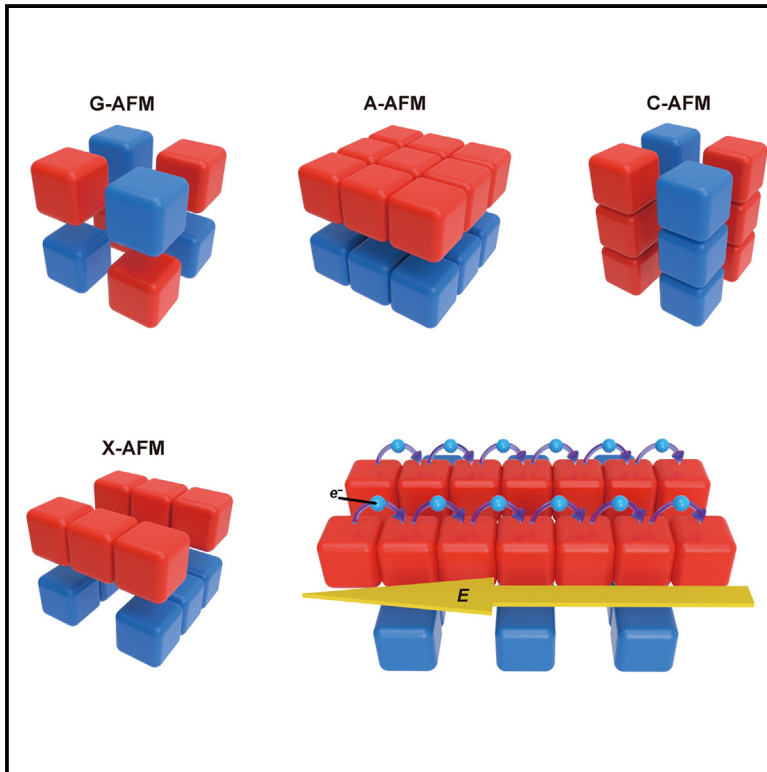


X-type stacking in cross-chain antiferromagnets

Graphical abstract



Authors

Shui-Sen Zhang, Zi-An Wang, Bo Li, ..., Evgeny Y. Tsymbal, Haifeng Du, Ding-Fu Shao

Correspondence

tsymbal@unl.edu (E.Y.T.),
duhf@hmfl.ac.cn (H.D.),
dfshao@issp.ac.cn (D.-F.S.)

In brief

Antiferromagnets consist of two or more ferromagnetically ordered sublattices that neutralize each other, rendering them inert to external stimuli. Zhang et al. show that selectively addressing sublattices—not present in conventional magnets—can be achieved in antiferromagnets with an uncharted X-type stacking, where two sublattices form a pattern of cross-chains. These X-type antiferromagnets allow spin current and thus spin torques on a single sublattice, enabling deterministic magnetic switching. This discovery offers avenues for novel fundamental physics and high-performance spintronic functionalities.

Highlights

- X-type stacking discovered in cross-chain antiferromagnets
- X-type antiferromagnets exhibit sublattice-selective spin-polarized transport
- Spin torques on a single sublattice for deterministic Néel vector switching
- β -Fe₂PO₅ is a representative high-temperature X-type antiferromagnet



Article

X-type stacking in cross-chain antiferromagnets

Shui-Sen Zhang,^{1,2,3} Zi-An Wang,^{2,3} Bo Li,⁴ Yuan-Yuan Jiang,^{2,3} Shu-Hui Zhang,⁵ Rui-Chun Xiao,⁶ Lan-Xin Liu,^{2,3} Xuan Luo,³ Wen-Jian Lu,³ Mingliang Tian,^{1,7} Yu-Ping Sun,^{1,3,8} Evgeny Y. Tsymbal,^{9,*} Haifeng Du,^{1,6,*} and Ding-Fu Shao^{3,10,*}

¹Anhui Province Key Laboratory of Low-Energy Quantum Materials and Devices, High Magnetic Field Laboratory, HFIPS, Chinese Academy of Science, Hefei, Anhui, China

²University of Science and Technology of China, Hefei, China

³Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei, China

⁴Institute for Advanced Study, Tsinghua University, Beijing, China

⁵College of Mathematics and Physics, Beijing University of Chemical Technology, Beijing, China

⁶Institute of Physics Science and Information Technology, Anhui University, Hefei, China

⁷School of Physics and Materials Science, Anhui University, Hefei, China

⁸Collaborative Innovation Center of Microstructures, Nanjing University, Nanjing, China

⁹Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE, USA

¹⁰Lead contact

*Correspondence: tsymbal@unl.edu (E.Y.T.), duhf@hmfl.ac.cn (H.D.), dfshao@issp.ac.cn (D.-F.S.)

<https://doi.org/10.1016/j.newton.2025.100068>

ACCESSIBLE OVERVIEW Physical phenomena in condensed matter typically arise from the collective effects of all atoms in a solid, while selectively addressing a single atomic sublattice is elusive. A prime example is antiferromagnetic materials, which consist of two or more ferromagnetically ordered sublattices that neutralize each other, rendering the antiferromagnets inert to external stimuli. If one of these sublattices could be selectively addressed, it would open exciting opportunities for exploring new physics and spintronic applications. This work illustrates such a remarkable property by introducing X-type antiferromagnetic stacking, an uncharted class of magnetic stacking in which two magnetic sublattices form a pattern of intersecting atomic chains. The associated cross-chain antiferromagnets with X-type stacking, dubbed X-type antiferromagnets, enable one magnetic sublattice to conduct while the other acts as an insulator, effectively combining both properties within the same material. Consequently, passing an electric current through X-type antiferromagnets exerts spin torque solely on a single magnetic sublattice, enabling deterministic switching of the antiferromagnetic domains. This discovery paves the way for exploring novel fundamental physics related to sublattice selectivity and opens an avenue for realizing advanced spintronic functionalities with enhanced performance.

SUMMARY

Physical phenomena in condensed matter normally arise from the collective effect of all atoms, while selectively addressing a lone atomic sublattice by external stimulus is elusive. The latter functionality may, however, benefit various applications, as the responses may differ when the external stimulus affects only a specific sublattice rather than the entire solid. Here, we introduce cross-chain antiferromagnets where the stacking of two magnetic sublattices forms a pattern of intersecting atomic chains, allowing for sublattice selectivity. We dub this antiferromagnetic (AFM) stacking X-type and demonstrate that it exhibits unique spin-dependent transport properties not present in conventional magnets. Through high-throughput analyses and computations, we unveil three prototypes of X-type AFM stacking and identify 15 X-type AFM candidates. Using $\beta\text{-Fe}_2\text{PO}_5$ as a representative X-type antiferromagnet, we predict sublattice-selective spin-polarized transport driven by the X-type stacking where one magnetic sublattice conducts, while the other does not. Consequently, a spin torque can be exerted solely on a single sublattice, leading to unconventional ultrafast dynamics of the Néel vector capable of deterministic switching of the AFM domains. Our work uncovers a previously overlooked type of magnetic moment stacking and reveals sublattice-selective physical properties promising for high-performance spintronic applications.



INTRODUCTION

The alignment of magnetic moments in magnetically ordered materials determines their physical properties. For example, ferromagnets have parallel-aligned magnetic moments that produce net magnetization, which can be controlled by an applied magnetic field and is responsible for various spin-dependent transport properties. In contrast, antiferromagnets exhibit magnetic orderings where atomic moments compensate for each other, resulting in zero net magnetization.^{1,2} Due to the obvious challenges in selectively addressing a single magnetic sublattice using conventional electric or magnetic means, antiferromagnets are often perceived as spin independent and less promising for applications.³

Despite this seemingly limiting constraint, a plethora of interesting and potentially useful properties of antiferromagnets have been discovered recently. Among these are spin currents, spin torques, and tunneling magnetoresistance effects^{4–18}—key phenomena of spintronics. These advances have been driven by symmetry-based analyses that have helped identify antiferromagnets with momentum-dependent spin polarizations, including spin-split collinear antiferromagnets,^{19–28} dubbed altermagnets,^{26,27} and some noncollinear antiferromagnets.^{4,7,14–16}

Although these newly discovered properties render antiferromagnets potentially useful,^{29,30} much more exciting opportunities for new physics and spintronic applications would emerge if one of the magnetic sublattices in antiferromagnets could be selectively addressed using electric means. However, this elusive perspective cannot be derived solely from the global symmetry of antiferromagnets, which relates their macroscopic properties to the spin-dependent electronic structure in momentum space. Instead, it requires a real space consideration of their magnetic sublattice stacking.

