Large magnetoresistance in an electric field controlled antiferromagnetic tunnel junction

Yurong Su¹, Jia Zhang²*, Jing-Tao Lü², Jeongmin Hong¹, and Long You¹*

¹School of Optical and Electronic Information, Huazhong University of Science and Technology, 430074 Wuhan, China

²School of Physics and Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, 430074 Wuhan, China

*jiazhang@hust.edu.cn;

*lyou@hust.edu.cn.

Large magnetoresistance effect controlled by electric field rather than magnetic field or electric current is a preferable routine for designing low power consumption magnetoresistance-based spintronic devices. Here we propose an electric-field controlled antiferromagnetic (AFM) tunnel junction with structure of piezoelectric substrate/Mn₃Pt/SrTiO₃/Pt operating by the magnetic phase transition (MPT) of antiferromagnet Mn₃Pt through its magneto-volume effect. The transport properties of the proposed AFM tunnel junction have been investigated by employing first-principles calculations. Our results show that a magnetoresistance over hundreds of percent is achievable when Mn₃Pt undergoes MPT from a collinear AFM state to a non-collinear AFM state. Band structure analysis based on density functional calculations shows that the large TMR can be attributed to the joint effect of significant different Fermi surface of Mn₃Pt at two AFM phases and the band symmetry filtering effect of the SrTiO₃ tunnel barrier. In addition, other than single-crystalline tunnel barrier, we also discuss the robustness of the proposed magnetoresistance effect by considering amorphous AlOₓ barrier. Our results may open perspective way for effectively electrical writing and reading of the AFM state and its application in energy efficient magnetic memory devices.

I. INTRODUCTION

A conventional magnetic tunnel junction (MTJ) with high tunnel magnetoresistance (TMR) consists of two ferromagnetic (FM) electrodes separated by an ultrathin insulating barrier. The TMR effect can be applied in various spintronic devices, for instance, magnetoresistive random access memories (MRAM), magnetic field sensors, read heads for hard drives, and spin logics [1-3]. At current stage,
electric current has been mainly used to manipulate the magnetization states in MTJs via spin-transfer-torque (STT) [4-6], spin-orbit torque [7-9] mechanisms or magnetic fields produced by current, which limits the energy efficiency of MTJ-based spintronic devices. Therefore, there have been great efforts aiming at electric field control of magnetic states instead of electric current. Voltage controlled magnetic anisotropy (VCMA) in perpendicularly magnetized CoFe(B)/MgO interface is one of the promising strategy [10-13]. However, the VCMA effect mainly relies on the electrostatic screening of magnetic electrodes at interface, and the voltage controlled effect alone is not sufficient for effectively manipulating magnetization state [10]. Alternative strategy towards electric-field control of TMR is to use ferroelectric barrier in a tunnel junction [14-16]. However, one of the main disadvantages of the ferroelectric tunnel junctions (FTJs) is the high resistance-area (R.A) product due to the existence of the critical thickness for the ferroelectric polarization of tunnel barrier [17].

Recently, an alternative route to obtain moderate TMR has been proposed via the magnetic phase transition (MPT) of a magnetic electrode [18,19]. A typical structure of this type of MTJ might be a sandwich structure of “metallic MPT-electrode/insulating tunnel barrier/non-magnetic metallic electrode”. The magnetoresistance will arise when the internal magnetic structure of MPT-electrode changes by external magnetic field, temperature, etc. For instance, the α'-FeRh electrode can be switched from G-type antiferromagnetic (AFM) to FM state via magnetic field (at the order of several Tesla), and over 20% TMR at room temperature has been demonstrated experimentally in α'-FeRh/MgO/γ-FeRh MTJ [18]. In the present work, we will focus on another more attractive metallic AFM MPT-material Mn3Pt and discuss the corresponding magnetoresistance effect.

As a well-studied MPT-materials, the ground magnetic state of cubic Cu3Au type Mn3Pt is triangular non-collinear AFM (D-phase). It shows a first-order magnetic transition from D-phase to the collinear AFM state (F-phase) when the temperature rises up to T\textsubscript{f}~365 K [20,21], and it further becomes paramagnetic when the temperature is high over T\textsubscript{f}~475 K. The magnetic structures of the two stable AFM states in bulk Mn3Pt are illustrated in Fig. 1(a). The non-collinear D phase state with the magnetic moments of the three Mn atoms in the unit cell establish a triangular arrangement within the (111) plane.

