

Rashba spin-orbit coupling in infinite-layer nickelate films on SrTiO₃(001) and KTaO₃(001)

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(Dated: March 2, 2023)

The impact of spin-orbit interactions in NdNiO₂/SrTiO₃(001) and NdNiO₂/KTaO₃(001) is explored by performing density functional theory simulations including a Coulomb repulsion term. Polarity mismatch drives the emergence of an interfacial two-dimensional electron gas in NdNiO₂/KTaO₃(001) involving the occupation of Ta 5*d* conduction-band states, which is twice as pronounced as in NdNiO₂/SrTiO₃(001). We identify a significant anisotropic k^3 Rashba spin splitting of the respective d_{xy} states in both systems that results from the broken inversion symmetry at the nickelate-substrate interface and exceeds the width of the superconducting gap. In NdNiO₂/KTaO₃(001), the splitting reaches 210 meV, which is comparable to Bi(111) surface states. At the surface, the Ni 3*d* _{x^2-y^2} -derived states exhibit a linear Rashba effect with $\alpha_R \sim 125$ meV Å, exemplifying its orbital selectivity. The corresponding Fermi sheets present a reconstructed circular shape due to the electrostatic doping, but undergo a Lifshitz transition towards a cuprate-like topology deeper in the film that coincides with a realignment of their spin texture. These results promote surface and interface polarity as interesting design parameters to control spin-orbit physics in infinite-layer nickelate heterostructures.

Spin-orbit coupling (SOC) correlates the electron spin and the crystal lattice and gives rise to a multitude of intriguing quantum phenomena. A prominent example is the Rashba effect [1], which originates from the broken inversion symmetry at interfaces and surfaces and is of fundamental relevance in spintronics, as it permits the electric control of the spin precession [2]. Moreover, it plays a key role in the quest to realize Majorana zero modes by exploiting the proximity effect between a material with strong SOC and a superconductor [3–5]. The pronounced coupling of lattice, orbital, spin, and charge degrees of freedom in transition metal oxides [6] renders them a particularly interesting platform to explore superconductivity in conjunction with a two-dimensional Rashba system. Paradigmatic is the LaAlO₃/SrTiO₃(001) interface [7–11], where the Rashba effect is considered to stabilize the emergent superconducting phase [12–14] and may reconcile superconductivity and magnetism [15, 16].

The very recent observation of superconductivity in Sr-doped NdNiO₂, PrNiO₂, and LaNiO₂ films grown on SrTiO₃(001) (STO) [17–20] sparked considerable interest in 3*d*⁹ infinite-layer (*ABO*₂) nickelates, which are formally isoelectronic to the cuprates [21–43]. However, superconductivity remained elusive in the respective bulk compounds so far [44, 45]. Early work unraveled the key role of the polar interface [46–50]: The polarity mismatch drives the formation of a two-dimensional electron gas (2DEG) in the substrate by occupation of the interfacial Ti 3*d* states [46, 50] that is considerably more pronounced than in LaAlO₃/STO(001) [10]. Therefore, these artificial oxides naturally host a 2DEG proximate to a novel class of superconductor.

An intriguing alternative to STO is KTaO₃ (KTO), which exhibits stronger spin-orbit interactions [51] and attracts increasing attention due to the emergence of superconductivity at different (111) and (110) heterointerfaces [52–54]. Moreover, 2DEGs have been reported in a variety of (001)-oriented perovskite systems [55–57].

Here we explore the impact of spin-orbit interactions in NdNiO₂/STO(001) and NdNiO₂/KTO(001) by performing density functional theory simulations including a Coulomb repulsion term in explicit film geometry. The distinct polar discontinuity at the Nd³⁺/(TiO₂)⁰ versus Nd³⁺/(TaO₂)¹⁺ interface results in the formation of a twice as pronounced 2DEG in the KTO system by occupation of Ta 5*d* conduction-band states, predominantly d_{xy} , which is accompanied by ferroelectric-like displacements of the Ta ions in the substrate. We find that the broken inversion symmetry at the surface and the interface gives rise to an anisotropic Rashba spin splitting that exceeds the size of the superconducting gap. Surprisingly, it reaches values at the KTO interface that are comparable to Bi(111) surface states. The Ti and Ta d_{xy} orbitals in the substrate exhibit a fundamentally different response to SOC than the Ni 3*d* _{x^2-y^2} orbitals in the film, i.e., a predominantly cubic versus linear momentum dependence of the spin splitting. We observe a substantial reconstruction of the Ni 3*d* _{x^2-y^2} -derived Fermi sheets at the surface due to the electrostatic doping, suggesting local modifications of the pairing mechanism. Layer-wise tracking of these states throughout the nickelate film unveils a Lifshitz transition towards a cuprate-like topology that coincides with a reorientation of their spin texture. These insights exemplify the impact of surface and interface polarity on spin-orbit-driven phenomena in infinite-layer nickelate heterostructures.

