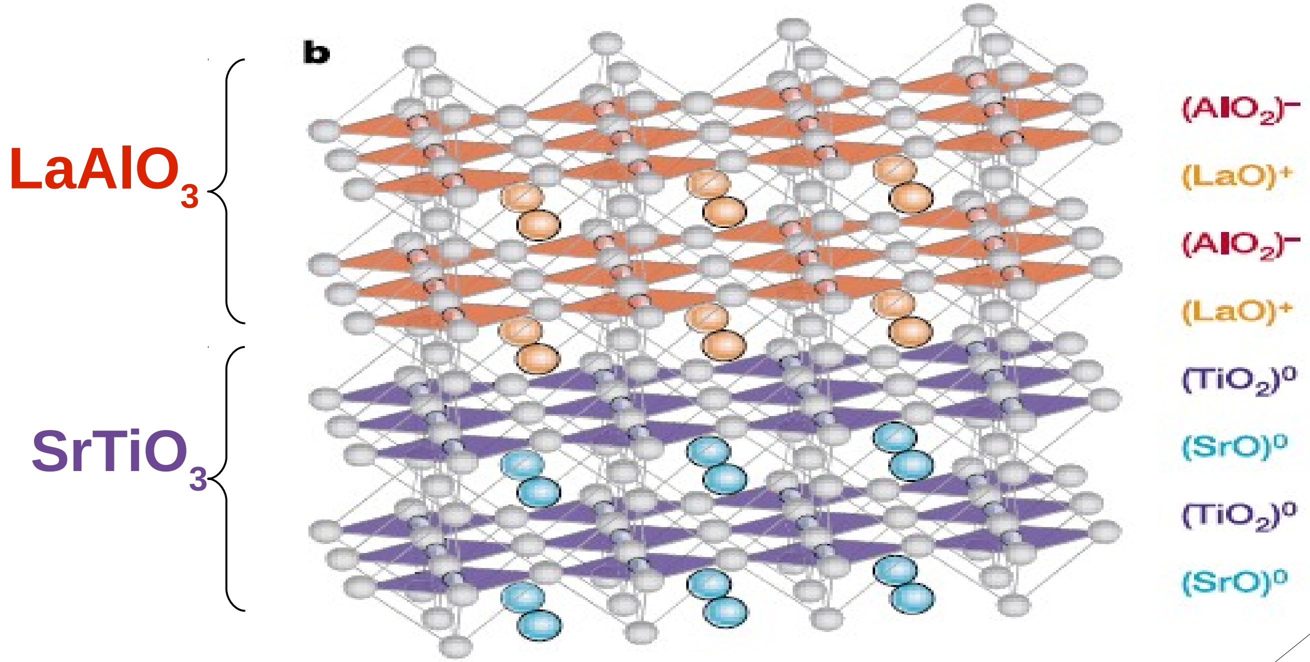
TWO-DIMENSIONAL CONDUCTIVITY AT $LaAlO_3/SrTiO_3$ INTERFACES

