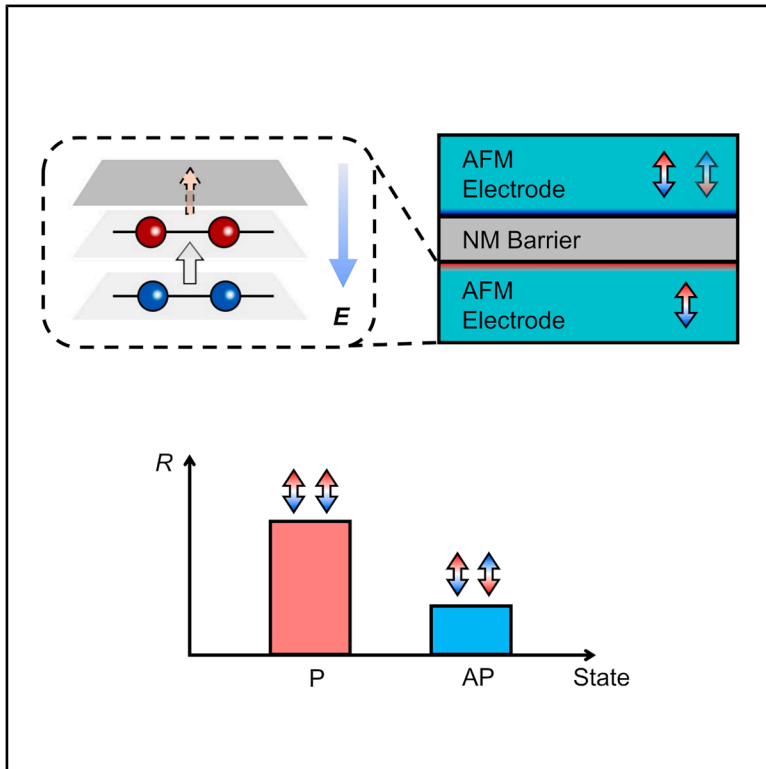


Interface-controlled antiferromagnetic tunnel junctions

Graphical abstract



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In brief

Antiferromagnetic tunnel junctions with spin-polarized interfaces enable large tunneling magnetoresistance and Néel vector switching, overcoming key limitations of conventional spintronics. Yang et al. present a scalable approach to ultrafast, high-density memory and computing devices by harnessing the often-overlooked interfacial spin polarization in van der Waals A-type antiferromagnets. Using doped Fe_4GeTe_2 as an example, the authors show that the compound exhibits magnetically active interfaces and generates strong spin-polarized currents along with sizable tunneling magnetoresistance effects, highlighting the significant potential of antiferromagnetic tunnel junctions.

Highlights

- Interface-driven tunneling magnetoresistance achieved in antiferromagnetic tunnel junctions
- Robust interface-driven spin currents demonstrated in van der Waals A-type antiferromagnets
- Doped Fe_nXTe_2 (X = Ge, Ga) systems are potential antiferromagnetic electrodes



Article

Interface-controlled antiferromagnetic tunnel junctions

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<https://doi.org/10.1016/j.newton.2025.100142>

ACCESSIBLE OVERVIEW Spintronics—a technology leveraging electron spin for faster, more efficient electronics—primarily relies on magnetic tunnel junctions (MTJs). While traditional MTJs use ferromagnets, switching to antiferromagnetic (AFM) materials could significantly boost device speed and storage density. Most AFM tunnel junctions (AFMTJs) to date have focused on spin-filtering barriers or bulk spin-dependent currents. This work highlights a promising, yet underexplored, approach: using certain AFM metals, such as doped Fe_4GeTe_2 , with magnetically active interfaces to generate strong spin-polarized currents and sizable tunneling magnetoresistance (TMR). Advanced simulations demonstrate that this design achieves a large negative TMR controlled solely by interface-driven spin currents. Crucially, these AFMTJs enable easy switching of the Néel vector, offering a practical route to ultrafast, high-density spintronic devices. This research broadens the toolkit for next-generation memory and computing and redefines how antiferromagnets can be harnessed by exploiting their often-overlooked interfacial properties—marking a step toward energy-efficient, scalable spin-based technologies.

SUMMARY

Magnetic tunnel junctions (MTJs) are essential components of high-performance spintronic devices. While conventional MTJs use ferromagnetic materials, antiferromagnetic (AFM) compounds can significantly increase operation speed and packing density. Current AFM tunnel junctions (AFMTJs) exploit antiferromagnets as spin-filter barriers or metal electrodes with bulk spin-dependent currents. Here, we highlight a largely overlooked AFMTJ prototype with bulk-spin-degenerate electrodes exhibiting A-type AFM stacking, forming magnetically uncompensated interfaces that enable spin-polarized tunneling currents and a sizable tunneling magnetoresistance (TMR). Using first-principles quantum-transport calculations and van der Waals (vdW) metal Fe_4GeTe_2 as an example, we demonstrate a large negative TMR from interfacial magnetic moment alignment. This prototype can also be realized with non-vdW A-type AFM metals featuring roughness-insensitive surface magnetization. Beyond TMR, these AFMTJs allow convenient switching of the Néel vector, opening new avenues for AFM spintronics based on interface-driven spin-dependent properties.



INTRODUCTION

Spintronics exploits spin-dependent transport properties for information processing and storage.¹ A key device in this field is the magnetic tunnel junction (MTJ), typically composed of two metallic ferromagnetic (FM) electrodes separated by a nonmagnetic (NM) insulating barrier.^{2–4} The tunneling conductance depends on the relative magnetization orientation of the electrodes, giving rise to the tunneling magnetoresistance (TMR) effect.^{5–7} Additionally, the tunneling spin-polarized currents can exert spin-transfer torque (STT) on FM magnetization, enabling its rotation and switching.^{8–10} A different approach employs spin-filter MTJs, where an insulating FM barrier layer controls spin-filter tunneling.^{11–16} Substantial efforts have been made to improve the density and operation speed of spintronic devices based on conventional MTJs. However, these MTJs suffer from the limitations associated with the stray fields and relatively slow (GHz frequency range) spin dynamics intrinsic to ferromagnets.

