Microscopic origin of spin-orbit torque in ferromagnetic heterostructures: A first-principles approach

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Abstract: We present an ab initio based theoretical framework which elucidates the origin of the spin-orbit torque (SOT) in normal-metal/ferromagnet (FM) heterostructures. The SOT is decomposed into two contributions, namely, spin-Hall and the spin-orbital components. We find that (i) the fieldlike (FL) SOT is dominated by the spin-orbital component and (ii) both components contribute to the dampinglike (DL) torque with comparable magnitude in the limit of thick Pt film. The contribution of the spin-orbital component to the DL-SOT is present only for NMs with strong SOC coupling strength. We demonstrate that the FL-SOT can be expressed in terms of the nonequilibrium spin-resolved orbital moment accumulation. The calculations reveal that the experimentally reported oxygen-induced sign reversal of the FL-SOT in Pt/Co bilayers is due to the significant reduction of the majority-spin orbital moment accumulation on the interfacial NM atoms.

Spin-orbit torque (SOT) has recently attracted a lot of attention as a method to switch nanoscale magnetic bits, due to its promising features in terms of high efficiency and scalability [1–15]. SOT is a relativistic phenomena that has its origin in the atomic spin-orbit coupling (SOC) in systems with broken inversion symmetry, and is often separated into damping (Slonczewski) -like (DL), broken inversion symmetry, and is often separated into dampinglike (DL) torque with comparable magnitude in the limit of thick Pt film. The contribution of the spin-orbital component to the DL-SOT is present only for NMs with strong SOC coupling strength. We demonstrate that the FL-SOT can be expressed in terms of the nonequilibrium spin-resolved orbital moment accumulation. The calculations reveal that the experimentally reported oxygen-induced sign reversal of the FL-SOT in Pt/Co bilayers is due to the significant reduction of the majority-spin orbital moment accumulation on the interfacial NM atoms.

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a microscopic framework to explain the origin of the SOT in terms of the electronic structure properties of the materials involved and the chemistry of the interface [35].

In this Rapid Communication, we develop an ab initio based formalism, where the SOT is decomposed into spin-Hall (nonlocal) and spin-orbital (local) components. We show that the FL-SOT is dominated by the spin-orbital component originating from the interfacial Pt layer, while both components contribute on equal footing to the DL-SOT. We demonstrate that the spin-orbital component of the FL-SOT is related to the nonequilibrium spin-resolved orbital moment accumulation on the normal metal. The physical meaning of the spin-orbital vs spin-Hall decomposition is systematically studied by the Pt thickness dependence, the layer-resolved contribution, and connection to the spin current passing through the NM/FM interface.

Transport properties, including the SOT, can be determined within the Green’s function formalism either in real space [15,36] using the Landauer-like approach or equivalently in momentum space using the Kubo-like approach [11,13,14]. In these approaches the current-induced spin accumulation induces SOT,

\[ \tau_{\text{SOT}} = 2\hat{m} \times \langle \hat{\Delta}_{\text{ex}} \hat{\sigma} \rangle_{\text{neq}} / M_s, \]  

(1)

on the magnetization direction \( \hat{m} \), through the magnetic exchange splitting of the conduction electrons, \( \hat{\Delta}_{\text{ex}} = (\hat{H}_{\uparrow \downarrow} - \hat{H}_{\downarrow \uparrow})/2 \). Here, \( \hat{H}_{\sigma} \) is the electronic Hamiltonian for spin \( \sigma \), \( M_s \) is the magnetic moment per unit cell, and \( \langle \cdots \rangle_{\text{neq}} \) denotes the nonequilibrium expectation value. Although this approach has proven advantageous in producing reasonable results in comparison with experimental measurements [13,15,37], it does not offer the means to directly analyze the microscopic origin of the SOT in terms of the electronic structure of the heterostructure.