Here, we introduce a new type of collinear antiferromagnetic (AFM) stacking in which two magnetic sublattices form a pattern of intersecting atomic chains. We refer to these associated cross-chain antiferromagnets as X-type antiferromagnets, which exhibit unique spin-dependent transport properties not observed in conventional magnets. Through high-throughput analyses and computations, we unveil three prototypes of X-type AFM stacking and identify 15 candidate materials. Using $\beta\text{-Fe}_2\text{PO}_5$ as a representative example, we predict that X-type AFM stacking supports sublattice-selective spin-dependent transport, where one magnetic sublattice conducts while the other does not, depending on the chosen transport direction. This distinctive property allows for a spin torque to be exerted solely on a single sublattice, resulting in unconventional ultrafast dynamics of the Néel vector capable of deterministic switching of the AFM order parameter. Our results highlight the unprecedented opportunities for both fundamental science and practical applications offered by X-type AFM stacking.

RESULTS

Conventional AFM stacking

Similar to ferromagnets and antiferromagnets being distinguished by their magnetic moment alignments, collinear antiferromagnets on their own are distinguished by different types of AFM stacking.

In general, an antiferromagnet is a magnetically ordered crystal characterized by three attributes: (1) equal magnitudes of magnetization of magnetic sublattices, $|\mathbf{m}_\alpha| = |\mathbf{m}_\beta|$, where α and β are sublattice indices; (2) vanishing net magnetization, $\mathbf{M} \propto \sum_\alpha \mathbf{m}_\alpha = 0$; and (3) a long-range AFM order, corresponding to a Heisenberg model with energy $H = - \sum_{\alpha \neq \beta} J_{\alpha\beta} \mathbf{m}_\alpha \mathbf{m}_\beta$ and a

negative exchange parameter $J_{\alpha\beta} < 0$ between different sublattices. In collinear antiferromagnets, the two magnetic sublattices can have different structures and stacking patterns. For example, Figures 1A–1C illustrate typical G-, A-, and C-types of AFM stacking, which have been originally proposed for simple cubic systems³¹ but are now widely used to characterize a broad range of antiferromagnets. For a G-type antiferromagnet, basic “building blocks” are isolated magnetic moments aligned antiparallel between all nearest neighbors (Figure 1A). In this sense, a G-type antiferromagnet can be considered “genuine” due to AFM coupling solely controlling this type of stacking, with ferromagnetic (FM) coupling playing a secondary role. On the contrary, for A-type or C-type antiferromagnets, where the building blocks are antiparallel-aligned two-dimensional (2D) FM-ordered layers (Figure 1B) or 1D FM-ordered atomic chains (Figure 1C). Such a classification has been used for over 70 years³¹ and involves other types of conventional AFM stacking, such as D-, E-, and F-types, which represent mixtures of parallel and orthogonal FM-aligned chains (D and F) combined with isolated magnetic moments antiparallel to all their nearest neighbors (E).

The classification of AFM stacking is useful to derive sublattice-dependent properties. As we discussed in our recent paper,¹⁷ some AFM crystals exhibiting a C-type AFM stacking, e.g., those that belong to the rutile family have small intra-sublattice distances resulting in strong intra-sublattice electron hopping between the neighboring sites. A similar property is expected for certain A-type antiferromagnets. Therefore, from the electronic transport perspective, such A-type and C-type antiferromagnets qualitatively represent FM-ordered sublattices electrically connected in parallel. They support staggered Néel spin currents capable of driving spin-transfer torques and sizable tunneling magnetoresistance (TMR) effects if used as electrodes in AFM tunnel junctions.^{17,18}

X-type AFM stacking

Antiferromagnets with stacking patterns other than those mentioned above may exhibit even more exciting spin-dependent transport phenomena. As an example, let us consider 1D FM-ordered chains of atoms with opposite magnetic moment orientations (denoted as FM_A and FM_B) as the basic building blocks of a new type of AFM stacking. Instead of alternating FM_A and FM_B chains parallel to each other as in the C-type stacking, the new stacking order hosts alternating layers of FM_A and FM_B chains parallel to each other within the plane but crossing in the adjacent layers (Figure 1D). Unlike the A-type AFM stacking with a similar FM ordering within the alternating planes, the new stacking has a sizable separation between the chains, making them rather isolated in each plane. This does not violate the three above-mentioned attributes of the AFM order and thus should exist in nature. Due to FM_A and FM_B chain

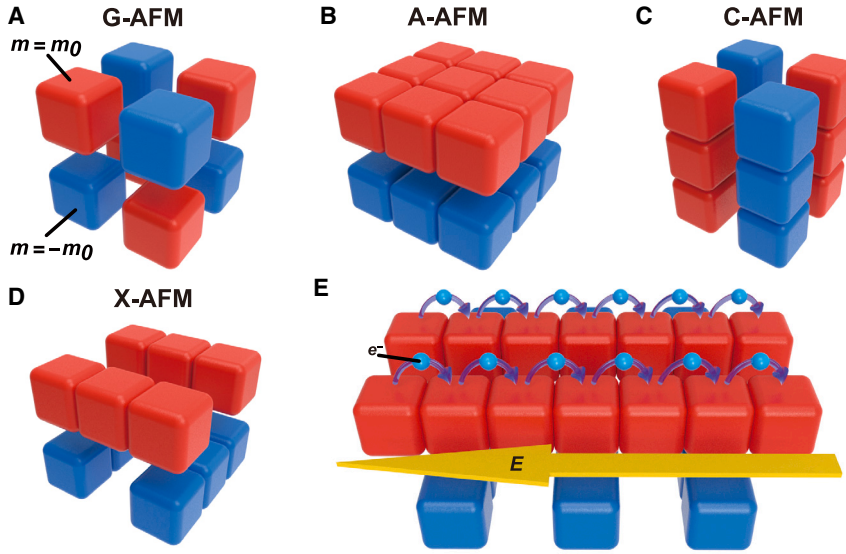


Figure 1. Building blocks for antiferromagnets

(A) A G-type AFM stacking with the isolated magnetic moments aligned antiparallel between all nearest neighbors.
(B) An A-type AFM stacking with the antiparallel-aligned FM layers.
(C) A C-type AFM stacking with the antiparallel-aligned FM chains.
(D) An X-type AFM stacking with the alternating layers of FM chains parallel to each other within the plane but crossing in the adjacent layers.
(E) The sublattice-selective spin transport allowed by X-type AFM stacking. The red and blue cubes represent the opposite magnetic sublattices. The yellow arrow represents an electric field parallel to the FM chains colored with red, and the blue balls and curved arrows represent the electric-field-driven electron hopping along the chains.

crossings in the antiferromagnets with such stacking, we dub them as cross-chain antiferromagnets, or X-type antiferromagnets for short.

The proposed X-type AFM stacking is expected to reveal unconventional transport properties never discovered before. Due to the pronounced anisotropy associated with the two cross-chain sublattices, X-type AFM metals are anticipated to exhibit strong anisotropy in their transport properties. For example, when applying an electric field along the FM_A direction, the FM_A chains are to be much more conductive for charge transport than the FM_B chains due to the strong intra-chain and weak inter-chain couplings (Figure 1E). In addition, due to the chains being FM ordered, the current flowing along the FM_A chain must be spin polarized. Therefore, unlike the A-type and C-type AFM stackings supporting staggered Néel spin currents on both sublattices, X-type AFM stacking is expected to support isolated Néel spin currents selectively flowing along a single sublattice, provided that the two chains are orthogonal. Similarly, when applying an electric field along the FM_B direction, oppositely spin-polarized Néel spin currents appear in the FM_B chains, while the FM_A chains become non-conducting.

