Theory of Spin-Orbit Coupling (SOC) at $LaAlO_3/SrTiO_3$ interfaces and $SrTiO_3$ surfaces

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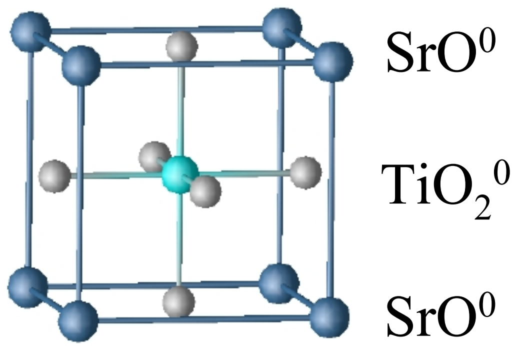
Two dimensional electron gas (2DEG) at $LaAlO_3/SrTiO_3$

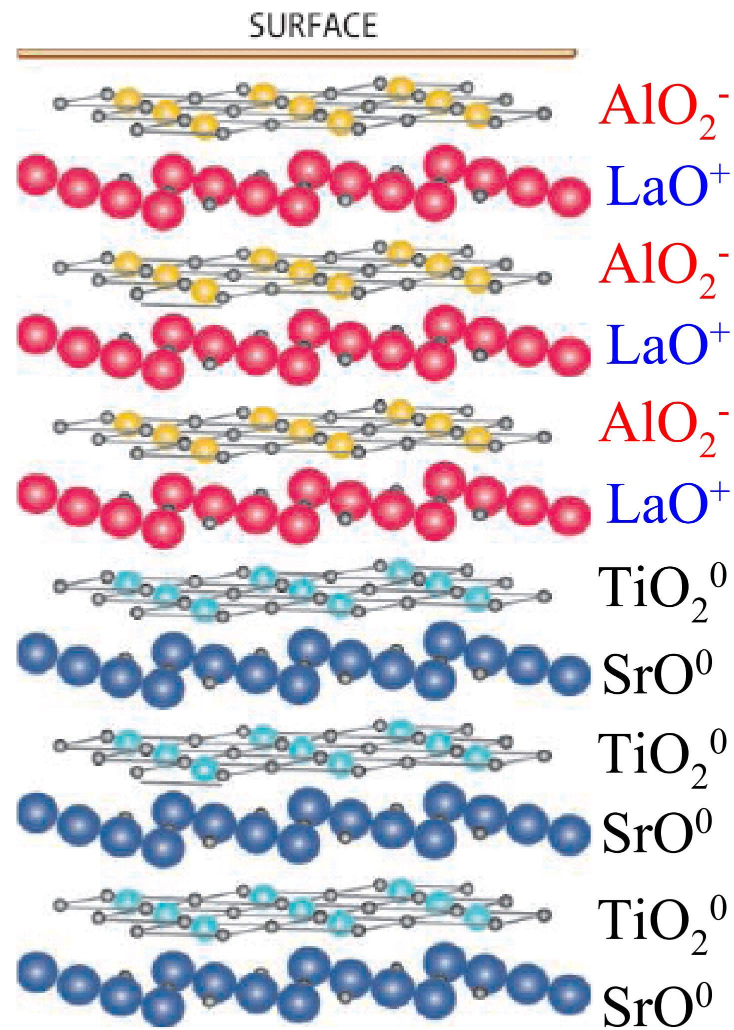
Bulk $SrTiO_3$(STO) ; $LaAlO_3$(LAO)



- Perovskite structure, no magnetic, band insulator

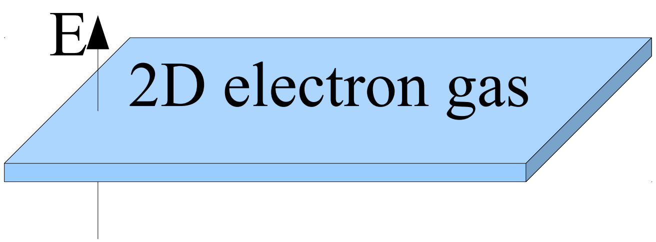
LAO/STO interface

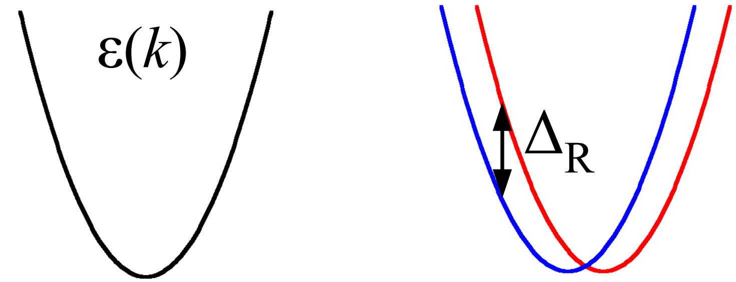
- Conducting, magnetic, superconducting, correlated, spin-orbit coupling....



A. Ohtomo and H. Y. Hwang Nature(2004)

Properties of 2DEG: Rashba spin splitting





(i)Space inversion symmetry $\varepsilon(\vec{k},\uparrow) = \varepsilon(-\vec{k},\uparrow)$ ✗

Time inversion symmetry $\varepsilon(\vec{k},\uparrow) = \varepsilon(-\vec{k},\downarrow)$

(ii)Spin orbit coupling $(\hbar/2m_e^2c^2)(\nabla V \times \vec{p})\cdot\vec{s}$

free 2DEG: $\Delta_R = 2\alpha_R k \quad \alpha_R = (\hbar/4m^2c^2)\mathrm{d}V(z)/\mathrm{d}z$

