

Possible flexoelectric origin of the Lifshitz transition in  
 $\text{LaAlO}_3/\text{SrTiO}_3$  interfaces

Amany Raslan and Bill Atkinson

PHYSICAL REVIEW B **98**, 195447 (2018)



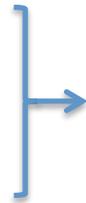
Shout out to: Patrick Lafleur, Kelsey Chapman



## SrTiO<sub>3</sub> Interfaces

Interface doping

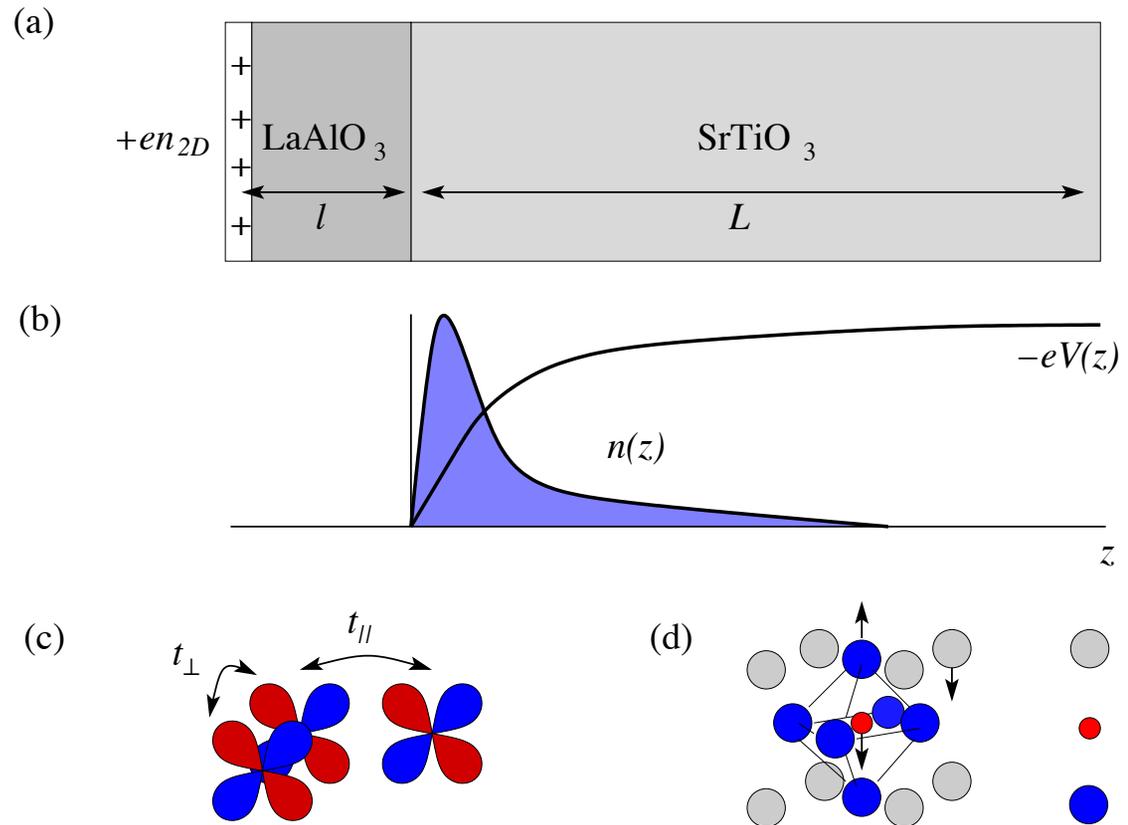
- polar catastrophe
- O-vacancies
- top gating



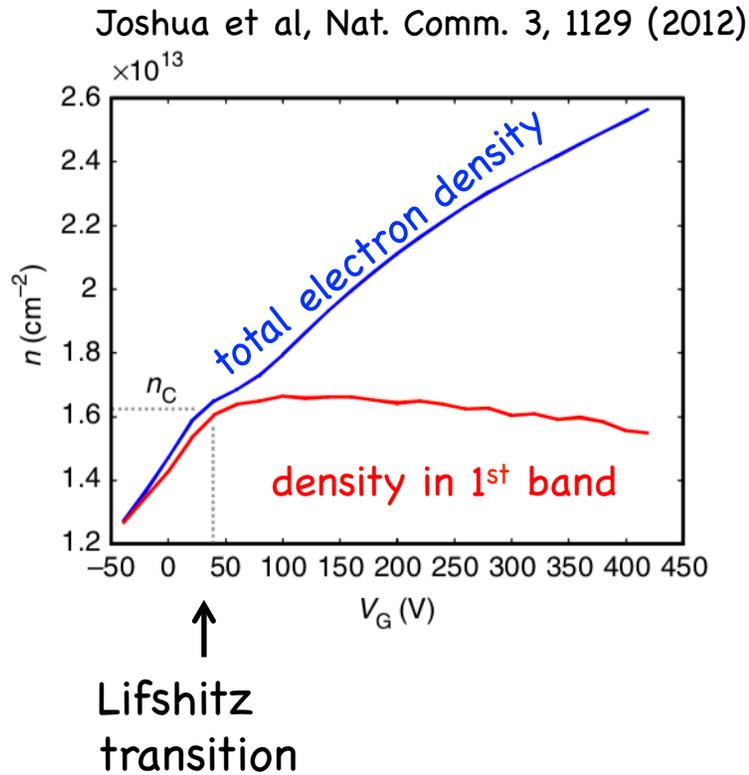
creates a confining potential

- quantum interface states
- semiclassical tails

2DEG occupies Ti  $t_{2g}$  orbitals  
( $d_{xy}$ ,  $d_{yz}$ ,  $d_{xz}$ )



