Unconventional spin-orbit torque in transition metal dichalcogenide/ferromagnet bilayers from first-principles calculations

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(Dated: May 5, 2020)

Motivated by recent observations of unconventional out-of-plane dampinglike torque in WTe2/Permalloy bilayer systems, we calculate the spin-orbit torque generated in two-dimensional transition metal dichalcogenide (TMD)/ferromagnet heterostructures using first-principles methods and linear response theory. Our numerical calculation of spin-orbit torques in WTe2/Co and MoTe2/Co heterostructures shows both conventional and novel dampinglike torques (torque per electric field) with comparable magnitude, around one hundred ℏ/2e (Ω⋅cm)^{-1}, for an electric-field applied perpendicular to the mirror plane of the TMD layer. To gain further insight into the source of dampinglike torque, we compute the spin current flux between the TMD and Co layers and find good agreement between the two quantities. This indicates that the conventional picture of dampinglike spin-orbit torque, whereby the torque results from the spin Hall effect plus spin transfer torque, largely applies to TMD/Co bilayer systems.

I. INTRODUCTION

Spin-orbit torque is an effect in which the application of an electric field induces the exchange of angular momentum between the crystal lattice and the magnetization of a magnetically ordered material. This exchange is mediated by spin-orbit coupling, and the effect offers a promising mechanism for energy-efficient electrical switching of thin film ferromagnets. The prototypical geometry of a spin-orbit torque-based device is shown in Fig. [1]. Charge current is applied in the plane of a heavy metal-ferromagnet bilayer, leading to magnetic dynamics and potentially switching of the ferromagnetic orientation. This geometry is quite distinct from the conventional spin transfer torque-based magnetic tunnel junctions, which utilize spin-polarized current flowing perpendicular to the materials’ interfaces. The geometry of devices which utilize spin-orbit torque enables separate electrical paths for writing and reading the magnetic information, which may be advantageous for applications.

The dependence of the spin-orbit torque on the magnetization orientation is determined by the system symmetry. In many devices studied to date (e.g., Co-Pt bilayers), the materials are deposited by sputtering and the film is effectively isotropic in the plane normal to the interface. This leaves the stacking direction (z) as the only symmetry broken direction. In the presence of an applied electric field E, and for the magnetization aligned to the E × z direction, the system is invariant under reflections about the plane spanned by E and z. This implies that the torque on the magnetization vanishes in this configuration, so that it is a fixed point for electric field-induced magnetic dynamics. This in turn implies that the spin-orbit torque for such a system can deterministically switch the magnetization between in-plane configurations.

Breaking the in-plane symmetry of the system removes this constraint on the form of the torque. In this case, the electric field-induced torque generally drives the magnetization to a point above or below the plane of the film (depending on the current polarity). This enables deterministic switching of perpendicularly magnetized thin film ferromagnets. This is of particular interest due to technological advantages of perpendicularly magnetized layers, such as improved switching speed and efficiency. The reduction of symmetry has been realized experimentally through a variety of means, such as the application of an in-plane magnetic field, the addition of in-plane magnetized layers (ferromagnetic or antiferromagnetic), or engineered structural asymmetry. Of relevance to this work is a series of recent experiments in which substrates with reduced crystal symmetry (transition metal dichalcogenides) were utilized to realize spin-orbit torques with a form that enables switching of perpendicular ferromagnets.

While symmetry dictates the form of the spin-orbit torque, quantifying its magnitude and identifying its microscopic origin require explicit calculation. Knowledge of these properties can aid in developing materials and device selection rules in order to optimize relevant figures of merit, such as switching efficiency. With this motivation, we report on first-principles calculations of electric-field induced spin-orbit torque in transition metal dichalcogenide/ferromagnet bilayers. Our numerical analysis demonstrates that a considerable out-of-plane dampinglike torque is generated in this low symmetry system. We also provide a general analysis of the symmetry-allowed torques for materials of this symmetry class. We compute the spin current flowing between layers in the heterostructure, and find that it provides the primary source of torque on the magnetic layer.

Our paper is organized as follows. In Sec. I we review
When an external electric field is applied, both the electrons’ distribution function and wave functions are modified. The linear response from the change of Fermi-Dirac distribution function is time-reversal odd within the relaxation time approximation, while the linear response from the change of electronic wave-function is time-reversal even. Using the Kubo formula, the even and odd torque (the torque per electric-field strength per area) under the external field in $x$-direction are expressed as:

$$\tau_{\text{even}} = 2e \sum_{k,n} f(E_{nk}) \frac{\text{Im} \langle \psi_{nk} | \frac{\partial H}{\partial k} | \psi_{mk} \rangle \langle \psi_{mk} | \mathbf{T} | \psi_{nk} \rangle}{(E_{nk} - E_{mk})^2 + \eta^2},$$

and

$$\tau_{\text{odd}} = \frac{e}{\pi} \sum_{k,n,m} \eta^2 \text{Re} \langle \psi_{nk} | \frac{\partial H}{\partial k} | \psi_{nk} \rangle \langle \psi_{nk} | \mathbf{T} | \psi_{mk} \rangle \langle \psi_{mk} | \psi_{nk} \rangle \delta_{mn},$$

where $|\psi_{nk}\rangle$ satisfy the steady state Schrodinger equation, $H_k |\psi_{nk}\rangle = E_{nk} |\psi_{nk}\rangle$, and are labeled by Bloch wave vector $k$ and band index $n$. In Eqs. 3-4, $e$ is the electron charge, $f(E)$ is the equilibrium Fermi-Dirac distribution function, $\mu$ is the chemical potential, and $\eta$ is the broadening parameter (note that $f$ depends on $\mu$). We use $k_B T = \eta = 25$ meV throughout the paper unless otherwise noted.