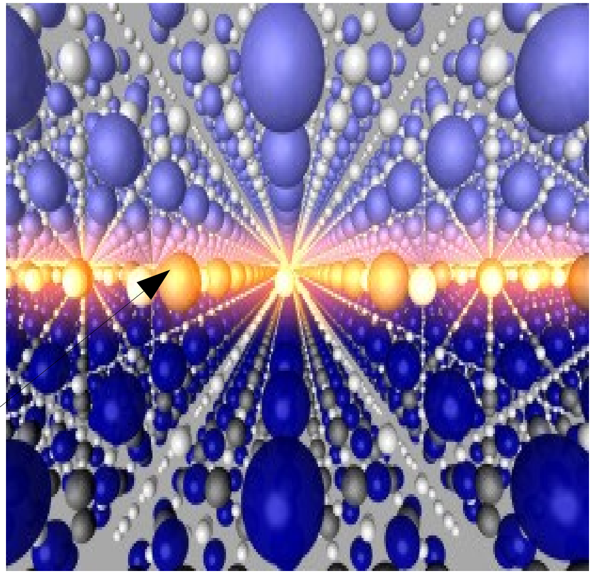
Amany Raslan

Material Science Program
Physics Department, Trent University

Supervisor
Dr. Bill Atkinson

LaAlO$_3$/SrTiO$_3$ INTERFACES

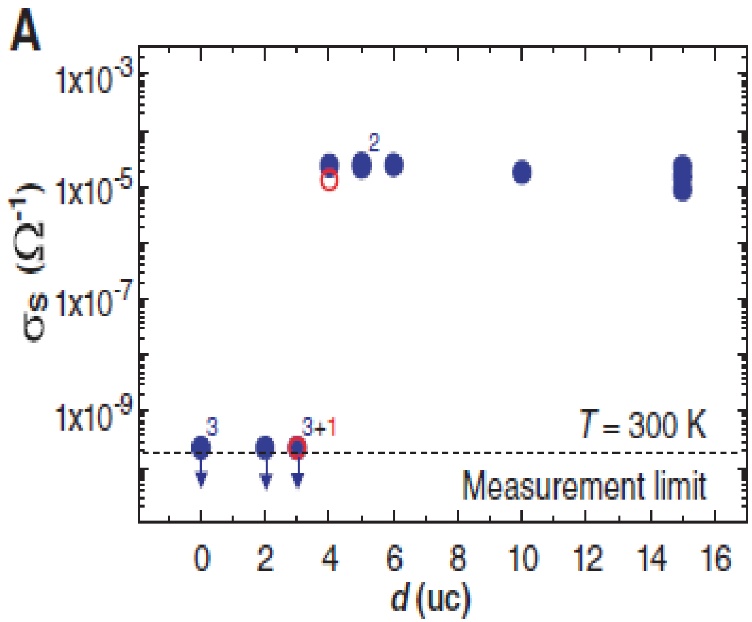




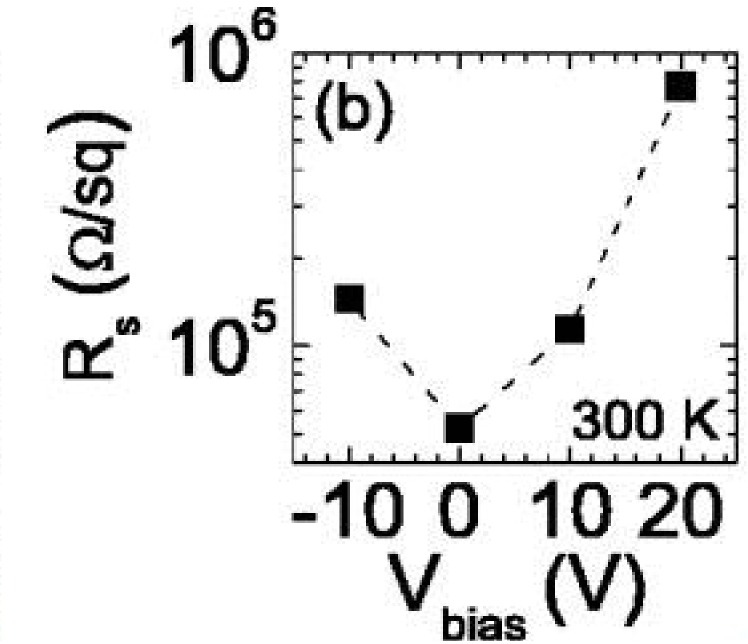
A. Ohtomo, H. Hwang, Nature 427, 423 (2004)

Conducting Interface OR Two-dimensional electron gas(2DEG)

Conductivity at the $LaAlO_3/SrTiO_3$ interface



S. Thiel et al., Science 313, 1942(2006)



F. Trier et al., App. Phys. Lett. 103(2013)

Study conductivity at the $LaAlO_3/SrTiO_3$ interface Theoretically

Theoretical Model

1- Write the Hamiltonian for the $SrTiO_3$ film

$$\hat{H} = \hat{H}_0 + \hat{V}_{ext} + \hat{V}_C$$

The non-interacting Hamiltonian

$$\hat{H}_0 = \sum_{ij} \sum_{\alpha,\beta} \sum_{\sigma} c^{\dagger}_{i\alpha\sigma} t_{i\alpha,j\beta} c_{j\beta\sigma}$$

