Lattice screening of the polar catastrophe
in \( \text{KNbO}_3/\text{BaTiO}_3 \) interfaces

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Financial support

Computing time:

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**Introduction**

The interface between insulators may lead to metallic states.

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**Ohtomo et al., Nature 427, 423 (2004)**

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

**Polar catastrophe**

**Existence of a critical thickness**

$n(\text{LAO})=4$

What happens if one or both materials are ferroelectric?
Introduction
Materials other than LaAlO$_3$ may lead to the polar catastrophe


Polar catastrophe

If a LaAlO$_3$ is substituted by a ferroelectric ...

Will there be 2DEG formation?
What is the interaction of the 2DEG with ferroelectricity?
Introduction

How can ferroelectrics influence the polar catastrophe?

Conducting charge density
\[ \sigma = \frac{e}{2a^2} \approx 50 \, \mu\text{C/cm}^2 \]
\[ a \approx 4.0 \, \text{Å} \]

Ferroelectric distortion induces surface charges

Full compensation when \( \Delta P \approx 50 \, \mu\text{C/cm}^2 \)

Can we alter the conducting charge density manipulating polarization?
First principles calculations using LDA


Integer number of the polar material cell

Stoichiometric vacuum-terminated slabs
First principles calculations using LDA

Symmetric structures

KNO(n)/BTO(m+0.5)/KNO(n)

max(m)=4

max(n)=5

Applied electric field

Asymmetric structures

KNO(n)/BTO(m)/KNO(n)

max(n)=4

max(m)=8

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Both the symmetric and asymmetric interfaces remain **insulating for any calculated size** and applied external field.

**Maximum system size:**
- Symmetric: 5/4.5/5
- Asymmetric: 4/8/4

**Maximum external field:** 0.1 eV/Å

Why do these interfaces remain insulating for thicknesses larger than that of LaAlO$_3$/SrTiO$_3$?
Is there a critical size for polar catastrophe in KNO?

Polar material

KO NbO$_2$ KO NbO$_2$ BaO TiO$_2$ BaO
-1 +1 -1 +1 +0 +0 +0

$\sigma = -\frac{1}{2}$

Electric field

$\sigma = \frac{1}{2}$

Polarization quenches polar catastrophe

Polarization quenches polar catastrophe

Electric fields simply vary polarization

Strong polarization: modulus equal in all interfaces independently of their size or type

Is there a critical size for the polar catastrophe in KNO?

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Is there a critical size for polar catastrophe in KNO?

The internal macroscopic field inside KNbO₃ is the same independently of the interface or thickness.

Asymmetric

<table>
<thead>
<tr>
<th>Potential</th>
<th>Asymmetric 4/8/4</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.025 eV/Å</td>
<td>0.025 eV</td>
</tr>
</tbody>
</table>

Electric field in LAO/STO (Lee et al. PRB 78, 193104 2008) 0.24 eV/Å

Critical thickness (BaTiO₃/KNbO₃) ≈ 130 Å

Critical thickness (SrTiO₃/LaAlO₃) ≈ 15 Å

Symmetric

<table>
<thead>
<tr>
<th>Potential</th>
<th>Symmetric 3/4.5/3</th>
</tr>
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<tbody>
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<td>0.025 eV/Å</td>
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</table>

Model:

Ferroelectric materials accumulate energy more slowly quenching polar catastrophe

ΔE

σ = -½

σ = +½

σₙ = \_P

σₙ = -P

Polar material

If interface is insulating and no external field D=0

KO NbO₂ KO NbO₂

BaO TiO₂ BaO

-1 +1 -1 +1 +0 +0 +0

KNO BTO KNO

KNO BTO KNO

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**Model:**
Is there a critical size for polar catastrophe in KNO?

If interface is insulating and no external field $D=0$

Bulk values must be recovered at certain thickness $D \neq 0$

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$\sigma_e = -\frac{1}{2} + P_1(\text{bulk})$

$\sigma_e = \frac{1}{2} - P_1(\text{bulk})$

$\sigma = -\frac{1}{2}$

$\sigma = +\frac{1}{2}$

$\sigma_T = -\frac{1}{2} + P_1(\text{bulk})$

$\sigma_T = \frac{1}{2} - P_1(\text{bulk})$

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2DEG in ferroelectric materials displays lower density

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Common wisdom: epitaxial BaTiO$_3$ under compressive in-plane strain stabilizes the tetragonal phase, with enhancement of $P_s$

Asymmetric

Symmetric

Enhancement of the remnant polarization

Enhancement of the transition temperature


In-plane polarization even under in-plane compressive strain

Localized on TiO$_2$/KO interfaces not present in NbO$_2$/BaO ones

What is the origin of this polarization?

At the interface new electrostatic conditions arise

In TiO$_2$/KO favor in-plane distortions

In NbO$_2$/BaO hinder in-plane distortions

Barrier: 16 meV

High dielectric constant
Conclusions

Critical width for polar catastrophe one order of magnitude larger in ferroelectric materials than in non-ferroelectric ones

\[ n(\text{LAO}) = 4 \text{ VS } n(\text{KNO}) \approx 30 \]

2DEG conducting density lower in ferroelectrics than in non-ferroelectrics

Electrostatic effects in the interface can be used to favor/hinder in-plane ferroelectricity

Thank you for your attention!

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