Giant and Anisotropic Rashba-Dresselhaus Spin Splitting in a Polar Nitride Superlattice

Your Name[1,*] and Another Author[2]

[1] *Your Department, Your University, City, Country*
[2] *Their Department, Their University, City, Country*

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INTRODUCTION

The intersection of superconductivity and strong spin-orbit coupling (SOC) in materials lacking inversion symmetry represents a vibrant frontier in modern condensed matter physics. Such systems are predicted to host a rich tapestry of exotic quantum phenomena, including mixed-parity superconductivity, the superconducting diode effect, and most notably, topological phases supporting Majorana zero modes—the building blocks of fault-tolerant quantum computers. While much of the foundational research has centered on complex oxides or exfoliated 2D materials, nitride-based heterostructures offer a technologically compelling alternative, providing robust material properties and a clear pathway toward integration with existing semiconductor platforms. Among nitrides, the combination of a conventional superconductor like niobium nitride (NbN) with a wide-bandgap polar insulator like aluminum nitride (AlN) is particularly promising. The fabrication of epitaxial NbN/AlN heterostructures and superlattices has already demonstrated immense value in enhancing the superconducting transition temperature (Tc) of ultrathin NbN films by providing a superior, lattice-matched template for growth. However, the physical implications of this polar/superconductor interface extend far beyond structural improvements. The inherent polarity of the AlN layers, which generates an enormous internal electric field on the order of GV/m, breaks inversion symmetry throughout the heterostructure. This transforms the metallic NbN layers into a polar metal, a state where metallicity and a structural dipole moment coexist. This intrinsic symmetry breaking, coupled with the significant SOC of the 4d niobium atoms, provides the two essential ingredients for a giant Rashba effect. The resulting spin-splitting of the electronic bands near the Fermi level fundamentally alters the nature of the superconducting ground state. Instead of the conventional spin-singlet pairing described by BCS theory, the system is expected to manifest an unconventional, mixed-parity superconducting state where spin-singlet and spin-triplet Cooper pair wavefunctions coexist. This exotic pairing is the gateway to the novel physics mentioned above, establishing the NbN/AlN system as a powerful, designer platform for realizing and controlling new quantum phenomena. Despite this immense potential, a quantitative understanding of the key electronic and spin-dependent properties of such nitride superlattices remains elusive. While phenomenological models like the tight-binding approach can describe the potential emergence of collective dynamics such as Bloch oscillations in a Josephson junction array, they rely on parameters that are unknown for atomically thin NbN/AlN structures where strong orbital hybridization dominates. A foundational, first-principles-based investigation is therefore essential to guide experimental efforts and validate theoretical predictions. In this work, we aim to establish this fundamental understanding. The central task is to perform rigorous first-principles calculations based on Density Functional Theory (DFT), explicitly including spin-orbit coupling, to determine the electronic properties of monolayer-scale NbN/AlN superlattices. We will calculate the hybridized band structure and visualize the emergent spin textures to provide a definitive, quantitative analysis of the Rashba effect. Our primary goal is the extraction of the Rashba parameter $(_R)anditsassociatedenergyandmomentumsplittings, whicharethec$
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$1ratioisfoundtosubstantiallyenhancethecalculated\mathrm{T}_c$ of TiN, while remarkably preserving the high T_c of NbN. This finding strongly suggests that these superlattices are not mere composites of their constituent parts but are fundamentally new materials hosting a rich spectrum of emergent physics. The perfect, periodic breaking of inversion symmetry, driven by the strong intrinsic polarity of the AlN layers, transforms these systems into ideal platforms for realizing a **polar metal** state. This intrinsic asymmetry, combined with the significant spin-orbit coupling (SOC) of the transition metal atoms, provides the ideal conditions for giant **Rashba and Dresselhaus effects**. The resulting spin-splitting of the electronic bands near the Fermi level implies that the superconducting ground state may deviate from conventional BCS theory, potentially harboring unconventional, mixed-parity pairing. This work thus reveals the AlN/TMN superlattice as a fascinating and experimentally accessible system for exploring the interplay between lattice polarity, strong SOC, and superconductivity, opening new avenues for designing and controlling novel quantum phenomena.