We assume $H$ is expressed in a tight-binding representation. In evaluating Eqs. 3 and 4, the velocity matrix operator is given by $\frac{\partial H}{\partial k} = \sum_{\mathbf{R}} \langle \mathbf{R} \rangle |\psi_{nk}\rangle \langle \psi_{nk} | e^{i \mathbf{k} \cdot \mathbf{R}} H_{\mathbf{R}}$, where $H_{\mathbf{R}}$ is the Hamiltonian matrix coupling the orbitals centered in the primary unit cell with orbitals centered in the unit cell displaced by $\mathbf{R}$. We include the atomic coordinate positions (i.e., the basis vectors of atoms within the unit cell) in the displacement vector $\mathbf{R}$. Within the LSDA approximation, we can rotate the magnetization direction by rotating the time-reversal odd component of real space tight-binding Hamiltonian.

We also evaluate the spin current flowing between the two layers of the heterostructure, whose evaluation we describe next. We write the Hamiltonian for the bilayer system as:

$$H = \begin{pmatrix} H_{\text{FM}} & t_{\text{TMD,FM}} \\ t_{\text{FM,TMD}} & H_{\text{TMD}} \end{pmatrix}$$

The diagonal elements of Eq. 5 describe intralayer (or “on-site”) contributions to the Hamiltonian. The off-diagonal elements describe the coupling (or “hopping”) between layers. The interlayer electron current operator $J$ is given by:

$$J = i \begin{pmatrix} 0 & t_{\text{FM,TMD}} \\ -t_{\text{TMD,FM}} & 0 \end{pmatrix}.$$

We denote the spin current flowing between layers as $Q$, whose vector direction specifies the spin polarization of...
the spin current. The spin current operator is the symmetrized product of the interlayer current and the spin operator:

$$Q_\alpha = \frac{1}{2} \left( \mathbf{S}_\alpha \mathbf{J} + \mathbf{J} \mathbf{S}_\alpha \right)$$  \hspace{1cm} (7)

To evaluate the electric field-induced spin current, we replace $\mathbf{J}$ with $Q$ in Eqs. 3 and 4.

**B. First principles calculations**

In this section we describe some details of the first principles calculations, which proceed in three steps: structural relaxation, Wannier projection, and evaluation of Eqs. 3 and 4 using the tight-binding Hamiltonian.

The structural relaxation itself is a two-step process, in which we first relax using the Vienna Ab initio Simulation Package (VASP)\textsuperscript{[29, 30]} and use this relaxed structure as input to a second structural relaxation in Quantum ESPRESSO\textsuperscript{[31]}. We find this is more efficient than exclusively using Quantum ESPRESSO for relaxation. In the VASP calculation, we use the PAW method\textsuperscript{[24]} with the Perdew-Burke-Ernzerhof Generalized-Gradient Approximation (PBE-GGA) functional\textsuperscript{[32]}. All structures are relaxed until the total energy converges to within $10^{-4}$ eV during the self-consistent loop, with forces converged to 0.1 eV/Å, while employing the Methfessel-Paxton method with a smearing of 0.2 eV width. The Brillouin zone is sampled with a $7 \times 4 \times 1$ Monkhorst Pack mesh\textsuperscript{[33]}. An energy cut-off of 450 eV is used for all calculations. Van der Waals interactions are accounted for by means of the Grimme (D2) scheme\textsuperscript{[34]}. The valence electron configuration for each metal considered are W:5d$^6$6s$^1$, Te:5s$^2$5p$^1$, Co:3d$^8$4s$^2$ and Mo:4d$^5$5s$^1$.

Prior to creating the TMD/Co systems, the lattice constants of the isolated TMD layer are optimized, resulting in $a = 0.349$ nm, $b = 0.625$ nm for WTe$_2$ and $a = 0.348$ nm, $b = 0.636$ nm for MoTe$_2$. The Co-TMD heterostructure consists of 1-2 monolayers of TMD stacked on a Co slab 3 layers thick with 4 Co atoms per layer. There is a large mismatch between TMD and Co lattice constants. In this work, we apply most of the strain to the Co layer (see Fig. 2), since we focus on retaining the crystal symmetry of the TMD layer, and experimental samples exhibit a lack of crystallinity in the ferromagnetic layer\textsuperscript{[19, 21]}. We replace W (Mo) and Te and restricted from movement (frozen) and the structure is relaxed again. The relaxed atomic positions are provided in Appendix B.