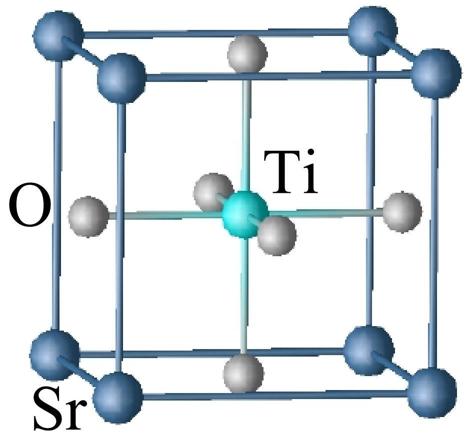
$\mathrm{E}\sim 100\ \mathrm{Volt/mm} \qquad \Delta_R \sim 10^{-8}\mathrm{meV}$

- $\Delta_R \sim$ meV
- $2\alpha k$ at $LaAlO_3/SrTiO_3$ interface (*Caviglia et.al.; Ben Shalom et.al.*)

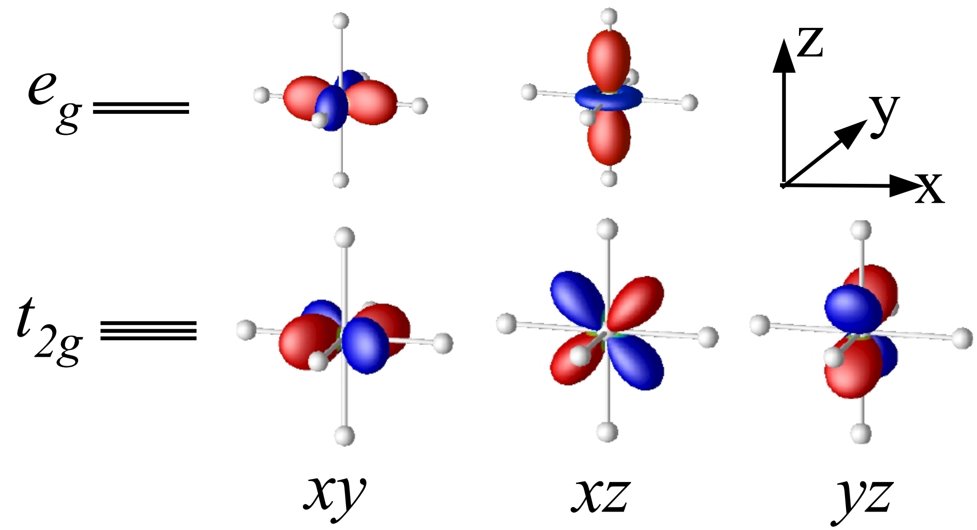
  $2\alpha k^3$ at $SrTiO_3$ surface (*Nakamura et.al.*)

