First-Principles Theory of Current-Induced Spin-Orbital Coupled Dynamics in Magnetic Heterostructures

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(Dated: April 14, 2020)

Motivated by the rising importance of understanding various competing mechanisms to the current-induced torque on magnetization in complex magnets, we develop a unified theory of current-induced spin-orbital coupled dynamics in magnetic heterostructures, which tracks the transfer of angular momentum between different degrees of freedom in solids: spin and orbital of the electron, lattice, and local magnetic moment. Based on the continuity equations for the spin and orbital angular momenta, we derive equations of motion that relate spin and orbital current fluxes and torques describing the transfer of angular momentum between different degrees of freedom, achieved in a steady state under an applied external electric field. Based on our first-principles implementation within the density functional theory, we apply our formalism to two different magnetic bilayers, Fe/W(110) and Ni/W(110), which are chosen such that the orbital and spin Hall effects in W have opposite sign and the resulting spin- and orbital-mediated torques can compete with each other. We find that while the spin torque arising from the spin Hall effect of W is the dominant mechanism of the current-induced torque in Fe/W(110), the dominant mechanism in Ni/W(110) is the orbital torque originating in the orbital Hall effect of the non-magnetic substrate. It leads to negative and positive effective spin Hall angles, respectively, which can be directly identified in experiments. This clearly demonstrates that our formalism is ideal for studying the angular momentum transfer dynamics in spin-orbit coupled systems as it goes beyond the “spin current picture” by naturally incorporating the spin and orbital degrees of freedom on an equal footing. Our calculations reveal that, in addition to the spin and orbital torque, other contributions such as the interfacial torque and self-induced anomalous torque within the ferromagnet are not negligible in both material systems. We propose a classification scheme for the mechanisms of the current-induced torque in magnetic bilayers and discuss experimental implications of our findings.

I. INTRODUCTION

The spin-orbit coupling (SOC) plays a central role in a plethora of intriguing phenomena occurring in magnetic multilayers [1]. The current-induced torque is one of the most important examples and a workhorse in the field of spin-orbitronics [2–3]. The current-induced torque allows not only for a fully electrical switching of the magnetization direction [4–8], but also for current-induced domain wall motion [9–12]. The former is a key element in the magnetic random access memory [13], and the latter can potentially be used for racetrack memory [14]. However, theoretical understanding of current-induced torque, especially its relation to the electronic structure, is rather unsatisfactory still: while various microscopic mechanisms have been proposed, quantification of the individual contributions is challenging both theoretically and experimentally.

In magnetic bilayers consisting of a nonmagnet (NM) and a ferromagnet (FM), the spin Hall effect (SHE) arising from the NM is considered to be one of the main mechanisms for generating a torque on the magnetization of the FM [3, 6]. That is, an electrical current in the NM induces a transverse spin current, which is injected into the FM and results in a torque. In this picture, the spin Hall conductivity (SHC) of the NM is assumed to be a bulk property, and the spin injection and resulting torque generation on the local magnetic moment is explained by the theory of the spin-transfer torque [15–16]. We denote such contribution due to spin injection from the NM as a spin torque (ST). This analysis considers the SOC only in the NM and neglects the SOC at the NM/FM interface. Moreover, current-induced effects from the FM are neglected. The SOC effect at the NM/FM interface has been considered to be another dominant mechanism and intensively investigated [17–25]. Since the Rashba-type interfacial states are formed at the NM/FM interface due to the broken inversion symmetry [26–28], scattering of electrons from the interface leads to finite spin density and current [24–25], which interacts with and exerts a torque on the local magnetic moments of the FM. We denote this contribution as interfacial torque (IT).

While the role of SOC in the FM has been considered to be negligible as compared to that of the SOC in NM which usually comprises heavy atomic species, it has been found that SOC in the FM can induce a sizable amount of self-induced
torque by the generation of the intrinsic spin current, e.g., via the SHE [29,31]. The corresponding torque contribution is called the anomalous torque (AT) in analogy to the anomalous Hall effect in the FM [30]. When inversion symmetry is present in a stand-alone FM, the net AT amounts to zero. However, in the NM/FM bilayer, where the inversion symmetry is broken at the interface, the AT may exert a torque comparable to the ST and IT. The above mechanisms arise from spin-dependent scattering in the bulk or at the interface, and rely on the concept of spin current or spin density.

Recently, a mechanism of the torque generation based on the orbital angular momentum (OAM) injection has been proposed [32]. This mechanism is fundamentally different from the other mechanisms in that it requires the consideration of the orbital part of the electron’s angular momentum, rather than its spin. Called the orbital torque (OT), it relies on two processes. First, the OAM or its current is generated, which can be achieved for instance by the orbital Hall effect (OHE) [33,36]. Second, the OAM is injected into the FM and transfers its angular momentum to the local magnetic moment. In this process, the injected OAM should couple to the spin such that the spin interacts with the local magnetic moment via the exchange interaction. Thus, it requires the SOC within the FM. Since the orbital Hall conductivity (OHC) can be truly gigantic, exceeding that of the SHC of heavy elements [33,34] by an order of magnitude, the OT contribution to the current-induced torque can be substantial. Moreover, since the OHE does not require the SOC, which is in contrast to the SHE, the OHC is gigantic even in light elements [35,36]. In NM/FM bilayers, the OHE and SHE coexist in the NM, especially when the NM consists of heavy elements. Thus, depending on the material combinations, the OT and ST may add up or cancel each other [32]. To enhance the torque efficiency of the device, it is favorable to have the same sign of the OT and ST.

On the other hand, the case when the sign of the OT and ST are opposite is of interest as well, because when the magnitude of the OT is larger than that of the ST, the sign of the measured effective spin Hall angle in the NM/FM bilayer will be opposite to the sign promoted by the SHC of the NM. Considering that the sign is a more robust quantity than the magnitude in torque measurements, such a sign change can serve as the first hint of an active OT mechanism.

It turns out that all of the above mentioned mechanisms (ST, IT, AT, and OT) contribute to both fieldlike torque (FLT) and dampinglike torque (DLT), often with comparable magnitudes. The former gives rise to a precessional motion of the magnetization with respect to the spin accumulation direction, and the latter leads the magnetization to point away/toward an effective field direction. This complicates the analysis of the experiments. Since previous theoretical models have been developed assuming a restricted setup and evaluated only specific contributions [24,29], e.g., when the SOC exists only at the interface, it is hard to compare magnitudes of different contributions directly. On the other hand, first-principles approaches often evaluate the total torque from linear response theory [37,42], which makes it hard to assess contributions by different mechanisms quantitatively.

Thus, it is necessary to develop a unified theory within which different mechanisms of the current-induced torque are classified and can be separately evaluated for a given system. This would bridge the gap between the theoretical pictures set up by models and first-principles calculations of real materials. The main difficulty here lies in the nonlocality of magnetoelectric coupling [43,44] and different sources of the SOC. The OT mechanism [32] is highly nonlocal in nature, with the orbital current converted into the spin current in the FM. In view of the existing analysis based on the spin current, the OT mechanism appears abnormal as the spin current seems to emerge out of nowhere, while in fact it originates in the orbital current. This implies that tracing only the spin current inevitably fails to describe the OT. In general, the spin is not conserved in the presence of SOC, and the spin current does not directly correspond to the spin accumulation or torque on the local magnetic moment [45]. However, it is important to realize that the angular momentum of the spin is not simply lost. Instead, it is transferred to other degrees of freedom. Therefore, a proper theory should track not only the flow of angular momentum in space, but also take into account the transfer between different degrees of freedom in solids: spin and orbital of the electron, lattice, and local magnetic moment.

Recent theories imply that the current-induced dynamics and transport of the spin in the presence of SOC originate in the orbital degrees of freedom [34,35]. For example, while the OHE occurs regardless of the SOC, the SHE is a consequence of the OHE by virtue of the SOC [35]. Depending on the correlation between the spin and OAM, the relative sign of the OHE and SHE may be the same or opposite, following the Hund’s rule behavior [34,35]. In this sense, the OHE is more fundamental than the SHE. In general, such a hierarchy is expected to be a rather universal feature. The reason is the following: in the microscopic Hamiltonian of the electrons in solids, the spin cannot interact with an external electric field unless the SOC is present. On the other hand, the orbital degree of freedom, originated in the real-space behavior of the wave functions and distribution of charge, directly couples to an external electric field. Hence, under the perturbation by an external electric field, the orbital dynamics is expected to occur prior to the spin dynamics and regardless of the SOC, and the spin dynamics becomes correlated with the orbital dynamics by the SOC. Therefore, the orbital degree of freedom should be explicitly incorporated into a theoretical formulation to properly describe the current-induced torque, or magnetoelectric coupling phenomena in general. This will help to achieve clarity in resolving various contributions to the current-induced torques.

In this paper, we develop a theoretical formalism that can track the flow and transfer of the angular momentum between spin and orbital degrees of freedom of electrons, lattice, and local magnetic moment in the presence of an external electric field. Following the continuity equations for the spin and OAM of the electron, which was outlined in Ref. [46], we clarify every channel for the angular momentum transfer: between spin-orbital, orbital-lattice, and spin-local magnetic moment. Then we derive equations of motion which hold in the steady state in the presence of an external electric field. For the angular momentum transfer between electron’s
spin and local magnetic moment, which is directly related to the current-induced torque, we propose criteria for classifying different microscopic mechanisms based on physical properties: whether the magnetoelectric coupling is of local or non-local nature and whether it originates in the atomic SOC of the NM or the FM. In this way, we classify the mechanism of the current-induced torque as ST, OT, IT, and AT, and separately evaluate them for a given system.

As a proof of principle, we implement our formalism in the density functional theory (DFT) framework, and perform first-principles calculations for two real material systems: Fe/W(110) and Ni/W(110), which are carefully chosen with the expectation that the ST and OT have an opposite sign in these bilayers. We show that the current-induced torque in Fe/W(110) is dominated by the ST contribution, that is, the spin current flux in Fe equals the torque acting on the local magnetic moment. As a result, the effective spin Hall angle is negative, as it is well known for W. On the other hand, we find that the OT is dominant over the ST in Ni/W(110). As a result, it leads to a positive sign of the effective spin Hall angle, which is opposite to the sign of the SHC in W. This peculiar result is due to a positive sign of the orbital Hall conductivity (OHC) in W. In Ni/W(110) it is found that angular momentum transfer from the orbital to the spin channel is pronounced in the FM, which is a crucial requirement for the OT mechanism. We attribute the different behavior of Fe/W(110) and Ni/W(110) to the difference in the correlation between the OAM and the spin in the FM, which is more pronounced in Ni/W(110) than in Fe/W(110). In addition, we find that the IT and AT are not negligible in both Fe/W(110) and Ni/W(110) as compared to the ST and OT. These results clearly demonstrate the advantages of our theoretical formalism tracking the flow and transfer of the angular momentum through various degrees of freedom. Moreover, a different sign of the effective spin Hall angle in two different systems can be readily measured in experiment.

The paper is organized as follows. In Sec. [II], we develop a theoretical formalism that describes angular momentum transfer between the spin and the OAM of the electron, lattice, and local magnetic moment in the steady state under an external electric field. In Sec. [III], we apply this formalism to perform a first principles study of current induced torques in Fe/W(110) and Ni/W(110) bilayers. We analyze the results and discuss various experimental implications in Sec. [IV]. Finally, Sec. [V] summarizes and concludes the paper.
II. THEORETICAL FORMALISM

A. Overview

In this section, we develop a theoretical formalism that describes angular momentum transfer between different degrees of freedom. Before presenting detailed equations, we provide a motivation and an overview of the formalism that we aim to derive. Figure 1 shows interactions between spin and orbital momenta of the electron, lattice, and local magnetic moment, each of which carry angular momentum in solids. Considering microscopic interactions, the electron’s spin interacts with the local magnetic moment via the exchange interaction, the electron’s orbital moment interacts with the lattice via the crystal field potential, and the electron’s spin and orbital momenta are coupled by the SOC. It is important to note that the local magnetic moment and the electron’s spin on the right column of Fig. 1 are related to magnetic excitations, i.e., in the absence of SOC they do not respond to an electric field. On the other hand, the electron’s orbital and the crystal lattice, in the left column of Fig. 1, react to an application of an external electric field, and their orbital dynamics couples to a magnetic field. Therefore, the electronic orbital degree of freedom is a core element in describing magnetoelectric coupling, e.g., the current-induced torque. Note that a charge excitation of the ions in the lattice is efficiently screened by the electrons in metals, which are our main interest in this paper. Moreover, we assume that the lattice degrees of freedom are frozen (absence of a phonon excitation) and we neglect a coupling between the ions and an external electric field. Therefore, according to this physical picture, the current-induced torque arises as follows: An external electric field excites the orbital dynamics, with which the spin dynamics is entangled by the SOC. The resulting spin dynamics alters the local magnetic moment by the exchange interaction.