Prototypes of X-type AFM stacking

Based on a high-throughput search within the dataset of the Materials Project,³² we have identified more than 600 crystals composed of alternating layers of chains parallel to each other within the plane but crossing in the adjacent layers. Assuming that the adjacent layers of chains are AFM coupled in these cross-chain crystals, we identify three prototypes of the X-type AFM stacking order (Figure 2). The first two prototypes, indicated as class I and class II, host the same magnetic unit cell as the crystal unit cell. They can be described by a minimum tight-binding toy model (Figures 2A and 2C) as follows:

$$H = H_{AA} + H_{BB} + H_{AB}, \quad (\text{Equation 1})$$

where H_{AA} (H_{BB}) is the Hamiltonian of an isolated FM chain A (B) and H_{AB} is the coupling between FM chains A and B:

$$\begin{aligned} H_{AA} &= t_{AA} \sum_{\alpha, \beta, \langle i, j \rangle} (c_{\alpha, i}^\dagger c_{\beta, j} + h.c.) - J \sum_{\alpha, j} c_{\alpha, j}^\dagger \sigma \cdot m_\alpha c_{\alpha, j} \\ &\quad + \varepsilon_0 \sum_{\alpha, j} c_{\alpha, j}^\dagger c_{\alpha, j}, \\ H_{BB} &= t_{BB} \sum_{\gamma, \delta, \langle i, j \rangle} (c_{\gamma, i}^\dagger c_{\delta, j} + h.c.) - J \sum_{\gamma, j} c_{\gamma, j}^\dagger \sigma \cdot m_\gamma c_{\gamma, j} \\ &\quad + \varepsilon_0 \sum_{\gamma, j} c_{\gamma, j}^\dagger c_{\gamma, j}, \text{ and} \\ H_{AB} &= t_{AB} \sum_{\alpha, \gamma, \langle i, j \rangle} (c_{\alpha, i}^\dagger c_{\gamma, j} + h.c.). \end{aligned} \quad (\text{Equation 2})$$

Here, α, β (γ, δ) denote atomic sites within a unit cell of the FM_A (FM_B) chain, i (j) are cell indices, t_{AA} (t_{BB}) is the intra-chain hopping parameter within the FM_A (FM_B) chain, t_{AB} is the hopping parameter between the FM_A and FM_B chains, J is the exchange parameter, ε_0 is the on-site energy, σ is the Pauli matrix vector, and m_α (m_γ) is the magnetic moment on the sites α (γ).

Within the X-type AFM stacking order of class I, FM_A and FM_B are connected by a symmetry operation $\hat{O}$ or $\hat{T}\hat{O}$, where $\hat{O}$ is a crystal symmetry such as a mirror/glide plane $\hat{M}_{\parallel}$ perpendicular to the x-y plane, a 2-fold rotation/screw axis $\hat{C}_{2\parallel}$ parallel to the x-y plane, or a 4-fold screw axis $\hat{C}_{4z}$ around the z direction, and $\hat{T}$ is time reversal (Figure 2A). These symmetries require $t_{AA} = t_{BB}$. This prototype of the X-type AFM stacking hosts alternating magnetic spin splitting (Figure 2B). Note that the stacking is not only defined by symmetry but involves the strength of interactions between the atomic planes and/or chains forming the structure; thus, it is evident that the symmetry group does not exclusively determine the stacking (see Figures S1 and S2 and Note S1).

The X-type AFM stacking order of class II, on the other hand, does not have a symmetry connection between FM_A and FM_B

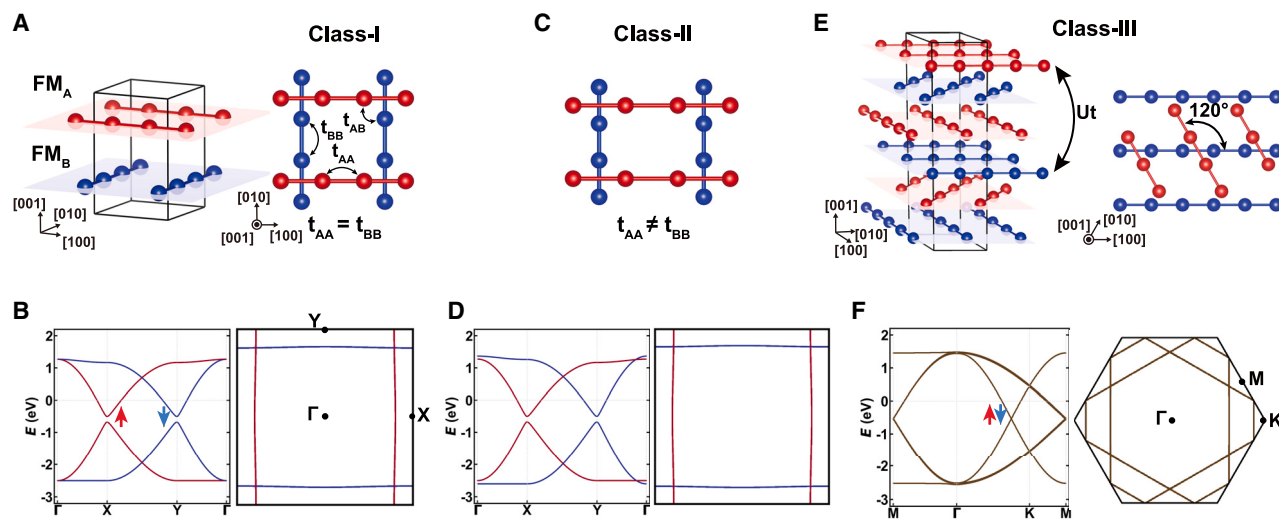


Figure 2. Prototypes of X-type AFM stacking

(A) The side view (left) and the top view (right) of the X-type AFM stacking of class I, where the magnetic unit cell is the same as the crystal unit cell and the FM_A and FM_B chains are connected by crystal symmetry, leading to equal intra-chain hopping.

(B) The band structure with an alternomagnetic spin splitting (left) and the associated Fermi surface (right) supported by the class I X-type AFM stacking with $t_{AA} = t_{BB}$.

(C) The top view of the X-type AFM stacking of class II, where the magnetic unit cell is the same as the crystal unit cell but the FM_A and FM_B chains are not connected by symmetry, leading to different intra-chain hopping.

(D) The band structure with a non-alternomagnetic spin splitting (left) and the associated Fermi surface (right) supported by the class II X-type AFM stacking with $t_{BB} = 1.05 t_{AA}$.

(E) The side view (left) and the top view (right) of the X-type AFM stacking of class III, where the magnetic unit cell doubles the crystal unit cell, resulting in the $\hat{U}\hat{t}$ symmetry combining spin rotation $\hat{U}$ and half-unit-cell translation $\hat{t}$.

(F) The spin degenerate band structure (left) and the Fermi surface (right) supported by class III X-type AFM stacking.

In the calculations (B, D, and F), we set $t_{AA} = 1$ eV, $t_{AB} = 0.3$ eV, $J = 3$ eV, and $\epsilon_0 = 2.5$ eV. $t_{AA} = t_{BB}$ is assumed in (F). The red and blue atomic chains in (A), (C), and (E) represent the opposite magnetic sublattices.

due to different intra-chain/inter-chain distances or relative rotations/distortions of the structural motifs of the chains (Figure 2C). This leads to a slightly different t_{AA} and t_{BB} . In this case, the spin degeneracy at the Γ point is removed (Figure 2D), indicating non-alternomagnetic spin splitting, as was discussed recently.³³

We note that the momentum-dependent spin splitting can be understood based on X-type AFM stacking in real space. For example, for X-type antiferromagnets with orthogonal cross-chains (Figures 2A and 2C) where the inter-chain hopping t_{AB} is not strong, in-plane electron hopping is confined within the chain. Therefore, the two spin-polarized bands contributed by FM_A (FM_B) are highly dispersive with a crossing in the Γ -X (Γ -Y) direction, but weakly dispersive with a large gap in the Γ -Y (Γ -X) direction (Figures 2B and 2D). This band structure indicates that it can be qualitatively considered as the superposition of the electronic structures of the isolated FM_A (FM_B) chains (see also Figures S3 and S4).

