Temperature-Dependent Band Structure of $LaAlO_3/SrTiO_3$ Interfaces

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$LaAlO_3/SrTiO_3$ Interfaces?

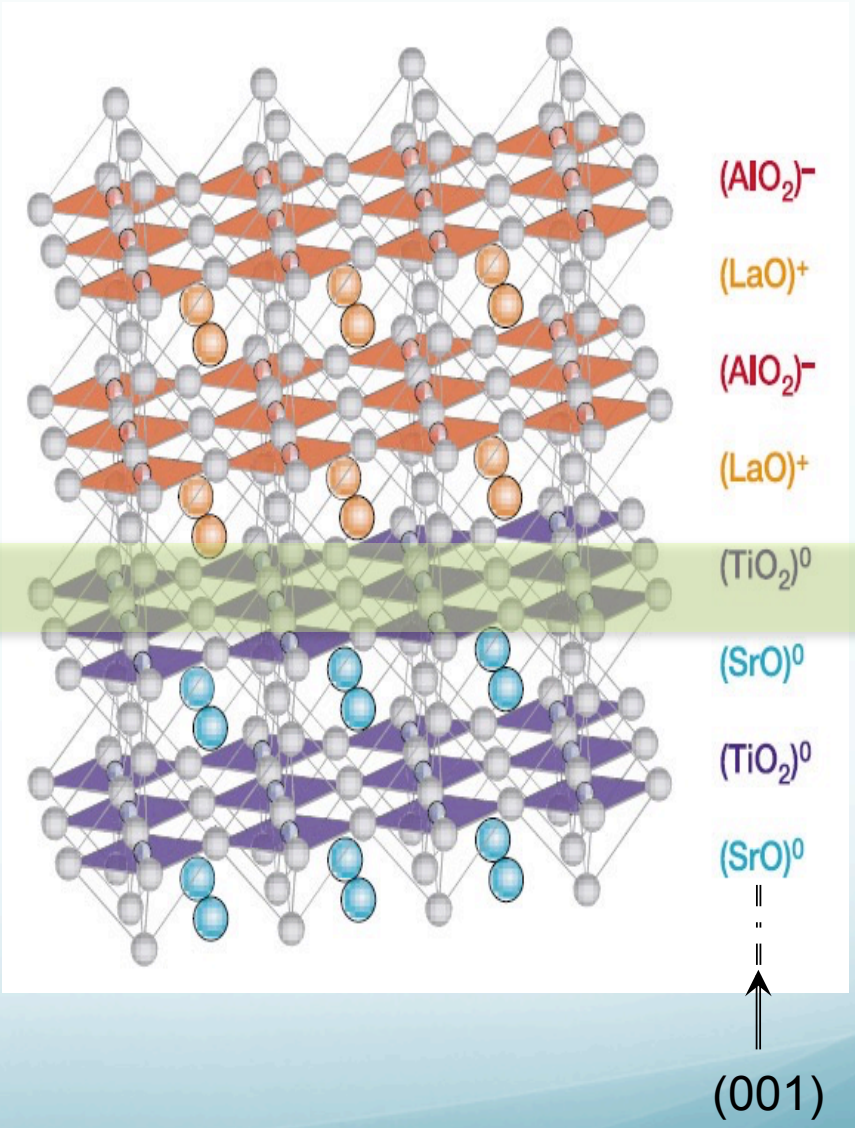
$LaAlO_3$:

Band insulator
E_G = 5.6eV

Metallic interface(2DEG)

$SrTiO_3$:

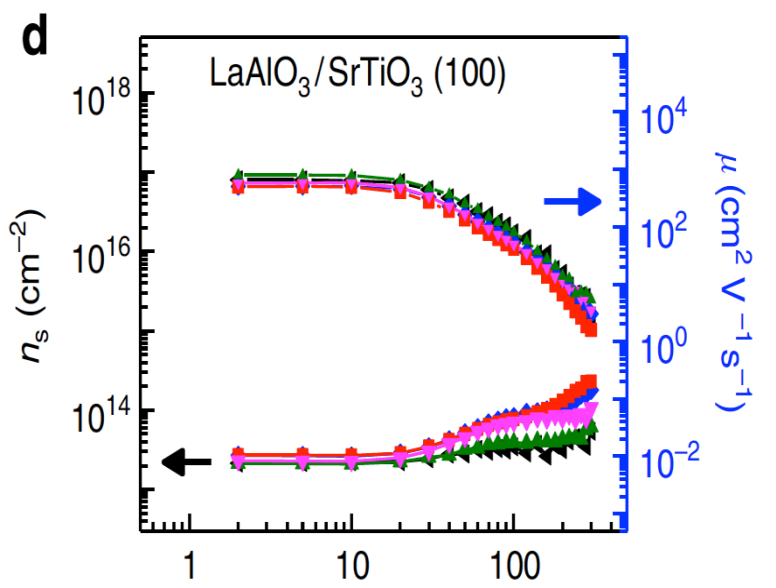
Band insulator
E_G = 3.25eV



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

Temperature effect on transport

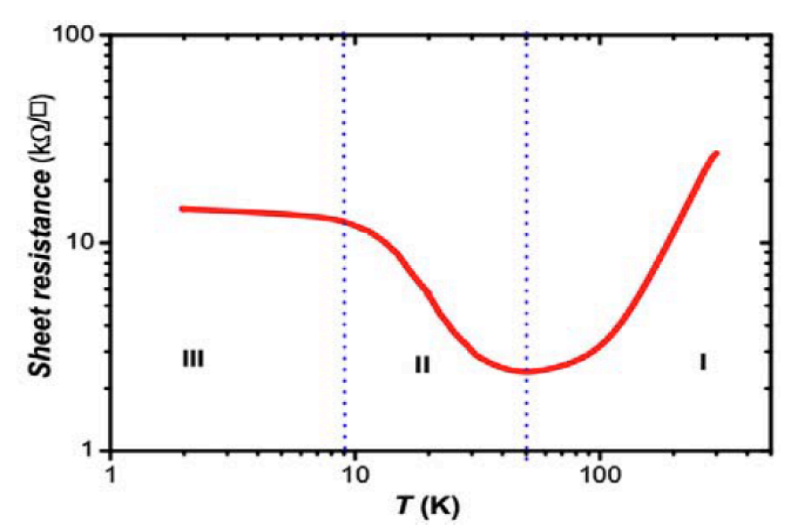
A. Annadi et. al., Nat. Com. (2013)



