The presence of large spin-orbit interaction at transition metal interfaces enables the emergence of a variety of fascinating phenomena that have been at the forefront of spintronics research in the past ten years. The objective of the present Chapter is to offer a review of these various effects from a theoretical perspective, with a particular focus on spin transport, chiral magnetism and their interplay. After a brief description of the orbital hybridization scheme at transition metal interfaces, we address the impact of spin-orbit coupling on the interfacial magnetic configuration, through the celebrated Dzyaloshinskii-Moriya interaction. We then discuss the physics of spin transport and subsequent torques occurring at these interfaces. We particularly address the spin Hall, spin swapping and inverse spin galvanic effects. Finally, the interplay between flowing charges and chiral magnetic textures as well as their induced dynamics are presented. We conclude this chapter by proposing some perspectives on promising research directions.

Keywords: Spin-Orbit Coupling, Spin Transfer Torque, Spin Hall Effect, Rashba effect, Dzyaloshinskii-Moriya interaction, Skyrmions
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1. Introduction

Spin-orbit coupling lies at the core of condensed matter. It is central to magnetism and spintronics, where it drives magnetic anisotropy [1], spin relaxation [2], magnetic damping [3], anisotropic magnetoresistance [4] and anomalous Hall effect [5]. Quite surprisingly, in spite of its already long history, this fundamental interaction has been pivotal to several revolutions in the past ten years. As a matter of fact, all the effects mentioned above exist in systems where inversion symmetry is preserved. But when inversion symmetry is broken, such as in certain classes of magnetic crystals or at interfaces, spin-orbit coupling triggers a number of fascinating phenomena such as antisymmetric magnetic exchange giving rise to topologically non-trivial magnetic textures, spin-momentum locking, spin-orbit torques, chiral magnetic damping etc. This broad area of research is called spin-orbitronics [6, 7].

Because of the coexistence of strong spin-orbit coupling and magnetism, transition metals have occupied a prominent position in the development of spin-orbitronics. The interplay between current-driven spin-orbit torques and chiral magnetic texture at transition metal interfaces has resulted in very fast current-driven magnetization reversal [8, 9, 10], ultrafast domain wall propagation [11, 12] and current-driven skyrmion motion [13, 14, 15, 16]. Ensuring a good control of these properties requires a fine understanding of the orbital hybridization occurring at the interface, as well as an accurate description of the various mechanisms at stake.

In this Chapter, we discuss the theoretical aspects of spin transport and magnetism at transition metal interfaces. Section 2 reviews the magnetism of bulk transition metals and transition metal interfaces and discuss the nature of the interfacial orbital hybridization in these systems. Section 3 addresses the microscopic origin of Dzyaloshinskii-Moriya interaction. Section 4 discusses the physics of spin-orbit torques, with a particular emphasis on spin Hall effect and inverse spin galvanic effect. Section 5 presents recent advances on the description of chiral magnets dynamics, and finally conclusions are given in Section 6.
2. Transition Metal Interfaces

2.1. The transition metal series

Transition metals occupy the central region of Mendeleev’s table, extending along three series from Sc $3d^14s^2$ to Cu $3d^{10}4s^1$ and Zn $3d^{10}4s^2$ ($3d$ series), from Y $4d^15s^2$ to Ag $4d^{10}5s^1$ and Cd $4d^{10}5s^2$ ($4d$ series), and from La $5d^16s^2$ to Au $5d^{10}6s^1$ and Hg $4d^{10}5s^2$ ($5d$ series). Because of the proximity in energy of the $(1-n)d$ and $ns$ shells, they display multiple oxidation states that make their chemistry particularly interesting, leading to a wide variety of transition metal oxides and organometallic compounds. While $M^{2+}$ and $M^{3+}$ oxidation states are quite common in the $3d$ series, higher oxidation states are more usual in the $4d$ and $5d$ series.

While magnetism in isolated transition metal ions is governed by Hund’s rules, the magnetic properties of bulk transition metals is determined by band magnetism and Stoner criterion [18]. In a nutshell, Stoner criterion states that magnetism emerges as a compromise between kinetic energy and exchange interaction. The criterion reads $In(\epsilon_F) > 1$, where $I$ is Stoner exchange parameter and $n(\epsilon_F)$ is the density of states at Fermi energy. To understand how bulk magnetism develops in transition metals, it is instructive to inspect the behavior of the density of states of their $d$ orbitals. As a simple rule of thumb, on the one hand, throughout one given series, the $d$-orbital becomes more localized as the electron number increases ($n4d^1\rightarrow n4d^{10}$) and correspondingly, the bandwidth...
decreases with the electron filling. On the other hand, upon increasing the series index \((3d^n \rightarrow 5d^n)\) the orbital gets more delocalized and as such more sensitive to the crystal field, resulting in \(d\)-orbital splitting and bandwidth broadening. This behavior is nicely represented by the evolution of the nearest neighbor hopping energies, as reported in Ref. [17] and collected in Fig. 1(a). It is clear that nearest neighbor hopping increases systematically from one series to another, \(t_{3d} > t_{4d} > t_{5d}\), but decreases when increasing the orbital filling within one given series. Of course this rule is simply qualitative, as the bandwidth also depends on the coordination number (it is larger for fcc than for bcc crystals for instance) and is influenced by \(spd\) hybridization as well [18]. Fig. 1(b) shows the behavior of Fermi level throughout the three series, where the maximum is obtained around half-filling of the \(d\) bands.

Figure 2: (a) Stoner exchange, (b) Stoner criterion and (c) spin-orbit coupling energy, as parametrized in Ref. [17]. As expected, Co, Fe and Ni are the only three elements fulfilling Stoner criterion in the bulk.

The systematic increase of the hopping parameters when increasing the shell index has a direct consequence in terms of magnetism. Indeed, the exchange integral \(I\) is an intra-atomic interaction, and it should scale with the localization of the orbital considered. Hence, one would expect \(I_{3d} > I_{4d} > I_{5d}\), as demonstrated in Fig. 2(a). Furthermore, since the density of states is roughly inversely proportional to the bandwidth, one expects \(n_{3d}(\epsilon_F) > n_{4d}(\epsilon_F) > n_{5d}(\epsilon_F)\) and naturally, \(3d\) elements are more likely to be magnetic than any other \(4d\) and \(5d\) elements. The calculated Stoner criterion for transition metals is reported in Fig. 2(b) and one can see that the criterion is in fact only satisfied for Fe, Ni and Co. Other \(3d\) elements such as Mn, Cr or V are not too far from fulfilling the Stoner criterion and indeed show enhanced susceptibility to magnetism. For instance, Mn and Cr (as well as \(\gamma\)-Fe) display antiferromagnetism. A phenomenological estimation can be obtained based on Bethe-Slater argument stating that antiferromagnetism occurs upon reducing the inter-atomic distance. This picture
is supported by \textit{ab initio} calculation on 3d monolayers deposited on 4d and 5d substrates \cite{19}.

Interestingly, Rh, Pd, and Pt are fairly close to fulfilling the Stoner criterion so that a slight modification of their environment (say, reduction of coordination number due to the presence of an interface) can lead to the onset of magnetism, as discussed below. Finally, of most importance for our topic, the atomic spin-orbit coupling also dramatically depends on the transition metal series, see Fig. 2(c). Indeed, the spin-orbit coupling parameter increases with $Z$, such that 5d transition metals possess a much larger spin-orbit coupling than their 4d and 3d counterparts. Combined with their high sensitivity to magnetism, this property makes 4d and 5d interfaces quite appealing for spin-orbitronics.

2.2. Magnetic properties of transition metal interfaces

At surfaces and interfaces, the coordination number reduces resulting in bandwidth narrowing for the out-of-plane orbitals [compare, for instance, the Co density of states reported on Fig. 4(a) and Fig. 4(c)]. As a result, the density of states at Fermi energy increases, which enhances Stoner criterion \cite{18}. When two transition metal surfaces are put in contact, the interfacial orbital overlap also modifies further the $d$-orbital bandwidth leading to significant change in the magnetic properties of the interface (see below).