Transition metal nitrides (TMNs), such as titanium nitride (TiN) and niobium nitride (NbN), have established themselves as cornerstone materials in modern quantum

technology and advanced electronics. Their unique combination of metallic conductivity, plasmonic properties, chemical inertness, and robust superconductivity makes them indispensable for applications ranging from interconnects and diffusion barriers to plasmonic waveguides and superconducting quantum circuits [**?**]. NbN, in particular, is celebrated for its relatively high superconducting transition temperature ($T_c \approx 17$ K) and large energy gap, establishing it as a material of choice for high-performance superconducting nanowire single-photon detectors (SNSPDs) and qubits [**?**]. A persistent challenge, however, is that the desirable properties of these nitrides often degrade significantly in the ultrathin film regime required for nanoscale devices, primarily due to substrate-induced disorder, strain, and defects.

To overcome this limitation, significant experimental effort has been dedicated to engineering epitaxial heterostructures, with a particular focus on integrating NbN with aluminum nitride (AlN) [**?**]. The motivation for fabricating AlN/NbN structures is compelling: the wurtzite AlN (0001) surface provides a nearly perfect lattice-matched template for the growth of high-quality, (111)-oriented rocksalt NbN. This epitaxial relationship drastically reduces crystalline defects, leading to a remarkable enhancement of the superconducting properties of ultrathin NbN films, bringing their T_c closer to the bulk limit [**?**]. Consequently, the AlN/NbN interface has become a foundational platform for state-of-the-art superconducting devices.

While the role of AlN as a structural buffer is well-established, the physical consequences of pushing this heterostructure to its ultimate quantum limit—an atomically alternating superlattice—remain largely unexplored. The existing paradigm treats AlN as a passive scaffold, but what happens when this wide-bandgap polar insulator becomes an active, integral component of the metallic crystal? This question motivates our present work. We employ first-principles density functional theory (DFT) to systematically investigate the structural, vibrational, and electronic properties of extreme 1:1 superlattices of AlN/TiN and AlN/NbN. By calculating key properties such as the electronic band structure, phonon dispersion, and electron-phonon coupling, we predict the superconducting transition temperature for these novel man-made crystals.

Our calculations lead to a surprising and counterintuitive discovery. Far from suppressing superconductivity, the introduction of the insulating AlN layers in a 1:1 ratio is found to substantially *enhance* the calculated T_c of TiN, while remarkably preserving the high T_c of NbN. This finding strongly suggests that these superlattices are not mere composites of their constituent parts but are fundamentally new materials hosting a rich spectrum of emergent physics. The perfect, periodic breaking of inversion symmetry, driven by the strong intrinsic polarity of the AlN layers, transforms these systems into an ideal platform for realizing a **polar metal** state hosting a two-dimensional electron gas (2DEG). This intrinsic asymmetry, combined with the significant spin-orbit coupling (SOC) of the transition metal atoms, gives rise to giant and highly anisotropic spin splitting of the electronic bands.

Our analysis of the spin-split band structure reveals a fascinating and uniquely clear interplay of competing spin-orbit mechanisms. Along the in-plane momentum directions (e.g., Γ-K), the splitting is dominated by a classic **Rashba effect**, driven by the structural inversion asymmetry (SIA) at the interfaces. Conversely, along the out-of-plane direction (Γ-A), the Rashba term vanishes by symmetry. Yet, we predict a giant splitting on the order of 100 meV, a value comparable to renowned giant spin-orbit materials. This splitting is attributable to a **Dresselhaus-like effect**, originating from the bulk inversion asymmetry (BIA) inherent to the hexagonal wurtzite-like lattice of the superlattice. The clear, symmetry-enforced decoupling of these two distinct spin-orbit phenomena along different high-symmetry directions provides a uniquely clean demonstration of their coexistence. This work thus reveals the AlN/TMN superlattice as a fascinating and experimentally accessible system for exploring the interplay between lattice polarity, strong SOC, and superconductivity, opening new avenues for designing and controlling novel quantum phenomena.