The F phase is a collinear magnetic structure with doubled unit cell along the c direction.

What’s more interesting, recent experiments demonstrate that being grown on a ferroelectric BaTiO\textsubscript{3} substrate, the transition temperature of Mn3Pt can be shifted upwards by applying electric field through BaTiO\textsubscript{3} substrate. Hence, the collinear F-phase of Mn3Pt can be driven into non-collinear D-phase by
applying an electric field on piezoelectric BaTiO$_3$ substrate above room temperature [22]. Therefore, it would be possible to design tunnel junctions by employing such electric field controlled MPT of Mn$_3$Pt as it is shown in Fig. 1(b). On the other hand, AFM materials are believed to be promising for applications in spintronic devices. However, the lack of efficient method for electrical control of AFM states is one of the main obstacle for their applications in magnetic memory devices. Therefore, the possibility of designing the electric field controlled AFM Mn$_3$Pt-based tunnel junctions with large TMR above room temperature may provide new avenue for AFM spintronics [23,24].

Now we will first briefly discuss the mechanism of electric field controlled MPT of Mn$_3$Pt on a piezoelectric substrate. The transition temperature $T_{tr}$ of Mn$_3$Pt between D and F phase has been found to be closely related to its lattice constant [25] due to the so-called “magneto-volume” effect [26]. The smaller lattice constant will result in higher transition temperature $T_{tr}$ of Mn$_3$Pt. When Mn$_3$Pt is grown on a piezoelectric substrate, for instance BaTiO$_3$, the applied electric field across BaTiO$_3$ will lead to the decrease of in-plane lattice constant due to the inverse piezoelectric effect, and correspondingly, the MPT temperature of Mn$_3$Pt will shift to a higher value. In consequence, the electric field can be applied to switch the magnetic phase of Mn$_3$Pt between collinear F phase and non-collinear D phase at certain temperature window as it has been demonstrated experimentally [22].

![Fig. 1](image_url)

Fig. 1. (a) The illustrations of the atomic and magnetic structures of AFM Mn$_3$Pt in D and F phases. The Pt atoms are in grey and the Mn atoms are in purple. The green arrows indicate the magnetic moment directions on Mn atoms. (b) The demonstration and operation principles of electric field driven MPT-TMR effect in a tunnel junction with a Mn$_3$Pt electrode.
A realistic Mn₃Pt-based AFM junction structure and its electric field driven operation principle is shown in Fig. 1(b). The whole Mn₃Pt/SrTiO₃/Pt tunnel junction can be grown on a piezoelectric substrate, for example, BaTiO₃. The electric field is applied between BaTiO₃ substrate and Mn₃Pt to write the AFM state of Mn₃Pt, and the tunnel resistance is measured between Mn₃Pt and Pt electrode across the SrTiO₃ tunnel barrier. By comparing with conventional MTJs and FTJs, the advantages of the proposed tunnel junctions are multifold including: (1) The magnetic phase of Mn₃Pt is controlled by electric field rather than magnetic field or electric current. In consequence, the proposed AFM MTJs may be more energy efficient in magnetoresistance based memory device. (2) The magnetoresistance is originating from the MPT of Mn₃Pt electrode and large TMR is optimistic. High TMR of the tunnel junctions will then be beneficial to its application in a memory device with high On/Off ratio. (3) The electric field controlled MPT is switched between two AFM phases, and the whole tunnel junction might be robust against the external magnetic field perturbation and suitable for high density non-volatile memory. (4) The proposed tunnel junction structure is simple with only one magnetic electrode and the switching speed should be fast due to the AFM phase transition.

The remaining key issue of the proposed AFM tunnel junction will then be the spin-dependent transport properties. Especially, the conductance (resistance) ratio of the tunnel junction when Mn₃Pt is in F and D-phase which is the main focus of the present work. In the past, there are also several experiments focusing on AFM tunnel junctions by using collinear antiferromagnet L₁₀-IrMn [27,28] or L₁₀-MnPt[29] as electrode. However, the magnetoresistances in those tunnel junctions which originates from the anisotropic electronic structure of antiferromagnets are relatively low (typically less than 10%). Hereafter, we will investigate the transport and the corresponding MPT-TMR effect in a Mn₃Pt/SrTiO₃/Pt tunnel junction through first-principles calculations.