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{figure3.png}
\caption{Schematic evolution of the $d$-orbital density of states upon increasing the orbital occupation for selected 3d and 5d monolayers. The energy position of the 3d orbitals are mostly governed by Hund’s rule, leading to a maximum spin-splitting for Mn elements and reduced spin-splitting at the two edges of the series, V and Ni. On the other hand, since 5d orbitals are much broader and governed by crystal field splitting, they do not show any splitting and are simply pushed below the Fermi level upon increasing the orbital occupation.}
\end{figure}

To better understand the orbital hybridization taking place at transition metal interfaces, let us consider the evolution of the energy position of the

\[ 6 \]
density of states of selected 3d and 5d monolayers, as illustrated on Fig. 3. Because of their large bandwidth, 4d and 5d elements do not show exchange splitting as expected and increasing the electronic filling pushes the density of states below the Fermi energy. As a results, Ag and Au display a d-orbital density of states located below Fermi energy. In contrast, 3d monolayers show a slightly different behavior. The density of states is also pushed down through Fermi level when increasing the number of electrons, but at the same time its exchange splitting also depends on orbital filling. When increasing the number of electrons from V to Mn, the exchange splitting increases while it decreases when going from Mn to Ni. This behavior can be understood following Hund’s third rule that governs magnetism in isolated ions [20, 21]: Mn ion has a high spin configuration with 5 unpaired electrons, while Ni and V ions have a low spin configuration. The consequence is that V and Ni, on both sides of the 3d series show a weak spin splitting while a large amount on one spin species is present at the Fermi level. In contrast, Mn has a large spin splitting but Fermi energy lies in-between the two spin species, leading to a reduced amount of 3d electrons at Fermi level.

Figure 4: Density of states of (a) bulk fcc Co, (b) Co overlayer and topmost Pt layer in Co/Pt(111) interface, and (c) Co overlayer and topmost Au layer in Co/Au(111) interface. The interfaces consist in one monolayer of Co deposited on six layers of Pt or Au. From Ref. [22].

Let us now consider the interface between 3d and 4(5)d layers. Because of the different in energy position of the 3d and 4(5)d states, different material combinations give rise to different hybridization schemes, as illustrated in Fig. 4. For instance, since the d-orbitals of Cu, Au and Ag are located far below Fermi level, they do not (or only very weakly) hybridize with the d-orbitals of the 3d elements deposited on top [Fig. 4(c)]. In contrast, other elements such as Pt or W possess a large density of states and are likely to hybridize strongly with the 3d overlayer [Fig. 4(b)]. Nonetheless, such hybridization depends on the 3d metal: it is stronger for elements at the edges of the 3d series (V, Ni), than for the ones in the center (Mn). The latter have much less 3d states available at Fermi energy due to the large exchange splitting, see Fig. 3.

An interesting consequence is that upon such an orbital hybridization, (i) the 4(5)d substrate becomes magnetized by proximity effect [23, 24, 25, 26], while
Figure 5: (Color online) Layer-resolved magnetic properties of the X/Co interfaces, where X is a heavy metal. (a) Spin and (b) orbital contributions to the magnetic moment for an in-plane magnetization. The left (right) panels represent the 4d (5d) metals, as indicated in the figure. The solid (dashed) line indicates the value for the bulk (freestanding layer of) Co. From Ref. [22].

(ii) the orbital moment of the 3d metal is enhanced. Metals with partially filled d shells acquire a large magnetic moment (Pt, Pd, Rh and Ir), which vanishes for metals with filled d shells (Au and Ag), as reported on Fig. 5(a). The magnetic moment is very small in the case of Tc, Ru, Os, and Re, but does not vanish. In addition, the transition metal interface acquires an induced orbital moment that is negative for Tc, Ru, Re, and Os, and positive at the interface with Rh, Pd, Ag, Ir, Pt, and Au, see Fig. 5(b).

2.3. Interfacial spin-orbit coupling

When an electron moves in an external electric field, or potential gradient, it experiences a magnetic field in its frame of motion, see Fig. 6(a). The coupling between this magnetic field and the spin degree of freedom (which is nothing but a Zeeman coupling) is the spin-orbit coupling given by $H_{so} = (\xi/h)\hat{\sigma} \cdot (\nabla \Phi \times \hat{p})$ ($\xi$ is the spin-orbit coupling strength in eV/m²). It couples the spin angular momentum $\hat{\sigma}$ to the gradient of the crystal field $\nabla \Phi$. In crystals, the potential is composed of the spherical atomic potential and the rest of the potential composing the crystal field. It turns out that the potential
gradient is particularly strong close to the atom nucleus, such that one can adopt the spherical approximation, $\nabla \Phi = (\partial_r \Phi / r) \hat{r}$. Hence, the spin-orbit coupling reduces to the well-known atomic Russell-Saunders form $\mathcal{H}_{so} = (\xi / \hbar) (\partial_r \Phi / r) \hat{L} \cdot \hat{\sigma}$, where $\hat{L} = \hat{r} \times \hat{p}$ is the orbital angular momentum. This form neglects the crystal contribution to the spin-orbit coupling but is usually sufficient to model spin-orbit physics.

$$\nabla \Phi = (\partial_r \Phi / r) \hat{r}.$$ 

$$\hat{L} = \hat{r} \times \hat{p}$$

Figure 6: (a) Schematics of spin-orbit coupling: an electron flowing in a potential gradient $-\nabla \Phi$ experiences a magnetic field $\sim -\nabla \Phi \times \mathbf{v}$ in its frame of motion. (b) Two-dimensional band structure of the free electron Rashba gas. The red and blue arrows indicate the spin orientation. (c) Schematics of the transition metal interface. (d) Band structure of Co/Ir(111) interface computed from first principles, when the magnetization of Co lies in-plane along $+x$ (red) and $-x$ (blue). From Ref. [22].

In solid state, the potential $\Phi$ arises from the ionic environment of the electron, i.e. crystal structure, defects, impurities etc. Therefore, through spin-orbit interaction, the information of this environment gets imprinted in the spin-dependent part of the wave function. In particular, in a solid possessing inversion symmetry ($\hat{H}_k = \hat{H}_{-k}$) in the presence of spin-orbit coupling, Kramers degeneracy imposes that the two following Bloch states must be degenerate

$$|k, n, +\rangle = [u_{k,n}^\uparrow | \uparrow \rangle + u_{k,n}^\downarrow | \downarrow \rangle] e^{ik \cdot r},$$

$$|k, n, -\rangle = [-u_{-k,n}^\downarrow | \uparrow \rangle + u_{-k,n}^\uparrow | \downarrow \rangle] e^{ik \cdot r}. $$

As a consequence, neither the spin angular momentum nor the linear momentum are good quantum numbers anymore. The impact of spin-orbit coupling on the band structure of bulk Pt is reported in Fig. 7. The spin-orbit coupling removes the band degeneracy away from the $\Gamma$ point and induces energy splitting of the
band structure. Because Pt has inversion symmetry, no splitting in momentum is observed.

Figure 7: (Color online) Electronic band structure of bulk Pt in the absence (a) and in presence of spin-orbit coupling (b). The red circle shows that around the Γ point, \( k = 0 \), no energy splitting is observed whereas away from it, the spin-orbit coupling induces energy splitting at the band-crossing points. Notice that the band structure is split only in energy, but not in momentum. (Courtesy from S. Grytsyuk)

What changes when going from the bulk to the interface? The usual way to look at the problem is by considering symmetry arguments. In such systems, the interface breaks the inversion symmetry along the normal to the interface, \( z \). Spatial inversion symmetry breaking allows the spin-orbit coupling to develop terms that are odd in momentum \( k \), which is well known since the pioneering work of Dresselhaus in bulk non-centrosymmetric semiconductors [27]. In the case of interfacial symmetry breaking, a simplistic picture suggests that the gradient of potential becomes \( \langle \xi \nabla V \rangle \approx -\alpha z \) and the spin-orbit coupling Hamiltonian reduces to \( \hat{H}_R \approx -\alpha \hat{\sigma} \cdot (z \times k) \), where \( \alpha \) is the so-called Rashba parameter, as originally proposed by Vas’ko [28] and studied by Bychkov and Rashba [29] in the context of low-doped two dimensional semiconducting quantum wells.

Figure 8: (a) Two-dimensional Fermi surface of Ir/Co(111) interface in \((k_x,k_y)\) plane, when the magnetization direction is along +\( x \) (red) or -\( x \) (blue). The distortion of the Fermi surface reflects the coupling between spin and momentum degrees of freedom [22]. (b) The \( x \)-component and (c) \( y \)-component of spin at Co/Pt(111) interface. The magnitude of each state’s spin is proportional to the dot size, and blue dots refer to positive value of the spin component, while red dots refer to negative values [30].
Although this picture is very popular and widely used in the literature, the actual origin of Rashba spin-orbit coupling is a bit more subtle. As mentioned above, in a crystal the potential gradient is dominated by the spherical atomic potential, so that the largest contribution to spin-orbit coupling comes from the nuclei themselves rather than from the crystal field. In other words, spin-orbit coupling is essentially of the Russell-Saunders form, $\hat{H}_{\text{so}} = (\xi/\hbar) (\partial/\partial r) \hat{\mathbf{L}} \cdot \hat{\mathbf{\sigma}}$.

