

# Inhomogeneous superconductivity in (001), (110), and (111) $\text{KTaO}_3$ two-dimensional electronic gases: Effect of electronic confinement on the transition temperature

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Experimental observations on  $\text{KTaO}_3$  superconductivity report widely different critical temperatures with a clear hierarchy among different crystallographic orientations. Accounting for spatial confinement, we connect the inhomogeneous superconducting order parameter with the spatial extent of the two-dimensional electron gas. We reproduce the observed hierarchy within a unified framework, based on a self-consistent tight-binding slab model with local spin-singlet  $s$ -wave pairing. The methods developed here can be readily extended to include more general interaction models, while still consistently including the characteristic spatial structure of the electron gas.

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**Introduction.** Two-dimensional electron gases (2DEGs) formed at oxide interfaces exhibit a unique interplay among confinement, orbital physics, spin-orbit coupling, and electronic correlations [1–10]. Heterostructures based on  $\text{KTaO}_3$  (KTO) oxides stand out owing to the strong spin-orbit coupling inherited from the Ta  $5d$  orbitals and a remarkable tunability of their electronic properties, such as superconductivity, by electrostatic gating and interface engineering [11–14]. The electronic structure of KTO 2DEGs is highly sensitive to the crystallographic orientation of the interface, with distinct energy and spin structures for the (001), (110), and (111) directions [15]. In particular, the (111) orientation exhibits a complex multiorbital structure associated with the trigonal symmetry of the interface, leading to unconventional spin-orbital locking and Berry curvature effects [16–23].

One of the most striking orientation-dependent features is the superconducting critical temperature [24–40]. In (001)-oriented 2DEGs, superconductivity emerges only within very limited experimental conditions at high doping (see Refs. [28,29]), and even then with a critical temperature  $T_c$  substantially lower than in the (110) and (111) interfaces. The microscopic origin of this anisotropy remains open: it is unclear whether the hierarchy [24–26] requires orientation-dependent pairing interactions or can arise from geometric confinement and multiorbital electronic structure alone, as

suggested by the observed correlation between higher  $T_c$  and stronger confinement [33].

Here, we address quantitatively the impact of spatial confinement and multiorbital electronic structure on the superconducting state across all orientations. We take as our starting assumption that the pairing interaction, electronic screening, and microscopic electronic couplings are orientation independent, and self-consistently obtain the critical temperature, accounting for a spatially dependent order parameter through a variational technique recently developed in Ref. [41]. We correctly recover the observed hierarchy of  $T_c$ , showing that accounting for the inhomogeneous nature of superconductivity is crucial to determine the character of the instability.

**Normal electronic state.** The microscopic electronic interactions are taken identical across all orientations: the unified geometry, from the underlying cubic structure to the projected crystallographic cuts, is shown in Fig. 1. While the (001) surface preserves the square symmetry, the (110) and (111) orientations lead to different symmetries and modified orbital overlap patterns.

The bulk electronic structure is described within a tight-binding model [21] in terms of the conducting  $t_{2g}$  orbitals denoted by  $\alpha \in \{1, 2, 3\} = \{x, y, z\}$ , corresponding to  $(d_{yz}, d_{zx}, d_{xy})$ ; each of the orbitals has an associated spin degree of freedom. The overall 2DEG Hamiltonian, depending on the two-dimensional quasimomentum  $\mathbf{k}$  in the plane of the 2DEG, reads

$$H = H_{\text{TB}} + H_{\text{SOC}} + H_{\text{dist}} + H_{\varphi}, \quad (1)$$

where  $H_{\text{TB}}$  is obtained by projecting the same microscopic three-dimensional (3D) bulk Hamiltonian along each crystallographic direction,  $H_{\text{SOC}}$  is the spin-orbit coupling term,  $H_{\text{dist}}$  the  $\mathbf{k} = \mathbf{0}$  crystal-field distortion, and  $H_{\varphi}$  the self-consistent electrostatic confinement potential. The latter is obtained from the Poisson equation using a direction-independent dielectric