II. CALCULATION METHODS

Experimentally, a Mn₃Pt film originally in the collinear F-phase with a = 3.875 Å, c = 3.850 Å can be switched to the non-collinear D-phase with a = 3.866 Å, c = 3.860 Å above room temperature by applying a moderate out-of-plane electric field $E = 4 \text{ kVcm}^{-1}$[22]. The corresponding experimental lattice constants of Mn₃Pt for two magnetic phases have been used in the present first-principles calculations. All the calculations in the present work are performed by employing the Quantum Espresso package[30] with the PBE-GGA (Perdew-Burke-Ernzerhof type of generalized-gradient-approximation) exchange
correlation potential[31] and ultrasoft pseudopotential[32] generated from PSlib0.3.1. A Monkhorst-Pack $k$-point mesh of $16 \times 16 \times 16$ and plane-wave cutoff 50 Ry are adopted for the self-consistent electronic structure calculations of bulk Mn$_3$Pt. The calculated ground state of bulk Mn$_3$Pt is D phase which has a total energy 1.01 eV per formula cell lower than the F phase, which agrees with the previous theoretical value [33]. The magnetic moment on Mn atom of D phase is 3.10 $\mu_B$ and it agrees well with the experimental value of 3.0 $\mu_B$[20,21]. For F phase, the Mn spins on the S-sites is 2.92 $\mu_B$ per Mn atom, and on the B-sites is nonzero, but has a small value of 0.11 $\mu_B$ along c axis, resulting a net magnetic moment and magnetization accordingly.

In order to calculate the electron transmission of Mn$_3$Pt/SrTiO$_3$/Pt tunnel junction, first, the electronic structures of the left Mn$_3$Pt electrode, the right Pt electrode, and the junction region in a Mn$_3$Pt/SrTiO$_3$/Pt supercell are separately self-consistently calculated. Then, the electron transmission is calculated by using a standard wave-function scattering method [32,34] in two-dimensional Brillouin zones (2DBZs) by matching the wave function between left and right electrodes. The ballistic Landauer conductance of the tunnel junction is calculated by summarizing the transmission over $200 \times 200$ $k/\mathbf{a}=(k_x, k_y)$ points in 2DBZ: $G = \frac{e^2}{h} \sum T(k_n)$, where $T(k_n)$ is the $k$-resolved transmission, $e$ is the elementary charge, and $h$ is the Planck constant.

### III. RESULTS AND DISCUSSIONS

The Fermi surface (FS) of electrode indicate the available Bloch states distributed over Brillouin zone for electron transmission, and it is crucial for electron transport of MTJs. Fig. 2(a) shows the side and top view (along $k_z$ direction) of the three-dimensional FSs for bulk Mn$_3$Pt in D and F phases. Both AFM phases have multiple bands and distributed over the 2DBZ, and the noteworthy difference of the two AFM phases is that there is no available Bloch state around the zone center for F phase while several Bloch states are present for D phase, which is evident from the top views shown in Fig. 2(a). This is one of the main reasons for the different transmission in Mn$_3$Pt-based MTJs and the resultant large magnetoresistance through SrTiO$_3$ barrier as we discuss later. The corresponding density of states for D phase and F phase are shown in Fig. 2(b). At Fermi energy, the F-phase has relative larger density of states than D-phase Mn$_3$Pt.
Fig. 2. (a) The side and top views of three-dimensional FSs for Mn$_3$Pt in D and F phases. The FSs are visualized by using Xcrysden package [35]. (b) Density of states (DOS) of bulk Mn$_3$Pt per formula cell for F (red) and D (blue) phases. The Fermi energy lies at zero as indicated by the vertical black dash line.

A Mn$_3$Pt/SrTiO$_3$/Pt MTJ is built and shown in Fig. 3(a). The tunnel junction consists of a semi-infinite Mn$_3$Pt electrode and SrTiO$_3$ tunnel barrier with a thickness of 2 unit cells (u.c.) stacked along the [001] direction. Perovskite oxide SrTiO$_3$ with lattice constant 3.905 Å is chosen as the tunnel barrier by considering its small lattice mismatch (< 1.0 %) with Mn$_3$Pt. In addition, Pt with lattice constant of 3.916 Å[36] serves as counter electrode which receives tunneling electrons from Mn$_3$Pt electrode. Therefore, the whole Mn$_3$Pt/SrTiO$_3$/Pt tunnel junction may be grown epitaxially with small lattice mismatch. The epitaxial relation between Mn$_3$Pt and SrTiO$_3$ might be Mn$_3$Pt(100)//SrTiO$_3$(100)//Pt[001] with the Ti atoms sit at the top of the Mn atoms. In the junction, the left lead consists of repeating unit
cells of Mn$_3$Pt and terminates on both ends with a Mn-Pt atomic layer. The SrTiO$_3$ layer is terminated on both sides with TiO$_2$ atomic plane. The oxygen atoms are connected with Mn and Pt atoms at the interface which is energy favorable [16].