That being said, close to an interface the wave function experiences symmetry breaking, such that the potential gradient gets imprinted in the wave function itself, rather than in the spin-orbit coupling Hamiltonian. This aspect was emphasized in an inspiring study by Bihlmayer et al. [31]. In a bulk crystal, the eigenstates are given by Bloch states. Close to the nucleus, the Bloch states are well represented by spherical harmonics, i.e. $s$, $p$ and $d$ orbitals. Close to an interface, the potential gradient mixes these orbitals such that a state with a predominantly $l$ character hybridizes with states of $l \pm 1$ characters.

In other words, $d$ and $p$ orbitals get mixed upon the potential gradient, such that the effective spin-orbit coupling, projected on the basis of the bulk Bloch states, becomes odd in momentum $k$. The sign of the potential gradient, and corresponding the charge imbalance around the nucleus, determines the sign of Rashba spin-orbit coupling [32, 33, 34, 35]. This results in quite a complex form of the band splitting. Indeed, while the initial Rashba model assumes a free electron gas with a circular Fermi surface, it is clear that transition metals display a much more complicated band structure, as illustrated on Fig. 8. However, in spite of this complexity, the overall physics associated with Rashba spin-orbit coupling is valid, as discussed in Section 4.

In a recent work, Grytsyuk et al. [22] have systematically calculated the $k$-asymmetric spin-splitting occurring at the interface between Co and transition metal substrates. In their method, the authors compute the effective momentum shift of the Fermi surface upon magnetization reversal [see Fig. 8(a)]. The results are reported on Fig. 9(a). It is remarkable that the spin-splitting follows roughly the charge transfer between the substrate and the Co overlayer shown.

Figure 9: (a) Effective momentum shift $\langle k_y \rangle$ for Co/X(111) interface and (b) corresponding charge transfer of the $d$-orbitals from the substrate to the Co overlayer. From [22].
in Fig. 8(b), as well as the Stoner criterion reported on Fig. 2(a,b). Indeed, the $k$-asymmetric spin-splitting is driven by the 4$d$ or 5$d$ orbitals (which possess the strongest spin-orbit coupling) and is therefore expected to be maximum with Pd and Pt substrates, respectively.
3. Dzyaloshinskii-Moriya Interaction

In the previous section, we discussed the onset of \(k\)-asymmetric spin-splitting at transition metal interfaces. We showed that this effect emerges from the cooperation between spin-orbit coupling and interfacial symmetry breaking, and is very sensitive to interfacial orbital hybridization. At magnetic interfaces, the interfacial spin-momentum locking results in antisymmetric exchange interaction that can stabilize chiral magnetic textures.

3.1. General principle

Magnetic materials lacking inversion symmetry can host chiral magnetic objects whose dynamics has attracted significant attention lately [36]. Fundamentally, chiral magnetic objects arise from the competition between ferro- or antiferromagnetic exchange (\(\sim J_{ij} S_i \cdot S_j\)) and a so-called antisymmetric exchange (\(\sim D_{ij} \cdot (S_i \times S_j)\)) [37, 38]. While the former tends to align neighboring spin in a collinear configuration, the latter tends to align neighboring spins perpendicular to each other, as illustrated on Fig. 10(a). As a result, spin-spirals or magnetic skyrmions can be achieved either as a ground state [39, 40, 41, 42, 43], or as metastable states [44, 45, 13, 14, 46, 47, 48]. An example of magnetic skyrmion is represented on Fig. 10(b). A crucial ingredient for the generation of such chiral textures is the Dzyaloshinskii-Moriya antisymmetric magnetic interaction (DMI) [37, 38] arising from spin-orbit coupling. Originally proposed in the context of Mott insulators [37, 38], weak metallic ferromagnets and spin glasses [49], it has recently been identified at transition metal interfaces, resulting in Néel domain walls [50, 51, 52], spin spirals [53, 54, 55, 56], and skyrmions with a defined chirality [43, 57]. In addition, DMI is known as the driving force for several magnetic phenomena such as spin glasses [49], magnon Hall effect [58], magnonic torque [59, 60], multiferroicity [61], and chiral molecular magnets [62, 63].

We also emphasize that non-collinear magnetic textures can also emerge out of frustration [65]. For instance, even in the presence of inversion symmetry, when all the nearest neighbor exchange interactions cannot be fulfilled simultaneously, it is often preferable for the magnetic structure to adopt a non-collinear configuration, see Fig. 10(c). However, since inversion symmetry is conserved, the non-collinear magnetic system is not chiral, i.e. the ground state is degenerate and comprises multiple configurations that are energetically equivalent. An example is the 120° spin spirals obtained in triangular lattices or the 3Q configuration obtained in Mn/Cu(111) bilayers [64, 66], see Fig. 10(d). This topic remains out of the scope of the present discussion.

3.2. Kashid’s trimer model

While the original theories of DMI apply in a context that is quite different from transition metal interfaces [38, 49], recent phenomenological models have explored the physics of DMI in metallic systems. Kim et al. [67] and Garate et al. [68] both proposed that Rashba or Dirac spin-orbit coupling in a two
Figure 10: (a) The combination between spin-orbit coupling, magnetism and inversion symmetry breaking at transition metal interfaces gives rise to non-collinear magnetic textures, such as, but not limited to, magnetic skyrmions, displayed in panel (b). (c) Alternatively, certain frustrated systems involving the competition between ferromagnetic and antiferromagnetic exchange interactions support non-collinear magnetic textures, such as multiple-Q spin spirals. Panel (d) shows the 3Q texture obtained in Mn/Cu(111) [64].

Dimensional electron gas can result in DMI. In these theories, the magnetization is modeled by localized $d$-type electrons, while the transport is due to the $s$-type electrons. Hence, through Rashba or Dirac spin-orbit coupling, the itinerant electrons mediate an antisymmetric exchange between the local magnetic moments. In this limit, DMI is of the form $E_{DM}\sim \mathbf{m} \cdot [\mathbf{z} \times \nabla] \times \mathbf{m}$. In other words, at interfaces, one expects that DMI creates an effective magnetic field $H_{DM}\sim \mathbf{m} \times (\mathbf{z} \times \mathbf{e}_i)$, where $\mathbf{e}_i$ is the direction of the magnetic texture. For perpendicularly magnetized materials, such a magnetic field favors Néel walls over Bloch walls [69], as observed experimentally a transition metal interfaces [50, 51, 52].

A finer "minimal" model was proposed by Kashid et al. [70]. In this approach, the authors consider a trimer, composed of two magnetic atoms (A and B) coupled to a non-magnetic atom (C) that possesses spin-orbit coupling [see Fig. 11(a)]. The magnetic atoms possess only $d_{xz}$ orbitals, while the non-magnetic atom possesses both $d_{xz}$ and $d_{yz}$. The Hamiltonian of the trimer reads

$$\hat{H} = \hat{H}_0 + \hat{H}_m + \hat{H}_{\text{hop}} + \hat{H}_{\text{so}},$$

where

$$\hat{H}_0 = \epsilon_A \hat{c}^\dagger_{xz,A} \hat{c}_{xz,A} + \epsilon_B \hat{c}^\dagger_{xz,B} \hat{c}_{xz,B} + \epsilon_C (\hat{c}^\dagger_{yz,C} \hat{c}_{yz,C} + \hat{c}^\dagger_{yz,C} \hat{c}_{yz,C})$$

$$\hat{H}_m = -\frac{J}{2} (\hat{c}^\dagger_{xz,A} (\mathbf{\sigma} \cdot \mathbf{m}_A) \hat{c}_{xz,A} + \hat{c}^\dagger_{xz,B} (\mathbf{\sigma} \cdot \mathbf{m}_B) \hat{c}_{xz,B}),$$

$$\hat{H}_{\text{hop}} = t_1 (\hat{c}^\dagger_{xz,A} \hat{c}_{xz,C} + \hat{c}^\dagger_{xz,B} \hat{c}_{xz,C}) + t_2 (\hat{c}^\dagger_{xz,A} \hat{c}_{yz,C} - \hat{c}^\dagger_{xz,B} \hat{c}_{yz,C}) + c.c.$$
scribes the intrinsic magnetic coupling on atoms A and B, where $m_{A,B} = (\cos \varphi, \pm \sin \varphi, 0)$ \cite{70}, and $\mathbf{H}_{\text{hop}}$ describes the hopping between the three atoms. The hopping energies, $t_1$ and $t_2$, are defined within Slater-Koster parametrization \cite{71},