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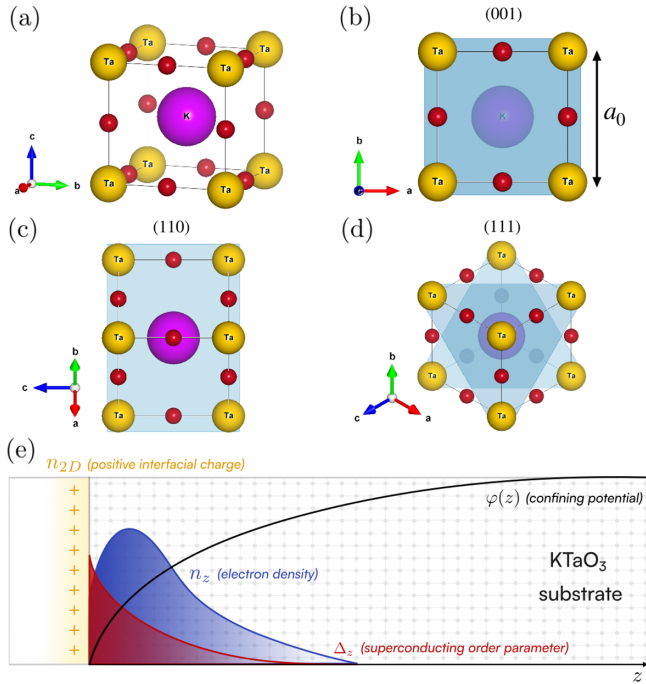


FIG. 1. (a) Cubic structure of KTO. (b)–(d) Top view of crystalline KTO along the (b) (001), (c) (110), and (d) (111) directions. The cubic lattice constant is  $a_0 = 3.988$  Å. (e) Schematic illustration of the inhomogeneous superconductivity induced by the electronic confinement.

function; details are given in the Supplemental Material (SM) [42] (see also Refs. [43–46] therein).

Figure 2 shows the resulting spatial profile of electron density of a slab of  $N_L = 51$  sites for different crystallographic orientations. The main control parameter is the total charge density  $n_{2D}$ , determining the filling of the system. In our model,  $n_{2D}$  is represented as a fixed positive sheet charge localized at the interface, which effectively accounts for the electrostatic origin of the 2DEG, including polar discontinuity, donor defects, deposited overlayers, or top-/ionic-liquid

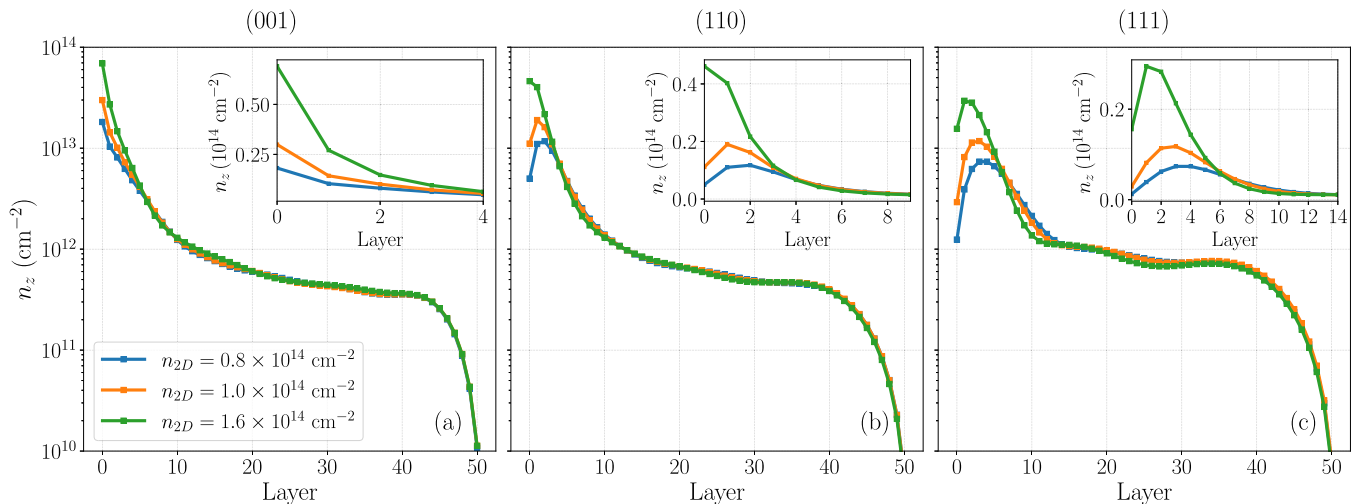


FIG. 2. Electron 2D density  $n_z$  for different benchmark values of  $n_{2D}$  at the (a) (001), (b) (110), and (c) (111) interfaces. The insets show the details close to the interfaces.