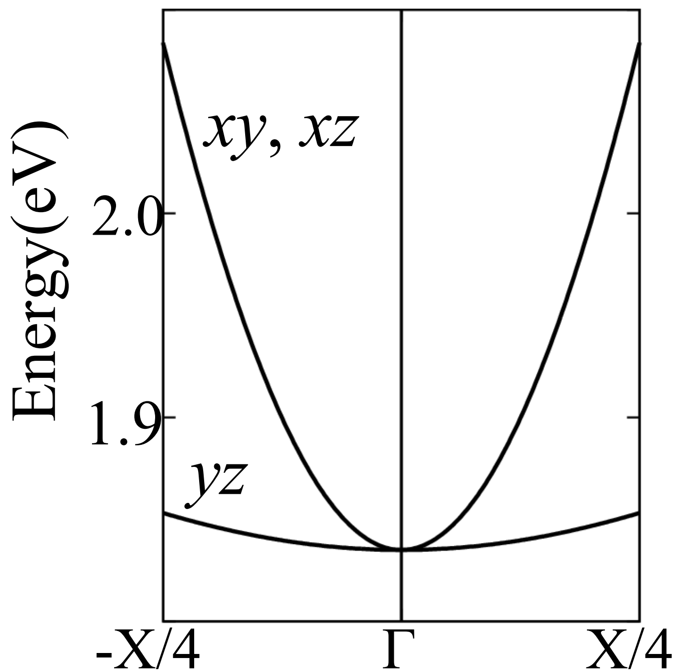
Band structure of bulk $SrTiO_3$

Bulk STO



TiO_6 crystal field splits Ti *d* orbitals

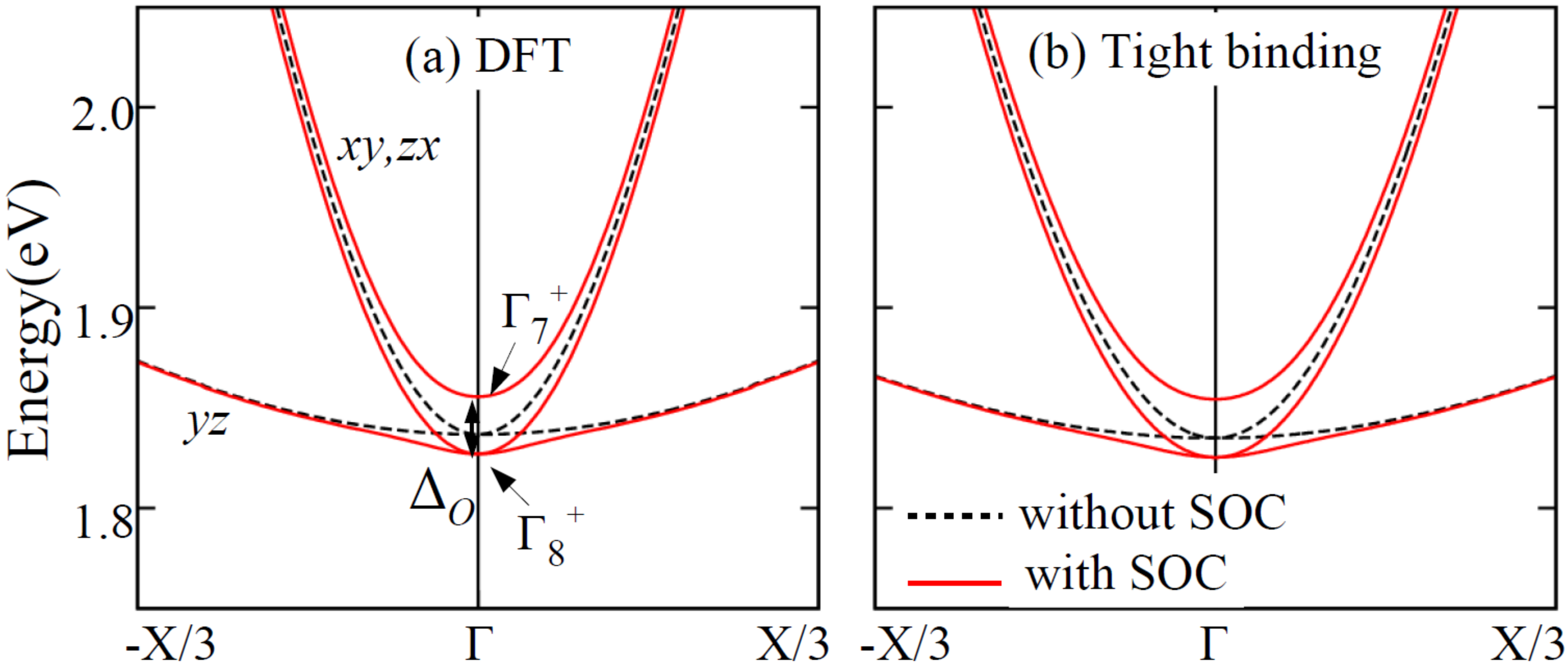




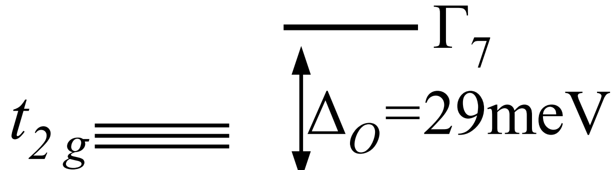
- three degenerate t_{2g} orbitals
- heavy carrier *yz* ($6.8m_e$), two light carriers xy and xz ($0.41m_e$)

Spin-orbit coupling (SOC) effects on bulk STO

Wien2k -->Wien2Wannier -->Wannier90

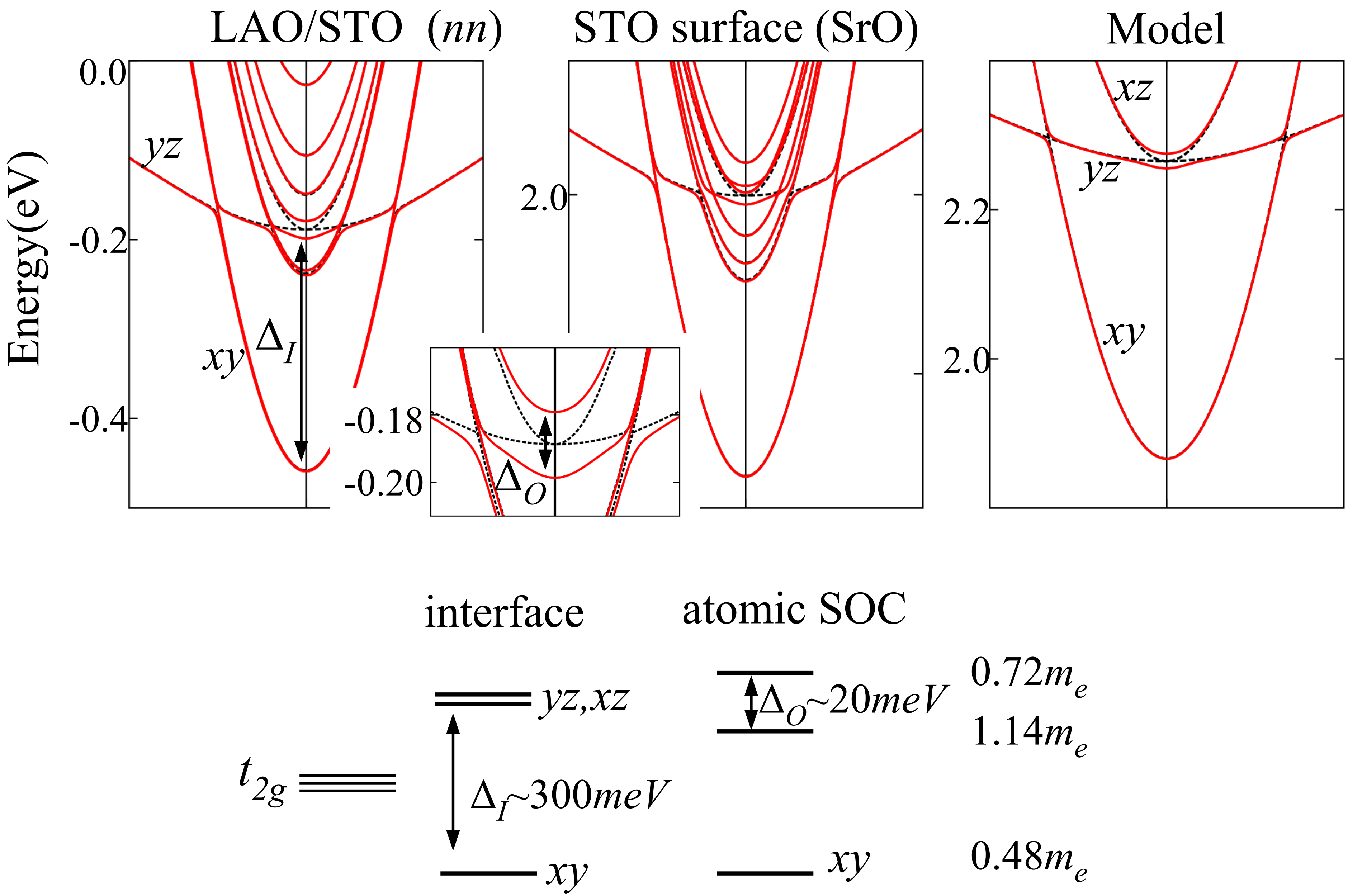


hopping t + atomic SOC $\xi \vec{l} \cdot \vec{s}$



$$\frac{1}{\sqrt{6}}\left(\pm i\, yz|\uparrow,\downarrow\rangle + zx|\uparrow,\downarrow\rangle + 2i\, xy|\downarrow,\uparrow\rangle\right)$$

