

Article

Multi-Interface Oxide Semiconductor Engineering in LAO/STO/LTO Heterostructures: A Self-Consistent Schrödinger–Poisson Study of Quantum Confinement, Enhanced 2DEG Carrier Density, and Tunable Transport

Basma Elzein ^{1,*} , Enrico Traversa ² and Ali Elrashidi ^{1,3}

¹ Department of Electrical Engineering, University of Business and Technology, Jeddah 23435, Saudi Arabia; a.elrashidi@ubt.edu.sa

² Department of Chemical Science and Technologies, University of Rome Tor Vergata, 00133 Rome, Italy; traversa@uniroma2.it

³ Department of Engineering Physics, Alexandria University, Alexandria 21544, Egypt

* Correspondence: basma@ieee.org

Abstract

Two-dimensional electron gases (2DEGs) at complex oxide interfaces have emerged as a promising platform for next-generation oxide semiconductor devices, owing to their tunable electronic properties and rich interfacial phenomena. In this work, a $\text{LaAlO}_3/\text{SrTiO}_3/\text{LaTiO}_3$ (LAO/STO/LTO) trilayer heterostructure is proposed and theoretically investigated using a self-consistent Schrödinger–Poisson framework to examine the effects of multi-interface engineering on quantum confinement and carrier transport. The proposed architecture combines polar-discontinuity-driven electronic reconstruction at the LAO/STO interface with charge-transfer-induced electron accumulation at the STO/LTO interface, forming two coupled 2DEG channels within the SrTiO_3 layer. Compared with conventional single-interface oxide heterostructures, the coupled-interface configuration significantly enhances sheet carrier density and electrical conductivity, with predicted carrier densities approaching 10^{14} cm^{-2} and gate-tunable conductivities in the range of 10^3 – 10^4 S cm^{-1} under idealized operating conditions. The effects of layer thickness, gate bias, temperature, and electrostatic coupling are systematically investigated to establish practical design guidelines for optimizing carrier confinement and transport. A sensitivity analysis incorporating interface trap densities up to $2 \times 10^{13} \text{ cm}^{-2}$ demonstrates that more than 60% of the ideal carrier population is retained under moderate defect concentrations, confirming the robustness of the proposed multi-interface strategy. Although the analytical model represents an upper-bound framework, its predictions are discussed in the context of experimentally relevant limitations, including interface roughness, oxygen vacancies, carrier trapping, and defect-induced scattering. Overall, the proposed LAO/STO/LTO heterostructure provides a predictive framework for engineering high-density, electrically tunable oxide 2DEGs for future nanoelectronic, terahertz, photonic, and energy-related applications.

Keywords: 2DEG; LAO/STO/LTO interfaces; Schrödinger–Poisson modeling; analytical model; oxide heterostructures; electricity generation; polar discontinuity; quantum confinement; perovskite interfaces



Received: 8 June 2026

Revised: 8 July 2026

Accepted: 15 July 2026

Published: 17 July 2026

Copyright: © 2026 by the authors.

Licensee MDPI, Basel, Switzerland.

This article is an open access article distributed under the terms and conditions of the [Creative Commons Attribution \(CC BY\)](https://creativecommons.org/licenses/by/4.0/) license.

1. Introduction

Two-dimensional electron gases (2DEGs) formed at complex oxide interfaces have emerged as a versatile platform for next-generation nanoelectronic and energy-conversion technologies [1]. In contrast to conventional semiconductor-based 2DEGs, complex oxide systems such as $\text{LaAlO}_3/\text{SrTiO}_3$ exhibit rich interfacial physics governed by polar discontinuities, strong electronic correlations, and large dielectric responses. These effects enable the formation of high-density, quantum-confined electron systems with tunable transport properties and strong coupling to external electromagnetic fields [2]. Furthermore, oxide 2DEGs exhibit a range of emergent phenomena, including electronic reconstruction, metal–insulator transitions, superconductivity, and spin–orbit coupling, which significantly expand their functional capabilities for advanced electronic and optoelectronic devices [3,4].

A wide variety of material platforms have been explored for realizing 2DEGs, including III–V semiconductor heterostructures, wide-bandgap III-nitrides, oxide interfaces, and two-dimensional materials. Among these, III–V systems such as $\text{AlGaAs}/\text{GaAs}$ provide ultra-high electron mobility and have played a central role in the development of quantum transport physics. However, their relatively small bandgap and limited breakdown field restrict their suitability for high-power and multifunctional applications. Similarly, III-nitride heterostructures such as AlGaN/GaN enable high carrier densities through polarization-induced charge accumulation and support high-frequency and high-power device operation. Nevertheless, these systems lack the strong electronic correlations and large dielectric tunability that are intrinsic to oxide-based 2DEGs [5–8].

In contrast, oxide heterostructures provide a fundamentally different mechanism for 2DEG formation, driven by polar discontinuity, orbital reconstruction, and interfacial charge transfer [9–11]. The $\text{LaAlO}_3/\text{SrTiO}_3$ interface represents the prototypical oxide 2DEG system [12], where a high-mobility electron gas forms when the LaAlO_3 layer exceeds a critical thickness [13], as first demonstrated by Ohtomo and Hwang [14]. Subsequent studies have revealed that this system supports a variety of correlated electronic phases, including superconductivity and magnetism, as well as strong coupling to lattice and optical excitations. These characteristics, combined with the large dielectric response of SrTiO_3 , make oxide interfaces highly attractive for tunable electronic and photonic applications [15].

Despite these advances, conventional bilayer oxide heterostructures remain fundamentally limited by single-interface charge transfer mechanisms, which constrain carrier confinement and electrostatic tunability [16].

Recent progress in complex oxide electronics has increasingly emphasized multi-interface engineering as a powerful approach for enhancing carrier confinement, interfacial charge transfer, and emergent quantum functionalities beyond those attainable in conventional single-interface heterostructures. Advances in buried perovskite interfaces have demonstrated room-temperature electron mobilities exceeding $100 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ through precise control of interface quality and epitaxial coupling, highlighting the importance of deliberate interface design in oxide 2DEG systems [17]. Moreover, defect and stoichiometry engineering in LAO/STO heterostructures has been shown to significantly improve carrier mobility and quantum transport behavior, providing additional routes for optimizing interfacial electronic properties [18]. Recent reviews have further emphasized that heterogeneous integration and cooperative interactions among multiple functional oxide layers offer new degrees of freedom for controlling charge transfer, orbital reconstruction, and electrostatic tunability in next-generation electronic and photonic devices [19]. These developments strongly motivate the present investigation of the $\text{LAO}/\text{STO}/\text{LTO}$ trilayer architecture, where polar discontinuity and correlated electron transfer act simultaneously to achieve enhanced carrier confinement and tunable transport characteristics.

In this work, a trilayer $\text{LaAlO}_3/\text{SrTiO}_3/\text{LaTiO}_3$ heterostructure is proposed to exploit the cooperative interaction between multiple interfaces for enhanced electron accumulation and control. A self-consistent analytical framework based on coupled Schrödinger–Poisson equations is developed to capture quantum confinement, electrostatics, and interfacial charge redistribution within a unified model. The proposed approach incorporates the effects of structural parameters, gate bias, and temperature, enabling a comprehensive description of carrier distribution and transport behavior. By leveraging multi-interface coupling, this work establishes a predictive framework for designing oxide-based 2DEG systems with enhanced tunability and functionality for nanoelectronic and energy-conversion applications.

2. Proposed Structure, Energy Band Diagram and Analytical Model

The coupled Schrödinger–Poisson equations presented in this work were solved using an in-house computational framework developed in MATLAB R2024b (version 24.2). The numerical implementation employs a self-consistent iterative procedure based on finite-difference discretization along the growth direction of the LAO/STO/LTO heterostructure.

2.1. Physical Structure, Modeling Assumptions and Device Structure and Gate Configuration

The proposed structure consists of a trilayer oxide heterostructure formed by LaAlO_3 (LAO), SrTiO_3 (STO), and LaTiO_3 (LTO). The formation of a two-dimensional electron gas (2DEG) at the interfaces arises from the combined effects of polar discontinuity at the LAO/STO interface and charge transfer at the STO/LTO interface, leading to strong electron confinement within the STO layer. At the LAO/STO interface, the alternating charged planes in LAO generate an internal electric field that drives electronic reconstruction once a critical thickness is reached [14]. Meanwhile, at the STO/LTO interface, electron transfer from the Mott-insulating LTO into STO further enhances carrier accumulation and contributes to the formation of a high-density 2DEG [20].

The energy band diagram of the LAO/STO/LTO heterostructure provides a clear physical interpretation of this mechanism. LAO, characterized by a wide band gap, exhibits a relatively high conduction band minimum, whereas STO has a smaller band gap with its conduction band located at lower energy. LTO, as a Mott insulator, contributes occupied Ti 3d states near the Fermi level. Due to band alignment, interfacial polarization, and electrostatic potential buildup, significant band bending occurs within the STO layer. In particular, the conduction band of STO bends downward near the STO/LTO interface and can fall below the Fermi level, forming a quantum well that confines electrons in the out-of-plane direction while allowing free in-plane transport. This results in the accumulation of a high-density electron gas localized within a narrow region of the STO layer, giving rise to a high mobility 2DEG.

The proposed trilayer architecture is illustrated in Figure 1, which depicts the LAO/STO/LTO configuration and the spatial localization of the two-dimensional electron gas (2DEG) within the SrTiO_3 layer. Figure 2 provides a comprehensive representation of the physical system considered in this work. Figure 2a presents the self-consistent energy-band diagram along the growth direction, highlighting the effects of band offsets, interfacial polarization, electrostatic potential, and charge transfer in driving band bending and stabilizing the coupled electron gases formed at the LAO/STO and STO/LTO interfaces. Figure 2b illustrates the corresponding gated device structure, consisting of a polar LaAlO_3 (LAO) layer deposited on a SrTiO_3 (STO) quantum-well region, followed by an electron-donor LaTiO_3 (LTO) layer. A metallic top electrode applies to the external gate voltage, V_G , while the bottom electrode is maintained at ground potential. The LAO/STO interface generates the first two-dimensional electron gas through polar discontinuity, whereas the

STO/LTO interface contributes a second electron channel through charge transfer from the Mott-insulating LTO layer. The electrostatic coupling between these interfaces forms the basis for the enhanced carrier confinement, conductivity modulation, and gate-tunable transport properties investigated in the present study.

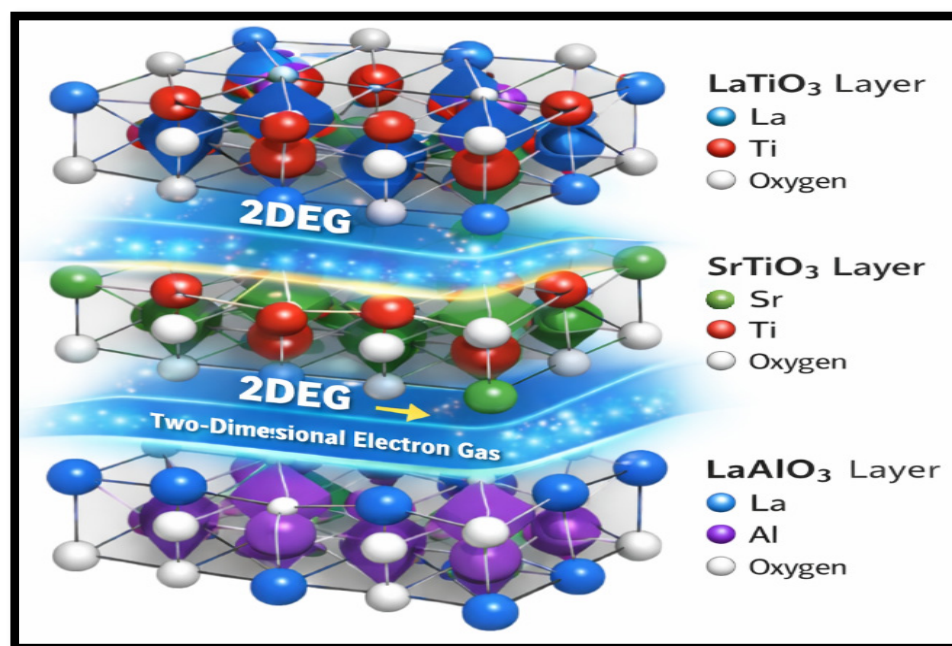


Figure 1. Proposed $\text{LaTiO}_3/\text{SrTiO}_3/\text{LaAlO}_3$ heterostructure showing the formation of dual 2DEG channels at the LTO/STO and STO/LAO interfaces. The atomic structure and elemental composition of each layer are illustrated.