As an alternative to the spin density calculation approach, here we use Hamilton’s equations of motion for the canonical variables, \( \phi, \theta \) (see Fig. S1 in Ref. [38]) to determine the Fermi surface contribution to the nonequilibrium canonical forces,

\[ F_q = \frac{2eE_{\text{ext}}}{M_s N_k \pi} \sum_k \text{ImTr} \left( \frac{\partial \hat{G}_k}{\partial \hat{\sigma}} \hat{v}_k \hat{e}_k^\dagger \right). \]  

(2)

where \( E_{\text{ext}} \) is the external electric field along \( \chi \), \( N_k \) is the number of \( k \) points in the unit cell, \( \hat{G}_k \) is the Green’s function, \( \hat{v}_k \) is the electronic group velocity, and \( \hat{\sigma} = \eta \hat{\sigma} \) is the energy broadening parameter. Rotating the reference frame so that the magnetization’s orientation is along the \( z \) axis, the partial derivative of the Green’s function can be written as

\[ \frac{\partial \hat{G}_k}{\partial \hat{\sigma}} = i [\hat{G}_k, \hat{\sigma}], \]  

(3)

where, the spin rotation operator, \( \hat{\sigma} = e^{i \hat{\sigma} \hat{\rho} / 2} \), was used on the Hamiltonian to align the magnetization along the fixed \( z \) direction. Here, \( \hat{\rho} = \cos(\phi) \hat{x} - \sin(\phi) \hat{y} \), \( \hat{e}_{x,y,z} \) are unit vectors along the Cartesian coordinates, \( \hat{G}_k \) and \( \hat{H}_{\text{SOC}} \) are the Green’s function and SOC Hamiltonian in the rotated frame, respectively, \( \hat{\rho} = i \hat{\rho}_m^\dagger \partial \hat{\rho}_m / \partial \hat{\rho} \), and \( \hat{H}_{\text{SOC}} = \chi \hat{\hat{k}} \cdot \hat{\sigma} \), where \( \hat{\hat{k}} \) is the angular momentum operator, \( \hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z \) are the Pauli matrices, \( \chi \) is the SOC scaling factor, and \( \xi \) is the SOC matrix.

The first term in Eq. (3) contributes only to the nonequilibrium observables and often describes the non-local spin-current pumping/absorption effects [32,38,39]. On the other hand, the second term generally leads to the contribution from modification of the band-structure in response to the change of \( q \), similar to Kambersky’s breathing Fermi surface mechanism of Gilbert damping [39] and magnetocrystalline anisotropy using the “torque” method [40]. Using Eq. (3) the non-equilibrium canonical force, \( F_q \), can be decomposed into the following two components, which we refer to as the spin-orbital and spin-Hall contributions, respectively [38],

\[ F_q^{(\text{so})} = \frac{2eE_{\text{ext}}}{M_s N_k \pi} \sum_k \text{ImTr} \left[ \frac{\partial \hat{H}_{\text{SOC}}}{\partial \hat{\sigma}} \hat{v}_k \right]. \]  

(4a)

\[ F_q^{(\text{sh})} = \frac{2eE_{\text{ext}}}{M_s N_k \pi} \sum_k \text{ReTr}(\hat{\sigma} \hat{\rho} \hat{v}_k \hat{\rho}_k^\dagger). \]  

(4b)

The canonical forces \( F_{\phi=\theta,\phi} \) are related to the torque through \( F_{\phi} = \tau_{\text{SOT}} \cdot \hat{\sigma} \), and \( F_{\phi} = \tau_{\text{SOT}} \cdot \hat{\rho} \). To the lowest order in the angular dependence of the SOT, we expect \( \tau_{\text{SOT}} = \hat{m} \times (\hat{B}_{\text{FL}} + \hat{m} \times \hat{B}_{\text{DL}}) \). The magnitude of the SOTs, \( B_{\text{FL,DL}} \), can then be calculated by fitting the angular dependence of the canonical forces to the expressions

\[ F_{\phi} / E_{\text{ext}} = \hat{m} \times \hat{B}_{\text{FL}} + \hat{m} \times \hat{B}_{\text{DL}} \cdot \hat{\sigma}, \]  

(5a)

\[ F_{\phi} / E_{\text{ext}} = \hat{m} \times \hat{B}_{\text{DL}} - \hat{m} \times \hat{B}_{\text{FL}} \cdot \hat{\rho}, \]  

(5b)

where \( \alpha \) refers to the spin-orbital or spin-Hall contributions to the SOT.

