

RESEARCH ARTICLE

Multiferroic Tunnel Junctions With Noncollinear Antiferromagnetic Electrodes

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ABSTRACT

Multiferroic tunnel junctions (MFTJs), comprising magnetic electrodes and an ultrathin ferroelectric tunnel barrier, hold great promise for the application in nonvolatile memory devices. Conventional MFTJs employ ferromagnetic (FM) electrodes, which are inherently vulnerable to stray magnetic fields and exhibit relatively slow operating speed. Here, we show, based on theoretical calculations, the feasibility of MFTJs with noncollinear antiferromagnetic (AFM) electrodes, which are expected to greatly enhance their performance. We design a $\text{Mn}_3\text{GaN}/\text{BaTiO}_3/\text{Mn}_3\text{ZnN}$ MFTJ, where noncollinear AFM antiperovskites Mn_3GaN and Mn_3ZnN serve as the electrodes separated by a ferroelectric BaTiO_3 tunnel barrier. Our first-principles quantum-transport calculations reveal sizable tunneling electroresistance (TER) and tunneling magnetoresistance (TMR) effects arising from the reversal of electric polarization of the ferroelectric barrier or the AFM Néel vectors of the electrodes, leading to four distinct resistance states. These phenomena are well explained by two key mechanisms: ferroelectricity-induced modulation of the interfacial electronic states, which controls the momentum-resolved transmission and underpins the TER effect; and spin-dependent matching of bulk electrode states, which drives the TMR effect. Our work paves a new pathway to realize high-performance MFTJs based on noncollinear antiferromagnets.

1 | Introduction

Spintronic devices harness the electron's spin degree of freedom for information storage and processing, making them promising candidates for next-generation low-power computing technologies [1, 2]. A prominent class of spintronic devices, magnetic tunnel junctions (MTJs), consists of ferromagnetic (FM) electrodes separated by a nonmagnetic insulating barrier and is widely used in magnetic random-access memories and magnetic-

field sensors due to their large magnetoresistive effects [3–5]. During operation, an electric current becomes spin-polarized as it passes through the first FM electrode, with electron spins aligning along its magnetization direction. The spin-polarized electrons then tunnel through the insulating layer to the second FM electrode, where the tunneling conductance depends sensitively on the relative magnetization alignment of the two FM electrodes. This phenomenon, known as the tunneling magnetoresistance (TMR) effect, underpins the operation of MTJ devices [6–8].

Over recent decades, ferroelectric (FE) materials have emerged as an important class of functional materials because of their promising potential in various technological applications [9–12]. Their intrinsic switchable spontaneous polarization makes them ideal candidates as a barrier in FE tunnel junctions (FTJs). In such devices, the FE barrier is sandwiched between two distinct metal electrodes. Different screening lengths of the two metal electrodes create asymmetry in the potential profile for opposite FE polarization directions, leading to polarization-dependent modulation of the effective barrier height [13, 14]. Consequently, the tunneling conductance of the FTJ exhibits strong dependence on the polarization orientation, manifesting a tunneling electroresistance (TER) effect.

A multiferroic tunnel junction (MFTJ) is formed when an FTJ incorporates two different types of FM electrodes [15–17]. Unlike MagnetoElectric Spin–Orbit (MESO) logic device [18, 19], which relies on strong magnetoelectric coupling so that ferroelectric polarization directly switches magnetic order, typically yielding only two stable states, MFTJs work in a fundamentally different regime. In an MFTJ, the relative magnetization alignment of two FM electrodes as well as the FE polarization direction of the barrier are largely decoupled and can be independently controlled, which enables the simultaneous manifestation of the TMR and TER effects. Therefore, multiple nonvolatile resistance states can be achieved, making MFTJs particularly promising candidates for next-generation nonvolatile memory applications [20–22]. Remarkably, MFTJs using conventional materials have recently been realized to operate at room temperature [23]. However, conventional MFTJs inevitably suffer from the limitations associated with the stray fields and relatively slow spin dynamics intrinsic to ferromagnets.