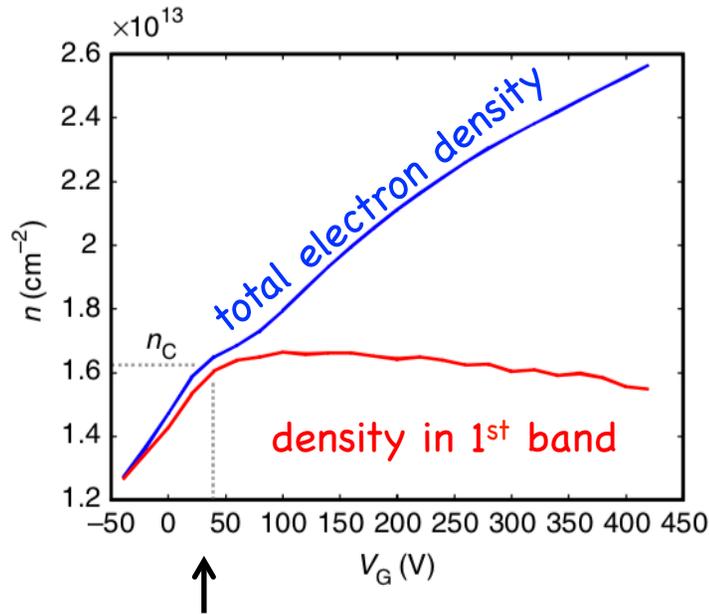
# Lifshitz Transition in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> Interfaces



See also:  
Smink et al, PRL **118**, 106401 (2017);  
PRB **97**, 245113 (2018)  
Wei Niu et al, Nano Lett. 2017, **17**, 6878–6885

# Lifshitz Transition in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> Interfaces

Joshua et al, Nat. Comm. 3, 1129 (2012)

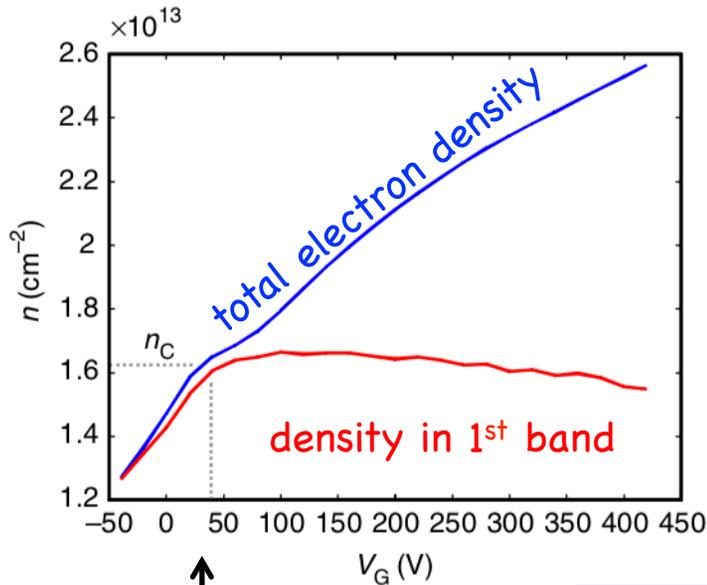


Key Question

- How does this transition happen?

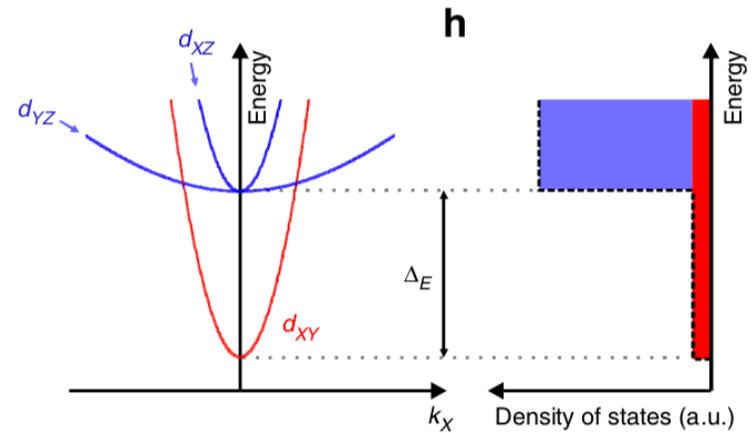
# Lifshitz Transition in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> Interfaces

Joshua et al, Nat. Comm. 3, 1129 (2012)



↑  
Lifshitz  
transition

Simple cartoon of what's happening



Does this cartoon match what you get from realistic calculations?

## Realistic calculations for an ideal interface

- tight-binding bands, fitted to experiments in bulk

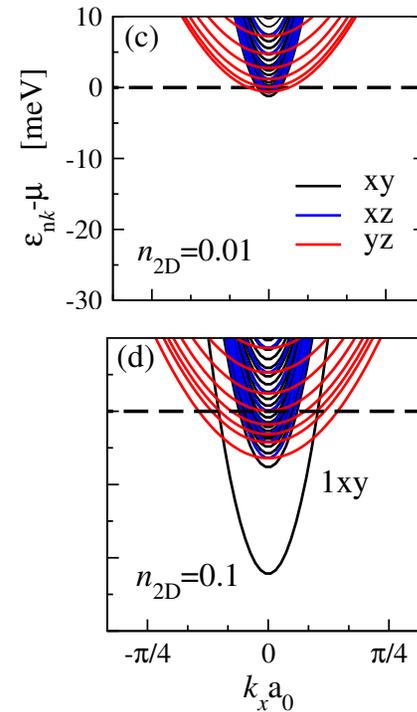
$$H_0 = - \sum_{\langle i,j \rangle, \alpha} t_{ij}^\alpha c_{i\alpha}^\dagger c_{j\alpha} - e \sum_{i\alpha} V_i n_{i\alpha}$$

- Landau-Ginzburg-Devonshire model for dielectric function, fitted to experiments in bulk

$$H_{lattice} = \frac{1}{2} \sum_{ij} D_{ij} P_i P_j + \frac{\gamma}{4} \sum_i P_i^4 - \sum_i E_i P_i$$

- solve self-consistent equations for potential, electron density, polarization in the interface geometry.