The relaxed structure provided by VASP serves as the initial configuration for the structural relaxation calculation in Quantum ESPRESSO. The optimized Co atoms form three flat layers consisting of 4 atoms per layer. To reduce the system size and computational load, we remove the top Co layer prior to relaxation in Quantum ESPRESSO. The relaxation calculation is non-relativistic and spin-polarized, and utilizes a $12 \times 6 \times 1$ Monkhorst Pack mesh\textsuperscript{[35]}, cutoff energy 1088 eV, total energy convergence threshold $1.36 \times 10^{-3}$ eV, force convergence threshold $2.57 \times 10^{-2}$ eV/Å.

With the optimized geometry of the heterostructure and the corresponding self-consistent ground state computed with Quantum ESPRESSO, we use Wannier90\textsuperscript{[36]} to obtain the real space tight-binding model in the basis of atomic orbitals. We project on to $d$ orbitals of transition metal atoms, $s$ and $p$ orbitals of chalcogen atoms, and $s, p, d$ orbitals of Co atoms. After obtaining the collinear spin-polarized Hamiltonian in the Wannier basis, we add the onsite spin-orbit coupling terms $\alpha \mathbf{L} \cdot \mathbf{S}$. Note that adding spin-orbit coupling "by hand" in this manner requires that Wannier orbitals are not localized, in order to ensure that they are spherical harmonics consistent with the standard representation of $\mathbf{L}$. The strength of the spin-orbit coupling parameter $\alpha$ is obtained by fitting the pristine spin-orbit coupled bands from Quantum ESPRESSO. We obtain $\alpha = [350, 100, 500, 70] \text{ meV}$ for W, Mo, Te, and Co, respectively. Note that the Wannier projection procedure breaks the mirror symmetry slightly, so we manually restore the mirror symmetry using procedures as described in Ref\textsuperscript{[37]}. We use a $k$-mesh of approximately $540 \times 300$ (similar integration steps in $k_x(k_y)$ direction) to evaluate Eqs. 3 and 4.

**III. RESULTS**

**A. Symmetry considerations**

We preface the presentation of numerical results with a review of the symmetry properties of the system,
which have been discussed in previous works[18,19,21]. In Appendix A, we present the fully general form of the current-induced torques for this system. In what follows we focus on the azimuthal angle dependence for in-plane magnetization orientations (along the equator of Fig. 3). We denote the out-of-plane and in-plane torque as follows:

\[
\tau_\perp = \tau_z, \quad \tau_\parallel = \tau_x \sin(\phi) - \tau_y \cos(\phi),
\]

where the azimuthal angle \(\phi\) defines the in-plane magnetization direction: \(M_x = M \cos \phi, M_y = M \sin \phi\). By examining the symmetry transformation of \(\tau_\perp\) and \(\tau_\parallel\) under an external field in \(x\)-direction, we find that both in-plane and out-of-plane torques are cosine functions. We group them into time-reversal even and odd parts:

\[
\tau_\perp = \sum_{n=0}^{\infty} B_{2n}^{\perp,\text{even}} \cos(2n\phi) + B_{2n}^{\perp,\text{odd}} \cos((2n+1)\phi)
\]

\[
\tau_\parallel = \sum_{n=0}^{\infty} B_{2n}^{\parallel,\text{odd}} \cos(2n\phi) + B_{2n}^{\parallel,\text{even}} \cos((2n+1)\phi)
\]

(10)

In this work we use the terms “time-reversal even torque” and “dampinglike torque” interchangeably, and also use the terms “time-reversal odd torque” and “fieldlike torque” interchangeably. The 1\(^{st}\) order contribution to the in-plane time-reversal even torque \(B_{1}^{\perp,\text{even}}\) is equivalent to the conventional dampinglike torque form, i.e., \(\mathbf{M} \times \mathbf{M} \times (\mathbf{E} \times \mathbf{z})\), and the 0\(^{th}\) order contribution to the out-of-plane time-reversal even torque \(B_{0}^{\perp,\text{even}}\) is the unconventional torque allowed only in the absence of mirror symmetry about the \(xz\) plane.

For an applied electric field in the \(y\)-direction, the torques take the form:

\[
\tau_\perp = \sum_{n=0}^{\infty} A_{2n}^{\parallel,\text{even}} \sin(2n\phi) + A_{2n+1}^{\parallel,\text{odd}} \sin((2n+1)\phi)
\]

\[
\tau_\parallel = \sum_{n=0}^{\infty} A_{2n}^{\parallel,\text{odd}} \sin(2n\phi) + A_{2n+1}^{\parallel,\text{even}} \sin((2n+1)\phi)
\]

(11)

For this direction of \(\mathbf{E}\) field, mirror symmetry about the \(yz\) plane is retained, and the torques assume a more conventional form. In particular there is no magnetization-independent out-of-plane dampinglike torque.