Orbital splitting at LAO/STO interfaces and STO surfaces



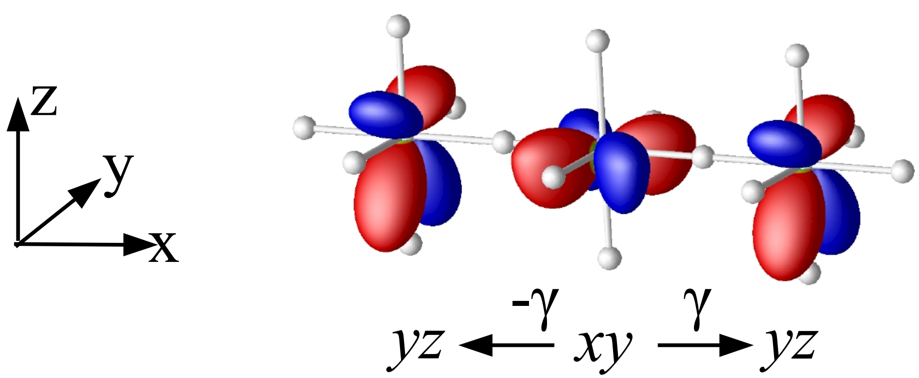
Model for Rashba spin splitting

$$H_0^i + H_\xi + H_\gamma$$

Free: $-2t_1 cos k_x - 2t_1 cos k_y - t_2 - 4t_3 cos k_x cos k_y$

atomic SOC:
$$\frac{\xi}{2}\begin{pmatrix} 0 & 0 & i & 0 & 0 & -1 \\ 0 & 0 & 0 & -i & 1 & 0 \\ -i & 0 & 0 & 0 & 0 & i \\ 0 & i & 0 & 0 & i & 0 \\ 0 & 1 & 0 & -i & 0 & 0 \\ -1 & 0 & -i & 0 & 0 & 0 \end{pmatrix}$$

interface asymmetry:
$$\gamma\begin{pmatrix} 0 & 0 & 2i\sin k_x \\ 0 & 0 & 2i\sin k_y \\ -2i\sin k_x & -2i\sin k_y & 0 \end{pmatrix}$$