Methodology. – We performed first-principles simulations in the framework of density functional theory (DFT [58]) as implemented in the *Vienna Ab initio Simulation Package* (VASP) [59, 60], employing the PBE exchange-correlation functional [61] and a wave-function cutoff of 520 eV. Static correlation effects were considered within the DFT+*U* formalism [62, 63] employing $U - J = 3$ eV at the Ni and Ti sites and $U - J = 1$ eV at the Ta sites, similar to previous work [25, 46, 50, 64–71]. Subsequent to a self-consistent calculation, we shift to a spinor representation, account for spin-orbit interactions, and thus obtain an updated electronic structure.

(NdNiO₂)₄/STO(001) and (NdNiO₂)₄/KTO(001) are mod-

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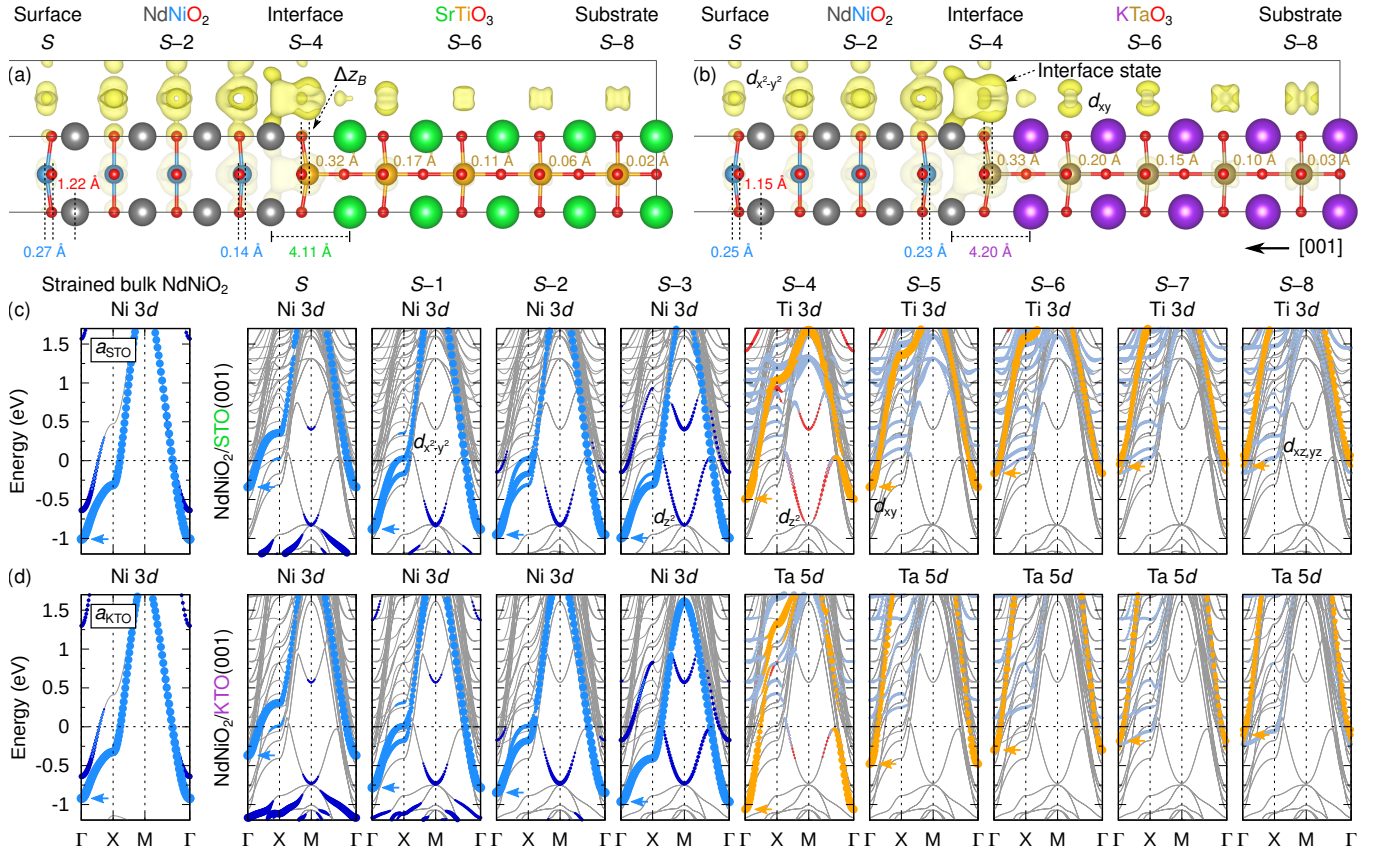