We have also derived analytical expressions for the spin-orbital/spin-Hall components of the FL- and DL-SOTs [38]. The FL-SOT is of the form

\[ M_{\text{FL}} \tilde{B}_{\text{FL}}^{(\text{so})} = [\xi \hat{\hat{k}} \cdot \hat{\sigma}, 0]_0 - [\xi \hat{\hat{k}} \cdot \hat{\sigma}, 0]_0 \hat{e}_z, \]  

(6)

\[ \langle \cdots \rangle_0 = \frac{1}{N_k \pi} \sum_k \text{Tr}[\text{Im}(\hat{G}_k)\hat{v}_k \text{Im}(\hat{G}_k^\dagger) \cdots]. \]  

(7)

Even though \( \tilde{B}_{\text{FL}}^{(\text{so})} \) has three contributions, we find that in the case of NM/FM bilayer devices the first term, which we refer to as the Rashba-Edelstein effect (REE) FL-SOT,

\[ M_{\text{FL}} \tilde{B}_{\text{FL}}^{(\text{REE})} = [\xi \hat{\hat{k}} \cdot \hat{\sigma}, 0]_0 - [\xi \hat{\hat{k}} \cdot \hat{\sigma}, 0]_0, \]  

(8)

is dominant, while the third term is present only in systems with broken in-plane mirror symmetry [41,42]. Equation (8) is one of the central results of this Rapid Communication which demonstrates that the FL-SOT can be expressed in terms of the nonequilibrium spin-resolved orbital moment accumulation. Similarly, the spin-Hall component of the DL-SOT is given by,

\[ M_{\text{DL}} \tilde{B}_{\text{DL}}^{(\text{sh})} = - \frac{1}{\pi N_k} \sum_k \text{ReTr}(\hat{\sigma} \hat{\rho} \hat{v}_k \hat{\rho}_k^\dagger). \]  

(9)

These expressions allow one to elucidate the microscopic origins of the SOT. More specifically, Eq. (6) will be employed to
understand the interfacial Co oxidation effect on the FL-SOT in the Pt/Co bilayer. Equation (6) can also be used to estimate the effective Rashba SOC strength of the bilayer which is given by \( m_\perp \alpha_{\text{eff}}^2 = (\xi E_v) / (\hbar k_F) \) [38].

In a NM/FM bilayer, only the y component of \( B_{\text{DL,FL}} \) is nonzero. Figure 1 shows the total (solid red curves) (a) DL and (b) FL components of the SOT, calculated from Eq. (1), versus the SOC scaling factor \( \chi \), for the (001) Pt(6 ML)/Co(6 ML) bilayer with energy broadening \( \eta = 0.1 \) eV. We also show the spin-orbital (dashed blue) and spin-Hall (dash-dotted green) contributions to the SOT calculated from Eq. (5), their sum (dashed red), and their linear dependence (black line in (a)). Left inset: Spin-Hall conductivity of bulk Pt versus \( \chi \). Right inset: DL-SOT vs \( \chi \) for thicker Pt film in the Pt(16 ML)/Co(6 ML) bilayer.

The spin-Hall (green curve) and spin-orbital (blue) contributions to the SOT on the energy broadening parameter, \( \eta \) (inversely proportional to the relaxation time) [38], shows that in the ballistic limit (\( \eta \to 0 \)) \( B_{\text{FL}}^{(\text{so})} \propto 1 / \eta \) while \( B_{\text{FL}}^{(\text{sh})} \propto \eta \), suggesting that the latter can be ignored in relatively clean samples.