### B. Numerical Results

We next turn to the calculation results. Fig. 3 shows the torque as a function of magnetization orientation for a heterostructure composed of one WTe\(_2\) layer and two layers of Co (as shown in Fig. 2). Figs. 3(a) and (c) show the dampinglike and fieldlike components of torque, respectively, for \(\mathbf{E}\) along \(x\). Recall that for this direction of \(\mathbf{E}\), all symmetries are broken and the form of the torque is unconstrained. The dampinglike torque drives the magnetization into a point in the \(yz\) plane. As discussed in the introduction, for this case an applied electric field can deterministically switch a perpendicularly magnetized layer due to the dampinglike torque driving the magnetization to a point in the northern or southern hemisphere. The fieldlike torque also vanishes at a point in the \(yz\) plane, although at a point different than for which the dampinglike torque vanishes. There is therefore no point at which the total electric field-induced torque vanishes.

Figs. 3(b) and (d) show the same data for \(\mathbf{E}\) along \(y\). This is a more conventional configuration in which there is a mirror plane symmetry with respect to the plane formed by \(z\) and \(\mathbf{E}\). The dampinglike torque drives the magnetization into the \(x\) direction and vanishes there due to the mirror symmetry \(x \rightarrow -x\). However we note that the dampinglike torque has substantial contributions from higher order terms, and is not well-described by the lowest order form \((\mathbf{M} \times \mathbf{M} \times \mathbf{x})\). The fieldlike torque is well described by the simple form \(\mathbf{M} \times \mathbf{x}\).

We next consider a series of systems in which we vary the TMD material type and thickness. We restrict our attention to the torque as a function of azimuthal angle \(\phi\) for in-plane magnetization directions, and only consider \(\mathbf{E}\) along \(x\). Fig. 4 shows \(\tau_\parallel\), \(\tau_\perp\) versus \(\phi\) for 1 and 2 layers of WTe\(_2\), and 1 and 2 layers of MoTe\(_2\), all with 2 layers of Co. For the WTe\(_2\) structures, going from 1 to 2 layers changes the sign of the out-of-plane torque \(\tau_\perp\) and decreases its magnitude. This is consistent with experimental observations[20] and indicates that, not surprisingly, the sign of \(\tau_\perp\) is determined by the direction of the electric field.
TABLE I. Table of fitting parameters based on Eq. (10) in five different heterostructures, given in units $\hbar/2e$ $(\Omega \cdot \text{cm})^{-1}$. For the WTe$_2$(1)/Co(2), we add an error bar from the Anderson disorder treatment described in the text. WTe$_2$(BA)/Co(2) and WTe$_2$(1)/Co(2) share a similar interfacial geometry (i.e., same direction of in-plane symmetry breaking).

|        | WTe$_2$(1)/Co(2) | WTe$_2$(BA)/Co(2) | WTe$_2$(BA)/Co(2) | MoTe$_2$(1)/Co(2) | MoTe$_2$(BA)/Co(2) |
|--------|------------------|-------------------|-------------------|------------------|-------------------|
| $B^\text{even}_0$ | $84\pm 50$       | $-52$             | $40$              | $39$             | $131$             |
| $B^\text{even}_1$ | $30\pm 28$       | $-63$             | $65$              | $11$             | $-22$             |
| $B^\text{odd}_0$ | $-146\pm 68$     | $-181$            | $-180$            | $-35$            | $135$             |
| $B^\text{even}_1$ | $15\pm 14$       | $28$              | $23$              | $19$             | $-18$             |
| $B^\text{odd}_0$ | $-301\pm 410$    | $922$             | $1165$            | $-1973$          | $-199$            |
| $B^\text{odd}_1$ | $-115\pm 77$     | $86$              | $-83$             | $-30$            | $-88$             |
| $B^\text{odd}_2$ | $57\pm 380$      | $-329$            | $238$             | $370$            | $624$             |
| $B^\text{odd}_3$ | $-107\pm 81$     | $74$              | $-79$             | $-56$            | $-29$             |

FIG. 4. (Color online) Azimuthal angle ($\phi$) dependence of torkances for (a) WTe$_2$(1)/Co(2), (b) WTe$_2$(AB)/Co(2), (c) MoTe$_2$(1)/Co(2), (d) MoTe$_2$(BA)/Co(2) at Fermi level. Red circles and blue squares denote out-of-plane torkance $\tau_\perp \equiv \tau_z$ and in-plane torkance $\tau_\parallel \equiv \tau_{x\parallel} \sin(\phi) - \tau_{x\perp} \cos(\phi)$ respectively. Dashed lines show the fitted results based on the symmetry constrained form Eq. (10) up to $n = 9$.

Consistent with this, we find that changing the order of stacking of WTe$_2$ from AB to BA changes the sign of the out-of-plane torque (see Fig. 5 for our definition of AB and BA stacking). The reduction in magnitude for $\tau_\perp$ with additional layers of WTe$_2$ can be expected because the two layers have opposite orientations of in-plane symmetry breaking. The out-of-plane torque due to the two layers should therefore exhibit partial cancellation, leading to a reduction in the overall magnitude. We find that $\tau_\parallel$ is relatively insensitive to the WTe$_2$ thickness.

For the MoTe$_2$ structures, we find somewhat different behavior: $\tau_\parallel$ and $\tau_\perp$ both increase in magnitude going from 1 to 2 layers of MoTe$_2$. It is surprising that $\tau_\perp$ increases with 2 layers, in light of the expected partial cancellation due to layers with opposite in-plane symmetry breaking, as described in the previous paragraph. However, the torque is quite sensitive to other features of the structure, which we discuss later.