An exception to this picture is a noncollinear magnet, where the OAM is associated with the scalar spin chirality or Skyrmion charge. Here, spin and orbital momenta may interact even without relativistic SOC. Although such topological OAM exhibits exotic dynamic phenomena associated with complex spin structures, we leave this case to future work.

In the rest of this section, we start from the effective single-particle Hamiltonian to separately define the SOC, the crystal field potential, and the exchange interaction, which is adapted for the DFT framework (Sec. II B). Then we derive the continuity equations for the spin and OAM in Sec. II C. In the continuity equations, rates for the changes of the spin and OAM are captured by the influxes of the spin and OAM as well as torques describing the angular momentum transfer between different degrees of freedom. To evaluate individual contributions appearing in the continuity equations under an external electric field, we consider interband and intraband contributions within the Kubo formula (Sec. II D). However, we point out that the interband contribution does not satisfy the stationary condition in the steady state (Sec. II E). To resolve this problem, we propose a balance-type equations that describe a relation between the interband and intraband contributions in the steady state, which we call the interband-intraband correspondence. The application of the interband-intraband correspondence to the continuity equations of the spin and OAM leads to the equations of motion (Sec. II F), which is the main result of this section. Meanwhile, the intraband contribution satisfies the stationary condition, for which we derive the equations of motion as well.

B. Effective Single-Particle Hamiltonian

Within the effective single-particle description, such as the Kohn-Sham treatment within the DFT, the general electronic Hamiltonian in a solid is formally written as

\[ \mathcal{H} = \int d^3r \Psi^\dagger(r) \left[ \frac{\mathbf{p}^2}{2m} + V_{\text{eff}}(r) \right] \Psi(r), \]

where \( \Psi(r) \) and \( \Psi^\dagger(r) \) are electron annihilation and creation field operators in the second quantization representation, respectively. Here, \( \mathbf{p} = -i\hbar \nabla_r \) is the momentum operator, \( \hbar \) is the reduced Planck constant, and \( m \) is the electron mass. The effective single-particle potential \( V_{\text{eff}}(r) \) can be divided into the SOC, \( V_{SO}(r) \), the exchange interaction, \( V_{XC}(r) \), and the spin-independent potential, \( V_0(r) \):

\[ V_{\text{eff}}(r) = V_{SO}(r) + V_{XC}(r) + V_0(r). \]

The SOC and exchange interaction are explicitly written as

\[ V_{SO}(r) = \beta \sigma \cdot \nabla_r V_0(r) \times \mathbf{p}, \]
\[ V_{XC}(r) = \mu_B \Omega_{XC}(r) \cdot \mathbf{\sigma}, \]

respectively. Here, \( \mathbf{\sigma} \) is the vector of the Pauli matrices representing the spin, \( \beta = \hbar/4m^2c^2 \) with the speed of light \( c \), \( \mu_B \) is the Bohr magneton, and \( \Omega_{XC}(r) \) is an effective magnetic field caused by the exchange interaction. Note that we construct \( V_{SO}(r) \) by neglecting \( V_{XC}(r) \) as an approximation. Note that the degrees of freedom of the lattice and the local magnetic moment are implicitly included in this description.

In the evaluation of operators we use symmetrized representations such that the hermiticity is kept in the numerical implementation. However, we present non-symmetrized forms throughout the paper for notational brevity.

C. Continuity Equations for Spin and Orbital Angular Momenta

Although the continuity equations for spin and OAM have been introduced, it assumes a LS coupling type of SOC. Thus, we present a detailed derivation for the general single particle Hamiltonian [Eqs. (1) and (2)] so as to arrive at expressions suitable for first principles calculations. In the Heisenberg picture (indicated by the hat symbol below), we define the OAM and spin density operators as

\[ \hat{I}(r, t) = \hat{\Psi}^\dagger(r, t) \mathbf{L} \hat{\Psi}(r, t), \]
\[ \hat{S}(r, t) = \hat{\Psi}^\dagger(r, t) \mathbf{S} \hat{\Psi}(r, t). \]
While the spin $\mathbf{S}$ is represented by the vector of the Pauli matrices $\mathbf{S} = (\hbar/2)\sigma$, evaluation of the OAM is nontrivial in periodic solids because the position $\mathbf{r}$ is ill-defined under periodic boundary conditions. Nonetheless, we can calculate the OAM with respect to the atomic spheres called muffin tins (MTs) centered at the positions of the atoms:

$$ L = \sum_{\mu} \mathbf{L}_{\mu}, \quad (6a) $$

$$ \mathbf{L}_{\mu} = \Theta(R_{\mu} - \mathbf{r}_{\mu}) (\mathbf{r}_{\mu} \times \mathbf{p}). \quad (6b) $$

Here, $\Theta(x)$ is the Heaviside step function, $\mu$ is the index of an atom in the unit cell whose center is located at $\mathbf{r}_{\mu}$, $\mathbf{r}_{\mu} = \mathbf{r} - \mathbf{r}_{\mu}$ is the displacement from the atom center, and $R_{\mu}$ is the radius of the muffin tin. This method is called atom-centered approximation (ACA), and it gives a reliable result when orbital currents are associated with partially localized $d$ or $f$ shells. Thus, the usage of the ACA is justified in magnetic bilayers consisting of transition metal elements, Fe/W(110) and Ni/W(110), which are in the focus of our study. However, the ACA neglects contributions from nonlocal currents, e.g., in Chern insulators and noncollinear magnets [53-56], and ultimately one should resort to the modern theory of orbital magnetization [54-56].

For the OAM and spin densities defined in Eq. (5), we can derive continuity equations from the Heisenberg equations of motion. These are formally written as

$$ \frac{\partial \mathbf{i}_{\alpha}(\mathbf{r}, t)}{\partial t} = \frac{1}{i\hbar} \left[ i_{\alpha}(\mathbf{r}, t), \mathcal{H}(t) \right] = -\nabla_{\mathbf{r}} \cdot \mathbf{Q}^{L\alpha}(\mathbf{r}, t) + \mathcal{T}^{L\alpha}(\mathbf{r}, t), \quad (7a) $$

$$ \frac{\partial \mathbf{S}_{\alpha}(\mathbf{r}, t)}{\partial t} = \frac{1}{i\hbar} \left[ \mathbf{S}_{\alpha}(\mathbf{r}, t), \mathcal{H}(t) \right] = -\nabla_{\mathbf{r}} \cdot \mathbf{Q}^{SO}(\mathbf{r}, t) + \mathcal{T}^{SO}(\mathbf{r}, t), \quad (7b) $$

where $\alpha = x, y, z$. Here,

$$ \mathbf{Q}^{L\alpha}(\mathbf{r}, t) = \frac{1}{2} \hat{\Psi}^{\dagger}(\mathbf{r}, t) \{ L_{\alpha}, \mathbf{v} \} \hat{\Psi}(\mathbf{r}, t), \quad (8a) $$

$$ \mathbf{Q}^{SO}(\mathbf{r}, t) = \frac{1}{2} \hat{\Psi}^{\dagger}(\mathbf{r}, t) \{ S_{\alpha}, \mathbf{v} \} \hat{\Psi}(\mathbf{r}, t), \quad (8b) $$

are orbital and spin current operators, respectively, where

$$ \mathbf{v} = \frac{i\hbar}{2m} \left( \nabla_{\mathbf{r}}^{L} - \nabla_{\mathbf{r}}^{R} \right) + \beta \sigma \times \nabla_{\mathbf{r}} V_{0}(\mathbf{r}) \quad (9) $$

is the velocity operator (\( \nabla_{\mathbf{r}}^{L} \) and \( \nabla_{\mathbf{r}}^{R} \) act on the left and on the right, respectively), and

$$ \mathcal{T}^{L}(\mathbf{r}, t) = \frac{1}{i\hbar} \hat{\Psi}^{\dagger}(\mathbf{r}, t) [\mathbf{L}, V_{eff}(\mathbf{r})] \hat{\Psi}(\mathbf{r}, t), \quad (10a) $$

$$ \mathcal{T}^{SO}(\mathbf{r}, t) = \frac{1}{i\hbar} \hat{\Psi}^{\dagger}(\mathbf{r}, t) [\mathbf{S}, V_{eff}(\mathbf{r})] \hat{\Psi}(\mathbf{r}, t) \quad (10b) $$

are torque operators for the OAM and spin, respectively.

The appearance of the torques in Eq. (7) signals the fact that the OAM and spin are not conserved. This implies that the angular momentum is transferred from the electron to other degrees of freedom as described in Fig. [1]. The electrons exchange orbital angular momentum with the lattice and with the electron’s spin via $V_{CF}(\mathbf{r})$ and $V_{SO}(\mathbf{r})$, respectively. Thus, the torque acting on the OAM of the electron is decomposed as

$$ \mathcal{T}^{L}(\mathbf{r}, t) = \mathcal{T}^{L}_{CF}(\mathbf{r}, t) + \mathcal{T}^{L}_{SO}(\mathbf{r}, t), \quad (11) $$

where

$$ \mathcal{T}^{L}_{CF}(\mathbf{r}, t) = \frac{1}{i\hbar} \hat{\Psi}^{\dagger}(\mathbf{r}, t) [\mathbf{L}, V_{0}(\mathbf{r}) + V_{XC}(\mathbf{r})] \hat{\Psi}(\mathbf{r}, t), \quad (12) $$

$$ \mathcal{T}^{L}_{SO}(\mathbf{r}, t) = \frac{1}{i\hbar} \hat{\Psi}^{\dagger}(\mathbf{r}, t) [\mathbf{L}, V_{SO}(\mathbf{r})] \hat{\Psi}(\mathbf{r}, t). \quad (13) $$

We denote $\mathcal{T}^{L}_{CF}(\mathbf{r}, t)$ as the crystal field torque and $\mathcal{T}^{L}_{SO}(\mathbf{r}, t)$ as the spin-orbital torque. On the other hand, the electron exchanges the spin angular momentum with the local magnetic moment and the electron’s orbital angular momentum via $V_{XC}(\mathbf{r})$ and $V_{SO}(\mathbf{r})$, respectively. Thus, the torque acting on the electron’s spin can be decomposed as

$$ \mathcal{T}^{S}(\mathbf{r}, t) = \mathcal{T}^{S}_{XC}(\mathbf{r}, t) + \mathcal{T}^{S}_{SO}(\mathbf{r}, t), \quad (14) $$

where

$$ \mathcal{T}^{S}_{XC}(\mathbf{r}, t) = \frac{1}{i\hbar} \hat{\Psi}^{\dagger}(\mathbf{r}, t) [\mathbf{S}, V_{XC}(\mathbf{r})] \hat{\Psi}(\mathbf{r}, t), \quad (15) $$

$$ \mathcal{T}^{S}_{SO}(\mathbf{r}, t) = \frac{1}{i\hbar} \hat{\Psi}^{\dagger}(\mathbf{r}, t) [\mathbf{S}, V_{SO}(\mathbf{r})] \hat{\Psi}(\mathbf{r}, t). \quad (16) $$

We denote $\mathcal{T}^{S}_{XC}(\mathbf{r}, t)$ as the exchange torque and $\mathcal{T}^{S}_{SO}(\mathbf{r}, t)$ as the spin-orbital torque. Note that $\mathcal{T}^{S}_{SO}(\mathbf{r}, t)$ and $\mathcal{T}^{S}_{SO}(\mathbf{r}, t)$ differ, and we specify them as the spin-orbital torques acting on the orbital and spin, respectively.

We have a few remarks on the different torques and their definitions. In the absence of the SOC, the spin-orbital torques vanish. Thus in a steady state, where $\langle \partial \mathbf{i}_{\alpha}(\mathbf{r}, t)/\partial t \rangle = 0$, Eq. (15) becomes $\langle \mathcal{T}^{S}_{XC}(\mathbf{r}, t) \rangle = \nabla_{\mathbf{r}} \cdot \langle \mathbf{Q}^{SO}(\mathbf{r}, t) \rangle$. Here, $(\cdots)$ represents expectation value in the steady state. This implies that the spin current divergence is absorbed by the local magnetic moment. Thus, this corresponds to the spin-transfer torque in the absence of the SOC. If we consider the opposite situation where the spin current flux is absent, occurring e.g. in atomically thin magnetic films, where the spin current effect can be neglected along the perpendicular direction to the film plane, Eq. (15) becomes $\langle \mathcal{T}^{S}_{XC}(\mathbf{r}, t) \rangle = -\langle \mathcal{T}^{S}_{SO}(\mathbf{r}, t) \rangle$. Thus, the exchange torque amounts to the spin-orbital torque. This is related to the widely used terminology, spin-orbit torque [17]. However, in our terminology, the net torque acting on the local magnetic moment is the exchange torque, which may differ from the spin-orbital torque due to the presence of the spin current flux. In general, both the spin current flux and spin-orbital torque contribute to the exchange torque.