The main results of the transport calculation are shown in Fig. 3(b) which displays the $k_\|$-resolved transmission for the junction with Mn$_3$Pt electrode in D and F phases. In the junction with D phase Mn$_3$Pt, an area has the largest transmission of $10^{-1}$ distributed around the 2DBZ center. In contrast, the FS of Mn$_3$Pt in F phase viewed along the [001] direction has holes in the zone center. There are no bulk states in both spin channels of F phase Mn$_3$Pt, which results in zero transmission around this area. Accordingly, the total transmission of the Mn$_3$Pt/SrTiO$_3$/Pt junction with D phase Mn$_3$Pt electrode is relatively larger than that with the F phase Mn$_3$Pt electrode. When the electric field is applied across piezoelectric substrate, the Mn$_3$Pt electrode undergoes a phase transition from F phase to D phase, consequently the tunneling junction undergoes a transition from high-resistance state to low-resistance state. The optimistic MPT-TMR can be defined as: $\text{MPT-TMR} = \frac{G_{D-phase} - G_{F-phase}}{\min(G_{F-phase}, G_{D-phase})} \times 100\%$. The electron transmission and the corresponding MPT-TMR are listed in Table 1. One can see that the MPT-TMR is over 500% by this definition.

![Atomic structure of Mn$_3$Pt/SrTiO$_3$/Pt junction](image)

**Fig. 3.** (a) The side view of the atomic structure of Mn$_3$Pt/SrTiO$_3$/Pt tunnel junction. (b) The electron transmission of Mn$_3$Pt/SrTiO$_3$/Pt MTJ with Mn$_3$Pt in D (left) and F (right) AFM phases, respectively. The color bar shows the intensity of transmission.

**Table 1.** The electron transmission of D-Mn$_3$Pt and F-Mn$_3$Pt per formula cell. The transmission of MTJ with paramagnetic Mn$_3$Pt (P-Mn$_3$Pt) electrode has also been listed for comparison.
Transmission for D-Mn₃Pt  |  Transmission for F-Mn₃Pt  |  Transmission for P-Mn₃Pt  |  MPT-TMR
--- | --- | --- | ---
Bulk-Mn₃Pt | 0.85 | 1.87 | — | -120%
Mn₃Pt/SrTiO₃/Pt | 2.5×10⁻² | 0.40×10⁻² | 0.90×10⁻² | 525%
Mn₃Pt/AlOₓ/Pt | — | — | — | -200%<sup>b</sup>

<sup>a</sup>For F-Mn₃Pt the transmissions for two spin channel are identical and for non-collinear D-Mn₃Pt the transmissions of the two spin channels are indistinguishable.

<sup>b</sup>Estimated from density of states at Fermi energy.

The large MPT-TMR in Mn₃Pt/SrTiO₃/Pt tunnel junction also partly relies on symmetry selective filtering effect in SrTiO₃ tunnel barrier. As it is shown in Fig. 4(a), similar to the band symmetry filtering effect in MgO[1] and spinel oxide MgAl₂O₄[37], the Bloch state with Δ₁ and Δ₅ symmetry has smallest decay rate within the bandgap of SrTiO₃. In consequence, the Bloch states around Γ point (zone center) may have relatively larger tunneling possibility. Fig. 4(b) shows complex wave vector with smallest imaginary part over the entire 2DBZ. It is clear that the slowest electron decay rate forms a cross shape around the Γ point. By comparing the FSs of D-Mn₃Pt and F-Mn₃Pt shown in Fig. 2(a), there is no available Bloch states of F-Mn₃Pt around Γ point while available Bloch states present for D-Mn₃Pt. In consequence, for D-Mn₃Pt/SrTiO₃/Pt tunnel junction, because of large transmission contribution from the Brillion zone center, the tunneling conductance should be much larger than that of F-Mn₃Pt/SrTiO₃/Pt MTJ, and lead to large positive MPT-TMR.