In addition, there is an X-type AFM stacking order of class III where the magnetic unit cell doubles the crystal unit cell, leading to the $\hat{U}\hat{t}$ symmetry combining spin rotation $\hat{U}$ and half-unit-cell translation $\hat{t}$ and compensating the magnetization (Figure 2E). This prototype is spin degenerate in the nonrelativistic limit, as shown in our model Hamiltonian calculation by introducing additional terms in Equation 1 coming from the isolated chains and their coupling (Figure 2F). The crystal structures supporting the

class III stacking can be found in trigonal and hexagonal systems where the adjacent cross-chains are connected by symmetry $\hat{T}\hat{C}_{3z}$ combining $\hat{T}$ and 3-fold screw axis $\hat{C}_{3z}$ (Figure 2E). Similar to class I and class II stackings, their band structures feature flat bands and band crossings (Figure 2F). The class III stacking also exhibits sublattice/chain selectivity: by applying an electric field perpendicular to two antiparallel chains in the cell, the staggered Néel spin currents can be selectively generated in the chains oblique to the electric field.

By calculating the exchange parameters of cross-chain materials based on 3d transition metals, we identify 15 X-type AFM candidates; among them, 13 belong to class I and 2 belong to class II, with 6 being experimentally available,^{34–40} as listed in Table 1 together with their spin space group^{41–43} (see also Figures S12–S27). We point out that more X-type antiferromagnets can be further designed, including those that belong to class III, by suitable element doping/substitution of cross-chain crystals in a material dataset. Below, we consider the class I X-type AFM candidate β -Fe₂PO₅^{39,40} as a representative example to demonstrate the sublattice-selective spin transport.

X-type AFM candidate β -Fe₂PO₅

Collinear antiferromagnet Fe₂PO₅ was discovered more than 30 years ago^{39,40,44} but remains not widely known. It has two polymorphs: the α phase, which has an orthogonal unit cell and a C-type AFM stacking below 250 K,⁴⁴ and the β phase, which

Table 1. Material candidates with X-type AFM stacking: Chemical formula, spin space group, Materials Project ID, and prototype class

Chemical formula	Spin space group	MP-ID	Prototype
Fe ₂ PO ₅ ³⁴	C ⁻¹ ₂ /C ^{∞m} ₁	mp-553913	class I
Co ₂ PO ₅	C ⁻¹ ₂ /C ^{∞m} ₁	mp-1272384	class I
KVAsO ₅ ³⁵	P ¹ _n ⁻¹ a ⁻¹ 2 ₁ ^{∞m} ₁	mp-1202651	class I
KVPO ₅ ³⁶	P ¹ _n ⁻¹ a ⁻¹ 2 ₁ ^{∞m} ₁	mp-19517	class I
SrV ₂ (PO ₅) ₂ ³⁷	F ⁻¹ d ¹ a ⁻¹ 2 ^{∞m} ₁	mp-559580	class I
CaNi ₂ (PO ₅) ₂	F ⁻¹ d ¹ a ⁻¹ d ^{∞m} ₁	mp-1378551	class I
Al(FeO ₂) ₂	I ⁻¹ 4 ₁ /a ^{∞m} ₁	mp-1248448	class I
VPbO ₂	I ⁻¹ 4 ₁ /a ^{∞m} ₁	mp-1208173	class I
Y(FeO ₂) ₂	I ⁻¹ 4 ₁ /a ^{∞m} ₁	mp-1405822	class I
Ca(CoO ₂) ₂	I ⁻¹ 4 ₁ /a ¹ m ⁻¹ d ^{∞m} ₁	mp-1406903	class I
Co ₂ PO ₅ ³⁸	I ⁻¹ 4 ₁ /a ¹ m ⁻¹ d ^{∞m} ₁	mp-1105140	class I
Fe ₂ PO ₅ ^{39,40}	I ⁻¹ 4 ₁ /a ¹ m ⁻¹ d ^{∞m} ₁	mp-18830	class I
VBiO ₂	I ⁻¹ 4 ₁ /a ¹ m ⁻¹ d ^{∞m} ₁	mp-1207870	class I
SrV ₂ (PO ₅) ₂	P ¹ ₁ ^{∞m} ₁	mp-723593	class II
Co ₂ PO ₅	I ¹ m ¹ m ¹ d ^{∞m} ₁	mp-1276873	class II

MP-ID, Materials Project ID.³²

represents an X-type AFM stacking.^{39,40} Figure 2A shows the crystal and magnetic structures of β -Fe₂PO₅, where the Fe atoms with upward and downward magnetic moments represent two magnetic sublattices denoted as Fe_A and Fe_B, respectively. The atomic structure of β -Fe₂PO₅ contains in-plane chains of face-sharing FeO₆ octahedra along the [100] and [010] directions of the tetragonal cell, which can be transformed to each other by the $\hat{T}\hat{C}_{4z}$ symmetry transformation, indicating class I X-type AFM stacking. The P atoms are located between these chains. The Fe ions have a mixed 2+/3+ valence and a small Fe-Fe intra-chain distance, favoring an intra-chain FM coupling via the double-exchange interaction.⁴⁵ These intersecting chains share common corners of the FeO₆ octahedra. The resulting Fe-O-Fe bond angle is $\sim 125^\circ$, leading to a super-exchange interaction that favors the inter-chain AFM coupling.⁴⁶ With a [001] directional Néel vector, β -Fe₂PO₅ belongs to the magnetic space group I4₁/am'd. A monoclinic distortion of β -Fe₂PO₅ reported at low temperatures³⁴ does not influence X-type AFM stacking. The uniqueness of X-type AFM stacking, metallic ground state, and Néel temperature $T_N = 408$ K,^{39,40} well above room temperature, make β -Fe₂PO₅ interesting for both fundamental studies and practical applications.

We perform first-principles density functional theory (DFT) calculations (see Figures S5–S7 and Tables S1 and S2) to explore the electronic and transport properties of β -Fe₂PO₅. Figures 3B and 3C show the calculated nonrelativistic band structure and Fermi surface of β -Fe₂PO₅ that reveal giant antiferromagnetic spin splitting⁴⁷ similar to that derived from our toy model (Figure 2B). To elucidate the spin-dependent transport properties, we calculate the bond transmission $T_{ij} = T_{ij}^\uparrow + T_{ij}^\downarrow$ and bond spin transmission $T_{ij}^s = T_{ij}^\uparrow - T_{ij}^\downarrow$ for transport along the [010] direction, where $\uparrow$ and $\downarrow$ denote the two spin channels and i and j are the atomic indices.⁴⁸ As is evident from Figures 3D and 3E, these quantities reflect the anticipated

chain-selective transport: both T_{ij} and T_{ij}^s are dominated by the Fe_A-Fe_A intra-chain bonds. It is notable that T_{ij}^s are negative, i.e., the spin current flows in the opposite direction to the charge current. This is due to the double-exchange interaction between Fe_A²⁺ and Fe_A³⁺ ions, which is mostly mediated by the hopping of electrons with the spins opposite to the Fe_A moments. As a result, the down-spin bands along the Γ -Y direction are highly dispersive (Figure 3B), leading to down-spin Fermi sheets representative of 1D transmission along the [010] direction (Figure 3B). On the other hand, although there are mobile up-spin electrons on the Fe_B chains to mediate the intra-chain double-exchange interaction, the weak inter-chain coupling due to the large Fe_A-Fe_B and Fe_B-Fe_B inter-chain distances leads to negligible T_{ij} and T_{ij}^s associated with Fe_B. Therefore, the dispersions of the up-spin bands are weak and have a large energy gap in the Γ -Y direction (Figure 3B). The transport spin polarization in this case is estimated to be as high as $\sim 68\%$ in the ballistic regime, which is further enhanced to $\sim 94\%$ in the diffusive regime, due to a small $T_{ij}^{(s)}$ associated with Fe_B being scattered out (see Figures S8–S10). Similarly, for transport along the [100] direction, the total transmission is majorly contributed by the hopping of up-spin electrons between intra-chain Fe_B atoms, corresponding to the band structure along the Γ -X direction and leading the up-spin Fermi surface sheets (Figures 3B and 3C). Therefore, the spin-split electronic structure of β -Fe₂PO₅ can be qualitatively considered as the superposition of the electronic structures of the isolated Fe_A and Fe_B chains, as expected based on our toy model.