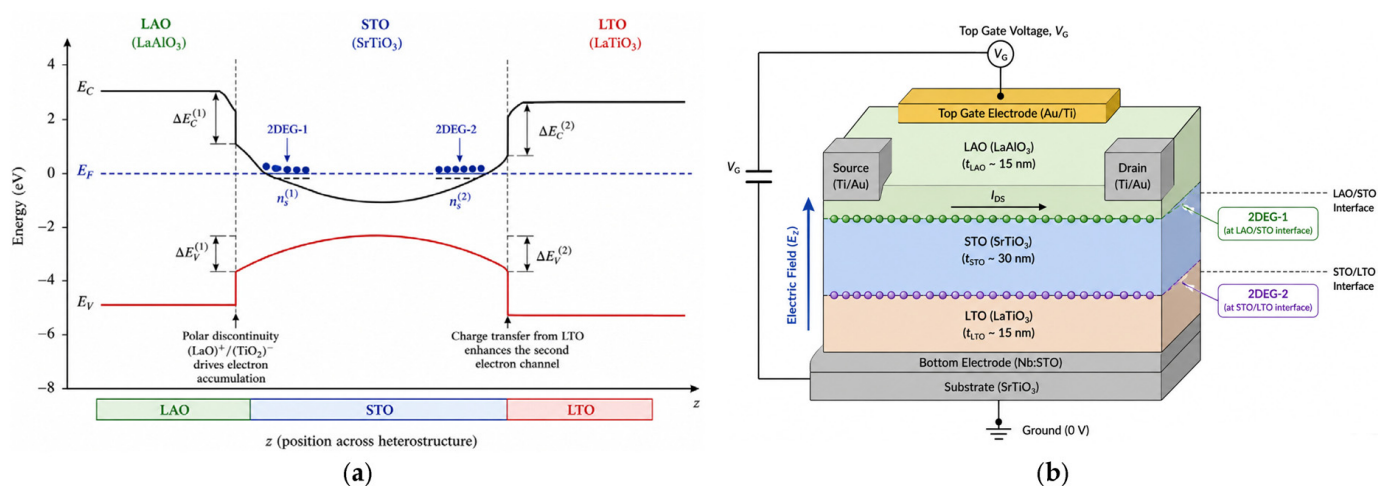


Figure 2. Gated LAO/STO/LTO trilayer heterostructure. (a) Energy-band diagram showing band bending, the Fermi-level reference, and the formation of two coupled 2DEGs within the STO layer due to polar discontinuity and LTO-induced charge transfer. (b) Device structure with a top-gate electrode, source/drain contacts, and coupled interfacial electron channels enabling gate-controlled transport and enhanced carrier confinement.

The analysis is performed under the following assumptions: electron motion is confined along the (z)-direction while remaining free in the in-plane directions; the 2DEGs are localized within the STO layer and described using the effective-mass approximation; a self-consistent electrostatic potential governs band bending and quantum confinement; and electron transport dominates, with hole contributions neglected throughout the analysis.

2.2. Analytical Model

The conduction band profile across the heterostructure is expressed as

$$E_c(z) = E_{c0}(z) - q\phi(z) \quad (1)$$

where $E_{c0}(z)$ represents the intrinsic conduction band edge including material-dependent band offsets, and $\phi(z)$ is the electrostatic potential.

The accumulation of interfacial charges induces band bending within the STO layer, resulting in the formation of a potential well that confines the electron gas. To accurately describe quantum confinement and electrostatic coupling, a self-consistent solution of the Schrödinger and Poisson equations is employed [21,22].

The electron states along the confinement direction are governed by

$$\left[-\frac{\hbar^2}{2} \frac{d}{dz} \left(\frac{1}{m^*} \frac{d}{dz} \right) + E_c(z) \right] \psi_i(z) = E_i \psi_i(z) \quad (2)$$

where m^* is the effective mass of electrons in STO, $\psi_i(z)$ is the wavefunction of the i -th subband, and E_i is the corresponding energy level.

The electrostatic potential is obtained from:

$$\frac{d}{dz} \left(\epsilon(z) \frac{d\phi(z)}{dz} \right) = -\rho(z) \quad (3)$$

where the charge density is defined as

$$\rho(z) = q[N_D^+(z) - n(z)] + \rho_{\text{int}} \quad (4)$$

Here, ρ_{int} represents the interface-induced charge density arising from polar discontinuity and charge transfer effects [14,23].

The coupled Schrödinger and Poisson equations are solved iteratively. An initial electrostatic potential is assumed, and the Schrödinger equation is solved to obtain the subband energies and wavefunctions. The resulting carrier density is then used in the Poisson equation to update the electrostatic potential. This procedure is repeated until convergence is achieved, ensuring consistency between quantum confinement and electrostatic interactions.

The spatial electron density is expressed as

$$n(z) = \sum_i n_i |\psi_i(z)|^2 \quad (5)$$

The sheet carrier density n_s , which is the primary quantity used in this work, is defined as

$$n_s = \int n(z) dz = \sum_i n_i \quad (6)$$

The subband population is determined using Fermi–Dirac statistics:

$$n_i = \frac{m^* k_B T}{\pi \hbar^2} \ln \left[1 + \exp \left(\frac{E_F - E_i}{k_B T} \right) \right] \quad (7)$$

Under strong confinement conditions, the lowest subband dominates ($n_s \approx n_1$). The electrical conductivity, σ , of the 2DEG is expressed as

$$\sigma = q n_s \mu \quad (8)$$

where the carrier mobility, μ , is given by

$$\mu = \frac{q\tau}{m^*} \quad (9)$$

Thus, the conductivity can be written as

$$\sigma = \frac{q^2 n_s \tau}{m^*} \quad (10)$$

The carrier mobility in oxide 2DEG systems is strongly influenced by several scattering mechanisms, including phonon scattering, charged impurity scattering, interface roughness scattering, oxygen-vacancy-related disorder, and structural defects at the heterointerfaces. In the present analytical framework, the relaxation time is treated as an effective parameter that captures the combined influence of these mechanisms. Therefore, the mobility values used in this study should not be interpreted as intrinsic bulk mobilities of LAO, STO, or LTO, but rather as effective 2DEG transport mobilities within the coupled interface region. The carrier mobility is influenced by multiple scattering mechanisms and is described using Matthiessen's rule:

$$\frac{1}{\mu_{\text{eff}}} = \frac{1}{\mu_{\text{ph}}} + \frac{1}{\mu_{\text{imp}}} + \frac{1}{\mu_{\text{IR}}} + \frac{1}{\mu_{\text{def}}} + \frac{1}{\mu_{\text{int}}} \quad (11)$$

where μ_{ph} is a phonon-limited mobility, μ_{imp} charged impurity scattering, μ_{IR} interface roughness scattering, μ_{def} defect/oxygen-vacancy-related scattering and μ_{int} interfacial disorder/cation intermixing contribution. Since the present work focuses on electrostatic confinement and carrier-density enhancement rather than microscopic scattering physics, these mechanisms are incorporated through an effective mobility/relaxation-time approximation. A fully field-dependent and interface-roughness-resolved mobility model is beyond the scope of the present analytical study and will be considered in future work.

Phonon scattering becomes dominant at elevated temperatures, leading to a reduction in mobility and consequently a decrease in conductivity, consistent with the observed trends in oxide-based 2DEG systems.

The application of an external gate voltage, V_g , modifies the electrostatic potential:

$$\phi(z) \rightarrow \phi(z) + V_g \quad (12)$$

This results in a shift in subband energies and an increase in carrier accumulation:

$$n_s(V_g) \propto \ln \left[1 + \exp \left(\frac{E_F + qV_g - E_1}{k_B T} \right) \right] \quad (13)$$

Therefore, increasing gate voltage enhances the sheet carrier density and improves conductivity, consistent with experimental observations.

The confinement of the electron gas is strongly dependent on the STO layer thickness t_{STO} . The ground-state energy level, E_1 , follows:

$$E_1 \propto \frac{\hbar^2}{2m^* t_{\text{STO}}^2} \quad (14)$$

An increase in thickness reduces quantum confinement, allowing greater carrier accumulation and resulting in enhanced conductivity, as demonstrated in the results section [24].

2.3. Simplified Analytical Expressions for Sheet Charge Density and Conductivity

The key parameter governing the performance of the 2DEG system is the sheet carrier density (n_s), which can be obtained from the self-consistent Schrödinger–Poisson formulation described previously. For practical analytical evaluation, n_s can be approximated using the ground subband population as follows [24]:

$$n_s = \frac{qm^*k_B T}{\pi \hbar^2} \ln \left(1 + \exp \left(\frac{E_F - E_1}{k_B T} \right) \right) \quad (15)$$

where $k_B T/q = V_T$ is the thermal voltage, E_F is the Fermi energy level, E_1 is the ground subband energy, and m^* is the effective electron mass.

For a completely ionized 2DEG layer, a simplified electrostatic approximation based on a parallel-plate capacitor model can be used to estimate the sheet charge density:

$$n_s = \frac{\epsilon_{\text{eff}}}{qt_{\text{eff}}} (V_g + V_{FB} - E_F) \quad (16)$$

where ϵ_{eff} and t_{eff} represent the effective permittivity and thickness of the heterostructure, V_g is the applied gate voltage, and V_{FB} is the flat-band voltage.

The model parameters used for the LAO, STO, and LTO layers are summarized in Table 1. The material parameters used in this study, including bandgap energy, Fermi level, and relative permittivity for LAO, STO, and LTO, are adopted from well-established experimental and theoretical studies on oxide heterostructures and their electronic properties [9,14].

Table 1. Model parameters for LAO, STO, and LTO layers.

Material	Bandgap E_g (eV)	Fermi Level E_F (eV)	Relative Permittivity ϵ_r
LTO	1.75	0.5	35
STO	3.2	1.6	300
LAO	5.6	3.2	24

The dielectric constants listed in Table 1 represent effective relative permittivity values adopted for the analytical simulation framework. They are not intended to reproduce the full static dielectric response of the bulk materials, particularly SrTiO_3 , whose permittivity is strongly temperature-, field-, strain-, and frequency-dependent. These values were selected to provide a simplified and computationally tractable approximation for comparing the relative electrostatic behavior of LAO, STO, and LTO within the coupled heterostructure model.

The carrier relaxation time τ is a key parameter in the Drude model, determined by carrier mobility and scattering mechanisms. In oxide-based 2DEG systems, τ is governed by electron–phonon interactions, defects, and interfacial effects. Reported studies on SrTiO_3 -based and correlated oxide interfaces indicate relaxation times in the range of 10^{-14} – 10^{-13} s [24], while optical and terahertz measurements further confirm Drude-like carrier dynamics in this regime [24]. In contrast, wide-bandgap oxides such as LaAlO_3 exhibit shorter relaxation times due to stronger scattering. Accordingly, the values used in this work $\tau_{\text{LTO}} \sim 10^{-14}$ s, $\tau_{\text{STO}} \sim 10^{-13}$ s, and $\tau_{\text{LAO}} \sim 10^{-15}$ s are consistent with reported transport behavior in oxide heterostructures [22].

3. Results and Analysis

It should be emphasized that the present simulations do not describe isolated bulk responses of LAO, STO, and LTO as independent materials. Rather, the Schrödinger–Poisson model is solved for the coupled LAO/STO/LTO heterostructure, and the reported quantities are interpreted in an interface-resolved manner. In this framework, the 2DEG forms exclusively on the STO side of the two heterointerfaces, namely LAO/STO and STO/LTO, where band bending, charge transfer, and electrostatic confinement collectively determine the carrier distribution. Accordingly, the calculated profiles represent interfacial contributions within the full stack, not standalone material-specific outputs.

3.1. Interface-Resolved Band Bending, Quantum Well Formation, and Carrier Localization

Figure 3 presents the conduction-band profile across the LAO/STO/LTO heterostructure obtained from the self-consistent Schrödinger–Poisson framework. Pronounced band bending occurs within the STO layer as a consequence of the combined effects of polar discontinuity at the LAO/STO interface and charge transfer from the Mott-insulating LTO layer, generating a built-in electrostatic field across the heterostructure. The resulting downward shift of the STO conduction band produces two asymmetric potential wells, with the deeper well located near the STO/LTO interface due to the additional electron injection provided by the partially filled Ti 3d states in LTO. This enhanced electrostatic coupling strengthens carrier confinement and promotes the formation of a high-density two-dimensional electron gas (2DEG).