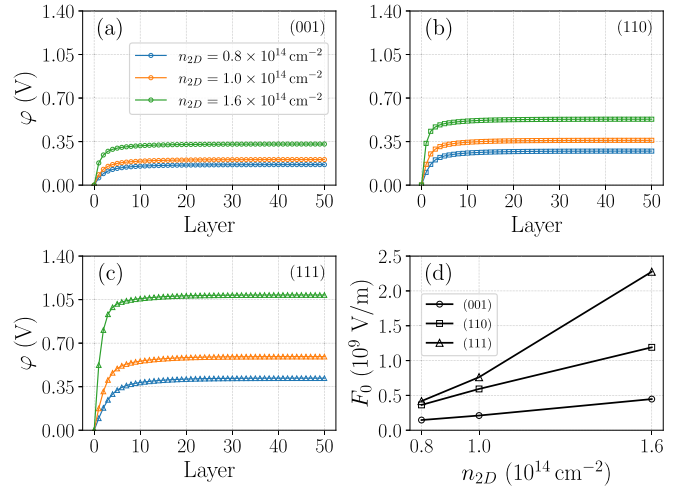


FIG. 3. (a)–(c) Potential barrier  $\varphi$  as a function of the layer position using different benchmark values of the positive charge density  $n_{2D}$  for the (a) (001), (b) (110), and (c) (111) directions. (d) Interfacial electric field  $F_0$  as a function of  $n_{2D}$  for (001), (110), and (111) directions.

gating [11,21,28,47,48]. The confinement is stronger in the (001) interface, with a stronger in-plane dispersion. Roughly, the number of layers within which the 2DEG is confined is  $\Delta N_{001} = 2$  for the (001) interface,  $\Delta N_{110} = 5$  for the (110) interface, and  $\Delta N_{111} = 10$  for the (111) interface. We stress that  $n_{2D}$  does not coincide with the charge density of a probed 2DEG, since it spreads along the slab. In turn, the electrostatic potential self-consistently produced at the interface has a quite different structure among the three interfaces. Figure 3 shows the electric potential and field for increasing density  $n_{2D}$ . For the same  $n_{2D}$ , the electric field increases from the (001) to the (110) to the (111) crystallographic cut, up to even a factor 4. The steepest electrostatic barrier occurs along the (111) direction, in spite of the 2DEG being less spatially confined here. In this case, the stronger confinement comes rather from the anisotropic dispersion, which favors out-of-plane hopping in the (111) orientation.