The strong intra-chain spin transmission supports highly spin-polarized Néel spin currents along the chains in β -Fe₂PO₅. These Néel spin currents are highly anisotropic due to the X-type AFM stacking. For example, an electric field along the [110] direction produces crossing Néel spin currents with opposite spin polarizations along the Fe_A and Fe_B chains. These currents can be decomposed into a transverse global spin current and the staggered longitudinal Néel spin current hidden in a globally spin-neutral current. On the other hand, when the electric field is along one of the chain directions ([100] or [010]), only the longitudinal chains are conductive, producing an isolated Néel spin current, while the transverse chains are almost insulating.

Spin torques on a single sublattice

The robust sublattice-selective spin-dependent transport property is very interesting, as it opens a possibility to realize sublattice-resolved spintronic phenomena. As an example, we show that X-type antiferromagnets, such as β -Fe₂PO₅, allow exerting a spin torque on a single magnetic sublattice. This can be achieved by passing an external spin current along one of the FM-chain directions or using an isolated Néel spin current on one type of FM chains in the presence of asymmetric boundary conditions to generate self-torque. Assuming that the current is flowing along the FM_A sublattice with magnetic moments $\mathbf{m}_A$ pointing in the +z direction, the associated magnetic dynamics of an X-type antiferromagnet can be described by the Landau-Lifshitz-Gilbert-Slonczewski equations^{49,50}:

$$\dot{\mathbf{m}}_A = \boldsymbol{\tau}_A^F + \boldsymbol{\tau}_A^D + \boldsymbol{\tau}_A^{FL} + \boldsymbol{\tau}_A^{DL} \text{ and}$$

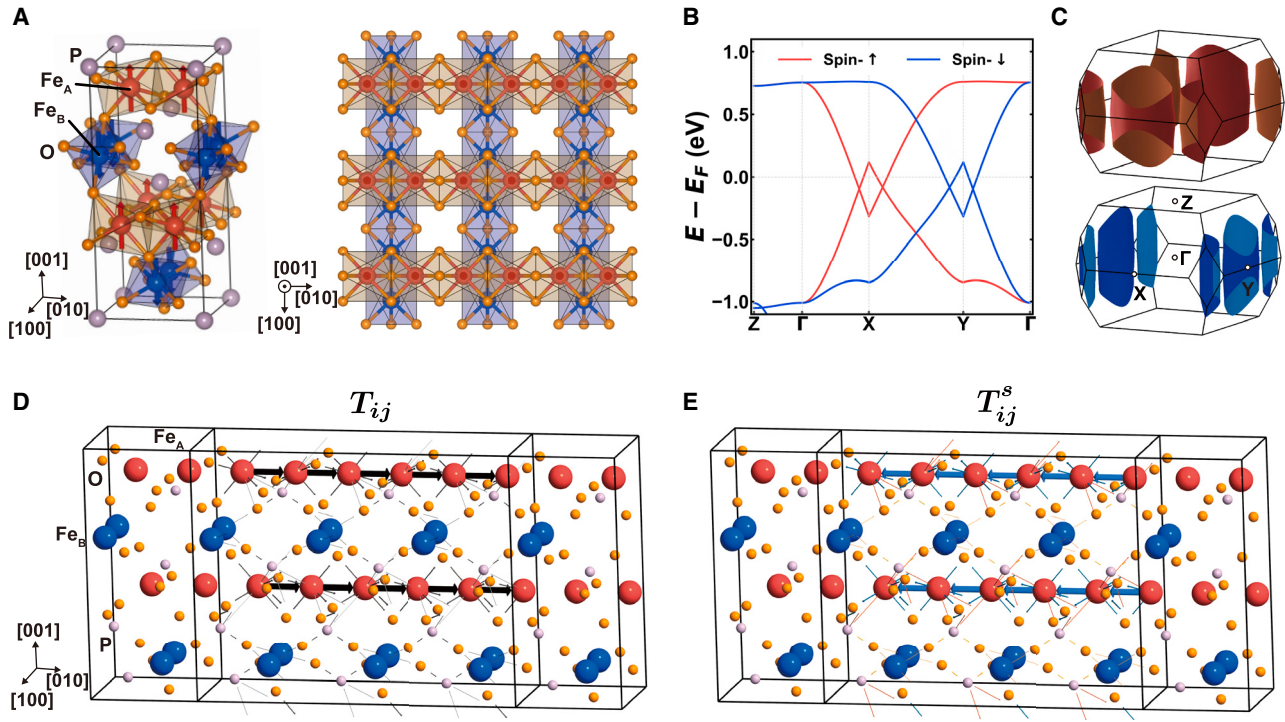


Figure 3. X-type antiferromagnet $\beta\text{-Fe}_2\text{PO}_5$

(A) Left: crystal and magnetic structures of $\beta\text{-Fe}_2\text{PO}_5$. Arrows denote the magnetic moments of Fe atoms. Right: top view of two bottom layers in the unit cell shown on the left. P atoms are ignored.

(B) Band structure of $\beta\text{-Fe}_2\text{PO}_5$.

(C) The up-spin (top) and down-spin (bottom) Fermi surfaces of $\beta\text{-Fe}_2\text{PO}_5$.

(D and E) Visualization of the calculated bond transmissions T_{ij} (D) and bond spin transmissions T_{ij}^s (E) of $\beta\text{-Fe}_2\text{PO}_5$. The directions of arrows indicate the sign of $T_{ij}^{(s)}$ between atoms i and j , i.e., a rightward (leftward) arrow implies that $T_{ij}^{(s)}$ is positive (negative). The width of the arrows is proportional to $\sqrt{|T_{ij}^{(s)}|}$. The spin-up (spin-down) magnetic moments, bands, and Fermi surfaces are colored with red (blue).

$$\dot{\mathbf{m}}_B = \boldsymbol{\tau}_B^F + \boldsymbol{\tau}_B^D. \quad (\text{Equation 3})$$