Mobility up to $10^4 cm^2/Vs$

Charge Density $\approx 10^{14}/cm^2$

V. K. Guduru et. al., J. KPS (2013)



Strong Temperature-dependent Resistance

Theoretical Model for temperature dependence is needed

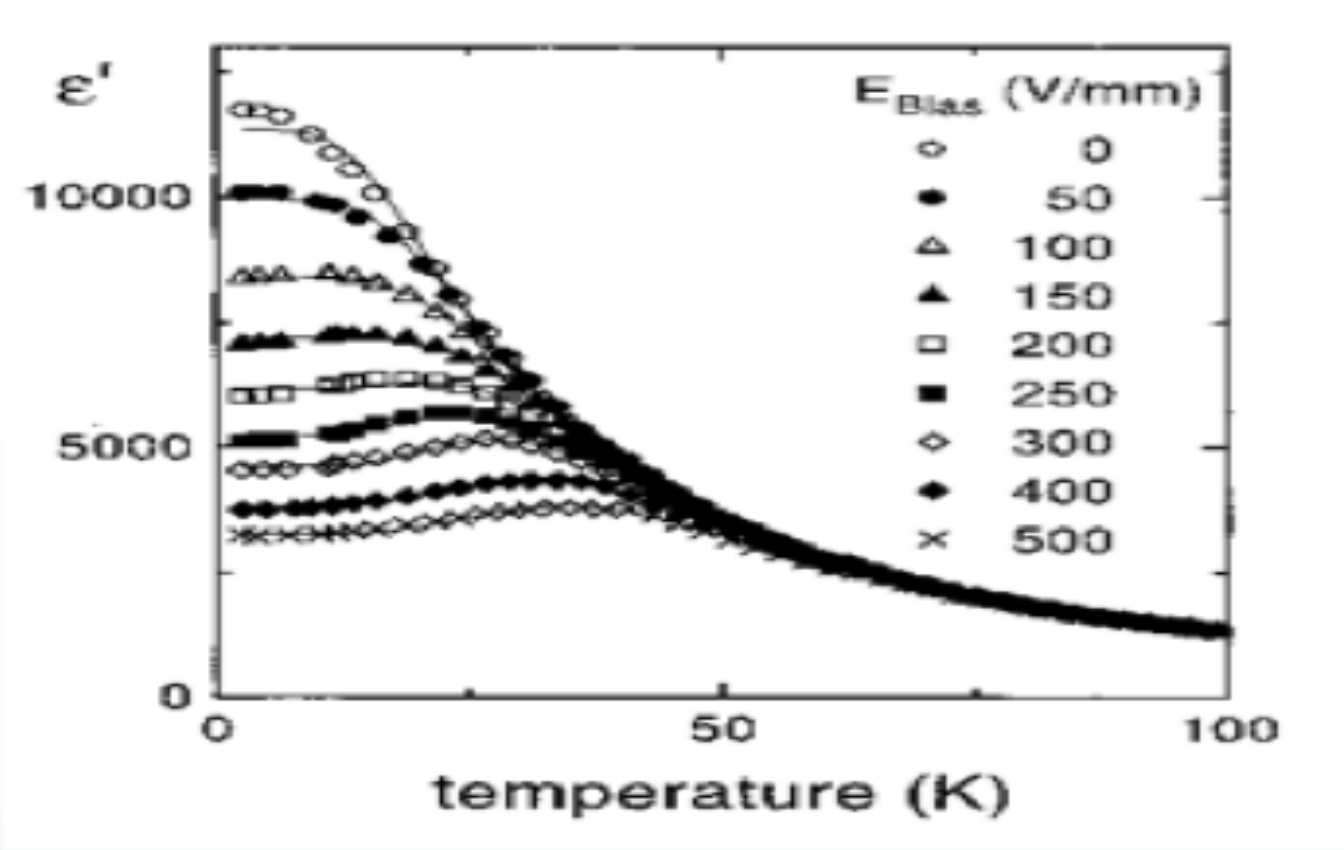
Our Goal

Develop a simple model to explore the temperature dependent electronic structure of the $LaAlO_3/SrTiO_3$ Interfaces.

Experimentally, the 2DEG reside in the Ti atoms at STO side

Temperature dependence of dielectric constant of the STO

J. Hemberger et. al., PRB, (1995)



Dielectric constant ε(STO) is a strong function in temperature and electric field

Theoretical Model

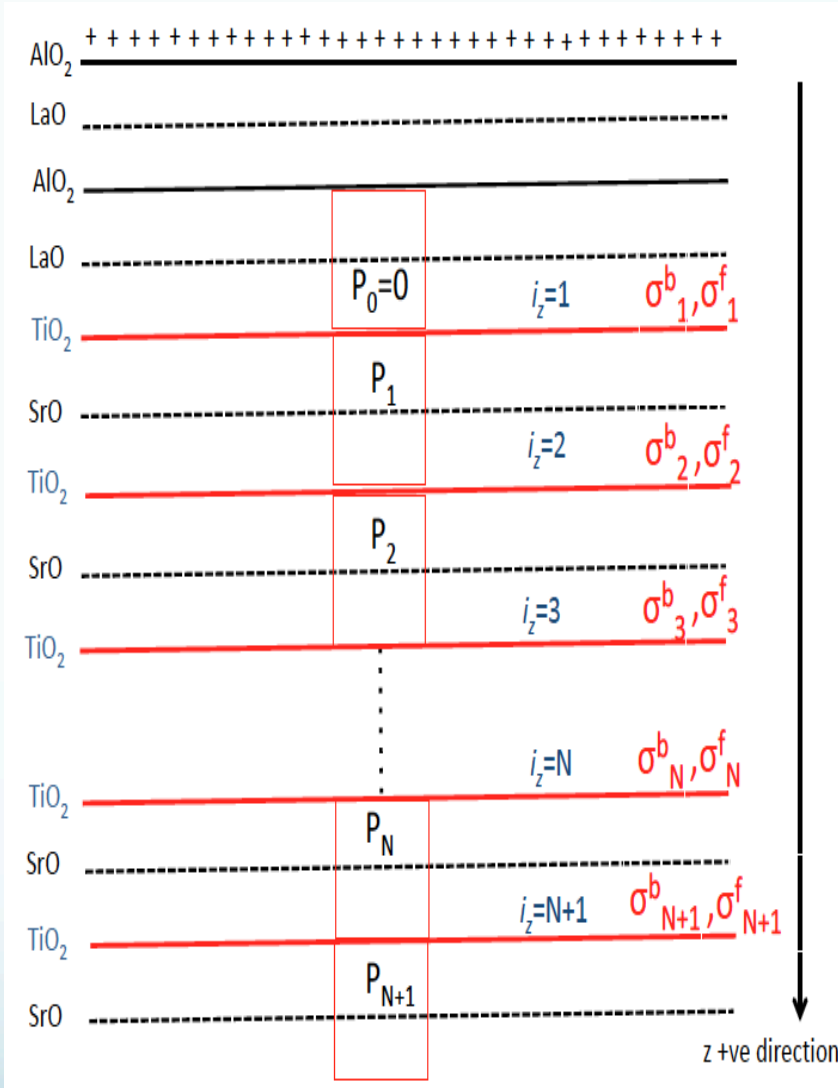
Our Assumptions:

- σ^s "+" at the LAO surface,
  That pulls e- from STO bulk to the interface "2DEGσ^f"
  And induces a polarization charge density "2D bound charge σ^b "

- Model only the 3d Ti t_{2g} orbitals (d_{xy}, d_{xz} and d_{yz})
- The model is discrete in the z-direction

Our boundary conditions:

- The polarization above the interface $P_0=0$
- The polarization at the bottom of STO $P_{N+1}=0$



Sketch of a model $LaAlO_3/SrTiO_3$ interface

Theoretical Model

The effective Hamiltonian for the $SrTiO_3$ electrons

$$\hat{H}^{\text{eff}} = \hat{H}_0 + \hat{V}^{\text{SC}}[\sigma^f, \sigma^b]$$

Electronic Kinetic term

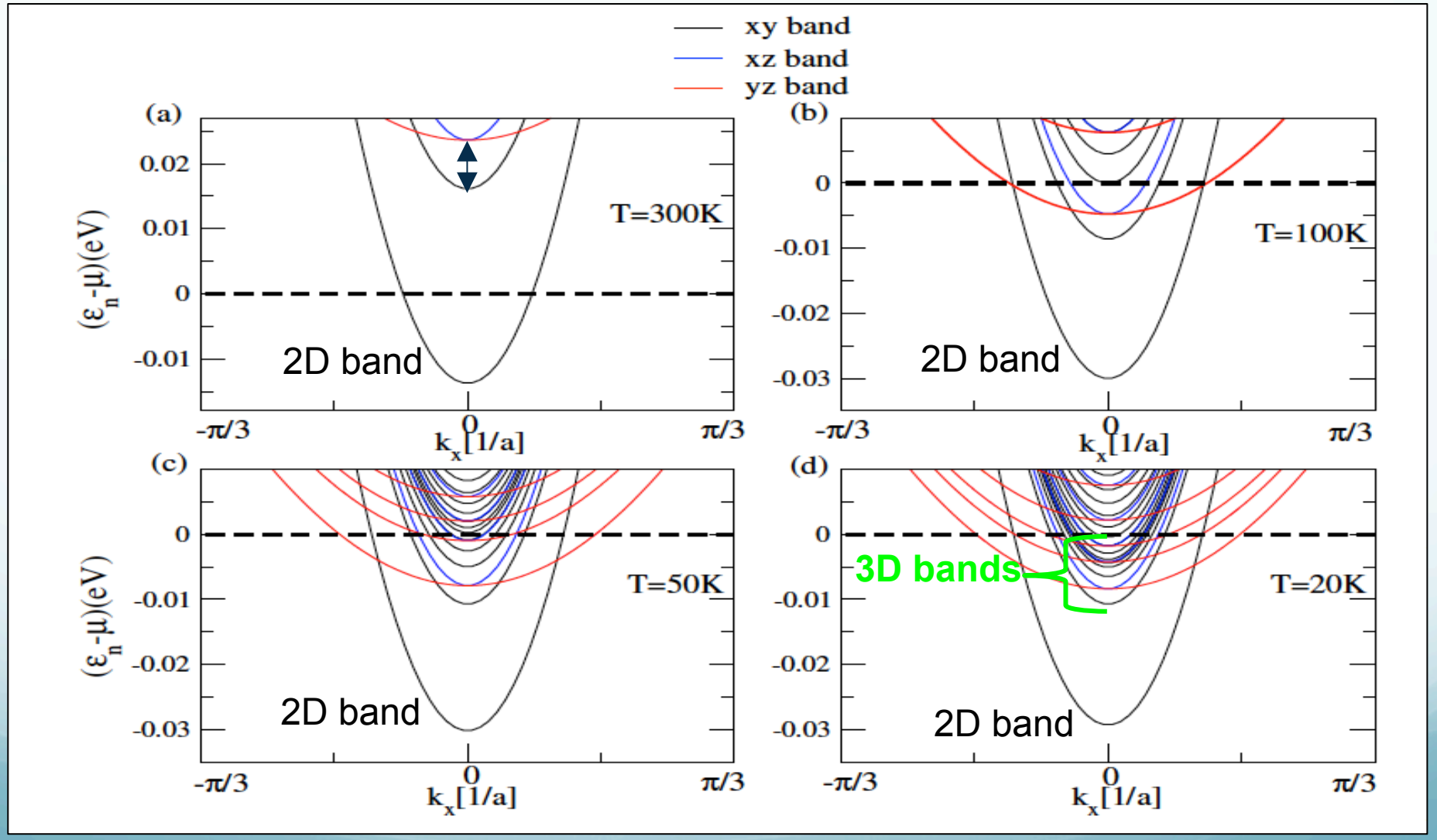
Coulomb Interaction term

- Employ Tight-binding Model for the hopping terms

- The interaction between the densities, σ^s ,σ^f ,σ^b
- It is temperature dependent term,
- Calculated self-consistently to find the 2DEG charge density σ^f and the polarization charge density σ^b

Results

The band structure changes with temperature



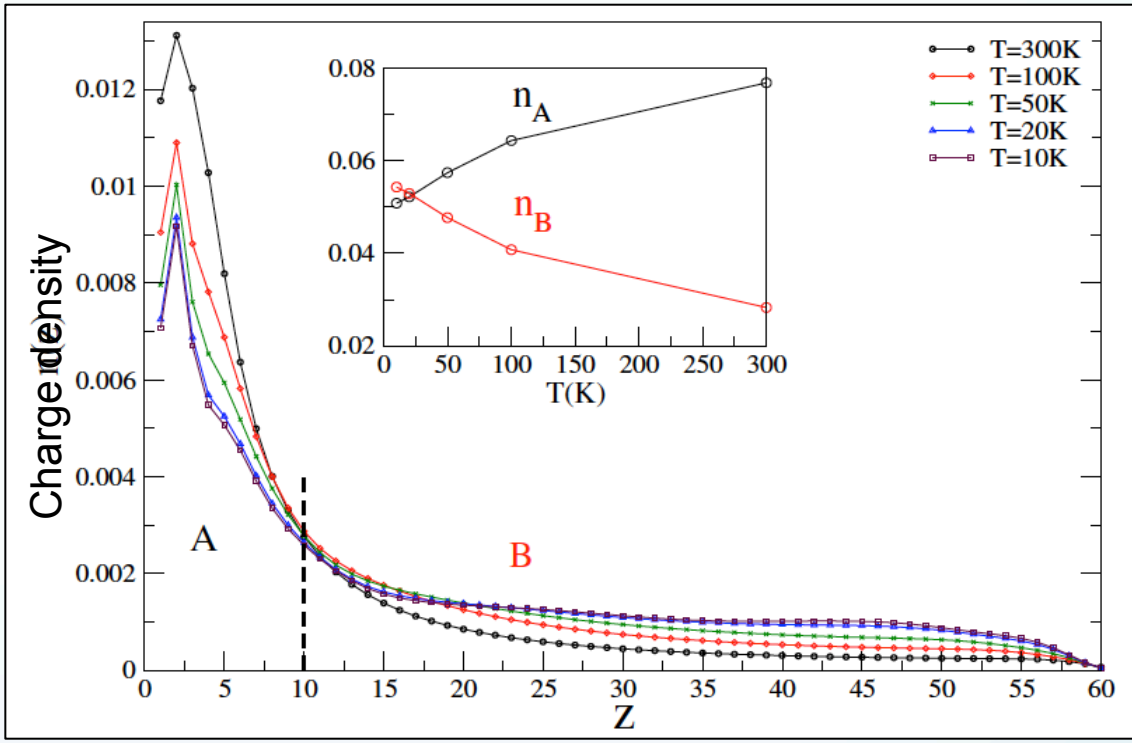
Self-consistence band structure for STO at several temperatures