We get additional insight from explicitly evaluating the torques in a simplified situation. Let us first consider the exchange torque. By using Eqs. (14) and (15), the exchange torque can be written as

$$ \mathcal{T}^{S}_{XC}(\mathbf{r}, t) = \mu_{B} \hat{\Psi}^{\dagger}(\mathbf{r}, t) [\sigma \times \Omega_{XC}(\mathbf{r})] \hat{\Psi}(\mathbf{r}, t), \quad (17) $$

in general. Thus, it describes a precession of the spin with respect to the direction of the exchange field. On the other
hand, by using Eqs. (3) and (16), the spin-orbital torque acting on the spin is formally written as
\[ \hat{T}^S_{SO}(r,t) = \beta \hat{\Psi}^\dagger(r,t) [\sigma \times \{ \nabla_r V_0(r) \times p \}] \hat{\Psi}(r,t). \]
(18)

Since it depends on the spatial gradient of \( V_0(r) \), the dominant contribution to it is concentrated near the atom centers, where \( V_0(r) \) is almost spherical. Thus, within the MTs, we can approximately write \( \nabla_r V_0(r) \approx \sum_\mu \Theta (r_\mu - r_\mu) [\partial V_0(r_\mu) / \partial r_\mu] \). Within this approximation
\[ V_{SO}(r) \approx \sum_\mu \hat{\Psi}^\dagger(r,t) [\xi_\mu(r_\mu) L_\mu \cdot \sigma] \hat{\Psi}(r,t). \]
(19)

Thus, the spin-orbital torque becomes
\[ \hat{T}^S_{SO}(r,t) \approx \sum_\mu \xi_\mu(r_\mu) (L_\mu \times \sigma), \]
(20)

where
\[ \xi_\mu(r_\mu) = \beta \frac{dV_0(r_\mu)}{dr_\mu} \]
(21)
is the strength of the SOC for the \( \mu \)-th atom. Therefore, Eq. (20) indicates that the spin-orbital torque describes a mutual precession between the OAM and the spin. That is,
\[ \hat{T}^S_{SO}(r,t) \approx -\hat{T}^L_{SO}(r,t). \]
(22)

While it is approximately true in most systems, we keep superscripts \( S \) and \( L \) separately, because \( \hat{T}^S_{SO}(r,t) \) and \( -\hat{T}^L_{SO}(r,t) \) differ in general due to nonspherical contributions to the \( V_{SO}(r) \).

Meanwhile, the crystal field torque cannot be expressed in simple terms. In general, it describes an angular momentum transfer between the lattice and the electronic OAM. It originates due to the breaking of the continuous rotation symmetry by the crystal field, which differentiates specific directions depending on the structure of the crystal, and leads to various anisotropic effects.

### D. Kubo Formula: Interband and Intraband Responses

The current-induced torque corresponds to the response of the exchange torque to an electric field, [Eqs. (15) and (17)]. One of the most widely used approaches for its calculation is the linear response theory, where often interband and intraband contributions are evaluated separately. The interband contribution originates in the change of a given state by a coherently superposition of the eigenstates for a given \( \mathbf{k} \): in response to an external electric field \( \mathbf{E} = \mathbf{E}_0 \mathbf{x} \) the periodic part of the Bloch state \( |u_{nk}\rangle \) changes as
\[ |u_{nk}\rangle \rightarrow |u_{nk}\rangle + |\delta u_{nk}\rangle, \]
(23)

where
\[ |\delta u_{nk}\rangle = i\hbar \mathbf{E}_0 \sum_{m \neq n} \frac{|u_{mk}\rangle \langle u_{mk}| v_\mathbf{k}(\mathbf{k}) |u_{nk}\rangle}{(E_{nk} - E_{mk} + i\eta)^2}. \]
(24)

Here, \( e > 0 \) is the absolute value of the charge of the electron, \( E_{nk} \) is the energy eigenvalue for the state \( |u_{nk}\rangle \). The infinitesimally small number \( \eta > 0 \) arises from the causality relation. That is, in describing time-evolution of the state, the electric field is adiabatically turned on from \( t = -\infty \) to \( t = 0 \) by the vector potential \( \mathbf{A}(t) = -te^{-it/\hbar} \mathbf{E}_0 \mathbf{x} \) such that \( \mathbf{E} = -\partial \mathbf{A}(t) / \partial t \). As a result, the interband response of an observable \( \mathcal{O} = S_0 \) or \( L_0 \) is given by
\[ \langle \mathcal{O} \rangle_{\text{inter}} = 2 \sum_{nk} f_{nk} \text{Re} \{ \langle u_{nk}| \mathcal{O}(\mathbf{k}) |u_{nk}\rangle \}, \]
(25)

where \( f_{nk} \) is the Fermi-Dirac distribution function for the state \( |u_{nk}\rangle \). By combining Eqs. (24) and (25) and manipulating the dummy indices \( n \) and \( m \), we arrive at
\[ \langle \mathcal{O} \rangle_{\text{inter}} = e\hbar \mathbf{E}_0 \sum_{n \neq m} \sum_{\mathbf{k}} (f_{nk} - f_{mk}) \]
\[ \times \text{Im} \left\{ \frac{\langle u_{nk}| \mathcal{O}(\mathbf{k}) |u_{mk}\rangle \langle u_{mk}| v_\mathbf{k}(\mathbf{k}) |u_{nk}\rangle}{(E_{nk} - E_{mk} + i\eta)^2} \right\}. \]
(26)

Here, we define \( \mathcal{O}(\mathbf{k}) = e^{-i\mathbf{k} \cdot \mathbf{r}} \mathcal{O}e^{i\mathbf{k} \cdot \mathbf{r}} \) in \( k \)-space for an arbitrary operator \( \mathcal{O} \). The interband contribution in Eq. (26) is also known as the intrinsic contribution since it depends only on the electronic structure, the eigenstates and their energy eigenvalues in the ground state.

On the other hand, the intraband response arises due to a shift of the Fermi surface by disorder scattering. The leading contribution arises from the change of the occupation function:
\[ \langle \mathcal{O} \rangle_{\text{Boltzmann}} = \sum_{nk} (f_{nk+\Delta k} - f_{nk}) \langle u_{nk}| \mathcal{O}(\mathbf{k}) |u_{nk}\rangle, \]
(27)

which is also referred to as Boltzmann-like contribution. Here, \( \Delta k = e\mathbf{E}_0 \tau / \hbar \) is the shift of the Fermi surface caused by the electric field \( \mathbf{E} = \mathbf{E}_0 \mathbf{x} \) and \( \tau \) is the momentum relaxation time. Up to linear order in \( \Delta k \), the shift of the Fermi-Dirac distribution function becomes
\[ f_{nk+\Delta k} - f_{nk} \approx \hbar \Delta k f'_{nk} \langle u_{nk}| v_\mathbf{k}(\mathbf{k}) |u_{nk}\rangle, \]
(28)

where \( f'_{nk} = \partial f_{nk} / \partial E_{nk} \). Thus, the intraband contribution can be written as
\[ \langle \mathcal{O} \rangle_{\text{Boltzmann}} = -e\hbar \mathbf{E}_0 \tau \sum_{nk} f'_{nk} \langle u_{nk}| \mathcal{O}(\mathbf{k}) |u_{nk}\rangle \]
\[ \times \langle u_{nk}| v_\mathbf{k}(\mathbf{k}) |u_{nk}\rangle. \]
(29)

Note that it is described by a single phenomenological parameter \( \tau \), which is assumed to be state-independent. As \( \tau \) increases, i.e., as the resistivity decreases, the intraband contribution linearly increases. In general, the momentum relaxation time depends on the particular state in the electronic structure. In FMs, for example, it is known that the momentum relaxation times of the majority and minority electrons are different, which plays an important role in understanding various magnetotransport effects. However, within the approach that we pursue here, as given by Eq. (29), we do not consider these effects.
In addition, there is another intraband response due to a change of the operator $O(k)$, which is given by

$$
\langle O \rangle_{\text{intra}}^{\text{extra}} = -\frac{eE_x \tau}{\hbar} \sum_{nk} f_{nk} \langle u_{nk} | \partial_{k_x} O(k) | u_{nk} \rangle.
$$

(30)

This contribution is often neglected because the operator $O(k)$ is assumed to be independent of $k$, which is the case for the spin. We note that it can be rewritten as

$$
\langle O \rangle_{\text{intra}}^{\text{extra}} = \sum_{nk} f_{nk} \langle u_{nk+\Delta k} | O(k+\Delta k) | u_{nk+\Delta k} \rangle
- \langle u_{nk} | O(k) | u_{nk} \rangle.
$$

(31)

by using

$$
\langle \partial_{k_x} u_{nk} | O(k) | u_{nk} \rangle + \langle u_{nk} | O(k) | \partial_{k_x} u_{nk} \rangle = 0.
$$

(32)

Thus, the extra intraband contribution describes the shift of the expectation value itself. Therefore, from Eqs. (29) and (30), the total intraband contribution becomes

$$
\langle O \rangle_{\text{intra}} = \langle O \rangle_{\text{intra}}^{\text{Boltzmann}} + \langle O \rangle_{\text{intra}}^{\text{extra}} = -\frac{eE_x \tau}{\hbar} \sum_{nk} \partial_{k_x} \left[ f_{nk} \langle u_{nk} | O(k) | u_{nk} \rangle \right].
$$

(33a)

and

$$
\langle O \rangle_{\text{intra}}^{\text{extra}} = \frac{1}{\tau} \langle O \rangle_{\text{intra}} = \left\langle \frac{dO}{dt} \right\rangle_{\text{intra}},
$$

(35)

with the proof presented in Appendix A. Physical meaning of Eq. (35) is the following. The right hand side of the equation describes intrinsic pumping of $O$, which depends only on the electronic structure. The left hand side of the equation is related to a relaxation process, which tend to suppress deviations from the equilibrium value of $O$. In the steady state, the intrinsic pumping and the relaxation rates are equal, thus $\langle O \rangle_{\text{intra}}$ is determined by the relaxation rate $\tau$. Therefore, Eq. (35) describes a balance between a tendency to increase $O$ by the intrinsic process and a relaxation rate by the extrinsic process. Meanwhile, the intraband contribution alone satisfies the steady state condition:

$$
\left\langle \frac{dO}{dt} \right\rangle_{\text{intra}} = 0.
$$

(36)

A proof of the stationary condition for the intraband contribution is given in Appendix B. Equations (35) and (36) are used to derive the equations of motion below.

### F. Steady State Equations of Motion for Spin and Orbital Angular Momenta

By applying the interband-intraband correspondence [Eq. (25)] to the continuity equations [Eq. (7)], we arrive at the following equations:

$$
\frac{1}{\tau} \left( l_\alpha (r) \right)_{\text{intra}} = -\nabla_r \cdot \left( Q^{L\alpha} (r) \right)_{\text{inter}} + \left( T^{L_{\alpha \beta}}_{CG} (r) \right)_{\text{inter}} + \left( T^{L_{\alpha \beta}}_{SG} (r) \right)_{\text{inter}},
$$

(37a)

$$
\frac{1}{\tau} \left( S_\alpha (r) \right)_{\text{intra}} = -\nabla_r \cdot \left( Q^{S\alpha} (r) \right)_{\text{inter}} + \left( T^{S_{\alpha \beta}}_{NC} (r) \right)_{\text{inter}} + \left( T^{S_{\alpha \beta}}_{SG} (r) \right)_{\text{inter}}.
$$

(37b)

Note that that the time dependence no longer appears since the equations describe the steady state. Also, the hat symbol for the Heisenberg picture is removed. Equation (37) relates the current fluxes and torques of the intrinsic origin to the intraband accumulation of the OAM and spin. Application of Eq. (36) leads to constraints between intraband contributions for the current fluxes and torques of the OAM and the spin:
The above equations constitute equations of motion for the spin and orbital angular momenta, which are coupled by the SOC, in the steady state reached after an external electric field has been applied. This is one of the main results of our work. Previous theories on the current-induced torque have focused on evaluating linear response of the exchange torque mechanism only. As an illustration, Fig. 2 shows a competition of the OAM and the spin are parallel to each other. When the injected spin in the FM exerts a torque directly, the injected OAM first couples to the spin and then exerts a torque on the local magnetic moment. We assume that the correlation between the OAM and the spin is positive in the FM, such that the directions of the OHC is by an order of magnitude larger than the SHC, two prototypical systems that satisfy these criteria. For W, the OHC is by an order of magnitude larger than the SHC, two prototypical systems that satisfy these criteria. For Fe/W(110) and Ni/W(110), respectively. Meanwhile, Fe/W(110) has been previously studied for the anisotropic Dzyaloshinskii-Moriya interactions for stabilizing the anti-Skyrmion [61].

The effective SOC strength — which incorporates not only the SOC itself but also band structure effect — can vary significantly. We expect that the effective SOC strength is much stronger in Ni than in Fe, and we show this by explicit calculations below.