In recent years, antiferromagnets have emerged as promising alternative electrodes in MTJs. They are free of stray magnetic fields, enabling much higher device density and minimal magnetic crosstalk. Meanwhile, they possess intrinsically ultrafast spin dynamics, allowing substantially faster Néel vector manipulation than conventional FM magnetization switching [24–27]. Substantial TMR values have been predicted theoretically in antiferromagnetic (AFM) tunnel junctions (AFMTJs), arising from symmetry-breaking electronic structures in the electrodes that enable momentum-dependent [28–31], sublattice-dependent [32, 33], or interface-dependent [34] transport spin polarization controllable by the AFM order parameter, i.e., the Néel vector. To date, however, only two experimental realizations of TMR using collinear AFM electrodes have been reported: one based on RuO_2 , which exploits transverse wave vectors ($k_{\parallel}$)-dependent spin splitting [35], and the other on $(\text{Fe,Co})_5\text{GeTe}_2$, which relies on interfacial spin polarization [36]. Notably, neither system exhibits TMR at room temperature, underscoring the need for further exploration of high-performance collinear AFM electrodes capable of sustaining robust TMR under ambient conditions.

On the contrary, noncollinear antiferromagnets—AFM materials that are characterized by three or more sublattices whose magnetic moments are arranged in noncollinear configurations—have shown great potential for spintronics [37]. In particular, noncollinear antiferromagnetic intermetallic compounds with Kagome lattices host spin-split band structures that can generate significant transport spin polarization [38, 39]. Despite

their noncollinearity, spin conservation is approximately maintained at specific $k_{\parallel}$, enabling substantial TMR in noncollinear AFMTJs [31, 40]. Current experimental demonstrations of TMR in noncollinear AFMTJs show sizable TMR ratios, while further optimization is required for these devices to become fully competitive with conventional MTJs [41–45]. Nevertheless, these results clearly establish the feasibility of this device architecture, and continued progress in interface and AFM material engineering will further improve their performance. Moreover, electrical switching of noncollinear AFM orders has been successfully achieved in spin–orbit torque (SOT) devices constructed with Mn-based noncollinear antiferromagnets, e. g., Mn_3Sn [46–49]. Most recently, spin-transfer torque (STT) and the STT-driven AFM switching have been experimentally demonstrated in a noncollinear AFMTJ [45], indicating strong compatibility with commercial spintronic technologies such as magnetic random-access memory (MRAM). Importantly, by integrating a ferroelectric tunnel barrier into such a junction, one can realize an MFTJ based on noncollinear antiferromagnets. This design combines spin-torque controllable Néel vector orientation with electric-field-switchable ferroelectric polarization, thereby enabling simultaneous exploitation of both TMR and TER effects. The resulting device supports multiple, nonvolatile resistance states, offering a promising platform for high-speed, high-density, low-power, multi-level memory applications.

In this work, we explore an MFTJ composed of typical noncollinear antiferromagnets Mn_3GaN and Mn_3ZnN as the electrodes and BaTiO_3 as an FE tunnel barrier. Based on first-principles quantum-transport calculations, we predict sizable TER and TMR effects arising from the reversal of FE polarization of the barrier or the Néel vectors of the electrodes and resulting in four distinct resistance states. The predicted transport properties of an MFTJ are well explained by two key mechanisms: ferroelectricity-induced modulation of interfacial electronic states, which governs the distribution of momentum-resolved transmission and underpins the TER effect; and spin-dependent matching of bulk electrode states, which drives the TMR effect. This work establishes a new route for achieving high-performance MFTJs utilizing noncollinear antiferromagnets.

2 | Results and Discussion

Figure 1 schematically illustrates the operational principle of an MFTJ with two different noncollinear (NC) AFM electrodes and an FE barrier, demonstrating how the tunneling conductance is collectively determined by the relative orientation of the Néel vectors in the two AFM electrodes and the direction of FE polarization. When the FE polarization direction is fixed, the TMR effect is governed by the relative Néel vectors alignment (parallel or antiparallel) between the AFM electrodes. Accordingly, when the relative orientation of the Néel vectors in the two AFM electrodes is fixed, the TER effect is obtained by reversing the FE polarization of the barrier. As a result, four possible resistance states in the MFTJ are expected.