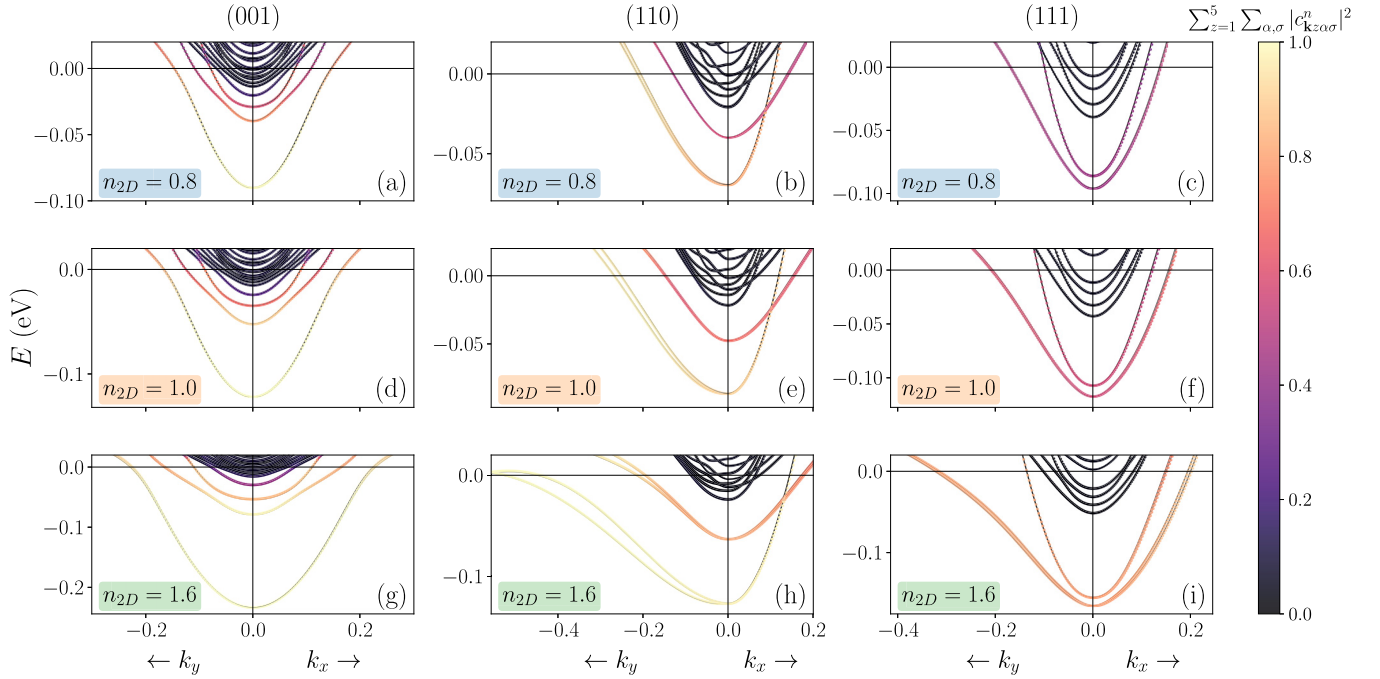


FIG. 4. Layer-resolved band structure of the KTO-based heterostructure along the (a), (d), (g) (001), (b), (e), (h) (110), and (c), (f), (i) (111) directions for positive charge densities (a)–(c)  $n_{2D} = 0.8 \times 10^{14} \text{ cm}^{-2}$ , (d)–(f)  $n_{2D} = 1.0 \times 10^{14} \text{ cm}^{-2}$ , and (g)–(i)  $n_{2D} = 1.6 \times 10^{14} \text{ cm}^{-2}$ . The color represent the probability to find a state over the first 5 layers. The quasi-momentum  $k_i$  is expressed in  $\text{\AA}^{-1}$ . The energy zero ( $E = 0$ ) is set to the self-consistent Fermi level obtained from the electrostatic screening simulations at each  $n_{2D}$ .

The overall properties of the normal state are contained in the band structure, which we show in Fig. 4. Energies are measured relative to the self-consistent chemical potential, so  $E = 0$  corresponds to the Fermi level at each  $n_{2D}$ . The projection of the bulk  $t_{2g}$  manifold onto the corresponding surface Brillouin zones produces markedly different dispersions depending on the interface orientation. For the (001) configuration, the bands exhibit a relatively stronger in-plane dispersion and a more clearly resolved confinement-induced subband structure. In contrast, the (110) and, even more prominently, the (111) orientations display a richer multi-orbital structure with enhanced band mixing and reduced effective confinement effects. Notably, even in the most localized (001) case, the chemical potential intersects bands belonging to the bulk continuum.

Finally, Fig. 5 shows density of states (DOS) as a function of the chemical potential and the local layer-resolved density of states (LDOS) evaluated at the self-consistent chemical potential for different values of the positive interface density  $n_{2D}$  and for the three crystallographic orientations. The LDOS is computed as

$$\text{LDOS}(z) = \sum_{n\alpha\sigma} \int \frac{d^2\mathbf{k}}{4\pi^2} \delta(E_{n\mathbf{k}}) |c_{\mathbf{k}z\alpha\sigma}^n|^2, \quad (2)$$

where  $E_{n\mathbf{k}}$  is the  $n$ th band energy measured from the self-consistent chemical potential, and  $c_{\mathbf{k}z\alpha\sigma}^n$  is the corresponding eigenvector component on layer  $z$ , orbital  $\alpha$ , and spin  $\sigma$ . In practice, the Dirac delta function is approximated by a Lorentzian broadening,  $\pi\delta(x) \approx \tau/(x^2 + \tau^2)$ , with  $\tau = 10^{-3} \text{ eV}$ .