These limitations of ferromagnets can be addressed by using antiferromagnetic (AFM) tunnel junctions (AFMTJs),¹⁷ as antiferromagnets exhibit ultrafast spin dynamics in the THz frequency range and produce no stray fields.^{18–20} However, due to their lack of net magnetization, antiferromagnets have long been considered inefficient as functional elements in MTJs. Nonetheless, over the past decade, two prototypes of AFMTJs demonstrating sizable TMR have been developed. Prototype I utilizes a thin layer of van der Waals (vdW) AFM insulator as a tunnel barrier (Figure 1A). This spin-filter AFMTJ employs an applied magnetic field to switch the AFM ordering of the barrier material into a metastable FM state, resulting in a giant spin-filter TMR effect.^{21–28} Although this FM state is volatile, it can be made non-volatile if the AFM layer has an in-plane Néel vector and is twisted.²⁹ Prototype II relies on a spin-dependent current originating from the AFM bulk electronic structure (Figure 1B).^{30–44} The TMR effect in these AFMTJs is associated with the momentum-dependent spin polarization of collinear spin-split antiferromagnets,^{45–55} now known as altermagnets,^{56,57} and noncollinear antiferromagnets.^{30–34} It can also arise from sublattice-dependent spin polarization determined by AFM stacking in real space.^{58,59} The specific growth direction of the AFM electrodes is critical to supporting the spin-dependent current. Recently, room temperature TMR has been demonstrated in AFMTJs with noncollinear AFM electrodes.^{35,36}

Although these AFMTJ prototypes are promising, they exclude a wide range of antiferromagnets that neither exhibit magnetic phase transitions nor support spin-dependent currents in their bulk. To address this limitation, we emphasize a previously discussed but largely overlooked AFMTJ prototype, where A-type AFM stacking of the electrodes creates magnetically uncompensated interfaces capable of generating spin-dependent tunneling currents and producing a sizable TMR effect (Figure 1C). Based on first-principles quantum-transport calculations and the two-dimensional (2D) vdW antiferromagnet Fe₄GeTe₂ as a representative A-type electrode, we demonstrate a large TMR solely attributed to the interface-driven tunneling spin current. Since A-type AFM stacking can potentially be realized in most antiferromagnets by selecting appropriate growth

orientations, we argue that this AFMTJ prototype can be created using a broad range of AFM metals with roughness-robust interfaces.

RESULTS

Stacking-dependent spin currents in antiferromagnets

Electric currents in collinear antiferromagnets can be intuitively described in terms of charge currents flowing within a given magnetic sublattice, i.e., the intra-sublattice currents, and those flowing between the two magnetic sublattices, i.e., the inter-sublattice currents.⁵⁸ The intra-sublattice currents are expected to be spin polarized, while the inter-sublattice currents are expected to be neutral. For example, in antiferromagnets with a G-type stacking, where the magnetic moments are aligned antiparallel between all nearest neighbors, the intra-sublattice currents are negligible due to the large hopping distance between the atoms that belong to the same sublattice. As a result, the net current is spin independent due to being contributed mainly by the inter-sublattice currents (Figure 1D). This is different from antiferromagnets with C-, X-, and A-type stackings, where the building blocks are FM chains or FM layers (Figures 1E–1G).^{59,60} For the C-type (A-type) stacking, an electric field parallel to the chains (layers) generates a globally spin-neutral current, representing a staggered Néel spin current flowing within the chains (layers), since the inter-sublattice currents are negligible (Figures 1E and 1G).⁵⁸ For the X-type stacking proposed recently, where FM chains of the two magnetic sublattices form a cross pattern, an electric field along one chain generates a net current that is majorly composed of an isolated Néel spin current on a single sublattice (Figure 1F).⁵⁹ The X-type stacking offers an intuitive picture of spin currents generated by altermagnetic^{56,57} and non-altermagnetic⁶¹ spin splitting.⁵⁹

This simple analysis suggests that the spin-dependent current, regardless of its net spin polarization, can be supported by an antiferromagnet if the intra-sublattice currents are much stronger than the inter-sublattice currents in the transport direction. C-, A-, and X-type antiferromagnets are thus suitable as electrodes in AFMTJs of prototype II (Figure 1B), where the transport spin polarization is generated in the bulk of AFM metals.^{17,58,59}

In addition to the bulk-induced spin polarization of AFM electrodes, the spin-dependent tunneling current in AFMTJs can be produced by their interfaces. For example, in a bulk A-type antiferromagnet, an out-of-plane electric field can only generate spin-neutral inter-sublattice currents (Figure 1H). However, when using such antiferromagnets as electrodes in a tunnel junction, the tunneling current is expected to be spin polarized due to the uncompensated magnetic moment of the interfacial layer. This property can be functionalized in AFMTJs of prototype III (Figure 1C). A notable difference between this and other AFMTJ prototypes is the TMR behavior. In prototypes I and II, an AFMTJ with the parallel (P)-aligned Néel vector always has higher conductance (G_P) than that with the antiparallel (AP)-aligned Néel vector (G_{AP}), resulting in a positive TMR ratio defined by $TMR = \frac{G_P - G_{AP}}{\min\{G_P, G_{AP}\}}$ (Figures 1A and 1B). On the contrary, in a prototype-III AFMTJ, it is the interface termination

