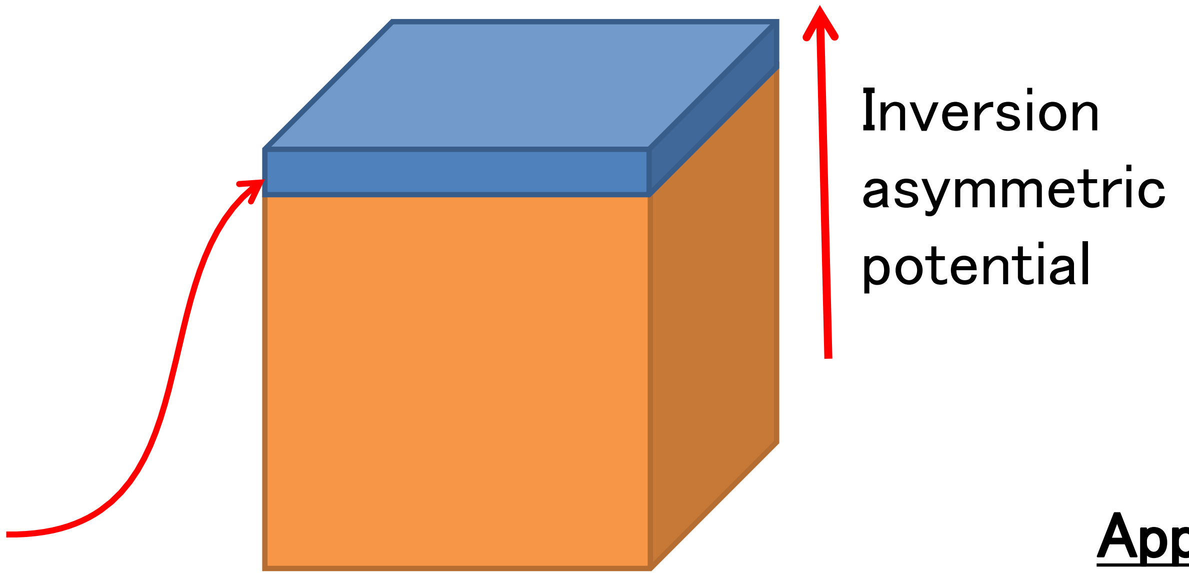
Y. Bychkov , E. Rashba JETP Lett. **39**, 78 (1984).

Hamiltonian with spin-orbit interaction

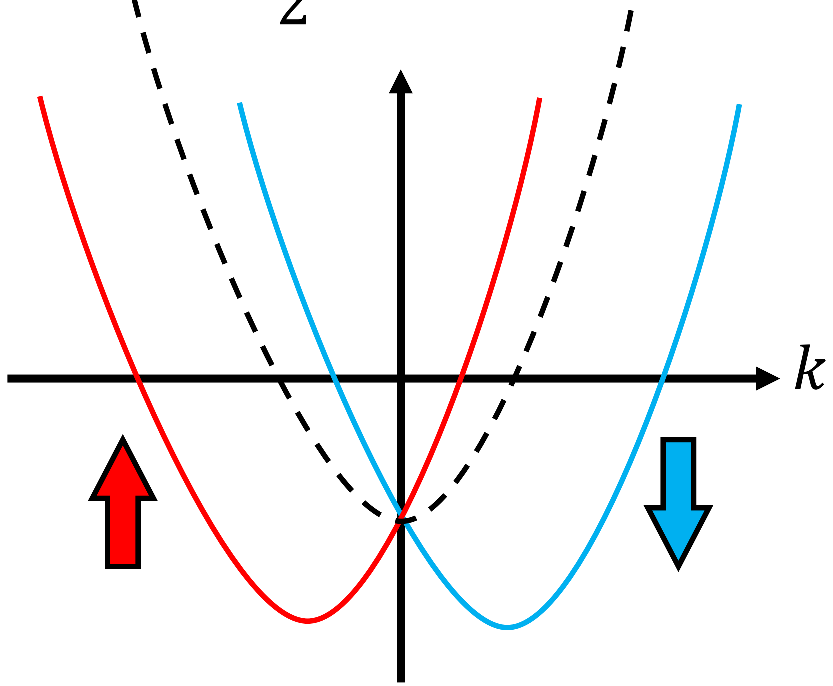
$$\hat{H} = -\frac{\nabla^2}{2} + V(r) + \frac{2}{c^2}(\nabla V(r) \times \boldsymbol{p}) \cdot \boldsymbol{s}$$

Confined 2D (Nearly Free) electrons

$$\hat{H}(\boldsymbol{k}) = \frac{\boldsymbol{k}^2}{2} + 2\alpha_R(\boldsymbol{e}_z \times \boldsymbol{k}) \cdot \boldsymbol{s}$$

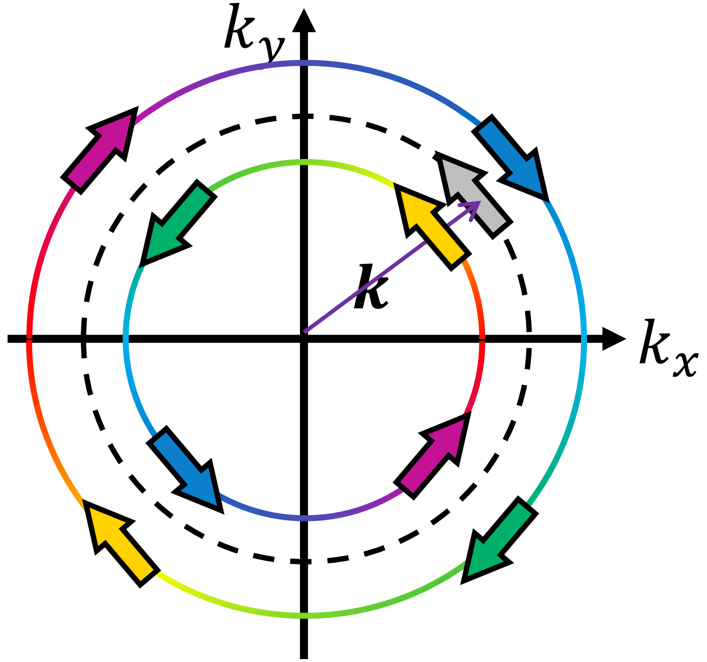


$$\varepsilon_k^{\pm} = \frac{\boldsymbol{k}^2}{2} \pm \alpha_R|\boldsymbol{k}|$$



$$\hat{H}_R(\boldsymbol{k}) = \boldsymbol{B}_R(\boldsymbol{k}) \cdot \boldsymbol{s}$$

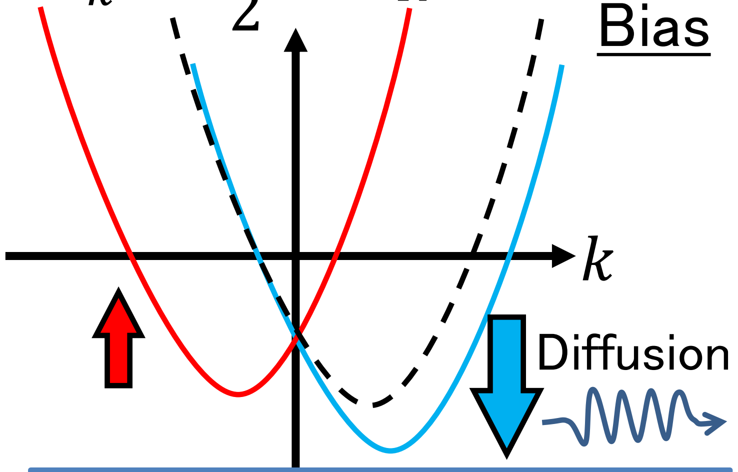
$$\boldsymbol{B}_R(\boldsymbol{k}) \equiv \alpha_R(\boldsymbol{e}_z \times \boldsymbol{k})$$



Application

$$\varepsilon_k^{\pm} = \frac{\boldsymbol{k}^2}{2} \pm \alpha_R|\boldsymbol{k}| + \boldsymbol{E} \cdot \boldsymbol{k}$$

Bias



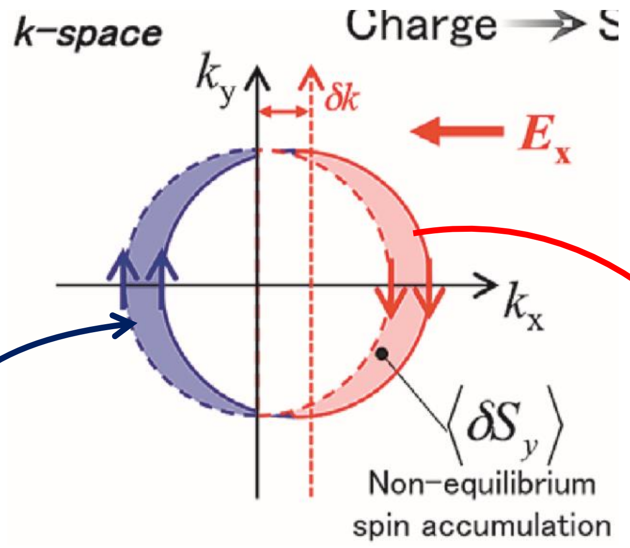
Spin-current generation
detection

Intro

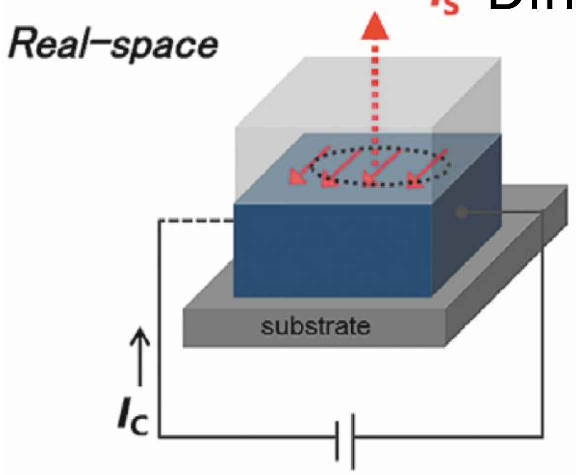
Application of Rashba effect

※Only large Fermi surface is drawn

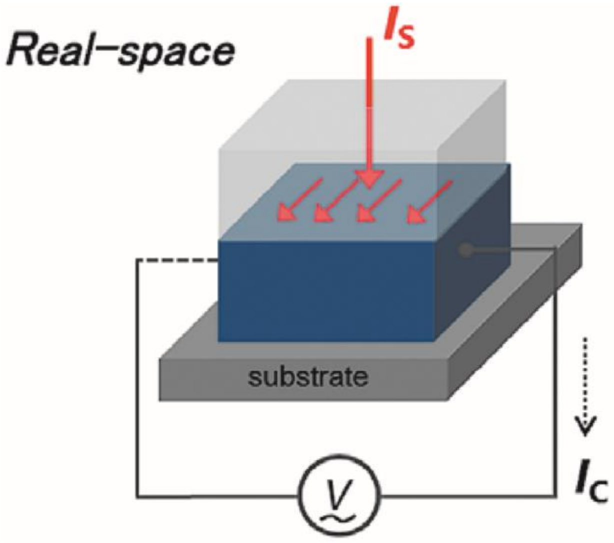
Generate spin current

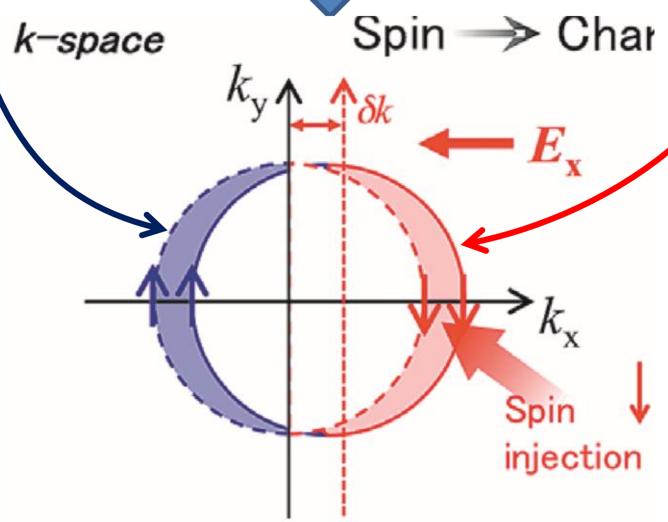


I_S Diffuse



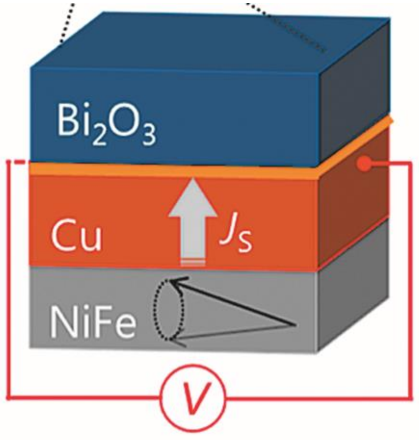
Detect spin current





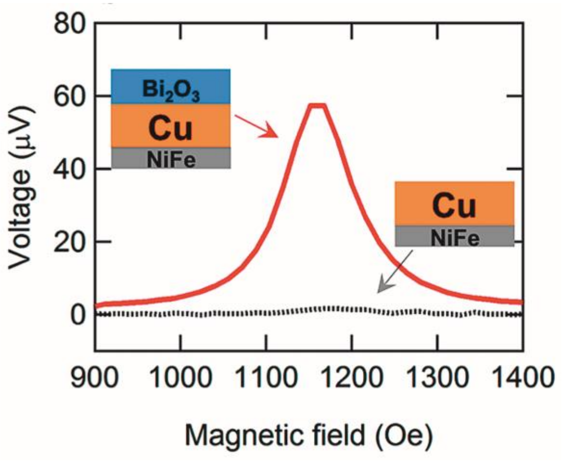
[K. Kondo, 日本物理学会誌 Vol. 72, No. 5, 2017]