![Fig. 4.](image-url)

Fig. 4. (a) The complex band structure of SrTiO₃ along [001] direction (k<sub>c</sub>=0). The real band and the imaginary band are plotted in red and blue, respectively. The top of the valence band is located at the zero energy. (b) The two dimensional complex band dispersion of SrTiO₃ at the middle of bandgap with smallest imaginary part χ in the unit of 2π/a).
It is worthwhile pointing out that SrTiO$_3$ may not be the unique tunnel barrier material suitable for the proposed tunnel junctions with Mn$_3$Pt electrode. Despite of the large MPT-TMR in the single-crystalline tunnel junction with SrTiO$_3$ barrier, it is also possible to fabricate a similar junction but with an amorphous barrier, for instance, AlO$_x$ barrier. By ignoring the difference of tunneling ability of each Bloch state, the electron transmission (or conductance) at zero bias is proportional to the density of states at Fermi energy of two electrodes as: 

$$ T \propto D_F(E_F)D_{Mn, Pt}(E_F) \cdot$$

A simple estimation of the MPT-TMR with amorphous AlO$_x$ barrier according to the density of states of F-Mn$_3$Pt and D-Mn$_3$Pt shown in Fig. 2(b) is around -200 % as it is listed in Table 1. Here the negative sign indicates a larger conductance of F-Mn$_3$Pt/AlO$_x$/Pt than D-Mn$_3$Pt/AlO$_x$/Pt MTJ.

The interfacial magnetic structure may be important for the spin-dependent transport and the resultant TMR in a MTJ [38]. In order to elucidate the effect of possible interface magnetic disorder, additional calculations are performed. Take the F-Mn$_3$Pt/SrTiO$_3$/Pt-MTJ for example, instead of perfect AFM interface magnetic structure (shown in Fig.5 (a)), we consider 1 u.c. (shown in Fig. 5(b)) and 4 u.c. (not shown) of paramagnetic Mn$_3$Pt present at the interface. The resultant electron transmission is listed in Table 2. Comparing with the perfect AFM ordered Mn$_3$Pt interface, paramagnetic Mn$_3$Pt present at the interface will lead to additional interface scattering and decrease of electron transmission. However, the MPT-TMR has been largely preserved due to the fact that the MPT-TMR mostly originates from the features of FS of bulk Mn$_3$Pt as we discuss previously. These results further confirm that the MPT-TMR should be robust against the imperfect interfacial magnetic structure.

![Fig. 5 Atomic structure of F-Mn$_3$Pt/SrTiO$_3$/Pt MTJ with perfect interface magnetic structure (a) and with 1 u.c. of paramagnetic Mn$_3$Pt interface (b). The arrows represent the magnetic moments.](image)

Table 2. The electron transmission of F-Mn$_3$Pt/SrTiO$_3$/Pt-MTJ per formula cell with different
In stoichiometry $\text{Mn}_3\text{Pt}/\text{BaTiO}_3$ system, the electric field control of MPT occurs above room temperature at around 360 K [22]. It may also be possible to further reduce the MPT temperature to room temperature (300 K) by choosing appropriate materials. For instance, it has been experimentally shown that the MPT temperature of non-stoichiometry $\text{Mn}_3\text{PtN}_x$ and $\text{Mn}_{3-x}\text{Pt}_{1+x}$ alloys [25,39,40] can be lowered down to room temperature, and theoretically shown that Mn-based antiperovskite nitrides [41] may have similar AFM phase transition. And also instead of $\text{BaTiO}_3$ substrate, an alternative piezoelectric substrate with a larger piezoelectric effect, for example, PMN-PT ($\text{Pb(Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$-$\text{PbTiO}_3$) [42] substrate may lead to a MPT at room temperature.

Moreover, the electronic structures of $\text{Mn}_3\text{Pt}$ in the non-collinear AFM D-phase and collinear AFM F-phase are significantly different and may lead to other different intrinsic physical properties beyond magnetoresistance effect in the studied $\text{Mn}_3\text{Pt}$-based MTJs. For example, it has been experimentally demonstrated that the non-collinear AFM D-phase has moderate anomalous Hall conductivity (AHE) while collinear AFM F-phase has zero AHE conductivity [22]. Thus one may expect different spin hall conductivity (or spin-hall angle) of $\text{Mn}_3\text{Pt}$ in two different AFM phases [43]. In addition, non-collinear and collinear AFM $\text{Mn}_3\text{Pt}$ may lead to different exchange bias effect in $\text{Mn}_3\text{Pt}/\text{FM}$ metal bilayer system. All these physical properties, can be controlled by electric field through inverse piezoelectric effect [22,44,45] and used in AFM spintronics [23,24].