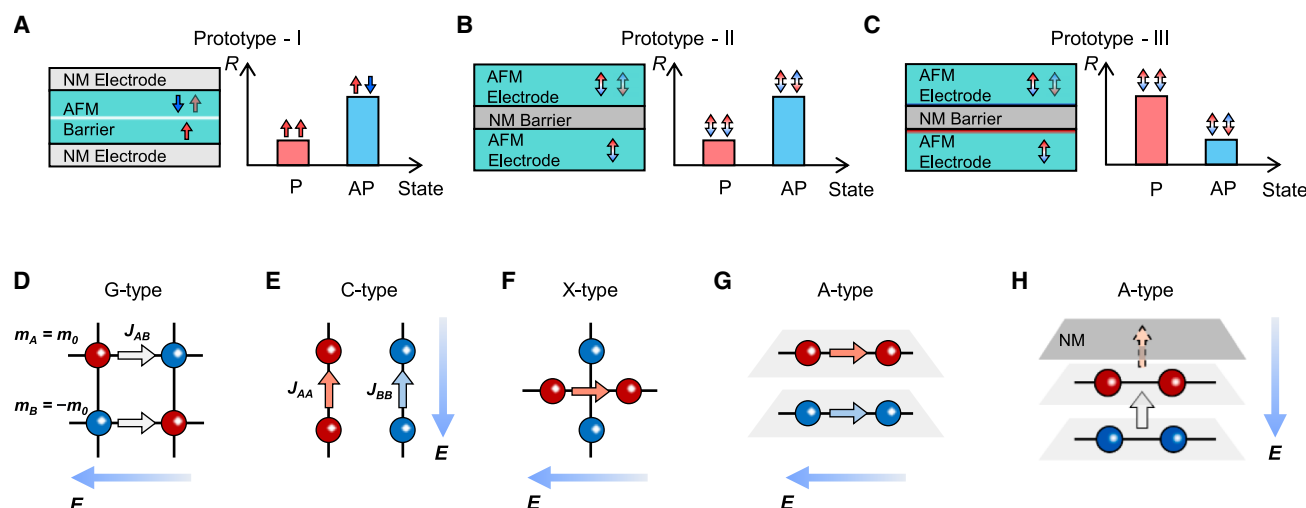


Figure 1. AFMTJ prototypes

(A) Prototype-I AFMTJs with NM electrodes and AFM barrier, where magnetic phase transition in the barrier controls the resistance states.
 (B) Prototype-II AFMTJs with AFM electrodes and NM barrier, where a match (mismatch) of the AFM bulk states results in low (high) resistance for the P (AP) state of the AFMTJ.
 (C) Prototype-III AFMTJs with AFM electrodes and NM barrier, where a match (mismatch) of the AFM interfacial states results in low (high) resistance for the AP (P) state.
 (D) G-type AFM stacking, where the net current is primarily determined by the spin-neutral inter-sublattice currents.
 (E) C-type AFM stacking, where the global current along the FM chain direction corresponds to staggered Néel spin currents.
 (F) X-type AFM stacking, where the global current along one of the chain directions is determined by an isolated Néel spin current.
 (G) A-type AFM stacking, where an in-plane net current represents staggered Néel spin currents.
 (H) A-type AFM stacking, where a magnetically uncompensated interface drives the spin-dependent tunneling current and generates TMR in prototype-III AFMTJs.

The spin-dependent currents in (E)–(G) can be used in prototype-II AFMTJs. In (D)–(H), the solid lines connect the nearest-neighbor atoms; the red and blue balls denote the opposite magnetic sublattices m_A and m_B , respectively; the hollow arrows denote the local currents between nearest-neighbor atoms; and the solid blue arrows denote the electric fields. Here, the gray color indicates the vanishing spin polarization of the inter-sublattice current J_{AB} , and the red and blue colors indicate the intra-sublattice currents J_{AA} and J_{BB} of opposite spin polarization, respectively.

that determines the TMR ratio rather than bulk electrodes. While a positive TMR is expected if the P (AP)-aligned Néel vector in the electrodes is associated with P (AP)-aligned interfacial magnetic moments, a negative TMR will occur if the P (AP)-aligned Néel vector corresponds to AP (P)-aligned interfacial moments (Figure 1C).

While prototype-III AFMTJs were proposed some time ago,^{62–64} their potential has largely been overlooked. This issue arose due to interface roughness, which was considered unavoidable and detrimental to interfacial spin polarization and the associated TMR. However, this problem may be solved by employing A-type antiferromagnets with roughness-insensitive surface magnetization coupled to the Néel vector.^{65–67} The most straightforward solution is to use A-type AFM electrodes composed of 2D vdW materials, where vdW gaps ensure flat surface terminations. These AFMTJs can be fabricated using vdW assembly techniques.

Interface effect on spin-dependent tunneling current

We first demonstrate the interface-driven spin-dependent transport of a representative vdW A-type AFM metal based on first-principles calculations. Figure 2A shows the structure of vdW metal Fe_4GeTe_2 , where each monolayer is centrosymmetric and has FM-aligned Fe moments. While Fe_4GeTe_2 is an FM ma-

terial, it is known that the A-type AFM ordering can be induced by Co doping.⁶⁸ In the following, for simplicity, we consider pristine Fe_4GeTe_2 with A-type AFM stacking as a representative electrode to demonstrate AFMTJs of prototype III. This simplification does not influence our conclusions because, as shown in Note S4, the effect of Co largely produces electron doping, and therefore, the results obtained for the AFM-ordered Fe_4GeTe_2 can be extrapolated to those for Co-doped Fe_4GeTe_2 by shifting the Fermi energy to higher energies.