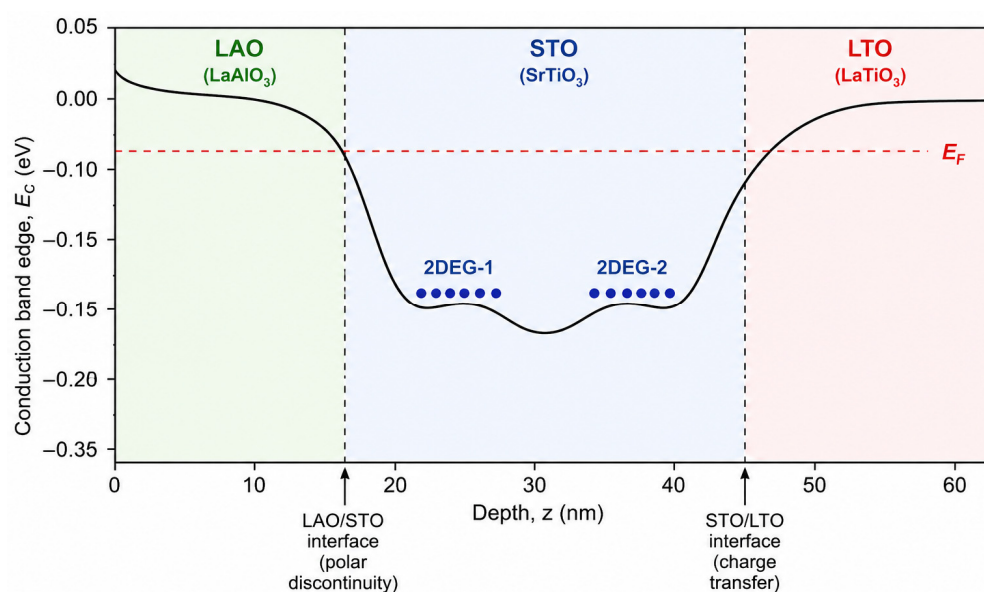


Figure 3. Conduction-band edge profile across the LAO/STO/LTO heterostructure showing the LAO/STO and STO/LTO interfaces, the Fermi-level reference (E_F), and the formation of two coupled 2DEGs within the STO layer due to polar discontinuity and LTO-induced charge transfer.

To further elucidate the interfacial origin of the electronic states, Figure 4 presents both the conduction-band edge profile (Figure 4a) and the corresponding carrier-density distribution (Figure 4b) across the complete heterostructure. Significant band bending is confined to the STO region, confirming that STO serves as the active layer hosting the electron gas. The potential well at the LAO/STO interface originates from the polar discontinuity associated with the alternating charged planes in LaAlO_3 , whereas the deeper well at the STO/LTO interface results from correlated charge transfer from LaTiO_3 . The coexistence of these mechanisms produces an asymmetric electrostatic landscape and demonstrates the cooperative coupling enabled by the trilayer architecture.

The carrier-density distribution in Figure 4b provides direct evidence of dual-interface electron accumulation. Two localized peaks are observed within the STO layer, corresponding to the LAO/STO and STO/LTO interfaces, respectively. The higher carrier concentration near the STO/LTO boundary indicates that charge transfer from LTO plays the dominant role in enhancing electron density, while the LAO/STO interface provides an additional transport channel. The rapid decay of carrier density away from the interfaces confirms that the 2DEG is an emergent interfacial phenomenon rather than a bulk property of the constituent materials. Consequently, the enhanced transport behavior of the proposed heterostructure originates from the cooperative interaction between the two coupled 2DEG channels.

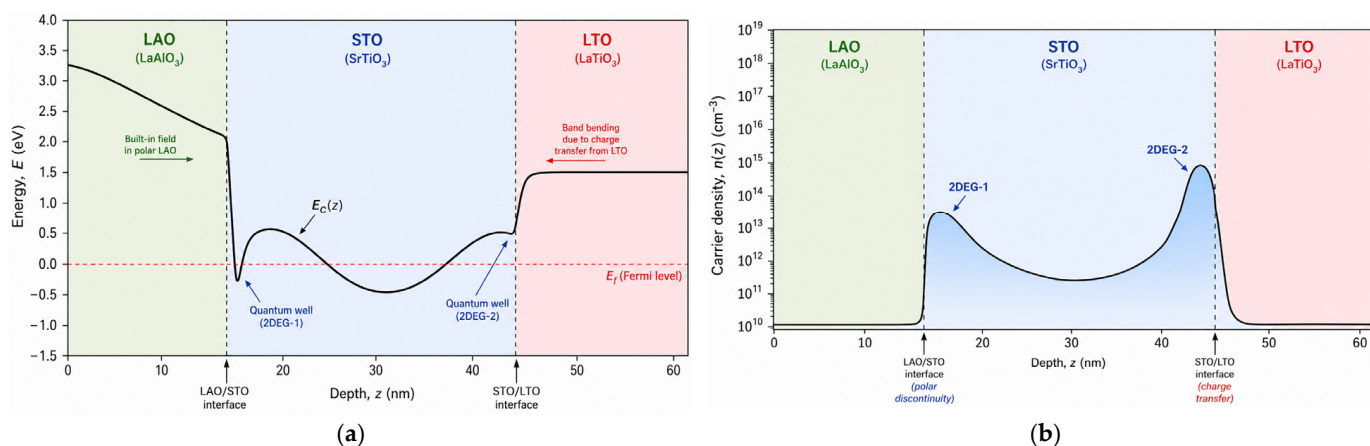


Figure 4. (a) Conduction-band edge profile showing band bending, the Fermi level, and the formation of two quantum wells (2DEG-1 and 2DEG-2) within the STO layer. The colored regions represent the LAO, STO, and LTO layers, while the dashed lines indicate the LAO/STO and STO/LTO interfaces. (b) Carrier-density profile showing two coupled 2DEGs within the STO layer. The dashed lines mark the interface boundaries, and the carrier-density peaks result from polar discontinuity and LTO-induced charge transfer.

3.2. Quantum Confinement, Wavefunction Localization, and Carrier Density Distribution

The calculated ground-state wavefunctions provide direct evidence of quantum confinement within the STO layer. As shown in Figure 5, the electron probability density, $|\psi_1(z)|^2$, is strongly localized near the heterointerfaces, with the degree of localization governed by the depth and asymmetry of the electrostatic potential wells established in the preceding section. The LTO-containing structure exhibits the strongest confinement, characterized by a rapid decay of the wavefunction away from the STO/LTO interface. This behavior is consistent with the formation of a triangular quantum well, where the internal electric field enhances electron localization and increases the occupation of low-energy subbands.

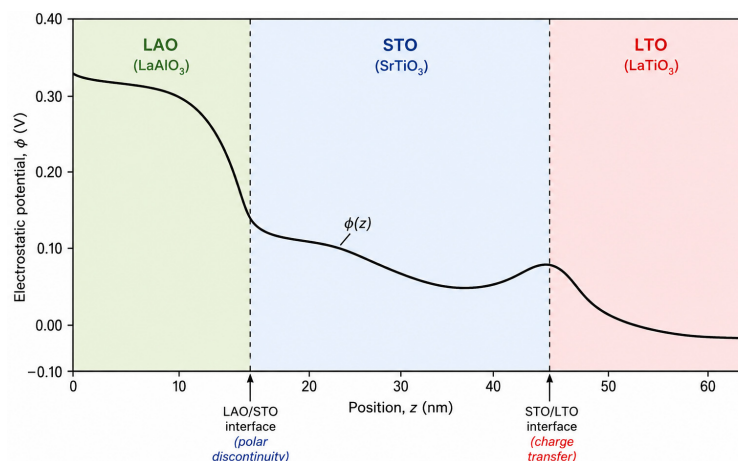


Figure 5. Electrostatic potential distribution across the LAO/STO/LTO heterostructure showing the influence of polar discontinuity at the LAO/STO interface and charge transfer at the STO/LTO interface on the self-consistent potential landscape and electron confinement within the STO layer.

The stronger confinement observed in the trilayer architecture directly contributes to improved electronic performance by increasing the effective sheet carrier density while preserving high in-plane mobility. The localization of the electronic states within a narrow region of the STO layer confirms the validity of the effective-mass approximation adopted in the analytical model and supports the self-consistent Schrödinger–Poisson description of the coupled interfaces.

The corresponding carrier-density distribution is presented in Figure 6. The spatial electron density exhibits pronounced localization within a few nanometers of the interfaces, with the highest concentration occurring near the STO/LTO boundary. This enhanced accumulation results from the cooperative interaction between the electron transfer supplied by the Mott-insulating LTO layer and the secondary carrier channel generated at the LAO/STO interface. Consequently, the trilayer configuration supports substantially higher carrier densities than conventional single-interface oxide heterostructures.

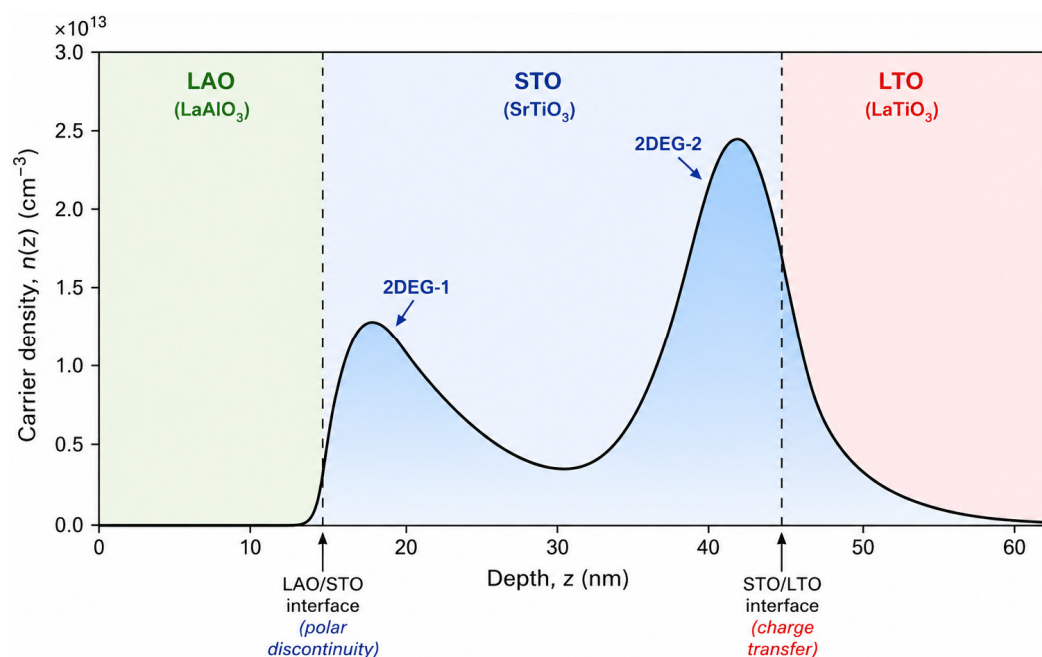


Figure 6. Carrier density profile across the LAO/STO/LTO heterostructure showing the formation of coupled 2DEGs at the LAO/STO and STO/LTO interfaces. Vertical dashed lines indicate the interface boundaries, while the enhanced electron accumulation within the STO region reflects the combined effects of polar discontinuity and LTO-induced charge transfer.

A strong correspondence between the wavefunction localization in Figure 5 and the carrier-density profile in Figure 6 is observed, demonstrating that the spatial distribution of electrons is governed primarily by quantum confinement within the STO layer. The rapid decay of carrier density away from the interfaces further confirms that the electron gas remains an interfacial phenomenon rather than a bulk property of the constituent oxides. These results validate the self-consistent analytical framework and establish the coupled LAO/STO/LTO architecture as an effective strategy for enhancing carrier confinement and transport tunability through multi-interface engineering.

3.3. Thickness Dependence of Sheet Carrier Density

As illustrated in Figure 7, the variation in sheet carrier density n_s with layer thickness reveals a strong dependence on quantum confinement. As the thickness increases, the electric field across the STO layer weakens, leading to a broader potential well and reduced carrier localization.

Consequently, n_s decreases monotonically with increasing thickness for all material configurations. This behavior reflects the inverse relationship between confinement strength and spatial extension of the electron gas.

Among the three cases, the LTO-based structure consistently maintains the highest n_s , as clearly shown in Figure 7, demonstrating its superior ability to sustain high carrier densities even at larger thicknesses.