We fit our first-principles numerical results with the symmetry constrained forms (Eq. (10)) to extract the values of out-of-plane and in-plane torkances for five structures. The two lowest order torkance conductivities are summarized in Table. II. Our numerical data conforms to the symmetry constrained forms with a sizable magnitude of constant out-of-plane torkance. Note that the numerical data contains small but finite symmetry-allowed higher order terms such as $\cos(2\phi)$ in the out-of-plane torkance.

To test the robustness of the computed torkance values with respect to disorder, we utilize an Anderson disorder treatment by adding a uniformly distributed random onsite potential $-V_m < V_i < V_m$ on all Co atoms. Fig. 6 shows the torkance coefficients versus Fermi energy for 40 realizations of random onsite potentials for the WTe$_2$(1)/Co(2) system. We find that adding a uniformly-distributed random onsite potential with relatively small magnitude (100 meV) has a noticeable impact on the computed value. The mean and standard deviation of the computed values are shown for WTe$_2$(1)/Co(2) in Table II. The standard deviation is substantial compared to the mean, underscoring the sensitivity of the computed values to details of the system. Note that we keep the chemical potential constant in different disorder realizations.
We note that the values obtained for the conventional dampinglike torque $B_0^{\perp}$-even are similar in magnitude to the bulk spin Hall conductivity computed for WTe$_2$ and MoTe$_2^{46}$. In the spin current + spin transfer torque picture, the unconventional out-of-plane dampinglike torque would arise from spin current flowing along the z-direction (or c-axis of the TMD), with spin polarization along the z-axis. As shown in Ref$^{[13]}$, this component of the bulk spin Hall conductivity is symmetry-forbidden in crystals with the symmetry of WTe$_2$. However, the non-symmorphic screw symmetry allows for a bulk spin current whose spin polarization along z alternates in sign between subsequent TMD layers (i.e., a staggered spin current). This staggered response has been discussed in general terms in Ref$^{[14]}$, and realized in various contexts, such as in the staggered Rashba-Edelstein effect present in CuMnA$^{[25]}$. We have performed preliminary calculations of this staggered out-of-plane spin Hall conductivity for bulk WTe$_2$ and MoTe$_2$ and compute conductivities which, although smaller than spin-orbit torque $B_0^{\perp}$-even, are within the same order of a few tens $(\hbar/2e) \cdot (\Omega \cdot \text{cm})^{-1}$. We leave this detailed analysis for future work. The correspondence between torque and spin current indicates that maximizing substrate material’s bulk spin Hall conductivity is a viable strategy for maximizing the spin-orbit torque in the corresponding heterostructure.

The overall magnitude of the unconventional dampinglike torque we compute (see Table [I]) is quite similar to the experimentally observed value of $(36 \pm 8) \cdot (\hbar/2e) \cdot (\Omega \cdot \text{cm})^{-1}$. This is substantially less than the value of dampinglike torque commonly observed and computed for the more conventional Co-Pt system, which is in the range $10^3 \cdot (\hbar/2e) \cdot (\Omega \cdot \text{cm})^{-1}$.$^{[11,24,52-53]}$ In light of the correspondence between spin current and spin-orbit torque described above, this difference can be understood as a consequence of the relatively moderate magnitude of bulk spin Hall conductivity in WTe$_2$. We hypothesize that this is traced back to the large distance between successive TMD layers along the c-axis, but again leave a systematic analysis for future work. We also note recent work which demonstrated magnetic switching using WTe$_2$ substrates$^{[52]}$, indicating that the conventional dampinglike torque in these materials may be sufficiently strong for applications. The magnitude of fieldlike torque we compute is also similar to that seen experimentally$^{[51,53]}$.
Appendix A: General symmetry analysis

In this Appendix we present the general form for the current-induced torque for a bilayer system whose only symmetry operation is mirror symmetry about the yz plane.

1. Symmetry-constrained effective magnetic field

Assume that an applied electric field (E) gives rise to an effective magnetic field (B) in a ferromagnetic system. To linear order in electric field, the response is given by

$$\mathbf{B} = \chi(\hat{\mathbf{m}})\mathbf{E}$$  \hspace{1cm} (A1)

where $\chi$ is a $3 \times 3$ tensor that depends on the magnetization direction $\hat{\mathbf{m}} = (\sqrt{1 - z^2} \cos(\phi), \sqrt{1 - z^2} \sin(\phi), z)$. The torque on the magnetization is given by

$$\tau = \hat{\mathbf{m}} \times \mathbf{B}$$  \hspace{1cm} (A2)

Since the unit vector $\hat{\mathbf{m}}$ is parameterized by $z$ and $\phi$, the general response tensor can be written as:

$$\chi(z, \phi) = \begin{pmatrix}
\chi_{11}(z, \phi) & \chi_{12}(z, \phi) & \chi_{13}(z, \phi) \\
\chi_{21}(z, \phi) & \chi_{22}(z, \phi) & \chi_{23}(z, \phi) \\
\chi_{31}(z, \phi) & \chi_{32}(z, \phi) & \chi_{33}(z, \phi)
\end{pmatrix}$$  \hspace{1cm} (A3)