In order to demonstrate such an MFTJ, we choose typical noncollinear AFM metals Mn_3GaN and Mn_3ZnN as electrodes [50, 51], with Néel temperatures reported to be up to 290 and 183 K [52, 53]. They crystallize in an antiperovskite structure

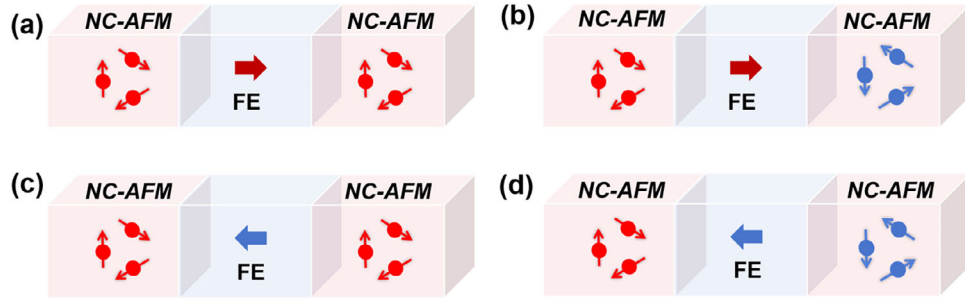


FIGURE 1 | Schematic diagrams of the MFTJ with noncollinear antiferromagnet (NC-AFM)/FE/NC-AFM structures. The electron tunneling schematic diagrams of the (a) the parallel state and (b) the antiparallel state for the FE layer polarized to the right, and (c) and (d) to the left.

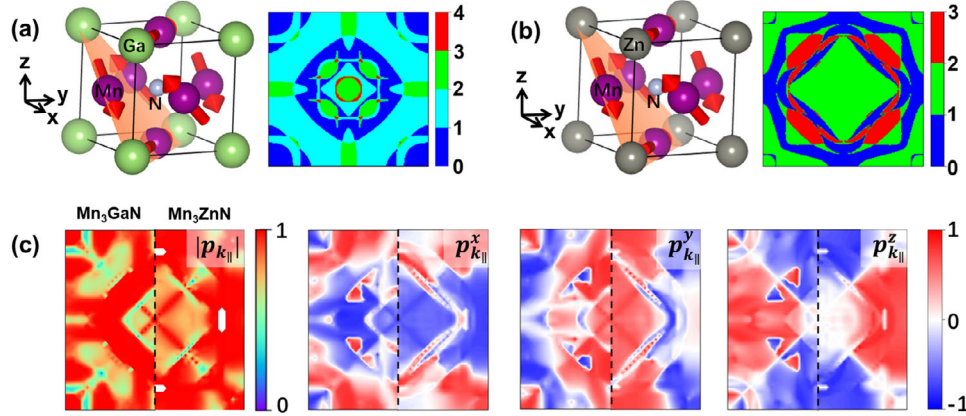


FIGURE 2 | Atomic structures with magnetic moment and conduction channels of NC-AFM (a) Mn_3GaN and (b) Mn_3ZnN . (c) The $k_{\parallel}$ -dependent spin-polarization components at E_F in the 2DBZ. The left half represents the spin polarization components of Mn_3GaN , while the right half represents the spin polarization components of Mn_3ZnN .

(Figure 2a,b) with lattice parameters closely matching those of widely used perovskite oxides, enabling high-quality epitaxy growth of the multilayer MFTJ stack [54–56]. Mn_3GaN and Mn_3ZnN exhibit a Γ_{5g} noncollinear AFM configuration (Figure 2a,b), where the Mn magnetic moments form a 120° clockwise configuration within (111) magnetic Kagome plane [50, 57]. This configuration lifts the Kramers spin degeneracy even in the absence of spin–orbit coupling (SOC), leading to spin-split band structures (Supplementary Figures S1a and S2a). The spin-resolved features of the band structures for Mn_3GaN and Mn_3ZnN are only weakly affected by SOC, indicating that the following results are qualitatively robust against SOC effects (Figures S6 and S7).

Figure 2a,b shows the calculated number of conduction channels of Mn_3GaN and Mn_3ZnN in the two-dimensional (2D) Brillouin zone (BZ). The number of conduction channels is the number of propagating Bloch states in the transport direction at the Fermi energy [58]:

$$N_{k_{\parallel}} = \frac{\hbar}{2} \sum_n \int |v_{nz}| \frac{\partial f}{\partial E_{nk}} dk_z \quad (1)$$

where E_{nk} is the energy of the n -th band, $v_{nz} = \frac{\partial E_{nk}}{\hbar \partial k_z}$ is the band velocity along the transport z direction, f is the Fermi distribution

function, and n and k denote the band index and the wave vector, respectively.