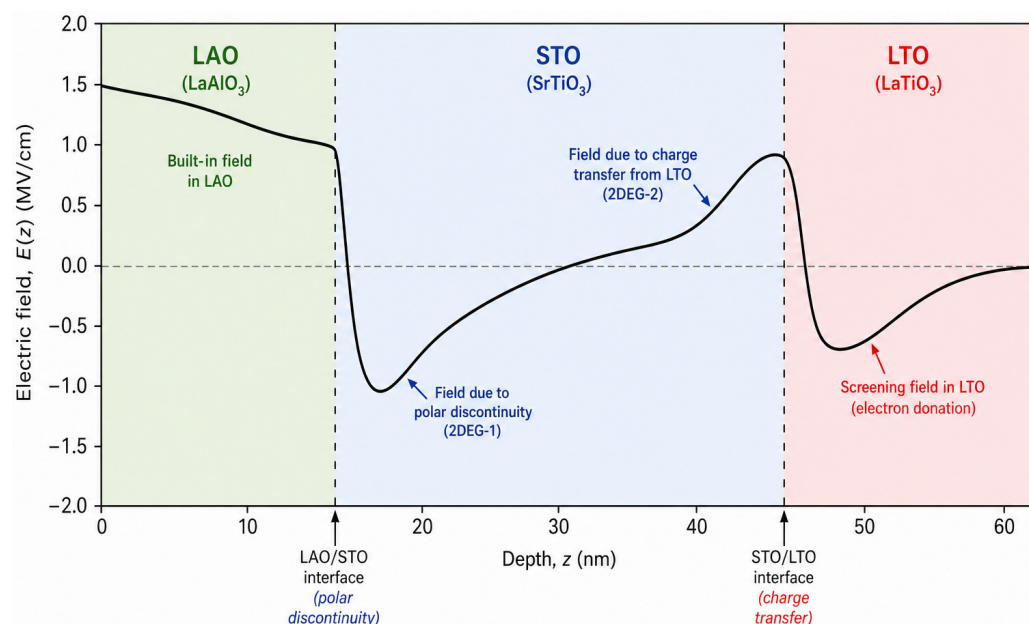


Figure 7. Electric field profile across the LAO/STO/LTO heterostructure showing the effects of intrinsic LAO polarity, polar discontinuity at the LAO/STO interface, and LTO-induced charge transfer at the STO/LTO interface. Vertical dashed lines indicate the interface boundaries, while the coupled electrostatic response within the STO layer promotes the formation of dual interfacial 2DEGs.

3.4. Electrostatic Tunability via Gate Voltage

Figure 8a–c illustrate the dependence of n_s on gate voltage V_g , highlighting the strong electrostatic tunability of the 2DEG. For all thicknesses, the sheet carrier density increases monotonically with increasing V_g , indicating effective modulation of the quantum well depth.

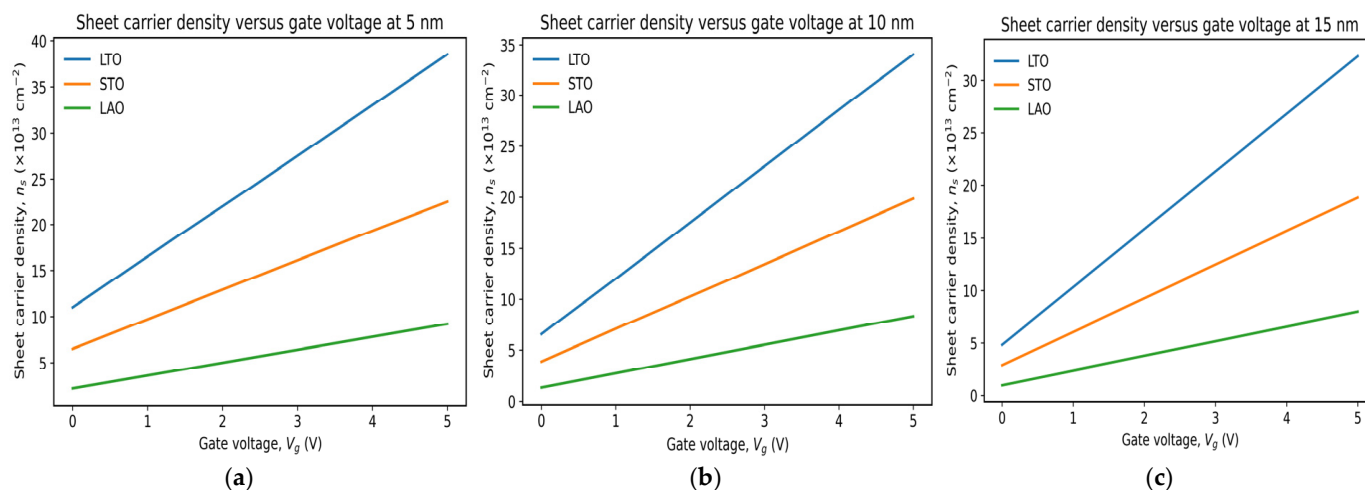


Figure 8. (a–c) Variation in sheet carrier density n_s as a function of gate voltage V_g for different layer thicknesses ((a) 5 nm, (b) 10 nm, and (c) 15 nm).

A positive gate voltage enhances the internal electric field, which lowers the conduction band and increases subband occupancy. This results in a higher carrier concentration at the interface, as clearly observed in Figure 8a–c.

The effect is more pronounced in thinner layers (Figure 8a), where the electric field is more effectively confined, leading to stronger modulation of the carrier density. In thicker layers (Figure 8b,c), although the tunability is preserved, the absolute values of n_s are lower due to reduced confinement. The maximum sheet carrier densities of LTO,

STO, and LAO at $V_g = 5$ V, are calculated $7.02 \times 10^{14} \text{ cm}^{-2}$ at 5 nm to $6.23 \times 10^{14} \text{ cm}^{-2}$ at 10 nm and $5.95 \times 10^{14} \text{ cm}^{-2}$ at 15 nm, confirming that reduced thickness enhances carrier accumulation due to stronger quantum confinement and electrostatic coupling.

It should be noted that the calculated sheet carrier density represents an idealized theoretical upper-bound obtained under the assumptions of defect-free interfaces, complete electrostatic confinement, and efficient charge transfer across the coupled LAO/STO and STO/LTO interfaces. Experimentally reported oxide 2DEG densities are commonly lower due to oxygen vacancies, interface roughness, cation intermixing, disorder, finite trap density, and scattering-related carrier localization. Therefore, the values reported here should be interpreted as predictive design limits rather than direct experimental expectations.

As shown in Figure 9, the total sheet carrier density decreases systematically with increasing thickness, dropping from $7.02 \times 10^{14} \text{ cm}^{-2}$ at 5 nm to $5.95 \times 10^{14} \text{ cm}^{-2}$ at 15 nm. This reduction in carrier density directly impacts the electrical conductivity, as described by $\sigma \propto n_s$. Consequently, the highest conductivity observed in Figure 9 for the 5 nm structure can be attributed to the enhanced carrier accumulation resulting from stronger quantum confinement and interfacial electrostatic coupling. In contrast, thicker structures exhibit reduced conductivity due to the spatial spreading of the electron gas and weakened electric field effects.

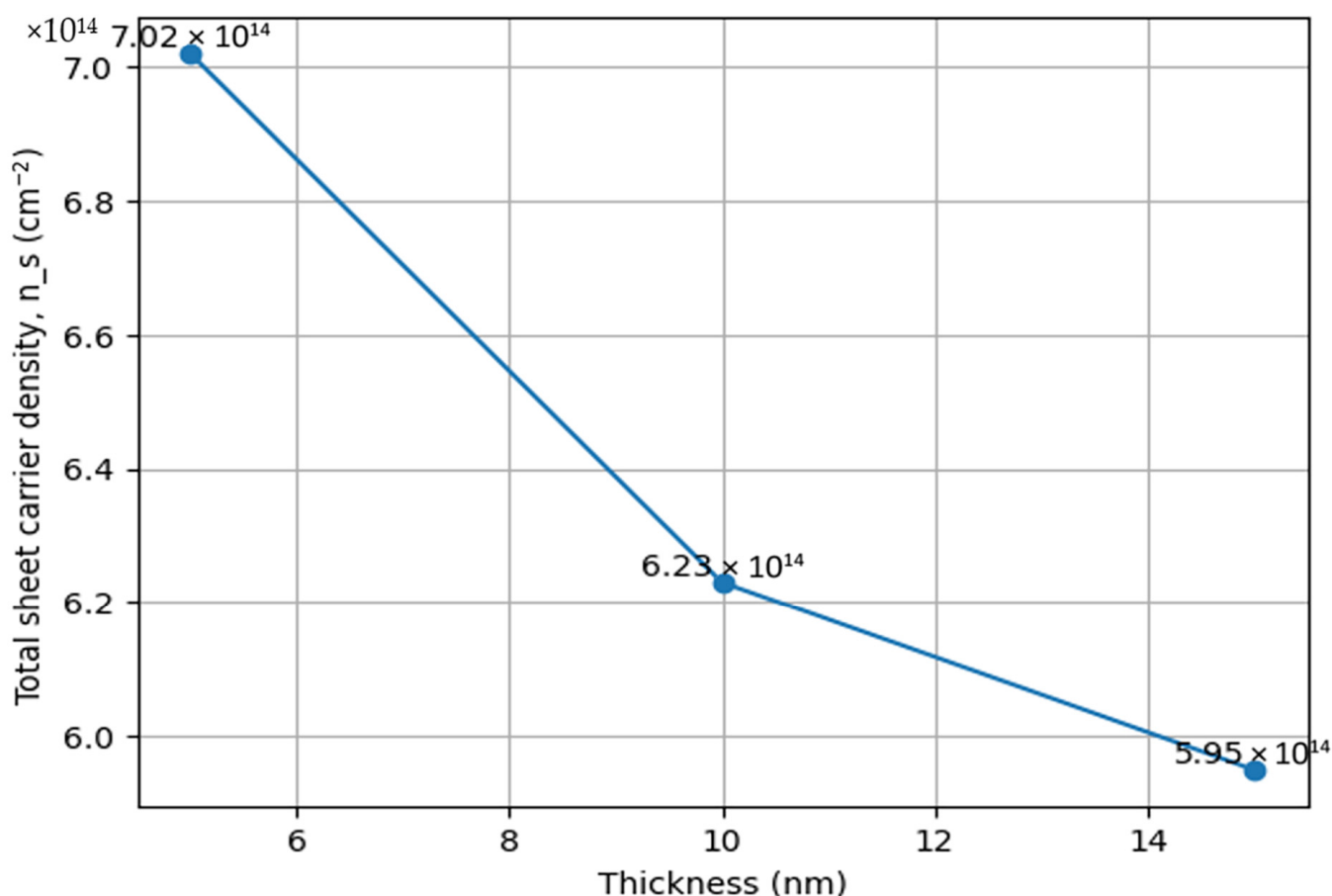


Figure 9. Total sheet carrier density of the LAO/STO/LTO heterostructure as a function of thickness at $V_g = 5$ V, obtained from the combined contributions of the LAO/STO and STO/LTO interfacial electron channels.

3.5. Electrical Conductivity and Transport Behavior

As shown in Figure 10, the electrical conductivity σ exhibits a strong dependence on gate voltage, following trends similar to the sheet carrier density. This confirms that transport in the 2DEG is primarily governed by carrier concentration.

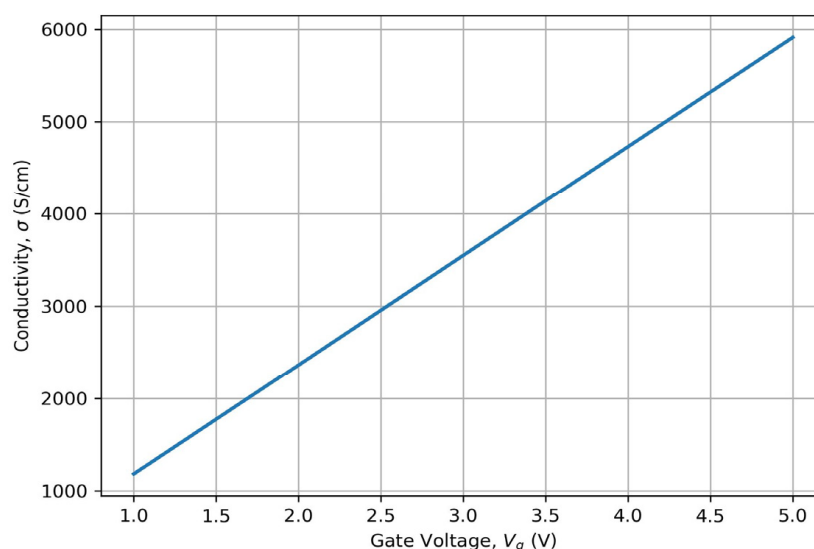


Figure 10. Dependence of electrical conductivity on gate voltage in the LAO/STO/LTO heterostructure. The solid line represents a linear fit to the analytical results, yielding $R^2 = 0.9987$, which indicates an excellent linear correlation within the investigated bias range.

The total conductivity increases nearly linearly with gate voltage due to the corresponding rise in the summed sheet carrier density. As shown in Figure 10, the conductivity increases from approximately 1.2×10^3 S/cm at $V_g = 1$ V to about 5.9×10^3 S/cm at $V_g = 5$ V. This behavior follows the direct proportionality $\sigma_{\text{total}} \propto n_s$, where increasing gate bias enhances charge accumulation at the interface, leading to improved charge transport. The maximum conductivity at $V_g = 5$ V corresponds to the highest total carrier density, confirming that electrostatic modulation plays a dominant role in controlling the electrical performance of the trilayer heterostructure. In contrast, the carrier mobility remains within the range of approximately 50–180 $\text{cm}^2/\text{V}\cdot\text{s}$ and exhibits weak dependence on gate voltage, reflecting its primary dependence on intrinsic material properties such as relaxation time and effective mass rather than carrier density.