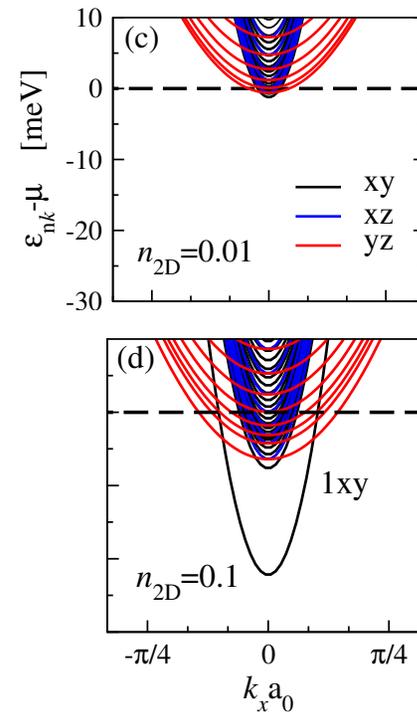
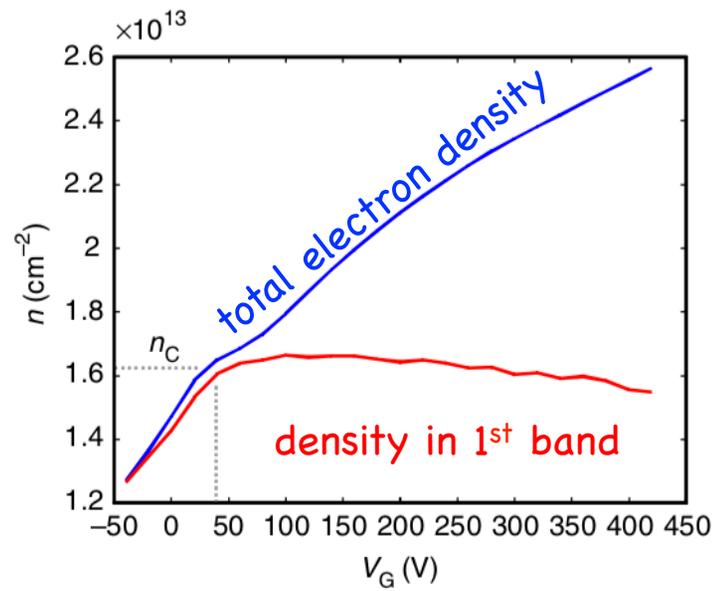
$$-\epsilon_\infty \frac{\partial^2 V}{\partial z^2} = -en(z) - \frac{\partial P}{\partial z} \quad (\text{Gauss' Law})$$



$$n_{2D} = 0.01$$

$$n_{2D} = 0.1$$

## Ideal Interface Model doesn't explain the transition



$$n_{2D} = 0.01$$

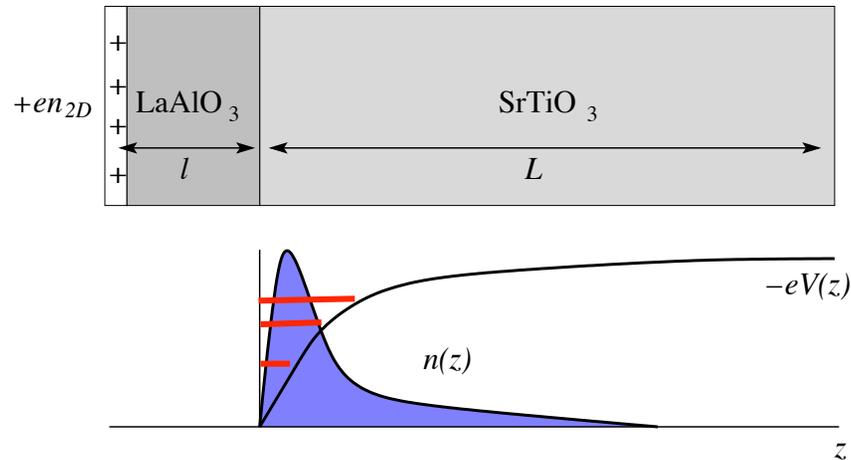
$$n_{2D} = 0.1$$

## Where does the 1xy state go?

Confining potential is proportional to  $n_{2D}$ .

At low  $n_{2D}$ , the electric field is strongly screened by  $\text{SrTiO}_3$ .

Electrons spread out into the semiclassical tails. Interface states disappear.



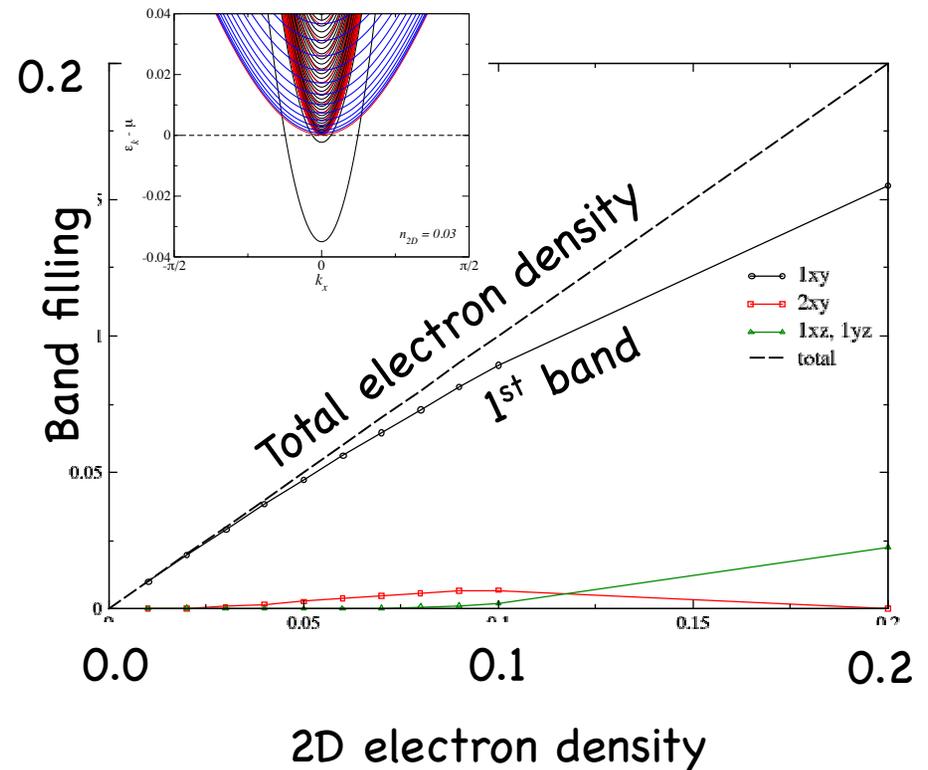
PHYSICAL REVIEW B **95**, 054107 (2017)  
PHYSICAL REVIEW B **95**, 054106 (2017)

## What is going on?

- Interface disrupts dielectric screening?