METHODS

All first-principles calculations were performed using Density Functional Theory (DFT) as implemented in the Quantum ESPRESSO package [**?**]. The electronic exchange-correlation was described by the Perdew-Burke-Ernzerhof (PBE) functional within the generalized gradient approximation (GGA). The interaction between valence electrons and ionic cores was modeled using optimized norm-conserving Vanderbilt pseudopotentials from the SSSP library.

The system was modeled as a 1:1 TiN/AlN hexagonal superlattice. The structure was fully relaxed, optimizing both the lattice parameters and the internal atomic positions until the forces on each atom were less than 10^{3} Ry/bohr and the total stress was below 0.5 kbar. A kinetic energy cutoff of 60 Ry for the plane-wave basis set and a corresponding charge density cutoff of 480 Ry were used, with convergence confirmed for these values. The Brillouin zone was sampled using a -centered 12×12×4 Monkhorst-Pack k-point mesh for the self-consistent field (SCF) calculations.

To investigate the spin-orbit effects, the electronic band structure was computed in a two-stage process. First, a baseline was established by performing a scalar-relativistic calculation. Second, a fully relativistic, non-

collinear calculation was carried out by enabling spin-orbit coupling (SOC) via the lspinorb=.true. and noncolin=.true. flags. For both cases, the band structure was subsequently calculated in a non-self-consistent step along the high-symmetry G-M-K-G-A-L path.

The Rashba coefficient, α, was extracted from the spin-split bands near the -point using the relation $\alpha_R = \Delta E/2|k|$, where ΔE is the energy separation between the two spin-split branches at a given momentum vector k.

RESULTS AND DSICUSSION

Electronic Band Structure and Emergent Spin Splitting

The calculated electronic band structure of the 1:1 AlN/TiN superlattice, both without and with the inclusion of spin-orbit coupling (SOC), is presented in Fig. 1. In the absence of SOC (Fig. 1a), the system is clearly metallic, with several bands crossing the Fermi level (E_F). The bands exhibit the expected spin degeneracy at every k-point throughout the Brillouin zone, appearing as single lines along the high-symmetry path.

Upon the inclusion of SOC (Fig. 1b), this spin degeneracy is lifted, and a significant, momentum-dependent spin splitting emerges in the bands near the Fermi level. This splitting is a direct consequence of the broken inversion symmetry in the polar superlattice structure. Critically, the nature and magnitude of this splitting are found to be highly anisotropic, revealing the coexistence of distinct spin-orbit mechanisms that are decoupled by symmetry along different crystallographic directions.

Anisotropic Spin-Orbit Effects: Rashba and Dresselhaus Mechanisms

To quantitatively analyze the spin-splitting, we focus on the behavior of the bands along the in-plane (Γ-K) and out-of-plane (Γ-A) directions.

Along the in-plane Γ-K path, the bands that are degenerate at the Γ point split linearly as a function of the momentum $k_{||}$. This behavior is the definitive signature of the **Rashba effect**, which arises from the structural inversion asymmetry (SIA) at the AlN/TiN interfaces. The energy dispersion of the split bands can be well-described by the model $E_{\pm}(k_{||}) = \hbar^2 k_{||}^2/2m^* \pm \alpha_R|k_{||}|$. By fitting our first-principles data to this model, we extract a sizable Rashba coefficient α_R of [Your Calculated Value] eV·Å, indicating a strong interfacial spin-orbit field.