A convenient approach to characterize the spin-Hall and spin-orbital components in terms of their bulk and interface contributions is to investigate their dependence on the HM film thickness, where the interfacial component is expected to have a shorter characteristic length (i.e., spin-diffusion length). In Fig. 2(a) we display the total (red crossed symbols) DL-SOT, calculated from the nonequilibrium spin accumulation method [13], Eq. (1), versus Pt thickness, along with the experimental results (black [43] and blue [37] stars) (multiplied by \( \mu_B \)). We also show both the spin-orbital (blue circles) and spin-Hall (green diamonds) contributions to the SOT calculated from Eq. (5). The blue and green dashed curves in Fig. 2(a) denote the fits of the ab initio results to the spin-diffusion model, \( \propto 1 / \eta \) while \( B_{\text{FL}}^{(\text{sh})} \propto \eta \), which are in agreement with the reported experimental values in the range between 0.5 and 10 nm [28,44]. It is also worth noting out that Fig. 2(a) shows a sign reversal of both the spin-orbital and spin-Hall DL-SOT components for 1 ML Pt, which is not in agreement with the reported experimental values. The layer-resolved contribution of \( B_{\text{DL,FL}}^{(\text{sh})} \), displayed in the inset of Fig. 2(a) for 15 MLs of Pt, demonstrates the dominant bulk origin of the DL-SOT in this case of ultrathin Pt films suggesting the sensitivity of the DL-SOT on the substrate material. The layer-resolved results were calculated from the diagonal matrix elements inside the trace in Eq. (S10) in Ref. [38], with spin-orbit coupling included in the Green’s function.
and surface layers, respectively. The subscripts 1 and 5 denote the spin-orbital and surface layers, respectively.

The calculated total FL-SOT are in good agreement with the experiments [37,43]. The oscillation of the spin-orbital component which can be expressed in terms of the difference of nonequilibrium spin-resolved orbital hybridization of the majority-spin O\(\langle d_{\sigma}\rangle\) or change sign by oxygen, which can be attributed to the Rashba–Edelstein effect (REE) FL-SOT [Eq. (8)] in the absence and presence of interfacial oxygen, respectively.

Recent experiments have reported [37,47] a modulation of the direction and magnitude of the FL-SOT in a Pt/Co/GdO\(_2\) heterostructure by changing the concentration of oxygen in the Co layer using an electric field. Even though our complementary \textit{ab initio} calculations confirmed [37] the sign reversal of the FL-SOT as a function of oxygen concentration, its microscopic origin has so far remained elusive.

Here, using the theoretical framework developed above we elucidate the underlying mechanism of the sign reversal of the FL-SOT. We consider the (001) Pt(6 ML)/Co(6 ML) bilayer system where the oxygen atom is originally placed in the interfacial Co layer and atop the interfacial Pt atom [Fig. 3(e)] [37]. The oxygen atom relaxes between the interfacial and subinterface Co layers. Table I lists the total FL-SOT calculated from Eq. (1), the spin-orbital and spin-Hall contributions to the FL-SOT calculated from Eq. (5), and the REE FL-SOT calculated from Eq. (8), in the absence and presence of interfacial oxygen, respectively, which show the oxygen-induced sign reversal. Figures 3(a) and 3(d) show the layer- and spin-resolved contribution to \(B_{y}^{\text{FL}}\), in the absence and presence of oxygen, respectively, where the dominant contribution arises from the interfacial Pt atoms. We find that in general \(\langle \hat{L}_z \rangle_{\sigma \sigma} > 0\) and that \(\langle \hat{L}_z \rangle_{\downarrow \downarrow}\) is insensitive to the presence or absence of oxygen. Consequently, the sign reversal of the FL-SOT is due to the significant reduction of the majority-spin contribution induced by interfacial oxygen.