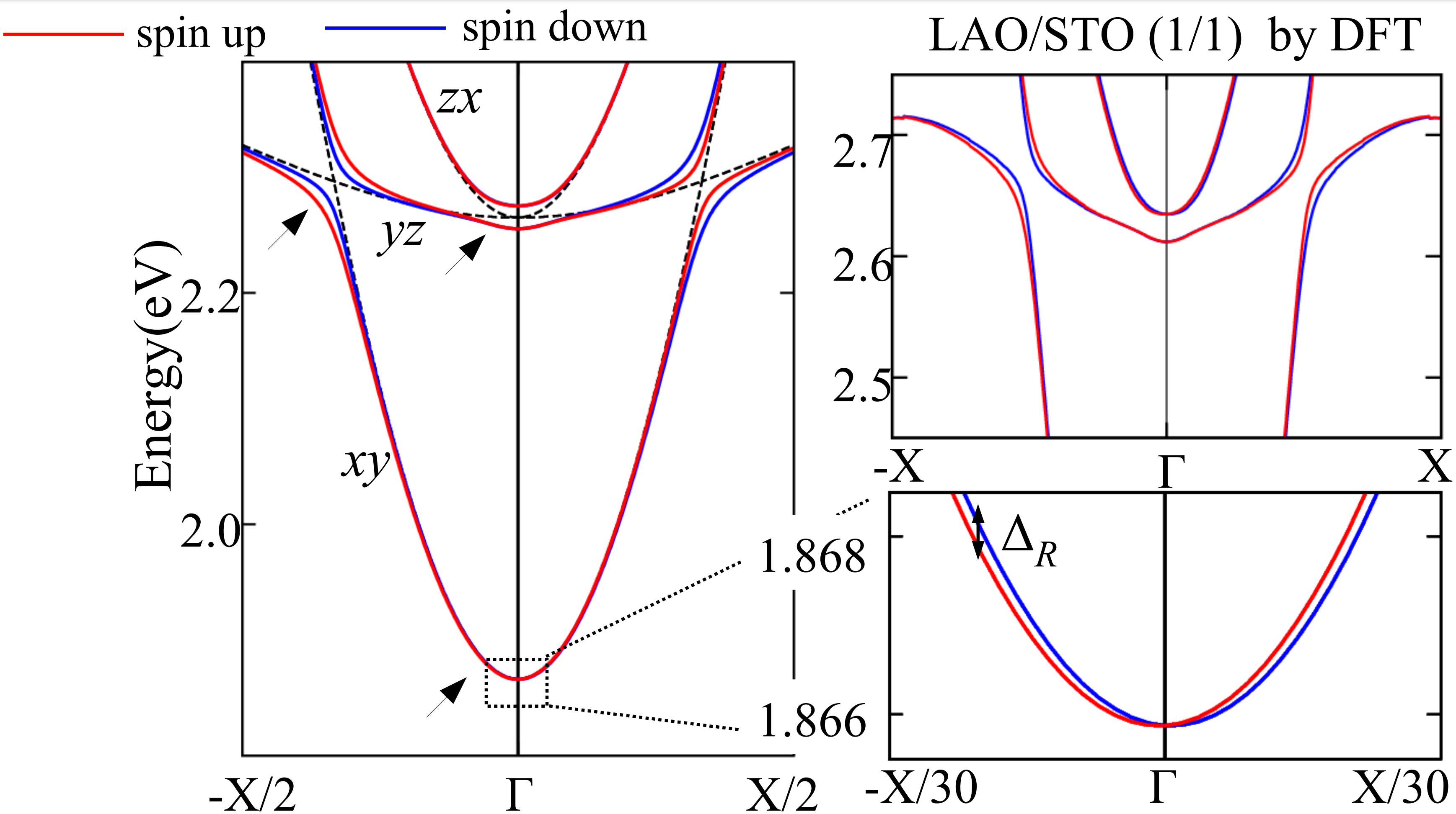


$$\gamma = \langle xy|H|yz(R)\rangle$$

0.02eV, interface layer

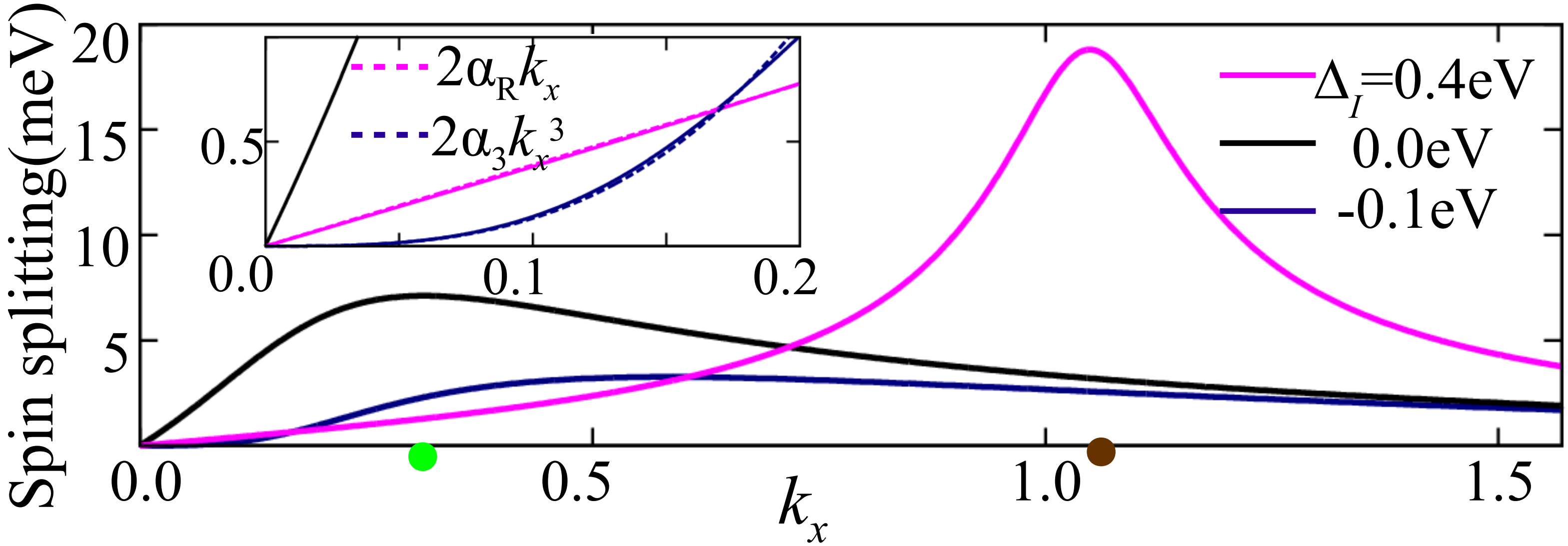
s-*p* electrons of Au surfaces *Lashell* et al.(1996); *Peterson* et al.(2000)

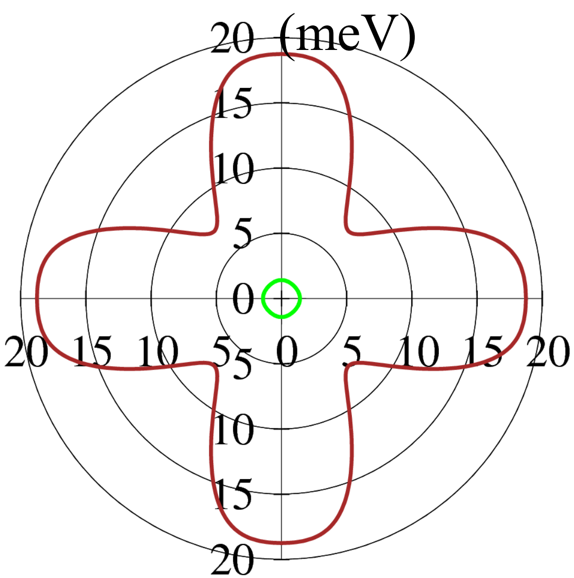
Spin splitting



- Γ, *xy* orbital: $\Delta_R = 2\alpha_R k$ $\alpha_R = 2a\xi\gamma/\Delta_I$
- Γ, *yz*/*xz* mixed orbitals: $2\alpha_3 k^3$
- *xy*-*yz* crossing point

spin splitting





$\Delta_R = 2\alpha_R k$

$\alpha_R = 0.76\times10^{-2}$eVÅ Δ_I=0.4eV

6.0×10^{-2}eVÅ Δ_I=0.0eV

$1\text{-}5\times10^{-2}$eVÅ (exp)