Therefore, we consider NM/FM bilayers where the NM exhibits an opposite sign of the OHE and SHE, while the FM is varied such that the strength of effective SOC is controlled. This leads us to the choice of Fe/W and Ni/W bilayers — two prototypical systems that satisfy these criteria. For W, the OHC is by an order of magnitude larger than the SHC, with opposite sign [33]. A reason for choosing Fe and Ni as FMs comes from the expectation that the orbital-to-spin conversion efficiency of the OT mechanism is much larger in Ni than it is in Fe. Moreover, both materials can be grown epitaxially along the [110] direction of the body-centered cubic (bcc) structure. We denote these systems as Fe/W(110) and Ni/W(110), respectively. Meanwhile, Fe/W(110) has been previously studied for the anisotropic Dzyaloshinskii-Moriya interactions for stabilizing the anti-Skyrmion [61].

Figures 2(a) and 2(b) respectively display side and top views of the FM/W(110) structure, where FM = Fe or Ni. We consider 8 layers of W and 2 layers of the FM. We denote the magnetic atom at the surface of the slab is marked as Fe2 and Ni2. For the bcc(110) stack of the W layers, we assume that the film follows the bulk lattice parameters of the bcc W, whose lattice constant is \(a = 3.190 \text{ Å}\) in the cubic unit cell convention. As a result, the distance between the neighboring layers of W is \(d_{W-W} = a/\sqrt{2} = 2.256 \text{ Å}\). The in-plane unit cell is of a rectangular shape, whose length along the [001] and [110] directions are \(a = 3.190 \text{ Å}\) and \(b = \sqrt{2a} = 4.511 \text{ Å}\), respectively. The layer distances between W-FM and FM-FM were optimized in order to minimize the total energy: \(d_{W-Fe} = 2.024 \text{ Å}\) and \(d_{Fe-Fe} = 1.744 \text{ Å}\) for Fe/W(110) and \(d_{W-Ni} = 1.909 \text{ Å}\) and \(d_{Ni-Ni} = 1.747 \text{ Å}\) for Ni/W(110). We assume that the local magnetic moment is oriented along the direction of \(-\hat{z}\), where \(\hat{z}\) is defined as the direction of the in-plane unit cell.

\[
-\mathbf{\nabla} \cdot \left\langle \mathbf{Q}_{\text{CF}}^{L} (\mathbf{r}) \right\rangle^{\text{intra}} + \left\langle T_{\text{CF}}^{L} (\mathbf{r}) \right\rangle^{\text{intra}} + \left\langle T_{\text{SO}}^{L} (\mathbf{r}) \right\rangle^{\text{intra}} = 0,
\]

(38a)

\[
-\mathbf{\nabla} \cdot \left\langle \mathbf{Q}_{\text{XC}}^{S} (\mathbf{r}) \right\rangle^{\text{intra}} + \left\langle T_{\text{XC}}^{S} (\mathbf{r}) \right\rangle^{\text{intra}} + \left\langle T_{\text{SO}}^{S} (\mathbf{r}) \right\rangle^{\text{intra}} = 0.
\]

(38b)
FIG. 3. (a) Crystal structure of FM/W(110), where FM = Fe or Ni. Side and top views are displayed on the left and right, respectively. (b) First Brillouin zone and high symmetry points of bcc(110) film. Electronic energy dispersion $E_{nk}$ and the spin-orbit correlation in the FM $(L \cdot S)_{nk}^{FM}$ for (c) Fe/W(110) and (d) Ni/W(110), which are represented by the line and color map, respectively. Note that $(L \cdot S)_{nk}^{FM}$ is much more pronounced in Ni compared to Fe near the Fermi energy $E_F$. Layer-resolved plots of the spin (blue squares) and orbital (red stars) moments for (e) Fe/W(110) and (f) Ni/W(110). Comparing Fe/W(110) and Ni/W(110), the spin moment in Fe is much larger than that in Ni, but the relative ratio of the orbital moment over the spin moment is much larger in Ni. This implies that the orbital degree of freedom is not frozen in Ni/W(110), while it is quenched in Fe/W(110).

### B. Spin-Orbit Correlation and Orbital Quenching

The calculated electronic band structures of Fe/W(110) and Ni/W(110) are shown in Figs. 3(c) and 3(d), respectively. On top of each energy band $E_{nk}$, the spin-orbit correlation in the FM $(L \cdot S)_{nk}^{FM}$ is shown in color, which is defined as

$$
(L \cdot S)_{nk}^{FM} = \sum_{z \in FM} \langle \psi_{nk} | P_z (L \cdot S) P_z | \psi_{nk} \rangle.
$$

Here, $| \psi_{nk} \rangle$ is the Bloch state of band $n$ at $k$-point $k$, and $P_z$ is the projection operator onto a layer at position $z$ inside the FM. It can be seen that near the Fermi energy $E_F$, the spin-orbit correlation is negligible in Fe/W(110). The hotspot is located about 1.0 eV below the Fermi energy, whose effect is negligible in the transport and dynamic phenomena. On the other hand, in Ni/W(110) the spin-orbit correlation is much more pronounced for states near the Fermi energy. The positive sign of this correlation tends to align the OAM and the spin in the same direction.

The difference in the spin-orbit correlation directly affects the orbital moment of the FM in equilibrium. In Figs. 3(e) and 3(f), spin and orbital magnetic moments are plotted in each layer for Fe/W(110) and Ni/W(110), respectively. Blue square symbols and red star symbols respectively indicate the spin and orbital moments. For Fe/W(110) [Fig. 3(e)], the magnitude of the spin moment is large: $+2.259 \ \mu_B$ and $+2.856 \ \mu_B$ for Fe1 and Fe2, respectively. On the other hand, the orbital moments of Fe1 and Fe2 are small: $+0.069 \ \mu_B$ and $+0.079 \ \mu_B$, respectively. The ratio of the orbital moment over the spin moment is 3.06 % and 2.76 % for Fe1 and Fe2, respectively, which is fairly small. Thus, the orbital magnetism is strongly quenched in Fe. This implies that even though the OAM may be injected into Fe, i.e., by the OHE of W, it is likely that most of the OAM is relaxed to the lattice through the crystal field torque [Eq. (12)] instead of being transferred to the angular momentum of the spin through the spin-orbital torque [Eq. (13)]. Therefore, in Fe/W(110), it is expected that the OT mechanism is not significant and the ST will be dominant, in accordance with common expectation. Meanwhile, we find proximity magnetism in W8 by the hybridization with Fe, where the spin and orbital moments are $-0.114 \ \mu_B$ and $-0.009 \ \mu_B$, respectively.

In contrast to Fe/W(110), Ni atoms in Ni/W(110) exhibit much smaller spin moment but relatively large orbital moment. The spin moments are $+0.146 \ \mu_B$, $+0.510 \ \mu_B$ and the orbital moments are $+0.023 \ \mu_B$, $+0.070 \ \mu_B$ for Ni1 and
We further decompose \( T^m \) into dampinglike (\( T_{DL} \)) and field-like (\( T_{FL} \)) components:

\[
T^m = T_{DL} \mathbf{m} \times (\mathbf{m} \times \hat{y}) + T_{FL} \mathbf{m} \times \hat{y} = -T_{DL} \mathbf{y} + T_{FL} \mathbf{x},
\]

For the orbital channel, these are interband responses of the spin current influx, which are closely related to that of the dampinglike torque. The analysis for \( L_x \) and \( S_y \) components of quantities from Eqs. \((37a)\) and \((37b)\), respectively, which is closely related to that of the dampinglike torque. The analysis for \( L_x \) and \( S_y \) from Eqs. \((38a)\) and \((38b)\) is presented in the Appendix \[E\]. In order to perform the decomposition of the computed quantities into contributions coming from each atomic layer, we adopt the tight-binding representation of the equations of motion, as explained in detail in Appendix \[E\]. In the tight-binding representation, we denote orbital and spin current influxes, which correspond to the first terms in the right hand side of Eqs. \((3a)\) and \((7b)\), as \( \Phi[Q_z^L] \) and \( \Phi[Q_z^S] \).

**D. Summary of the Result**

In Secs. \[III_E\] and \[III_F\] we present detailed results of the first-principles calculations for Fe/W(110) and Ni/W(110) bilayers, respectively, and evaluate each term in Eq. \((37)\). For the orbital channel, these are interband responses of the orbital current influx \( \Phi[Q_z^L] \), the crystal field torque \( T_{CF} \), the spin-orbital torque \( T_{SO} \), and the intraband response of the orbital accumulation \( L_y \), divided by momentum-relaxation time \( \tau \). For the spin channel, these are interband responses of the spin current influx \( \Phi[Q_z^S] \), the exchange torque \( T_{XC} \), the spin-orbital torque \( T_{SO} \), and the intraband response of the spin accumulation \( S_y \), divided by \( \tau \). We find that in both Fe/W(110) and Ni/W(110), the equations of motion given by Eq. \((37)\) are satisfied.

By evaluating these quantities, we aim to understand the main mechanism of the current-induced torque on the local magnetic moment. This leads to a negative effective spin Hall angle, as it is well-known for W. On the other hand, in Ni/W(111), there is a significant contribution of the spin-orbital torque to the magnetization torque.
hand, in Ni/W(110), the effective spin Hall angle is found to be positive in sign. We find that the $\langle T_{SO}^{S_H} \rangle_{\text{inter}}$ dominates over $\langle T_{SO}^{Q} \rangle_{\text{inter}}$ [Fig. 5(b)], which signifies that the simple spin injection picture does not hold. Instead, $\langle T_{SO}^{Q} \rangle_{\text{inter}}$ is associated with pronounced $\langle T_{SO}^{S} \rangle_{\text{inter}}$. Thus, we conclude that the orbital-to-spin conversion in Ni plays a crucial role in generating a torque on the local magnetic moment. Furthermore, we also find that the sign of $\langle T_{SO}^{Q} \rangle_{\text{inter}}$ in Ni is abnormal: it is opposite to the sign predicted from the SHE in W. This implies that the orbital current injected from W is converted into the spin current in Ni, in accord to the mechanism displayed in Fig. [5]. Detailed analysis confirms that the OT is the dominant mechanism of current-induced torque in Ni/W(110).

Meanwhile, for the response of quantities associated with the orbital channel, we find in both Fe/W(110) and Ni/W(110) that $\langle T_{CF}^{L} \rangle_{\text{inter}} \approx 0$, suggesting that the injected OAM is mostly transferred to the lattice. Nonetheless, in Ni/W(110), $\langle T_{CF}^{L} \rangle_{\text{inter}}$ is suppressed near the Fermi energy, which opens a channel for the angular momentum transfer from the orbital to spin via $\langle T_{CF}^{L} \rangle_{\text{inter}}$. Since the orbital response is larger than the spin response by an order of magnitude, $\langle T_{SO}^{S} \rangle_{\text{inter}} \approx -\langle T_{CF}^{L} \rangle_{\text{inter}}$ becomes a dominant contribution in the spin channel.

### E. Fe/W(110)

In Fig. 5(a), spatial profiles of individual terms appearing in Eq. (37a) are shown for $L_y$. We find that $\langle T_{CF}^{L} \rangle_{\text{inter}}$ (blue squares) is negative near W1 and positive at W8, which corresponds to a positive sign of the OHC. In concurrence with $\langle T_{CF}^{L} \rangle_{\text{inter}}$, $\langle T_{CF}^{L} \rangle_{\text{inter}}$ (purple diamonds) appears in the opposite sign. However, $\langle T_{SO}^{L} \rangle_{\text{inter}}$ (red stars) is much smaller than $\langle T_{CF}^{L} \rangle_{\text{inter}}$ and $\langle T_{CF}^{L} \rangle_{\text{inter}}$. This means that most of the orbital current influx is absorbed by the lattice. Meanwhile, the sum of $\langle T_{SO}^{L} \rangle_{\text{inter}}$ and the total torque $\langle L_y \rangle_{\text{inter}} = \langle T_{SO}^{L} \rangle_{\text{inter}} + \langle T_{CF}^{L} \rangle_{\text{inter}}$ (cyan crosses), which corresponds to the right hand side of Eq. (37a), matches $\langle L_y \rangle_{\text{inter}} / \tau$ (black dashed line), which corresponds to the left hand side of Eq. (37a). This confirms the validity of the equation of motion Eq. (37a). Slight deviations are due to a finite $\eta$ parameter assumed in the calculation of the interband responses by Eq. (26) (Appendix C).