Once again, the LDOS shows increasing delocalization from the (001) to the (110) to the (111) configuration. Even though the DOS of the (001) and (110) is larger compared to the (111), the distribution of the available states along the system is displaced differently. As a benchmark, we also show the sum over the first ten layers of the LDOS, since experimentally angle-resolved photoemission spectroscopy (ARPES) measurements can only probe surface properties. This feature has a direct bearing on the superconducting instability: in a Bardeen-Cooper-Schrieffer (BCS)-like framework the superconducting gap grows with the density of states of the normal-state system. At the level of the bare DOS, one would therefore expect a higher  $T_c$  for the (001) interface. However, the superconducting instability is spatially inhomogeneous and is controlled by a surface-weighted DOS. As shown below, this reverses the expectation and yields the highest  $T_c$  for the (111) interface.

*Superconducting instability.* Starting from a bulk three-dimensional description of a local attractive four-fermion Hamiltonian, inhomogeneous superconductivity is described within a mean-field approximation as

$$H_S = -U \sum_{\mathbf{k} \in \frac{1}{2}\text{BZ}} \sum_{z\alpha} (\Delta_z c_{\mathbf{k}z\alpha\uparrow}^\dagger c_{-\mathbf{k}z\alpha\downarrow}^\dagger + \text{H.c.}) + \mathcal{A} \sum_z U \Delta_z^2, \quad (3)$$

where  $\Delta_z = \langle c_{iz\alpha\uparrow} c_{iz\alpha\downarrow} \rangle$ . Here,  $i$  is the in-plane real-space coordinate,  $U$  is the effective pairing interaction strength, taken to be the same for all slab configurations, and  $\mathcal{A}$  accounts for the different interface unit-cell areas associated with the various interface orientations, as we report in detail in SM [42]. We consider here a *phonon-mediated pairing*