α → Ti t_{2g} orbitals, d_{xy} , d_{xz} and d_{yz}

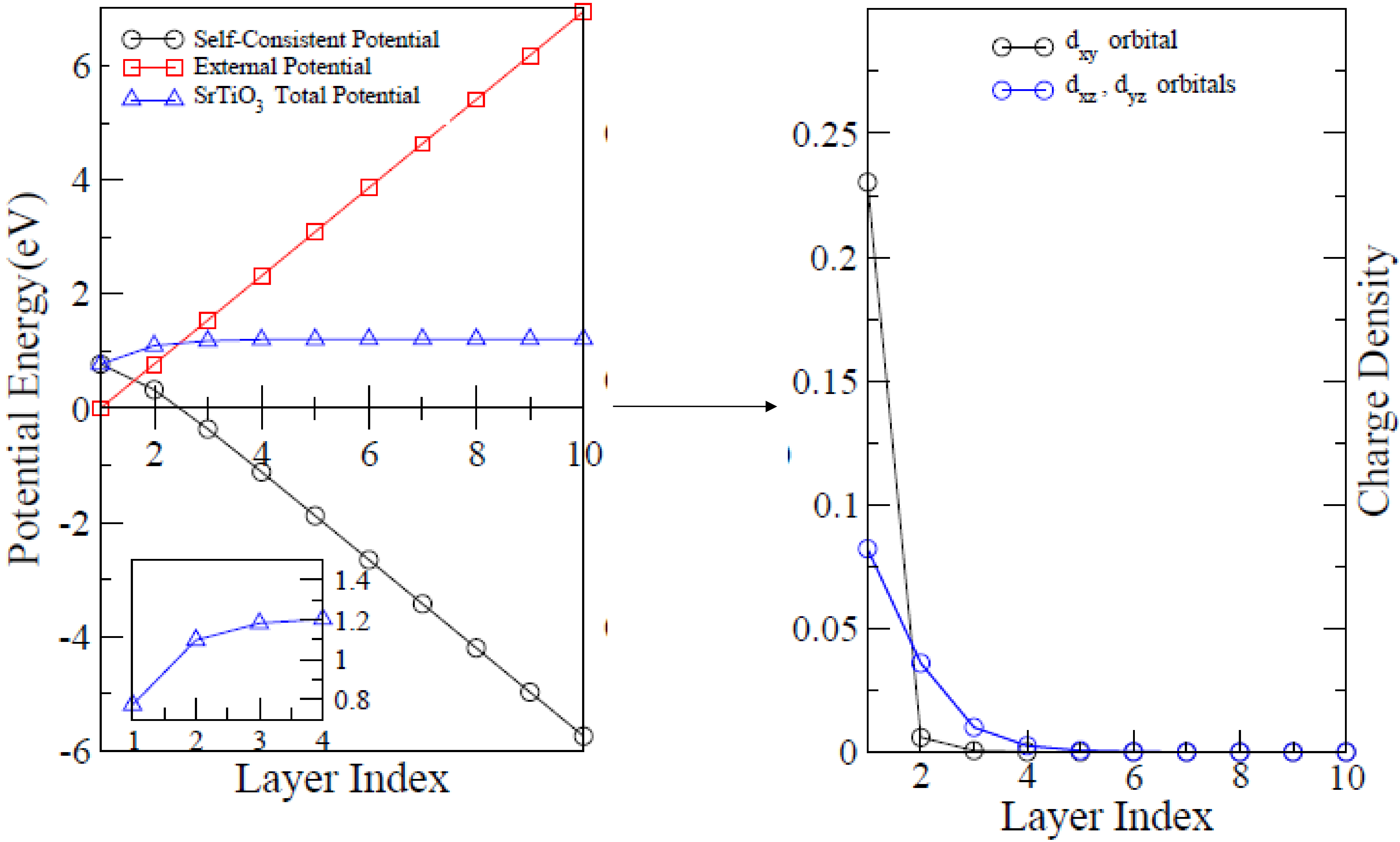
The Coulomb potential energy

$$\hat{V}_C = \frac{-e^2 a}{2\epsilon_0 k} \sum_{i_z\alpha\sigma} \sum_{j_z} \sum_{\beta} (|i_z - j_z| - j_z) n_{j_z\beta\sigma} \hat{n}_{i_z\alpha\sigma}$$