Analogously, spatial profiles of the individual terms appearing in Eq. (37b), related to the spin degree of freedom, are displayed in Fig. 5(b). We remark that the responses related to spin are an order of magnitude smaller than those related to the orbital channel in Fig. 5(a). This is natural since the spin dynamics is caused by the orbital dynamics that occurs first. From the sign of $\langle T_{SO}^{S} \rangle_{\text{inter}}$ (light blue squares), which is positive near W1 and negative near W8, we conclude that the sign of the SHC is negative. Only in Fe layers, $\langle T_{XC}^{S} \rangle_{\text{inter}}$ (orange circles) is sizable, where the exchange interaction is dominant. Overall positive sign of $\langle T_{XC}^{S} \rangle_{\text{inter}}$ in Fe layers corresponds to negative sign of the effective spin Hall angle. We observe a strong correlation between $\langle T_{SO}^{S} \rangle_{\text{inter}}$ and $\langle T_{SO}^{S} \rangle_{\text{inter}}$. This implies that the spin current influx is mostly transferred to the local magnetic moment, which agrees with the ST mechanism. Meanwhile, $\langle T_{SO}^{S} \rangle_{\text{inter}}$ (dark red stars) is much smaller, but not negligible. The sum of $\langle T_{SO}^{S} \rangle_{\text{inter}}$ and the total torque on the spin $\langle T_{SO}^{S} \rangle_{\text{inter}} + \langle T_{XC}^{S} \rangle_{\text{inter}}$ (green crosses), the right
hand side of Eq. (37b), corresponds to $\langle S_y \rangle^{\text{intra}} / \tau$ on the left hand side (black dashed line).

A pronounced value of $\langle \Phi[Q^{S_y}] \rangle^{\text{inter}}$ near the Fe layers, compared to its value at W1, may seem anomalous [Fig. 5(b)]. However, it can be understood by looking at $\langle S_y \rangle^{\text{intra}}$, which exhibits a much more pronounced magnitude in W1 and W2, as compared to its value in Fe1 and Fe2. That is, in Fe1 and Fe2, the spin current is efficiently absorbed by the FM instead of inducing the spin accumulation. The situation is opposite in W1 and W2, where such spin current absorption is not possible, and the spin current simply results in spin accumulation. A similar behavior, where the spin current is strongly enhanced near the FM interface, has been also predicted in Py/Pt [62] and in Co/Pt [38].

To understand the predicted behavior in terms of the electronic structure, we present the Fermi energy dependence of the computed quantities in Figs. 5(c) and 5(d) for spin and orbital channels, respectively, where a superscript FM means that it is summed over Fe1 and Fe2 layers. To arrive at these plots, we intentionally varied the Fermi energy $E_F$ from $-2$ eV to $+2$ eV with respect to the true Fermi energy $E_F^{\text{true}}$, assuming that the crystal potential remains invariant when $E_F$ changes. For the orbital channel [Eq. (37a) and Fig. 5(c)], we observe that $\langle \Phi[Q^{S_y}] \rangle^{\text{inter}}$ (blue solid line) and $\langle T_{\text{CF}}^{\text{inter}} \rangle$ (purple solid line) tend to cancel each other. Meanwhile, $\langle T_{\text{SO}}^{\text{inter}} \rangle$ (red solid line) is smaller than the rest of the contributions. Thus, most of the OAM is transferred to the lattice instead of the spin. We find that the equation of motion [Eq. (37a)] is valid over the whole range of $E_F$, which is opposite to the negative sign of the SHC in W. This means $\langle \Phi[Q^{S_y}] \rangle^{\text{inter}}$ (light blue solid line) and $\langle T_{\text{CF}}^{\text{inter}} \rangle$ (blue squares) does not exhibit a close correlation with $\langle S_y \rangle^{\text{intra}}$, which is negative. Meanwhile, $\langle T_{\text{SO}}^{\text{intra}} \rangle$ (dark red solid line) is positive in sign according to $\langle \Phi[Q^{S_y}] \rangle^{\text{inter}}$. As in the case of Fe/W(110), $\langle \Phi[Q^{S_y}] \rangle^{\text{inter}}$ and $\langle T_{\text{CF}}^{\text{intra}} \rangle$ (orange solid line) are different in sign, implying that the OAM is transferred to the lattice. Thus, $\langle T_{\text{SO}}^{\text{inter}} \rangle$ (red stars) is much smaller. These features are similar to those we found in Fe/W(110). The interband-intraband correspondence between $\langle L_y \rangle^{\text{intra}} / \tau$ (black dashed line) and the sum of $\langle \Phi[Q^{S_y}] \rangle^{\text{inter}}$ and total torque $\langle T_{\text{CF}}^{L_y} \rangle$ (cyan crosses) is also preserved.

On the other hand, as shown in Fig. 7(b), spatial profiles of spin quantities are significantly different from those of Fe/W(110). First, we notice that $\langle \Phi[Q^{S_y}] \rangle^{\text{inter}}$ (light blue squares) does not exhibit a close correlation with $\langle T_{\text{SO}}^{\text{intra}} \rangle$ (orange circles). Moreover, the sign of $\langle T_{\text{XC}}^{\text{inter}} \rangle$ is negative. This means positive effective spin Hall angle in Ni/W(110), which is opposite to the negative sign of the SHC in W. This is in contrast to the common interpretation that the spin Hall angle is a property of the NM, regardless of the FM. Second, $\langle T_{\text{SO}}^{\text{inter}} \rangle$ (dark red stars) is comparable to the rest of the contributions, indicating the importance of SOC in Ni. Meanwhile, the interband-intraband correspondence stands (green crosses for the sum of $\langle \Phi[Q^{S_y}] \rangle^{\text{inter}}$ and $\langle T_{\text{CF}}^{L_y} \rangle$), and a black dashed line for $\langle S_y \rangle^{\text{intra}} / \tau$.

The Fermi energy dependence of the computed quantities, shown in Figs. 7(c) and 7(d) for orbital and spin channels respectively, provides a detailed information on the overall trend. Although $\langle \Phi[Q^{S_y}] \rangle^{\text{inter}}$ and $\langle T_{\text{CF}}^{L_y} \rangle$ have opposite sign, their magnitudes differ we find that $\langle T_{\text{SO}}^{L_y} \rangle$ is very pronounced near the Fermi energy, with corresponding peak.

FIG. 6. Fermi energy dependence of interband responses of the spin current influx $\Phi[Q^{S_y}]$ (light blue solid line), spin-orbital torque $T_{\text{SO}}^{L_y}$ (dark red solid line), and exchange torque $T_{\text{CF}}^{L_y}$ (orange solid line), which are summed over the Fe layers in Fe/W(110). (a) The result when SOC is on in W and off in Fe, and (b) the result when SOC is off in W and on in Fe.

F. Ni/W(110)

In Figs. 7(a) and 7(b) we show the plots of layer-resolved individual terms appearing in the equation of motion [Eq. (37)] for the $y$ component of the orbital and spin parts, respectively, in Ni/W(110). In Fig. 7(a), we find that the OHC is positive in sign according to $\langle \Phi[Q^{S_y}] \rangle^{\text{inter}}$ (blue squares). As in the case of Fe/W(110), $\langle \Phi[Q^{S_y}] \rangle^{\text{inter}}$ and $\langle T_{\text{CF}}^{\text{inter}} \rangle$ (purple diamonds) are only different in sign, implying that the OAM is transferred to the lattice. Thus, $\langle T_{\text{SO}}^{\text{inter}} \rangle$ (red stars) is much smaller. These features are similar to those we found in Fe/W(110). The interband-intraband correspondence between $\langle L_y \rangle^{\text{intra}} / \tau$ (black dashed line) and the sum of $\langle \Phi[Q^{S_y}] \rangle^{\text{inter}}$ and total torque $\langle T_{\text{CF}}^{L_y} \rangle$ (cyan crosses) is also preserved.
indicated with a black arrow [Fig. 7(c)]. Since the response of the spin quantities is an order of magnitude smaller than that for the orbital channel, the pronounced spin-orbital torque, which is still much smaller than \( \langle Q^{S}_{y} \rangle_{\text{inter}} \) and \( \langle T^{S}_{X_C} \rangle_{\text{inter}} \), can have a significant effect on the dynamics of spin. In accordance with the increase of \( \langle T^{S}_{X_C} \rangle_{\text{inter}} \), \( \langle T^{L}_{y} \rangle_{\text{inter}} \) is significantly decreased near the Fermi energy. This implies that a channel for the OAM transfer to the lattice is suppressed.

As a result, the response of spin in Ni/W(110) exhibits a much more rich and complicated behavior when compared to Fe/W(110) [Fig. 7(d)]. We first notice that the correlation between \( \langle Q^{S}_{z} \rangle_{\text{inter}} \) (light blue solid line) and \( \langle T^{S}_{X_C} \rangle_{\text{inter}} \) (orange yellow solid line) is no longer present. Moreover, with the negative drop of \( \langle T^{S}_{X_C} \rangle_{\text{inter}} \), corresponding to the positive sign of the effective spin Hall angle, there is an associated positive peak from \( \langle T^{S}_{SO} \rangle_{\text{inter}} \) (dark red solid line), which is indicated with a black arrow. This indicates that the spin is transferred from the orbital rather than spin current influx. Therefore, the OAM is responsible for the current-induced torque in Ni/W(110). Meanwhile, the interband-intraband correspondence (green solid line for the sum of \( \langle Q^{S}_{y} \rangle_{\text{inter}} \) and \( \langle T^{S}_{S} \rangle_{\text{inter}} \) and black dashed line for \( \langle S_{y} \rangle_{\text{intra}}/\tau \)) is satisfied.

As we have done for Fe/W(110), we switch on and off the SOC separately for W and Ni atoms in Ni/W(110) as well, showing the results in Fig. 8. In Fig. 8(a), the Fermi energy dependence of \( \langle Q^{S}_{y} \rangle_{\text{inter}} \), \( \langle T^{S}_{SO} \rangle_{\text{inter}} \), and \( \langle T^{S}_{X_C} \rangle_{\text{inter}} \) is shown when the SOC of W is on and the SOC of Ni is off. First of all, we find that \( \langle T^{S}_{X_C} \rangle_{\text{inter}} \) is positive at the Fermi energy, which is opposite to the full-SOC case [Fig. 7(d)]. In this case, we find a strong correlation between \( \langle Q^{S}_{y} \rangle_{\text{inter}} \) and \( \langle T^{S}_{X_C} \rangle_{\text{inter}} \). Thus, the negative sign of the effective spin Hall angle is caused by the spin injection from the SHE of W. However, such correlation is not as perfect as in the case of Fe/W(110) [Fig. 6(a)]. We attribute such difference to an interfacial mechanism, where the torque is generated regardless of the spin current. Meanwhile, \( \langle T^{S}_{S} \rangle_{\text{inter}} \) is negligible since the SOC of Ni is off.

When the SOC is off in W and on in Ni, we still find nontrivial features in \( \langle Q^{S}_{y} \rangle_{\text{inter}} \), \( \langle T^{S}_{SO} \rangle_{\text{inter}} \), and \( \langle T^{S}_{X_C} \rangle_{\text{inter}} \), which is in contrast to Fe/W(110) [Fig. 8(b)]. This is due to nontrivial spin-orbit correlation of Ni shown in Fig. 8(d). Moreover, \( \langle T^{S}_{X_C} \rangle_{\text{inter}} \) is negative at the Fermi energy. We find that nontrivial peak features [black arrows in Fig. 7(d)] are reproduced in this calculation. Thus, we confirm that the latter peaks originate in the SOC of Ni. To further clarify the microscopic mechanisms, we apply the external electric field in W only [Fig. 8(c)] or Ni only [Fig. 8(d)] when the SOC of the W is off and the SOC of Ni is on, which correspond to the OT and the AT contributions, respectively (more details can be found in the Appendix C). In both cases, \( \langle T^{S}_{X_C} \rangle_{\text{inter}} \) exhibits a negative drop near \( E_F \approx 0.15 \text{ eV} \), which is correlated with a positive peak of \( \langle T^{S}_{SO} \rangle_{\text{inter}} \). This implies that for both cases the angular momentum transfer from the orbital channel to the spin channel is crucial. The difference is that for the OT mechanism, Fig. 8(c), \( \langle Q^{S}_{y} \rangle_{\text{inter}} \) exhibits a positive peak at the Fermi energy (marked with a black arrow), which comes from the conversion of the orbital current into the spin current by the SOC of Ni. We find that it is correlated with a shoulder feature of \( \langle T^{S}_{X_C} \rangle_{\text{inter}} \) at the Fermi energy (marked with a black arrow). Such peak of \( \langle Q^{S}_{y} \rangle_{\text{inter}} \) implies that in the OT mechanism, there are two different microscopic channels for

FIG. 7. Electric response of \( S_y \) and \( S_y \) current influxes - \( \Phi[Q^{L}_{y}] \) and \( \Phi[Q^{S}_{y}] \) - and various torques - \( T^{L}_{SO}, T^{L}_{CF}, T^{S}_{SO}, \) and \( T^{S}_{X_C} \) - arising from the interband processes and accumulation, and arising from the intraband processes (divided by \( \tau \)) in Ni/W(110). Spatial profiles for (a) orbital and (b) spin quantities at the true Fermi energy \( E_F = E_F^{\text{true}} \). Fermi energy dependence for (c) orbital and (d) spin quantities, summed over the FM layers (Ni1 and Ni2). Note that the sum of the interband responses of the orbital/spin current influx and the total torque \( T^{L}_{y} = T^{S}_{SO} + T^{S}_{CF} \) and \( T^{S}_{y} = T^{S}_{SO} + T^{S}_{X_C} \) for orbital and spin, respectively) matches with the intraband response of the orbital/spin accumulation divided by \( \tau \).
the orbital-to-spin conversion: one for the spin converted from the OAM via \( (T_{SO}^{y})_{\text{inter}} \), and the other for the conversion of the orbital current into the spin current followed by the spin-transfer torque. Meanwhile, in Fig. 8(d), which corresponds to the AT mechanism, \( (\Phi Q_{z}^{x})_{\text{inter}} \) is not very pronounced, and only the peak of \( (T_{SO}^{x})_{\text{inter}} \) is observed (indicated with a black arrow). The negative sign of \( (T_{SO}^{y})_{\text{inter}} \) (positive sign of the effective spin Hall angle) is due to a positive sign of the SHE in Ni. We also find that even within the AT mechanism, the orbital-to-spin conversion via \( (T_{SC}^{y})_{\text{inter}} \) is crucial. Therefore, we conclude that in Ni/W(110) the OT and AT are the first and the second dominant mechanisms for the torque generation on the local magnetic moment.