Measurement of Spin current → Charge current



No inverse spin Hall effect

No spin current in Bi_2O_3



J. Sánchez, *et al.*, Nat. Commun. **4**, 2944 (2013).

Intro

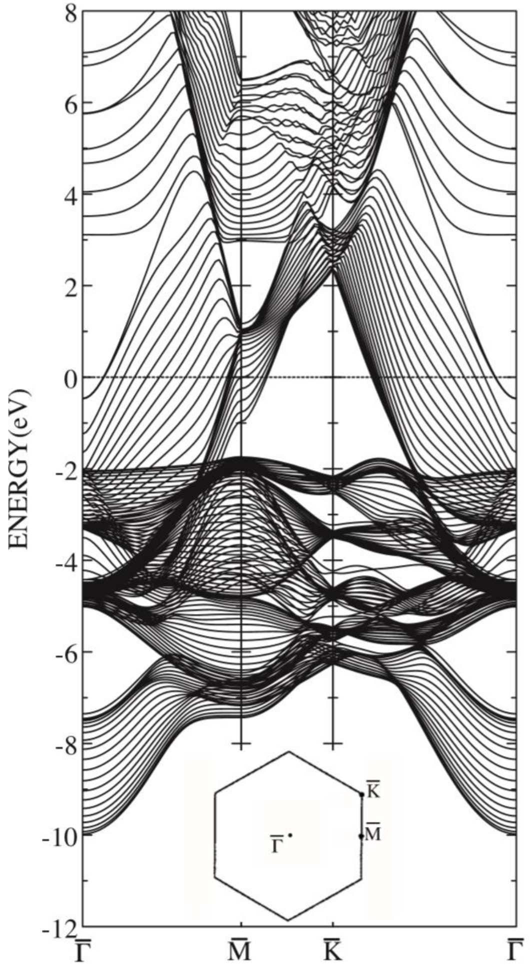
Origin of potential gradient

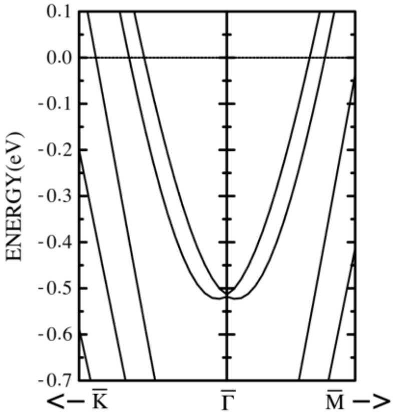
Au(111), Ag(111), Sb(111)
23 layer slab

M. Nagano, *et al.*, J. Phys.: Condens. Matter **21**, 064239 (2009).

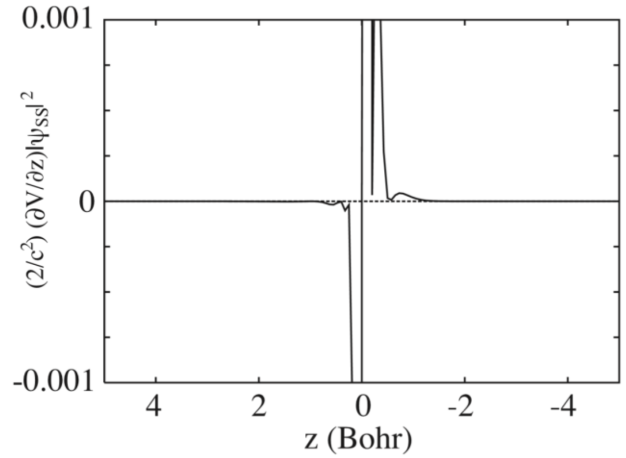
- SOC : Second variational
- FLAPW

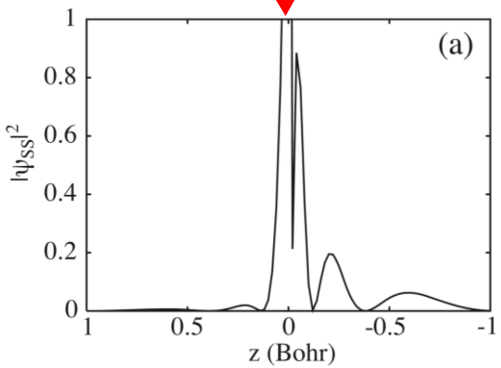
$$\Delta\varepsilon_R = \langle \psi_{SS}^{k_\parallel} | \hat{H}_R | \psi_{SS}^{k_\parallel} \rangle = |\boldsymbol{k}_\parallel| \int d^3r \, \frac{2}{c^2} \frac{\partial V}{\partial z} \left| \psi_{SS}^{k_\parallel} \right|^2$$

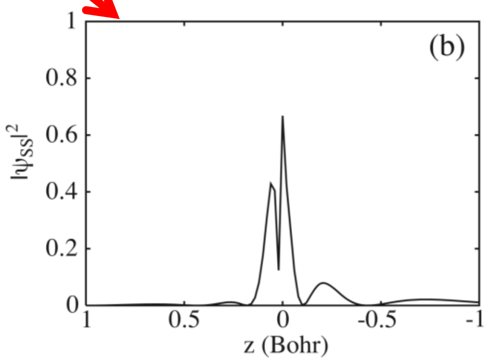


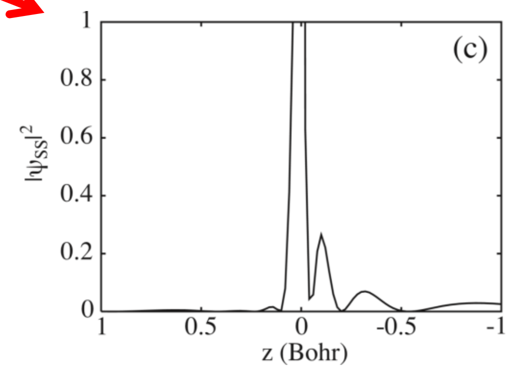


		$_{71}$Au(111)	$_{47}$Ag(111)	$_{51}$Sb(111)
Δk_R	$\bar{\Gamma}\bar{M}$	27.8	—	20.5
(10^{-3} Å^{-1})	$\bar{\Gamma}\bar{K}$	27.8	—	21.2
ζ_l	p	6.34	1.90	2.27
(eV)	d	0.79	0.27	0.52
Component	s	1.3	0.7	3.3
(%)	p	4.7	4.6	9.8
	d	2.5	0.8	—









Large SOI +
Asymmetry of WF

Intro

Material with Large Rashba Splitting

Au(111) surface state

S. LaShell, *et al.*, PRL **77**, 3419 (1996).

$$\alpha_R = 0.33 \text{ eV} \cdot \text{Å}$$

Bi surface alloy

$\sqrt{3} \times \sqrt{3}$ R30° Bi/Ag(111)

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

$$\alpha_R = 3.05 \text{ eV} \cdot \text{Å}$$

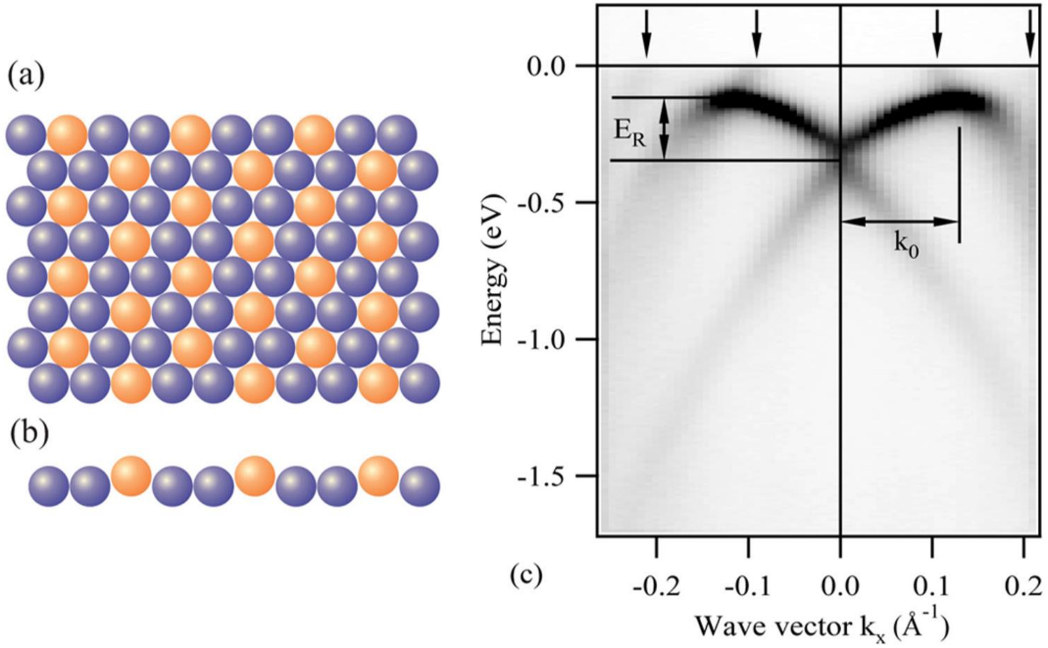
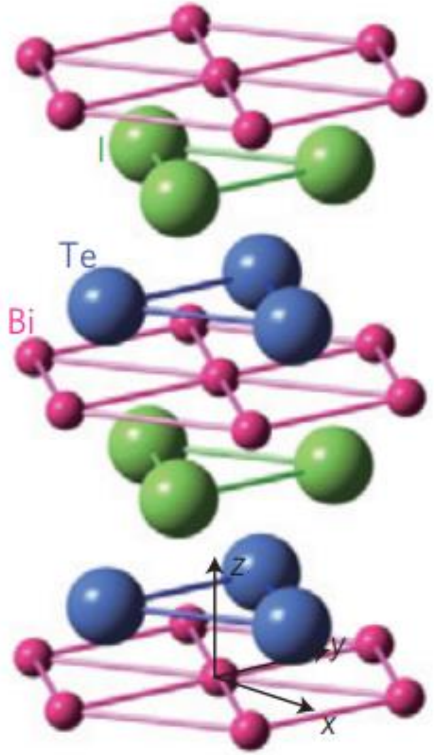


Table 1 | Selected materials and parameters characterizing spin band splitting: the momentum offset k_0 ($Å^{-1}$), Rashba energy E_R (meV) and Rashba parameter α_R (eV Å).

Sample	k_0	E_R	α_R	Reference
Surface state				
Au(111)	0.012	2.1	0.33	5
Bi(111)	0.05	14	0.55	16
1/3 ML Bi on Ag surface alloy	0.13	200	3.05	7
Interface				
InGaAs/InAlAs	0.028	<1	0.07	4
QW state				
Pb thin film (6–22 ML)	0.035	≲10	0.04	36
Bi thin film (7–40 BL)	–	–	–	18,37
1 ML Bi on Cu	N/A	N/A	2.5	20
Bulk				
BiTeI	0.052	100	3.8	This work

For the Bi thin-film system in refs 18,37, the splitting was observed only for the surface states, not for the QW subband states. ML, monolayer.



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

Table 2
Rashba parameters in the Bi/M alloys: α_R is the Rashba coefficient, E_R the Rashba energy, k_R the Rashba momentum offset.

M	Cu	Ag	Au	Ni	Co	Fe
Upper splitting						
k_R($Å^{-1}$)	0.036	0.075	0.046	0.067	0.077	0.082
E_R(eV)	0.068	0.123	0.044	0.135	0.140	0.139
α_R(eV·Å)	3.76	3.28	1.91	4.05	3.71	3.40
Lower splitting						
k_R($Å^{-1}$)	0.072	0.124	0.206	0.094	0.113	0.115
E_R(eV)	0.093	0.177	0.168	0.107	0.112	0.067
α_R(eV·Å)	2.59	2.85	1.63	2.28	1.98	1.17

N. Yamaguchi, F. Ishii, J. Crys. Growth **468**, 688 (2017)

Intro

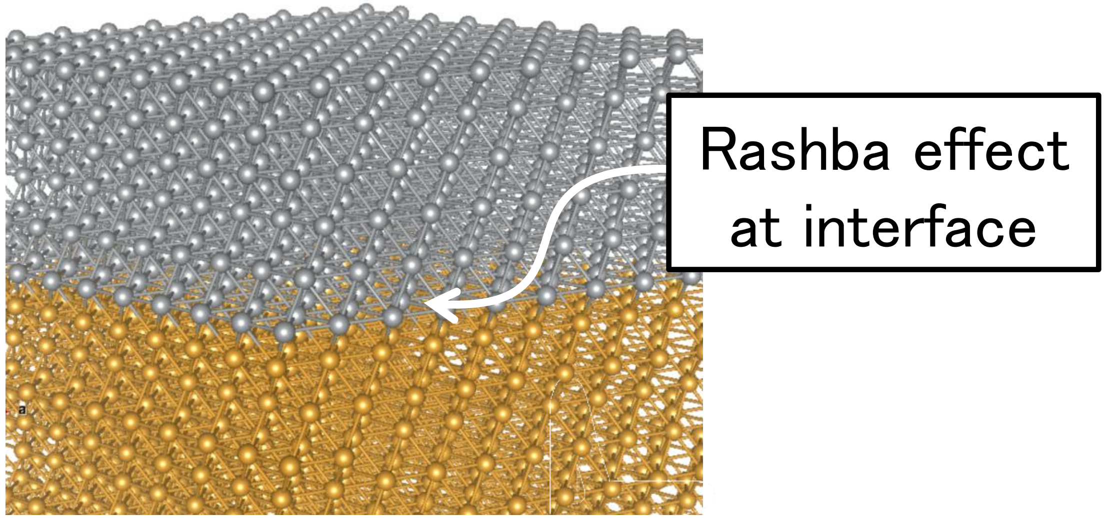
Ag/Au(111) : Purpose of study

High-resolution spin-decomposed ARPES

Au(111) : $\alpha_R = 330$ meV・Å

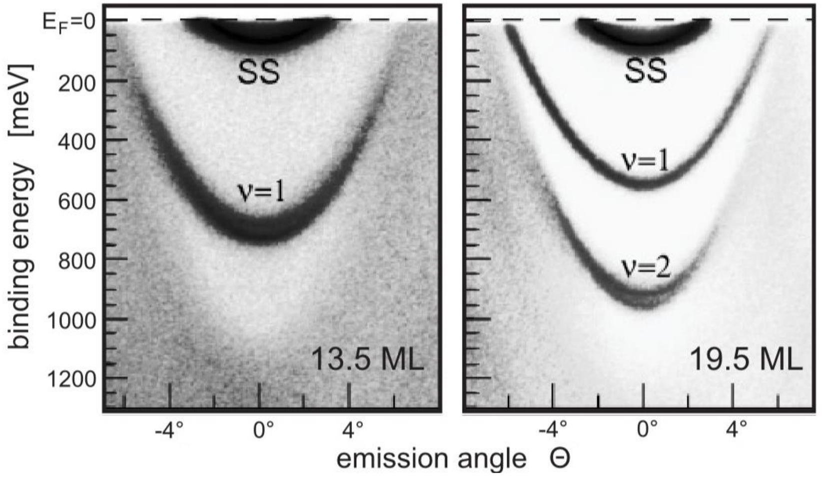
Ag(111) : $\alpha_R = 31$ meV・Å

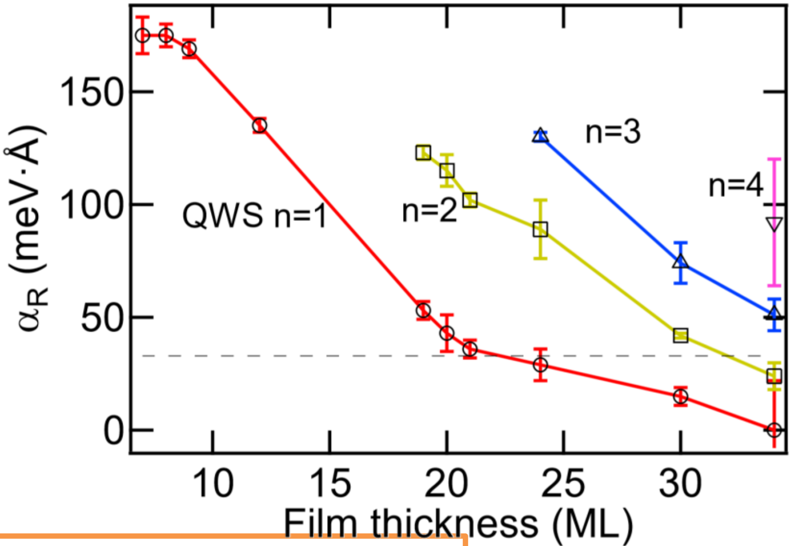
K. Yaji *et al.*, PRB **98**, 041404 (2018).