The external potential energy due to the charge at the $LaAlO_3$ surface

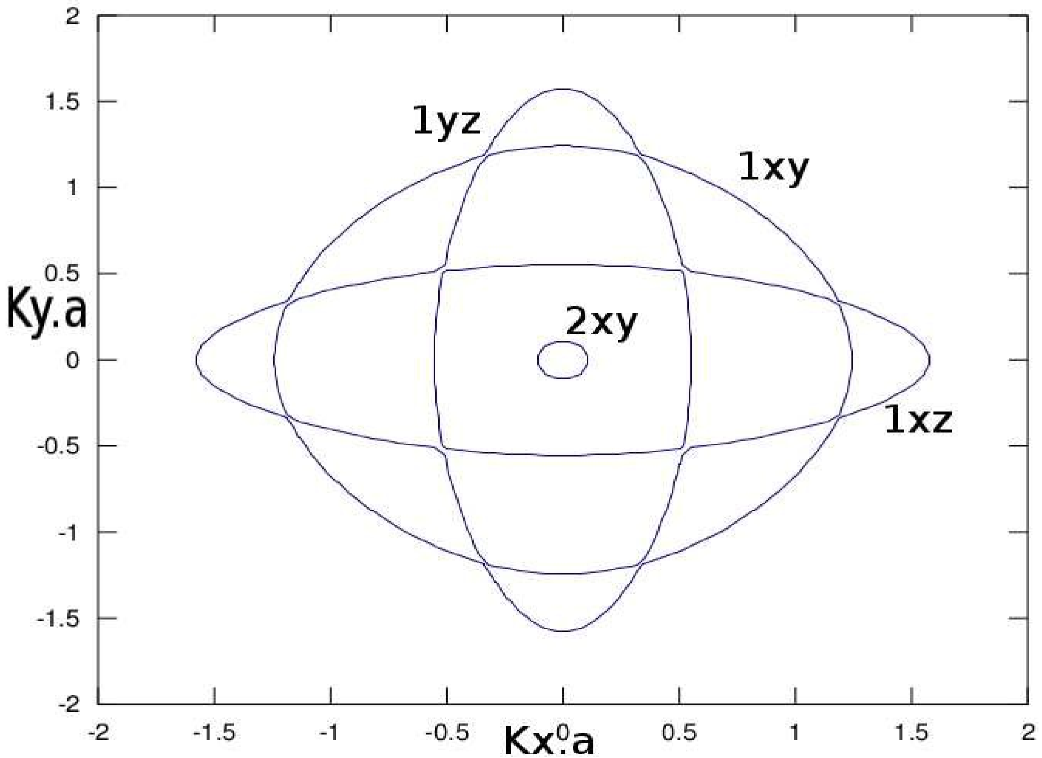
$$\hat{V}_{\text{ext}} = \sum_{i_z\alpha\sigma} \varphi^{\text{ext}}_{i_z\alpha} \hat{n}_{i_z\alpha\sigma}$$

Self-Consistent Results



The self-consistent solutions for the total potential energy and the charge density inside the $SrTiO_3$ film

Theoretical Model



- There are four occupied bands, two with d_{xy} orbital character, and one each with d_{xz} and d_{yz} orbital character.

Fermi surfaces for a Fermi energy E_f = 0.15eV

The next step is study the contribution of these four occupied bands to the interface conductivity

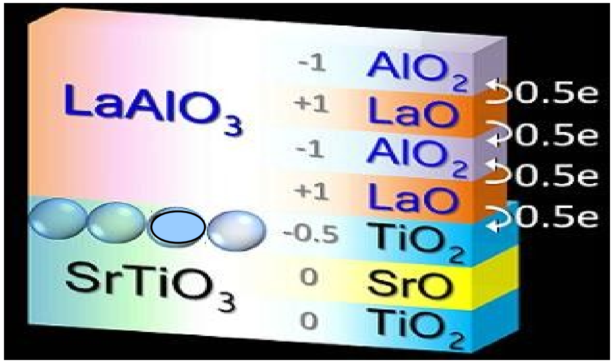
Theoretical Model

2- Develop the model for impurities to study the interface conductivity

We assume that

- A low density of point-like impurities with Potential $\tilde{V}_{\mathrm{imp}}$