The A-type AFM stacking of bulk Fe_4GeTe_2 is characterized by the coexistence of inversion symmetry $\hat{P}$ and combined symmetry $\hat{P}\hat{T}\hat{t}$ in bulk material, where $\hat{T}$ is the time-reversal symmetry and $\hat{t}$ is the translation symmetry. A thin film of Fe_4GeTe_2 with an even number of monolayers, however, is non-centrosymmetric and hosts combined $\hat{P}\hat{T}$ symmetry. These symmetries enforce the spin-degenerate electronic structure of both bulk (Figure 2B) and even-monolayer films of Fe_4GeTe_2 . Despite this spin degeneracy, when an electric field is applied in the plane, staggered Néel spin currents are generated along the P-aligned FM-ordered monolayers of Fe_4GeTe_2 .⁵⁸ The situation is different when an electric field is applied out of the plane. As seen from Figure 2C, the Fermi surface of bulk Fe_4GeTe_2 is spin degenerate along the out-of-plane direction. At the same time, due to alternating magnetic moments along the c axis (Figure 2A), there

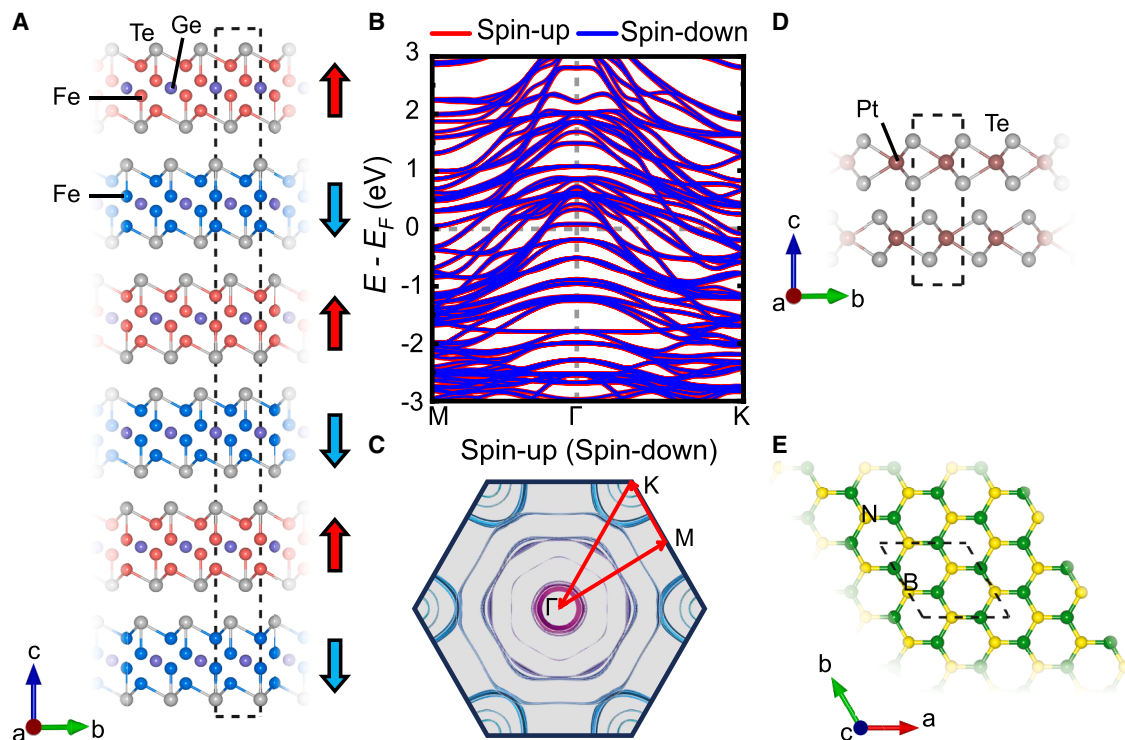


Figure 2. 2D vdW materials for prototype-III AFMTJs

(A) Side view of the 2D vdW A-type AFM metal Fe_4GeTe_2 . Fe atoms are indicated by red (blue) balls that have positive (negative) magnetic moments. (B and C) The spin-resolved band structure (B) and top view of the Fermi surface (C) of bulk Fe_4GeTe_2 .

(D and E) Atomic structure of 2D vdW metal 2H- PtTe_2 (D) and insulator BN (E). Pt, Te, B, and N atoms are indicated by brown, gray, yellow, and green balls, respectively.

are no Néel spin currents along the out-of-plane direction, indicating spin-independent transport. As a result, no bulk contribution to the spin dependence of the tunneling current is thus expected when using Fe_4GeTe_2 as the electrodes in AFMTJs.

To reveal the interface effect on spin-polarized tunneling, we construct a tunnel junction $\text{PtTe}_2/[\text{Fe}_4\text{GeTe}_2]_n/\text{BN}/\text{PtTe}_2$ (Figure 3A), where NM vdW metal 2H- PtTe_2 (Figure 2D)⁶⁹ is used as a lead, NM insulating monolayer BN (Figure 2E)⁷⁰ is used as a barrier, and n -monolayer Fe_4GeTe_2 is used as a spacer layer. The Néel vector of Fe_4GeTe_2 is set parallel to the magnetic moments of the interfacial monolayer (Figure 3B). Figure 3C shows the monolayer-resolved density of states of this heterostructure. We find that a wide band gap of BN is well maintained, and the Fermi energy E_F is located deeply inside the band gap.

We first calculate the transmission of the tunnel junction with an infinite n , which corresponds to a $\text{Fe}_4\text{GeTe}_2/\text{BN}/\text{PtTe}_2$ junction where the left electrode is bulk Fe_4GeTe_2 . Despite the spin-degenerate Fermi surface in bulk Fe_4GeTe_2 (Figure 2C), we find that the $\vec{k}_{\parallel}$ -dependent transmissions $T_{\parallel}^{\sigma}(\vec{k}_{\parallel})$ are different for the up-spin ($\sigma = \uparrow$) and down-spin ($\sigma = \downarrow$) channels (Figure 3D), leading to a finite $\vec{k}_{\parallel}$ -dependent spin polarization $p_{\parallel}(\vec{k}_{\parallel}) = \frac{T_{\parallel}^{\uparrow} - T_{\parallel}^{\downarrow}}{T_{\parallel}^{\uparrow} + T_{\parallel}^{\downarrow}}$ (Figure 3E).