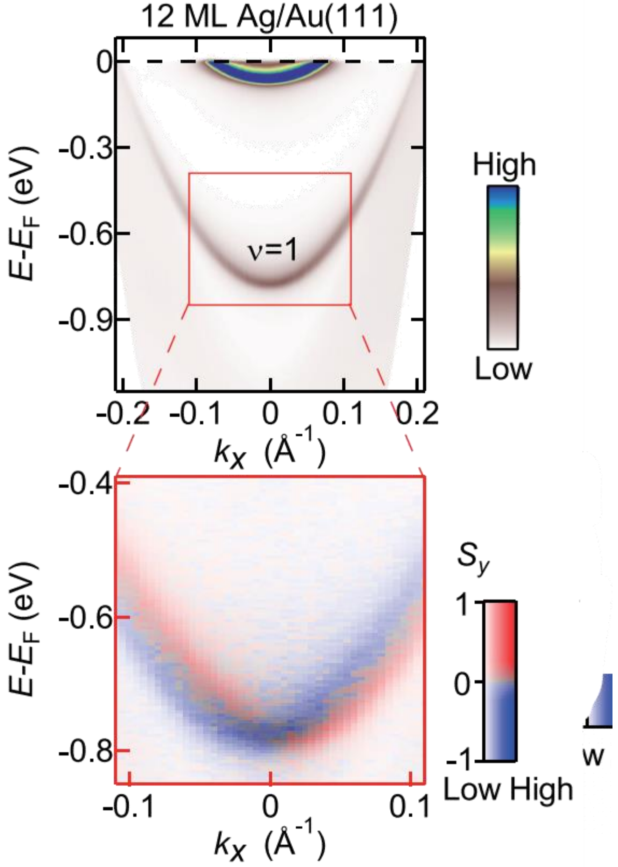


Ag/Au(111) : Quantum well states confined in Ag region

T. Miller, *et al.*, PRL 61, 1404 (1988). F. Forster, *et al.* PRB 84, 075412 (2011).







Purpose : Reveal the mechanism of this trend

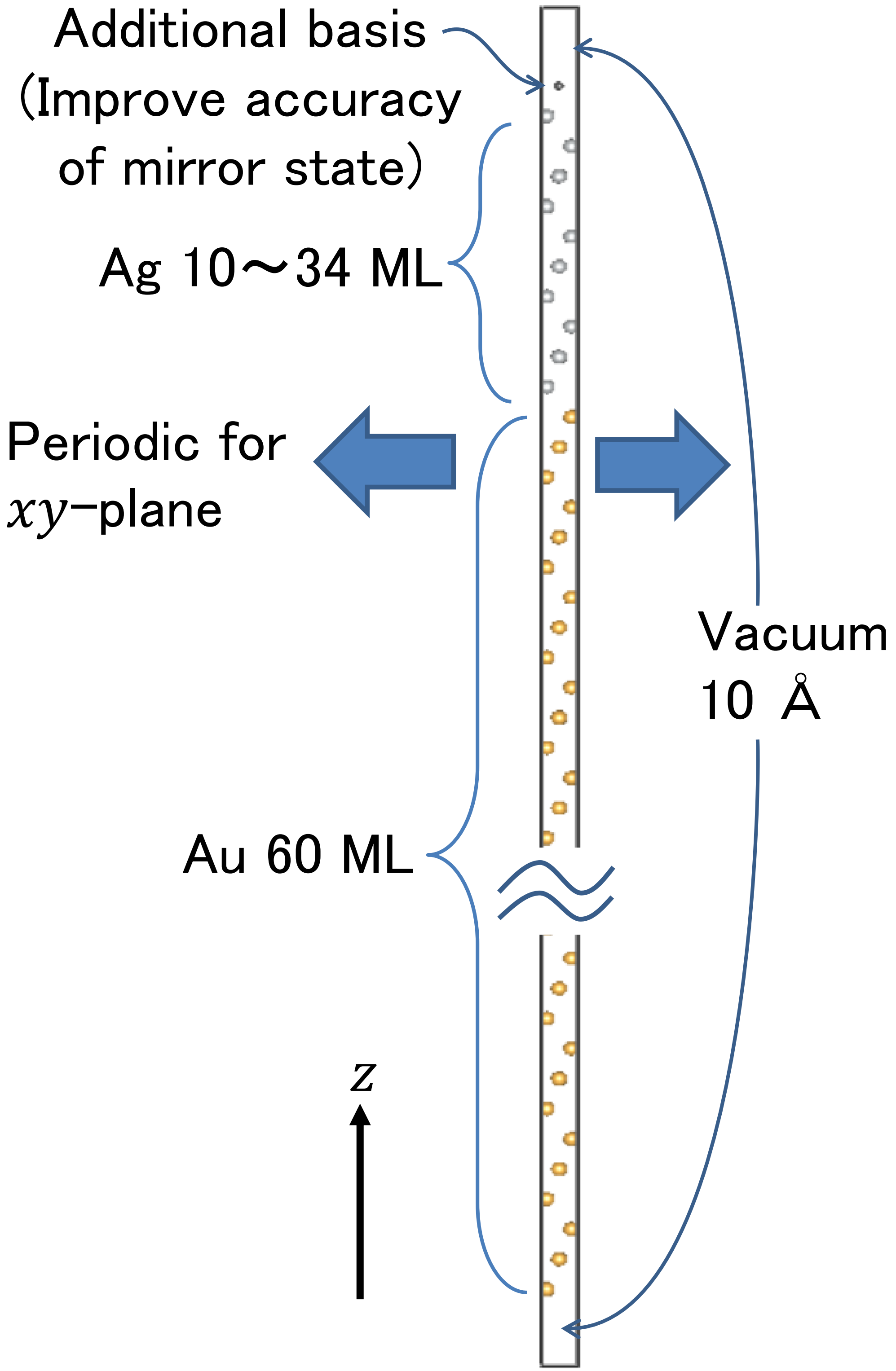
- The shape of the quantum well state
- The effect of Au-SOI at the boundary atom
- How well states (not surface state) feel the Rashba effect

R. Noguchi, K. Kuroda, M. Kawamura, K. Yaji, A. Harasawa, T. Iimori, S. Shin, F. Komori, T. Ozaki, T. Kondo PRB **104**, L180409 (2021).

Example

QWS in Ag/Au(111)

- DFT code : OpenMX
- GGA-PBE functional
- ρ cutoff : 300 Ry
- Broadening : 5000 K (0.03 Ry)
- $\mathbf{k}$-grid : 14 × 14 × 1
- Spin-orbit
- Au 60 ML
  - Basis
    - Au7.0-s4p3d2f1
    - Ag7.0-s2p2d2f1
  - With structure optimization

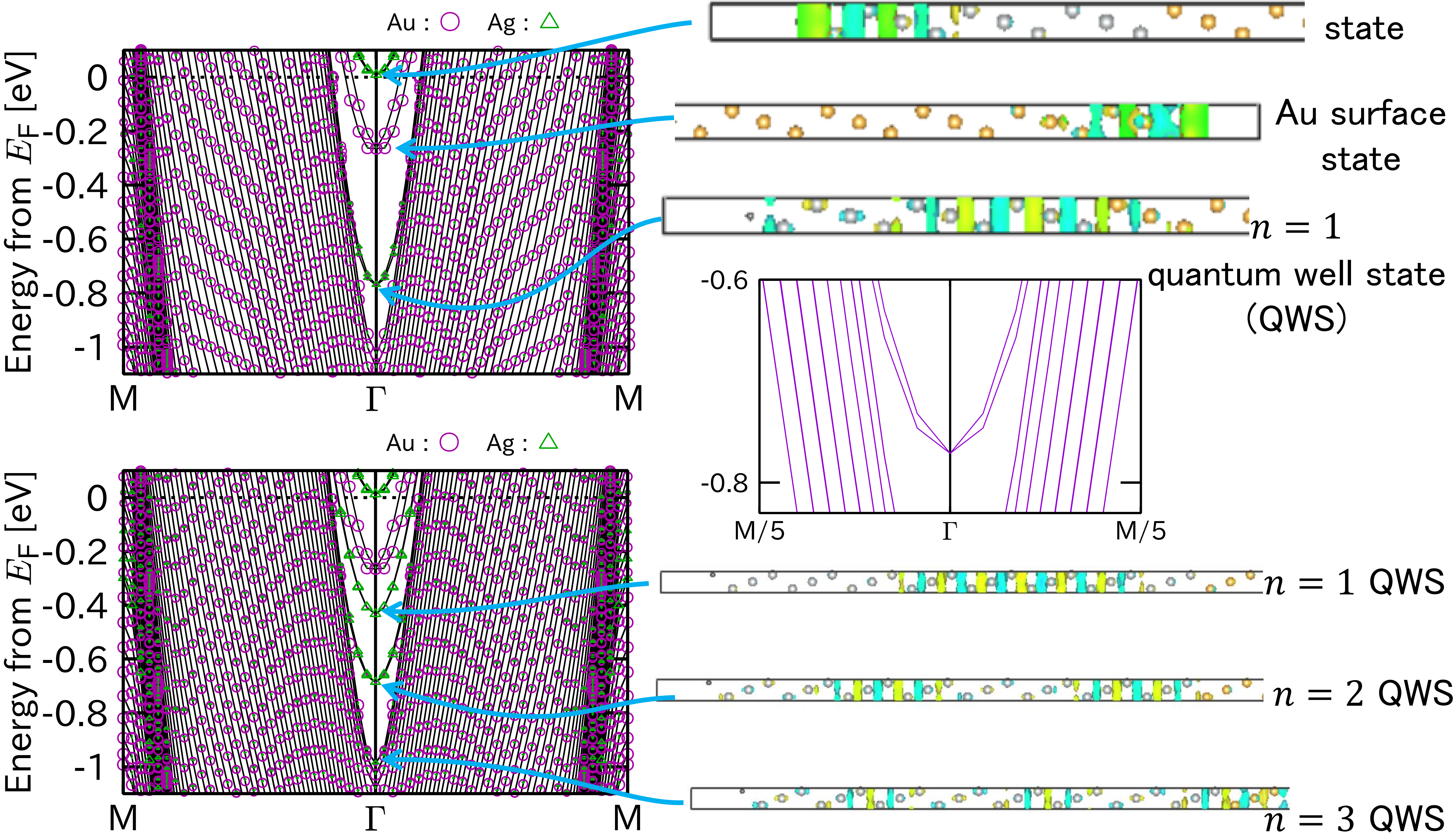


Result

Band structure and well states

Ag10ML
on
Au(111)

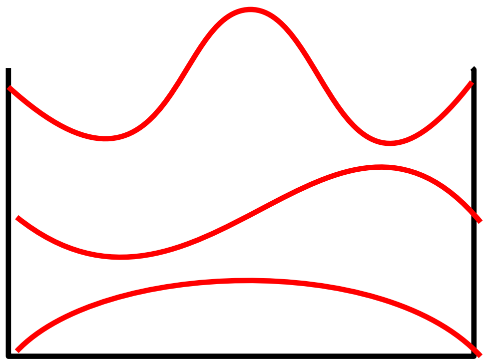
Ag24ML
On
Au(111)