Here, $\boldsymbol{\tau}_\alpha^F \propto -\mathbf{m}_\alpha \times \mathbf{H}_{\text{eff},\alpha}$ and $\boldsymbol{\tau}_\alpha^D \propto \mathbf{m}_\alpha \times \dot{\mathbf{m}}_\alpha = -\mathbf{m}_\alpha \times (\mathbf{m}_\alpha \times \mathbf{H}_{\text{eff},\alpha})$ are the precession and damping torques on sublattice α induced by the intrinsic effective field $\mathbf{H}_{\text{eff},\alpha}$, respectively, and $\boldsymbol{\tau}_\alpha^{FL} \propto -\mathbf{m}_\alpha \times \mathbf{H}_{\text{st}}$ and $\boldsymbol{\tau}_\alpha^{DL} \propto -\mathbf{m}_\alpha \times (\mathbf{m}_\alpha \times \mathbf{H}_{\text{st}})$ are the field-like and damping-like torques driven by a spin-torque effective field $\mathbf{H}_{\text{st}}$ oriented toward the $-z$ direction. Since $\mathbf{H}_{\text{eff},\alpha}$ includes the anisotropy field $\mathbf{H}_{K,\alpha}$ and the exchange field $\mathbf{H}_{E,\alpha}$, the $\boldsymbol{\tau}_\alpha^F$ and $\boldsymbol{\tau}_\alpha^D$ can be further decomposed as $\boldsymbol{\tau}_\alpha^F = \boldsymbol{\tau}_{K,\alpha}^F + \boldsymbol{\tau}_{E,\alpha}^F$ and $\boldsymbol{\tau}_\alpha^D = \boldsymbol{\tau}_{K,\alpha}^D + \boldsymbol{\tau}_{E,\alpha}^D$, where the subscripts K and E denote the associated torques driven by $\mathbf{H}_{K,\alpha}$ and $\mathbf{H}_{E,\alpha}$, respectively. Due to $\mathbf{H}_{E,\alpha}$ being much larger than $\mathbf{H}_{K,\alpha}$, $\boldsymbol{\tau}_\alpha^F \approx \boldsymbol{\tau}_{E,\alpha}^F$ and $\boldsymbol{\tau}_\alpha^D \approx \boldsymbol{\tau}_{E,\alpha}^D$ when $\mathbf{m}_A$ and $\mathbf{m}_B$ are not perfectly antiparallel. Figures 4A and 4B schematically show how these torques affect the dynamics of $\mathbf{m}_A$ and $\mathbf{m}_B$. When the isolated spin-torque-carrying effective field $\mathbf{H}_{\text{st}}$ is applied solely to $\mathbf{m}_A$, the associated damping-like torque $\boldsymbol{\tau}_A^{DL}$ pulls $\mathbf{m}_A$ away from the easy axis toward the $-z$ direction. This creates canting between $\mathbf{m}_A$ and $\mathbf{m}_B$, and hence, $\mathbf{H}_{E,\alpha}$ exerts non-zero torques $\boldsymbol{\tau}_\alpha^F$ and $\boldsymbol{\tau}_\alpha^D$ on both moments $\mathbf{m}_A$ and $\mathbf{m}_B$. The torque $\boldsymbol{\tau}_\alpha^F$ generates oscillations of the Néel vector, while the torque $\boldsymbol{\tau}_B^D$ pulls

$\mathbf{m}_B$ toward the $+z$ direction even without the assistance of an external spin torque (see Note S9). Using realistic parameters $|\mathbf{H}_{K,\alpha}| = 2$ T, $|\mathbf{H}_{E,\alpha}| = 100$ T, and a damping factor of 0.01 (for simulations with different parameters, see Figure S11), we find that $\mathbf{H}_{\text{st}}$ much smaller than $\mathbf{H}_{K,\alpha}$ ($0.17|\mathbf{H}_{K,\alpha}| < |\mathbf{H}_{\text{st}}| < 0.24|\mathbf{H}_{K,\alpha}|$) is sufficient to switch the Néel vector (Figure 4C). The switching trajectory is similar to that for the spin-transfer torque in ferromagnets,^{49,50} indicating the decisive role of the damping-like torque $\boldsymbol{\tau}_A^{DL}$. Since this $\mathbf{H}_{\text{st}}$ can be driven by an external spin current, the AFM domains can be aligned according to the spin polarization of the external spin source. This solves the challenging problem of AFM spintronics where measurable time-reversal-odd properties (e.g., TMR in AFM tunnel junctions) are strongly diminished by misaligned domains.

Interestingly, we find that a larger $\mathbf{H}_{\text{st}}$ ($|\mathbf{H}_{\text{st}}| > 0.24|\mathbf{H}_{K,\alpha}|$) can drive ultrafast oscillations of the Néel vector (Figure 4D). This is because of the much stronger canting of $\mathbf{m}_A$ and $\mathbf{m}_B$ that produces a large out-of-plane component of $\boldsymbol{\tau}_A^F$ competing with $\boldsymbol{\tau}_A^{DL}$. This property distinguishes the dynamics of X-type antiferromagnets from other antiferromagnets, where full switching and ultrafast oscillations cannot be generated using the same type of spin torques.^{9,10,51}

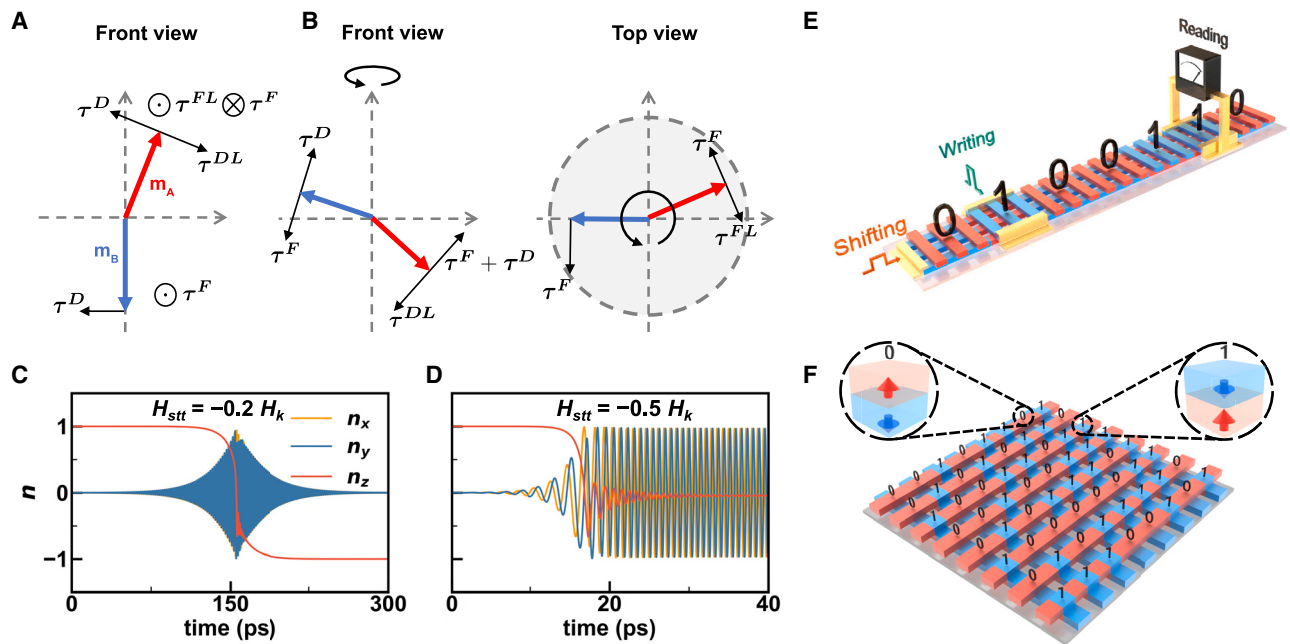


Figure 4. Sublattice-selective spin torques and their implications for spintronics

(A) Vectors of magnetic moments and spin torques in the initial process of spin dynamics.

(B) Vectors of magnetic moments and spin torques in the process of Néel vector oscillations driven by the single-sublattice spin torque: front (left) and top (right) views.

(C and D) Simulated dynamics of the x, y, and z components of the normalized Néel vector n under the current-induced spin-torque effective field $H_{st} = -0.2 H_K$ (C) and $H_{st} = -0.5 H_K$ (D).

(E) Schematic of an X-type racetrack memory. Here, the colored bars denote FM_A and FM_B chains of an X-type antiferromagnet, where the upward (downward) magnetic moments are denoted by red (blue). In this schematic, we assume with a slight exaggeration that the electrodes contact three chains.

(F) Schematic of X-type AFM stacking with crossing atomic chains forming an intrinsic crossbar array. Each bar is composed of a bunch of parallel chains, and the red and blue colors denote upward and downward moment orientations in these chains, respectively. The gaps between these bars are the chains not connected to the electrodes. The AFM domains at the intersections of these bars represent 0 and 1 bits.

DISCUSSION

Among the 15 antiferromagnets with X-type AFM stacking that we identified, 11 are metallic and, hence, expected to exhibit the properties discussed in this work. For the remaining 4 insulating X-type antiferromagnets, sublattice-selective transport properties associated with magnon excitations are possible,⁵² offering promising opportunities for spintronics with low-energy dissipation and long coherence lengths.