IV. DISCUSSION

A. Classifying Mechanisms of the Current-Induced Torque

In Sec. III we found that the ST provides the dominant contribution to the current-induced torque in Fe/W(110) according to the correlation between the exchange torque and the spin current influx from W, which is reflected in the negative effective spin Hall angle [Fig. 6(a)]. In Ni/W(110), on the other hand, the OT is found to be the most dominant contribution. The evidence for the OT is provided by pronounced peaks in the spin-orbital torque and the spin current influx that suggests a positive effective spin Hall angle, associated with the exchange torque [Fig. 6(c)]. However, we also observed that the AT can be associated with the spin-orbital torque [Fig. 8(d)] because the self-induced spin accumulation in the FM results from the current-induced OAM. A crucial difference between the OT and AT is that while the OT is due to an electrical current flowing in the NM, the AT is due to an electrical current passing through the FM. In this respect, only the OT is important for memory applications where the ferromagnetic layer must be patterned to form a physically separate memory cell, whereas both OT and AT are important for applications based on magnetic textures (i.e., domain walls and Skyrmions) for which such patterning is not necessary.

Based on these findings, we propose a classification scheme for various mechanisms of the current-induced torque. We consider two independent criteria: (1) whether it is an effect due to SOC in the NM or the FM, and (2) whether it is due to electrical current flowing in the NM or in the FM. Figure 9 presents a table of the mechanisms of the current-induced torque, where the row classifies whether the SOC originates in the NM or in the FM, and the column classifies whether the nature of the torque response is nonlocal or local. We define the nonlocal and local nature of the torque as the response arising in the FM from the electrical current flowing in the NM and the torque arising in the FM from the electrical current flowing in the NM, respectively. Thus, we classify microscopic mechanisms of the current-induced torque as follows:

- **ST** (nonlocal, NM-SOC origin): Electric current flowing in the NM generates a transverse spin current via the SHE. The spin current is injected to the FM and transferred to the local magnetic moment.

- **OT** (nonlocal, FM-SOC origin): Electric current flowing in the NM generates a transverse orbital current via the SHE. The orbital current is injected into the FM and interacts with the spin in the FM via SOC. The converted spin or current generate a torque on the local magnetic moment.

- **IT** (local, NM-SOC origin): Electric current flowing in the FM scatters from the NM/FM interface. By the SOC of the NM, the interfacial scattering may alter the direction of the spin, i.e., by spin-orbit filtering or spin-orbit precession. The reflected spin exerts torque on the local magnetic moment.
FIG. 9. Classification of the mechanisms of the current-induced torque. The row represents the origin of SOC in either the NM or in the FM. The column represents the locality of the torque: i.e., whether the torque acting on the FM originates from the electrical current flowing in the NM (nonlocal) or in the FM itself (local). The red arrows represent the spin, and the blue arrows represent the OAM. The local magnetic moment is represented with a big yellow arrow.

- AT (local, FM-SOC origin): Electric current flowing in the FM induces transverse spin current via the SHE. As the inversion symmetry is broken by the NM/FM interface, spin accumulation at the top and at the bottom of the FM become asymmetric, leading to a finite torque on the local magnetic moment.

We remark that our definition of the IT is restricted rather than general. With the general definition, we neglect an effect of the current flowing in the NM in the proximity of the interface. For example, the spin Hall or orbital Hall current in the NM may be enhanced near the interface, but we include this effect into the definition of the ST or the OT, respectively. Thus, the definition of the IT agrees with the picture that spin-orbit effects in the FM originate in the proximity-induced SOC from the NM. Meanwhile, we emphasize that not only the OT but also all the other mechanisms involve an excitation of the OAM or its current, because electric response of the spin follows the orbital response via SOC. For example, we have seen that the AT contribution in Ni/W(110) is associated with a colossal spin-orbital torque [Fig. 8(d)].

Next, we attempt to disentangle each of the contributions in the current-induced torque of Fe/W(110) and Ni/W(110). For this, we apply an external electric field in the NM (8 layers of W) or in the FM (2 layers of Fe or Ni). We note that this is an approximate measure since an electric current may flow in the FM(NM) although an electric field is applied only to the NM (FM) layer, as the electronic wave functions are delocalized across the film. Meanwhile, the disentanglement of the sources of SOC is achieved not by turning on and off SOC in the NM or FM, because it modifies the electronic structure profoundly, but by performing the same calculation for an auxiliary system in which the sign of the SOC strength is opposite to the original value. For example, we rely on the property that the sign of the OT and AT should become opposite after flipping the sign of SOC in the FM. Thus, we can extract the NM-SOC contribution and FM-SOC contribution by comparing the original system with the auxiliary system. We emphasize that with this procedure, the sum of the individual contributions equals the total current-induced torque. For more details on the procedure, see Appendix G.

In Figs. 10(a) and 10(b) we show the decomposition of the total dampinglike torque in Fe/W(110) and Ni/W(110), respectively, into separate contributions. In Fe/W(110), the ST is the most dominant contribution. However, our analysis reveals that the IT is not negligible, accounting for about 35% of the ST. Overall, the ST and IT are larger than the OT and AT, implying that the SOC in W is more important than that in Fe. In Ni/W(110), the OT is the most dominant contribution. The second largest contribution is the AT, which accounts for about a half of the OT. The magnitude of the IT is not much smaller, reaching as much as 37% of the magnitude of the OT. Overall, the OT and AT are dom-
dominant over the ST and IT in Ni/W(110). This suggests that the SOC in Ni is more important than the SOC in W in this system, in contrast to an intuitive expectation that SOC in 3d FMs plays a minor role as compared to the SOC of the heavy element. These results are consistent with our analysis of the results presented in Figs. [6] and [8].

B. Experiments and Materials

Although the effective spin Hall angle measured in experiments is the sum of all contributions to the torque on the local magnetic moment, it has been assumed that it is a property of the NM in NM/FM bilayers, which can be incorrect. For example, we have shown that the current-induced torque depends on the choice of the FM in FM/W(110), where FM = Fe or Ni. In this case, it is due to an opposite sign of the OHE and SHE in W, and the resulting orbital-to-spin conversion efficiencies are different for Fe and Ni. As a result, even the sign of the effective spin Hall angle changes: from negative for Fe/W(110) to positive for Ni/W(110). We believe that such change-of-sign behavior can be directly measured in experiments. More concretely, we suggest performing a spin-orbit torque experiment on an FeNi alloy in order to observe the effective spin Hall angle change as the alloying ratio varies, with the effective spin Hall angle turning zero at a certain critical concentration. We speculate that this behavior would be observed in other systems where the OHE competes with the SHE. For example, among 5d elements, Hf, Ta, and Re exhibit gigantic OHC, whose sign is opposite to that of the SHC. Such behavior holds in general for groups 4-7 among transition metals. For 3d elements, such as Ti, V, Cr, and Mn, the SHC is much smaller than that of 5d elements, while the OHC is almost as large as in 5d elements. Thus, the OT contribution is expected to be more pronounced than the ST contribution when the nominally non-magnetic substrate is made of 3d elements, as compared to the systems where the NM is made of 5d elements. Therefore, alloying not only the FM but also the NM provides a useful knob for observing competing mechanisms of the current-induced torque.

Layer thickness dependence of the spin-orbit torque has been measured in Ta/CoFeB/MgO [63] and Hf/CoFeB/MgO [64], where the sign of the current-induced torque was found to change when the thickness of Ta or Hf was as small as \( \sim 1 - 2 \) nm. The origin of the sign change has been attributed to the competition between the bulk and interfacial mechanisms, which correspond to the ST and IT mechanisms in our terminology. Recently, such behavior has also been observed in a similar system Zr/CoFeB/MgO [65], where a much lighter 4d element Zr was used instead of a 5d element. Due to a negligible SHC of Zr as compared to the OHC, it has been proposed that the sign change occurs due to a competition between the ST and OT, instead of the competition between the ST and IT. Detailed investigation of these systems by our method may reveal the origin of the sign change.

Another widely-studied system in spintronics is a Pt-based magnetic heterostructures. Due to a large SHC of Pt [66], the ST is assumed to be the most dominant mechanism of the torque in Pt-based systems [5]. In Pt/Co, however, theoretical analysis revealed that the interfacial SOC contributes significantly to the fieldlike torque [21, 67]. On the other hand, the dampinglike torque is attributed to the ST mechanism [37, 67], which is also supported by experiments [68]. Hiroki et al. compared Pt/Ni and Pt/Fe bilayers, finding that the current-induced torque strongly depends on the choice of the FM [69]. According to their interpretation, while the bulk effect is dominant in Pt/Ni, a pronounced interface effect in Pt/Fe not only leads to fieldlike torque but also suppresses the spin current injection from Pt, which leads to a distinct FM dependence of the torque [69]. A similar conclusion has also been drawn in an experiment by Zhu et al., where the interfacial SOC has been varied by choosing different samples and annealing conditions [70]. Further investigation of the exact mechanism in these systems by theory is required.

For the study of the interplay between the spin and orbital degrees of freedom transition metal oxides (TMOs) may present a very fruitful playground. In TMOs, a strong entanglement of the spin, orbital, and charge degrees of freedom has been intensively studied in the past [71-73]. For example, magnetic properties of TMOs are heavily affected by the orbital physics not only via the effect of SOC but also because of the anisotropic exchange interactions caused by the shape of participating orbitals [71]. However, most studies on the TMOs have focused on their ground state properties, such as various competing magnetic phases. We expect that the investigation of the spin-orbital entangled dynamics would provide crucial insights into understanding the complex physics of TMOs.

V. CONCLUSION

Motivated by various proposed mechanisms of the current-induced torques, which are challenging to disentangle both theoretically and experimentally, we developed a theory of current-induced spin-orbital coupled dynamics in magnetic heterostructures, which tracks the transfer of the angular momentum between different degrees of freedom in solids: spin and orbital of the electron, lattice, and local magnetic moment. By adopting the continuity equations for the orbital and spin
angular momentum [Eq. (7)], we derive equations for the angular momentum dynamics in the steady state reached when an external electric field is applied, which provide relations between interband and intraband contributions to the current influx, torques, and accumulation of the spin and orbital angular momentum [Eqs. (37) and (38)].

This formalism is particularly useful for the detailed study of the microscopic mechanisms of the current-induced torque and we used its first principles implementation to investigate the spin-orbit torque origins in Fe/W(110) and Ni/W(110) bilayers. In Fe/W(110), we observe a strong correlation between the spin current influx and the exchange torque, which is a key characteristic of the ST mechanism. On the other hand, such correlation is not observed in Ni/W(110). Instead, we observe a pronounced correlation between the exchange torque and the spin-orbital torque, indicating the transfer of angular momentum from the orbital to the spin channel. Moreover, the spin current influx exhibits a sign opposite to that of the SHE in W. This leads us to a conclusion that the OT is dominant in Ni/W(110).

We further propose a classification scheme of the different mechanisms of current-induced torque based on the criteria of whether the scattering source is in the NM-SOC or the FM-SOC, and whether the torque response is of local or nonlocal nature (Fig. 2). This analysis also confirms that the ST and OT are the most dominant mechanisms in Fe/W(110) and Ni/W(110), respectively. However, we also find that the other contributions, IT and AT, are not negligible as well. Our formalism enables an analysis of the angular momentum transport and transfer dynamics in detail, which clearly goes beyond the “spin current picture”. Since it treats the spin and orbital degrees of freedom on an equal footing, it is ideal for systematically studying the spin-orbital coupled dynamics in complex magnetic heterostructures.