Figure 1. Optimized geometry of (a) (NdNiO₂)₄/STO(001) [46] and (b) (NdNiO₂)₄/KTO(001), together with the electron density integrated between -0.75 eV and the Fermi energy. (c,d) The corresponding layer-resolved band structures (here from DFT+ U without SOC) show the polarity-driven emergence of an interfacial 2DEG in both substrates by occupation of Ti 3d and Ta 5d conduction-band states, respectively (orange arrows), as well as the electrostatic modulation of the Ni 3d states in the polar infinite-layer nickelate film (blue arrows). Light- and dark-blue bands depict Ni $d_{x^2-y^2}$ and d_{z^2} states; orange, gray-blue, and red bands depict Ti and Ta d_{xy} , $d_{x^2-y^2}$, and d_{z^2} states; and the thin gray lines represent the total band structure of the supercells. Results for strained bulk NdNiO₂ are provided as reference (left panels).

eled in explicit film geometry by using tetragonal supercells, fixing the in-plane lattice parameter to $a_{\text{STO}} = 3.905$ Å and $a_{\text{KTO}} = 3.988$ Å [54], respectively. The supercells are symmetric, consisting in total of 9.5 unit cells of substrate, 4 + 4 unit cells of infinite-layer nickelate film, and about 20 Å of vacuum region.

The Brillouin zone was sampled employing a $16 \times 16 \times 1$ Monkhorst-Pack $\vec{k}$ -point grid [72] in conjunction with a Gaussian smearing of 0.005 Ry. The ionic positions were accurately optimized, reducing ionic forces below 1 mRy/a.u.

Ionic relaxations and electronic reconstruction. – Figures 1(a) and (b) show the optimized geometry of (NdNiO₂)₄/STO(001) [46] and (NdNiO₂)₄/KTO(001), respectively. The apical A-site distances are significantly enhanced at the interface (S-4) to $d_{\text{Nd-Sr}} = 4.11$ Å for STO and even $d_{\text{Nd-K}} = 4.20$ Å for KTO. This observation can be attributed to the electrostatic doping [46] and resembles the increased La-Sr distance at the n -type LaNiO₃/STO(001) interface (~ 4.06 Å) [66, 73, 74]. Conversely, the distance between the surface NiO₂ layer (S) and the subsurface Nd layer is considerably contracted to $d_{\text{Nd-O}} = 1.22$ Å (STO) and

1.15 Å (KTO).

Both systems exhibit a prominent buckling of the NiO₂ layers at the surface (S) [Figs. 1(a,b)], the Ni ions being displaced outwards from the respective oxygen layer by $\Delta z_B = 0.27$ Å (STO) and 0.25 Å (KTO). At the interface (S-3), the Ni displacements point inwards and are more distinct, i.e., 0.14 Å (STO) and 0.23 Å (KTO). Furthermore, the Ti and Ta ions show a sizable inwards ferroelectric-like displacement of $\Delta z_B \sim 0.3$ Å in layer S-4 that decays with increasing distance from the interface. Close comparison of the two systems reveals consistently larger displacements Δz_B in the KTO substrate, even though bulk KTO is cubic and paraelectric down to at least 4.2 K [54, 75, 76]. In summary, these results point to a substantial difference between the two materials combinations.