In addition to the existing X-type antiferromagnets, X-type AFM stacking may also occur in magnets that are not naturally AFM. For example, one can design X-type ferrimagnets with AFM stacking of cross-chains composed of different magnetic elements. Furthermore, synthetic X-type antiferromagnets can be engineered to possess the same advantages as their natural counterparts.

From a technological perspective, X-type AFM stacking presents an unprecedented approach for non-volatile memories. In an X-type antiferromagnet, it is possible to selectively nucleate and move domains via spin torques by passing an isolated Néel spin current or an external spin current along a designated FM_A or FM_B chain (Figure 4E). This capability promises the development of ultrafast X-type racetrack memory, where oppositely magnetized AFM domains can serve as “0” and “1” bits of information (Figure 4E). Moreover, X-type AFM stacking, characterized

by crossing chains of magnetic atoms, forms an intrinsic crossbar array that is widely utilized in magnetic random-access memories (MRAMs) (Figure 4F). Assuming a bilayer array of $\beta\text{-Fe}_2\text{PO}_5$ with one bit area containing a domain of 50×50 intersecting chains, the associated storage density is $\sim 15 \text{ Tb/in}^2$, which is promising for future big data applications.

Overall, X-type AFM stacking signifies an exciting area of research for fundamental science and offers an attractive new paradigm for AFM spintronics. The predicted sublattice-selective electronic transport carrying isolated Néel spin currents has multiple important implications, including spin torques exerted on a single magnetic sublattice, unconventional ultrafast spin dynamics, and deterministic switching of AFM domains. These unprecedented functionalities promise new AFM spintronic devices that can be employed in non-volatile memories with ultra-high density and ultrafast switching speeds. We hope that our theoretical results will inspire experimentalists in this field to explore the properties of X-type AFM stacking relevant to spintronics and beyond.

METHODS

Details regarding the methods can be found in the [supplemental information](#).

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. 2021YFA1600200), the National Natural Science Funds for Distinguished Young Scholars (grant no. 52325105), the National Natural Science Foundation of China (grant nos. 12274411, 12241405, and 52250418), the Basic Research Program of the Chinese Academy of Sciences (CAS) 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. S.-S.Z. performed the primary calculations and simulations. S.-S.Z., Z.-A.W., and B.L. performed analytical analysis of spin-torque dynamics. S.-S.Z., Z.-A.W., B.L., Y.-Y.J., S.-H.Z., R.-C.X., L.-X.L., X.L., W.-J.L., M.T., Y.-P.S., E.Y.T., H.D., and D.-F.S. analyzed the results. S.-S.Z., E.Y.T., H.D., 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.2025.100068>.

Received: November 27, 2024

Revised: February 4, 2025

Accepted: March 18, 2025

Published: April 11, 2025

REFERENCES

- Néel, L. (1932). Propriétés magnétiques du manganèse et du chrome en solution solide étendue. *J. Phys. Radium* 3, 160.
- Néel, L. (1952). Antiferromagnetism and Ferrimagnetism. *Proc. Phys. Soc.* 65, 869–885.
- Nobel Foundation (1972). Nobel Lectures - Physics : Including Presentation Speeches and Laureates' Biographies, 1963–1970. 4 (Elsevier Pub. Co. for the Nobel Foundation).
- Železný, J., Zhang, Y., Felser, C., and Yan, B. (2017). Spin-Polarized Current in Noncollinear Antiferromagnets. *Phys. Rev. Lett.* 119, 187204.
- Naka, M., Hayami, S., Kusunose, H., Yanagi, Y., Motome, Y., and Seo, H. (2019). Spin current generation in organic antiferromagnets. *Nat. Commun.* 10, 1–8.
- González-Hernández, R., Šmejkal, L., Výborný, K., Yahagi, Y., Sinova, J., Jungwirth, T., and Železný, J. (2021). Efficient Electrical Spin Splitter Based on Nonrelativistic Collinear Antiferromagnetism. *Phys. Rev. Lett.* 126, 127701.
- Gurung, G., Shao, D.-F., and Tsymbal, E.Y. (2021). Transport spin polarization of noncollinear antiferromagnetic antiperovskites. *Phys. Rev. Mater.* 5, 124411.
- Ma, H.-Y., Hu, M., Li, N., Liu, J., Yao, W., Jia, J.-F., and Liu, J. (2021). Multifunctional antiferromagnetic materials with giant piezomagnetism and noncollinear spin current. *Nat. Commun.* 12, 2846.
- Železný, J., Gao, H., Výborný, K., Zemen, J., Mašek, J., Manchon, A., Wunderlich, J., Sinova, J., and Jungwirth, T. (2014). Relativistic Néel-Order Fields Induced by Electric Current in Antiferromagnets. *Phys. Rev. Lett.* 113, 157201.
- Manchon, A., Železný, J., Miron, I.M., Jungwirth, T., Sinova, J., Thiaville, A., Garello, K., and Gambardella, P. (2019). Current-induced spin-orbit torques in ferromagnetic and antiferromagnetic systems. *Rev. Mod. Phys.* 91, 035004.
- Wadley, P., Howells, B., Železný, J., Andrews, C., Hills, V., Campion, R.P., Novák, V., Olejník, K., Maccherozzi, F., Dhesi, S.S., et al. (2016). Electrical switching of an antiferromagnet. *Science* 351, 587–590.
- Shao, D.-F., Zhang, S.-H., Li, M., Eom, C.-B., and Tsymbal, E.Y. (2021). Spin-neutral currents for spintronics. *Nat. Commun.* 12, 7061.
- Šmejkal, L., Hellenes, A.B., González-Hernández, R., Sinova, J., and Jungwirth, T. (2022). Giant and Tunneling Magnetoresistance in Unconventional Collinear Antiferromagnets with Nonrelativistic Spin-Momentum Coupling. *Phys. Rev. X* 12, 011028.
- Dong, J., Li, X., Gurung, G., Zhu, M., Zhang, P., Zheng, F., Tsymbal, E.Y., and Zhang, J. (2022). Tunneling Magnetoresistance in Noncollinear Antiferromagnetic Tunnel Junctions. *Phys. Rev. Lett.* 128, 197201.
- Qin, P., Yan, H., Wang, X., Chen, H., Meng, Z., Dong, J., Zhu, M., Cai, J., Feng, Z., Zhou, X., et al. (2023). Room-temperature magnetoresistance in an all-antiferromagnetic tunnel junction. *Nature* 613, 485–489.
- Chen, X., Higo, T., Tanaka, K., Nomoto, T., Tsai, H., Idzuchi, H., Shiga, M., Sakamoto, S., Ando, R., Kosaki, H., et al. (2023). Octupole-driven magnetoresistance in an antiferromagnetic tunnel junction. *Nature* 613, 490–495.
- Shao, D.-F., Jiang, Y.-Y., Ding, J., Zhang, S.-H., Wang, Z.-A., Xiao, R.-C., Gurung, G., Lu, W.-J., Sun, Y.-P., and Tsymbal, E.Y. (2023). Néel Spin Currents in Antiferromagnets. *Phys. Rev. Lett.* 130, 216702.
- Shao, D.-F., and Tsymbal, E.Y. (2024). Antiferromagnetic tunnel junctions for spintronics. *npj Spintronics*. 2, 13.
- Wu, C., Sun, K., Fradkin, E., and Zhang, S.-C. (2007). Fermi liquid instabilities in the spin channel. *Phys. Rev. B* 75, 115103.
- Hayami, S., Yanagi, Y., and Kusunose, H. (2019). Momentum-Dependent Spin Splitting by Collinear Antiferromagnetic Ordering. *J. Phys. Soc. Jpn.* 88, 123702.
- Yuan, L.-D., Wang, Z., Luo, J.-W., Rashba, E.I., and Zunger, A. (2020). Giant momentum-dependent spin splitting in centrosymmetric low-Z antiferromagnets. *Phys. Rev. B* 102, 014422.
- Yuan, L.-D., Wang, Z., Luo, J.-W., and Zunger, A. (2021). Prediction of low-Z collinear and noncollinear antiferromagnetic compounds having momentum-dependent spin splitting even without spin-orbit coupling. *Phys. Rev. Mater.* 5, 014409.
- Hayami, S., Yanagi, Y., and Kusunose, H. (2020). Bottom-up design of spin-split and reshaped electronic band structures in antiferromagnets without spin-orbit coupling: procedure on the basis of augmented multipoles. *Phys. Rev. B* 102, 144441.
- Liu, P., Li, J., Han, J., Wan, X., and Liu, Q. (2022). Spin-Group Symmetry in Magnetic Materials with Negligible Spin-Orbit Coupling. *Phys. Rev. X* 12, 021016.
- Mazin, I.I., Koepmick, K., Johannes, M.D., González-Hernández, R., and Šmejkal, L. (2021). Prediction of unconventional magnetism in doped FeSb₂. *Proc. Natl. Acad. Sci. USA* 118, e2108924118.