Each component can be expanded in terms of real spherical harmonics,

$$\chi_{ij}(z, \phi) = \sum_{l=0}^{\infty} \sum_{m=0}^{l} P_{l}^{m}[z] \left( \alpha_{l,i,j}^{m} \cos(m\phi) + \beta_{l,i,j}^{m} \sin(m\phi) \right)$$  \hspace{1cm} (A4)

where $\alpha_{l,i,j}^{m}$ and $\beta_{l,i,j}^{m}$ are constant coefficients and $P_{l}^{m}$ are the associated Legendre polynomials. We rewrite this expression for convenience as

$$\chi(z, \phi) = \sum_{l=0}^{\infty} \sum_{m=0}^{l} c_{l}^{m}(z, \phi) A_{l}^{m} + s_{l}^{m}(z, \phi) B_{l}^{m}$$  \hspace{1cm} (A5)

where

$$c_{l}^{m}(z, \phi) = P_{l}^{m}[z] \cos(m\phi)$$  \hspace{1cm} (A6)

$$s_{l}^{m}(z, \phi) = P_{l}^{m}[z] \sin(m\phi)$$  \hspace{1cm} (A7)

and

$$A_{l}^{m} = \begin{pmatrix}
\alpha_{l,11}^{m} & \alpha_{l,12}^{m} & \alpha_{l,13}^{m} \\
\alpha_{l,21}^{m} & \alpha_{l,22}^{m} & \alpha_{l,23}^{m} \\
\alpha_{l,31}^{m} & \alpha_{l,32}^{m} & \alpha_{l,33}^{m}
\end{pmatrix}, \quad B_{l}^{m} = \begin{pmatrix}
\beta_{l,11}^{m} & \beta_{l,12}^{m} & \beta_{l,13}^{m} \\
\beta_{l,21}^{m} & \beta_{l,22}^{m} & \beta_{l,23}^{m} \\
\beta_{l,31}^{m} & \beta_{l,32}^{m} & \beta_{l,33}^{m}
\end{pmatrix}$$  \hspace{1cm} (A8)

The purpose of rewriting the response tensor was to separate the functional dependence on magnetization direction $(z, \phi)$ with the matrix structure $(A_{l}^{m}, B_{l}^{m})$.

2. Transforming the response tensor

In general, the response tensor transforms under some orthogonal transformation matrix $R$ as follows:

$$\chi' = \operatorname{det}[R] R \chi R^{T}.$$  \hspace{1cm} (A9)
Under this transformation, $\chi$ becomes

$$\chi' = -R\chi R^T = \begin{pmatrix} -\chi_{11} & \chi_{12} & \chi_{13} \\ \chi_{21} & -\chi_{22} & -\chi_{23} \\ \chi_{31} & -\chi_{32} & -\chi_{33} \end{pmatrix} \tag{A11}$$

To transform functions of magnetization, we note that the magnetization transforms like a pseudovector, which means that for a $yz$ mirror plane transformation, $z' = -z$ and $\phi' = -\phi$. Thus:

$$c^m_l(z', \phi') = P^m_l[-z] \cos(-m\phi) = (-1)^{l+m} c^m_l(z, \phi) \tag{A12}$$
$$s^m_l(z', \phi') = P^m_l[-z] \sin(-m\phi) = (-1)^{l+m} s^m_l(z, \phi) \tag{A13}$$

where we have used the identity $P^m_l[-z] = (-1)^{l+m} P^m_l[z]$. To obtain the symmetrized response tensor, we simply add the transformed tensor to the original tensor, since $R$ and $I_{3x3}$ are the only members of the symmetry group:

$$\chi_S(z, \phi) = \chi(z, \phi) + \chi'(z', \phi')$$
$$= \sum_{l=0}^{\infty} \sum_{m=0}^{l} c^m_l(z, \phi) \left( A^m_l + (-1)^{l+m+1} RA^m_l R^T \right) + s^m_l(z, \phi) \left( B^m_l + (-1)^{l+m} RB^m_l R^T \right) \tag{A14}$$

3. Condensed form of response tensor

The response tensor derived in the last section contains matrices given by $A^m_l + (-1)^{l+m+1} RA^m_l R^T$ and $B^m_l + (-1)^{l+m} RB^m_l R^T$. Depending on the value of $l$ and $m$, these matrices take either of the following forms:

$$S^m_l = \begin{pmatrix} a^m_l & 0 & 0 \\ 0 & c^m_l & f^m_l \\ 0 & h^m_l & i^m_l \end{pmatrix} \quad T^m_l = \begin{pmatrix} 0 & b^m_l & c^m_l \\ 0 & d^m_l & 0 \\ 0 & g^m_l & 0 \end{pmatrix} \tag{A15}$$