- Impurities lie at the interface



The relative two-dimensional conductivity of each occupied band as a function in $\tilde{V}_{\mathrm{imp}}$

$$\sigma_{xx}^{(n)}(\tilde{V}_{imp}) = \sqrt{\frac{m_y^n}{m_x^n}}\frac{\varepsilon_f^n}{\gamma^n(\tilde{V}_{imp})}$$

$$\sigma_{xx}^{(n)}(\tilde{V}_{imp}) = \sqrt{\frac{m_y^n}{m_x^n}} \frac{\varepsilon_f^n}{\gamma^n(\tilde{V}_{imp})}$$

Where

$\sigma_{xx}^{(n)}$ The two-dimensional conductivity due to band n

$\sqrt{\frac{m_y^n}{m_x^n}}$ The effective mass ratio for band n

$\varepsilon_f^n = (\varepsilon_f - \varepsilon_{n0})$ The relative Fermi energy to the bottom of the band n

γ^n The scattering rate for electrons in band n

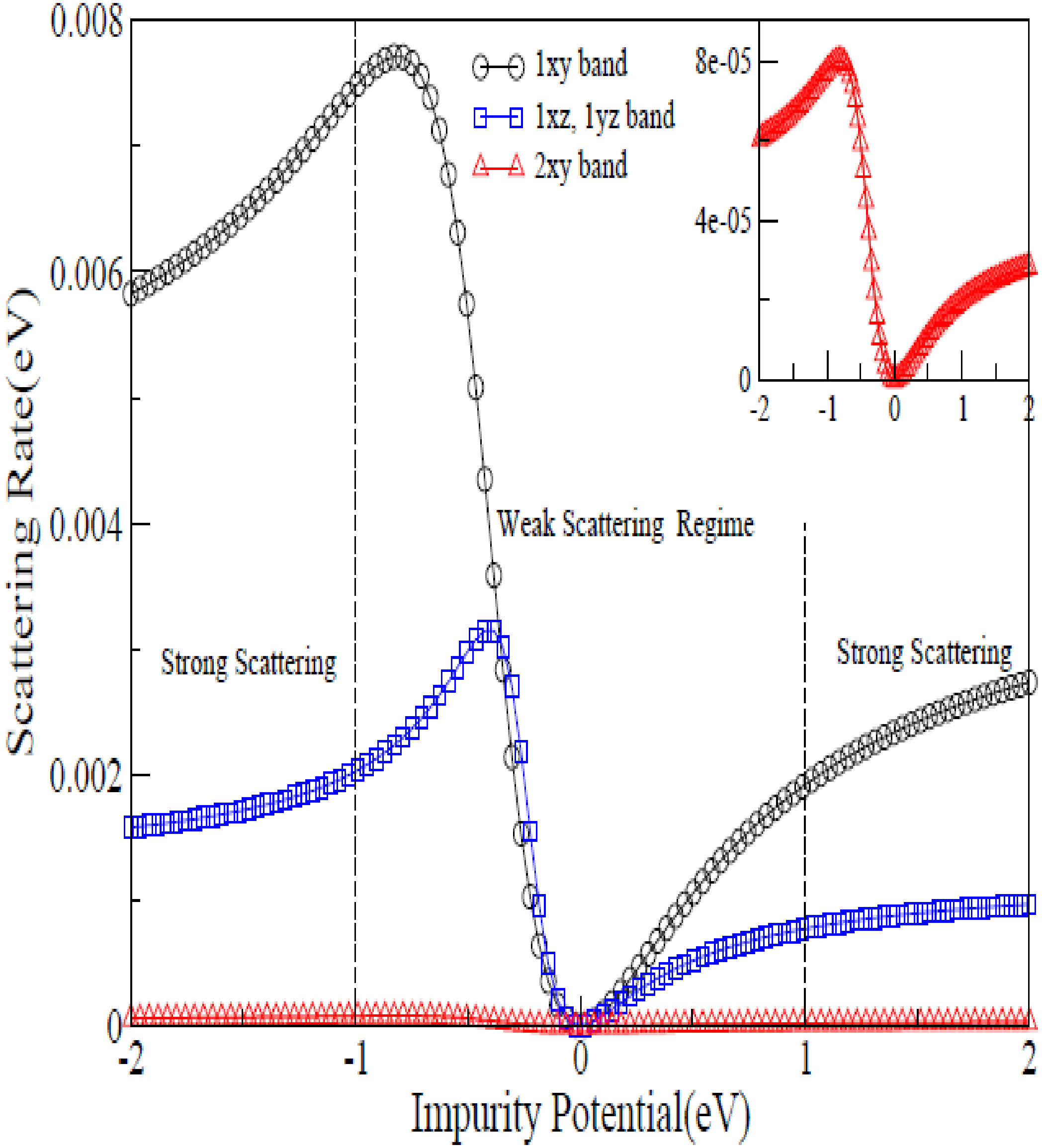
$$\gamma^n(\tilde{V}_{\text{imp}}) = -cIm \sum_{\alpha} |\psi_{1\alpha n}(\Gamma)|^2 t_{1\alpha,1\alpha}(\tilde{V}_{\text{imp}})$$