Since the bulk electronic structure of Fe_4GeTe_2 is spin degenerate, the predicted spin polarization is solely driven by the uncompensated magnetic moments at the interface of Fe_4GeTe_2

with BN. Overall, we find that $T_{\parallel}^{\uparrow}(\vec{k}_{\parallel}) > T_{\parallel}^{\downarrow}(\vec{k}_{\parallel})$ for most $\vec{k}_{\parallel}$, resulting in the total transmission being much larger for the up-spin channel ($T^{\uparrow}$) than for the down-spin channel ($T^{\downarrow}$) and the net spin polarization $p = \frac{T^{\uparrow} - T^{\downarrow}}{T^{\uparrow} + T^{\downarrow}} = 84\%$ at E_F . As is evident from Figure 3F, p is maintained to be large and positive within a wide energy window around E_F .

We then calculate the spin-dependent transmission of the $\text{PtTe}_2/[\text{Fe}_4\text{GeTe}_2]_n/\text{BN}/\text{PtTe}_2$ tunnel junction with a finite n . As seen from Figure 3G, the Fe_4GeTe_2 spacer layer in the 2D limit ($n = 1$) produces a small p due to the interfacial monolayer being proximitized with PtTe_2 . For $n \geq 2$, p increases and converges to the value of bulk Fe_4GeTe_2 when $n = 6$. We find that p at E_F is always positive regardless of n being odd or even. These facts demonstrate the interface origin of the spin-polarized current.

TMR in AFMTJs with Fe_4GeTe_2 electrodes

The sizable interface effect on the spin-dependent tunneling current indicates that Fe_4GeTe_2 can be used in electrodes of prototype-III AFMTJs. We thus construct the $\text{PtTe}_2/(\text{Fe}_4\text{GeTe}_2)_n/\text{BN}/(\text{Fe}_4\text{GeTe}_2)_m/\text{PtTe}_2$ AFMTJ, as shown in Figures 4A and 4B. We first calculate the transmission of the AFMTJ with the same Fe_4GeTe_2 spacer layer thickness on the two sides ($n = m$). Figure 4C shows the $\vec{k}_{\parallel}$ -dependent transmissions, $T_{\beta}^{\sigma}(\vec{k}_{\parallel})$ and

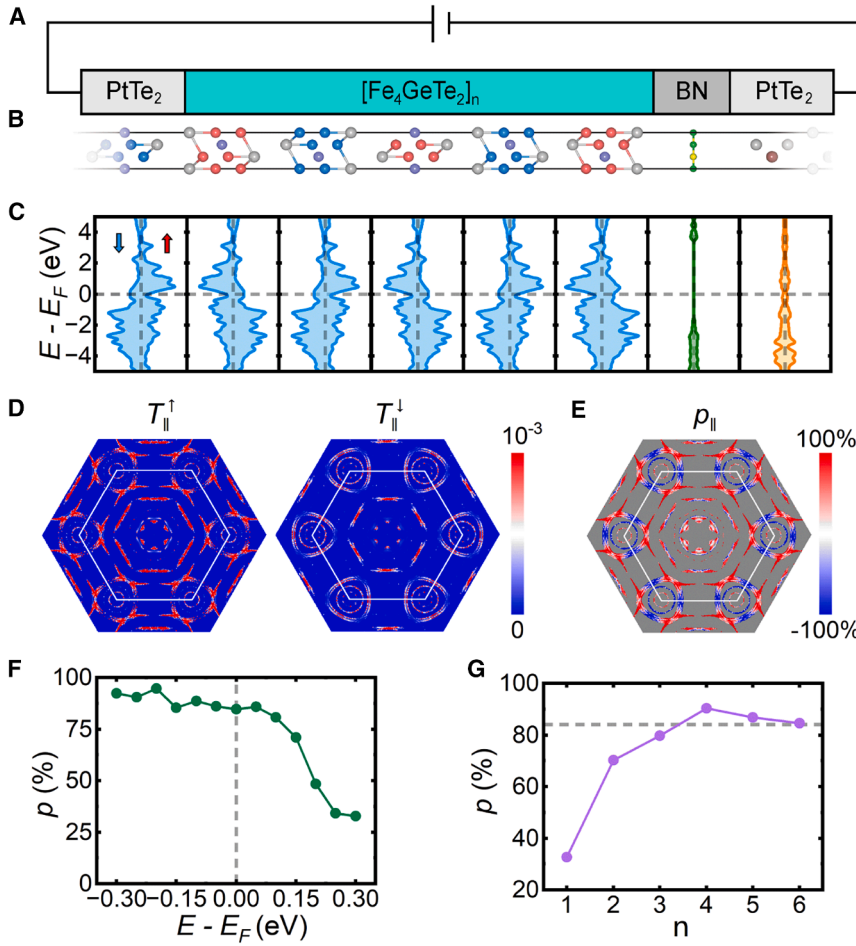


Figure 3. Interfacial effect on spin-dependent current

(A) Schematic of the PtTe₂/[Fe₄GeTe₂]_n/BN/PtTe₂ tunnel junction.

(B and C) Atomic structure (B) and monolayer-resolved density of states (C) of the tunnel junction.

(D–F) Spin- and $\vec{k}_{\parallel}$ -dependent transmissions $T_{\parallel}^{\uparrow}(\vec{k}_{\parallel})$ and $T_{\parallel}^{\downarrow}(\vec{k}_{\parallel})$ (D), $\vec{k}_{\parallel}$ -dependent spin polarization $p_{\parallel}(\vec{k}_{\parallel})$ at Fermi energy E_F (E), and total transport spin polarization p as a function of energy (F) in Fe₄GeTe₂/BN/PtTe₂ tunnel junction.