$\Delta_R = 2\alpha_3 k^3$

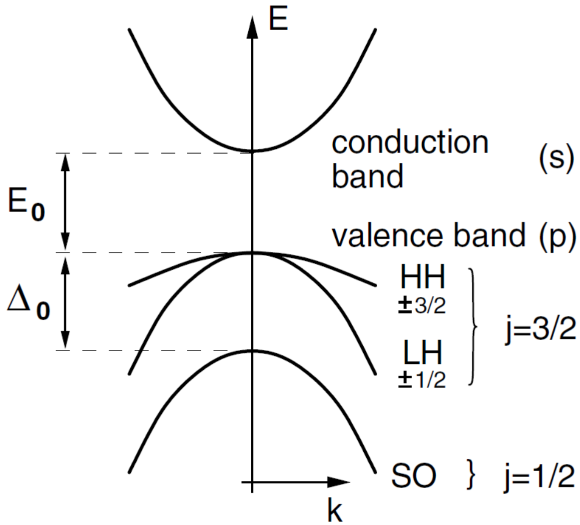
$\alpha_3 =$ 4eVÅ^3

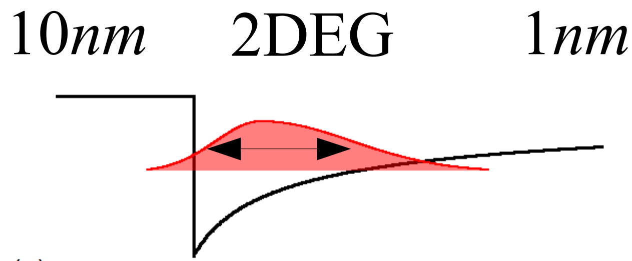
1-2eVÅ^3 (exp)

Anisotropic spin splitting->AMR (exp)?

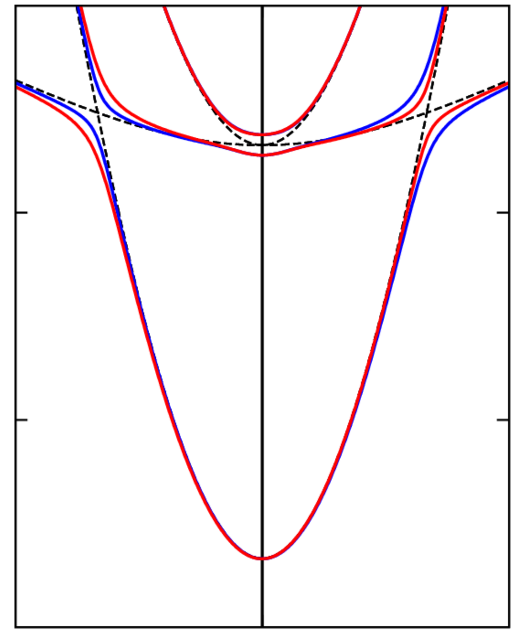
Comparison: semiconductor and oxide heterostructures

$GaAs/Al_xGa_{1-x}As$





LAO/STO



single orbital Rashba
nearly free electron

fitting parameter or *kp* method

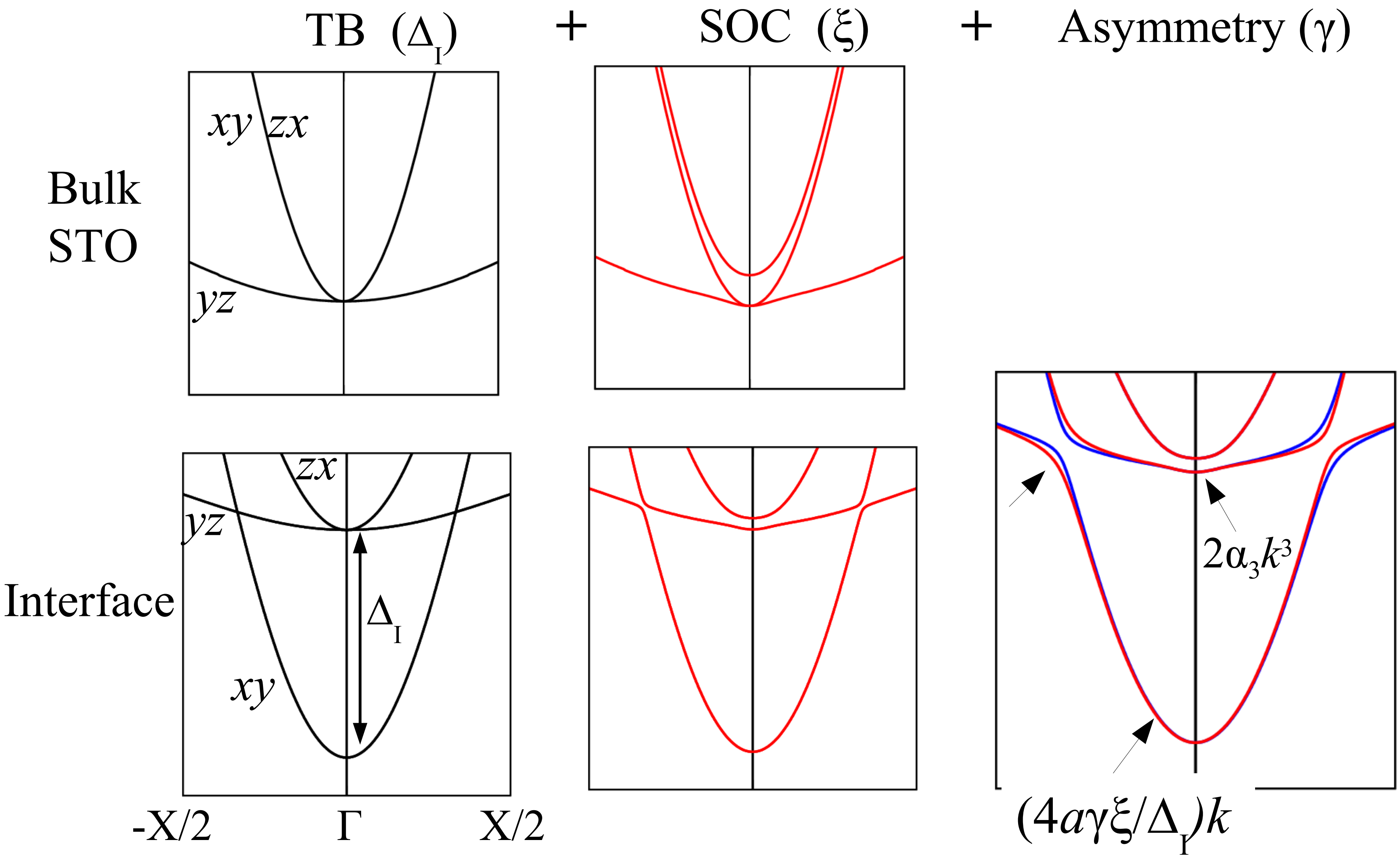
multi-orbital
magnetic, superconducting,
correlated, and spin-orbit coupling