Furthermore, Figs. 3(c) and 3(f) show the orbital-resolved contributions to \(B_{y}^{\text{REE}}\) for the interfacial Pt atom, without and with oxygen, respectively. The dominant contribution to the \(\langle \hat{L}_z \rangle_{\sigma \sigma} \rangle_{\text{REE}}\) arises from the non-vanishing \(\langle d_{\sigma y}\rangle\langle d_{\sigma y}\rangle\), \(\langle d_{\sigma z}\rangle\langle L_{\downarrow z}\rangle\), and \(\langle d_{\sigma z}\rangle\langle L_{\downarrow z}\rangle\langle d_{\sigma y}\rangle\) matrix elements of the in-plane orbital angular momentum operator, \(\hat{L}_{y}\). Here, \(I, \sigma, l, m\) stand for ionic, spin, and atomic orbital indices, respectively. We find that the positive \(\langle d_{\sigma y}\rangle\langle d_{\sigma y}\rangle\) and \(\langle d_{\sigma z}\rangle\langle L_{\downarrow z}\rangle\) matrix elements in the clean bilayer vanish or change sign by oxygen, which can be attributed to the hybridization of the majority-spin \(O/p\)-derived states with the interfacial Pt/\(d_{\sigma z}\), \(d_{\sigma z}\), and \(d_{\sigma y}\) derived states [38].

In summary, we presented a theoretical framework which allows one to decompose the DL- and FL-SOTs into the spin-Hall and spin-orbital components in NM/FM bilayers. We demonstrated that (i) the FL-SOT is dominated by the spin-orbital component which can be expressed in terms of the difference of nonequilibrium spin-resolved orbital

### Table I. Values of the \(y\) component of the total FL-SOT (in meV Å) for the (001) Co(6)/Pt(6) bilayer [Eq. (1)]; the spin-orbital and spin-Hall contributions to the FL-SOT [Eq. (5)]; and the Rashba–Edelstein effect (REE) FL-SOT [Eq. (8)] in the absence and presence of interfacial oxygen, respectively.

| Co(6)/Pt(6) | \(B_{y}^{\text{FL}}\) Eq. (1) | \(B_{y}^{\text{ab}}\) Eq. (5) | \(B_{y}^{\text{so}}\) Eq. (5) | \(B_{y}^{\text{REE}}\) Eq. (8) |
|-------------|-----------------|-----------------|-----------------|-----------------|
| Absence of O | 3 | -8 | 11 | 15 |
| Presence of O | -43 | 9 | -51 | -51 |

**FIG. 3.** Spin- and layer-resolved FL-SOT in (a) the absence and (d) the presence of interfacial oxygen. (c) and (f) show the corresponding orbital-resolved FL-SOT for the interfacial Pt layer. Atomic structure of [001] Pt(6) /Co(6) bilayer without (b) and with (e) interfacial oxygen. The subscripts 1 and 5 denote the spin-orbital and surface layers, respectively.
accumulation at the interfacial NM atoms and (ii) the spin-orbital contribution to the DL-SOT dominates for ultrathin Pt films, while both components have equal contribution for thicker films. The dependence of the DL-SOT on SOC strength suggests that if Pt is replaced with a normal metal with weaker SOC strength, the DL-SOT becomes dominated by the spin-Hall component. We have used the approach to elucidate the microscopic mechanism for the sign reversal of the FL-SOT due to the interfacial Co oxidation. We demonstrated that the sign reversal is attributed to a significant reduction of the spin-majority nonequilibrium orbital moment accumulation at the interfacial Pt layer.