Results

As the temperature is lowered, the electrons are less confined to the interface

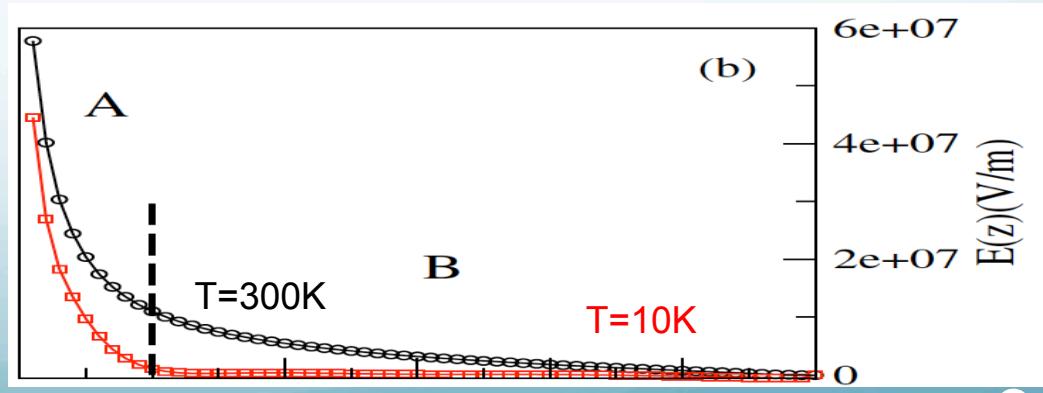
- Most of the electrons are confined to the interface within the first 10 layers (region A)

Strong electric field at the interface



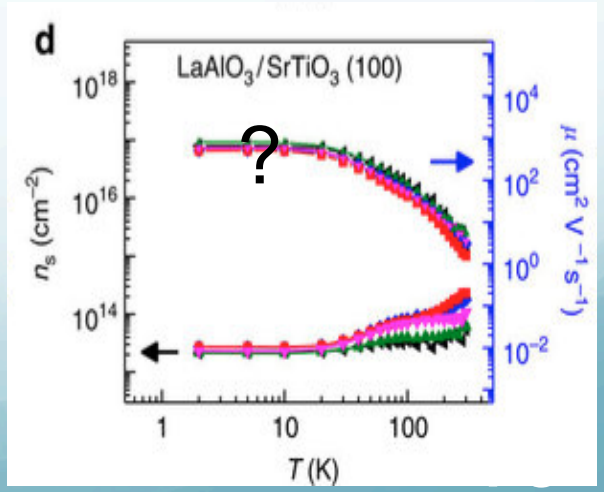
- There is always long tail of electrons(region B)

The electric field decays slowly into the STO bulk



Summery

- ➔ We introduced a simple model for studying the electronic structure of LAO/STO interface at different temperatures.
- ➔ The band structure does change with temperature.
- ➔ As the temperature is lowered, the character of the electron gases changes from 2D to a mixture of 2D and 3D.
- ➔ The electrons spreads into the bulk of STO at low temperature
- ➔ Our next step, use these results to understand one of the interface transport properties, such as the mobility



Thank You