**Approach:** Reduce dielectric screening in the top few layers. Electric field at interface is weakly screened.

- ✓ Gives a single bound state at low charge density.
- ✧ No abrupt Lifshitz transition!

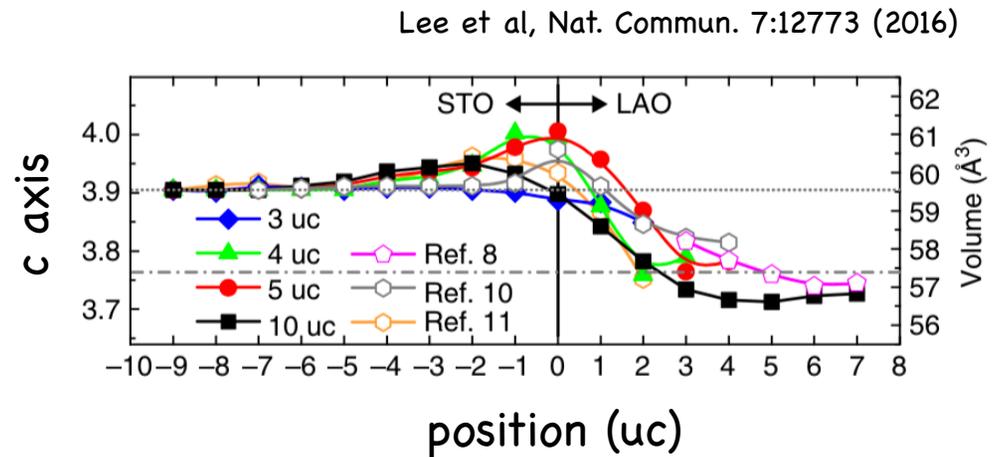


## Interfacial Strains

$$H_{lattice} = \frac{1}{2} \sum_{ij} \tilde{D}_{ij} P_i P_j + \frac{\gamma}{4} \sum_i P_i^4 - \sum_i \tilde{E}_i P_i$$

$$\tilde{E}_i = E_i + f_{11} \left. \frac{\partial \eta}{\partial z} \right|_i$$

$$\tilde{D}_{ij} = D_{ij} - 2g_{11} \delta_{i,j} \eta_i$$

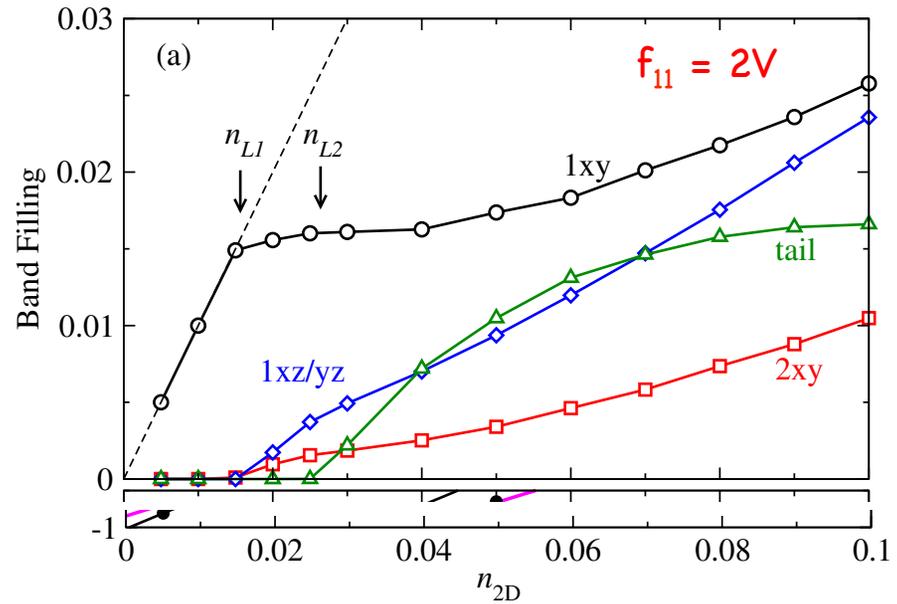


**electrostriction:** coupling between strain and (polarization)<sup>2</sup>

**flexoelectricity:** coupling between polarization and strain gradient

## Interfacial Strains

- If  $f_{11} > 0$  then the lattice strain creates a region of negative polarization near the interface.
- Switches direction when electric field exceeds threshold.



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## Caveat

- Mechanism requires  $f_{11} > 0$ .
  - **experiments** are hard!
    - Zubko, Catalan, & Tagantsev, Ann. Rev. Mater. Res. 43, 387 (2013)
  - **calculations** predict negative  $f_{11}$  in bulk STO
    - Stengel PRB 92, 205115 (2013)
    - Hong & Vanderbilt PRB 88, 045114 (2011)
  - **however** - surface contributions and screening from 2DEG should be large;  $f_{11}$  might be different at the SrTiO<sub>3</sub> interface than in bulk

## Why this is interesting:

- The new idea in this work is that lattice **strain gradients** may be used to manipulate 2DEGs.