first principle tight-binding

Book “Spin–Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems” by Winkler (2003)

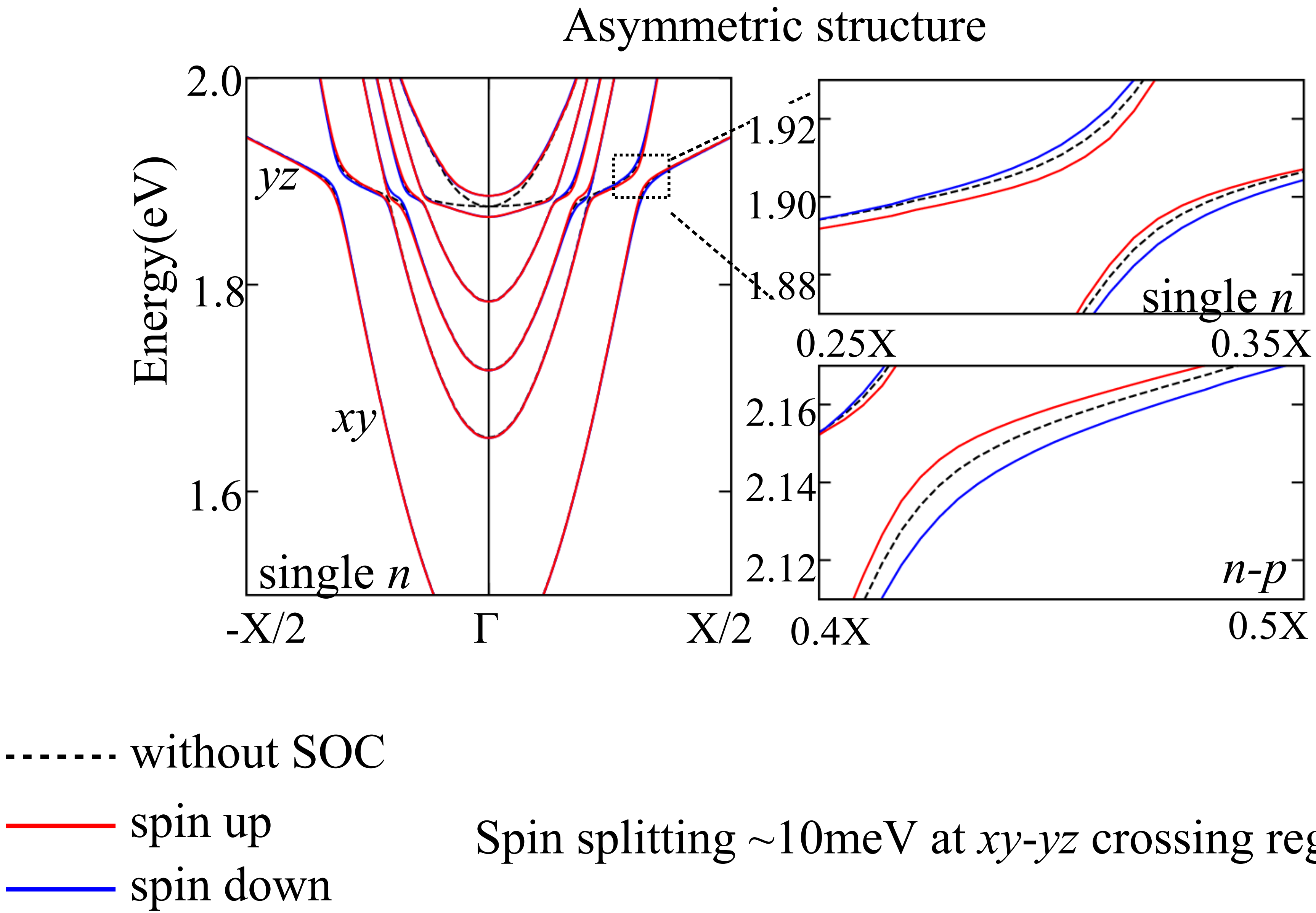
J. Mannhart and D. G. Schlom, Science (2010).