The vertical ionic displacements are a sensitive response to the internal electric fields [46, 50]. This becomes evident in Figs. 1(c) and (d), which compare the layer-resolved DFT+ U electronic structure of the two systems. Similar to NdNiO₂/STO(001), the polar discontinuity at the NdNiO₂/KTO(001) interface drives the formation of a 2DEG

due to the occupation of Ta 5d conduction-band states in the substrate, predominantly the planar d_{xy} orbitals, which are bent down by -1.06 eV at the Γ point in layer $S - 4$. This electronic reconstruction and the orbital order present at the Ti and Ta sites are clearly visible in the electron density [Figs. 1(a,b)]. For comparison, the respective Ti 3d states bend down by -0.49 eV (-0.55 eV in Ref. [46]). The strongly enhanced Ta 5d occupation relative to Ti 3d can be traced back to the distinct $3+/1+$ versus $3+/0$ interface polarity. The band bending decays exponentially with increasing distance from the interface, paralleling the evolution of the ferroelectric-like displacements Δz_B . Hence, the potential well confining the 2DEG is considerably more asymmetric in NdNiO₂/KTO(001) than in NdNiO₂/STO(001). A concomitant electrostatic modulation of the Ni 3d states leads to an overall charge depletion (hole doping) in the polar films for both systems, particularly near the surface [Figs. 1(c,d)].

Anisotropic and orbital-selective Rashba effect. – We now explore the impact of SOC on the electronic structure at the surface of the nickelate film and in the 2DEG near the interface, where the electronic reconstruction is most pronounced. The polar discontinuities result in strong electric fields perpendicular to the basal conduction plane that are perceived as magnetic fields by a moving electron and thus couple to its spin. Specifically, this gives rise to the Rashba effect, which can be described by $H_R = \alpha_R(\vec{e}_z \times \vec{k}) \cdot \vec{\sigma}$, where $\vec{\sigma}$ is the Pauli vector and α_R is the Rashba coupling constant. The latter is a measure of the SOC strength and depends on the local electric fields [77]. It lifts the spin degeneracy of the bands and manifests as a linear splitting $\Delta(k) = 2\alpha_R k$ for a free-electron 2DEG model. First-principles simulations provide a more comprehensive perspective and allow us to explore the Rashba effect layer resolved, specifically the aspect of anisotropy, higher-order k^3 effects, and the distinct response of the different transition-metal d orbitals.

Figure 2(a) shows the Ni- $3d_{x^2-y^2}$ -derived surface state in layer S , exemplarily for NdNiO₂/STO(001); we obtained similar results for NdNiO₂/KTO(001). The characteristic Rashba shape emerges around the Γ point in the basal plane: The quasi-parabolic band splits into two distinct cones of opposite spin (represented here by different colors). The spin splitting is anisotropic, reflecting the fourfold D_{4h} symmetry of the structure, and amounts to $\Delta = 33$ meV along Γ -X and 36 meV along Γ -M at the Fermi level. This corresponds to a wave vector of $\Delta k_{\parallel} \sim 0.02 \text{ \AA}^{-1}$, which is surprisingly larger than $\Delta k_{\parallel} \sim 0.01 \text{ \AA}^{-1}$ calculated for the polar KTO(001) surface [51], even though NdNiO₂ consists of much lighter elements and shows negligible impact of SOC in the bulk [78].

Next, we investigate the state in the first substrate layer [$S - 4$; Figs. 2(b) and (c)]. Around the Γ point, it exhibits a quasi-parabolic dispersion, indicative of the 2DEG, and predominantly d_{xy} orbital character. In NdNiO₂/STO(001) [Fig. 2(b)], the Rashba splitting at the Fermi level amounts to $\Delta = 16$ meV along Γ -X and 11 meV along Γ -M, which is smaller than the results obtained for the surface state. Interestingly, along Γ -M, the bands bend down again after initially rising to ~ 0.05 eV, concomitantly changing their predomi-