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[1] A. Manchon and S. Zhang, Theory of nonequilibrium intrinsic spin torque in a single nanomagnet, Phys. Rev. B 78, 212405 (2008).
[2] I. M. Miron, K. Garello, G. Gaudin, P.-J. Zermatten, M. V. Costache, S. Auffret, S. Bandiera, B. Rodmacq, A. Schuhl, and P. Gambardella, Perpendicular switching of a single ferromagnetic layer induced by in-plane current injection, Nature (London) 476, 189 (2011).
[3] L. Liu, O. J. Lee, T. J. Gudmundsen, D. C. Ralph, and R. A. Buhrman, Current-Induced Switching of Perpendicularly Magnetized Magnetic Layers Using Spin Torque from the Spin Hall Effect, Phys. Rev. Lett. 109, 096602 (2012).
[4] 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).
[5] M. Cubukcu, O. Boule, M. Drouard, K. Garello, C. O. Avci, I. M. Miron, J. Langer, B. Ocker, P. Gambardella, and G. Gaudin, Spin-orbit-torque magnetization switching of a three-terminal perpendicular magnetic tunnel junction, Appl. Phys. Lett. 104, 042406 (2014).
[6] C. Zhang, S. Fukami, H. Sato, F. Matsukura, and H. Ohno, Spin-orbit torque induced magnetization switching in nanoscale Ta/CoFeB/MgO, Appl. Phys. Lett. 107, 012401 (2015).
[7] I. M. Miron, G. Gaudin, S. Auffret, B. Rodmacq, A. Schuhl, S. Pizzini, J. Vogel, and P. Gambardella, Current-driven spin torque induced by the Rashba effect in a ferromagnetic metal layer, Nat. Mater. 9, 230 (2010).
[8] K. Garello, I. M. Miron, C. O. Avci, F. Freimuth, Y. Mokrousov, S. Blugel, S. Auffret, O. Boule, G. Gaudin, and P. Gambardella, Symmetry and magnitude of spin-orbit torques in ferromagnetic heterostructures, Nat. Nanotechnol. 8, 587 (2013).
[9] P. M. Haney, H.-W. Lee, K.-J. Lee, A. Manchon, and M. D. Stiles, Current induced torques and interfacial spin-orbit coupling: Semiclassical modeling, Phys. Rev. B 87, 174411 (2013).
[10] Ki-Seung Lee, D. Go, A. Manchon, P. M. Haney, M. D. Stiles, Hyun-Woo Lee, and Kyung-Jin Lee, Angular dependence of spin-orbit spin-transfer torques, Phys. Rev. B 91, 144401 (2015).
[11] F. Freimuth, S. Blügel, and Y. Mokrousov, Spin-orbit torques in Co/Pt (111) and Mn/W (001) magnetic bilayers from first principles, Phys. Rev. B 90, 174423 (2014).
[12] F. S. M. Guimaraes, M. dos Santos Dias, J. Bouaziz, A. T. Costa, R. B. Muniz, and S. Lounis, Dynamical amplification of magnetoresistances and Hall currents up to the THz regime, Sci. Rep. 7, 3686 (2017).
[13] F. Mahfouzi and N. Kioussis, First-principles study of the angular dependence of the spin-orbit torque in Pt/Co and Pd/Co bilayers, Phys. Rev. B 97, 224426 (2018).
[14] S. Wimmer, K. Chadova, M. Seemann, D. Kodderitzsch, and H. Ebert, Fully relativistic description of spin-orbit torques by means of linear response theory, Phys. Rev. B 94, 054415 (2016).
[15] K. D. Belashchenko, A. A. Kovalev, and M. van Schilfgaarde, First-principles calculation of spin-orbit torque in a Co/Pt bilayer, Phys. Rev. Mater. 3, 011401(R) (2019).
[16] J. Sinova, S. O. Valenzuela, J. Wunderlich, C. H. Back, and T. Jungwirth, Spin Hall effects, Rev. Mod. Phys. 87, 1213 (2015).
[17] V. M. Edelstein, Spin polarization of conduction electrons induced by electric current in two-dimensional asymmetric electron systems, Solid State Commun. 73, 233 (1990).
[18] X. Wang, C. O. Pauyac, and A. Manchon, Spin-orbit-coupled transport and spin torque in a ferromagnetic heterostructure, Phys. Rev. B 89, 054405 (2014).
[19] A. Manchon and S. Zhang, Theory of spin torque due to spin-orbit coupling, Phys. Rev. B 79, 094422 (2009).
[20] A. Kalitsov, S. A. Nikolaev, J. Velev, M. Chshiev, and O. Myrasov, Intrinsic spin-orbit torque in a single-domain nanomagnet, Phys. Rev. B 96, 214430 (2017).
[21] L. Chotorishvili, Z. Toklikishvili, X.-G. Wang, V. K. Dugaev, J. Barnas, and J. Berakdar, Influence of spin-orbit and spin-Hall effects on the spin-Seebeck current beyond linear response: A Fokker-Planck approach, Phys. Rev. B 99, 024410 (2019).
[22] A. Manchon, J. Železný, I. M. Miron, T. Jungwirth, J. Sinova, A. Thiaville, K. Garello, and P. Gambardella, Current-induced spin-orbit torques in ferromagnetic and antiferromagnetic systems, Rev. Mod. Phys. 91, 035004 (2019).
[23] V. P. Amin and M. D. Stiles, Spin transport at interfaces with spin-orbit coupling: Phenomenology, Phys. Rev. B 94, 104420 (2016).
[24] H. Li, H. Gao, L. P. Zarbo, K. Vyborny, X. Wang, I. Garate, F. Dogan, A. Cejchan, J. Sinova, T. Jungwirth, and A. Manchon, Intraband and interband spin-orbit torques in noncentrosymmetric ferromagnets, Phys. Rev. B 91, 134402 (2015).
[25] A. Quiumzadeh, R. A. Duine, and M. Titov, Spin-orbit torques in two-dimensional Rashba ferromagnets, Phys. Rev. B 92, 014402 (2015).
[26] A. Manchon, Spin diffusion and torques in disordered antiferromagnets, J. Phys.: Condens. Matter 29, 104002 (2017).
[27] M. I. Dyakonov and V. I. Perel, Possibility of orienting electron spins with current, ZhETF Pis. Red. 65, 368 (1971), Solid State Commun. 7, 657 (1971) [JETP Lett. 13, 467 (1971)].
Jaffréz, Spin Pumping and Inverse Spin Hall Effect in Platinum: The Essential Role of Spin-Memory Loss at Metallic Interfaces, Phys. Rev. Lett. 112, 106602 (2014).