Conclusion: orbital and spin splittings

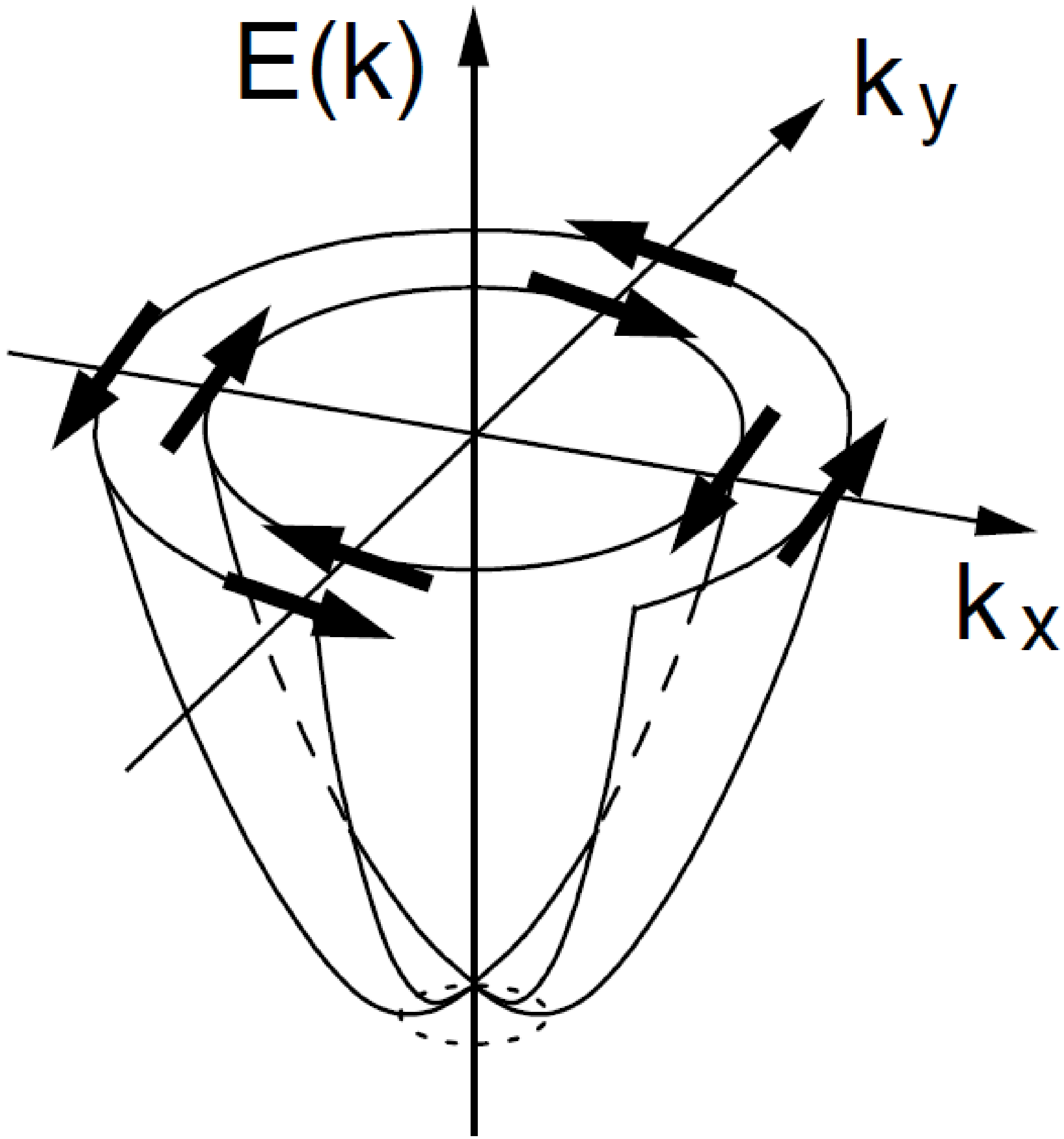


Zhicheng Zhong, Anna Toth, and Karsten Held PRB 87 161102(R) (2013)

Spin splitting at LAO/STO interfaces and STO surfaces



Spin splitting ~10meV at *xy*-*yz* crossing region?


E(k)
k y
k x

Oxide Interfaces—An Opportunity for Electronics

J. Mannhart* and D. G. Schlom*

	GaAs - $Al_xGa_{1-x}As$	$LaAlO_3$ - $SrTiO_3$
Carrier density n (without gate field)	several 10^{10} - several $10^{11}/cm^2$	several 10^{13} $/cm^2$
Sheet resistance ρ (H=0)	order of 10-100 Ω/□ (low T, samples with high-μ)	~ 200 Ω/□ (4.2 K) ~ 20 kΩ/□ (300 K)
Thickness d	order of 10 nm	~ 10 nm (4.2 K) ≲ 4 nm, possibly 0.4 nm (300 K)
Equivalent volume carrier concentration	order of 10^{17} $/cm^3$	order of 10^{20} $/cm^3$
Typical thicknesses of the host layers in heterojunctions (*e.g.*, cap layers)	tens of nanometer	≥ 1.6 nm $LaAlO_3$ (4 unit cells)
Hall mobility μ	≳ 10^7 cm^2/Vs (4.2 K)	≲ 1000 cm^2/Vs (4.2 K) ≲ 10 cm^2/Vs (300 K)
Effective mass m of carriers at interface	$m_e \sim 0.07\ m_0$	$m_e \sim 3\ m_0$
Mean scattering time τ, mean free path	100 psec, order of 100 µm	psec, tens of nm (4.2 K)
v_F	~ 3×10^7 cm/s	several 10^6 cm/s
Magnetic flux density inducing quantum Hall filling factor v =1	order of 10 T	order of 1000 T
Energy dependence of density of states $N(E)$	step function of 2-DEG (ideal case)	complex function reflecting the $N(E)$-dependence of the Ti-, La-, and O-ions

$GaAs$ - $Al_xGa_{1-x}As$	$LaAlO_3$ - $SrTiO_3$
• two-dimensional electron gas (2-DEG); • quantum well induced by band bending; • 2D-subbands of nominally free electrons	• two-dimensional electronic liquid (2-DEL); • metal-insulator transition at a few 10^{12} /cm^2; quantum well structure as shown in Fig. 4; • 2D-subbands composed of ionic orbital states with local character (*e.g.*, Ti 3*d*, La 5*d*, O 2*p*); • 2D-superconducting ground state; • strong spin-orbit coupling.