Using this observation, we can rewrite the response tensor one last time in matrix form as

$$\chi_S(z, \phi) = \sum_{l=0}^{\infty} \sum_{m=0}^{l} P^m_l[z] \left( s^m_l(\phi) S^m_l + t^m_l(\phi) T^m_l \right) \tag{A16}$$

where

$$s^m_l(\phi) = \begin{cases} \cos(m\phi) & \text{for } l, m = \text{ even/odd or odd/even} \\ \sin(m\phi) & \text{for } l, m = \text{ even/even or odd/odd} \end{cases} \tag{A17}$$
$$t^m_l(\phi) = \begin{cases} \sin(m\phi) & \text{for } l, m = \text{ even/odd or odd/even} \\ \cos(m\phi) & \text{for } l, m = \text{ even/even or odd/odd} \end{cases} \tag{A18}$$

We have arrived at the final form of the general response tensor. For a given $l$ and $m$, the contribution to each element of $\chi$ contains either $\sin(m\phi)$ or $\cos(m\phi)$ but not both. This is the main consequence of the symmetry $x \rightarrow -x$. Note that the matrix $T^m_0$ gives the magnetization-independent contribution ($l = 0, m = 0$) to $\chi$. In general, the matrices $S^m_l$ and $T^m_l$ are odd and even with respect to the mirror plane transformation $x \rightarrow -x$ respectively.

4. Symmetry-constrained torque

The torque can be written in terms of its own response tensor $\chi^T$ defined as follows

$$\tau = \hat{m} \times B \tag{A19}$$
$$= \hat{m} \times \chi E \tag{A20}$$
$$= \chi^T E \tag{A21}$$

where $\chi^T_{il} = \epsilon_{ijk} \hat{m}_j \chi_{kl}$. Replacing the coordinate $z$ with $\theta$, where $z = \cos(\theta)$, one can then show that

$$\chi^T(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=0}^{l} P^m_l[\cos(\theta)] \left( a^m_l A^m_l(\theta, \phi) + c^m_l E^m_l(\theta, \phi) + h^m_l H^m_l(\theta, \phi) + b^m_l B^m_l(\theta, \phi) + d^m_l D^m_l(\theta, \phi) + g^m_l G^m_l(\theta, \phi) \right) \tag{A22}$$
where (assuming an in-plane electric field, i.e. $E_z = 0$):

$$\chi_{xx}^{T}(\pi/2, \phi) = \sum_{l=0}^{\infty} \sum_{m=0}^{l} P_l^m[0] \left( s_l^m A_{l,xx}^m(\pi/2, \phi) + d_l^m t_l^m(\phi) \right),$$  

$$\chi_{zz}^{T}(\pi/2, \phi) = \sum_{l=0}^{\infty} \sum_{m=0}^{l} P_l^m[0] \left( -a_l^m s_l^m(\phi) \sin(\phi) + d_l^m t_l^m(\phi) \cos(\phi) \right),$$

Note that the assumption of an in-plane electric field means that the coefficients $c_l^m$, $f_l^m$, and $i_l^m$ are no longer relevant to the torque. The expansion provided here captures all the consequences of symmetry, but is obviously quite complicated because that there are only two symmetry operations in the symmetry group. For each $l$ and $m$, there are six independent parameters given by $a_l^m$, $e_l^m$, $h_l^m$, $b_l^m$, $d_l^m$, and $g_l^m$. The functions that contain the magnetization dependence are labeled accordingly.

5. Simpler expression for the out-of-plane torque

An out-of-plane ($z$) torque of some kind is required to switch ferromagnetic layers with perpendicular magnetic anisotropy. In the low symmetry system we have studied here, such out-of-plane torques are non-vanishing. For an in-plane magnetization (i.e., $\theta = \pi/2$), the response tensor element relating an electric field along $\hat{\mathbf{e}}$ with the out-of-plane torque $\tau_z$ is

$$\chi_{zz}^{T}(\pi/2, \phi) = \sum_{l=0}^{\infty} \sum_{m=0}^{l} P_l^m[0] \left( s_l^m A_{l,zz}^m(\pi/2, \phi) + d_l^m t_l^m(\phi) \right),$$

where we have used Eqs. [A22], [A23], and [A24]. We note that $P_l^m[0]$ is nonzero only when $l$ and $m$ are both even or both odd, which gives

where $s_l^m(\phi)$ and $t_l^m(\phi)$ are replaced with $\sin(m\phi)$ and $\cos(m\phi)$ in the first line using Eqs. A17 and A18. The last line is obtained using trigonometric summation identities. Note the second summation operator runs only over even(odd) values of $m$ for even(odd) values of $l$.

Finally, we note that the above expression contains several redundancies, because the $l$ dependence has dropped out and all integer multiples of $\phi$ are present somewhere in the sum. This yields

$$\chi_{zz}^{T}(\pi/2, \phi) = \sum_{m=0}^{\infty} n_m \cos(m\phi)$$

where we have absorbed the redundant sums over coefficients $a_l^m$ and $d_l^m$ into $n_m$.