$$
    t_1 = \cos^2 \theta V_{dd\pi} + \sin^2 \theta V_{dd\delta},
$$

$$
    t_2 = \sin \theta \cos \theta (V_{dd\pi} - V_{dd\delta}),
$$

where $V_{dd\pi}$ and $V_{dd\delta}$ are the Slater-Koster parameters and $\theta$ is the angle represented on Fig. 11(a). For simplicity, the direct hopping between A and B is discarded. Finally, the spin-orbit coupling is only active on the non-magnetic atom C, and mixes orbitals $d_{xz}$ and $d_{yz}$,

$$
    \mathbf{H}_{\text{so}} = \frac{i \xi}{2} \left( (\hat{c}^\dagger_{xz,C})^\dagger \hat{c}^\dagger_{yz,C} - (\hat{c}^\dagger_{yz,C})^\dagger \hat{c}^\dagger_{xz,C} \right) + \text{c.c.}
$$

Since DMI is, to the lowest order, linear in spin-orbit coupling, one can get an estimate of its strength by computing

$$
    E_{\text{DM}} = \int_{-\infty}^{\epsilon_F} d\epsilon \text{Tr}[\hat{\rho}_0 \mathbf{H}_{\text{so}}],
$$

where $\hat{\rho}_0$ is the density matrix in the absence of spin-orbit coupling. By looking at the form of the spin-orbit coupling term, Eq. (8), one realizes that in order to obtain large DMI, the unperturbed eigenstate should possess both $d_{xz}$ and $d_{yz}$ characters with opposite spins. As a result, DMI stems from (i) non-collinear magnetism (both up and down spins are present), as well as (ii) symmetry breaking (that mixes $d_{xz}$ and $d_{yz}$ orbitals). The former is obtained by taking $\varphi \neq 0$, while the latter requires $t_2 \neq 0$. Moreover, condition (i) implies that half metals (where only one spin species is present at Fermi energy) are unlikely to show DMI. In summary, in this model $E_{\text{DM}}$ is very sensitive to the hybridization between the spin-mixed orbitals, $d_{xz,A(B)}$, and the spin-orbit coupled orbitals, $d_{xz,C}$ and $d_{yz,C}$.

Let us now explore the outcomes of this model. For the calculation, we take the same parameters as in Ref. \cite{70}: $V_{dd\pi} = 0.8$ eV, $V_{dd\delta} = -0.07$ eV, $\theta = \pi/3$, $\epsilon_A = \epsilon_B = 0$, $J = 1.125$ eV, and the Fermi energy is $\epsilon_F = 1.14$ eV. We also take a canted magnetic configuration by setting $\varphi = \pi/4$, which provides the maximum DMI energy. Finally, we take an energy broadening $\Gamma = 0.025$ eV to perform the energy integral. The spin- and orbital-resolved density of states are reported on Fig 11(b)-(e) when modifying the relative energy shift $\epsilon_C - \epsilon_A$. Three main situations can be obtained. When $\epsilon_C - \epsilon_A = 0$, the non-magnetic orbitals are located in-between the majority and minority states of the magnetic atoms such that their overlap remains weak [Fig 11(b)]. When lowering the onsite energy of the non-magnetic orbitals, they get closer to Fermi level and approach the energy level of the minority spins, such that their overlap increases [Fig 11(c,d)]. When exceeding $\epsilon_C - \epsilon_A \approx 1$ eV, the non-magnetic orbitals are pushed above the Fermi energy and the orbitals of the magnetic ions remain mostly unperturbed [Fig 11(d)].
Figure 11: (a) Schematics of Kashid’s trimer model. (b)-(e) Orbital-resolved density of states for different relative energy shift between the magnetic and non-magnetic orbitals. The blue lines refer to the magnetic orbitals $d_{xz,A} + d_{xz,B}$, the solid red lines correspond to the non-magnetic orbital $d_{xz,C}$ and the dashed red lines to $d_{yz,C}$. The parameters are given in the text.

Figure 12(a) displays the DM energy $E_{DM}$ as a function of the relative energy shift, $\epsilon_C - \epsilon_A$. The vertical lines correspond to the cases reported on Fig. 11(c,d,e). $E_{DM}$ remains vanishingly small as long as the non-magnetic orbital remain in-between the magnetic orbitals, $\epsilon_C - \epsilon_A < 0.5$ eV [Fig. 11(a)], then increases moderately when the non-magnetic orbital start overlapping with the magnetic ones, close to Fermi energy [Fig. 11(b)]. When the non-magnetic orbital enters in resonance with the minority bands, around 0.9 eV, a transition occurs from positive to negative DMI. It reverses back to positive DMI when further lowering the non-magnetic orbital energy and eventually vanishes when the non-magnetic orbitals are expelled above Fermi level. The change of sign of DMI can be analyzed by tracking the density of states of $d_{yz,C}$ at Fermi energy. As explained above, since DMI scales with $d_{xz,C}$-$d_{yz,C}$ orbital mixing, it depends on the amount majority versus minority $d_{yz,C}$ orbitals at Fermi level. This quantity is very sensitive to the details of the orbital hybridization, as shown in these calculations.

Since the physics of orbital hybridization is quite complex, it is reasonable to seek for a macroscopic quantity that correlates with $E_{DM}$. Let us define two such quantities, the induced magnetic momentum on the non-magnetic ion $m_C$
and the charge transfer between the magnetic and non-magnetic ions \( \Delta n \),

\[
m_C = \int_{-\infty}^{\epsilon_F} d\epsilon \text{Tr}[\hat{\rho}_C^F \hat{\sigma}_z], \tag{10}
\]

\[
\Delta n = \int_{-\infty}^{\epsilon_F} d\epsilon \text{Tr}[\hat{\rho}_B^0 + \hat{\rho}_0^H - \hat{\rho}_C^0]. \tag{11}
\]

These two quantities are reported on Fig. 12(b) and (c). We observe two remarkable features. First both positive maxima of \( E_{DM} \) at \( \epsilon_C - \epsilon_A \approx 0.8 \text{ eV} \) and \( 1.08 \text{ eV} \) correspond to a negative maximum in induced magnetization. Second, the largest \( E_{DM} \) value is reached around \( \epsilon_C - \epsilon_A \approx 0.93 \), which corresponds to a local minimum in \( m_C \) and a vanishing \( \Delta n \). What we wish to emphasize here is that there is no straightforward, systematic correlation between \( E_{DM} \) and either induced magnetization or charge imbalance, even in this simple model.

Another interesting study is to vary the symmetry breaking. To do so, we simply vary the angle \( \theta \) in the range \( \pm \pi/3 \), assuming that the overlap integrals,
and $V_{dd\delta}$ remain unmodified. The results for $E_{DM}$, $m_C$ and $\Delta n$ are reported on Fig. 12(d)-(f). The DMI is clearly antisymmetric, while the induced magnetism and charge imbalance remain symmetric. Again, a correlation between these three quantities can be found for some specific points [denoted by the vertical lines in Fig. 12(d)-(f)], but no systematic rule of thumb can be determined, highlighting the complexity of the phenomena involved.

The analysis of Kashid’s trimer model reveals the high sensitivity of DMI to the specific orbital hybridization scheme present at interfaces. As such, one would expect an even more complex behavior when performing multiple-orbital calculations. That being said, since the evolution of the $d$-bands shows some systematic trends across the transition metal series, as discussed in details in Section 2, one could optimistically hope that such trends reflect in the magnitude of DMI.

### 3.3. First principles methods

In density function theory, DMI energy can be estimated by calculating the energy of the magnetic system in the presence of a spin spiral. Indeed, the impact of DMI on spin spirals resembles the influence of Rashba coupling on itinerant electrons: it distorts their energy dispersion \[72\]. The momentum shift of this dispersion provides a measurement of DMI. The main technical difficulty when using density functional theory is to accurately evaluate the energy of the system in the presence of both spin-spiral (i.e. non-collinear magnetism) and spin-orbit coupling (the spin is not a good quantum number anymore). Indeed, building a spin-spiral in real space is restricted to short wave lengths (typically less than 10 atoms \[73\]) and becomes computationally prohibitive in the long-wavelength limit. This goes without mentioning the specific issues related to the application of the local magnetic field constraining the spin direction \[73\]. An alternative powerful approach employs the generalized Bloch theorem \[74, 75\] that allows studying the spin spiral in the reciprocal space \[76\]. In that case, the DMI energy can be calculated for the whole range of spin-spiral wavelengths, from $q = 0$ (ferromagnetic) to $q = \pi/a$ (antiferromagnetic), up to the first order perturbation in spin-orbit coupling \[77, 78\]. Here $a$ is the lattice constant of the crystal unit cell. This is the method we will be using below.