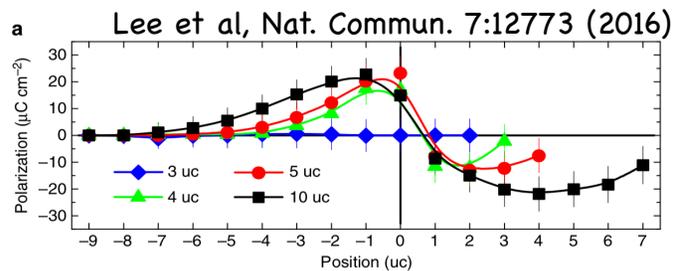
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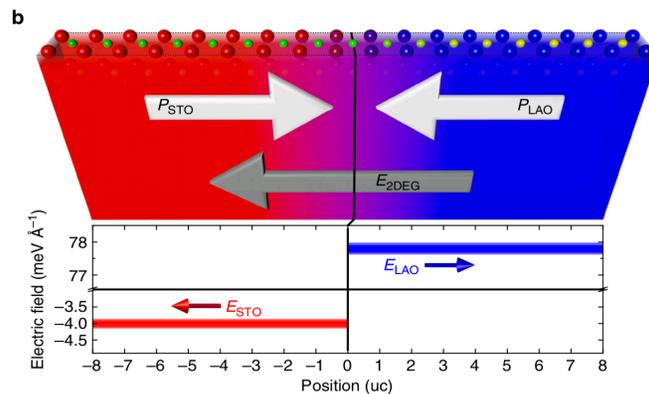
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## Polarization at an ungated interface

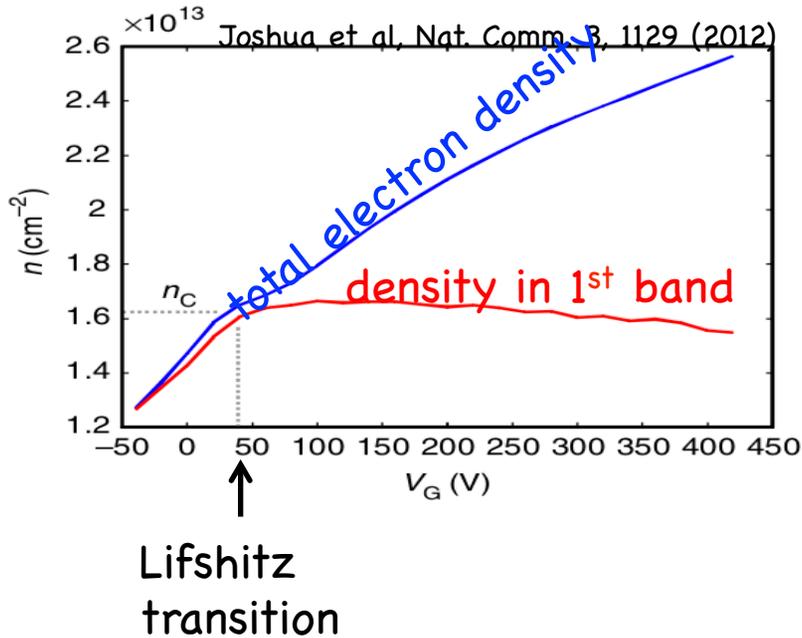


(STEM-HAADF)

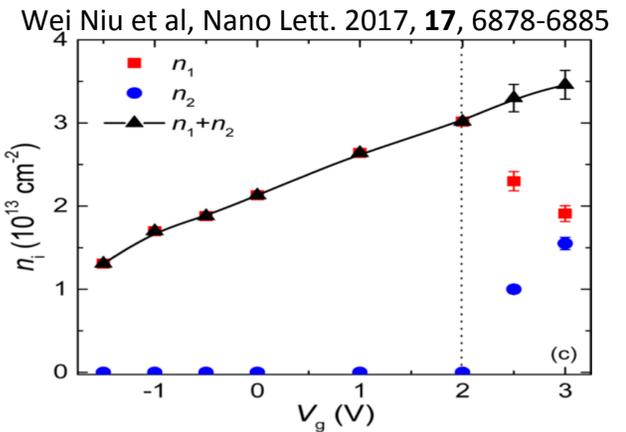
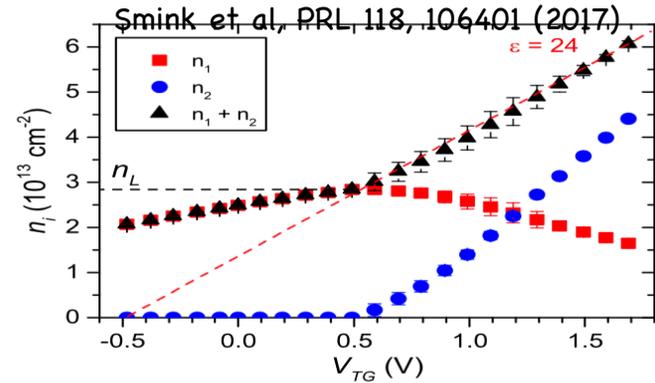


Key question: does the polarization reverse at the Lifshitz transition?

# Ideal interface not consistent with expts!



Why only a single occupied band at low  $n_{2D}$ ?  
 Why is the transition abrupt?



# SrTiO<sub>3</sub> is almost ferroelectric

## Dielectric Properties of SrTiO<sub>3</sub> at Low Temperatures

T. Sakudo and H. Unoki

*Electrotechnical Laboratory, Tanashi, Tokyo, Japan*

(Received 8 February 1971)

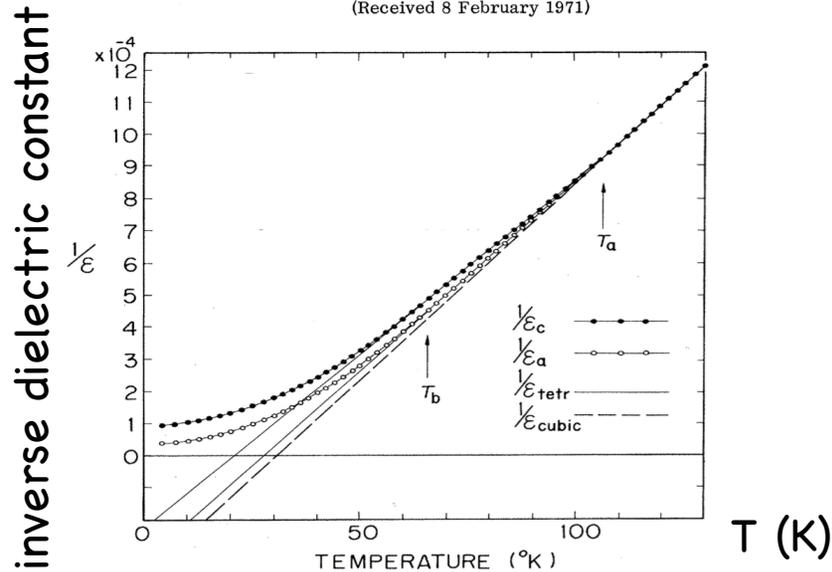


FIG. 3. Inverse dielectric constants as function of temperature. Between  $T_a$  and  $T_b$ , both  $\epsilon_a^{-1}$  and  $\epsilon_c^{-1}$  follow straight lines which are denoted as  $\epsilon_{\text{tetr}}^{-1}$ . Inset:  $(\epsilon_i^{-1} - \epsilon_{\text{tetr}}^{-1})^{1/2}$  versus temperature, open and solid circles corresponding to  $\epsilon_a$  and  $\epsilon_c$ , respectively.