Impurity density (c)

Impurity at the interface in orbital α ($t_{1\alpha,1\alpha}$)

How γ^n Changes with $\tilde{V}_{\text{imp}}$?!

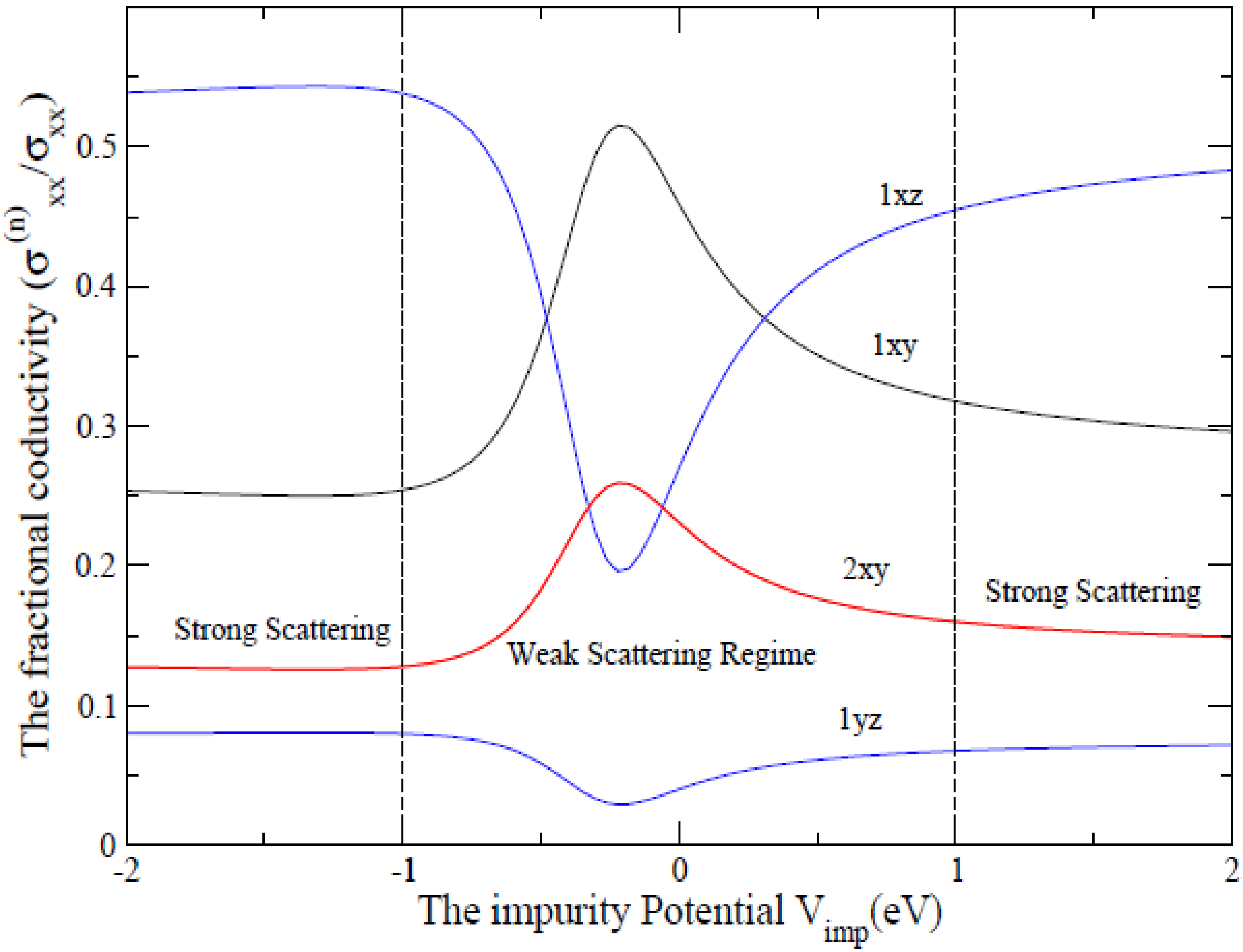
$$\gamma^n(\tilde{V}_{\text{imp}}) = -c Im \sum_{\alpha} |\psi_{1\alpha n}(\Gamma)|^2 t_{1\alpha,1\alpha}(\tilde{V}_{\text{imp}})$$