Besides the generalized Bloch theorem and constrained spin-spiral methods, two other approaches have been proposed lately. Freimuth et al. \[79, 80\] developed a linear response theory that provides an estimation of the DMI in the limit $q \to 0$. The authors demonstrated that at 0K, DMI can be written

$$D_{ij} = \frac{\hbar}{2\pi\Omega} \Re \int d\epsilon f(\epsilon) (\epsilon - \epsilon_F) \text{Tr}[\hat{T}_i \hat{G}^R \hat{\nu}_j \hat{G}^R - \hat{T}_i \partial_\epsilon \hat{G}^R \hat{\nu}_j \hat{G}^R],$$

(12)

where $\hat{\nu}$ is the velocity operator, $\hat{G}^R = (\epsilon - \hat{H} - \hat{\Sigma}^R)^{-1}$ is the retarded perturbed Green’s function of the system ($\Sigma^R$ being the retarded self-energy including disorder etc.), $f(\epsilon)$ is Fermi-Dirac distribution, $\Omega$ is the volume of the unit cell, $\Re$ takes the real part and Tr denotes the trace. Here $\hat{T} = \mu_B \mathbf{B} \times \sigma$, is the torque operator between the electron spin and the exchange field, $\mu_B$ is
Bohr’s magneton. In this definition, \( D_{ij} \) is in eV m\(^{-2}\). This formula involves the summation over all the states located below Fermi level. Physically, Eq. (12) describes the Fermi sea contribution of an equilibrium torque \( \mathcal{T} \) induced by electrons flowing with a velocity \( \mathbf{v} \). A similar physical picture has been proposed by Kikuchi et al. [81], where spin-orbit coupling enables the flow of an equilibrium spin current that interacts with spin spirals and induces a "Doppler shift", corresponding to the DMI. In Kikuchi’s picture, the problem boils down to calculating the equilibrium spin current \( \mathbf{J}_s \) that interacts with the magnetic texture through the DM energy term

\[
\mathcal{H}_{\text{DM}} = \langle \hbar \rangle \int_\Omega \mathbf{m} \cdot [(\mathbf{J}_s \cdot \nabla) \times \mathbf{m}] d^3r, \tag{13}
\]

where \( \mathbf{J}_s \) is a 3×3 tensor in the spin⊗real space. Notice that in the above expression, the projection \( \mathbf{J}_s \cdot \nabla \) is taken on the real space coordinates, such that this term is a 3-component vector.

### 3.4. DMI at 3d/5d interfaces

There are many reports on the spin textures in 3d/5d multilayered material stacks and interfaces [82, 53, 54, 43, 55, 56], and several models have been developed to explain the physics of DMI [77, 78, 70, 73, 83, 84]. In spite of this intense effort, the various aspects of the physics underlying the onset of DMI and its behavior are not well understood. More specifically, the DMI in 3d/5d interfaces depends sensitively on the details of the electronic structure, in which the high complexity of interfacial hybridization hinders the development of qualitative and quantitative predictions in these material combinations. In this regard, controlling the sign and magnitude of DMI represents an outstanding challenge.

![Figure 13](image-url)
for modern magnetism. For this reason, a universal phenomenological description of the DMI in transition-metal interfaces is required to simplify the complex physical picture, and can provide significant guidance for designing new interfaces and especially controlling their spin textures. From a fundamental point of view, we believe that predicting the general trend is extremely important to understand the underlying physical mechanisms of DMI. Therefore, it is instructive to develop a new physical picture by predicting the chemical trend of DMI across the majority of 3d/5d interfaces. In this Section, we review a systematic investigation of DMI for 3d metals (V, Cr, Mn, Fe, Co, Ni) as overlayers on 5d substrates (W, Re, Os, Ir, Pt, Au) [21]. The calculations are performed using density functional theory within the local density approximation to the exchange correlation functional [85], using the full potential linearized augmented plane wave method in film geometry [86] as implemented in the Jülich density functional theory code FLEUR [87]. The DMI energy is computed to the first order in spin-orbit coupling within the framework of the generalized Bloch theorem [64, 78].

In Fig. 13 we summarize our results of total DMI energy $D_{\text{tot}}$ as a function of the 3d overlayer element for various 5d substrates. According to our calculations, regardless of the sign found in Co/Re(0001) and Co/Ir(111) interfaces, the DMI shows a clear variation with respect to the 3d filling where the Mn overlayer has the largest values and it gradually decreases for chemical elements on both sides of Mn in the 3d transition metal row of the periodic table. This variation is actually very surprising since it reveals an interesting chemical trend, in which the DMI across the 3d/5d interfaces clearly follows Hund’s first rule [88] with a tendency similar to their magnetic trends in either the unsupported monolayers or ultrathin films [see Fig. 13(a)] [21]. Since the energy term resulting from this interaction is proportional to $M^2$, this correlation holds true and remains unchanged when considering the ratio of DMI divided by the square of the magnetic moment $M^2_{3d/5d}$ for all studied 3d/5d interfaces [see Fig. 13(b)]. Indeed, this appears consistent with the behavior observed in low-dimensional systems whose spin moments as a function of the number of d electrons are well described by Hund’s first rule [88, 20, 19] as shown in Fig. 13(b). The only exception is 3d/Au(111) systems where the magnitude of DMI is very small, independent of the 3d overlayer. Despite the large spin-orbit coupling of Au compared with all 5d substrates, the weak DMI seems unusual but can be understood on the basis of its electronic configuration, in which the 5d shells are completely occupied [see Figs. 3 and 13(a)]. The latter indicates that the DMI depends critically not only on spin-orbit coupling and breaking of the inversion symmetry, but also on the 5d wave function localization of the chosen substrate. It is also worthwhile to note that most of 3d/5d interfaces have a positive sign of DMI, such that the left- or right-rotating character of the spin spiral depends on their ferro- or antiferromagnetic ground state [see Fig. 13(a)] [21].

These remarkable findings reveal the existence of magnetically correlated behavior between the DMI and spin magnetic moment. Furthermore, this trend was not expected since the other magnetic interactions, magnetic anisotropy energy and Heisenberg exchange interaction, behave differently and show a com-
pletely different chemical trend when moving along the 3d elements [18]. More specifically, although the magnetic anisotropy contributes to the magnetic energies, it does not show a positive correlation with magnetic moment of 3d/5d thin films. For instance, Mn systems have the smallest magnetic anisotropies but the largest magnetic moment. In the same way, the Heisenberg-type exchange interaction parameter $J$ is also independent of $M$, being smaller for Mn than for Co. Obviously, the nearest-neighbor exchange interaction ($J_1$) for 3d transition metals follows perfectly the Bethe-Slater curve and not Hund’s first rule [89]. Further, this fact is also surprising as it is opposite to what is expected from the knowledge of magnetism in bulk and thin films. For instance, such uncorrelated behavior has also been recently observed in the skyrmion phase of Mn$_{1-x}$F$_x$Ge by Gayles et al. [83], where the strength of DMI does not show any correlation with the magnetic moment of the 3d transition metal. This provides additional evidence for a violation of direct relation of magnetic moment and DMI in alloy systems.

Since the relation between interfacial DMI and local magnetic moments of 5d substrate has been so controversially debated lately, we emphasize here that the DMI shows no direct correlation with the proximity induced magnetism in 5d across the 3d/5d interfaces [21]. Indeed, the 5d states are degenerate and partially occupied due the strong crystal-field splitting or large bandwidth, irrespective of deposited 3d overlayer on the top, in good agreement with the experimental observations [90] and previous theoretical studies [18, 73]. This result is in contrast, however, with recent experiment by Ryu et al. [91] who claim that DMI should scale with the induced magnetization of the heavy metal.