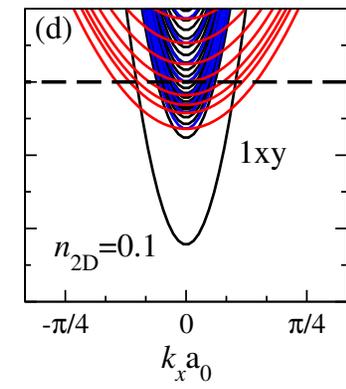
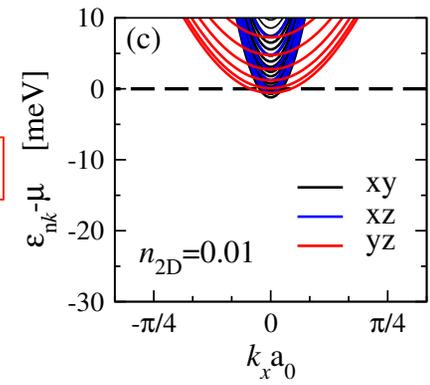
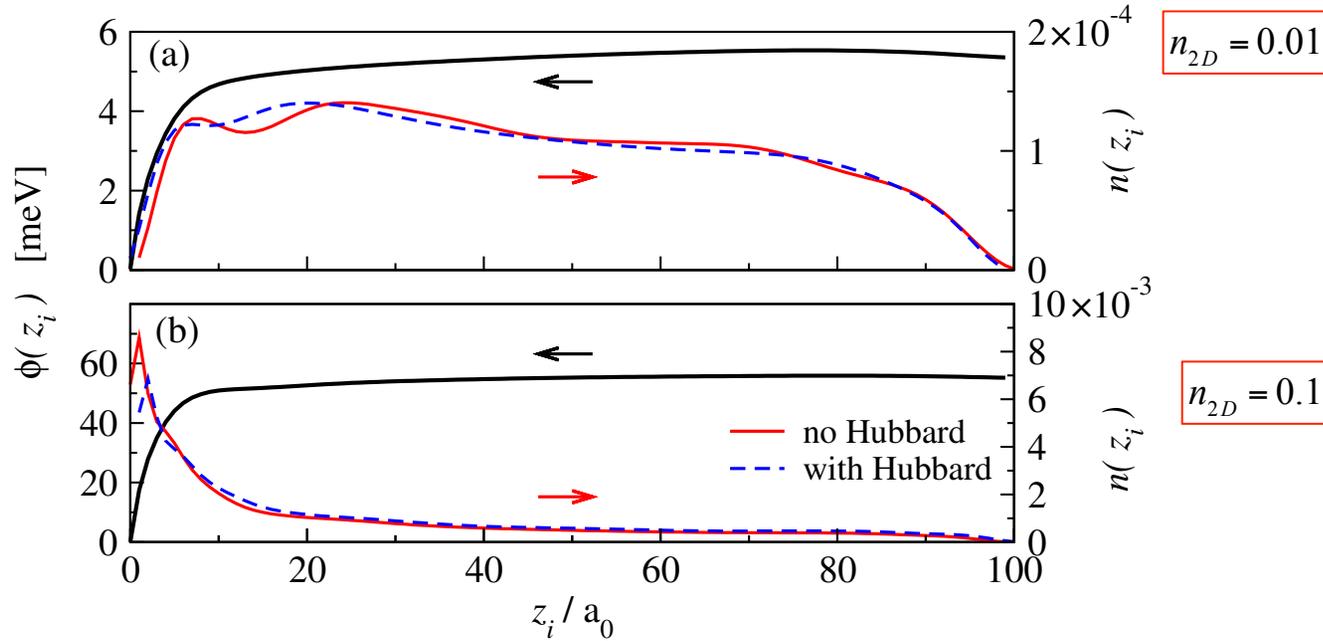
Polarization depends strongly on

- Temperature
- Electric field
- Wavevector

## Doping and the ideal interface

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 PHYSICAL REVIEW B **95**, 054106 (2017)

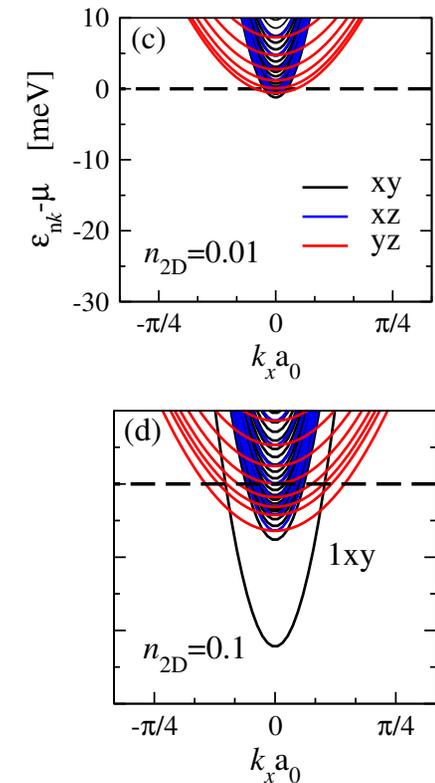
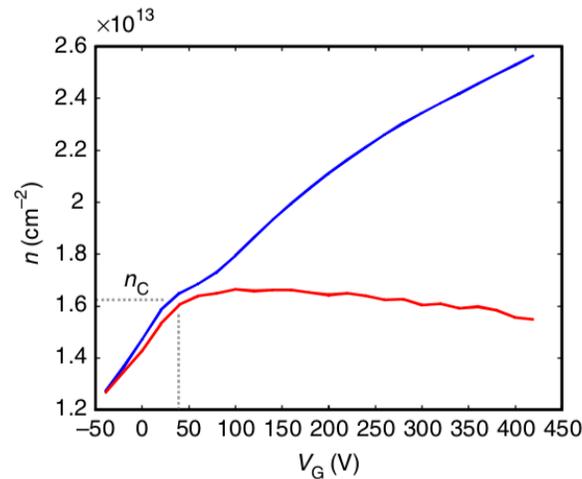
- ignore disorder
- dielectric function of surface is same as the bulk
- all model parameters obtained by fitting to experiments!