3.6. Temperature-Dependent Transport Properties

As illustrated in Figure 11a,b, the temperature dependence of mobility and conductivity provides insight into the dominant scattering mechanisms. The mobility decreases with increasing temperature due to enhanced phonon scattering, which reduces carrier relaxation time.

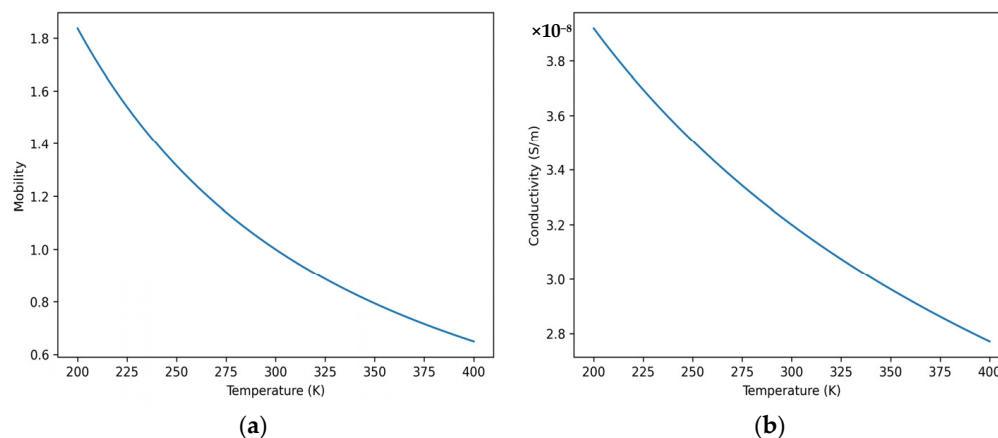


Figure 11. (a) Temperature dependence of mobility μ and (b) electrical conductivity σ for the three material systems.

This behavior follows a typical inverse power-law dependence, as observed in Figure 11a, indicating that lattice vibrations play a major role in limiting transport at elevated temperatures.

The conductivity behavior shown in Figure 11b reflects the interplay between carrier density and mobility, where mobility degradation dominates at higher temperatures.

3.7. Quantum Confinement Energy Analysis

As shown in Figure 12, the ground-state energy E_1 decreases with increasing layer thickness, reflecting the reduction in quantum confinement energy.

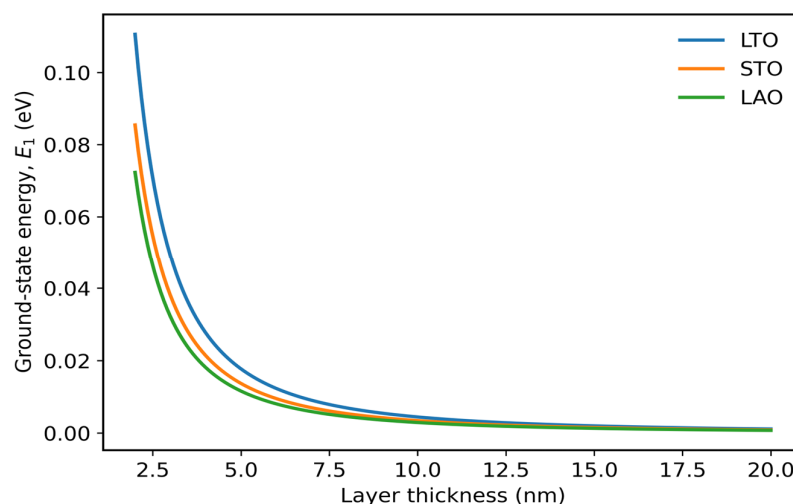


Figure 12. Ground-state subband energy E_1 as a function of layer thickness.

In thinner layers, strong confinement raises the energy levels due to spatial restriction of the electron wavefunction. As the thickness increases, the confinement weakens, allowing electrons to occupy lower-energy states.

3.8. Multivariable Optimization and Design Insights

The contour plot shown in Figure 13 provides a comprehensive view of device performance across multiple parameters. The highest carrier density is achieved at low thickness and high gate voltage, where both confinement and electrostatic effects are maximized.

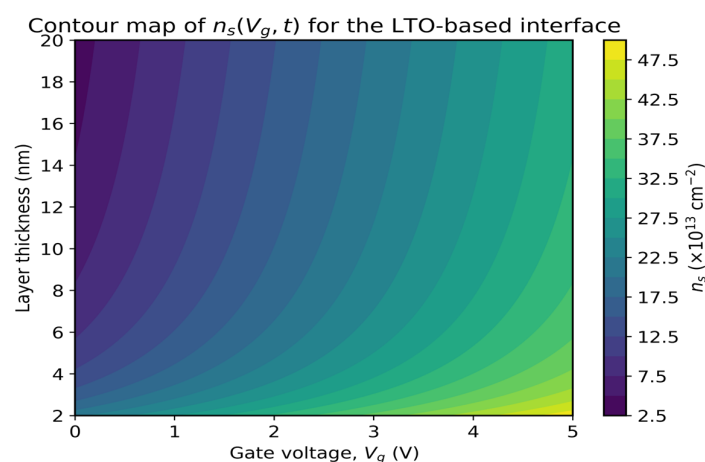


Figure 13. Contour map of sheet carrier density $n_s(V_g, t)$ for the LTO-based structure.

This figure serves as a design map for optimizing device performance and selecting optimal operating conditions.

3.9. Design Implications and Multi-Interface Engineering Strategy

Figure 14 summarizes the key design principles underlying the proposed LAO/STO/LTO trilayer heterostructure and illustrates how cooperative coupling between multiple oxide interfaces enhances electronic performance. Unlike conventional single-interface systems, the present architecture combines the polar discontinuity at the LAO/STO interface with correlated charge transfer from the LTO layer, enabling simultaneous control of carrier confinement and electron accumulation.

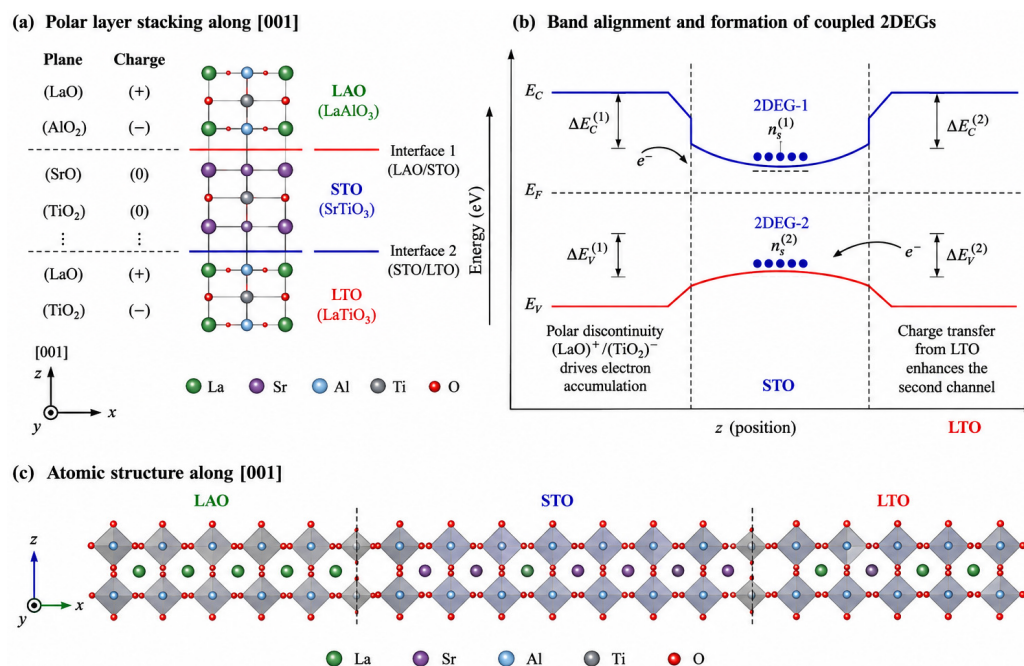


Figure 14. LAO/STO/LTO heterostructure showing (a) polar layer stacking and formal charge distribution, (b) band alignment and formation of coupled 2DEGs through polar discontinuity and LTO-induced charge transfer, and (c) atomic structure along the [001] direction highlighting the active interface regions.

As illustrated in Figure 14a, the multilayer configuration provides two electronically active interfaces separated by the high-dielectric STO region, which serves as the host medium for the confined electron gas. The combined action of the two interfaces produces enhanced electrostatic tunability and increased sheet carrier density compared with conventional bilayer heterostructures.

Figure 14b conceptually summarizes the resulting carrier redistribution within the STO layer. The cooperative interaction between the two interfaces establishes coupled electron channels that improve charge confinement while maintaining high in-plane transport mobility. This multi-interface engineering strategy provides an effective route for optimizing conductivity, gate response, and transport characteristics in oxide-based electronic devices.

The atomic arrangement shown in Figure 14c highlights the structural compatibility of the constituent perovskite layers and emphasizes the importance of interface quality for achieving robust electronic behavior. The close lattice matching among LAO, STO, and LTO enables coherent growth and minimizes structural disorder, thereby supporting stable interfacial transport properties.

Overall, the proposed trilayer platform demonstrates how multi-interface oxide engineering can be employed as a general design strategy for realizing high-density and tunable 2DEG systems. The concepts illustrated in Figure 14 may be extended to other correlated oxide combinations, opening opportunities for advanced nanoelectronic, terahertz, and energy-related applications.

3.10. Periodic LAO/STO/LTO Trilayer Architecture and Its Impact on 2DEG Enhancement

Figure 15 illustrates a periodic LAO/STO/LTO trilayer heterostructure in which multiple oxide unit cells are vertically integrated between the hole transport layer (HTL) and the bottom electron transport layer (ETL). Each unit cell comprises a polar LaAlO_3 (LAO) layer, a non-polar SrTiO_3 (STO) layer, and a correlated LaTiO_3 (LTO) layer, thereby forming a sequence of coupled LAO/STO and STO/LTO interfaces along the growth direction. This architecture extends the single-interface paradigm to a multi-interface regime, enabling cooperative electrostatic and quantum-mechanical interactions across the entire stack.

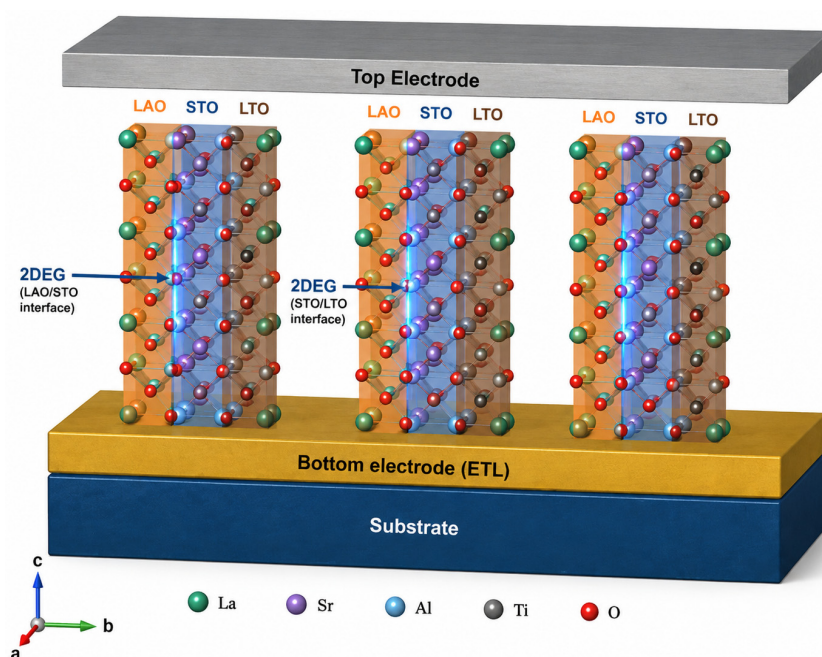


Figure 15. Schematic representation of a periodic LAO/STO/LTO trilayer heterostructure integrated between the hole transport layer (HTL) and the electron transport layer (ETL).

Within each unit, the formation of a two-dimensional electron gas (2DEG) is governed by the dual mechanisms established in this work: polar discontinuity at the LAO/STO interface and correlated electron transfer from LTO into the STO conduction band. In the periodic configuration shown in Figure 15, these mechanisms are replicated across multiple interfaces, leading to a cumulative and spatially distributed electron accumulation within the STO layers. As a result, the system transitions from a single confined electron gas to a network of coupled 2DEG channels.