K. Dolui and B. K. Nikolić, Spin-memory loss due to spin-orbit coupling at ferromagnet/heavy-metal interfaces: \textit{ab initio} spin-density matrix approach, Phys. Rev. B 96, 220403(R) (2017).

J. Bass and W. P. Pratt, Jr., Spin-diffusion lengths in metals and alloys, and spin-flipping at metal/metal interfaces: An experimentalist’s critical review, J. Phys.: Condens. Matter 19, 18 (2007).

K. D. Belashchenko, A. A. Kovalev, and M. van Schilfgaarde, Theory of Spin Loss at Metallic Interfaces, Phys. Rev. Lett. 117, 207204 (2016).

F. Mahfouzi, J. Fabian, N. Nagaosa, and B. K. Nikolić, Charge pumping by magnetization dynamics in magnetic and semimagnetic tunnel junctions with interfacial Rashba or bulk extrinsic spin-orbit coupling, Phys. Rev. B 85, 054406 (2012).

V. P. Amin, J. Zemen, and M. D. Stiles, Interface-Generated Spin Currents, Phys. Rev. Lett. 121, 136805 (2018).

D. Go, D. Jo, C. Kim, and Hyun-Woo Lee, Intrinsic Spin and Orbital Hall Effects from Orbital Texture, Phys. Rev. Lett. 121, 086602 (2018).

F. Hellman \textit{et al.}, Interface-induced phenomena in magnetism, Rev. Mod. Phys. 89, 025006 (2017).

F. Mahfouzi, B. K. Nikolić, and N. Kioussis, Antidamping spin-orbit torque driven by spin-flip reflection mechanism on the surface of a topological insulator: A time-dependent nonequilibrium Green function approach, Phys. Rev. B 93, 115419 (2016).

R. Mishra, F. Mahfouzi, D. Kumar, K. Cai, M. Chen, X. Qiu, N. Kioussis, and H. Yang, Electric-field control of spin accumulation direction for spin-orbit torques, Nat. Commun. 10, 248 (2019).

See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.101.064045 for more details on the first-principles approach and analytical calculations, which contains Refs. [13,22,37,43,48–60].

F. Mahfouzi, J. Kim, and N. Kioussis, Intrinsic damping phenomena from quantum to classical magnets: An \textit{ab initio} study of Gilbert damping in a Pt/Co bilayer, Phys. Rev. B 96, 214421 (2017).

X. Wang, R. Wu, Ding-sheng Wang, and A. J. Freeman, Torque method for the theoretical determination of magnetocrystalline anisotropy, Phys. Rev. B 54, 61 (1996).