Discuss

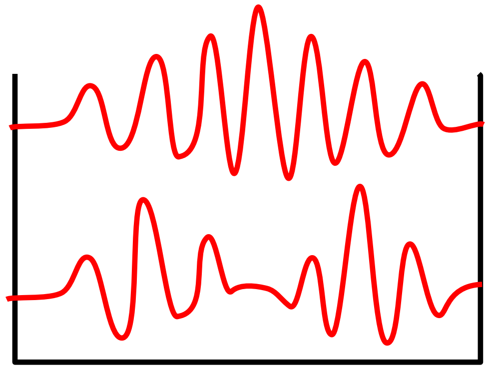
Energy level of QWS

Normal QWS



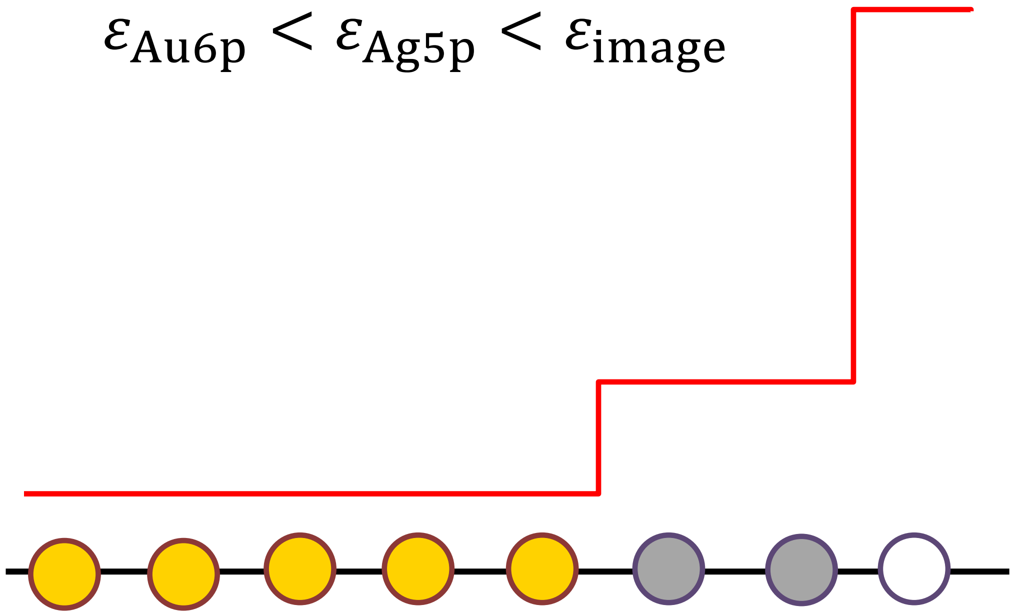
$\varepsilon_1 < \varepsilon_2 < \varepsilon_3 < \cdots$

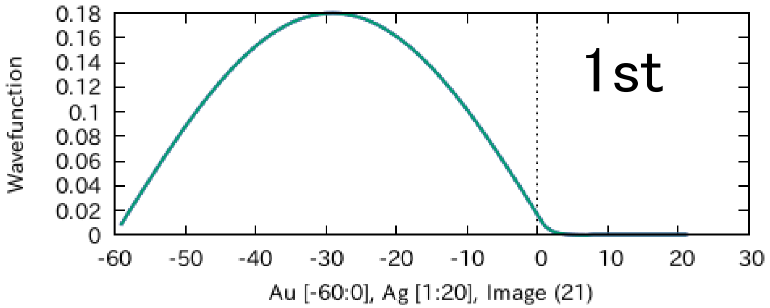
This case

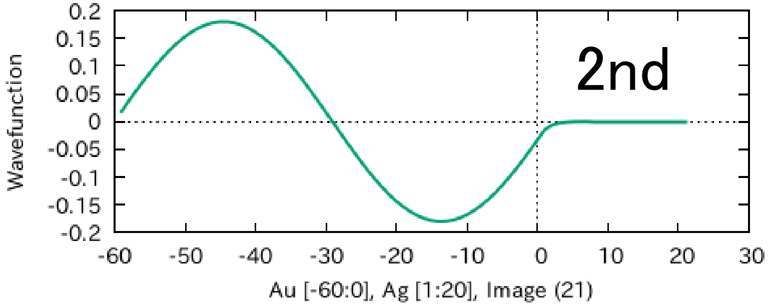


$\varepsilon_1 > \varepsilon_2 > \varepsilon_3 > \cdots$

$\varepsilon_{\mathrm{Au6p}} < \varepsilon_{\mathrm{Ag5p}} < \varepsilon_{\mathrm{image}}$







Au : 60 sites

Ag : 20 sites

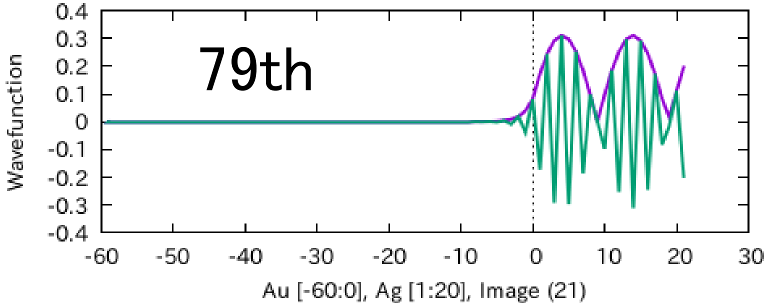
Image : 1site

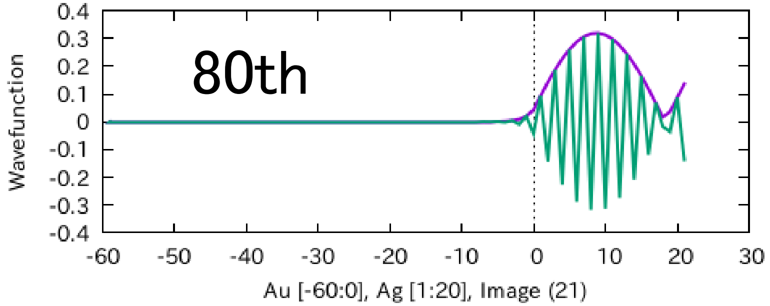
$t = -3$

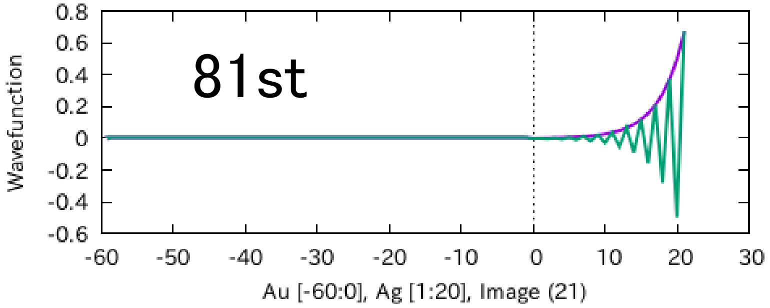
$\varepsilon_{\mathrm{Au}} = 0$

$\varepsilon_{\mathrm{Ag}} = 2$

$\varepsilon_{\mathrm{image}} = 6$

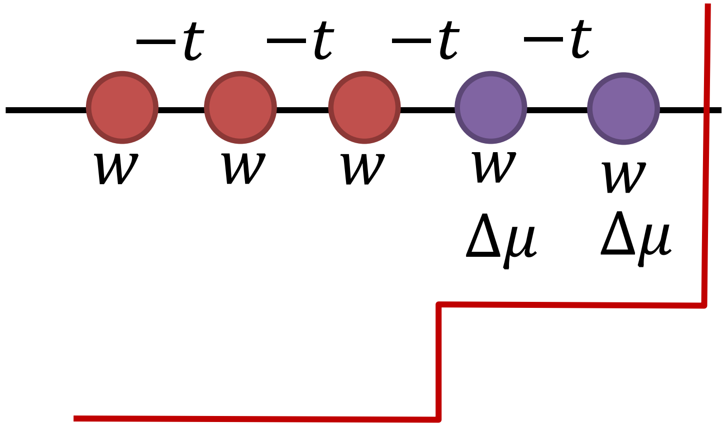






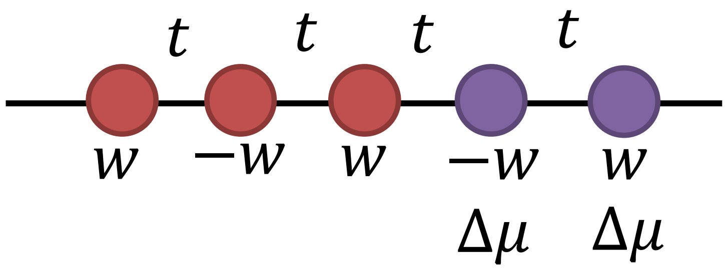
Discuss

Tight-binding

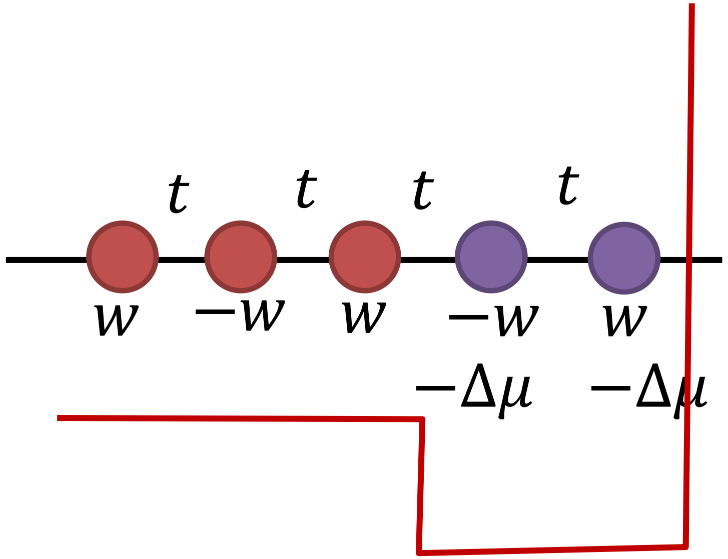


$$H = \begin{pmatrix} 0 & -t & 0 & 0 & 0 \\ -t & 0 & -t & 0 & 0 \\ 0 & -t & 0 & -t & 0 \\ 0 & 0 & -t & \Delta\mu & -t \\ 0 & 0 & 0 & -t & \Delta\mu \end{pmatrix}$$

Same spectrum



$$H_{\text{staggered}} = \begin{pmatrix} 0 & t & 0 & 0 & 0 \\ t & 0 & t & 0 & 0 \\ 0 & t & 0 & t & 0 \\ 0 & 0 & t & \Delta\mu & t \\ 0 & 0 & 0 & t & \Delta\mu \end{pmatrix}$$



$$H_{\text{stag,inv}} = \begin{pmatrix} 0 & t & 0 & 0 & 0 \\ t & 0 & t & 0 & 0 \\ 0 & t & 0 & t & 0 \\ 0 & 0 & t & -\Delta\mu & t \\ 0 & 0 & 0 & t & -\Delta\mu \end{pmatrix} = -H$$

Inverted spectrum

Result

Rashba split vs ML

R. Noguchi, M. Kawamura, *et al.*, PRB **104**, L180409 (2021).

Reproduce experimental results

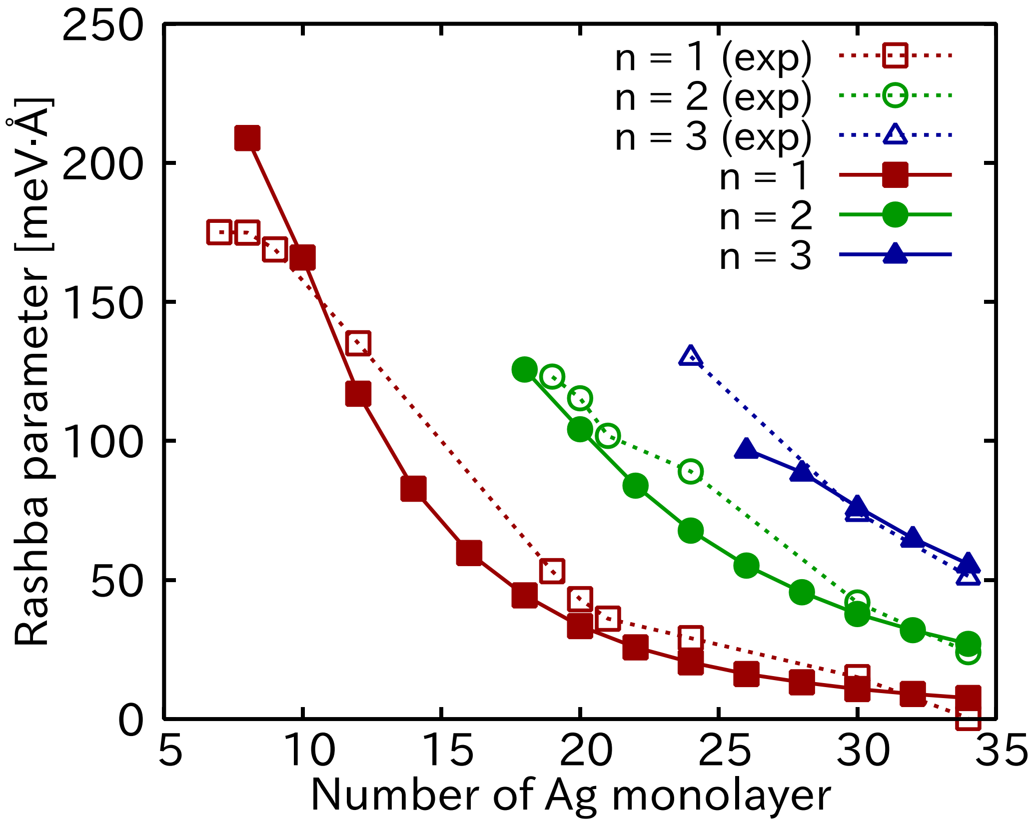
Next

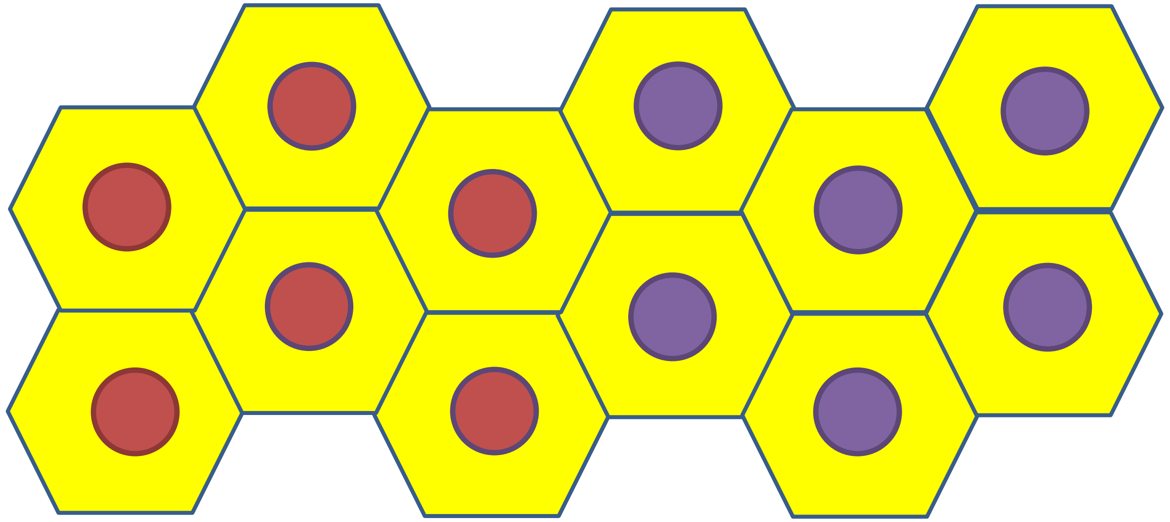
Investigate ML and well state dependence of the splitting

$$\hat{H} = -\frac{\nabla^2}{2} + V(r) + \frac{2}{c^2}(\nabla V(r) \times \boldsymbol{p}) \cdot \boldsymbol{s}$$