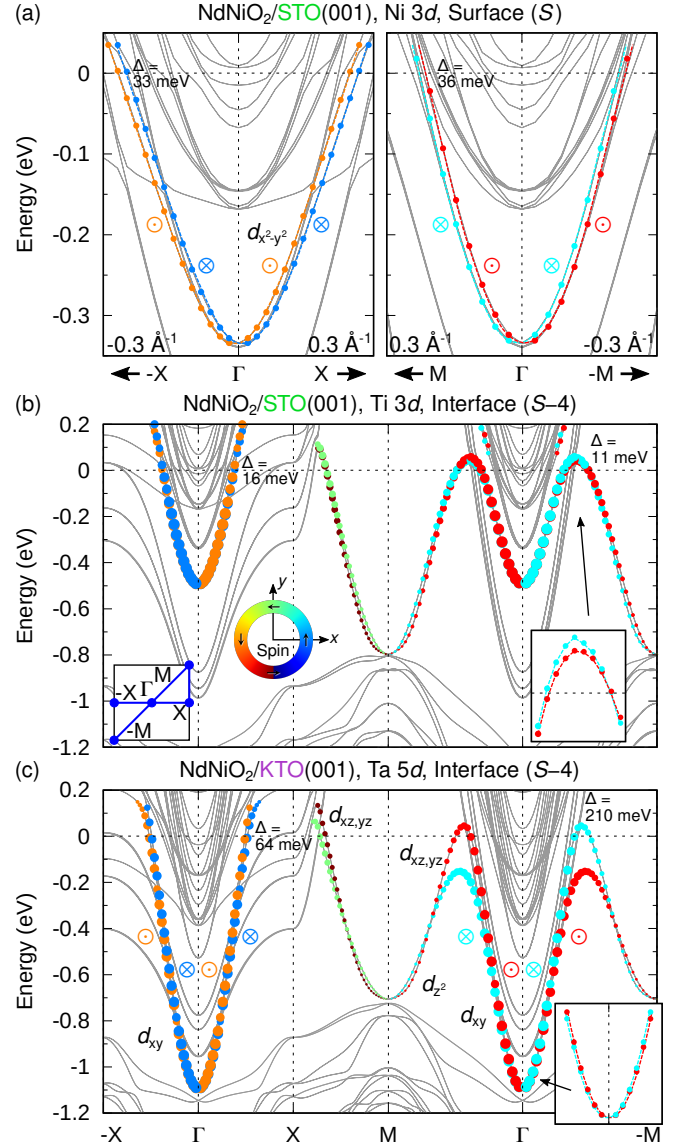


Figure 2. DFT+U+SOC surface and interface electronic structure in NdNiO₂/STO(001) and NdNiO₂/KTO(001). The colored points represent the orbital projections, while the color encodes the spin direction in the xy plane. The splitting of bands with opposite spin is clearly visible (e.g., blue vs. orange and cyan vs. red points). (a) The Ni- $3d_{x^2-y^2}$ -derived surface state (S), plotted exemplarily for NdNiO₂/STO(001) along two directions, displays the characteristic Rashba shape around the Γ point. (b,c) The interface state ($S - 4$) exhibits a similar effect, but with a massively boosted splitting in NdNiO₂/KTO(001). Intriguingly, the outer Ta 5d cone does not cross the Fermi energy along Γ -M, in sharp contrast to the inner cone. This behavior is fundamentally distinct from NdNiO₂/STO(001).

nant orbital character from Ti d_{xy} to Ti $d_{xz,yz}$ and finally to Ni d_{z^2} at the M point. In contrast, the corresponding state in layer $S - 5$ presents a consistently parabolic dispersion around the Γ point [cf. Figs. 1(c,d)].

For NdNiO₂/KTO(001) [Fig. 2(c)], the dispersion of the interface state is qualitatively similar to NdNiO₂/STO(001). However, the splitting along Γ -X is considerably enhanced

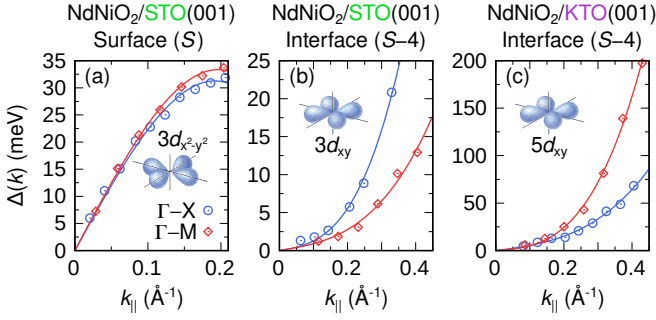


Figure 3. Momentum-resolved spin splitting $\Delta(k)$ around the Γ point for selected layers of (a,b) $\text{NdNiO}_2/\text{STO}(001)$ and (c) $\text{NdNiO}_2/\text{KTO}(001)$ from DFT+ U +SOC (symbols; cf. Fig. 2). The lines represent fits to $\Delta(k) = 2\alpha_R k + 2\tilde{\alpha}_R k^3$ (Table I). The qualitative differences between the three panels reflect the orbital selectivity of the anisotropic Rashba effect at the surface versus interface, as well as the role of lighter versus heavier substrate elements.