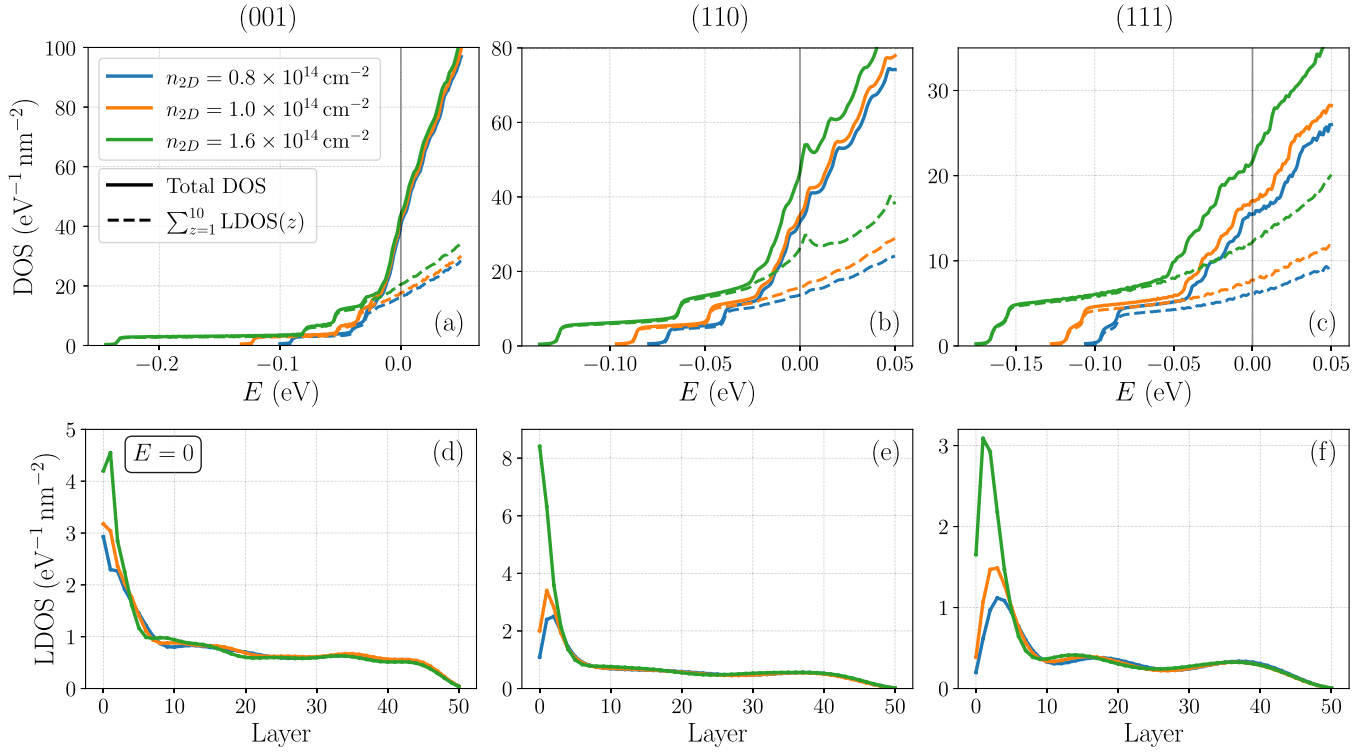


FIG. 5. (a)–(c) Density of states (solid lines) and the sum over the first ten layers of the layer-resolved density of states (dashed lines) as a function of energy. (d)–(f) Layer-resolved density of states at the self-consistent chemical potential. (a) and (d), (b) and (e), and (c) and (f) correspond to the (001), (110), and (111) orientations, respectively.

*mechanism*, which should be regarded as a lower bound for the predicted  $T_c$  within this singlet  $s$ -wave model. In this case, the interaction  $U$  is taken to be nonzero only within an energy shell of width  $\hbar\omega_i$  around the Fermi level, where  $\omega_i$  is a characteristic frequency scale typical of phonon-mediated superconductivity (e.g., the Debye frequency or the frequency of soft modes [24,49]). In the SM [42], we also consider an *instantaneous pairing mechanism*, with  $U$  constant over the full energy range, which gives an upper bound for  $T_c$ . Since the results are qualitatively unchanged, we focus here on the standard retarded case. In Eq. (3),  $\Delta_z$  depends explicitly on  $z$ , to reflect the breaking of translational invariance from the confining potential (See Fig. 1). To mimic the spatial profile of the electronic density in Fig. 2, we use a variational ansatz  $\Delta_z = \Delta e^{-z/z_0}$  in terms of the parameters  $\Delta$  and  $z_0$  describing amplitude and penetration of the order parameter across the material. Different variational profiles could be introduced, but the exponential ansatz provides the minimal parametrization needed to retain the relevant physical ingredient, namely the spatial extension  $z_0$  of the superconducting condensate. To determine the self-consistent variational parameters, we minimize the free-energy functional

$$F = 3U \sum_{z=0}^{N_L-1} \Delta^2 e^{-2z/z_0} - \frac{\mathcal{P}}{\beta} \sum_n \int d^2\mathbf{k} \{ \ln[2 + 2 \cosh(\beta \lambda_{n\mathbf{k}})] - \ln[2 + 2 \cosh(\beta E_{n\mathbf{k}})] \}, \quad (4)$$

where  $\beta = 1/k_B T$ , the factor 3 accounts for the three orbital degrees of freedom,  $n$  labels the normal-state bands, and  $\mathcal{P}$  is geometry dependent, with  $\mathcal{P}_{001} = 1/(4\pi^2)$ ,  $\mathcal{P}_{110} = \sqrt{2}/(4\pi^2)$ , and  $\mathcal{P}_{111} = 27/(8\pi^2)$  (see SM [42]). The Bogoliubov–de Gennes (BdG) eigenvalues are

$$\lambda_{n\mathbf{k}} = \sqrt{E_{n\mathbf{k}}^2 - U^2 \Delta^2 f_{n\mathbf{k}}^2(z_0)}, \quad (5)$$

where  $f_{n\mathbf{k}}(z_0) = \sum_{\alpha\sigma} |c_{\mathbf{k}z\alpha\sigma}^n|^2 e^{-z/z_0}$  weights the normal-state eigenvector across the slab.

The critical interaction  $U$  is obtained from the superconducting instability in the limit  $\Delta \rightarrow 0$ , imposing

$$\frac{\partial^2 F}{\partial G^2} = 0, \quad \frac{\partial F}{\partial z_0} = 0,$$

with  $G = U \Delta$ .