ACKNOWLEDGMENTS

D.G. thanks insightful comments from discussions with Gustav Bihlmayer, Mathias Kläui, OukJae Lee, Kyung-Whan Kim, and Daegan Jeo. K.-J. L., J.-P. H., and Y. M. acknowledge discussions with Mark Stiles. J.-P. H., and Y. M. additionally acknowledge discussions with Jairo Sinova. We gratefully acknowledge the Jülich Supercomputing Centre for providing computational resources under project jiff40.

D.G. and H.-W. Lee were supported by SSTF (Grant No.BA-1501-07). We also acknowledge funding under SPP 2137 “Skyrmionics” (project MO 1731/7-1) and TRR 173 – 268565370 (project A11) of the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation).

Appendix A: Interband-Intraband Correspondence

Here we provide a proof of Eq. (35). From Eqs. (29), (30), and (33), the left hand side of Eq. (35) is written as

$$\frac{1}{\tau} \left\langle O \right\rangle_{\text{intra}}^{\text{inter}} = -\frac{e\hbar}{\tau} \sum_{n,k} \left[ \partial_{k_x} f_{nk} \langle u_{nk} | O(k) | u_{nk} \rangle \right]$$

$$+ f_{nk} \langle u_{nk} | \partial_{k_x} O(k) | u_{nk} \rangle .$$

where we used

$$\frac{\partial f_{nk}}{\partial k_x} = \frac{\partial f_{nk}}{\partial E_{nk}} \frac{\partial E_{nk}}{\partial k_x} = f'_{nk} \frac{\hbar}{\tau} \langle u_{nk} | v_x(k) | u_{nk} \rangle .$$

Application of integration by parts to the first term in Eq. (A1) leads to

$$\frac{1}{\tau} \left\langle O \right\rangle_{\text{intra}}^{\text{inter}} = \frac{e\hbar}{\tau} \sum_{n,k} \sum_{m \neq m} (f_{nk} - f_{mk})$$

$$\times \left\langle \partial_{k_x} u_{nk} | u_{mk} \right\rangle \left\langle u_{mk} | O(k) | u_{mk} \right\rangle .$$

It can be rewritten as

$$\frac{1}{\tau} \left\langle O \right\rangle_{\text{intra}}^{\text{inter}} = \frac{e\hbar}{\tau} \sum_{n,k} \sum_{m \neq m} (f_{nk} - f_{mk})$$

$$\times \left\langle \partial_{k_x} u_{nk} | u_{mk} \right\rangle \left\langle u_{mk} | O(k) | u_{mk} \right\rangle .$$

By using identities

$$\left\langle \partial_{k_x} u_{nk} | u_{mk} \right\rangle = \frac{\hbar}{E_{nk} - E_{mk}} \left\langle u_{nk} | v_x(k) | u_{mk} \right\rangle .$$

and

$$\left\langle u_{mk} | O(k) | u_{mk} \right\rangle = \frac{i\hbar}{E_{nk} - E_{mk}} \left\langle u_{mk} | (1/\hbar) O(k) H(k) | u_{mk} \right\rangle ,$$

for $n \neq m$, we have

$$\frac{1}{\tau} \left\langle O \right\rangle_{\text{intra}}^{\text{inter}} = \frac{e\hbar}{\tau} \sum_{n,k} \sum_{m} (f_{nk} - f_{mk}) \mathrm{Im} \left[ \left\langle u_{nk} | v_x(k) | u_{mk} \right\rangle \left\langle u_{mk} | (1/\hbar) O(k) H(k) | u_{mk} \right\rangle \right]$$

$$\times \left( E_{nk} - E_{mk} \right)^2$$

$$\times \left( E_{nk} - E_{mk} + i\eta \right)^2$$

$$\times \left( E_{nk} - E_{mk} + i\eta \right)^2$$

$$\times \left( E_{nk} - E_{mk} + i\eta \right)^2$$

$$\times \left( E_{nk} - E_{mk} + i\eta \right)^2$$

$$\times \left( E_{nk} - E_{mk} + i\eta \right)^2$$

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$$\times \left( E_{nk} - E_{mk} + i\eta \right)^2$$

$$\times \left( E_{nk} - E_{mk} + i\eta \right)^2$$

$$\times \left( E_{nk} - E_{mk} + i\eta \right)^2.$$
This proves Eq. \([35]\).

\[
\left\langle \frac{d\mathcal{O}}{dt} \right\rangle_{\text{intra}} = -\frac{e\mathcal{E}_x T}{i\hbar^2} \sum_{nk} \partial_{k_x} \langle u_{nk}|[\mathcal{O}(\mathbf{k}), \mathcal{H}(\mathbf{k})]|u_{nk}\rangle.
\]

Because

\[
\langle u_{nk}|[\mathcal{O}(\mathbf{k}), \mathcal{H}(\mathbf{k})]|u_{nk}\rangle = 0 \tag{B2}
\]

for any Hermitian operator \(\mathcal{O}\), we have

\[
\left\langle \frac{d\mathcal{O}}{dt} \right\rangle_{\text{intra}} = 0. \tag{B3}
\]

**Appendix C: Computational Method**

First-principles calculation consists of three steps. The first step is calculation of the electronic structure from the DFT. In this step, we obtain Bloch states and their energy eigenvalues. The second step is to obtain maximally-localized Wannier functions (MLWFs) starting from the Bloch states obtained in the first step. Once the MLWFs are found, matrix elements of all relevant operators (Hamiltonian, position, spin, and orbital) are expressed within the basis set of the MLWFs. Thus, a tight-binding model is obtained. The last step is evaluation of the interband and intraband responses of the individual terms in the equations of motion [Eqs. \([37]\) and \([38]\)] by solving the tight-binding model obtained from the second step.

The electronic structure of FM/W(110) (FM=Fe or Ni), whose lattice structure is shown in Fig. 3, is calculated self-consistently in the film mode of the full-potential linearized augmented plane wave method [74] from the code FLEUR [75]. We use Perdew-Burke-Ernzerhof exchange-correlation functional within the generalized gradient approximation [76]. Muffin-tin radii of the FM and W atoms are set to 2.1\(a_0\) and 2.5\(a_0\), respectively, where \(a_0\) is the Bohr radius. The plane wave cutoff is set to 3.8\(a_0^{-1}\). The Monkhorst-Pack \(k\)-mesh of 24 \times 24 are sampled from the first Brillouin zone. The SOC is treated self-consistently within the second variation scheme. The layer distances \(d_{\text{FM-FM}}\) and \(d_{\text{W-FM}}\) are optimized such that the total energy is minimized. The optimized values for Fe/W(110) are \(d_{\text{Fe-Fe}} = 1.744\ \text{Å}\) and \(d_{\text{W-Fe}} = 2.024\ \text{Å}\), and those for Ni/W(110) are \(d_{\text{Ni-Ni}} = 1.747\ \text{Å}\) and \(d_{\text{W-Ni}} = 1.909\ \text{Å}\).

In order to obtain MLWFs, we initially project the Bloch states onto \(d_{xy}\), \(d_{xz}\), \(d_{yz}\), and \(s_p d_2\) trial orbitals for each atom, and minimize their spreads using the code WANNIER90 [77]. We obtain in total 180 MLWFs out of 360 Bloch states, that is, 18 MLWFs for each atom. For the disentanglement of the inner and outer spaces, we set the frozen window as 2 eV above the Fermi energy. The Hamiltonian, position, spin, and orbital operators, which are evaluated beforehand within the Bloch basis, are then transformed to the basis of MLWFs, and the tight-binding model is obtained.

**Appendix B: Stationary Condition of the Intraband Contribution**

For a proof of Eq. \([36]\), we apply Eq. \([33b]\) to \(d\mathcal{O}/dt\):

\[
\forall z \in \{\text{FM}\}, \quad v_x^z = \sum_{z'\in\text{FM}} P_{z'z} v_{x}^{z'}, \tag{C1a}
\]

\[
\forall z \in \{\text{W}\}, \quad v_x^z = \sum_{z'\in\text{W}} P_{z'z} v_{x}^{z'}, \tag{C1b}
\]

where \(P_{z'}\) is the projection onto the MLWFs located in a layer whose index is \(z\). We confirm that the 18 MLWFs are well localized in each layer. Note that Eq. \([C1]\) is defined such that

\[
v_x = v_x^\text{FM} + v_x^\text{W}. \tag{C2}
\]

**Appendix D: Symmetry Analysis**

In Sec. \([IIIc]\) we state that only \(y\) and \(x\) components are nonzero in Eqs. \([37]\) and \([38]\), respectively. Here, we prove this by symmetry argument. Two important symmetries present in FM/W(110), where the magnetization is pointing the \(z\) direction, are \(T\) and \(M_y\) symmetries. Here, \(\mathcal{T}\) is the time-reversal operator and \(M_y(y)(z)\) is the mirror reflection operator along the direction of \(x(y)\). Since all the terms appearing in the same equation should transform in the same way, we consider only the response of a torque operator

\[
T^J = \frac{dJ}{dt} \tag{D1}
\]

for a general angular momentum operator \(J\), which can be either orbital and spin origin. To find symmetry constraints on the interband [Eq. \([26]\)] and intraband [Eq. \([33b]\)] responses, we first investigate how matrix elements of \(v_x\) and \(T^J\) transform. We define \(U_T\) and \(U_{M_y(y)}\) as Hilbert space representations of \(T\) and \(M_{x(y)}\), respectively. Note that \(T\) transforms \(v_x\) and \(T^J\) as

\[
U_T^{-1} v_x U_T = -v_x, \tag{D2}
\]
and
\[ U^{-1}_T T^J U_T = + T^J, \] (D3)
respectively. On the other hand, \( \mathcal{M}_x \) and \( \mathcal{M}_y \) symmetries transform \( v_x \) and \( T^J \) as
\[ U^{-1}_{\mathcal{M}_x} v_x U_{\mathcal{M}_x} = - v_x, \] (D4a)
\[ U^{-1}_{\mathcal{M}_y} v_x U_{\mathcal{M}_y} = + v_x, \] (D4b)
and
\[ U^{-1}_{\mathcal{M}_x} T^J_x U_{\mathcal{M}_x} = + T^J_x, \] (D5a)
\[ U^{-1}_{\mathcal{M}_x} T^J_y U_{\mathcal{M}_x} = - T^J_y, \] (D5b)
\[ U^{-1}_{\mathcal{M}_x} T^J_z U_{\mathcal{M}_x} = - T^J_z, \] (D5c)
\[ U^{-1}_{\mathcal{M}_y} T^J_x U_{\mathcal{M}_y} = - T^J_x, \] (D5d)
\[ U^{-1}_{\mathcal{M}_y} T^J_y U_{\mathcal{M}_y} = + T^J_y, \] (D5e)
\[ U^{-1}_{\mathcal{M}_y} T^J_z U_{\mathcal{M}_y} = - T^J_z. \] (D5f)

As a result, \( \mathcal{T}_M \) and \( \mathcal{M}_y \) symmetries transform \( v_x \) and \( T^J \) as
\[ U^{-1}_{\mathcal{T}_M} v_x U_{\mathcal{T}_M} = + v_x, \] (D6a)
\[ U^{-1}_{\mathcal{T}_M} v_x U_{\mathcal{T}_M} = - v_x, \] (D6b)
and
\[ U^{-1}_{\mathcal{T}_M} T^J_x U_{\mathcal{T}_M} = + T^J_x, \] (D7a)
\[ U^{-1}_{\mathcal{T}_M} T^J_y U_{\mathcal{T}_M} = - T^J_y, \] (D7b)
\[ U^{-1}_{\mathcal{T}_M} T^J_z U_{\mathcal{T}_M} = - T^J_z, \] (D7c)
\[ U^{-1}_{\mathcal{T}_M} T^J_x U_{\mathcal{T}_M} = - T^J_x, \] (D7d)
\[ U^{-1}_{\mathcal{T}_M} T^J_y U_{\mathcal{T}_M} = + T^J_y, \] (D7e)
\[ U^{-1}_{\mathcal{T}_M} T^J_z U_{\mathcal{T}_M} = - T^J_z. \] (D7f)

where \( U_{\mathcal{T}M_x(y)} = U_T U_{\mathcal{M}_x(y)} \). Note that \( \mathcal{T} \) and \( \mathcal{M}_x(y) \) commute each other.

We remark that \( U_T \) and \( U_{\mathcal{M}_x(y)} \) are anti-unitary and unitary operators, respectively. Thus, \( U_{\mathcal{T}M_x(y)} \) is anti-unitary. For an arbitrary anti-unitary operator \( \Theta \), a matrix element of an operator \( \mathcal{O} \) satisfies
\[ \langle \Theta \phi | \mathcal{O} | \psi \rangle = \langle \phi | (\Theta^{-1} \mathcal{O} \Theta) | \psi \rangle^*. \] (D8)

Thus, combining this result with Eqs. (D6) and (D7) provides constraints on the interband [Eq. (26)] and intraband [Eq. (33b)] contributions.