- Similar dependences of all bands on
- Two Scattering regimes:
  - Weak Scattering
  - Strong Scattering
- 1xy band largest scattering rate
- 2xy band smallest scattering rate
- 1xz & 1yz bands same scattering rate

The Fractional Conductivity

$$\sigma_{xx}^{(n)}(\tilde{V}_{imp}) = \sqrt{\frac{m_y^n}{m_x^n}} \frac{\varepsilon_f^n}{\gamma^n(\tilde{V}_{imp})}$$

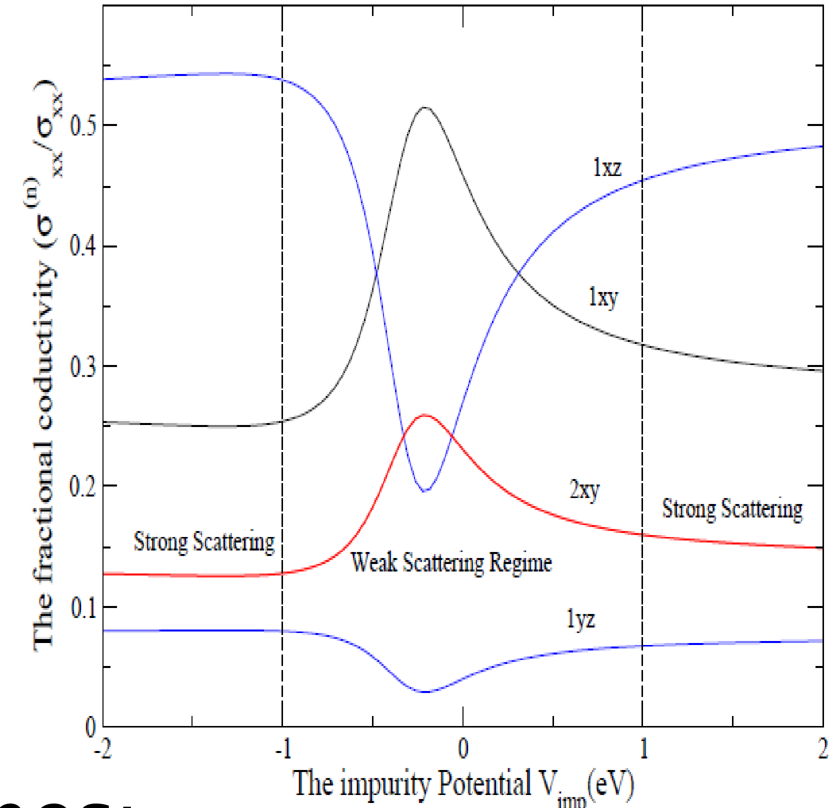


Band	$\sqrt{\frac{m_y}{m_x}}$	$\epsilon_f^n(eV)$
$1xy$	1	0.319
$1yz$	0.385	0.069
$1xz$	2.597	0.069
$2xy$	1	0.001

Three parameters control the contribution of each band to the total two-dimensional conductivity

Summary

* The contribution of the occupied bands to the interface
conductivity depends on three main parameters;
The impurity potential
The effective mass ratios
The relative Fermi energy