For phonon-mediated pairing mechanism Eq. (4) can be written as

$$F(z_0) \approx 3 \frac{G^2}{U} \frac{1 - e^{-2N_L/z_0}}{1 - e^{-2/z_0}} - G^2 \frac{\mathcal{P}}{2} \rho(z_0) \int_{-\omega_i}^{\omega_i} \frac{dE}{E} \tanh\left(\frac{\beta E}{2}\right), \quad (6)$$

where

$$\rho(z_0) = \sum_n \int d^2\mathbf{k} \delta(E_{n\mathbf{k}}) f_{n\mathbf{k}}^2(z_0) \quad (7)$$

is the density of states at the Fermi level weighted by the factor  $f_{n\mathbf{k}}^2(z_0)$ . Thus, the instability reflects a balance between the

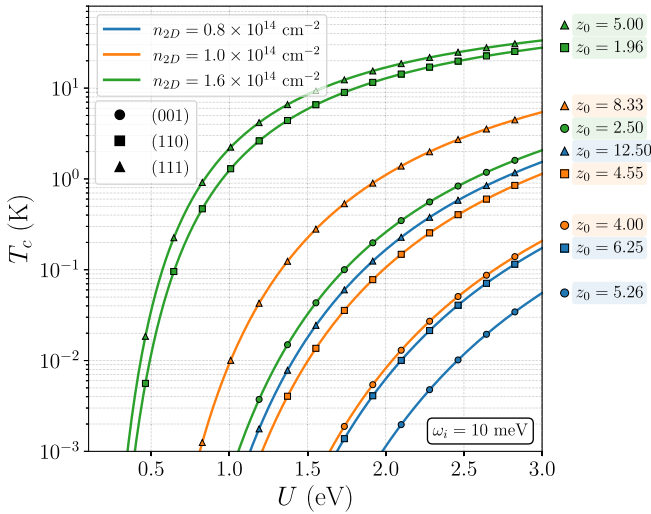


FIG. 6. Critical temperature  $T_c$  as a function of the interaction strength  $U$  for the (001) (circles), (110) (squares), and (111) (triangles) interfaces in the phonon-mediated pairing scenario. The self-consistent penetration length  $z_0$  is indicated at the end of each curve.

overlap-weighted DOS and the cost of extending the condensate across the slab.

Since  $U$  is fixed for all interfaces, the differences among the  $T_c$  we recover across different orientations arise purely from electronic properties. We use  $\hbar\omega_i = 10$  meV as a representative phonon scale, although  $\omega_i$  may also depend on the interface orientation [24,25]. The resulting  $T_c(U)$  is shown in Fig. 6.

At fixed electronic density, a clear hierarchy emerges among the three orientations: the (111) interface exhibits the highest  $T_c$  and the largest penetration length, while the (001) orientation shows the lowest critical temperature, namely

$$T_c^{(001)} < T_c^{(110)} < T_c^{(111)}.$$

Moreover, there exists a range of interaction strengths for which  $T_c^{(111)} \approx 1$  K,  $T_c^{(110)} \approx 0.1$  K, while the (001) interface does not display a superconducting instability within accessible temperatures, consistent with experimental data in Refs. [24,25]. Differences among the carrier densities in the various orientations—with the (111) interface typically hosting the largest two-dimensional electron density—may further enlarge the allowed range of  $U$ . Generally, increasing the electronic density leads to stronger confinement and a reduction in  $z_0$ . The role of inhomogeneity is indeed quite crucial: allowing for a spatially varying order parameter naturally captures the correct hierarchy of critical temperatures across different orientations, while also highlighting that the spatial extent of superconductivity can be sizable in these systems. In the SM [42] we present a representative case where the penetration depth  $z_0$  is not determined self-consistently, showing how this affects the results.

**Discussion.** We have systematically investigated the superconducting instability arising from the electronic properties of the 2DEG at (001), (110), and (111) KTaO<sub>3</sub>-based interfaces. To isolate the role of crystallographic orientation, we have employed a tight-binding model with identical bulk hopping

amplitudes for all three geometries. The self-consistent confining potential has been computed for a large number of layers, using the same dielectric function fitted to experimental ARPES data [15,18] and considering representative values of the positive interface density  $n_{2D}$ .