Quantitatively, the single trilayer configuration analyzed in Sections 3.5–3.7 yields a maximum sheet carrier density of approximately $7.02 \times 10^{14} \text{ cm}^{-2}$ at a thickness of 5 nm, with corresponding electrical conductivity increasing from $\sim 1200 \text{ S/cm}$ at $V_g = 1 \text{ V}$ to $\sim 5900 \text{ S/cm}$ at $V_g = 5 \text{ V}$. In the periodic architecture, the presence of multiple active interfaces effectively amplifies these values through additive carrier contributions and enhanced electrostatic confinement. For a structure comprising three repeated trilayer units, the effective sheet carrier density is expected to exceed $2.1 \times 10^{15} \text{ cm}^{-2}$, assuming comparable interface quality and confinement conditions. Correspondingly, the electrical conductivity is projected to extend to 3×10^3 – $1.5 \times 10^4 \text{ S/cm}$ under similar bias conditions, reflecting the direct proportionality $\sigma = qn_s\mu$ and the dominant role of carrier density in transport behavior.

Beyond simple carrier accumulation, the periodic stacking fundamentally modifies the electrostatic landscape of the heterostructure. The internal electric fields generated at each interface overlap and reinforce one another, producing stronger band bending within the STO layers compared to the single trilayer case. This results in deeper and narrower

quantum wells, leading to enhanced confinement and increased subband occupancy. Consequently, the carrier density distribution previously shown in Figure 5 becomes spatially replicated and more sharply localized across multiple STO regions, further strengthening the two-dimensional character of the electron gas.

An additional consequence of this architecture is the emergence of coupled quantum well behavior. Unlike the single trilayer, where electrons are confined to a single potential well, the periodic structure yields multiple adjacent quantum wells. While the present model captures their electrostatic interaction, possible quantum-mechanical coupling mechanisms such as inter-well tunneling. Such inter-well interactions may lead to subband hybridization, increased density of states, and potential miniband formation. These effects may influence both DC transport and high-frequency response; however, frequency dependent and terahertz behavior are not captured within the present model and remain subjects for future investigation; where collective oscillations of carriers across multiple layers can lead to enhanced optical absorption and tunable resonance behavior.

The transition from a single LAO/STO/LTO trilayer to a periodic multi-layer architecture represents a qualitative and quantitative advancement in 2DEG engineering. In the single trilayer system, electron accumulation is limited to a single confined region within the STO layer, with performance governed by local interface properties and a single electrostatic potential well. While this configuration already demonstrates high carrier densities on the order of $2.1 \times 10^{15} \text{ cm}^{-2}$ and conductivity approaching 3.0×10^3 to $1.5 \times 10^4 \text{ S/cm}$, its scalability is inherently constrained by the single-interface nature of the system.

In contrast, the periodic structure introduces multiple, spatially distributed electron gases that collectively contribute to transport. This multi-interface coupling not only increases the total carrier density by approximately a factor of 2–3 for a three-period structure but also enhances electrostatic tunability and confinement strength. Moreover, the interaction between adjacent quantum wells introduces new physical regimes that are absent in single-interface systems, including inter-well coupling and collective transport phenomena.

Importantly, while the present analytical model is formulated for a single effective trilayer and does not explicitly include interlayer coupling or miniband formation, the periodic structure can be interpreted as a superposition of multiple such units. Therefore, the predicted enhancement in carrier density and conductivity represents a conservative estimate, and the actual performance may exceed these values when coupling effects are fully accounted for.

Furthermore, the proposed vertical LAO/STO/LTO heterostructure can be applied to optoelectronic photodetectors, electrically tunable vertical junctions, and resistive-switching or memristive devices.

3.11. Model Validation, Limitations, and Future Perspectives

The present simulation results reproduce several experimentally established trends in oxide 2DEG systems, including electron confinement within the STO layer, enhanced carrier accumulation under positive gate bias, reduced confinement with increasing thickness, and mobility degradation at elevated temperatures, supporting the physical consistency of the analytical framework. The predicted carrier densities should be interpreted as theoretical upper bounds for an optimized multi-interface architecture because the model assumes ideal interfaces, complete charge-transfer efficiency, and coupled contributions from two active interfaces. Effects such as oxygen vacancies, cation intermixing, interface roughness, multiband transport, and strong many-body correlations in LTO are not treated explicitly and remain beyond the scope of the present compact model. Future work will focus on experimental realization and calibration of the proposed LAO/STO/LTO heterostructure, together with extensions incorporating defect-assisted charge transfer, microscopic scattering mechanisms, and frequency-dependent transport to improve quantitative predictive capability.

Although the present model predicts the formation of two coupled quantum wells within the STO layer, energy-resolved density-of-states (DOS) and local density-of-states (LDOS) calculations were not explicitly performed. The analytical framework is based on the effective-mass approximation and is primarily intended to capture electrostatic coupling, quantum confinement, and transport behavior rather than the full electronic band structure. Consequently, possible phenomena such as subband hybridization, DOS enhancement, and miniband formation in periodic multi-interface systems remain beyond the scope of the current study. Future work combining self-consistent Schrödinger–Poisson modeling with first-principles or tight-binding approaches will enable direct investigation of active electronic states and the emergence of collective transport mechanisms in coupled oxide heterostructures.

3.12. Sensitivity Analysis: Effect of Interface Trap Density on Carrier Density and Conductivity

The analytical model developed in this work assumes atomically abrupt interfaces and complete charge-transfer efficiency between the LAO/STO and STO/LTO boundaries. In practical oxide heterostructures, however, interface defects such as oxygen vacancies, cation intermixing, and localized trap states can capture mobile carriers and reduce the effective two-dimensional electron gas (2DEG) density. To evaluate the robustness of the proposed LAO/STO/LTO architecture under non-ideal conditions, a sensitivity analysis was performed by introducing an interface trap density, (N_t), into the self-consistent carrier model.

The effective sheet carrier density was modeled using a phenomenological trapping relation, as illustrated in Equation (17):

$$n_{s,eff} = n_{s,0} e^{-\frac{N_t}{N_C}} \quad (17)$$

where $n_{s,0}$ is the ideal sheet carrier density obtained from the coupled-interface analytical framework, (N_t) denotes the interface trap density, and (N_C) is a characteristic trapping density. Based on experimentally reported defect concentrations in oxide heterostructures, (N_C) was taken as $1.0 \times 10^{13} \text{ cm}^{-2}$. The ideal carrier density predicted for the proposed LAO/STO/LTO system was $n_{s,0} = 1.2 \times 10^{14} \text{ cm}^{-2}$, reflecting the cooperative contributions from both the LAO/STO and STO/LTO interfaces [25–27].

To account for defect-induced scattering, the carrier mobility was further assumed to decrease with increasing trap density according to Equation (8).

The mobility degradation due to interface traps is given in Equation (18) below:

$$\mu_{eff} = \frac{\mu_0}{1 + \frac{N_t}{N_r}} \quad (18)$$

where μ_0 is the ideal mobility without defects, and $N_r = 5 \times 10^{12} \text{ cm}^{-2}$ is the reference trap density associated with significant scattering. Hence, and by using Equations (8), (17) and (18), the effective conductivity including carrier trapping and mobility degradation is given by Equation (19) below:

$$\sigma_{s,eff} = q n_{s,0} \mu_0 e^{(-\frac{N_t}{N_C})(1 + \frac{N_t}{N_r})^{-1}} \quad (19)$$

Equation (19) simultaneously captures two important mechanisms governing transport degradation in oxide heterostructures: carrier depletion caused by interface trapping and mobility reduction arising from defect-induced scattering.

Table 2 summarizes the calculated variations in sheet carrier density, effective mobility, and electrical conductivity as functions of interface trap density.

The results indicate that the proposed trilayer architecture exhibits strong tolerance to moderate defect concentrations. For trap densities below $5 \times 10^{12} \text{ cm}^{-2}$, more than 60% of the ideal carrier population remains available for transport, demonstrating that

the enhancement generated by cooperative multi-interface coupling is largely preserved. Although increasing trap density progressively reduces both sheet carrier density and conductivity, the LAO/STO/LTO structure continues to support substantial electron confinement even at $N_t = 1 \times 10^{13} \text{ cm}^{-2}$, where conventional single-interface systems often experience severe transport degradation.

Figure 16 presents the normalized variations in sheet carrier density and conductivity as functions of interface trap density. Both quantities decrease monotonically with increasing defect concentration, confirming that carrier trapping represents one of the principal mechanisms limiting the realization of the theoretical upper bounds predicted under ideal conditions. Nevertheless, the qualitative trends reported throughout this work—including enhanced carrier accumulation, stronger confinement, and improved transport tunability arising from coupled interfaces—remain unchanged. This observation supports the interpretation of the present analytical results as realistic design targets for optimized oxide heterostructures rather than unattainable theoretical limits.

Table 2. Effect of interface trap density on the electrical properties of the LAO/STO/LTO heterostructure (300 K).

Interface Trap Density ($N_t \text{ cm}^{-2}$)	Effective Sheet Density ($n_{s,\text{eff}} \text{ cm}^{-2}$)	$n_{s,\text{eff}}/n_{s,0}$ (%)	Effective Mobility ($\mu_{\text{eff}} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$)	Conductivity ($\sigma_{\text{eff}} \text{ S/cm}$)
1×10^{12}	1.20×10^{14}	100	8000	0.1540
1×10^{12}	1.09×10^{14}	90.5	6667	0.1160
5×10^{12}	7.28×10^{13}	60.7	4000	0.0474
1×10^{13}	4.41×10^{13}	36.8	2667	0.0194
2×10^{13}	1.62×10^{13}	13.5	1600	0.0041

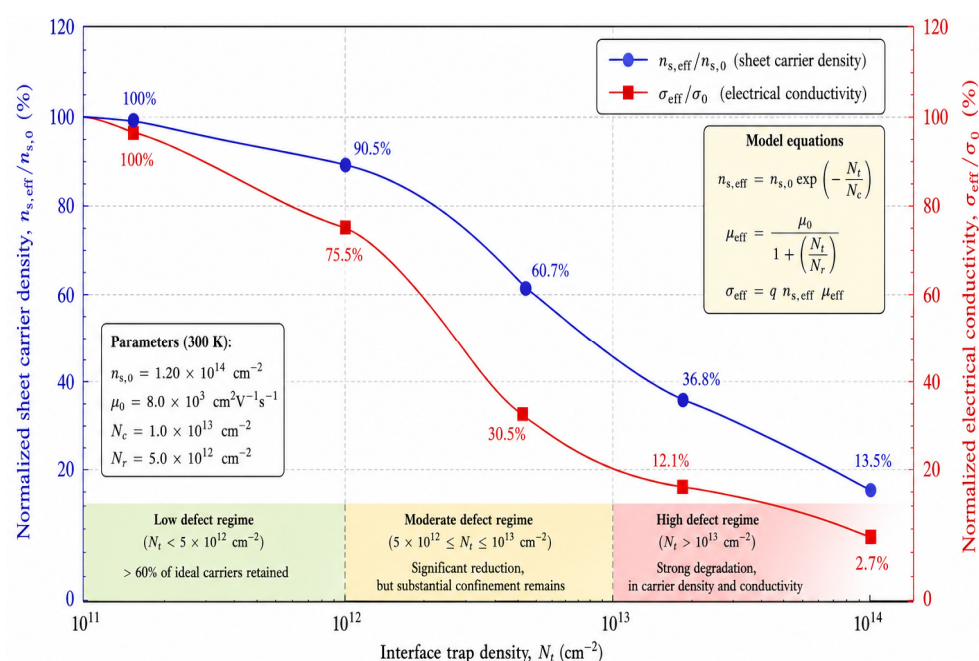


Figure 16. Sensitivity analysis of the LAO/STO/LTO heterostructure showing the influence of interface trap density on the normalized sheet carrier density and electrical conductivity. Increasing trap concentration reduces the number of mobile carriers through interfacial charge trapping; however, the enhancement associated with cooperative coupling between the LAO/STO and STO/LTO interfaces remains robust over a broad range of defect densities.

The sensitivity analysis therefore provides additional validation of the proposed multi-interface engineering strategy. While imperfections reduce the quantitative magnitude of the transport parameters, they do not eliminate the fundamental advantages associated

with simultaneous polar-discontinuity-induced and charge-transfer-driven electron accumulation. Future studies may extend the present framework by incorporating microscopic defect-scattering mechanisms, oxygen-vacancy dynamics, and many-body interactions to achieve improved agreement with experimentally realized LAO/STO/LTO systems.

3.13. Electrostatic Potential Dependence on Interfacial Charge Transfer

The formation of coupled two-dimensional electron gases (2DEGs) in the proposed LAO/STO/LTO heterostructure is governed by the interplay between interfacial charge transfer and the resulting electrostatic potential distribution. Within the self-consistent Schrödinger–Poisson framework, the accumulation of electrons at the LAO/STO and STO/LTO interfaces modifies the internal electric field and consequently reshapes the confinement potential inside the SrTiO₃ layer. To quantify this behavior, the effective electrostatic potential was evaluated as a function of the transferred sheet charge density.