In collinear magnets, the $k_{\parallel}$ -dependent transport spin polarization is defined as the normalized difference between the number of up- and down-spin conduction channels: $p_{k_{\parallel}} = \frac{N_{k_{\parallel}}^{\uparrow} - N_{k_{\parallel}}^{\downarrow}}{N_{k_{\parallel}}}$. In noncollinear antiferromagnets, however, the effective spin polarization becomes a vector and is defined by [31].

$$p_{k_{\parallel}} = \frac{\sum_n s_{nk_{\parallel}}}{\sum_n |s_{nk_{\parallel}}|} \quad (2)$$

where the spin of a propagating Bloch state ψ_{nk} is the average of the spin expectation value at the Fermi surface

$$s_{nk_{\parallel}} = \frac{l_z}{2\pi} \int \psi_{nk} |s| \psi_{nk} \delta(E_{nk} - E_F) dk_z \quad (3)$$

and l_z is the out-of-plane lattice constant along the transport direction.

Figure 2c presents a comparison of the $k_{\parallel}$ -dependent spin polarization $p_{k_{\parallel}}$ for Mn_3GaN and Mn_3ZnN showing their magnitudes $p_{k_{\parallel}}$ and Cartesian components $p_{k_{\parallel}}^i$ ($i = x, y, z$) and revealing strong effective spin polarization of the two materials. As has been discussed in ref. [31], for the Γ_{5g} configuration, the $p_{k_{\parallel}}^x$

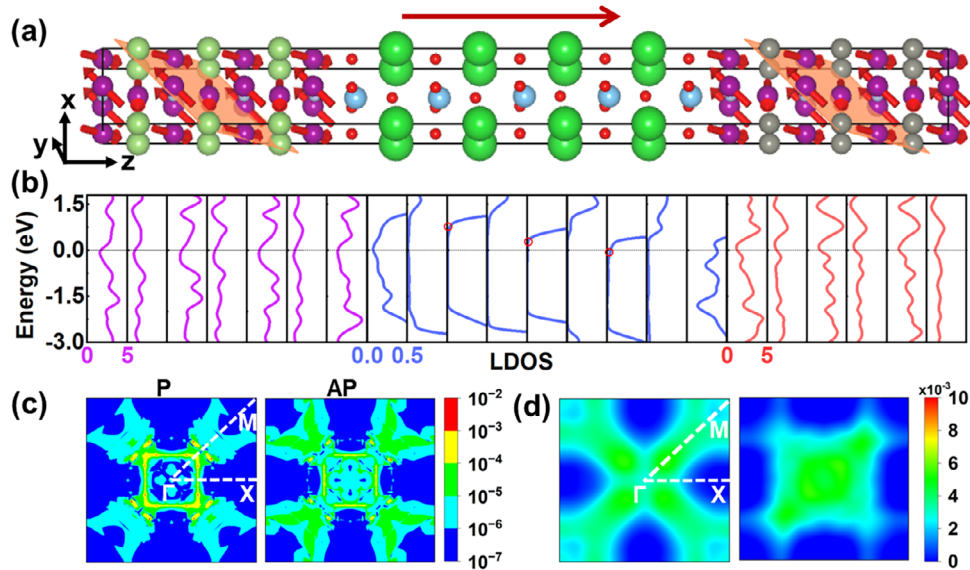


FIGURE 3 | (a) Atomic structure and (b) LDOS of the Mn₃GaN/BaTiO₃/Mn₃ZnN heterostructure at FER (FE polarization points to the right) state. (c) The $k_{||}$ -dependent transmission of Mn₃GaN/BaTiO₃/Mn₃ZnN MFTJ in 2DBZ for the P and AP states at the FER state. (d) The $k_{||}$ -resolved DOS of Ti atoms at the left and right interfaces of the BaTiO₃ barrier.