(G) Total transport spin polarization p at E_F as a function of different layers n in PtTe₂/[Fe₄GeTe₂]_n/BN/PtTe₂ tunnel junction. These results suggest the giant and robust spin polarizations of the interface-driven tunneling currents.

nant contribution of the interfacial magnetic moments rather than bulk effects. Moreover, we find that the TMR ratio can be further enhanced by increasing the thickness of the BN barrier (see Note S2).

DISCUSSION

Previous theoretical calculations of spin transport in AFMTJs^{62–64,71} have predicted either very small zero-bias TMR^{62–64} or TMR oscillating in sign as a function of energy.⁷¹ These results indicate competing bulk- and interface-

induced contributions to the spin polarization of the tunneling current. In some cases, TMR is dominated by a spin-neutral contribution from the bulk electrodes, leading to small TMR, while in others, the spin-dependent bulk contribution opposes the interface-driven spin polarization, causing TMR to oscillate in sign with energy. This behavior is illustrated in our modeling of a hypothetical Cr/Si/Cr AFMTJ (see Note S8), where TMR oscillates in sign as a function of energy but can be made positive or negative across all energies by applying strain that enhances or reduces the bulk-controlled spin-dependent current, respectively. In contrast, the prototype-III AFMTJs designed in our work exhibit large TMR solely controlled by interface magnetic moments, showing no sign change as a function of energy.

The robustness of the predicted TMR against the position of the Fermi energy implies similar behavior in realistic AFMTJs based on Fe₄GeTe₂ electrodes doped with Co, which is necessary to induce antiferromagnetism in Fe₄GeTe₂. Since Co doping adds valence electrons and raises the Fermi energy, we calculated the transport properties of PtTe₂/[(Fe_{0.67}Co_{0.33})₄GeTe₂]_n/BN/[(Fe_{0.67}Co_{0.33})₄GeTe₂]_m/PtTe₂ AFMTJs, explicitly modeling Co doping by the virtual crystal approximation. The results closely align with those obtained for Fe₄GeTe₂-based AFMTJs, as discussed in Note S4. Moreover, prototype-III AFMTJs can be realized using A-type AFM electrodes beyond Fe₄GeTe₂.

$T_{AP}^{\alpha}(\vec{k}_{\parallel})$, for the P and AP states, respectively, for the AFMTJ with $n = m = 2$. It is seen that $T_P^{\downarrow}(\vec{k}_{\parallel}) = T_P^{\uparrow}(\vec{k}_{\parallel})$, which is due to the $\hat{P}\hat{T}$ symmetry being preserved in the AFMTJ with the P-aligned Néel vector (Figure 4B). The interfacial magnetic moments are AP aligned in this case, suppressing the spin-dependent tunneling current. At the same time, we find that $T_{AP}^{\downarrow}(\vec{k}_{\parallel})$ is enhanced and $T_{AP}^{\uparrow}(\vec{k}_{\parallel})$ reduced for the AP state due to the interfacial moments being P aligned (Figure 4C). These results indicate that the alignment of the interfacial moments controls the spin-dependent tunneling current in this AFMTJ. As a result, the total transmission for the P state (T_P) appears to be much smaller than that for the AP state (T_P) (Figure 4D). The predicted TMR ratio is $\text{TMR} = \frac{T_P - T_{AP}}{\min\{T_P, T_{AP}\}} = -300\%$ at E_F . The large negative TMR is sustained within a broad energy window around E_F (Figure 4D).

For an Fe₄GeTe₂ spacer layer thickness of $n = m = 4$ and 6, we obtain TMR ratios of about -250% and -360% , respectively (Figure 4E). For bulk Fe₄GeTe₂ representing the left electrode ($n = \infty$) and a thin Fe₄GeTe₂ spacer layer in the right electrode (m is small), the TMR ratios are predicted to be between -150% and -300% (Figure 4E). These results indicate the minor influence of Fe₄GeTe₂ layer thickness on TMR due to the domi-

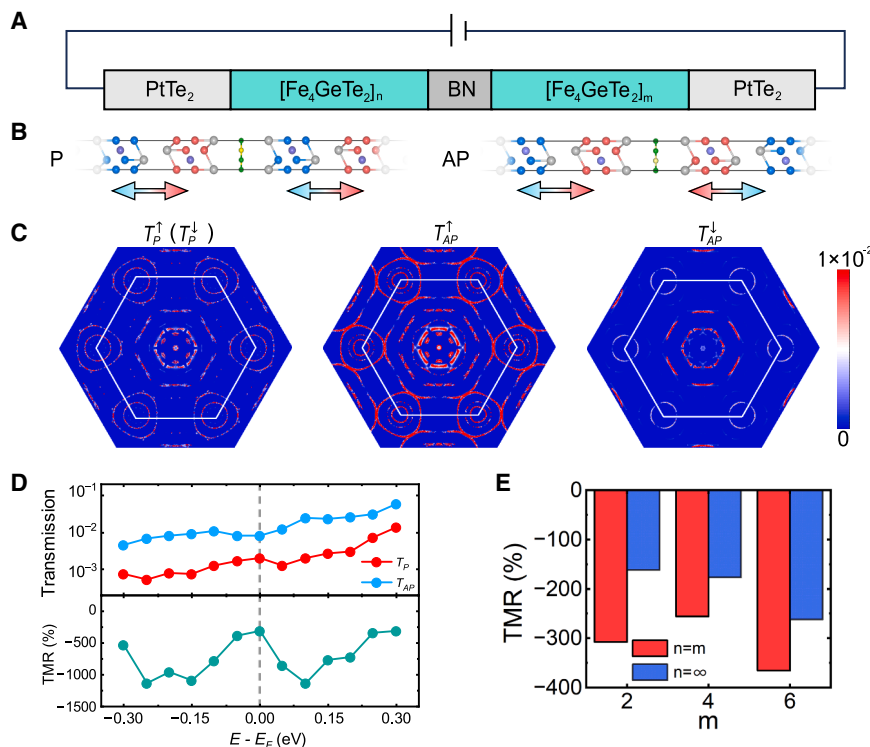


Figure 4. TMR of PtTe₂/(Fe₄GeTe₂)_n/BN/(Fe₄GeTe₂)_m/PtTe₂ AFMTJ

(A and B) Schematics of the AFMTJ (A) and its structure for P and AP states (B).