**IV. SUMMARY**

In summary, by employing first-principles calculations we have investigated the transport properties of MTJs by using an AFM electrode $\text{Mn}_3\text{Pt}$, which can be transformed from collinear AFM F-phase to non-collinear AFM D-phase by applying electric field across piezoelectric substrate. Our results show that the magnetoresistance ratio in a $\text{Mn}_3\text{Pt}/\text{SrTiO}_3/\text{Pt}$ tunnel junction can reach hundreds of percent, making it promising for application in low-power consumption memory devices. The MPT-TMR in the proposed single crystalline MTJ originates from the cooperative effect of different Fermi surfaces of

| Interfacial magnetic structure | Transmission     | MPT-TMR  |
|-------------------------------|------------------|----------|
| 1 u.c. $\text{P-Mn}_3\text{Pt}$ | $0.11 \times 10^{-2}$ | +2173%   |
| 4 u.c. $\text{P-Mn}_3\text{Pt}$ | $0.28 \times 10^{-2}$ | +793%    |
Mn$_3$Pt in two AFM phases and the band symmetry filtering effect of SrTiO$_3$ barrier. This would make the MPT-TMR robust against the possible interface magnetic structure disorder. In addition, by estimating from the density of states, a similar tunnel junction with amorphous AlO$_x$ barrier also has large MPT-TMR. Such electric field controlled MPT-TMR effect is expected in a class of similar materials beyond Mn$_3$Pt. Moreover, the electric-field controlled MPT of Mn$_3$Pt can be largely extended to other electric-controlled phenomenon beyond MPT-TMR including anomalous Hall, spin Hall, exchange bias, etc. This work may stimulate the future experimental investigations on the MPT-TMR mechanism and the application of Mn$_3$Pt and similar materials in AFM spintronics.

ACKNOWLEDGMENTS

Jia Zhang and Long You are supported by the National Natural Science Foundation of China with grant No. 11704135, 61674062 and 61821003. The calculations in this work are partly performed at National Supercomputer Center in Tianjin, TianHe-1(A) China.