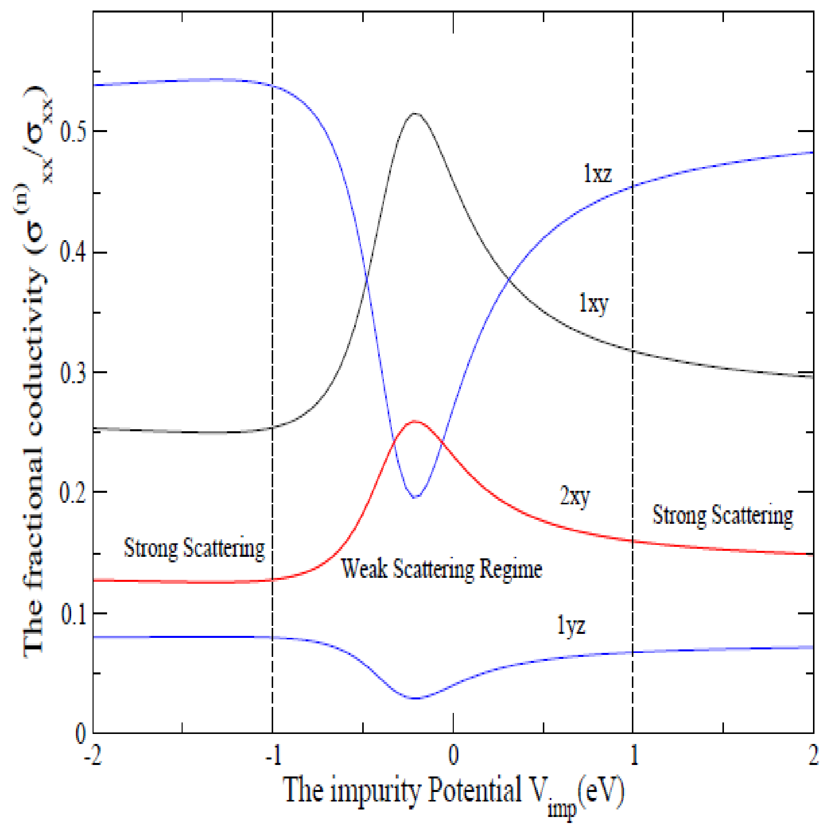


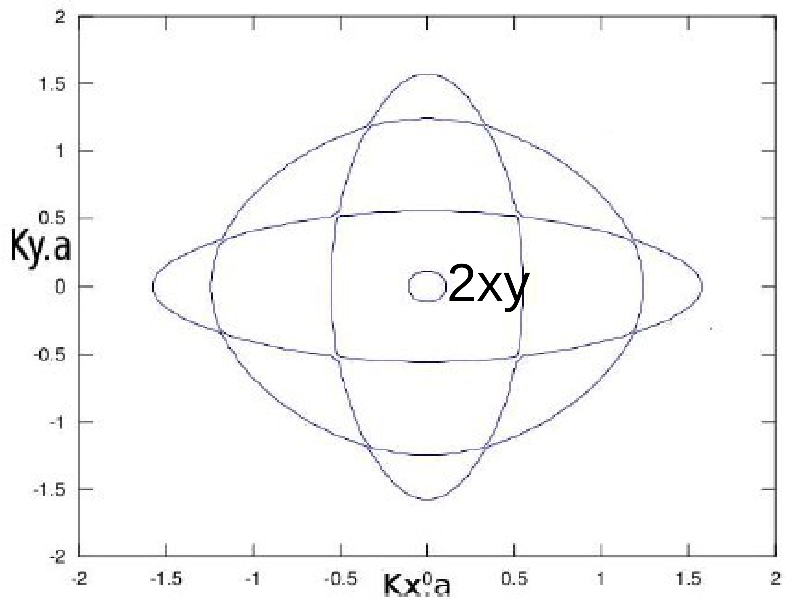
*There are two scattering regimes:
the weak scattering regime in which the 1xy and 2xy band contributions are dominant, and

the strong scattering regime in which the 1xz band has the largest fractional conductivity.

Summary

*The 2xy band makes a remarkably large contribution to the two-dimensional conductivity, even though it has the smallest Fermi surface.





THANK YOU