The above discussion demonstrates that varying the orbital hybridization between the 3d overlayer and the 5d substrate impacts the DMI and the other magnetic interactions differently in those systems. More specifically, since the DMI emerges from a complex interplay between (i) the degree of spin polarization of the 3d/5d interface atoms and their band filling, (ii) the strength of spin-orbit coupling in the underlying heavy metal 5d substrate, and (iii) the inversion symmetry breaking at the interface, one does not necessarily expect a direct correlation between the magnetism of the 3d overlayer and the DMI. This lack of correlation confirms our previous conclusions based on Kashid’s model. In the following, we will explain in more detail the physical reasons behind the unexpected trend, pointing out the importance of this magnetic correlation from the electronic point of view.

The microscopic origin of the correlation displayed in Fig. 13 clearly involves the impact of the 3d-orbital magnetization and their electron filling on DMI, which, however, affects significantly the overlayer-substrate hybridization and consequently the magnetic coupling between the 3d atoms in the monolayer plane. This can be understood by examining the energetic positions of 3d/5d states and their spin-flip mixing processes. Indeed, as explained in the previous Section, we remind that the antisymmetric exchange mechanism, as an excitation signature, requires spin-flip transitions between occupied and unoccupied states through spin-orbit active 5d states. Of course, this requires certain level of hybridization with the 3d orbitals, since the energetic band alignment of the
$3d$-$5d$ interface states around the Fermi energy controls the magnetic coupling of deposited $3d$ atoms and, consequently, the DMI.

Figure 14: Left side: filling with electrons of $3d$ transition metal elements into the five $3d$-orbitals according to Hund’s first rule, spin-up and -down are shown by red and blue arrows, respectively. On the right side we show the spin-split band positions of $3d$ states with respect to $5d$-W states. Note, since the $5d$ bandwidth is significantly larger than the crystal field splitting the $5d$ states are degenerate at the Fermi level. $\Delta_{CF}$ indicates the crystal-field splitting between the $t_{2g}$ and $e_g$ shells. From [21].

This fact is reflected, for instance, by the electronic configurations of the $3d$ orbitals and their spin-split band positions with respect to $5d$ W states, see Fig. 14. Inspecting this figure in more detail, one can see that the band lineups of $3d$ and $5d$ states reveal two interesting features, which are essentially similar to a first approximation. First, the W surface is weakly polarized where the $5d$ states are degenerate and partially filled, consistent with the fact that those configurations of the outer electrons shell are dominated by the significant large bandwidth or by the crystal-field splitting. Note that the number of available $5d$ states near the Fermi level and their bandwidth are fixed for a certain substrate depending on their filling. Second, the electron filling of the $3d$ orbitals, according to Hund’s first rule, fits well the band alignment of $3d$ states around the Fermi level, as shown in Fig. 14. At this stage, it is important to stress out that the $3d$-$5d$ majority and minority spin states and their exchange-splitting gap are energetically aligned according to their calculated band structure, as depicted on Fig. 14, right side. The latter is found to be consistent with the electronic occupation of $3d$-$5d$ (in first approximation) spin channels (Fig. 14, left side) and thus obeying both crystal field splitting and Hund’s first rule.
In this context, since the 5d bandwidth is significantly larger than the crystal-field splitting and the 5d states are weakly polarized (degenerate and partially filled), the overall physics of the predicted trend in Fig. 13 is mostly governed by the band lineup of 3d spin channels, themselves determined by Hund’s first rule. Therefore, in a simple picture one can easily explain this fact for all 3d elements.

By comparing the early and late 3d overlayers, V and Ni respectively, one can observe that both spin channels are mostly either occupied or unoccupied; their band alignment with respect 5d states is energetically unfavorable and, consequently, the spin-flip excitation processes are not allowed. As a result, the DMI is weak in both cases since this mechanism requires the availability of 3d electrons, occupied and unoccupied, to facilitate the spin-flip process which is crucial for the appearance of the DMI. Proceeding from Ni to Co overlayer, the DMI remains relatively weak because of the small amount of unoccupied minority 3d states. Keep in mind that the degeneracy of 5d spin channels is not lifted by the presence of any 3d overlayer on the top, despite the overlap of the relatively more extended 5d wave function of the W substrate with the wave functions of 3d overlayers. In other words, since the 5d orbitals are more extended than 3d ones, these orbitals are only weakly perturbed by the adsorption of 3d elements. On the other hand, since the DMI is weaker it is more sensitive to the detail of the orbital hybridization between the substrate and the overlayer, resulting in a change of handedness of the magnetic structure. This actually happens for Ni/5d and V/5d interfaces on both sides of this trend, as well as for Co overlayer. This also holds true for Au substrate, because the 5d states lie far below the Fermi level (the bonding character is less clear for the involved states) the DMI is weaker and therefore shows variations in the sign as a function of the 3d overlayer (Fig. 13, yellow line). Such an oscillation in sign has been analyzed extensively for Mn$_{1−x}$Fe$_x$Ge by Gayles et al. [83] and has also been identified in the trimer model developed by Kashid et al. [70], where the sign and magnitude of DMI depend on the shifts of the single-particle energies with respect to the scalar-relativistic eigenvalues due to spin-orbit coupling ($\delta\epsilon_{\nu\nu} = \delta\epsilon_{\nu\nu}^{\text{SOC}} - \delta\epsilon_{\nu\nu}^{\text{SR}}$) in the energy range around the Fermi level [70].

According to perturbation theory, the 5d orbitals "spin-orbit active states" are responsible for the spin-orbit coupling matrix elements $H_{\nu\nu}(L)$ and make essential contributions to DMI [see Fig. 6(a)]. However, despite the weak spin-orbit coupling in the 3d overlayer their intra-atomic exchange field can easily modify the electronic structure around the Fermi energy and consequently change the strength of the DMI. One may conclude that the spin-orbit-induced energy shift of the highest occupied orbital depends sensitively on the charge rearrangement between the 3d orbitals of opposite spin and, hence, Hund’s first rule. In the following, we will demonstrate how the spin-flip excitations through spin-orbit coupling in half-filled or high spin 3d overlayer make the largest contribution to the DMI.

The situation is completely different when moving to half-filled 3d transition metals. In the case of Mn overlayer, the filling of the five Mn 3d orbitals adopts a stable "high spin state" due to the small crystal field splitting between the
The spin-up (spin-down) channels are entirely occupied (unoccupied) and all transitions contribute to the DMI through the intermediate spin-orbit active 5d states. In other words, the 3d-5d-3d electron hopping is facilitated, resulting in a large DMI [92]. Therefore, the Mn/5d interfaces, in particular Mn/W(001), shows the largest magnetic antisymmetric exchange. When the DMI is strong enough to compete against the Heisenberg exchange and magnetic energy anisotropy, complex spin textures are more likely to appear. The latter holds true especially since the Heisenberg-type exchange interaction is independent of the magnetic moment \( M \), and is smaller for Mn than for Co according to the Bethe-Slater curve. This result is in good agreement with the experimental observation of Bode et al. [53], who demonstrated for the first time that the strong DMI in Mn monolayer on a W(110) substrate can stabilize long-range spin spirals. Also, by combining spin polarized scanning tunneling microscopy and ab-initio theory, a unique rotational sense as a left-rotating cycloidal spin spiral was also found by Ferriani et al. [54].

The situation is almost similar for the half-filled Fe and Cr atoms but the exchange splitting is reduced, where most of the Fe spin-down (Cr spin-up) states are still unoccupied (occupied). This fact clearly explains the sensitivity of the DMI to the choice of the 3d overlayer and the degree of hybridization with 5d states (see, e.g., [93]). Recently, a similar trend for Mn, Co and Ni chains on Pt(111) step edge was found by Schweflinghaus et al. [92]. Concerning the sign of \( D \) in the half-filled 3d shells (Fe, Mn, Cr), the DMI prefers to maintain its left-hand chirality (left rotating). In general, although some subtleties can be observed when the DMI is small as discussed above, the atomic Hund’s first rule overall gives a clear trend of the overlayer dependence of the DMI.