to $\Delta = 64$ meV, which is four times as high as for the STO system. This demonstrates that shifting from $Z_{\text{Ti}} = 22$ to $Z_{\text{Ta}} = 73$ promotes the impact of SOC substantially. An additional contribution stems from the stronger asymmetry of the confining potential well in $\text{NdNiO}_2/\text{KTO}(001)$ owing to the distinct interface polarity [Fig. 1(d)]. Intriguingly, we observe a spin splitting of $\Delta = 210$ meV along Γ - M , which is 19 times as high as for the STO system and reminiscent of $\text{Bi}(111)$ surface states (~ 0.2 eV [79]; $Z_{\text{Bi}} = 83$). Even the shape of the spin-split bands bears striking resemblance to $\text{Bi}(111)$. A notable difference, however, is the suppressed contribution of the counter-clockwise Ta $5d$ cone to the Fermi surface, in sharp contrast to the clockwise cone [Fig. 2(c)]. We verified this result, which is fundamentally distinct from $\text{NdNiO}_2/\text{STO}(001)$, by performing fully self-consistent SOC calculations. Compellingly, the pristine KTO(001) surface lacks a comparable effect and exhibits a much smaller spin splitting [51].

Motivated by this observation, we analyze the momentum-resolved spin splitting $\Delta(k)$ of the states shown in Fig. 2 along two directions from the Γ point to roughly the Fermi wave

vector k_F in Fig. 3. The data points show a clear nonlinearity, but can be accurately fitted to $\Delta(k) = 2\alpha_R k + 2\tilde{\alpha}_R k^3$ despite the broad k range. The three panels reveal the complexity of the Rashba effect in infinite-layer nickelate heterostructures. First, they underpin that $\Delta(k)$ is anisotropic and generally more pronounced along Γ - M . Surprisingly, $\text{NdNiO}_2/\text{STO}(001)$ shows an inverted behavior in layer $S-4$, with a stronger splitting along Γ - X [Fig. 3(b)]. Second, the $d_{x^2-y^2}$ -derived states in the nickelate film exhibit a fundamentally distinct response to SOC than the d_{xy} -derived states in the substrate, albeit both are planar. At the surface, the linear term is very strong ($\alpha_R \sim 125$ meV $\text{\AA}$, Table I). Simultaneously, $\tilde{\alpha}_R \sim -1.1$ eV $\text{\AA}^3$ is highly negative due to a profound nonlinearity for $k > 0.1$ $\text{\AA}^{-1}$ [Fig. 3(a)]. In sharp contrast, the substrate layers feature a dominant k^3 term with positive $\tilde{\alpha}_R$ [Figs. 3(b,c), Table I]. The linear term is at least one order of magnitude smaller than at the surface and decays with increasing distance to the interface. Despite this orbital selectivity, α_R is not fully quenched by symmetry, as suggested for the KTO(001) surface [51]. Finally, the role of heavier versus lighter substrate elements manifests in massively enhanced Rashba constants α_R and $\tilde{\alpha}_R$ near the $\text{NdNiO}_2/\text{KTO}(001)$ interface (Table I), in line with the boosted splittings Δ discussed above. For instance, α_R differs by one order of magnitude. Interestingly, the massive splitting of 210 meV observed along Γ - M in the KTO system is perfectly captured by the fit [Fig. 3(c)] and thus emerges as strong nonlinear k^3 response ($\tilde{\alpha}_R \sim 1.2$ eV $\text{\AA}^3$) of the d_{xy} orbitals.

At the $\text{NdNiO}_2/\text{KTO}(001)$ interface, α_R reaches ~ 24 meV $\text{\AA}$ (Table I), which compares favorably to ~ 20 meV $\text{\AA}$ for $\text{LaAlO}_3/\text{STO}(001)$ determined from magnetotransport measurements [13]. Moreover, all Rashba splittings observed here exceed ~ 4 meV reported for $\text{LaAlO}_3/\text{STO}(001)$ [13]. In particular, they are one or two orders of magnitude larger than the superconducting gap, which amounts to 2-4 meV in 12-25% Sr-doped NdNiO_2 films on $\text{STO}(001)$ according to scanning tunneling spectroscopy [29]. Therefore, spin-orbit effects turn out to be a key ingredient in describing the interactions between the superconducting infinite-layer nickelate film and the 2DEG in the substrate.