As an illustration, let us demonstrate that both interband and intraband contributions vanishes for \( T^J \). We consider \( \mathcal{T}_M \) symmetry at first. By this, matrix elements of \( v_x \) and \( T^J \) transform as
\[ \langle U_{\mathcal{T}_M} \psi_{mk} | v_x | U_{\mathcal{T}_M} \psi_{mk} \rangle = \langle \psi_{mk} | v_x | \psi_{mk} \rangle, \] (D9)
and
\[ \langle U_{\mathcal{T}_M} \psi_{mk} | T^J | U_{\mathcal{T}_M} \psi_{mk} \rangle = - \langle \psi_{mk} | T^J | \psi_{mk} \rangle, \] (D10)
where \( k' = (+k_x, -k_y, -k_z) \). On the other hand, \( \mathcal{M}_y \) symmetry gives
\[ \langle U_{\mathcal{M}_y} \psi_{mk} | v_x | U_{\mathcal{M}_y} \psi_{mk} \rangle = - \langle \psi_{mk} | v_x | \psi_{mk} \rangle, \] (D11)
and
\[ \langle U_{\mathcal{M}_y} \psi_{mk} | T^J | U_{\mathcal{M}_y} \psi_{mk} \rangle = - \langle \psi_{mk} | T^J | \psi_{mk} \rangle, \] (D12)
where \( k'' = (-k_x, +k_y, -k_z) \).

A constraint for the interband contribution for \( T^J \) [Eq. (26)] is given by \( \mathcal{T}_M \) symmetry:

\[
\langle T^J \rangle_{\text{inter}} = e \hbar E_x \sum_{n \neq m} \sum_k (f_{nk'} - f_{mk'}) \text{Im} \left[ \frac{\langle U_{\mathcal{T}_M} \psi_{nk} | T^J | U_{\mathcal{T}_M} \psi_{mk} \rangle \langle U_{\mathcal{T}_M} \psi_{mk} | v_x | U_{\mathcal{T}_M} \psi_{nk} \rangle}{(E_{nk'} - E_{mk'} + i\eta)^2} \right] \] (D13a)
\[
eq e \hbar E_x \sum_{n \neq m} \sum_k (f_{nk'} - f_{mk'}) \text{Im} \left[ \frac{\langle \psi_{mk'} | T^J | \psi_{nk'} \rangle \langle \psi_{nk'} | v_x | \psi_{mk'} \rangle}{(E_{nk'} - E_{mk'} + i\eta)^2} \right] \] (D13b)
\[
eq e \hbar E_x \sum_{n \neq m} \sum_k (f_{mk} - f_{nk}) \text{Im} \left[ \frac{\langle \psi_{nk} | T^J | \psi_{mk} \rangle \langle \psi_{mk} | v_x | \psi_{nk} \rangle}{(E_{mk} - E_{nk} + i\eta)^2} \right] \] (D13c)
\[= - \langle T^J \rangle_{\text{inter}} \] (D13d)

in the limit \( \eta \to 0^+ \). Thus, \( \langle T^J \rangle_{\text{inter}} \) is forbidden by \( \mathcal{T}_M \) symmetry. In Eq. (D13a), we used the fact that the linear response can also be written in terms of the transformed states.

Note that we use the Bloch state representation instead of their periodic parts. For the intraband contribution, we have the following constraint by \( \mathcal{T}_M \) symmetry:
small in general, only near the true Fermi energy it is sup-
torque. Although the spin-orbital torque is not particularly
dependence plots in Fig. 11 also show the cancellation behaviors
and quenching of the orbital moment. Fermi energy depen-
dence to small spin-orbit correlation in Fe [Fig. 3(c)]
Therefore, both interband and intraband responses for $T_{J_z}$
vanishes by the symmetries. By the procedure for different
components of the torque, we arrive at the conclusion that
the presence of $\mathcal{T}_{M_x}$ and $\mathcal{T}_{M_y}$ symmetries allows only
$\langle T_{J_z} \rangle_{\text{inter}}$ and $\langle T_{J_z} \rangle_{\text{intra}}$ to be nonzero.

**Appendix E: Intraband Response**

In Fig. [11] intraband contributions appearing in Eq. (38)
are plotted for each layer of Fe/W(110). We confirm that the
sum of the current influx and torques vanishes for the intra-
band contributions, respectively for the orbital and spin, which
confirms Eq. (38). For the orbital [Fig. [11](a)], we find that
$\langle \Phi(Q_z^L) \rangle_{\text{intra}}$ tends to cancel with $\langle T_{L_{CF}} \rangle_{\text{intra}}$
and $\langle T_{SO} \rangle_{\text{intra}}$ is small. Meanwhile, for the spin, not only
$\langle \Phi(Q_z^S) \rangle_{\text{intra}}$ and $\langle T_{XC} \rangle_{\text{intra}}$ but also $\langle T_{SO} \rangle_{\text{intra}}$ are of comparable magnitudes, which is distinct from the interband response [Fig.
3(b)]. However, near the Fe layers, $\langle T_{SO} \rangle_{\text{intra}}$ is small, and
$\langle T_{SO} \rangle_{\text{intra}}$ tends to cancel with $\langle \Phi(Q_z^S) \rangle_{\text{intra}}$. We attribute
this behavior to small spin-orbit correlation in Fe [Fig. 3(c)],
and quenching of the orbital moment. Fermi energy dependence
plots in Fig. [11] also show the cancellation behaviors
between the orbital current influx and crystal field torque,
and between the spin current influx and the exchange
torque. Although the spin-orbital torque is not particularly
small in general, only near the true Fermi energy it is sup-
pressed. Therefore, the FLT originates in the spin current
injection (ST mechanism).

In Ni/W(110), for the orbital, $\langle \Phi(Q_z^E) \rangle_{\text{intra}}$ and $\langle T_{CF} \rangle_{\text{intra}}$
cancel each other, with small magnitude of $\langle T_{SO} \rangle_{\text{intra}}$ [Fig.
12(a)]. For the spin, on the other hand, as well as
$\langle \Phi(Q_z^L) \rangle_{\text{intra}}$, $\langle T_{SO} \rangle_{\text{intra}}$ contributes to $\langle T_{XC} \rangle_{\text{intra}}$, in compara-
ble magnitudes [Fig. 12(b)]. This is due to pronounced
spin-orbit correlation of Ni at the Fermi energy [Fig. 3(d)].
The Fermi energy dependence plots in Figs. 12(c) and 12(d)
also show that the spin-orbital torque is nonnegligible at the
Fermi energy. Therefore, in Ni/W(110), the FLT is a com-
bined effect of the spin injection and the SOC. Such behavior
has also been observed in Pt/Co [67].

To clarify microscopic mechanisms of different origins, we
disentangle the FLT into the ST, OT, IT, and IT, analogously
to Fig. [10] For Fe/W(110) [Fig. [13](a)], we find that the ST
is the most dominant contribution, as expected. On the other
hand, for Ni/W(110) [Fig. [13](b)], not only the ST but also the
AT significantly contributes. This is due to pronounced spin-
orbit correlation in Ni. Meanwhile, we also find that the IT is
not negligible.
FIG. 12. Electric response of current influxes \(-\Phi[Q^L_y]\) and \(\Phi[Q^S_y]\) and various torques \(-T^L_y, T^L_y, T^L_{SO},\) and \(T^{SO}_{XC}\) arising from the intraband process in Ni/W(110). Spatial profiles for (a) the orbital and (b) the spin at true Fermi energy \(E_F = E_F^{true}\). Fermi energy dependences for (c) the orbital and (d) the spin, which are summed over the FM layers (Ni1 and Ni2).

Appendix F: Tight-binding Representation of the Continuity Equation

Here, we derive a tight-binding representation of the current influx and torque appearing in the continuity equation \([\text{Eq. (7)}]\). To do this, we first define \(P_z\) as a projection operator onto a set of MLWFs located near a layer whose index is \(z\). Then, for the spin operator \(S\), we define

\[
S(z) = \frac{1}{2} [SP_z + P_zS] \quad \text{(F1)}
\]

as the spin operator at \(z\), such that

\[
S = \sum_z S(z). \quad \text{(F2)}
\]

The Heisenberg equation of motion for \(S(z)\) is written as

\[
\frac{dS(z)}{dt} = \frac{i}{\hbar} [S(z), \mathcal{H}] \quad \text{(F3a)}
\]

\[
= \frac{1}{2i\hbar} [SP_z, P_zS, \mathcal{H}] \quad \text{(F3b)}
\]

\[
= \frac{1}{2i\hbar} \{ [S, \mathcal{H}]P_z + S[P_z, \mathcal{H}] \}
\]

\[
+ [P_z, \mathcal{H}]S + P_z[S, \mathcal{H}] \}
\]

\[
= T^S(z) + \Phi[j^S](z). \quad \text{(F3c)}
\]

We define local torque operator at \(z\) by

\[
T^S(z) = \frac{1}{2i\hbar} [SP_z + P_zS], \quad \text{(F4a)}
\]

\[
= \frac{1}{2} [T^SP_z + P_zT^S], \quad \text{(F4b)}
\]

where

\[
T^S = \frac{1}{i\hbar} [S, \mathcal{H}] \quad \text{(F5)}
\]

is the total torque operator, and we define

\[
\Phi[j^S](z) = \frac{1}{2i\hbar} \left\{ [P_z, \mathcal{H}]S + S[P_z, \mathcal{H}] \right\} \quad \text{(F6)}
\]

the spin current influx at \(z\).

Although \(\Phi[j^S](z)\) may not seem intuitive, it corresponds to an usual definition of the spin current influx. To demonstrate this point, we consider the case where \(P = \langle r | r \rangle\) and \(\mathcal{H} = -\hbar^2 \nabla^2 / 2m\), where \(\langle r |\) is an eigenket for the position operator \(r\). Then \(\Phi[j^S]\) becomes

\[
\Phi[j^S] = \frac{1}{2i\hbar} \left\{ [r | r \rangle \langle r | \mathcal{H}S - H | r \rangle \langle S | r \rangle + S | r \rangle \langle r | \mathcal{H} - S \mathcal{H} | r \rangle \langle r | \right\}. \quad \text{(F7)}
\]

FIG. 13. Disentanglement of the FLT into the ST, OT, IT, and AT, for dampinglike component in (a) Fe/W(11) and (b) Ni/W(110). In both systems, the ST is most dominant mechanism. We note that the AT is not negligible in Ni/W(110).
Thus, a matrix element between states $\phi$ and $\psi$ is written as

$$
\langle \phi | \Phi [j^S] | \psi \rangle = \frac{i\hbar}{2m} \left\{ \phi^*(r) S [\nabla_r^2 \psi(r)] - [\nabla_r^2 \phi^*(r)] S \psi(r) \right\} \quad (F8a)
$$

$$
= -\nabla_r \cdot (\langle \phi | j^S | \psi \rangle) \quad (F8b)
$$

where

$$
\langle \phi | j^S | \psi \rangle = -\frac{i\hbar}{2m} \left\{ \phi^*(r) S [\nabla_r \psi(r)] + [\nabla_r \phi^*(r)] S \psi(r) \right\}.
$$

(F9)

From Eq. (F9), we find that this is consistent with usual definition of the spin current $j^S = S \otimes (p/m)$. Therefore, Eq. (F6) can be understood as an operator of the spin current influx to the subspace defined by the projection $P_z$.

### Appendix G: Disentangling Different Contributions of the Current-Induced Torque

To disentangle different contributions of the torque (Figs. 10 and 13), we utilize a property that upon changing the sign of the SOC constant the OT and AT flip their signs while the signs of the ST and IT remain invariant. That is, the total exchange torque is decomposed as the sum of the NM-SOCs and FM-SOC contributions

$$
\langle T_{XC}^S \rangle_{tot} = \langle T_{XC}^S \rangle_{NM} + \langle T_{XC}^S \rangle_{FM}.
$$

(G1)

In an auxiliary system where the sign of the SOC is flipped in the FM atoms, the exchange torque becomes

$$
\langle T_{XC}^S \rangle_{aux} = \langle T_{XC}^S \rangle_{NM} - \langle T_{XC}^S \rangle_{FM}.
$$

(G2)

Thus, the NM-SOC contribution is written as

$$
\langle T_{XC}^S \rangle_{NM} = \frac{1}{2} \left[ \langle T_{XC}^S \rangle_{tot} + \langle T_{XC}^S \rangle_{aux} \right],
$$

(G3)

and the FM-SOC contribution is written as

$$
\langle T_{XC}^S \rangle_{FM} = \frac{1}{2} \left[ \langle T_{XC}^S \rangle_{tot} - \langle T_{XC}^S \rangle_{aux} \right].
$$

(G4)

Then, by applying the electric field only in the NM or FM layers by Eq. (C1), we can separately evaluate the ST, OT, AT, and IT.
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