In order to further understand the chemical trend of DMI across the 3d/5d interfaces, it is instructive to consider the charge transfer and induced dipole moment since the interfacial orbital hybridization in those systems is quite different in term of their bonding character. For the sake of clarity, we focus on 3d MLs on Au(111) and W(001) as the two extreme cases on both sides of the trend. We first consider the charge density difference computed in the following manner: \( \Delta \rho(r) = \rho_{\text{tot}}(r) - \left[ \rho_{5d}(r) + \rho_{3d}(r) \right] \), where \( \rho_{\text{tot}}(r) \), \( \rho_{5d}(r) \), and \( \rho_{3d}(r) \) are the charge density distributions of the conjugate system, W or Au substrate, and 3d overlayer, respectively, each in the precise position they adopt in the adsorption configuration. The dipole moment \( \mu(z) \) induced by 3d adsorption can be obtained by integrating the half-cell volume along the \( z \)-direction

\[
\mu(z) = \frac{1}{n} \int_{-c}^{-c+z/2} \int_{z'} \Delta \rho(z', \mathbf{r}) d\mathbf{r},
\]

where \( z/2 \) is half the length of the supercell, \( c \) is the distance from the topmost layer to the middle of the slab, and \( n \) is the number of 3d adatoms per unit cell. Note that the planar averaged charge density difference \( \Delta \rho(z') \) is \( \Delta \rho(r) \) integrated over lateral coordinates \( x \) and \( y \) for each \( z \) plane.

The DMI and the corresponding dipole moment values for 3d/Au(111) and 3d/W(001) are reported in Fig. 15. We find a pronounced correlation between the electric dipole moment and DMI in both cases, indicating that the physical
Figure 15: Correlation between Dzyaloshinskii-Moriya interaction (DMI) and the electric surface dipole moment (Dm) for 3d transition metal monolayers on Au (111) (a) and W (001) (b) substrates.

The mechanism responsible for DMI is intimately related to interfacial charge transfer between the 3d overlayer and the 5d substrate close to the Fermi level. More specifically, by changing the electronic occupation of the 3d-orbitals the 3d-5d hybridization-driven effects such as symmetry of surface wave-function comes into play which is also crucial for the appearance of the DMI and can be easily influenced by changes in surface dipole moment. At first glance, the dipole moment in 3d/W(001) interfaces, displayed in Fig. 15(b), is much more revealing than 3d/Au(111) Fig. 15(a). According to this figure, since the 5d states are partially filled the origin of this effect can be easily understood on the basis of the symmetry of 3d orbitals and their energetic positions upon hybridization with 5d orbitals. In the case of W(001) surface, apart from Mn overlayer, switching from V to Ni moves up the Fermi level across the 3d bands of transition metal adatoms, in which the Fermi energy is located inside one of the spin subbands and charge transfer occur depending on their filling. As a consequence the surface dipole moment increases the interface symmetry, thereby reducing the DMI energy for 3d elements on both side of Mn atom. Interestingly, the trend of the electric dipole moment shows an inverse correlation with the DMI. However, in the case of Mn/W(001) the Mn majority d band is nearly filled and the minority d band is nearly empty, resulting in a large interlayer distance [93]. As a result, the dipole moment becomes weaker and the large asymmetry of the 5d surface state wave function remains unaffected, which contributes strongly to DMI in presence of large spin-orbit coupling. In contrast, for the 3d/Au(111) interfaces, the dipole moments remain small while DMI almost vanishes [Fig. 15(a)]. Obviously, this is a consequence of the weak hybridization between 3d overlayer and the deeper 5d-states of Au substrate. More specifically, the changes in the DMI strength and induced dipole moment over the range of the 3d series are only of the order of ~ 2 meV nm and ~ 0.1 Debye, respectively.

The above results support the physical picture that DMI is not only driven by the spin-orbit coupling of 5d substrate and the inversion symmetry breaking
but also by the contribution of the intra-atomic exchange field of 3d overlayer which is responsible for the correlated behavior. In this context, these findings are consistent with atomic Hund’s rule-type arguments [88] where the maximum of the magnetic moment occurs for half band-filling of d states and, hence, the spin-flip excitation process necessary for DMI is larger in the presence of spin-orbit coupling.

3.5. Controlling DMI

According to the previous Section, we demonstrated that the magnetic interactions depend sensitively on the band alignment of 3d and 5d spin channels, where a tiny modification of those states at the Fermi level can dramatically impact the induced dipole moment and consequently the DMI. Therefore, controlling the electric dipole moment, using various tunable physical effects as external perturbations, e.g., temperature, strain, electric or magnetic field, doping, electrolyte charging etc., could allow manipulation of the complex spin textures at the atomic scale and, thus, potentially enables predicting and engineering new exotic magnetic phases.

In this respect, we present a new physical process to fine tune the DMI by controlling the electrical dipole moment of 3d/5d interfaces via adsorption of electronegative atoms. In order to validate this idea we demonstrate that the sign and strength of the DMI at asymmetric magnetic ultrathin films can be tailored by manipulating the oxygen coverage as a capping layer. In principle, the concept of surface functionalization is more general and not limited to only adatoms whose electronegativity is larger than that of ferromagnet, but can be extended for other electropositive adsorbates. An analogue mechanism based on the concept of surface-charging effect has been successfully applied to tune the magnetic anisotropy energy [94].

Among these adsorbates we have specially chosen the oxygen in this study for the following reasons: (i) from the experimental point of view, the absorption of a very small amount of oxygen is certainly unavoidable during the growth process, and this can happen even under high vacuum conditions, (ii) most first principles calculations on DMI were focused on clean surfaces without oxidants, and (iii) since the oxygen is an electronegative atom, the charge transfer toward oxygen should be significant and, consequently, the interfacial electric dipole moment can be easily tuned by the degree of surface oxidation. In this context, the presence of oxygen at the surface should not be considered as a serious obstacle for growing magnetic nanodevices, but it can prove very useful as a tunable parameter for the functionalization of their magnetic interactions [95, 96, 97]. For instance, the oxidation of CoFeB layer at certain level of oxygen coverage can greatly tune the magnetic anisotropy [98, 99], magnetoresistance properties [100, 101], and spin-orbit torque [102]. Recently, Krupin et al. [103] have also demonstrated a change of Rashba splitting and its sign when oxygen adsorbed on the top of Gd(0001) surface. Furthermore, recent ab initio study by Yuan et al. [104] demonstrated that manipulating the oxygen concentration on Pt-nanojunction can tune the sign and magnitude of DMI and, consequently, leads to the formation of spin-spirals with different sense of rotations.
For the sake of clarity, we consider the oxygen adsorption on Fe/Ir(001) as a prototype interface of complex magnetic oxides. As a matter of fact, this interface has attracted much attention lately because its strong DMI can promote in a great variety of complex magnetic phases, such as skyrminons or homochiral spin spirals [105, 43, 55, 66, 21, 70]. More specifically, because of the degeneracy of the nearest-neighbor exchange interactions, FM and AFM coupling of the deposited Fe atoms, in clean Fe/Ir(001) interface we believe that the electric dipole moment induced by oxygen adsorption is useful to control the competition between Heisenberg exchange interaction, magnetic energy anisotropy, and DMI.

In Figure 16(b), we show the variation of DMI and the electric dipole moment as a function of oxygen coverage. We find a clear chemical tendency when varying the oxygen coverage on Fe/Ir(001), in which the magnitude and sign of DMI are strongly correlated with the induced electric dipole moment. This fact actually depends on the balance of the interfacial charge transfer between both Fe-Ir and Fe-O layers, as shown in Fig. 16(a). Indeed, oxygen with O-2\textit{p} orbital affects the energetic ordering of Fe-3\textit{d} spin channels with respect to the Fermi level and, consequently, controls the hybridization between Fe-3\textit{d} and Ir-5\textit{d} states and their band lineup. Physically, this correlation is very interesting since the electric dipole moment also depends sensitively on relative energy position of 3\textit{d} and 5\textit{d} states around the Fermi energy. The latter demonstrates the close link between the DMI and dipole moment depending on the charge rearrangement between the 3\textit{d} and 5\textit{d} spin channels and their energetic position.

The most striking feature in Fig. 16(b) is the sign variation of DMI with increasing the O coverage beyond 0.25 ML. More specifically, the magnetic chirality exhibits an oscillatory behavior between the left and right hand, accompanied by a significant reduction in magnitude of DMI for higher coverages compared to clean surface. These trends are found to be consistent with the energetic shift of the Fermi level $\epsilon_F$ with respect to unperturbed one $\epsilon_0^F$ for spin spiral of wave vector $q' = 0.25 \frac{2\pi}{a'}$ [see Fig. 16(c)]. Note that the $\epsilon_0^F$ and $\epsilon_F$ are the Fermi levels obtained without and with spin-orbit coupling, respectively. It is interesting to note that the weak surface dipole moment and DMI at 0.75 ML is traced back to the significant reduction of the electrostatic interactions between the adsorbed oxygen atoms. As a result, surface depolarization occurs because of inversion direction of the dipole moment, indicating that a partial electron charge is transferred from the oxygen overlayer back to Fe atoms. This behavior is clearly visible when inspecting the charge density difference at the neighboring O (2-3) atoms in Fig. 16(e) compared to 0.25 ML in Fig. 16(d).