In the normal state, the (111) orientation exhibits the steepest electrostatic barrier, even though its 2DEG is less spatially confined. This unusual behavior arises from dominant out-of-plane hopping, unlike the (001) and (110) orientations where stronger in-plane dispersion promotes interface localization. The interplay between electronic screening and anisotropic dispersion ultimately produces a stronger electric field at the (111) interface.

We have studied the onset of superconductivity using an inhomogeneous mean-field singlet  $s$ -wave pairing interaction. Allowing the superconducting order parameter to vary across the slab, we reproduce the experimentally observed hierarchy of critical temperatures, with the (111) orientation consistently displaying the highest  $T_c$ . This hierarchy is robust across two limiting pairing scenarios: a phonon-mediated (retarded) mechanism and a local instantaneous (nonretarded) interaction, which provide a lower and upper bound on the superconducting instability within our model. In particular, in the retarded case the results do not depend sensitively on the choice of cutoff frequency, further supporting the geometric origin of the predicted hierarchy. Importantly, the hierarchy of critical temperatures is not set by the interfacial electric field alone. Although the (111) interface has the strongest field, its superconducting profile is more extended across the slab. Thus,  $T_c$  is controlled not simply by electrostatic confinement, but by the redistribution of low-energy spectral weight and its overlap with the layer-dependent pairing profile.

In contrast to standard hard-wall descriptions of confinement-induced superconductivity [50–53], our mechanism relies on the smooth spatial variation of the confining potential, emphasizing the role of geometry-dependent confinement and a multiorbital band structure in oxide-interface superconductivity. This is consistent with experiments on LaAlO<sub>3</sub>/SrTiO<sub>3</sub>, where superconductivity correlates with the occupation of confinement-induced subbands and with the shape of the confining potential, rather than with carrier density alone [54].

Both the normal-state analysis and the superconducting treatment have allowed us to isolate the effects arising purely from geometric constraints and electronic structure, showing that this mechanism is sufficient to account for the qualitative hierarchy of  $T_c$  without introducing orientation-dependent microscopic parameters. In realistic systems, however, additional effects may further enhance the differences among orientations. Different surface orientations may involve distinct impurity concentrations, low-temperature lattice distortions, hopping amplitudes, dielectric responses, phonon spectra, and carrier densities, with the (111) interface typically hosting the largest 2DEG density [24,25]. These effects may affect the hierarchy of  $T_c$  predicted here and should be included for a fully quantitative description. Another limitation concerns the spatial distribution of compensating charges. Here, the positive charge is assumed to be localized at the interface, whereas in real oxide interfaces donor defects and trapped electronic charges may extend into the substrate, modifying

the confinement potential [55,56]. Including these contributions in the Poisson equation, as well as a systematic treatment of back gating, is a natural extension of the present model and may quantitatively affect both  $T_c$  and the effective superconducting thickness. Our prediction could be further tested experimentally by extracting the effective superconducting thickness from the anisotropy of the upper critical field. In Ref. [32], a thickness  $d \approx 1.25$  nm was inferred for the (111) interface, consistent in order of magnitude with the characteristic extension  $z_0 \approx 5$  layers obtained in our benchmark calculation at  $n_{2D} = 1.6 \times 10^{14}$  cm $^{-2}$ .

Finally, our analysis has been restricted to singlet  $s$ -wave pairing. Although alternative pairing symmetries have been proposed for KTO-based systems [13,37,40],  $s$ -wave pairing is expected to remain the most robust channel in the experimentally relevant dirty regime, where higher-angular-momentum components are typically suppressed. More generally, the present framework is not tied to a specific symmetry of the order parameter. Its key ingredients—namely the multiorbital electronic structure and the finite dispersion along the  $z$  direction—govern the spatial extension of the 2DEG and thus directly affect the superconducting instability, by controlling both the spatial distribution of the condensate and the structure of the pairing kernel. The formalism can be straightforwardly generalized by considering more variational parameters and other pairing symmetries [57], allowing one to investigate how the symmetry of the

order parameter modifies both its spatial profile and the resulting instability, including in the dynamic regime [58,59]. In this context, confinement plays a central role by setting the spatial structure of the electronic states participating in pairing.

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*Data availability.* The data are available upon reasonable request from the authors.

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