Rashba splitting from SOI term

$$\Delta\varepsilon_R \approx \int d^3r \frac{2}{c^2}(\nabla V(r) \times \boldsymbol{p}) \cdot \boldsymbol{s}\, |\varphi(r)|^2$$





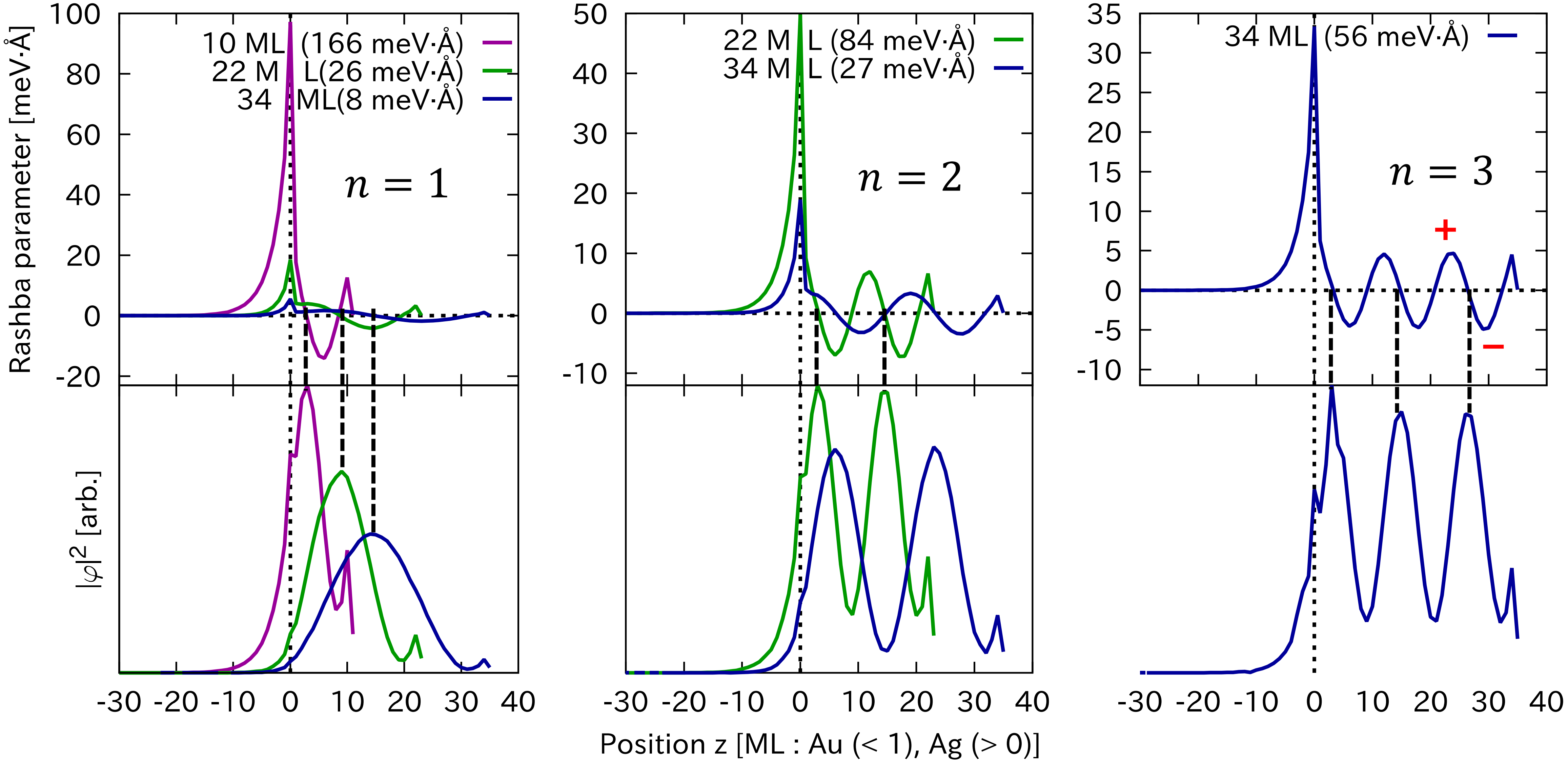
Decompose integration into contributions from each atom

※ Decomposition method is not unique

Result

Split vs $|\varphi(r)|^2$

$$\Delta\varepsilon_R = \int d^3r \frac{2}{c^2}(\nabla V(r) \times \boldsymbol{p}) \cdot \boldsymbol{s}\, |\varphi(r)|^2$$



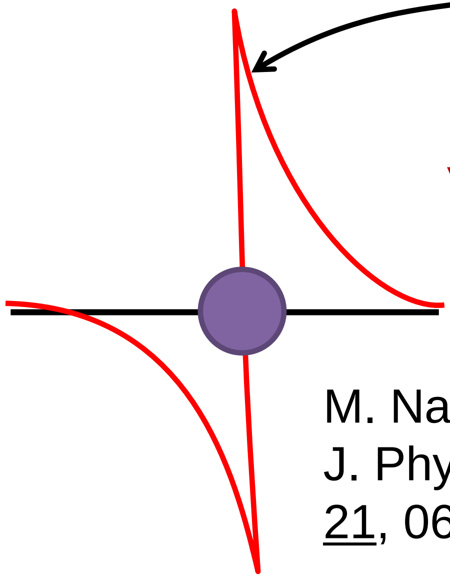
Peak of $|\varphi(r)|^2$ → Node of decomposed splitting $\Delta\varepsilon_i$

Slope of $|\varphi(r)|^2$ → Peak of decomposed splitting $\Delta\varepsilon_i$ (Opposite sign)

Result

Mechanism

$$\Delta\varepsilon_R = \int d^3r\, \frac{2}{c^2}\left(\nabla V(\mathbf{r}) \times \boldsymbol{p}\right) \cdot \boldsymbol{s}\, |\varphi(\mathbf{r})|^2$$
$$\approx \left|\boldsymbol{k}_\parallel\right| \int d^3r\, \frac{1}{c^2}\frac{\partial V}{\partial z}|\varphi(\mathbf{r})|^2$$

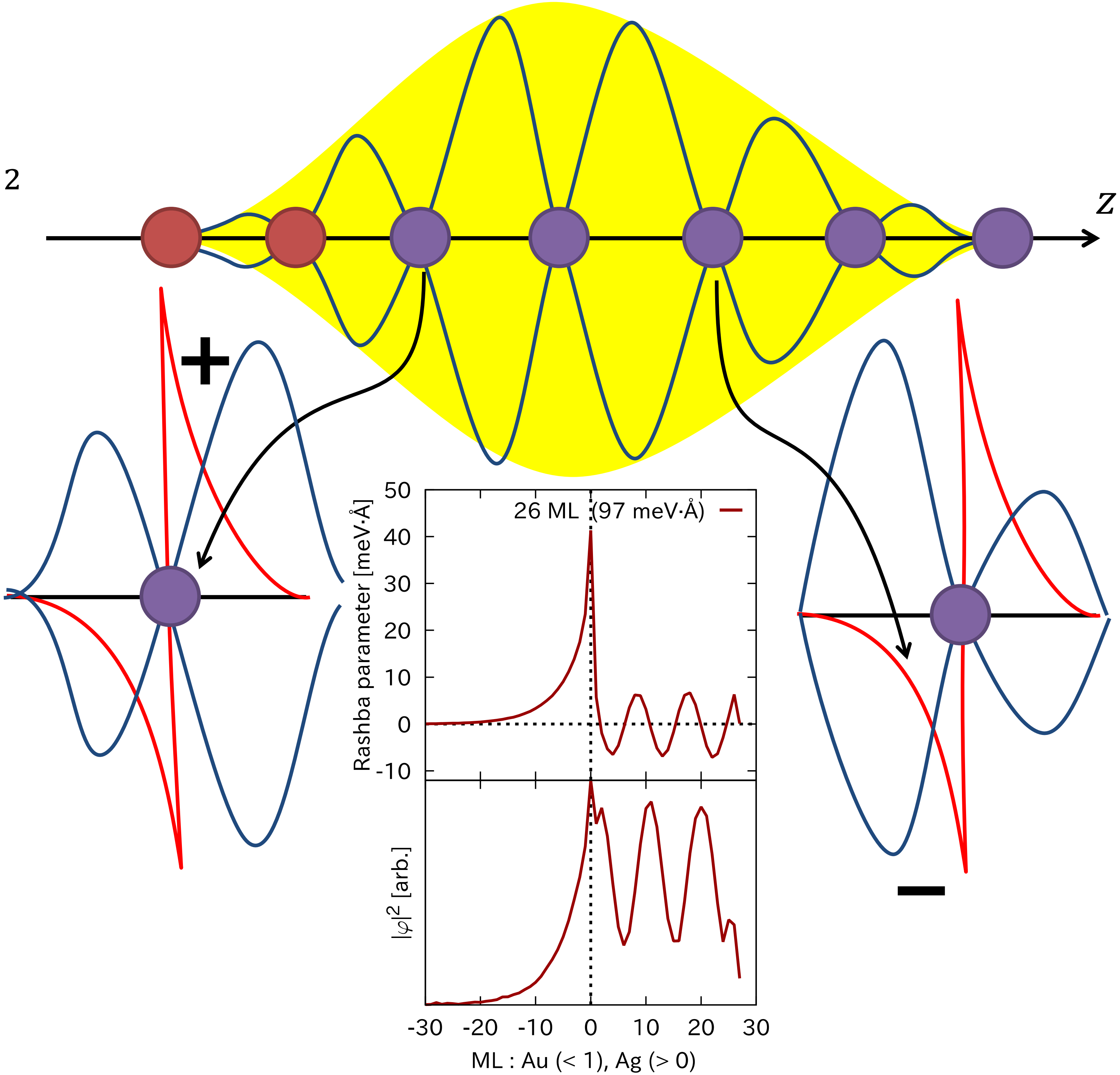


Large in the **vicinity of atoms**

M. Nagano *et al.*,
J. Phys.: Condens. Matter
21, 064239 (2009).

$$\varphi(\mathbf{r}) \approx \varphi_{pz}(\mathbf{r})\varphi_{\text{envelope}}(z)$$

$$\Delta\varepsilon_i \propto \left\langle \frac{\partial V}{\partial z} z \left|\varphi_{pz}\right|^2 \right\rangle \frac{d\left|\varphi_{\text{envelope}}\right|^2}{dz}$$



Result

Split vs $|\varphi(r)|^2$ at boundary Au and Ag

$$\Delta\varepsilon_{\mathrm{R}} \approx \int dz \left\langle \frac{\partial V}{\partial z} z \left|\varphi_{pz}\right|^2 \right\rangle \frac{d\left|\varphi_{\mathrm{emvelope}}\right|^2}{dz} \qquad \langle \delta V \rangle \equiv \left\langle \frac{\partial V}{\partial z} z \left|\varphi_{pz}\right|^2 \right\rangle$$

R. Noguchi, M. Kawamura, *et al.*, PRB **104**, L180409 (2021).

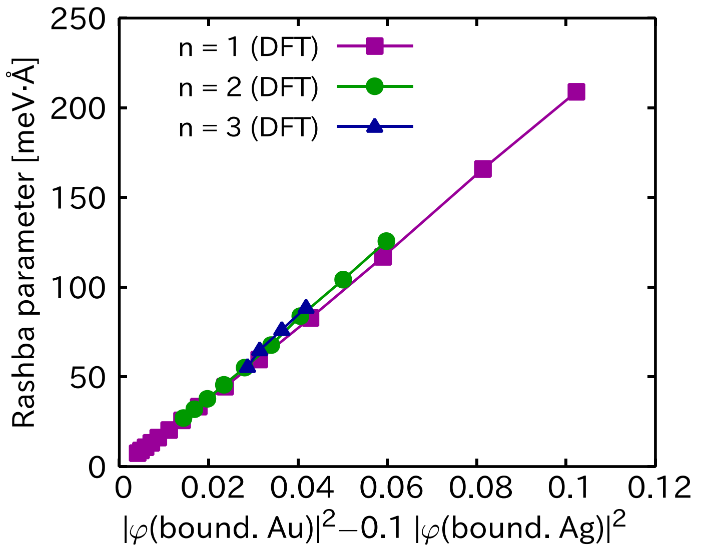
$$\approx \langle \delta V \rangle_{\mathrm{Au}} \int_{-\infty}^{0} \frac{\partial\left|\varphi_{\mathrm{emvelope}}\right|^2}{\partial z} + \langle \delta V \rangle_{\mathrm{Ag}} \int_{0}^{\infty} \frac{\partial\left|\varphi_{\mathrm{emvelope}}\right|^2}{\partial z}$$

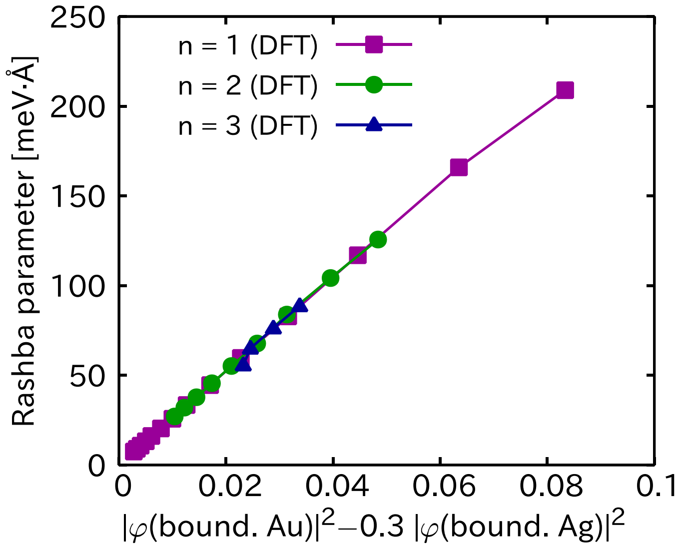
$$= \langle \delta V \rangle_{\mathrm{Au}} \left|\varphi_{\mathrm{emvelope}}(0)\right|^2 - \langle \delta V \rangle_{\mathrm{Ag}} \left|\varphi_{\mathrm{emvelope}}(0)\right|^2$$