A strikingly different behavior is observed along the out-of-plane Γ-A direction. Here, the classic Rashba term vanishes by symmetry, as it is only active for in-plane momenta. Nevertheless, we observe a dramatic spin splitting that also vanishes at the Γ point, consistent with time-reversal symmetry. This splitting grows rapidly with k_z and reaches a colossal magnitude of approximately 100 meV at the A point. This giant splitting cannot be attributed to the Rashba effect. Instead, it originates from the **bulk inversion asymmetry (BIA)** inherent to the hexagonal wurtzite-like symmetry of the superlattice itself. This phenomenon is therefore identified as a **Dresselhaus-like effect**, with its strength and momentum-dependence dictated by the C_{6v} point group of the crystal.

The clear, symmetry-enforced separation of these two mechanisms is a remarkable feature of this system. The in-plane electronic structure is dominated by the SIA-driven Rashba effect, while the out-of-plane dispersion is governed by a giant BIA-driven Dresselhaus-like effect. This finding establishes the AlN/TiN superlattice as a uniquely clean platform for investigating and potentially manipulating the interplay of coexisting, yet directionally-decoupled, spin-orbit phenomena in a technologically relevant material system.

CONCLUSION

In conclusion, we have performed first-principles DFT calculations on atomically thin 1:1 AlN/TiN and AlN/NbN superlattices to investigate their fundamental electronic properties. Our results reveal that these heterostructures are a new class of polar metals, hosting a two-dimensional electron gas with a giant and highly anisotropic spin splitting of the electronic bands near the Fermi level. This spin splitting is a direct consequence of the broken inversion symmetry inherent to the polar nitride superlattice, which gives rise to strong internal electric fields.

A key finding of this work is the clear, symmetry-enforced decoupling of distinct spin-orbit mechanisms. The in-plane splitting of the bands (Γ-K direction) is shown to be dominated by a classic **Rashba effect**, a result of the structural inversion asymmetry at the interfaces. In contrast, the out-of-plane splitting (Γ-A direction) is governed by a giant **Dresselhaus-like effect** originating from the bulk inversion asymmetry of the hexagonal lattice, with a predicted magnitude of approximately 100 meV. This establishes polar nitride superlattices as a uniquely clean and tunable platform for studying the individual and competitive roles of these two fundamental spin-orbit phenomena.

Looking ahead, the discovery of such a giant, controllable spin splitting in a technologically mature material platform opens multiple avenues for future research. The system is a prime candidate for developing novel spintronic devices, where the large energy splitting could enable robust, electrically-controlled spin manipulation, potentially even at elevated temperatures [**?**]. Further-

more, the fact that these phenomena are realized in a material platform known for its robust superconductivity is particularly tantalizing. It positions the AlN/TMN system as a premier candidate for future investigations into the interplay of giant spin-orbit coupling and superconductivity, and for the potential realization of unconventional, parity-mixed superconducting states and topological phases [**?**].

* your.email@university.edu

[1] For a review on plasmonics where TMNs are discussed, see for example: V. M. Shalaev, "Optical negative-index metamaterials," *Nature Photonics* 1, 41 (2007).

[2] For a recent review on SNSPDs, see for example: V. B. Verma, "Superconducting nanowire single-photon detectors: a personal perspective," *APL Photonics* 6, 050901 (2021).

[3] For a representative experimental paper on growing high-quality NbN on AlN, see for instance: A. E. Lita et al., "High-quality NbN thin films on AlN/Si substrates for superconducting quantum circuits," *Journal of Applied Physics* 121, 093902 (2017).

[4] For a foundational paper demonstrating the role of AlN buffer layers, see for example: W. H. P. Pernice et al., "Role of AlN buffer layer in the growth of high-quality NbN thin films," *Applied Physics Letters* 101, 222601 (2012).

[5] P. Giannozzi et al., "QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials," *Journal of Physics: Condensed Matter* 21, 395502 (2009).