## Doping and the ideal interface

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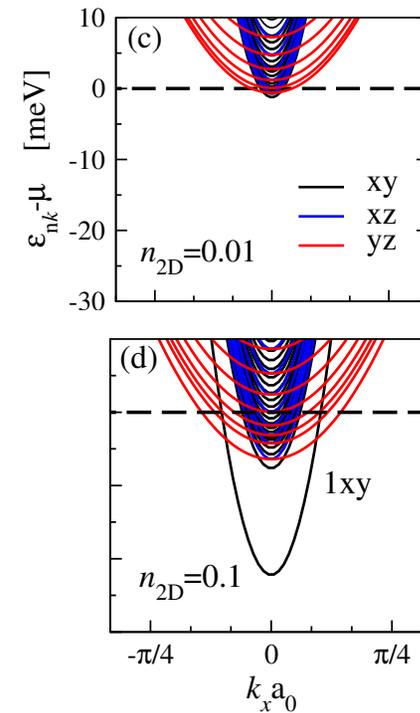
- ignore disorder
- dielectric function of surface is same as the bulk
- all model parameters obtained by fitting to experiments!
- Ideal interface model predicts deconfinement of 2DEG at low doping
- large number of occupied bands.
- No Lifshitz transition!



## According to the Ideal Interface Model ...

- Why only a single occupied band at low  $n_{2D}$ ? **Multiple bands are occupied.**
- Why is the transition abrupt? **There is no abrupt transition.**
- Why does the filling of the 1<sup>st</sup> band saturate? **It doesn't.**

Ideal interface model does not explain experiments.

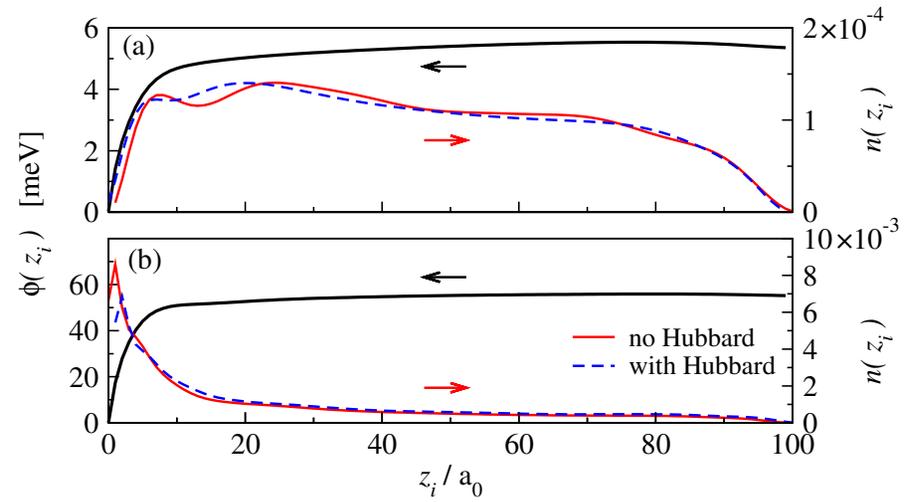


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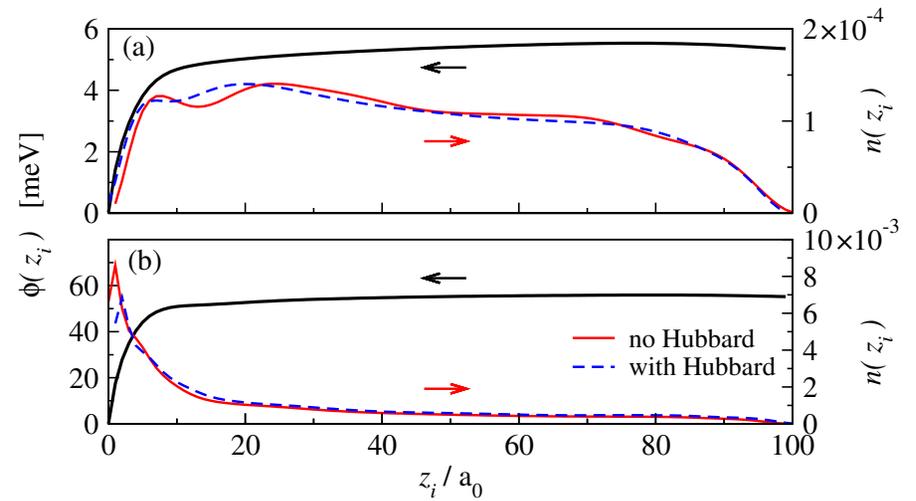
What is going on?

- Missing Hubbard interactions?