References:
[1]. W. H. Butler, X.-G. Zhang, T. C. Schulthess, and J. M. MacLaren, Spin-dependent tunneling conductance of Fe/MgO/Fe sandwiches, Phys. Rev. B 63, 054416 (2001).
[2]. S. S. P. Parkin, C. Kaiser, A. Panchula, P. M. Rice, B. Hughes, M. Samant, and S.-H. Yang, Giant tunneling magnetoresistance at room temperature with MgO(001) tunnel barriers, Nat. Mater. 3, 862 (2004).
[3]. S. Yuasa, T. Nagahama, A. Fukushima, Y. Suzuki, and K. Ando, Giant room-temperature magnetoresistance in single-crystal Fe/MgO/Fe magnetic tunnel junctions, Nat. Mater. 3, 868 (2004).
[4]. J. C. Slonczewski, Current-driven excitation of magnetic multilayers, J. Magn. Magn. Mater. 159, L1 (1996).
[5]. L. Berger, Emission of spin waves by a magnetic multilayer traversed by a current, Phys. Rev. B 54, 9353 (1996).
[6]. Z. Diao, Z. Li, S. Wang, Y. Ding, A. Panchula, E. Chen, L.-C. Wang, and Y. Huai, Spin-transfer torque switching in magnetic tunnel junctions and spin-transfer torque random access memory, J. Phys.: Condens. Matter 19, 165209 (2007).
[7]. L. Liu, C.-F. Pai, Y. Li, H. W. Tseng, D. C. Ralph, and R. A. Buhrman, Spin-Torque Switching with the Giant Spin Hall Effect of Tantalum, Science 336, 555 (2012).
[8]. C.-F. Pai, L. Liu, Y. Li, H. W. Tseng, D. C. Ralph, and R. A. Buhrman, Spin transfer torque devices utilizing the giant spin Hall effect of tungsten, Appl. Phys. Lett. 101, 122404 (2012).
[9]. A. Brataas, A. D. Kent, and H. Ohno, Current-induced torques in magnetic materials, Nat. Mater. 11, 372 (2012).
[10]. W.-G. Wang, M. Li, S. Hageman, and C. L. Chien, Electric-field-assisted switching in magnetic tunnel junctions, Nat. Mater. 11, 64 (2012).
[11]. Y. Shiota, T. Nozaki, F. Bonell, S. Murakami, T. Shinjo, and Y. Suzuki, Induction of coherent magnetization switching in a few atomic layers of FeCo using voltage pulses, Nat. Mater. 11, 39–43 (2012).
[12]. F. Matsukura, Y. Tokura, and H. Ohno, Control of magnetism by electric fields, Nat. Nanotech. 10, 209 (2015).
[13] E. Y. Tsymbal, Electric toggling of magnets, Nat. Mater. 11, 12 (2012).
[14] E. Y. Tsymbal and H. Koh lstedt, Tunneling across a ferroelectric, Science 313, 181 (2006).
[15] J. P. Velev, C-G. Duan, J. D. Burton, A. Smogunov, M. K. Niranjan, E. Tosatti, S. S. Jaswal, and E. Y. Tsymbal, Magnetic Tunnel Junctions with Ferroelectric Barriers: Prediction of Four Resistance States from first principles, Nano. Lett. 9, 1 (2009).
[16] J. P. Velev, C. G. Duan, K. D. Belashchenko, S. S. Jaswal, and E. Y. Tsymbal, Effect of Ferroelectricity on Electron Transport in Pt/BaTiO$_3$/Pt Tunnel Junctions, Phys. Rev. Lett. 98, 137201 (2007).
[17] G. Gerra, A. K. Tagantsev, N. Setter, and K. Parlinski, Ionic Polarizability of conductive metal oxide and critical thickness for ferroelectricity in BaTiO$_3$, Phys. Rev. Lett. 96, 107603 (2006).
[18] X. Z. Chen, J. F. Feng, Z. C. Wang, J. Zhang, X. Y. Zhong, C. Song, L. Jin, B. Zhang, F. Li, M. Jiang, Y. Z. Tan, X. J. Zhou, G. Y. Shi, X. F. Zhou, X. D. Han, S. C. Mao, Y. H. Chen, X. F. Han, and F. Pan, Tunneling anisotropic magnetoresistance driven by magnetic phase transition, Nat. Commun. 8, 449 (2017).
[19] J. Zhang, X. Z. Chen, C. Song, J. F. Feng, H. X. Wei, and J.-T. Lü, Giant tunnel magnetoresistance with a single magnetic phase-transition electrode, Phys. Rev. Appl. 9, 044034 (2018).
[20] E. Krén, G. Kádár, L. Pál, and P. Szabó, Investigation of the first-order magnetic transformation in Mn$_3$Pt, J. Appl. Phys. 38, 1265 (1967).
[21] E. Krén, G. Kádár, L. Pál, J. Sólyom, P. Szabó, and T. Tarnóczi, Magnetic structures and exchange interactions in the Mn-Pt system, Phys. Rev. 171, 574–585 (1968).
[22] Z. Q. Liu, H. Chen, J. M. Wang, J. H. Liu, K. Wang, Z. X. Feng, H. Yan, X. R. Wang, C. B. Jiang, J. M. D. Coey, and A. H. MacDonald, Electrical switching of the topological anomalous Hall effect in a non-collinear antiferromagnet above room temperature, Nat. Electron. 1,172–177 (2018).
[23] V. Baltz, A. Manchon, M. Tsai, T. Moriyama, T. Ono, and Y. Tserkovnyak, Antiferromagnetic spintronics, Rev. Mod. Phys. 90, 015005 (2018).
[24] T. Jungwirth, X. Marti, P. Wadley, and J. Wunderlich, Antiferromagnetic spintronics, Nat. Nanotechnol. 11, 231 (2016).
[25] H. Yasui, T. Kaneko, H. Yoshida, S. Abe, K. Kamigaki and N. Mori, Pressure dependence of magnetic transition temperatures and lattice parameter, J. Phys. Soc. Jpn 56, 12 (1987).
[26] E. Mendive-Tapia and J. B. Staunton, Ab initio theory of the Gibbs free energy and a hierarchy of local moment correlation functions in itinerant electron systems: The magnetism of the Mn$_3$A materials class, Phys. Rev. B 99, 144424 (2019).
[27] B. G. Park, J. Wunderlich, X. Marti, V. Holý, Y. Kurosaki, M. Yamada, H. Yamamoto, A. Nishide, J. Hayakawa, H. Takahashi, A. B. Shick, and T. Jungwirth, A spin-valve-like magnetoresistance of an antiferromagnet-based tunnel junction, Nature Mater. 10, 347 (2011).
[28] Y. Y. Wang, C. Song, B. Cui, G. Y. Wang, F. Zeng, and F. Pan, Room-temperature perpendicular exchange coupling and tunneling anisotropic magnetoresistance in an antiferromagnet-based tunnel junction, Phys. Rev. Lett. 109, 137201 (2012).
[29] H. Yan, Z. Feng, S. Shang, X. Wang, Z. Hu, J. Wang, Z. Zhu, H. Wang, Z. Chen, H. Hua, W. Lu, J. Wang, P. Qin, H. Guo, X. Zhou, Z. Leng, Z. Liu, C. Jiang, M. Coey, and Z. Liu, A piezoelectric, strain-controlled antiferromagnetic memory insensitive to magnetic fields, Nat. Nanotechnol. 14, 131 (2019).
[30] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, et. al., Quantum Espresso: a modular and open-source software project for quantum simulations of materials, J. Phys.: Condens. Matter 21, 395502 (2009).
[31] J. P. Perdew, K. Burke, and M. Ernzerhof, Generalized gradient approximation made simple. Phys. Rev. Lett. 77, 3865 (1996).
[32] D. Vanderbilt, Soft self-consistent pseudopotentials in a generalized eigenvalue formalism, Phys. Rev. B 41,
[33]. Y. Kota, H. Tsuchiura, and A. Sakuma, Ab-Initio study on the magnetic structures in the ordered Mn:Pt alloy, IEEE Trans. On. Mag. 44, 3131(2008).