(C) Calculated $\vec{k}_{\parallel}$ -resolved transmission (T) at E_F for P and AP states and for the case of $n = m = 2$.

(D) Total transmission for P and AP states (top) and TMR ratio (bottom) as functions of energy for $n = m = 2$, indicating the large TMR sustained within a broad energy window around E_F .

(E) TMR ratio for $n = m$, which remains sizable for different thicknesses of electrodes.

A-type AFM phases with high Néel temperatures have been reported in 2D vdW AFM metals Fe₅GeTe₂⁷² and Fe₃GeTe₂,⁷³ which can be modified by appropriate doping. Fe_nGeTe₂ and Fe_nGaTe₂ ($n = 3, 4$, and 5) have already been employed as FM electrodes in conventional MTJs.^{73–80} Implementing their AFM phases in prototype-III AFMTJs is thus straightforward using similar techniques.

Furthermore, electrodes for prototype-III AFMTJs can be fabricated from three-dimensional (3D) AFM metals that exhibit roughness-insensitive surface (interface) magnetization due to symmetry.^{65–67} In these antiferromagnets, the surface magnetization is coupled to the Néel vector, so switching the Néel vector reverses the interface magnetic moments, resulting in the TMR effect predicted in this work. This significantly broadens the range of materials suitable for prototype-III AFMTJs.

Importantly, from a device application perspective, writing the appropriate magnetic state in prototype-III AFMTJs is much more convenient than in the other two prototypes. Since the TMR effect is only weakly dependent on the AFM spacer thickness, one can design AFMTJs with an odd number of AFM monolayers in one electrode to induce finite magnetization in the AFM spacer layer. This property allows efficient switching of the Néel vector in this layer by applying a magnetic field (Figure 5A).

Moreover, the write-in operation in prototype-III AFMTJs can be achieved electrically using spin torques. Deterministic switching of the Néel vector in an antiferromagnet can be produced by the Néel spin torques arising from staggered spin polarization on two magnetic sublattices⁵⁸ or by the torque generated from spin polarization acting solely on a single magnetic sublattice.⁵⁹ Both

approaches can be realized in vdW AFMTJs. Firstly, an out-of-plane tunneling spin current exerts a spin-transfer torque expected to primarily accumulate within the interfacial monolayer of the A-type AFM spacer due to the large interlayer distance. This is supported by our calculations, shown in Figure S8A (see Note S6), and mimics the torque on a single magnetic sublattice when the A-type AFM spacer is ultra-thin, consisting of only two monolayers (Figure 5B). Secondly, an in-plane current in the A-type electrode can generate Néel torques (Figure 5C) via staggered Néel spin current⁵⁸ and/or the Edelstein effect.^{81,82} The former is supported by the A-type stacking, while the latter arises from the $\hat{P}\hat{T}$ symmetry usually preserved in A-type antiferromagnets, as reflected in the layer-resolved spin textures shown in Figure S8B (see Note S6). Furthermore, it is noted that the switching of an A-type vdW antiferromagnet via the spin Hall effect has recently been experimentally demonstrated.⁸³

The convenient control of the Néel vector state makes prototype-III AFMTJs promising for high-performance spintronic devices. In particular, we envision an AFM racetrack memory, where AFM domains can be nucleated and moved via the Néel spin torques (Figure 5D) and detected via the TMR response from an AFMTJ integrated into the racetrack (Figure 5E).

Finally, we highlight several challenges worth investigating for the practical applications of prototype-III AFMTJs. First, our calculations fixed the in-plane lattice constant of the AFMTJs to that of Fe₄GeTe₂, resulting in strains of -6.7% on BN and 1.5% on PtTe₂. While this did not affect our key results, since PtTe₂ remained metallic and BN retained a large band gap, the strain from lattice mismatch could produce wrinkling and buckling of the layers,⁸⁴ potentially impacting device performance. Second, defects and disorder are unavoidable in real materials. Although we showed that TMR is robust to disorder by introducing effective energy-level broadening within the Green's function formalism, this approach does not capture resonant tunneling effects due to localized defect states in the barrier.^{85–87} Exploring these effects would be valuable in future studies. Lastly, our calculations for the PtTe₂/[Fe₄GeTe₂]₂/BN/[Fe₄GeTe₂]₂/PtTe₂ AFMTJ reveal a decrease in TMR from