## What is going on?

- Missing Hubbard interactions?
  - too weak



## What might be going on?

### Gauss' Law:

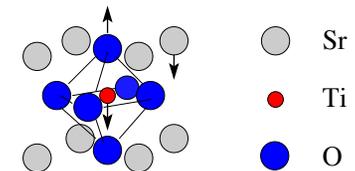
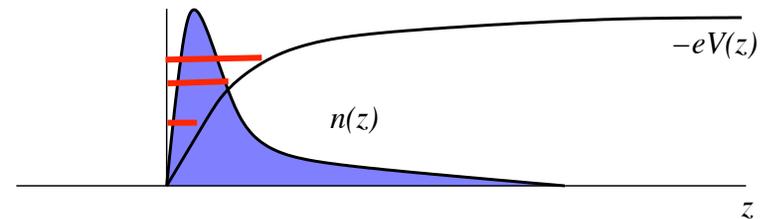
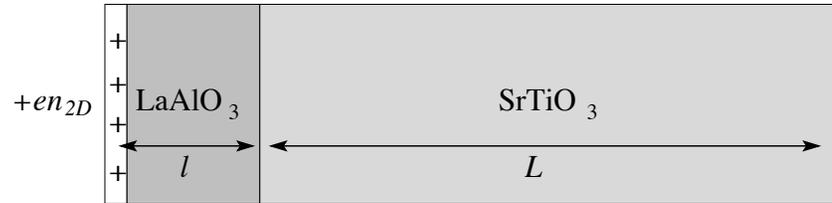
$$-\epsilon_{\infty} \frac{\partial^2 V}{\partial z^2} = -en(z) - \frac{\partial P}{\partial z}$$

### Schrodinger Equation:

$$H_0 = - \sum_{\langle i,j \rangle, \alpha} t_{ij}^{\alpha} c_{i\alpha}^{\dagger} c_{j\alpha} - e \sum_{i\alpha} V_i n_{i\alpha}$$

### Landau-Ginzburg-Devonshire model for dielectric:

$$H_{lattice} = \frac{1}{2} \sum_{ij} D_{ij} P_i P_j + \frac{\gamma}{4} \sum_i P_i^4 - \sum_i E_i P_i$$



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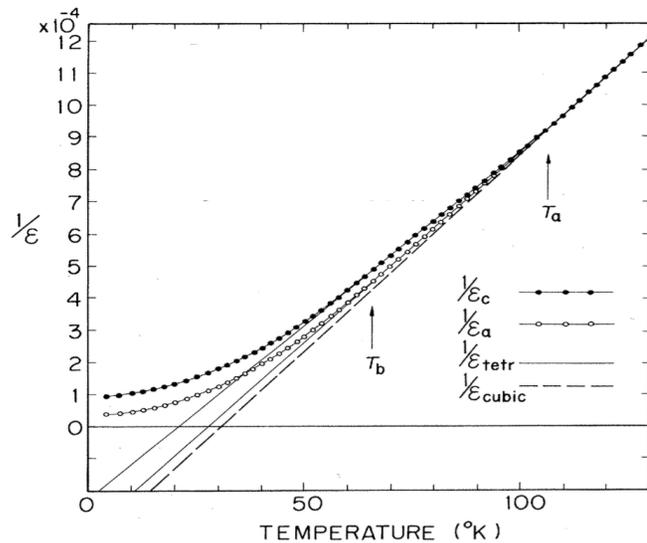
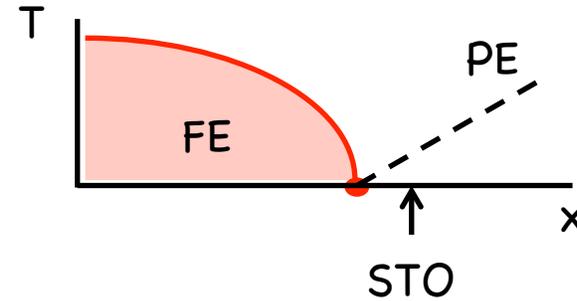


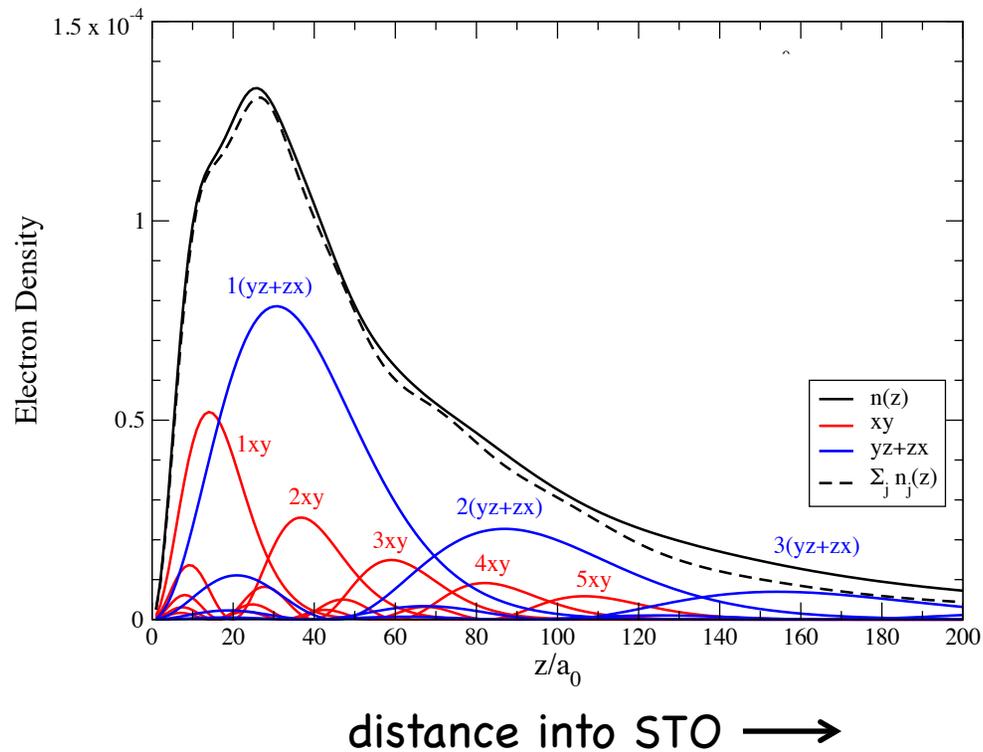
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Polarization depends strongly on

- Temperature
- Electric field
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## Structure of the 2DEG in the SrTiO<sub>3</sub> Substrate



### Key Points:

- multiple occupied sub-bands
- interface breaks degeneracy b/w  $d_{xy}$  and  $d_{yz,xz}$  orbitals
- interfacial states come mostly from 1xy, 2xy, 1xz, and 1yz states