($p_{k_{||}}^y$) components are expected to exhibit the relationship $p_{k_x, k_y}^x = -p_{k_y, k_x}^x$ and possess same signs in a prominently large region around $k_y = 0$ ($k_x = 0$). At the same time $p_{k_{||}}^z$ is expected to vanish along the diagonals k_{110} and $k_{\bar{1}10}$, due to the mirror symmetry $\hat{M}_{110}$ and two-fold rotation symmetry $\hat{C}_{110}$. These features are indeed observed in Figure 2c for both Mn₃GaN and Mn₃ZnN. Regions within the 2D BZ exhibiting nearly perfect spin polarization correspond to spin-conserving states and thus should be carefully inspected, as they play a key role in enabling TMR [31]. Notably, in both materials, a nearly perfect spin polarization appears across broad areas of the 2DBZ, particularly along the $k_x = 0$ and $k_y = 0$ lines away from the zone center, as well as some scattered regions adjacent to the $k_x = \pm k_y$ diagonals, in excellent agreement with previous studies using different computational approaches [31].

From the above discussion of the spin polarization distribution, it can be readily inferred that the regions of nearly perfect spin polarization in the two antiferromagnets largely overlap. This overlap is expected to play a dominant role in controlling the transport properties of an AFMTJ with these electrodes. To illustrate this, we construct a Mn₃GaN/BaTiO₃/Mn₃ZnN heterostructure that consists of a 4.5 unit-cell (u. c.) BaTiO₃ (001) sandwiched between 3.5 u. c. Mn₃GaN (001) and 3 u. c. Mn₃ZnN (001) (see Figure 3a for rightward polarization and Figure 4a for leftward). The magnetic configurations of bulk Mn₃GaN and Mn₃ZnN, as well as those of the Mn₃GaN/BaTiO₃/Mn₃ZnN superlattices under parallel and antiparallel Néel-vector alignments, are presented in the supplemental information (Figure S5). We assume a fixed in-plane lattice constant of 3.94 Å (corresponding to the theoretical value of the lattice constant of BaTiO₃, which is commonly used as a substrate), providing lattice mismatches below 3% (Table S1), thus showing the possibility of epitaxial growth of the heterostructure [55, 56]. The Mn₂N/TiO₂ interface is adopted, as it exhibits the lowest energy among all interfacial configurations, and the A₂N/BO₂ (A and B are

transition metal elements) termination has been experimentally demonstrated at antiperovskite/perovskite interfaces [56]. The reversal of FE polarization induces asymmetry in the relative displacements of Ti–O (Ba–O) atoms (Figure S3) as well as in the electrostatic potential (Figure S4) at the interface for opposite polarization directions. The atomic positions of the heterostructure are relaxed, and the layer-resolved density of states (LDOS) ensures that the BaTiO₃ barrier layer remains insulating (Figures 3b and 4b).

We first investigate the transport properties of the Mn₃GaN/BaTiO₃/Mn₃ZnN MFTJ with a rightward polarization. Figure 3b shows the LDOS of the MFTJ heterostructure where the Néel vectors of the two electrodes are parallel (P). We find that both the left and right interfacial TiO₂ layers exhibit nonzero LDOS contributed by d_{xz} and d_{yz} orbitals at the Fermi level (E_F) (Figure S10), resulting from interfacial hybridization between Mn and Ti atoms. For the atomic layers of BaTiO₃ away from the interfaces, the band edges, i.e., the conduction band minimum (CBM) and the valence band maximum (VBM), shift monotonically to lower energies from left to right, which is attributed to the depolarizing electric field and the associated band bending.

Figure 3c shows the $k_{||}$ -dependent transmission ($T_{k_{||}}$) for the parallel (P) and antiparallel (AP) alignments of the Néel vector of the electrodes. We find that the distributions of $T_{k_{||}}$ exhibit similar patterns for both alignments, which is inconsistent with the bulk conduction channels of the electrodes shown in Figure 2a,b, particularly around the regions near $k_x = 0$ and $k_y = 0$. At the same time, we see that these patterns align with the $k_{||}$ -resolved LDOS at E_F of the two interfacial TiO₂ layers (Figure 3d) and total $k_{||}$ -resolved LDOS of Ti atoms in the barrier layer (Figure S9), indicating that the interfacial hybridization controls the overall transmission in the MFTJ. On the other hand, notable differences persist between the transmission patterns for the P and AP states, especially within a square-like region