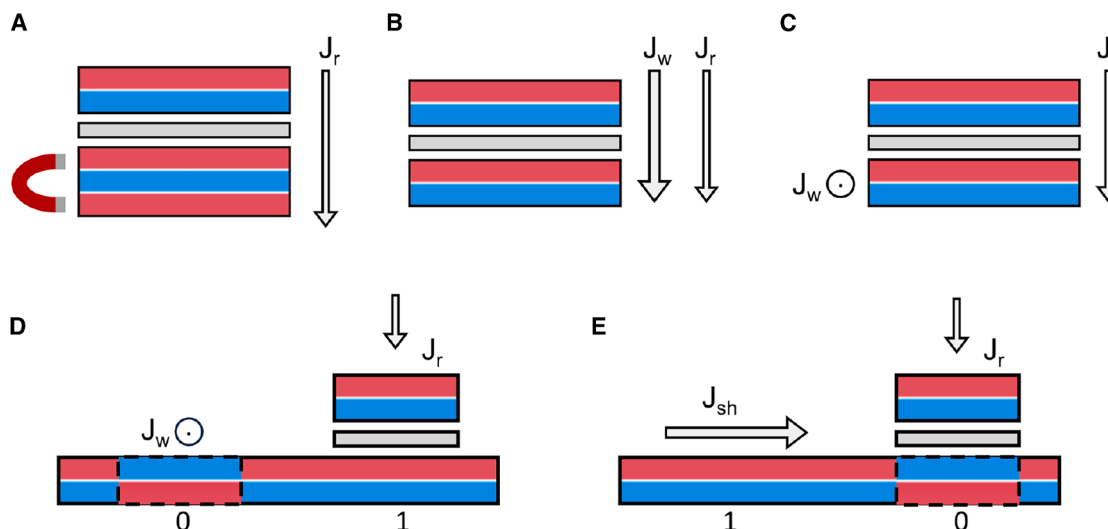


Figure 5. Write-in and readout of the prototype III of AFMTJs

The gray stripe denotes the NM barrier. The red and blue stripes denote the layers in A-type AFM electrodes with positive and negative moments, respectively.

(A) The switching of the bottom odd-layer electrode by a magnetic field.

(B) The switching of the bottom electrode by a spin-transfer torque via an out-of-plane writing current J_w .

(C) The switching of the bottom electrode by the Néel torques via an in-plane J_w .

(D and E) An AFM racetrack memory made of an A-type antiferromagnet, where the AFM domains are created by an in-plane J_w (D) and transported by an in-plane shifting current J_{sh} (E). An AFMTJ is implemented for detecting the domain via an out-of-plane reading current J_r . The 0 and 1 represent low- and high-resistance states, respectively. The arrows denote the currents, where the widths of arrows qualitatively represent the associated current densities.

–300% to –40% when a bias voltage of 0.1 V bias voltage is applied. While this does not preclude practical observations of TMR, there is room for improvement to match the performance of commercial MTJs.⁸⁸

Overall, AFMTJs with spin-degenerate A-type AFM electrodes can produce a sizable TMR due to the spin-polarized tunneling current driven by the uncompensated interfacial magnetic moments coupled to the Néel vector. The A-type AFM stacking ensures the convenient switching of the Néel vector, providing the means to achieve parallel and antiparallel states in these AFMTJs. With these functionalities, this prototype of AFMTJs allows employing a broad range of available vdW AFM metals in high-performance spintronic devices.

METHODS

First-principles calculations of the electronic structure are performed within the density functional theory (DFT)⁸⁹ using the projector augmented-wave (PAW)⁹⁰ method implemented in the VASP code.^{91,92} The plane-wave cutoff energy is 500 eV, and k -point meshes of about $12 \times 12 \times 1$ are used in the calculations. The exchange and correlation effects are treated within the generalized gradient approximation (GGA) developed by Perdew-Burke-Ernzerhof (PBE).⁹³ The semiempirical DFT-D3 method parameterizing the vdW correction is used in calculations.⁹⁴

The non-equilibrium Green's function formalism (DFT+NEGF approach)^{95,96} is used to calculate quantum transport, which is implemented in QuntumATK.⁹⁷ The cutoff energy of 80 Ry, the nonrelativistic Fritz-Haber Institute (FHI) pseudopotentials, and

$\vec{k}$ -point meshes of $11 \times 11 \times 101$ for Fe_4GeTe_2 -based AFMTJs are used for self-consistent calculations. The $\vec{k}$ -resolved transmission is calculated using 401×401 k -points in the 2D Brillouin zone (BZ).

RESOURCE AVAILABILITY

Lead contact

Further information and requests for resources and reagents should be directed to and will be fulfilled by the lead contact, Ding-Fu Shao (dfshao@issp.ac.cn).

Materials availability

This study did not generate new unique materials.

Data and code availability

All data needed to evaluate the conclusions in the paper are present in the paper and/or the supplemental information. Additional data related to this paper are available from the authors upon reasonable request.

ACKNOWLEDGMENTS

This work was supported by the National Key R&D Program of China (grant no. 2024YFB3614101), the National Natural Science Foundation of China (grants nos. 12274411, 12241405, and 52250418), the Basic Research Program of the Chinese Academy of Sciences Based on Major Scientific Infrastructures (grant no. JZHKYPT-2021-08), and the CAS Project for Young Scientists in Basic Research (grant no. YSBR-084). E.Y.T. acknowledges support from the Division of Materials Research of the National Science Foundation (NSF grant no. DMR-2316665). Computations were performed at the Hefei Advanced Computing Center.

AUTHOR CONTRIBUTIONS

D.-F.S. conceived and supervised this project. L.Y. performed the primary calculations and simulations. L.Y., Y.-Y.J., and X.-Y.G. performed analyses of the TMR effect. L.Y., Y.-Y.J., X.-Y.G., S.-H.Z., R.-C.X., W.-J.L., L.W., Y.-P.S., E.Y.T., and D.-F.S. analyzed the results. L.Y., Y.-Y.J., X.-Y.G., E.Y.T., and D.-F.S. wrote the manuscript. All authors contributed to the final version of the manuscript.

DECLARATION OF INTERESTS

The authors declare that they have no competing interests.

SUPPLEMENTAL INFORMATION

Supplemental information can be found online at <https://doi.org/10.1016/j.newton.2025.100142>.

Received: October 28, 2024

Revised: February 26, 2025

Accepted: May 26, 2025

Published: June 23, 2025

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