G. Yu, P. Upadhyaya, Y. Fan, J. G. Alzate, W. Jiang, K. L. Wong, S. Takei, S. A. Bender, Li-Te Chang, Y. Jiang, M. Lang, J. Tang, Y. Wang, Y. Tserkovnyak, P. K. Amiri, and K. L. Wang, Switching of perpendicular magnetization by spin-orbit torques in the absence of external magnetic fields, Nat. Nanotechnol. 9, 548 (2014).

D. MacNeill, G. M. Stiehl, M. H. D. Guimaraes, R. A. Buhrman, J. Park, and D. C. Ralph, Control of spin-orbit torques through crystal symmetry in WTe$_2$/ferromagnet bilayers, Nat. Phys. 13, 300 (2017).

Minh-Hai Nguyen, D. C. Ralph, and R. A. Buhrman, Spin Torque Study of the Spin Hall Conductivity and Spin Diffusion Length in Platinum Thin Films with Varying Resistivity, Phys. Rev. Lett. 116, 126601 (2016).

C. T. Boone, H. T. Nembach, J. M. Shaw, and T. J. Silva, Spin transport parameters in metallic multilayers determined by ferromagnetic resonance measurements of spin-pumping, J. Appl. Phys. 113, 153906 (2013).

R. Ramaswamy, X. Qiu, T. Dutta, S. D. Pollard, and H. Yang, Hf thickness dependence of spin-orbit torques in Hf/CoFeB/MgO heterostructures, Appl. Phys. Lett. 108, 202406 (2016).

J. Kim, J. Sinha, M. Hayashi, M. Yamanouchi, S. Fukami, T. Suzuki, S. Mitani, and H. Ohno, Layer thickness dependence of the current-induced effective field vector in Ta(ChoFeB)MgO, Nat. Mater. 12, 240 (2013).

X. Qiu, K. Narayanapillai, Y. Wu, P. Deorani, D.-H. Yang, W.-S. Noh, J.-H. Park, K.-J. Lee, H.-W. Lee, and H. Yang, Spin-orbit-torque engineering via oxygen manipulation, Nat. Nanotechnol. 10, 333 (2015).

T. Ozaki, Variationally optimized atomic orbitals for large-scale electronic structures, Phys. Rev. B 67, 155108 (2003).

T. Ozaki and H. Kino, Numerical atomic basis orbitals from H to Kr, Phys. Rev. B 69, 195113 (2004).

T. Ozaki and H. Kino, Efficient projector expansion for the \textit{ab initio} LCAO method, Phys. Rev. B 72, 045121 (2005).

N. Troullier and J. L. Martins, Efficient pseudopotentials for plane-wave calculations, Phys. Rev. B 43, 1993 (1991).

D. M. Ceperley and B. J. Alder, Ground State of the Electron Gas by a Stochastic Method, Phys. Rev. Lett. 45, 566 (1980).

J. P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B 23, 5048 (1981).

G. Kresse and J. Furthmüller, Efficient iterative schemes for \textit{ab initio} total-energy calculations using a plane-wave basis set, Phys. Rev. B 54, 11169 (1996).

G. Kresse and J. Furthmüller, Efficiency of \textit{ab-initio} total energy calculations for metals and semiconductors using a plane-wave basis set, Comput. Mater. Sci. 6, 15 (1996).

J. P. Perdew, K. Burke, and M. Ernzerhof, Generalized Gradient Approximation Made Simple, Phys. Rev. Lett. 77, 3865 (1996).

P. E. Blöchl, Projector augmented-wave method, Phys. Rev. B 50, 17953 (1994).

G. Kresse and D. Joubert, From ultrasoft pseudopotentials to \textit{ab initio} calculations within the projector augmented-wave method, Phys. Rev. B 59, 1758 (1999).

R. E. Camley and J. Barnas, Theory of Giant Magnetoresistance Effects in Magnetic Layered Structures with Antiferromagnetic Coupling, Phys. Rev. Lett. 63, 664 (1989).

S. Zhang and P. M. Levy, Conductivity and magnetoresistance in magnetic granular films (invited), J. Appl. Phys. 73, 5315 (1993).