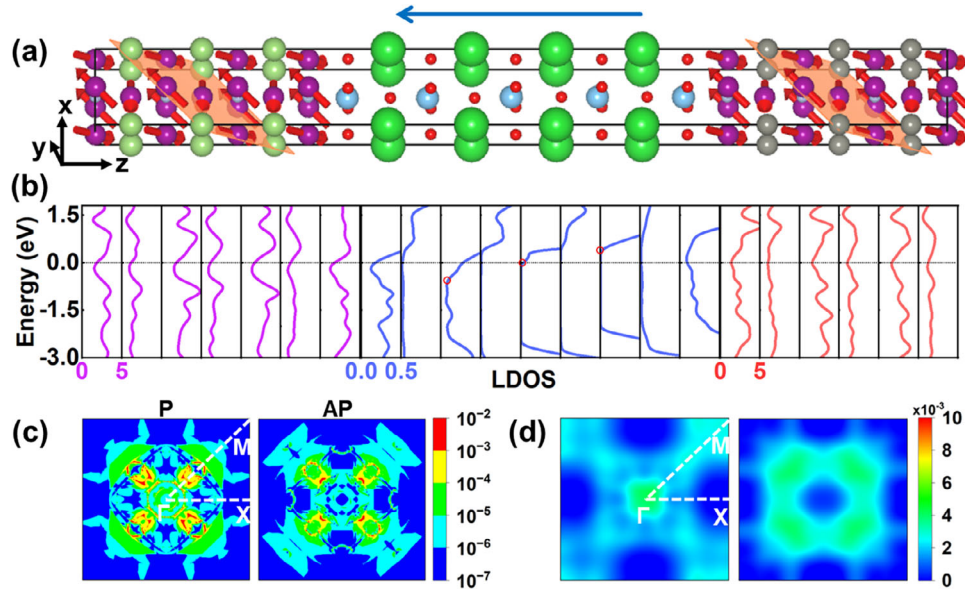


FIGURE 4 | (a) Atomic structure and (b) LDOS of the $\text{Mn}_3\text{GaN}/\text{BaTiO}_3/\text{Mn}_3\text{ZnN}$ heterostructure at FEL (FE polarization points to the left) state. (c) The $k_{\parallel}$ -dependent transmission of $\text{Mn}_3\text{GaN}/\text{BaTiO}_3/\text{Mn}_3\text{ZnN}$ MFTJ in 2DBZ for the P and AP states at the FEL state. (d) The $k_{\parallel}$ -resolved DOS of Ti atoms at the left and right interfaces of the BaTiO_3 barrier.

TABLE 1 | The total transmission (T) for leftward/rightward (FEL/FER) polarization state and parallel/antiparallel (P/AP) Néel vectors alignment of $\text{Mn}_3\text{GaN}/\text{BaTiO}_3/\text{Mn}_3\text{ZnN}$ MFTJs, and the resulting TER and TMR ratios.

T (10^{-5})	P	AP	TMR (%)
FER	1.4	1.0	40%
FEL	12.9	3.2	303.1%
TER (%)	821.4%	220%	

around the zone center, where $T_{k_{\parallel}}$ is large for the P state but much smaller for the AP state (Figure 3c). Table S3 and Figure S11 illustrate that the square-like regions dominate the total transmission coefficient. This can be understood by comparing the matching condition of $p_{k_{\parallel}}$ between Mn_3GaN and Mn_3ZnN for the respective states illustrated in Figure 2a,b and Figure S8. By calculating the total transmission T for the two states (Table 1), a sizable TMR ratio of 40% is derived using the definition $\text{TMR} = \frac{T_P - T_{AP}}{T_{AP}}$.

When the polarization is reversed to the left, we find that while the two interfacial TiO_2 layers remain metallic, the variation of band edges for the inner layers of BaTiO_3 shows an opposite trend compared to the rightward polarization, i.e., the shift to higher energies from right to left. Notably, the CBM of the second TiO_2 layer from the left interface is shifted below E_F , resulting in a finite LDOS at E_F for this layer (Figure 4b). This implies a reduced tunneling barrier width in the $\text{Mn}_3\text{GaN}/\text{BaTiO}_3/\text{Mn}_3\text{ZnN}$ MFTJ for the leftward polarization. The transmission patterns can be understood by considering the $k_{\parallel}$ -resolved interfacial LDOS and the matching of $p_{k_{\parallel}}$ between the electrodes. A large TMR ratio of 303.1% is obtained for this polarization state. Remarkably, due to the reduced tunneling barrier width, the transmission is

much more pronounced than that for the rightward polarization (Table 1). The resulting TER ratio is defined as $\text{TER} = \frac{|T_{\leftarrow} - T_{\rightarrow}|}{\min(T_{\leftarrow}, T_{\rightarrow})}$ [59] reaches 821.4% and 220% for the P and AP states, respectively, where $T \rightarrow (T \leftarrow)$ is the total transmission at E_F when the FE polarization orientation points to rightward (leftward). Moreover, we have explicitly verified the robustness of our conclusions by varying the BaTiO_3 barrier thickness from 4.5 to 6.5 unit cells (Table S2).