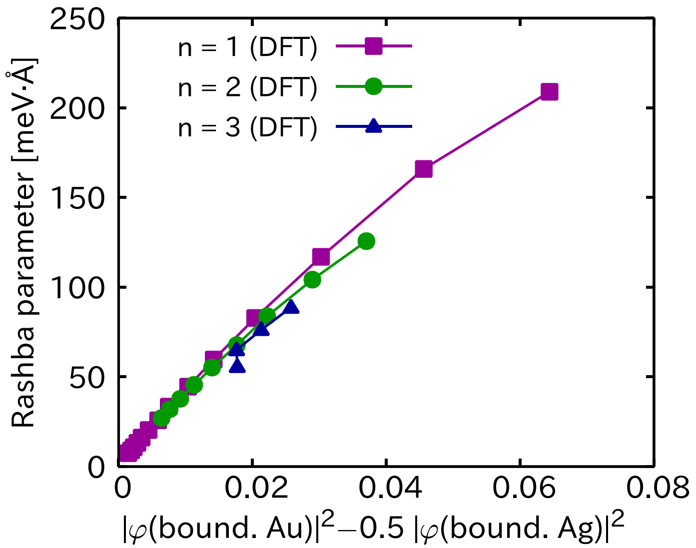
$$\frac{\alpha_{\mathrm{R,Ag}}}{\alpha_{\mathrm{R,Au}}} = \frac{31\mathrm{meV}\cdot\text{Å}}{330\mathrm{meV}\cdot\text{Å}} \approx 0.1$$

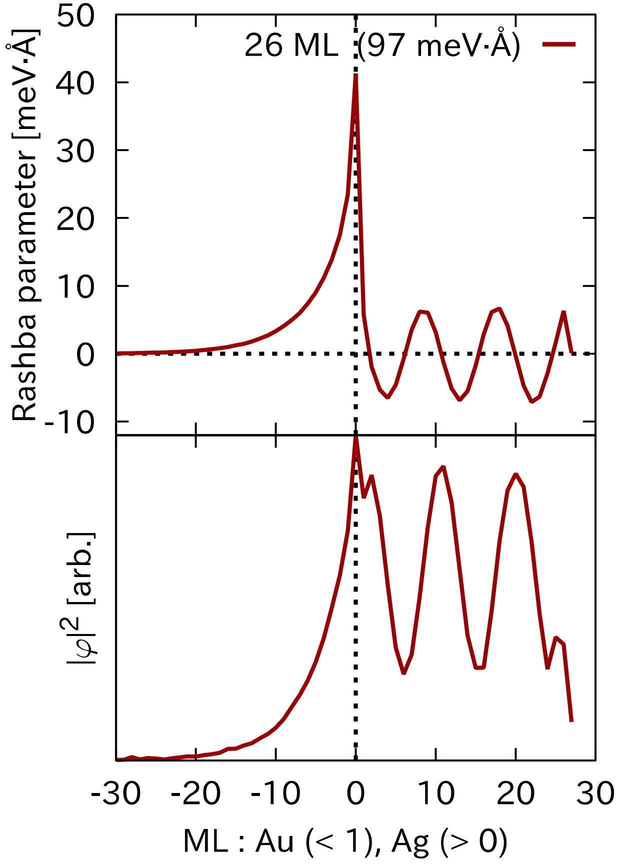
SOI coupling constant
Au(6p) : Ag(5p) ≈ 1 : 0.3

1 : 0.5 → ×









Further question and motivation

M. Nagano, *et al.*, J. Phys.: Condens. Matter **21**, 064239 (2009).

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u(z)$$

2D nearly free electronic state

$$\Delta\varepsilon_R = \langle \psi_{\mathbf{k}} | \hat{H}_{\mathrm{SOC}} | \psi_{\mathbf{k}} \rangle = |\boldsymbol{k}| S_{xy} \int dz 2 \left\langle \frac{\partial V}{\partial z} \right\rangle_{xy} |u(z)|^2$$

- Since the wavefunction of a realistic system is not like the 2D free electronic state
- The applicability of the earlier study is unclear.
- We need to fill the gap between the atomic SOC and Rashba interaction term.
- precise theoretical model to capture the wide range of behavior of QWSs system will be derived.

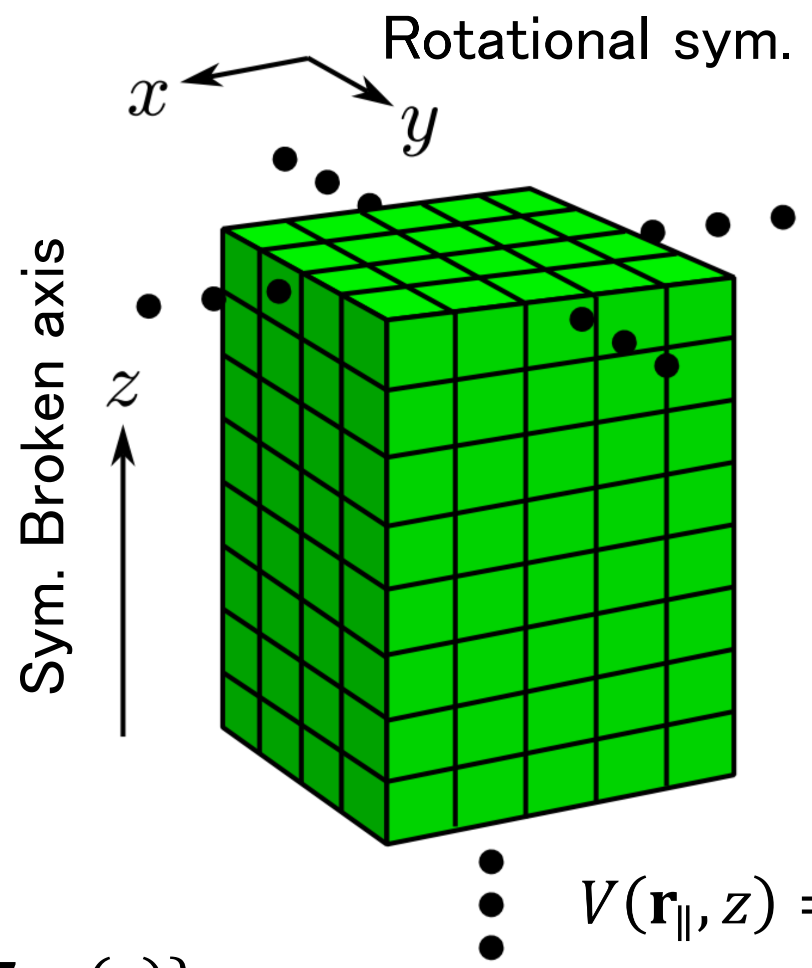
Theory

Spin-orbit coupling and symmetry-broken system

SOC part of Hamiltonian $\hat{H}^{SOC}_{\sigma\sigma'} = 2(\nabla V(\mathbf{r}) \times \mathbf{p}) \cdot \mathbf{s}_{\sigma\sigma'}$

Uniform spin wavefunction $\begin{pmatrix} \psi_{\mathbf{k}\uparrow}(\mathbf{r}) \\ \psi_{\mathbf{k}\downarrow}(\mathbf{r}) \end{pmatrix} = e^{i\mathbf{k}\cdot\mathbf{r}} \begin{pmatrix} \chi_{\mathbf{k}\uparrow} \\ \chi_{\mathbf{k}\downarrow} \end{pmatrix} u_{\mathbf{k}}(\mathbf{r})$

$$\left(-\frac{(\nabla + i\mathbf{k})^2}{2} + V(\mathbf{r})\right) u_{\mathbf{k}}(\mathbf{r}) = \varepsilon^0_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r})$$



$$\varepsilon^{SOC}_{\mathbf{k}} = \mathbf{s}_{\mathbf{k}} \cdot \int d^3r 2\nabla V(\mathbf{r}) \times \{\mathbf{k}|u_{\mathbf{k}}(\mathbf{r})|^2 - iu^*_{\mathbf{k}}(\mathbf{r})\nabla u_{\mathbf{k}}(\mathbf{r})\}$$

$$= 2\mathbf{s}_{\mathbf{k}} \cdot \int d^3r\{\nabla V(\mathbf{r}) \times \mathbf{k}|u_{\mathbf{k}}(\mathbf{r})|^2 + iV(\mathbf{r})\nabla u^*_{\mathbf{k}}(\mathbf{r}) \times \nabla u_{\mathbf{k}}(\mathbf{r})\}$$

$$V(\mathbf{r}_\parallel, z) = V(-\mathbf{r}_\parallel, z)$$

$$u^*_{\mathbf{k}}(\mathbf{r}_\parallel, z) = u_{-\mathbf{k}}(\mathbf{r}_\parallel, z) = u_{\mathbf{k}}(-\mathbf{r}_\parallel, z)$$

$$(\chi^*_{\mathbf{k}\uparrow}, \chi^*_{\mathbf{k}\downarrow}) \begin{pmatrix} \mathbf{s}_{\uparrow\uparrow} & \mathbf{s}_{\uparrow\downarrow} \\ \mathbf{s}_{\downarrow\uparrow} & \mathbf{s}_{\downarrow\downarrow} \end{pmatrix} \begin{pmatrix} \chi_{\mathbf{k}\uparrow} \\ \chi_{\mathbf{k}\downarrow} \end{pmatrix}$$

Re←Gauss theorem & anti sym. of ×

Expansion of $u_{\mathbf{k}}(\mathbf{r})$ for $\mathbf{k}$

$$u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{0}}(\mathbf{r}) + \sum_i k_i \partial_{k_i} u_{\mathbf{k}}(\mathbf{r})\Big|_{\mathbf{k}=\mathbf{0}} + \sum_{ij} k_i k_j \partial_{k_i}\partial_{k_j} u_{\mathbf{k}}(\mathbf{r})\Big|_{\mathbf{k}=\mathbf{0}} + O(k^3)$$

Real

$$\partial_{k_i} u_{\mathbf{k}=\mathbf{0}}(\mathbf{r}) = i\left(-\frac{\boldsymbol{\nabla}^2}{2} + V(\mathbf{r}) - \varepsilon_{\mathbf{k}=0}\right)^{-1} \partial_{r_i} u_{\mathbf{0}}(\mathbf{r})$$

Imaginary

$$\partial_{k_i}\partial_{k_j} u_{\mathbf{k}=\mathbf{0}}(\mathbf{r})$$

Real

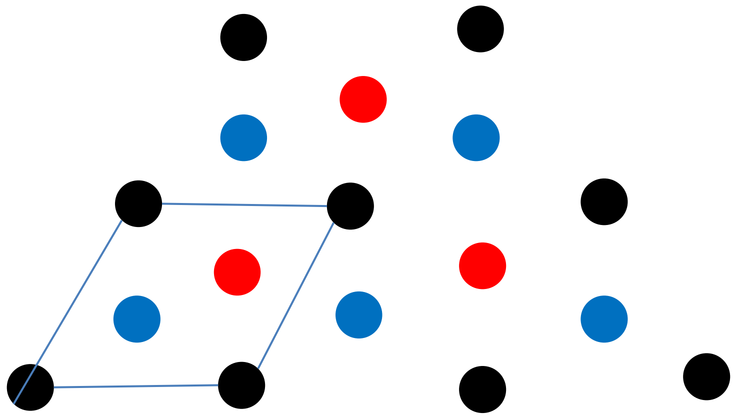
$$= i\left(-\frac{\boldsymbol{\nabla}^2}{2} + V(\mathbf{r}) - \varepsilon_{\mathbf{k}=0}\right)^{-1} \left\{\left(\partial_{k_i}\partial_{k_j}\varepsilon_{\mathbf{k}=0} - \delta_{ij}\right) u_{\mathbf{0}}(\mathbf{r}) + i\partial_{r_j}\partial_{k_i} u_{\mathbf{k}=\mathbf{0}}(\mathbf{r}) + i\partial_{r_i}\partial_{k_j} u_{\mathbf{k}=\mathbf{0}}(\mathbf{r})\right\}$$

$$u^*_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{0}}(\mathbf{r}) - \sum_i \partial_{k_i} u_{\mathbf{k}}(\mathbf{r})\Big|_{\mathbf{k}=\mathbf{0}} + \sum_{ij} \partial_{k_i}\partial_{k_j} u_{\mathbf{k}}(\mathbf{r})\Big|_{\mathbf{k}=\mathbf{0}} + O(k^3)$$

$$\varepsilon^{\mathrm{SOC}}_{\mathbf{k}} = 2\mathbf{s}_{\mathbf{k}} \cdot \int d^3r \left\{\boldsymbol{\nabla} V(\mathbf{r}) \times \mathbf{k}|u_{\mathbf{0}}(\mathbf{r})|^2 + 2iV(\mathbf{r})\boldsymbol{\nabla} u_{\mathbf{0}}(\mathbf{r}) \times \boldsymbol{\nabla} \sum_i k_i \partial_{k_i} u_{\mathbf{k}=\mathbf{0}}(\mathbf{r})\right\} + O(k^3)$$

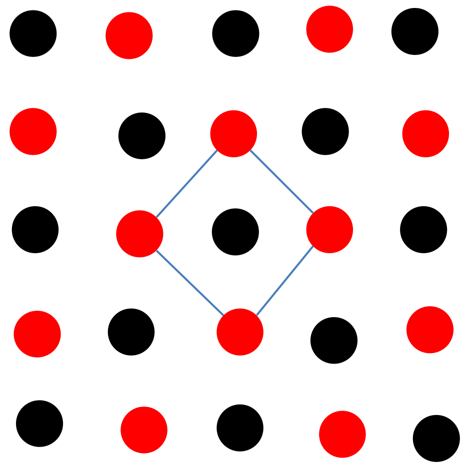
Symmetry

(111) surface of fcc lattice



3-fold + 3 mirrors

(100) surface of cubic lattice



4-fold + 4 mirrors

Symmetry op.