Appendix B: Notes on First principles calculations details

The atomic configurations of the relaxed structures are shown in the following tables. The unit of length for lattice vectors $\mathbf{a}_i$ is Angstrom, and fractional coordinates are shown.

| TABLE II. Atomic Positions of WTe$_2$(1)/Co(2) and MoTe$_2$(1)/Co(2) |
|-------------------------------------------------------------|
| $a_1$ | 3.4895 | 0 | 0 | $a_1$ | 3.4814 | 0 | 0 |
| $a_2$ | 0 | 6.254 | 0 | $a_2$ | 0 | 6.3562 | 0 |
| $a_3$ | 0 | 0 | 45 | $a_3$ | 0 | 0 | 39.9653 |
| W | 0.0 | 0.0608 | 0.2651 | Mo | 0.0 | 0.3244 | 0.3805 |
| W | 0.5 | 0.4169 | 0.2615 | Mo | 0.5 | 0.6915 | 0.3771 |
| Te | 0.0 | 0.6639 | 0.2954 | Te | 0.5 | 0.4256 | 0.4289 |
| Te | 0.5 | 0.1541 | 0.3088 | Te | 0.0 | 0.9346 | 0.4148 |
| Te | 0.0 | 0.3212 | 0.2170 | Te | 0.5 | 0.0750 | 0.3428 |
| Te | 0.5 | 0.8085 | 0.2311 | Te | 0.0 | 0.5872 | 0.3278 |
| Co | 0.0 | 0.3240 | 0.1720 | Co | 0.5 | 1.0842 | 0.2804 |
| Co | 0.5 | 0.5821 | 0.1720 | Co | 0.0 | 0.5885 | 0.2784 |
| Co | 0.0 | 0.8215 | 0.1755 | Co | 0.0 | 0.3277 | 0.2791 |
| Co | 0.0 | 0.0642 | 0.1727 | Co | 0.0 | 0.8452 | 0.2775 |
| Co | 0.0 | 0.3218 | 0.1354 | Co | 0.5 | 0.3318 | 0.2370 |
| Co | 0.0 | 0.8239 | 0.1340 | Co | 0.0 | 0.5837 | 0.2374 |
| Co | 0.5 | 0.5827 | 0.1344 | Co | 0.5 | 0.8424 | 0.2359 |
| Co | 0.5 | 0.0643 | 0.1351 | Co | 0.0 | 1.0892 | 0.2356 |
TABLE III. Atomic Positions of WTe$_2$(AB)/Co(2), WTe$_2$(BA)/Co(2), and MoTe$_2$(BA)/Co(2)

| $a_1$ | 3.4895 | 0 | 0 | 3.4895 | 0 | 0 | 3.4814 | 0 | 0 |
|-------|--------|---|---|--------|---|---|--------|---|---|
| $a_2$ | 0 | 6.254 | 0 | 0 | 6.254 | 0 | 0 | 6.3562 | 0 |
| $a_3$ | 0 | 0 | 45 | 0 | 0 | 45 | 0 | 0 | 39.9653 |

W 0.0 0.0628 0.4207 0.5 0.9473 0.4207 Mo 0.5 0.1807 0.5489
W 0.5 0.9466 0.2680 0.0 0.5929 0.4161 Mo 0.0 0.8196 0.5442
W 0.0 0.5917 0.2641 0.0 0.0629 0.2677 Mo 0.0 0.3294 0.3829
W 0.5 0.4171 0.4161 0.5 0.4177 0.2639 Mo 0.5 0.6967 0.3794
Te 0.0 0.1992 0.2337 0.5 0.3346 0.4505 Te 0.0 0.0782 0.5972
Te 0.5 0.8134 0.3869 0.5 0.8508 0.4642 Te 0.5 0.5722 0.5824
Te 0.0 0.3211 0.3725 0.0 0.1968 0.3869 Te 0.0 0.4292 0.5120
Te 0.5 0.6877 0.2196 0.5 0.6895 0.3725 Te 0.5 0.9224 0.4958
Te 0.0 0.6667 0.4506 0.0 0.6655 0.2973 Te 0.5 0.4323 0.4316
Te 0.5 0.3441 0.2975 0.5 0.1579 0.3117 Te 0.0 0.9406 0.4160
Te 0.0 0.8515 0.3120 0.5 0.8104 0.2335 Te 0.5 0.9807 0.3450
Te 0.5 0.1589 0.4642 0.5 0.3218 0.2194 Te 0.0 0.5921 0.3301
Co 0.5 0.9424 0.1750 0.5 0.8206 0.1779 Co 0.5 1.0775 0.2826
Co 0.0 0.6844 0.1746 0.0 0.5807 0.1744 Co 0.5 0.5883 0.2808
Co 0.5 0.4258 0.1749 0.5 0.3225 0.1744 Co 0.0 0.3233 0.2824
Co 0.0 0.1848 0.1780 0.0 0.6362 0.1751 Co 0.0 0.8416 0.2789
Co 0.0 0.4250 0.1372 0.0 0.3204 0.1378 Co 0.5 0.3285 0.2402
Co 0.0 0.9428 0.1374 0.0 0.5758 0.2739 Co 0.0 0.5758 0.2399
Co 0.5 0.6843 0.1380 0.5 0.5814 0.1369 Co 0.5 0.8385 0.2374
Co 0.0 0.1845 0.1367 0.5 0.6630 0.1375 Co 0.0 1.0891 0.2378

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