3 | Conclusions

In summary, we have designed a $\text{Mn}_3\text{GaN}/\text{BaTiO}_3/\text{Mn}_3\text{ZnN}$ multiferroic tunnel junction based on noncollinear antiferromagnetic electrodes and systematically investigated its electronic and transport properties using first-principles calculations. Our results reveal sizable tunneling electroresistance and tunneling magnetoresistance effects driven by the reversal of either the ferroelectric polarization of the barrier or the Néel vector of the electrodes, leading to four distinct resistance states. These effects are governed by two key mechanisms: (i) ferroelectricity-induced modulation of interfacial electronic states, which controls the momentum-dependent transmission and underpins the TER effect; and (ii) spin-dependent matching of bulk electrode states, which gives rise to the TMR effect.

We acknowledge that several experimental challenges may arise in realizing such devices, including the relatively low Néel temperatures of the electrodes, potential leakage currents associated with oxide tunnel barriers, and the intrinsically weak magnetic anisotropy typical of noncollinear AFM systems. These issues may be resolved through appropriate materials engineering and optimization of growth processes. Therefore, our $\text{Mn}_3\text{GaN}/\text{BaTiO}_3/\text{Mn}_3\text{ZnN}$ heterostructure provides a representative and promising model platform for AFM-based MFTJs, and the physical mechanisms and design principles revealed

here are expected to remain applicable to other noncollinear AFM materials with higher Néel temperatures and enhanced anisotropy, and optimized barrier-electrode combinations once they are experimentally realized.

Our predicted TER and TMR values are comparable to those reported for previously demonstrated FM-based MFTJs [21, 23, 60–63]. In addition, employing noncollinear AFM electrodes eliminates stray magnetic fields and offers intrinsic terahertz spin dynamics, thereby enabling higher device integration density together with ultrafast electrical manipulation [24–27]. Thus, overall, our findings demonstrate the potential of MFTJs based on noncollinear antiferromagnets for next-generation ultrafast spintronic applications, offering a pathway to overcome intrinsic limitations of ferromagnets while retaining compatibility with perovskite oxide integration.

4 | Computational Detail

We employ density functional theory (DFT) as implemented in Vienna Ab-initio Simulation Package (VASP) [64–66] for the calculation of the electronic structure of the Mn_3GaN , Mn_3ZnN , BaTiO_3 , and the associated MFTJ heterostructures. The exchange correlation potential is described through the Perdew-Burke-Ernzerhof (PBE) formula within the generalized gradient approximation (GGA) [67]. A cutoff energy for the plane-wave expansion is set to 500 eV, and the k-point grids of $10 \times 10 \times 10$ and $10 \times 10 \times 1$ are adopted when calculating the bulk and heterostructure properties, respectively. Transport properties are calculated using the nonequilibrium Green's function formalism (DFT+NEGF approach), as implemented in Synopsys QuantumATK [68–70]. The cut-off energy of 100 Ry, the nonrelativistic Fritz-Haber Institute (FHI) pseudopotentials [71], and k-point meshes of $11 \times 11 \times 101$ for $\text{Mn}_3\text{GaN}/\text{BaTiO}_3/\text{Mn}_3\text{ZnN}$ MFTJ are used for self-consistent calculations. Transmission is calculated using k-point meshes of 201×201 in the 2DBZ of $\text{Mn}_3\text{GaN}/\text{BaTiO}_3/\text{Mn}_3\text{ZnN}$ MFTJ. The GGA+U method [72, 73] with $U_{\text{eff}} = 8$ eV on Ti 3d orbitals is employed in the above calculations to avoid the well-known deficiency of underestimated bandgap and thus the proximity of the conduction band minimum with the E_F in Ti-based oxides in heterostructures. To prevent the artificial over-localization of the itinerant Mn-3d states, no Hubbard U is applied on Mn, consistent with the previous first-principles studies of metallic Mn-based noncollinear antiferromagnets [74].

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Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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