[34]. A. Smogunov, A. D. Corso, and E. Tosatti, Ballistic conductance of magnetic Co and Ni nanowires with ultrasoft pseudopotentials, Phys. Rev. B 70, 045417 (2004).

[35]. http://www.xcrysden.org/.

[36]. P. Haas, F. Tran, and P. Blaha, Calculation of the lattice constant of solids with semilocal functionals, Phys. Rev. B 79, 085104 (2009).

[37]. J. Zhang, X.-G. Zhang, and X. F. Han, Spinel oxides: Δ1 spin-filter barrier for a class of magnetic tunnel junctions, Appl. Phys. Lett. 100, 222401 (2012).

[38]. J. Zhang, Y. Wang, X.-G. Zhang, and X. F. Han, Inverse and oscillatory magnetoresistance in Fe/MgO/Cr/Fe magnetic tunnel junctions, Phys. Rev. B 82, 134449 (2010).

[39]. E. Krén, E. Zsoldos, M. Barberon, and R. Fruchart, Magnetic properties of the Mn3PtNx system, Solid State Commun. 9, 27–31 (1971).

[40]. E. Krén, G. Kádár, L. Pál, J. Sólyom, and P. Szabó, Magnetic structures and magnetic transformations in ordered Mn3(Rh, Pt) alloys, Phys. Lett. 20, 331 (1966).

[41]. J. Zemen, E. Mendive-Tapia, Z. Gercsi, R. Banerjee, J. B. Staunton, and K. G. Sandeman, Frustrated magnetism and caloric effects in Mn-based antiperovskite nitrides: Ab initio theory, Phys. Rev. B 95, 184438 (2017).

[42]. S. Park and T. R. Shroult, Ultrahigh strain and piezoelectric behavior in relaxor based ferroelectric single crystals, J. Appl. Phys. 82, 1804 (1997).

[43]. W. Zhang, M.B. Jungfleisch, W. Jiang, J. E. Pearson, and A. Hoffmann, Spin Hall Effects in Metallic Antiferromagnets, Phys. Rev. Lett. 113, 196602 (2014).

[44]. S. M. Wu, S. A. Cybart, D. Yi, J. M. Parker, R. Ramesh, and R. C. Dynes, Full electric control of exchange bias, Phys. Rev. Lett. 110, 067202 (2013).

[45]. X. He, Y. Wang, N. Wu, A.N. Caruso, E. Vescovo, K. D. Belashchenko, P. A. Dowben, and C. Binek, Robust isothermal electric control of exchange bias at room temperature, Nat. Mater. 9, 579 (2010).