$$u_{\mathbf{0}}(\hat{R}\mathbf{r}) = u_{\mathbf{0}}(\mathbf{r})$$

$$\nabla_{\mathbf{r}} u_{\mathbf{0}}(\mathbf{r}) \to \hat{R}^{-t} \nabla_{\mathbf{r}} u_{\mathbf{0}}(\hat{R}\mathbf{r})$$

$$\nabla_{\mathbf{k}} u_{\mathbf{k}=\mathbf{0}}(\hat{R}\mathbf{r}) = \hat{R}^{-t} \nabla_{\mathbf{k}} u_{\mathbf{k}=\mathbf{0}}(\mathbf{r})$$

$$\varepsilon_{\mathbf{k}}^{\mathrm{SOC}} = 2\mathbf{s}_{\mathbf{k}} \cdot (\mathbf{e}_z \times \mathbf{k}) \int d^3r \left\{ \frac{\partial V(\mathbf{r})}{\partial z} |u_{\mathbf{0}}(\mathbf{r})|^2 + iV(\mathbf{r}) \left(\frac{\partial u_{\mathbf{0}}(\mathbf{r})}{\partial z} \nabla_{\mathbf{r}} \cdot \nabla_{\mathbf{k}} u_{\mathbf{k}=\mathbf{0}}(\mathbf{r}) - \nabla_{\mathbf{r}} u_{\mathbf{0}}(\mathbf{r}) \cdot \frac{\partial \nabla_{\mathbf{k}} u_{\mathbf{k}=\mathbf{0}}(\mathbf{r})}{\partial z} \right) \right\} + O(k^3)$$

Intrinsic magnetic field in $x - y$ plane and parallel to $\mathbf{e}_z \times \mathbf{k}$

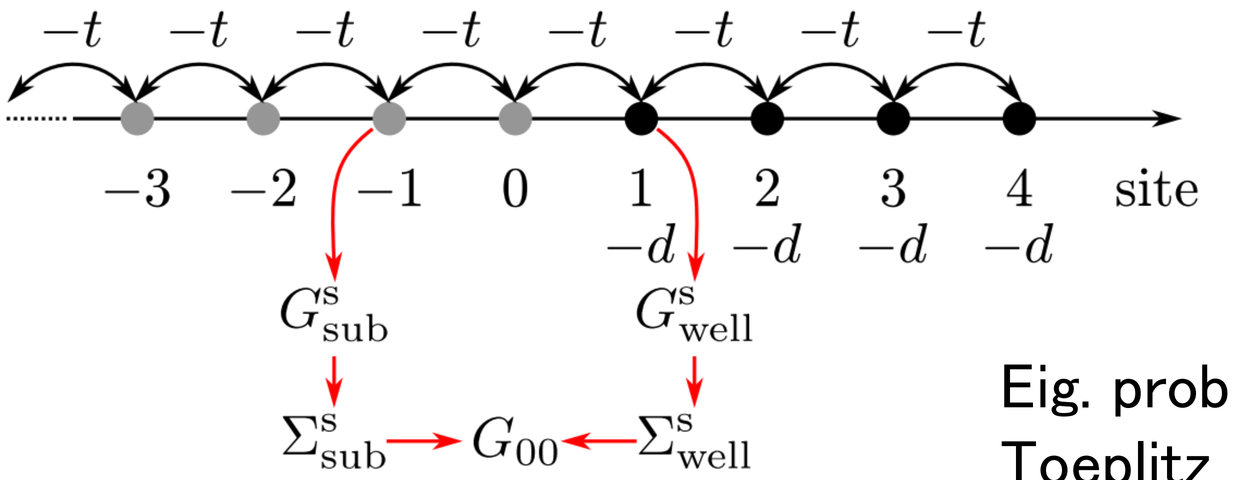
Assuming $\nabla_{\mathbf{k}} u_{\mathbf{k}=\mathbf{0}}(\mathbf{r}) = 0$, this becomes Nagano's formula

Theory

Tight-binding model

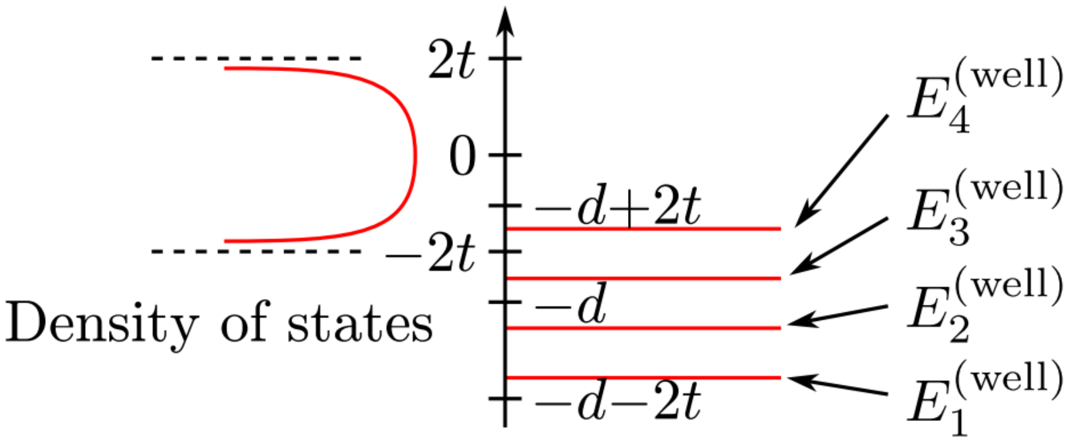
$$|u_{env}(z_b)|^2 \approx |\langle 0|u_n\rangle|^2 = \mathrm{Res}_{\varepsilon=\varepsilon_n}[G_{00}(\varepsilon)]$$

$$G_{00}(\varepsilon) = \frac{1}{\varepsilon - \Sigma^{\mathrm{s}}_{\mathrm{sub}} - \Sigma^{\mathrm{s}}_{\mathrm{well}}}$$



$$E_n^{(\mathrm{well})} \equiv -d - 2t\cos\left(\frac{n\pi}{N_{\mathrm{well}}+1}\right)$$

Eig. problem of Toeplitz matrix



$$e_2 \equiv \frac{2t^2}{N_{\mathrm{well}}+1}\sin^2\left(\frac{n\pi}{N_{\mathrm{well}}+1}\right)$$

$$e_1 \equiv \frac{1}{2}\left(E_n^{(\mathrm{well})} + \sqrt{E_n^{(\mathrm{well})2} - 4t^2}\right)$$

$$e_0 \equiv \frac{1}{2} + \frac{E_n^{(\mathrm{well})}}{2\sqrt{E_n^{(\mathrm{well})2} - 4t^2}}$$

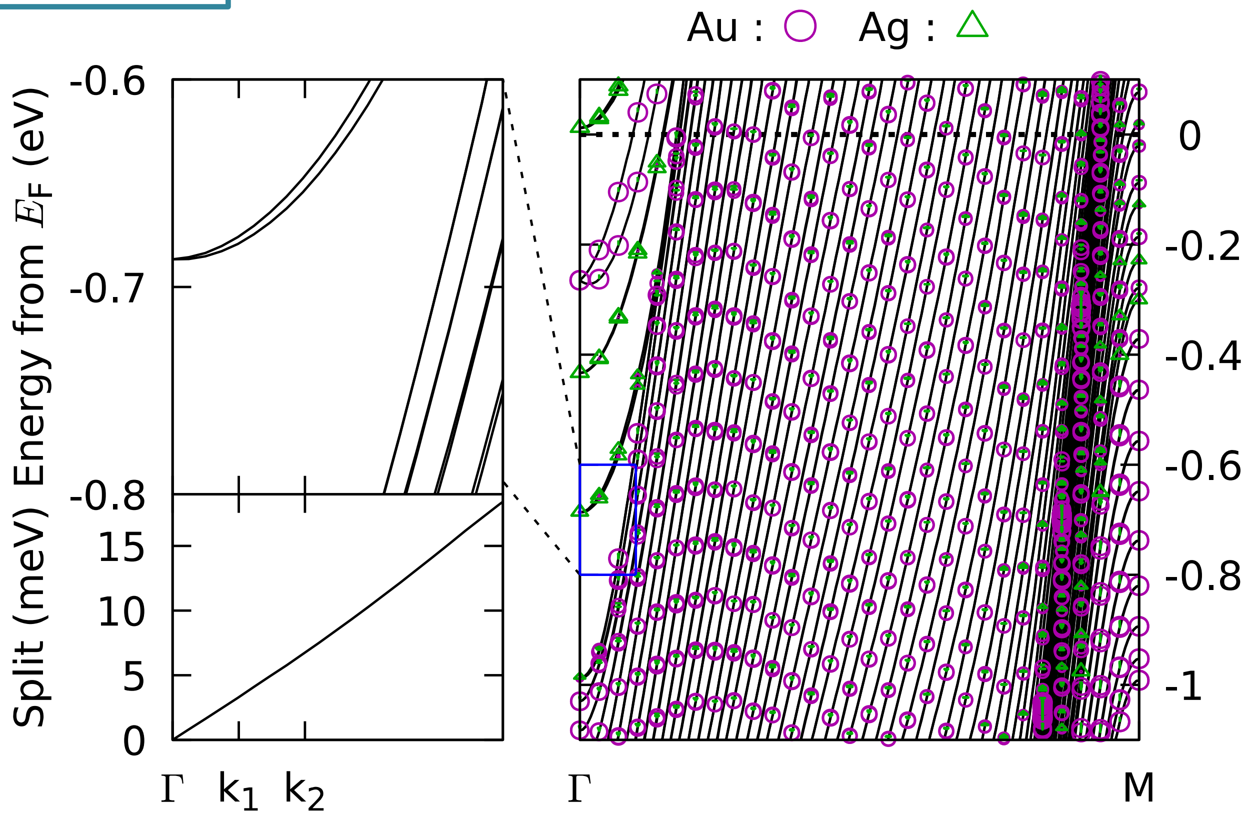
$$\mathrm{Res}_{\varepsilon=\varepsilon_n}[G_{00}(\varepsilon)] = \frac{\sqrt{4e_2(1-e_0) + \left(e_1 - E_n^{(\mathrm{well})}\right)^2} - \left(e_1 - E_n^{(\mathrm{well})}\right)}{2(1-e_0)\sqrt{4e_2(1-e_0) + \left(e_1 - E_n^{(\mathrm{well})}\right)^2}}$$