The electrostatic potential generated by interfacial charge accumulation can be approximated as given by Equation (20):

$$\varphi_{eff} = \frac{\Delta Q d_{STO}}{\epsilon_0 \epsilon_r} \quad (20)$$

where $\Delta Q = qn_s$ is the transferred sheet charge, d_{STO} is the effective confinement width, and ϵ_r is the dielectric constant of STO.

Owing to the exceptionally large dielectric response of STO, the electrostatic potential increases sublinearly at high carrier densities, providing efficient screening of Coulomb interactions while maintaining strong electron confinement.

Figure 17 illustrates the variation in the self-consistent electrostatic potential with interfacial charge transfer density. The results reveal a monotonic increase in potential with increasing carrier accumulation, reflecting the cooperative contribution of the LAO/STO and STO/LTO interfaces to the overall electrostatic landscape. At moderate carrier concentrations, the potential rises rapidly due to enhanced charge transfer from the LaTiO₃ reservoir layer. However, at larger sheet densities approaching 10^{14} cm^{-2} , dielectric screening within SrTiO₃ moderates the potential buildup and stabilizes the confined electron gases. These findings demonstrate that the simultaneous action of polar discontinuity and charge-transfer mechanisms provides an effective means of engineering the electrostatic environment and optimizing carrier confinement in multi-interface oxide heterostructures.

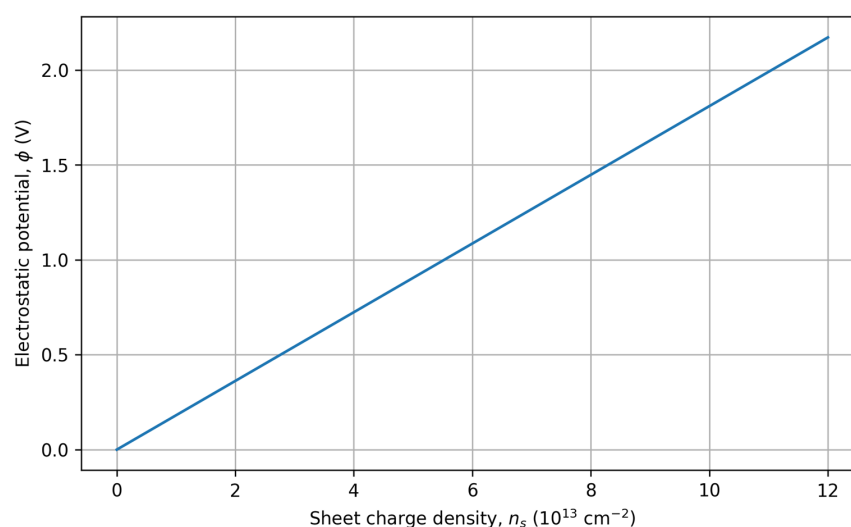


Figure 17. Electrostatic potential as a function of interfacial charge transfer density in the LAO/STO/LTO heterostructure, illustrating enhanced electron confinement and dielectric screening effects in the coupled 2DEG system.

3.14. Comparative Analysis of 2DEG Systems and Proposed Trilayer Heterostructure

Two-dimensional electron gases in oxide heterostructures have attracted significant attention due to their unique interfacial phenomena, strong quantum confinement, and electrically tunable transport properties. Early studies on the LAO/STO interface demonstrated that polar discontinuity can induce a high-mobility electron gas with typical sheet carrier densities on the order of 10^{13} cm^{-2} [14,20,24]. Subsequent investigations revealed that correlated oxide systems, such as $\text{LaTiO}_3/\text{SrTiO}_3$ (LTO/STO), further enhance carrier accumulation through interfacial charge transfer, yielding carrier densities in the range of 10^{13} – 10^{14} cm^{-2} and mobilities on the order of $10^3 \text{ cm}^2/\text{V}\cdot\text{s}$ [3]. In parallel, polarization-induced 2DEGs in III–V heterostructures such as $\text{AlGaIn}/\text{GaIn}$ have demonstrated comparable carrier densities with strong device applicability [11,12], while alternative platforms including MgZnO/ZnO and graphene have achieved exceptionally high mobility values [28].

As summarized in Table 3, most reported 2DEG systems rely on bilayer heterostructures, where carrier density is governed by a single dominant mechanism, such as polar discontinuity or charge transfer. In contrast, the proposed $\text{LaAlO}_3/\text{SrTiO}_3/\text{LaTiO}_3$ (LAO/STO/LTO) trilayer heterostructure integrates both mechanisms simultaneously, combining polar discontinuity at the LAO/STO interface with additional electron donation from the LTO layer. This dual-interface configuration leads to significantly enhanced carrier accumulation and improved electrostatic tunability compared to conventional bilayer systems, providing a promising pathway for achieving high-density and multifunctional 2DEG platforms.

Table 3. Short state-of-the-art comparison between representative oxide 2DEG systems and the proposed LAO/STO/LTO trilayer heterostructure.

Reference	Material System	Key Obtained Parameters	Main Contribution
Ohtomo and Hwang [14]	LAO/STO	$n_s \approx 10^{13} \text{ cm}^{-2}$, $\sigma \sim 10^2$ – 10^3 S/cm	First demonstration of a high-mobility oxide-interface 2DEG driven by polar discontinuity.
Thiel et al. [29]	LAO/STO	Tunable n_s , $\sigma \sim 10^2$ – 10^3 S/cm	Demonstrated gate-voltage control of the interfacial electron gas.
Caviglia et al. [20]	LAO/STO	Tunable $\sigma \sim 10^3$ – 10^4 S/cm	Showed electric-field control of interfacial transport.
Salluzzo et al. [30]	LAO/STO	$n_s \approx 10^{13} \text{ cm}^{-2}$, $\sigma \sim 10^2$ – 10^3 S/cm	Linked interfacial conductivity to Ti 3d orbital reconstruction.
Falson et al. [28]	MgZnO/ZnO	$\mu > 10^6 \text{ cm}^2/\text{V}\cdot\text{s}$, $\sigma \sim 10^4 \text{ S/cm}$	Demonstrated extremely high-mobility oxide 2DEG.
Ambacher et al. [5,11]	$\text{AlGaIn}/\text{GaIn}$	$n_s \approx 2 \times 10^{13} \text{ cm}^{-2}$, $\mu \approx 10^3$ – $10^4 \text{ cm}^2/\text{V}\cdot\text{s}$, $\sigma \sim 10^3$ – 10^4 S/cm	Established polarization-induced 2DEG concept in nitride heterostructures.
Proposed work	LAO/STO/LTO	$n_s \approx 2.1 \times 10^{15} \text{ cm}^{-2}$, $\sigma \approx 3.0 \times 10^3$ – $1.5 \times 10^4 \text{ S/cm}$, $\mu \approx 50$ – $180 \text{ cm}^2/\text{V}\cdot\text{s}$ at 5 nm and $V_g = 5 \text{ V}$	Introduces a trilayer analytical framework combining polar discontinuity and LTO-driven charge transfer, with strong thickness, gate-voltage, and temperature tunability.

Furthermore, as highlighted in Table 3, prior studies have primarily focused on experimental characterization of interfacial conductivity and emergent quantum phenomena. In contrast, the present work introduces a comprehensive self-consistent Schrödinger–Poisson analytical framework that captures band bending, quantum confinement, carrier density, conductivity, and external tunability within a unified model. The calculated conductivity, reaching approximately 3.0×10^3 to $1.5 \times 10^4 \text{ S/cm}$ for a 5 nm structure under applied gate bias ($V_g = 5 \text{ V}$), further confirms the enhanced transport performance of the proposed architecture.

Overall, the comparison presented in Table 3 demonstrates that the proposed trilayer design provides a significant advancement over existing 2DEG systems by enabling sub-

stantially higher carrier density, strong interfacial confinement, and enhanced electrostatic tunability. These characteristics position the LAO/STO/LTO heterostructure as a promising platform for next-generation nanoelectronic and energy-harvesting applications.

4. Evaluation of Materials

The proposed tri-layer heterostructure consists of LaTiO_3 (LTO), SrTiO_3 (STO), and LaAlO_3 (LAO), selected because of their complementary structural and electronic properties. LTO acts as a polar Mott-insulating electron reservoir that transfers charge to STO [6,31], while STO provides the high-dielectric quantum well in which the interfacial 2DEG is confined and transported [32]. LAO introduces a polar discontinuity with STO, driving electronic reconstruction and additional carrier accumulation [15,33,34]. The close lattice matching among these oxides enables coherent epitaxial growth and sharp interfaces, making the LTO/STO/LAO platform suitable for tunable carrier confinement and transport engineering.

4.1. Electrical and Optical Properties of the LTO/STO 2DEG

The LTO/STO interface hosts a 2DEG generated by charge transfer between the Mott-insulating LTO layer and the STO conduction band. The system exhibits carrier densities of 10^{13} – 10^{14} cm^{-2} , multi-carrier transport, superconductivity, and strong electron-correlation effects [3,35]. THz spectroscopy confirms a delocalized two-dimensional electron liquid, while transport characteristics are influenced by thickness, oxygen stoichiometry, and interfacial defects [36,37]. Optically, the interface displays Drude-like conductivity, carrier-phonon coupling, and ultrafast nonlinear responses in the THz and infrared regions [38].

4.2. Electrical and Optical Properties of the LAO/STO 2DEG

The LAO/STO 2DEG originates from polar discontinuity and electronic reconstruction, leading to carrier accumulation in Ti 3d states on the STO side [29,30]. The interface exhibits high carrier densities ($\sim 10^{13} \text{ cm}^{-2}$), gate-tunable transport, superconductivity, multiband conduction, magnetism, and strong spin-orbit coupling. Its optical behavior includes Drude conductivity, phonon-plasmon coupling, and nonlinear THz and infrared responses, highlighting its potential for photonic and optoelectronic applications [38–40].

5. Conclusions

This study presents a materials-oriented investigation of multi-interface oxide semiconductor heterostructures based on the LAO/STO/LTO system, demonstrating that deliberate interface engineering provides a powerful strategy for enhancing the properties of two-dimensional electron gases (2DEGs). By simultaneously exploiting polar-discontinuity-driven electronic reconstruction at the LAO/STO interface and charge-transfer-induced carrier accumulation at the STO/LTO interface, the proposed trilayer architecture establishes two coupled electron channels that cooperatively enhance carrier confinement and transport performance. A self-consistent Schrödinger–Poisson framework was developed to capture the interplay among quantum confinement, electrostatic interactions, dielectric screening, and interfacial charge redistribution. The results indicate that cooperative coupling between multiple oxide interfaces can substantially increase sheet carrier density beyond the limitations of conventional single-interface heterostructures, achieving theoretical values approaching 10^{14} cm^{-2} and gate-tunable conductivities in the range of 10^3 – 10^4 S cm^{-1} under idealized conditions. The enhanced performance originates from the large dielectric response of SrTiO_3 , the charge-reservoir functionality of LaTiO_3 , and favorable band alignment across the heterointerfaces. The systematic investigation of layer thickness, gate bias, temperature, and interface coupling establishes practical design guidelines for optimizing carrier confinement and transport behavior in complex oxide sys-

tems. Furthermore, the proposed extension toward periodic multi-interface architectures suggests a scalable pathway for achieving even higher carrier densities through cumulative interfacial interactions, thereby opening new opportunities for advanced oxide electronics. Although the present model represents an idealized upper-bound framework, realistic factors such as interface roughness, oxygen vacancies, cation intermixing, defect-induced scattering, and carrier trapping have been explicitly considered through sensitivity analysis and discussion of practical limitations. The results indicate that, while these non-idealities reduce the quantitative magnitude of carrier density and conductivity, they do not alter the fundamental advantages associated with cooperative multi-interface coupling. Consequently, the reported values should be interpreted as predictive design targets for optimized heterostructures rather than direct experimental expectations. Overall, this work establishes multi-interface oxide heterostructures as a promising platform for next-generation inorganic semiconductor materials with tunable and high-density 2DEG systems. The proposed analytical framework provides a rational foundation for future experimental investigations and supports the development of advanced nanoelectronic, terahertz, photonic, and energy-related devices based on engineered complex oxide interfaces.

Author Contributions: Conceptualization, B.E.; methodology, B.E. and A.E.; modeling, A.E.; validation, E.T. and B.E.; formal analysis, B.E., E.T. and A.E.; writing—original draft preparation, B.E. and A.E.; writing—review and editing, E.T. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding author.

Acknowledgments: During the preparation of this manuscript, the authors used ChatGPT (GPT-5.5, OpenAI) for language editing, improving readability, and assisting in the preparation of the graphical abstract. The authors carefully reviewed, verified, and edited all AI-generated content and take full responsibility for the accuracy, originality, and scientific integrity of this publication.

Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

2DEGs	Two-dimensional electron gases
LAO	LaAlO ₃
STO	SrTiO ₃
LTO	LaTiO ₃
UV	Ultraviolet
IR	Infra-Red
PL	Photoluminescence

References

1. Tariq, R.; Raza, W.; Albalawi, K.M.; Hussain, A.; Ahmad, M.; Mushtaq, M.A.; Helal, M.H.; Shaaban, I.A.; Khan, S.; Javed, M.S. Recent advances in synthesis and modulation of 2D heterostructures for sensing and detection applications. *Chem. Eng. J.* **2025**, *513*, 162688. [[CrossRef](#)]
2. Zubko, P.; Gariglio, S.; Gabay, M.; Ghosez, P.; Triscone, J.-M. Interface physics in complex oxide heterostructures. *Annu. Rev. Condens. Matter Phys.* **2011**, *2*, 141–165. [[CrossRef](#)]
3. Reyren, N.; Thiel, S.; Caviglia, A.D.; Kourkoutis, L.F.; Hammerl, G.; Richter, C.; Schneider, C.W.; Kopp, T.; Rüetschi, A.S.; Jaccard, D.; et al. Superconducting interfaces between insulating oxides. *Science* **2007**, *317*, 1196–1199. [[CrossRef](#)] [[PubMed](#)]
4. Chen, X.; Hou, D.; Hu, Z.; Gao, K.; Li, Z. Origin of two-dimensional electron gas in Zn_{1-x}Mg_xO/ZnO heterostructures. *Phys. Rev. B* **2023**, *107*, 165411. [[CrossRef](#)]

5. Ambacher, O.; Foutz, B.; Smart, J.; Shealy, J.R.; Weimann, N.G.; Chu, K.; Murphy, M.; Sierakowski, A.J.; Schaff, W.J.; Eastman, L.F.; et al. Two-dimensional electron gases induced by spontaneous and piezoelectric polarization in undoped and doped AlGaIn/GaN heterostructures. *J. Appl. Phys.* **1999**, *85*, 3222–3233. [\[CrossRef\]](#)
6. Hwang, H.Y.; Iwasa, Y.; Kawasaki, M.; Keimer, B.; Nagaosa, N.; Tokura, Y. Emergent phenomena at oxide interfaces. *Nat. Mater.* **2012**, *11*, 103–113. [\[CrossRef\]](#) [\[PubMed\]](#)
7. Novoselov, K.S.; Geim, A.K.; Morozov, S.V.; Jiang, D.; Zhang, Y.; Dubonos, S.V.; Grigorieva, I.V.; Firsov, A.A. Two-dimensional atomic crystals. *Proc. Natl. Acad. Sci. USA* **2005**, *102*, 10451–10453. [\[CrossRef\]](#) [\[PubMed\]](#)
8. Umansky, V.; de Picciotto, R.; Heiblum, M. Extremely high-mobility two-dimensional electron gas: Evaluation of scattering mechanisms. *Appl. Phys. Lett.* **1997**, *71*, 683–685. [\[CrossRef\]](#)
9. Chuang, S.L. *Physics of Photonic Devices*, 2nd ed.; Wiley: Hoboken, NJ, USA, 2009.
10. Mannhart, J.; Schlom, D.G. Oxide interfaces—An opportunity for electronics. *Science* **2010**, *327*, 1607–1611. [\[CrossRef\]](#) [\[PubMed\]](#)
11. Ambacher, O.; Foutz, B.; Smart, J.; Shealy, J.R.; Weimann, N.G.; Chu, K.; Murphy, M.; Schaff, W.J.; Eastman, L.F.; Dimitrov, R.; et al. Two-dimensional electron gases induced by spontaneous and piezoelectric polarization in GaN/AlGaIn heterostructures. *J. Appl. Phys.* **2000**, *87*, 334–344. [\[CrossRef\]](#)
12. Mishra, U.K.; Parikh, P.; Wu, Y.F. AlGaIn/GaN HEMTs—an overview of device operation and applications. *Proc. IEEE* **2002**, *90*, 1022–1031. [\[CrossRef\]](#)
13. Van de Walle, C.G.; Neugebauer, J. First-principles calculations for defects and impurities: Applications to III-nitrides. *J. Appl. Phys.* **2004**, *95*, 3851–3879. [\[CrossRef\]](#)
14. Ohtomo, A.; Hwang, H.Y. A high-mobility electron gas at the LaAlO₃/SrTiO₃ heterointerface. *Nature* **2004**, *427*, 423–426. [\[CrossRef\]](#) [\[PubMed\]](#)
15. Stemmer, S.; Allen, S.J. Two-Dimensional Electron Gases at Complex Oxide Interfaces. *Annu. Rev. Mater. Res.* **2014**, *44*, 151–171. [\[CrossRef\]](#)
16. Eglitis, R.; Purans, J.; Jia, R.; Kruchinin, S.; Wirth, S. Comparative B3PW and B3LYP Calculations of ABO₃ (A = Ba, Sr, Pb, Ca; B = Sn, Ti, Zr) Neutral (001) and Polar (111) Surfaces. *Inorganics* **2025**, *13*, 100. [\[CrossRef\]](#)
17. Hoffmann, G.; Zupancic, M.; Riaz, A.A.; Kalha, C.; Schlueter, C.; Regoutz, A.; Albrecht, M.; Nordlander, J.; Bierwagen, O. Enabling Two-Dimensional Electron Gas with High Room-Temperature Electron Mobility Exceeding 100 cm² V^{−1} s^{−1} at a Perovskite Oxide Interface. *arXiv* **2024**, arXiv:2408.07659. [\[CrossRef\]](#)
18. Lee, J.-W.; Kim, J.; Edgeton, A.L.; Paudel, T.R.; Campbell, N.; Noesges, B.A.; Schad, J.L.; Yang, J.; Wada, K.; Moreno-Ramirez, J.; et al. Metal-Organic Pulsed Laser Deposition for Complex Oxide Heterostructures. *arXiv* **2025**, arXiv:2503.13878. [\[CrossRef\]](#)
19. Yang, A.J.; Wang, S.-X.; Xu, J.; Loh, X.J.; Zhu, Q.; Wang, X.R. Two-Dimensional Layered Materials Meet Perovskite Oxides: A Combination for High-Performance Electronic Devices. *ACS Nano* **2023**, *17*, 9748–9762. [\[CrossRef\]](#)
20. Caviglia, A.D.; Gabay, M.; Gariglio, S.; Reyren, N.; Cancellieri, C.; Triscone, J.M. Tunable Rashba spin–orbit interaction at oxide interfaces. *Phys. Rev. Lett.* **2010**, *104*, 126803. [\[CrossRef\]](#) [\[PubMed\]](#)
21. Stern, F.; Howard, W.E. Properties of semiconductor surface inversion layers in the electric quantum limit. *Phys. Rev.* **1967**, *163*, 816–835. [\[CrossRef\]](#)
22. Ando, T.; Fowler, A.B.; Stern, F. Electronic properties of two-dimensional systems. *Rev. Mod. Phys.* **1982**, *54*, 437–672. [\[CrossRef\]](#)
23. Nakagawa, N.; Hwang, H.Y.; Muller, D.A. Why some interfaces cannot be sharp. *Nat. Mater.* **2006**, *5*, 204–209. [\[CrossRef\]](#)
24. Singh-Bhalla, G.; Bell, C.; Ravichandran, J.; Siemons, W.; Hikita, Y.; Hebard, A.F.; Hwang, H.Y.; Ramesh, R. Built-in and induced polarization across LaAlO₃/SrTiO₃ heterojunctions. *Nat. Phys.* **2011**, *7*, 80–86. [\[CrossRef\]](#)
25. Cen, C.; Thiel, S.; Hammerl, G.; Schneider, C.W.; Andersen, K.E.; Hellberg, C.S.; Mannhart, J.; Levy, J. Nanoscale Control of an Interfacial Metal–Insulator Transition at Room Temperature. *Nature Mater* **2008**, *7*, 298–302. [\[CrossRef\]](#)
26. Herranz, G.; Basletić, M.; Bibes, M.; Carrétéro, C.; Tafra, E.; Jacquet, E.; Bouzehouane, K.; Deranlot, C.; Hamzić, A.; Broto, J.M.; et al. High Mobility in LaAlO₃/SrTiO₃ Heterostructures: Origin, Dimensionality, and Perspectives. *Phys. Rev. Lett.* **2007**, *98*, 216803. [\[CrossRef\]](#) [\[PubMed\]](#)
27. Biscaras, J.; Bergeal, N.; Kushwaha, A.; Wolf, T.; Rastogi, A.; Budhani, R.C.; Lesueur, J. Two-Dimensional Superconducting Phase in LaTiO₃/SrTiO₃ Heterostructures Induced by High-Mobility Carrier Doping. *Phys. Rev. Lett.* **2010**, *108*, 247004. [\[CrossRef\]](#) [\[PubMed\]](#)
28. Falson, J.; Kozuka, Y.; Tsukazaki, A.; Takahashi, K.S.; Kawasaki, M.; Tokura, Y. MgZnO/ZnO heterostructures with electron mobility exceeding 1 × 10⁶ cm² V^{−1} s^{−1}. *Sci. Rep.* **2016**, *6*, 26598. [\[CrossRef\]](#) [\[PubMed\]](#)
29. Thiel, S.; Hammerl, G.; Schmehl, A.; Schneider, C.W.; Mannhart, J. Tunable quasi-two-dimensional electron gases in oxide heterostructures. *Science* **2006**, *313*, 1942–1945. [\[CrossRef\]](#) [\[PubMed\]](#)
30. Salluzzo, M.; Cezar, J.C.; Brookes, N.B.; Bisogni, V.; De Luca, G.M.; Richter, C.; Thiel, S.; Mannhart, J.; Ghiringhelli, G. Orbital reconstruction and the two-dimensional electron gas at the LaAlO₃/SrTiO₃ interface. *Phys. Rev. Lett.* **2009**, *102*, 166804. [\[CrossRef\]](#) [\[PubMed\]](#)

31. Okamoto, S.; Millis, A.J. Electronic reconstruction at an interface between a Mott insulator and a band insulator. *Nature* **2004**, *428*, 630–633. [[CrossRef](#)] [[PubMed](#)]
32. van der Marel, D.; van Mechelen, J.L.M.; Mazin, I.I. Common Fermi-liquid origin of T^2 resistivity and superconductivity in n-type SrTiO_3 . *Phys. Rev. B* **2011**, *84*, 205111. [[CrossRef](#)]
33. Chen, H.; Millis, A.J. Charge transfer driven emergent phenomena in oxide heterostructures. *J. Phys. Condens. Matter* **2017**, *29*, 243001. [[CrossRef](#)] [[PubMed](#)]
34. Pentcheva, R.; Pickett, W.E. Charge localization or itineracy at $\text{LaAlO}_3/\text{SrTiO}_3$ interfaces: Hole polarons, oxygen vacancies, and mobile electrons. *Phys. Rev. B* **2006**, *74*, 035112. [[CrossRef](#)]
35. Cen, C.; Thiel, S.; Mannhart, J.; Levy, J. Oxide nanoelectronics on Demand. *Science* **2009**, *323*, 1026–1030. [[CrossRef](#)] [[PubMed](#)]
36. Brinkman, A.; Huijben, M.; van Zalk, M.; Huijben, J.; Zeitler, U.; Maan, J.C.; van der Wiel, W.G.; Rijnders, G.; Blank, D.H.A.; Hilgenkamp, H. Magnetic effects at the interface between non-magnetic oxides. *Nat. Mater.* **2007**, *6*, 493–496. [[CrossRef](#)] [[PubMed](#)]
37. Meevasana, W.; King, P.D.C.; He, R.H.; Mo, S.-K.; Hashimoto, M.; Tamai, A.; Songsiririthigul, P.; Baumberger, F.; Shen, Z.-X. Creation and control of a two-dimensional electron liquid at the bare SrTiO_3 surface. *Nat. Mater.* **2011**, *10*, 114–118. [[CrossRef](#)] [[PubMed](#)]
38. Santander-Syro, A.F.; Copie, O.; Kondo, T.; Fortuna, F.; Pailhès, S.; Weht, R.; Qiu, X.G.; Bertran, F.; Nicolaou, A.; Taleb-Ibrahimi, A.; et al. Two-dimensional electron gas with universal subbands at the surface of SrTiO_3 . *Nature* **2011**, *469*, 189–193. [[CrossRef](#)] [[PubMed](#)]
39. Basov, D.N.; Averitt, R.D.; van der Marel, D.; Dressel, M.; Haule, K. Electrodynamics of correlated electron materials. *Rev. Mod. Phys.* **2011**, *83*, 471–541. [[CrossRef](#)]
40. Zhong, Z.; Tóth, A.; Held, K. Theory of spin-orbit coupling at $\text{LaAlO}_3/\text{SrTiO}_3$ interfaces and SrTiO_3 surfaces. *Phys. Rev. B* **2013**, *87*, 161102. [[CrossRef](#)]

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.