Lifshitz transition and spin texture. – Finally, we investigate the Fermi surface and the corresponding spin texture of $\text{NdNiO}_2/\text{STO}(001)$ and $\text{NdNiO}_2/\text{KTO}(001)$. Figure 4 disentangles the d -orbital contributions from subsequent BO_2 layers, similar to the layer-resolved band structure in Fig. 1. Owing to the electrostatic doping, each layer exhibits a distinct sheet of unique shape. Spin-orbit interactions generally split each contribution into two sheets of opposite spin, e.g., clockwise versus counter-clockwise spin rotation, which is indicative of the underlying Rashba spin-orbit physics [80].

At the surface of the nickelate film (S), we observe a significantly reconstructed Ni- $3d_{x^2-y^2}$ -derived sheet of almost circular shape centered around the Γ point. The reconstruction can be attributed to the electrostatic doping and suggests a substantial modification of the the local pairing mechanism (e.g., to s -wave [81]), which may be key in the interpretation of scanning tunneling spectroscopy results [29]. This is

Table I. Rashba constants α_R (meV $\text{\AA}$) and $\tilde{\alpha}_R$ (meV $\text{\AA}^3$) obtained by fitting the DFT+ U +SOC data for the surface and two substrate layers near the interface (cf. Fig. 3). Additionally, the corresponding spin splitting energy Δ (meV) at the Fermi level is provided.

System Layer	Orbital	— Γ - X —			— Γ - M —		
		Δ	α_R	$\tilde{\alpha}_R$	Δ	α_R	$\tilde{\alpha}_R$
NdNiO ₂ /STO(001)							
S	Ni $3d_{x^2-y^2}$	33	123	-1116	36	128	-1107
$S-4$	Ti $3d_{xy}$	16	3.9	251	11	3.8	79
$S-5$	Ti $3d_{xy}$	8	2.4	278	10	1.5	405
NdNiO ₂ /KTO(001)							
S	Ni $3d_{x^2-y^2}$	32	119	-1092	35	123	-1052
$S-4$	Ta $5d_{xy}$	64	24	355	210	14	1185
$S-5$	Ta $5d_{xy}$	15	14	409	36	11	972

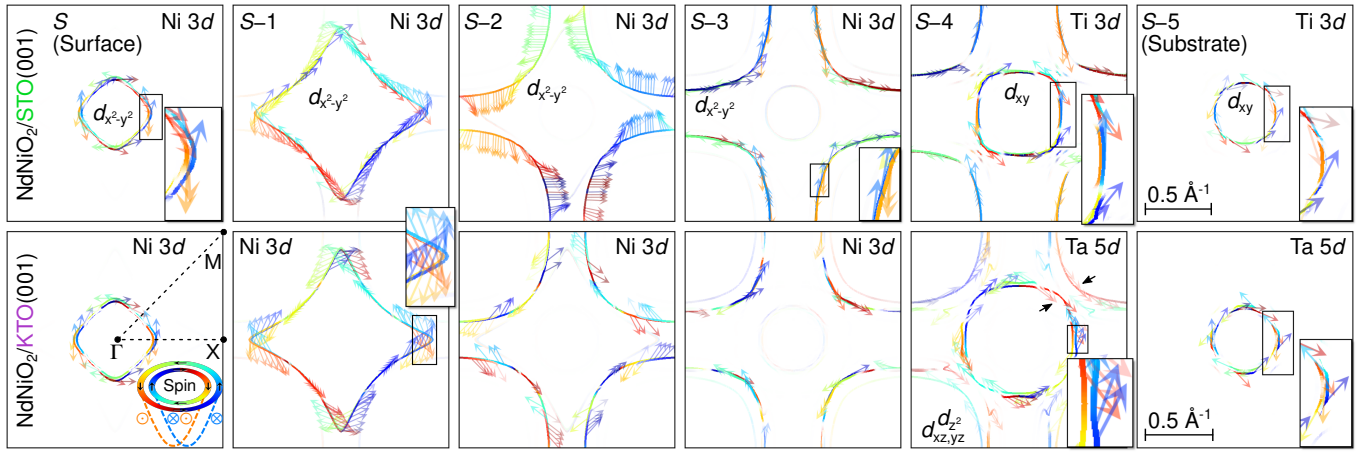


Figure 4. Layer-resolved Fermi surface of $(\text{NdNiO}_2)_4/\text{STO}(001)$ (top) and $(\text{NdNiO}_2)_4/\text{KTO}(001)$ (bottom). The line intensity represents the respective d orbital character, whereas the color and arrows indicate the basal spin direction (cf. Fig. 2). The reconstructed $\text{Ni } 3d_{x^2-y^2}$ -derived Fermi sheet at the surface undergoes a Lifshitz transition towards a cuprate-like topology deeper in the film, accompanied by a realignment of the spin texture. Spin-orbit interactions generally split each contribution into two distinct sheets of opposite spin. An exception are the 'single-band' zones along Γ - M resulting from the suppression of the counter-clockwise Ta $5d$ cone at the interface [black arrows; cf. Fig. 2(c)].