26. Šmejkal, L., Sinova, J., and Jungwirth, T. (2022). Beyond Conventional Ferromagnetism and Antiferromagnetism: A Phase with Nonrelativistic Spin and Crystal Rotation Symmetry. *Phys. Rev. X* 12, 031042.
27. Šmejkal, L., Sinova, J., and Jungwirth, T. (2022). Emerging Research Landscape of Altermagnetism. *Phys. Rev. X* 12, 040501.
28. Yuan, L.-D., and Zunger, A. (2023). Degeneracy Removal of Spin Bands in Collinear Antiferromagnets with Non-Interconvertible Spin-Structure Motif Pair. *Adv. Mater.* 35, 2211966.
29. Jungwirth, T., Marti, X., Wadley, P., and Wunderlich, J. (2016). Antiferromagnetic spintronics. *Nat. Nanotechnol.* 11, 231–241.
30. Baltz, V., Manchon, A., Tsoi, M., Moriyama, T., Ono, T., and Tserkovnyak, Y. (2018). Antiferromagnetic spintronics. *Rev. Mod. Phys.* 90, 015005.
31. Wollan, E.O., and Koehler, W.C. (1955). Neutron Diffraction Study of the Magnetic Properties of the Series of Perovskite-Type Compounds $[(1-x)\text{La}, x\text{Ca}]\text{MnO}_3$. *Physiol. Rev.* 100, 545–563.
32. Jain, A., Ong, S.P., Hautier, G., Chen, W., Richards, W.D., Dacek, S., Cholia, S., Gunter, D., Skinner, D., Ceder, G., and Persson, K.A. (2013). Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. *APL Mater.* 1, 011002.
33. Yuan, L.-D., Georgescu, A.B., and Rondinelli, J.M. (2024). Nonrelativistic Spin Splitting at the Brillouin Zone Center in Compensated Magnets. *Phys. Rev. Lett.* 133, 216701.
34. Elkaim, E., Berar, J.F., Gleitzer, C., Malaman, B., Ijjaali, M., and Lecomte, C. (1996). Occurrence of a monoclinic distortion in $\beta\text{-Fe}_2\text{PO}_5$. *Acta Crystallogr. B* 52, 428–431.
35. Belkhir, S., Mezaoui, D., and Roisnel, T. (2012). $\text{K}_2\text{V}_2\text{O}_7(\text{AsO}_4)_2$. *Acta Crystallogr.* 68, i54.
36. Benhamada, L., Grandin, A., Borel, M.M., Leclaire, A., and Raveau, B. (1991). KVPO_5 , an intersecting tunnel structure closely related to the hexagonal tungsten bronze. *Acta Crystallogr. C* 47, 1138–1141.
37. Berrah, F., Leclaire, A., Borel, M.-M., Guesdon, A., and Raveau, B. (1999). A new vanadium(IV) monophosphate, $\text{Sr}(\text{VO})_2(\text{PO}_4)_2$, isotypic with $\text{Ca}(\text{VO})_2(\text{PO}_4)_2$. *Acta Crystallogr. C* 55, 288–291.
38. Wang, G., Valldor, M., Spielberg, E.T., and Mudring, A.-V. (2014). Ionothermal Synthesis, Crystal Structure, and Magnetic Study of $\text{Co}_2\text{PO}_4\text{OH}$ Isostructural with Caminite. *Inorg. Chem.* 53, 3072–3077.
39. Ech-Chahed, B., Jeannot, F., Malaman, B., and Gleitzer, C. (1988). Préparation et étude d'une variété basse température de l'oxyphosphate de fer de valence mixte $\beta\text{Fe}_2(\text{PO}_4)\text{O}$ et de $\text{NiCr}(\text{PO}_4)\text{O}$: Un cas d'échange électronique rapide. *J. Solid State Chem.* 74, 47–59.
40. Ijjaali, M., Mallaman, B., and Gleitzer, C. (1990). Stability, Structure Refinement, and Magnetic Properties of $\beta\text{-Fe}_2\text{PO}_5$. *J. Solid State Chem.* 86, 195–205.
41. Xiao, Z., Zhao, J., Li, Y., Shindou, R., and Song, Z.-D. (2024). Spin Space Groups: Full Classification and Applications. *Phys. Rev. X* 14, 031037.
42. Chen, X., Ren, J., Zhu, Y., Yu, Y., Zhang, A., Liu, P., Li, J., Liu, Y., Li, C., and Liu, Q. (2024). Enumeration and Representation Theory of Spin Space Groups. *Phys. Rev. X* 14, 031038.
43. Jiang, Y., Song, Z., Zhu, T., Fang, Z., Weng, H., Liu, Z.-X., Yang, J., and Fang, C. (2024). Enumeration of Spin-Space Groups: Toward a Complete Description of Symmetries of Magnetic Orders. *Phys. Rev. X* 14, 031039.
44. Warner, J.K., Cheetham, A.K., Cox, D.E., and Von Dreele, R.B. (1992). Valence contrast between iron sites in $\alpha\text{-Fe}_2\text{PO}_5$ - a comparative study by magnetic neutron and resonant x-ray-powder diffraction. *J. Am. Chem. Soc.* 114, 6074–6080.
45. Zener, C. (1951). Interaction between the d-Shells in the Transition Metals. II. Ferromagnetic Compounds of Manganese with Perovskite Structure. *Phys. Rev.* 82, 403–405.
46. Anderson, P.W. (1950). Antiferromagnetism. Theory of Superexchange Interaction. *Phys. Rev.* 79, 350–356.
47. He, T., Zhang, X., Meng, W., Jin, L., Dai, X., and Liu, G. (2019). Topological nodal lines and nodal points in the antiferromagnetic material $\beta\text{-Fe}_2\text{PO}_5$. *J. Mater. Chem. C* 7, 12657–12663.
48. Solomon, G.C., Herrmann, C., Hansen, T., Mujica, V., and Ratner, M.A. (2010). Exploring local currents in molecular junctions. *Nat. Chem.* 2, 223–228.
49. Slonczewski, J.C. (1996). Current-driven excitation of magnetic multilayers. *J. Magn. Magn. Mater.* 159, L1–L7.
50. Zhang, S., Levy, P.M., and Fert, A. (2002). Mechanisms of spin-polarized current-driven magnetization switching. *Phys. Rev. Lett.* 88, 236601.
51. Cheng, R., Daniels, M.W., Zhu, J.-G., and Xiao, D. (2015). Ultrafast switching of antiferromagnets via spin-transfer torque. *Phys. Rev. B* 91, 064423.
52. Wang, Z.-A., Li, B., Zhang, S.-S., Lu, W.-J., Tian, M., Sun, Y.-P., Tsymbal, E.Y., Wang, K., Du, H., and Shao, D.-F. (2025). Giant uncompensated magnon spin currents in X-type magnets. Preprint at arXiv. <https://doi.org/10.48550/arXiv.2502.13511>.