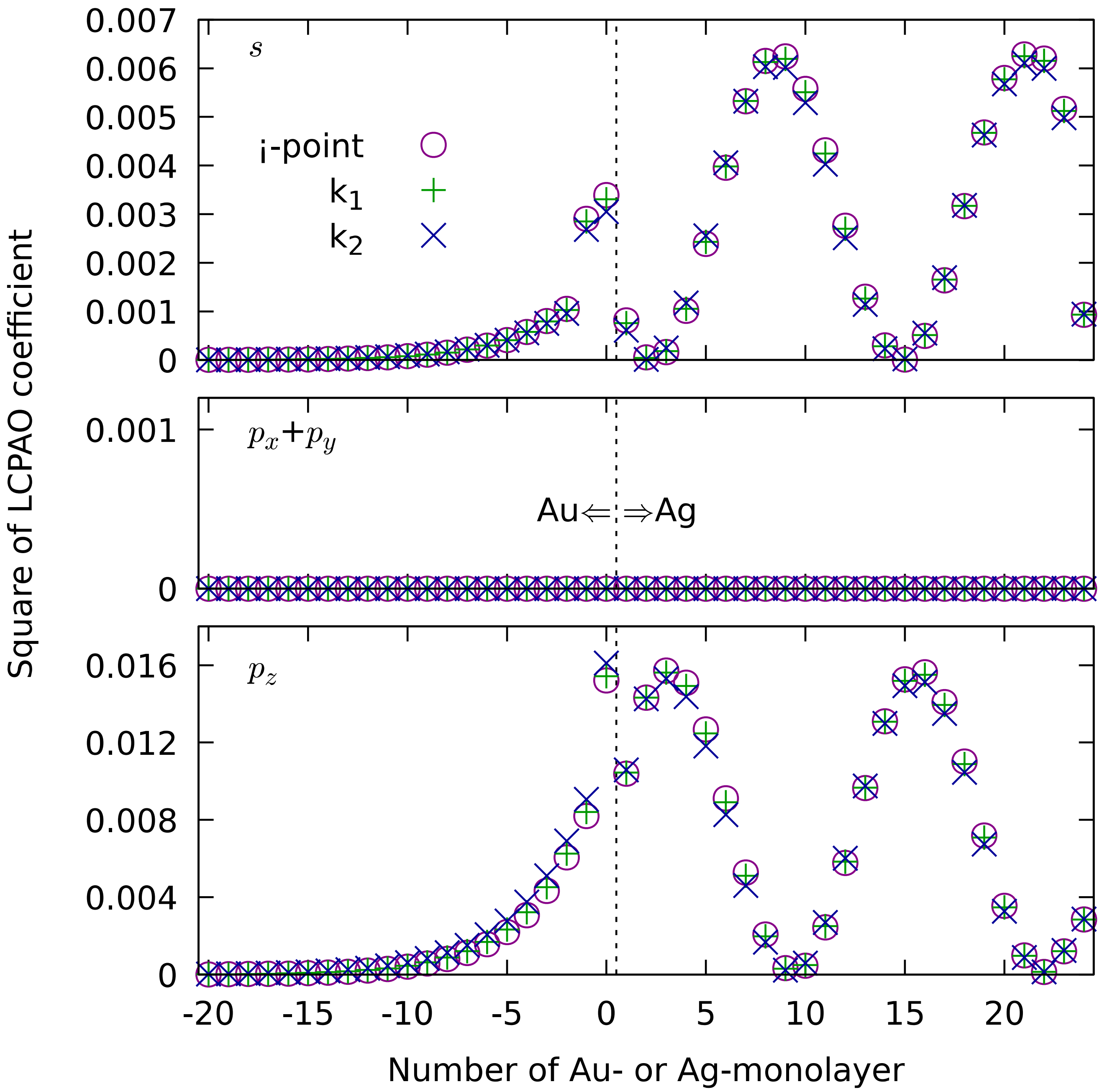
Function of d/t

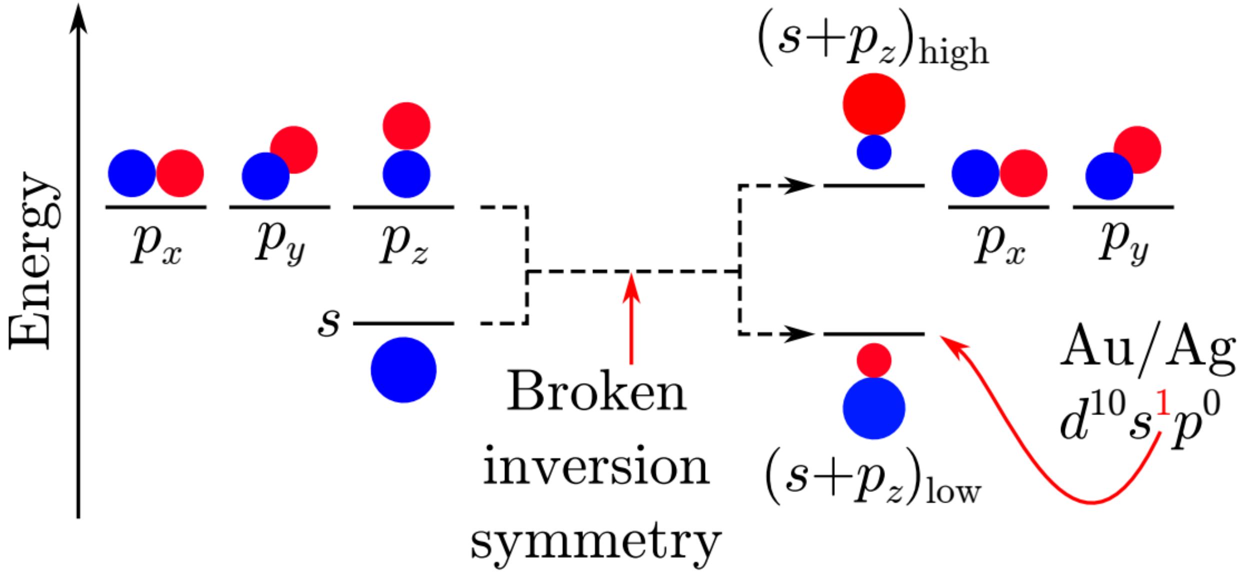
$$\alpha_R \approx \alpha_R^{\mathrm{V}}\mathrm{Res}_{\varepsilon=\varepsilon_n}[G_{00}(\varepsilon)]$$

Example

Band structure and orbital character



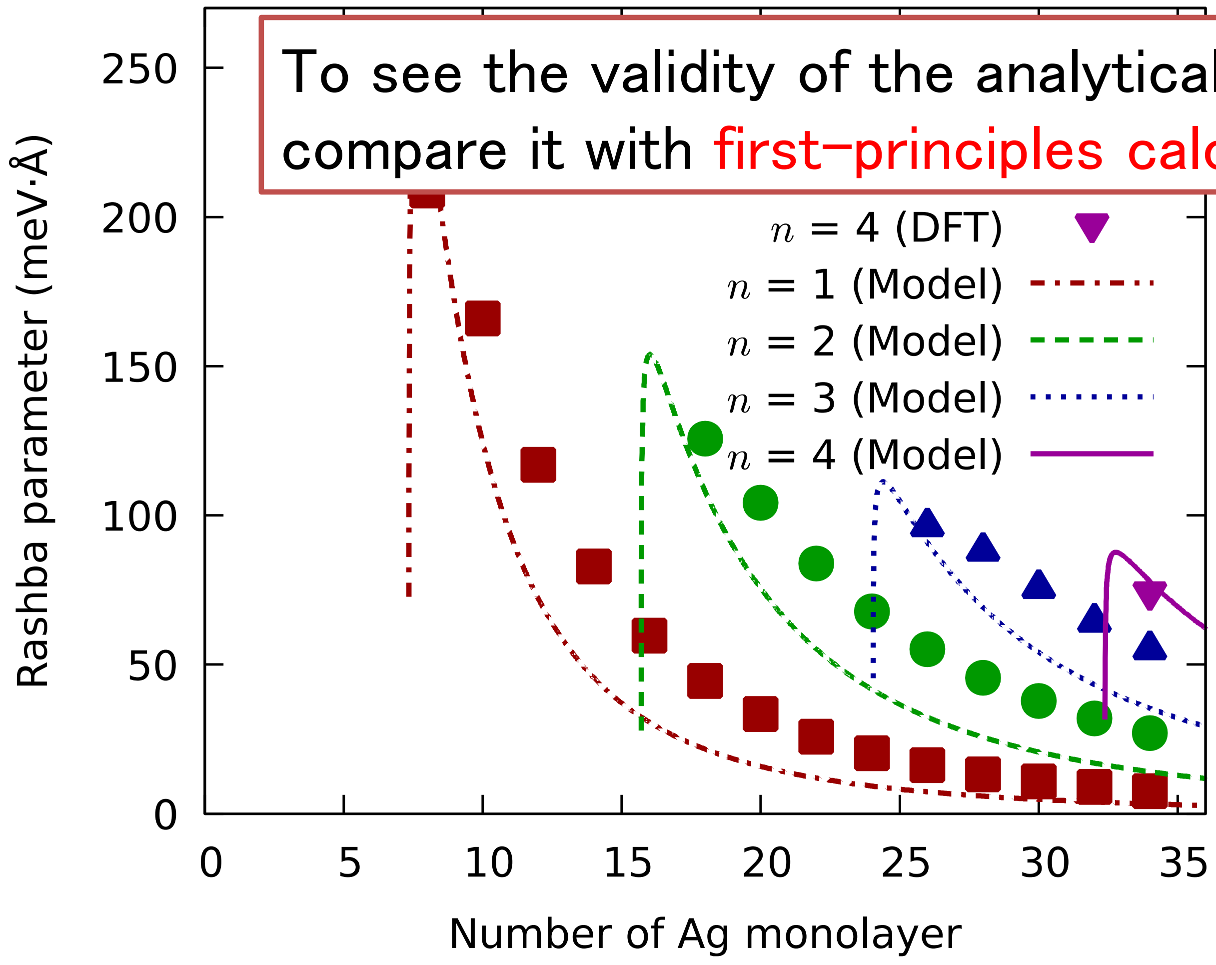


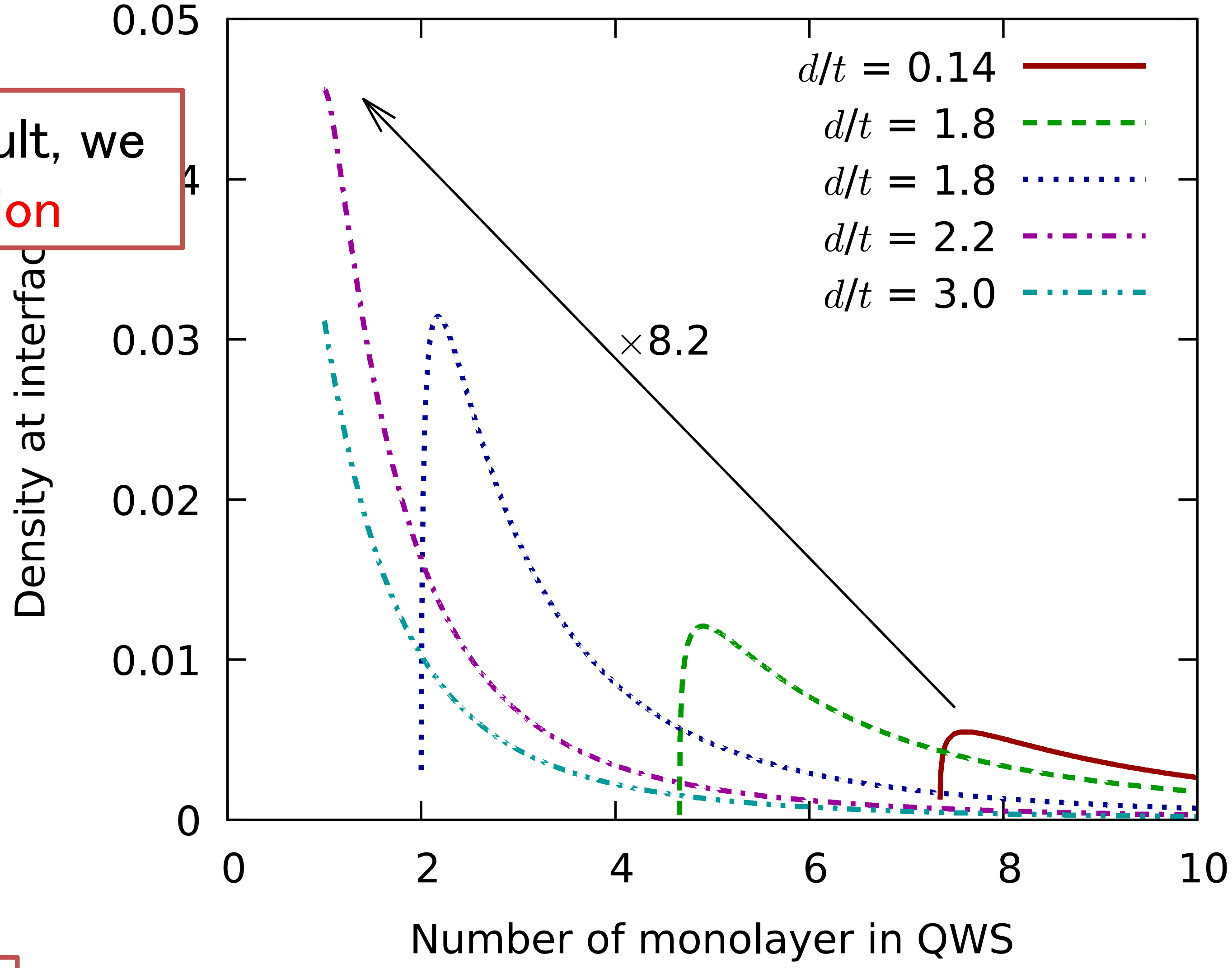


Validity and efficiency of analytical formula

Example

To see the validity of the analytical result, we compare it with first-principles calculation





$$\alpha_R \approx \alpha_R^{\mathrm{V}} \mathrm{Res}_{\varepsilon=\varepsilon_n}[G_{00}(\varepsilon)]$$

α_R^{V} =47,000 (meV・Å), d/t =0.14

Two fitting params.

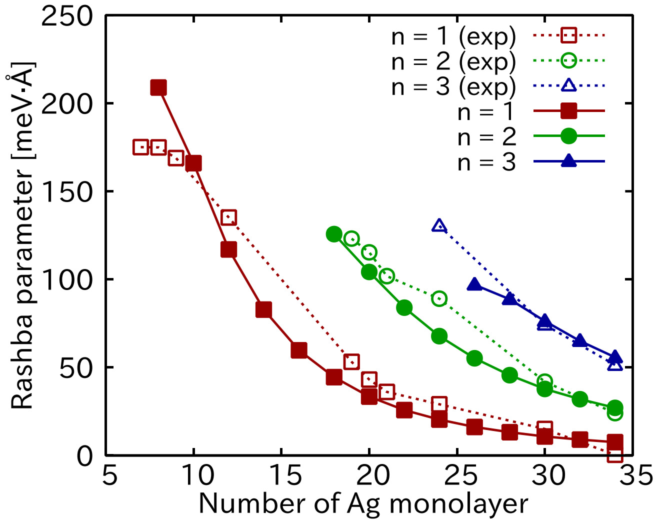
Max. at $N_{\mathrm{well}} = 1$

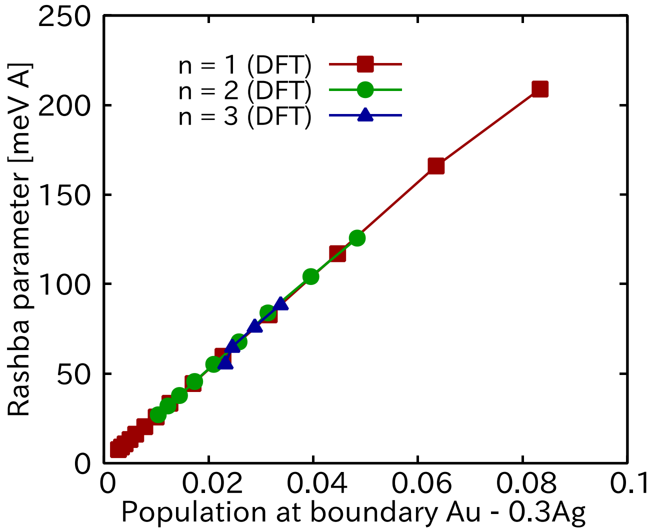
Bi(1/3ML) surface alloy : C. R. Ast, *et al.*, PRL 98, 186807 (2007).

Bi (1ML) on Cu(111) : S. Mathias, et al., PRL **104**, 066802 (2010).

Summary

- We computed Ag/Au(111) slab model (Au 60 ML + Ag 6～34 ML).
- We reproduced quantitatively the experimental Rashba splitting (the same ML number and well state dependence).





  - We decomposed the splitting parameter α_R into contributions from each atom.
  - α_R can be estimated with $|\varphi(r)|^2$ at boundary–Au/Ag and $\langle \partial V / \partial z \rangle$ of each element. Therefore the Rashba effect mainly occurs at the boundary of this system.
  - We constructed minimum tight–binding model which can explain the trend of α_R.

R. Noguchi, K. Kuroda, M. Kawamura, K. Yaji, A. Harasawa, T. Iimori, S. Shin, F. Komori, T. Ozaki, T. Kondo, PRB **104**, L180409 (2021).

- We construct the theory to obtain the $\mathbf{k}$–linear Rashba splitting energy systematically from the SOC.
- Then, we derive a minimum model that captures the Rashba effect in QWS using a one–dimensional tight–binding model and the Green's function method.
- Our theory qualitatively fits the first–principles result of a realistic Ag/Au(111) system using only two fitting parameters.