of particular relevance since, based on these measurements, it has recently been argued that the superconductivity in infinite-layer nickelates is of conventional type [82]. On the other hand, the considerable Ni-O buckling at the surface (cf. Fig. 1) rather evokes parallels to Fe-based superconductors [83].

From layer $S-1$ to layer $S-2$, a topological transition of the Fermi sheets to a cuprate-like shape occurs. This Lifshitz transition [84] is accompanied by a reorientation of the spins, which ultimately form a closed loop around the M point ($S-3$). The Fermi sheets are degenerate for layer $S-2$, whereas layers $S-1$ and $S-3$ present a clear Rashba splitting.

At the interface ($S-4$), the d_{xy} -derived 2DEG sheets centered around the Γ point are combined with $d_{xz,yz}$ and d_{z^2} contributions centered around the M point. The enhanced splitting in $\text{NdNiO}_2/\text{KTO}(001)$ is clearly visible (cf. Table I). Interestingly, 'single-band' zones emerge along Γ - M due to the suppression of the counter-clockwise Ta $5d$ cone [black arrows in Fig. 4]. In turn, weak $d_{xz,yz}$ signatures appear around the X point that are absent in the STO system. The overall shape of the Fermi sheet and its spin texture is reminiscent of the oxygen-deficient (i.e., n -type) $\text{STO}(001)$ surface [85]. Finally, layer $S-5$ presents a quasi-circular Rashba-split 2DEG sheet of exclusive d_{xy} character centered around the Γ point.

Summary. – We investigated the impact of spin-orbit interactions in $\text{NdNiO}_2/\text{SrTiO}_3(001)$ and $\text{NdNiO}_2/\text{KTaO}_3(001)$ in explicit film geometry. First-principles simulations unraveled that the distinct polarity mismatch at the $\text{Nd}^{3+}/(\text{TiO}_2)^0$ versus $\text{Nd}^{3+}/(\text{TaO}_2)^{1+}$ interface results in the emergence of a two-dimensional electron gas (2DEG) in $\text{NdNiO}_2/\text{KTaO}_3(001)$ that is twice as pronounced as in $\text{NdNiO}_2/\text{SrTiO}_3(001)$ and involves the occupation of Ta $5d$ conduction-band states, pre-

dominantly d_{xy} . Ferroelectric-like displacements of the Ta ions in the substrate act as a fingerprint of this electronic reconstruction. We identified an anisotropic Rashba spin splitting of the states at the surface and the interface that exceeds the size of the superconducting gap, which establishes spin-orbit effects as crucial ingredient in describing the superconductor–2DEG coupling. At the KTaO_3 interface, the splitting reaches 210 meV, which is reminiscent of $\text{Bi}(111)$ surface states. The predominantly cubic momentum dependence of the spin splitting exhibited by the substrate Ti and Ta d_{xy} states contrasts with a strong linear component presented by the Ni $3d_{x^2-y^2}$ orbitals in the film, which exemplifies the orbital selectivity of the Rashba effect. Finally, we observed a reconstructed, quasi-circular Ni $3d_{x^2-y^2}$ -derived Fermi sheet at the surface owing to the electrostatic doping, which undergoes a Lifshitz transition towards a cuprate-like topology and a concomitant realignment of its spin texture deeper in the film. These results suggest surface and interface polarity as promising control parameters to tune spin-orbit physics in infinite-layer nickelate heterostructures.

ACKNOWLEDGMENTS

This work was funded by the National Science Foundation via grant No. NSF-DMR-2118718, which is gratefully acknowledged. The author thanks Armin Sahinovic, Dr. Okan Köksal, Prof. Rossitza Pentcheva, Prof. Richard Hennig, and Prof. Peter Hirschfeld for their support and numerous discussions.

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