First principles calculations by Zhang et al. [106] also reported almost similar effect that can be obtained at oxygen rich condition. This mechanism principally drives the induced electric dipole moment and the resulting oscillatory variation of DMI as a function of oxygen coverage. Therefore, our findings demonstrate that the existence of a charge accumulation and depletion at the surface of 3\textit{d}/5\textit{d} systems is very efficient in controlling the work function [see Fig. 16(b)]. The latter plays an important role to control the induced electric dipole moment and thus the sign and strength of DMI.
Figure 16: Correlation between Dzyaloshinskii-Moriya interaction (DMI) and the electric surface dipole moment (Dm). (a) Planar averaged charge density difference $\Delta \rho(z)$ for the adsorption of O on Fe/Ir(001) at different coverages. The dashed red (O), blue (Fe), and gray (Ir-surface) lines show the approximate equilibrium position on the fully relaxed surface. O coverage dependence of the change in the surface dipole moment (Dm), DMI (b) and relative Fermi energy (c). Isosurface plot of the charge density difference $\Delta \rho(r)$ for 0.25(d) and 0.75ML(e), red and blue surfaces depict the region of charge accumulation and depletion, respectively. The selected surfaces correspond to the charge isodensity of $1.2 \times 10^{-2} e/\text{Å}^3$. From [84].

From the above discussion, we conclude that the DMI is a subtle physical mechanism that depends sensitively on the details of the electronic band structure around the Fermi level. This holds particularly true since the DMI involves transitions from the occupied states spin-up to the unoccupied states spin-down and vice versa. As long as the influence of oxygen on the orbital occupation is strong, the positions of these states can be shifted to higher or lower energies depending on the oxygen coverage on top. On the other hand, we emphasize that the energy shift due to the spin-orbit coupling correction also depends on the resulting charge rearrangement between 3d/5d orbitals of opposite spin, as discussed in the previous Section. Finally, since controlling the magnetic interactions, in particular the DMI, has been investigated only recently, we anticipate that the prediction and design of complex spin textures via surface functionalization are likely to have major impact in the near-future.
4. Spin-Orbit Torques

4.1. Overview

Let us now turn our attention towards the non-equilibrium properties of transition metal interfaces. In magnetic bilayers composed of a (metallic or insulating) magnet deposited on top of a heavy metal (W, Pt, Bi$_2$Se$_3$, WTe$_2$ etc.), the flowing charges experience spin-charge conversion mechanisms that produce a non-equilibrium spin accumulation at the interface with the ferromagnet, such that an overall torque is exerted on the magnetization. This effect, called spin-orbit torque, has been initially observed in transition metal bilayers [107, 108, 8, 9, 109] and bulk non-centrosymmetric magnets [110, 111, 112], and recently extended to a wide variety of transition metal bilayers [113, 109, 67, 114, 115, 116], oxide interfaces [117, 102, 118], thick multilayers [119, 120], magnetic insulators deposited on heavy metals [121, 122, 123], as well as ferromagnets deposited on topological insulators [124, 125, 126, 127], and Weyl semimetals [128].

Overall, the experiments confirm that the torque is of the form $\tau = \tau_{DL} m \times \left( [z \times u] \times m \right) + \tau_{FL} m \times (z \times u)$, where $z$ is the normal to the interface and $u$ is the direction of injection of the flowing charges. The first term $\sim \tau_{DL}$ is the damping-like torque while the second term $\sim \tau_{FL}$ is called the field-like torque. Both damping-like and field-like torques are present in most of the systems involving heavy metals. Uncovering the physical mechanisms that sustain the spin-orbit torque is quite challenging, as many effects are present in such ultrathin systems. In a nutshell, two main effects have been pointed out originally: the inverse spin-galvanic effect, localized at the interface between the heavy metal (or the oxide) and the ferromagnet, and the spin Hall effect present in the bulk of the heavy metal, as illustrated on Fig. 17. As explained in more details below, the former generates a field-like torque [129, 130, 131] $\sim m \times (z \times u)$, while the spin Hall effect generates a damping-like torque [108, 132] $\sim m \times ([z \times u] \times m)$. However, only a few systems, such as the Ti/NiFe/AlOx trilayers from Emori et al. [118], can be reasonably well explained by these two scenarios. In most cases, both torques are observed and their materials dependence raises many questions concerning the physical mechanism at their origin. More recently, two additional mechanisms have been proposed: the magnetoelectric effect and the spin swapping effect. The former is a correction to the inverse spin galvanic effect when inversion symmetry breaking, spin-orbit coupling and magnetic exchange are present on the same orbitals, and generates a damping-like torque [133, 134, 135]. The latter is a correction to the spin Hall effect and only survives in ultrathin multilayers as thin as the mean free path [136]. It creates a field-like torque.

Our objective is to present these various mechanisms, and discuss their physical origin and their impact on the spin-orbit torque. We first address the physics of spin Hall and spin swapping in Section 4.2, and discuss the physics of inverse spin galvanic effect and magnetoelectric effect in Section 4.3.
Figure 17: (Color online) In magnetic bilayers involving a ferromagnet deposited on a heavy metal, two main spin-charge conversion mechanisms occur: the inverse spin galvanic effect (also called the Rashba or Rashba-Edelstein effect), and the spin Hall effect. While the inverse spin galvanic effect directly generates a non-equilibrium spin density, \( \delta S \sim z \times u \), at the interface with the ferromagnet, the spin Hall effect induces a spin current in the bulk of the heavy metal. This spin current creates a non-equilibrium spin accumulation that diffuses into the ferromagnet. The two mechanisms give rise, at the lowest order, to a field-like (orange arrow) and damping-like torque (green arrow), respectively.

4.2. Spin Hall and swapping effects

Spin Hall effect is the conversion of a unpolarized charge flow \( j_e \) into a chargeless spin current \( j_s \). In the bulk, it reads \( e \mathcal{J}_s = \theta_{sh} \sigma \otimes \sigma \times j_e \), where \( \sigma \) is the polarization of the spin current. We remind that the spin current \( j_s \) is a \( 3 \times 3 \) tensor in spin and real space. \( \theta_{sh} \) is called the spin Hall angle and quantifies the charge-to-spin conversion efficiency. This effect was predicted originally by D’yakonov and Perel [137, 138] and revived about twenty years ago by Hirsch [139] and Zhang [140]. It has initially been observed optically in semiconductors [141, 142] and measured electrically in transition metals [143, 144]. Since then, spin Hall effect has drawn a massive amount of attention [145, 146, 147, 148, 149] as it offers a convenient way to generate pure spin currents, enabling non-local spin logic [150] as well as promoting spin-orbit torques [8, 108, 9].

Computing non-equilibrium properties of non-collinear magnetic systems in the presence of spin-orbit coupling is in itself a significant challenge since neither the linear momentum nor the spin angular momentum are good quantum numbers in this case. Different approaches have been proposed to tackle this problem. The "simplest" microscopic multi-orbital approach is probably the one adopted by Tanaka et al. [151] and Kontani et al. [152, 153] for noble metals.
The authors use a tight-binding model accounting for a minimum set of orbitals (e.g. 5s, 5p and 4d orbitals for 4d noble metals) to calculate the bulk intrinsic spin Hall effect using Kubo formula. This model allows for a rather transparent analysis of the origin of the orbital and spin Hall effects. Computation of intrinsic spin Hall effect based on the Berry phase formula and using ab initio methods has been achieved by Yao et al. [154, 155] and Guo et al. [156, 157]. These studies have been recently extended to account for both extrinsic and intrinsic effects [158, 159, 160, 161] (see also Ref. [162]). In these works, the band structure was obtained through fully relativistic Korringa-Kohn-Rostoker method (see for instance Ref. [163]) and the transport properties were evaluated either through Boltzmann equation [158, 159] or Kubo-Streda formula [160, 161]. While these different works have shed light on extrinsic and intrinsic spin Hall effects in metals and semiconductors, they focus on bulk materials and do not address the torque arising from spin Hall effect.

We emphasize straightaway that the spin Hall effect is the time-reversal counterpart of the anomalous Hall effect [5]. Therefore, both effects encompass the same classes of mechanisms. In the theoretical investigation of spin Hall effect, two classes of mechanisms have been identified. In the first case, the separation between opposite spins occurs upon scattering against spin-orbit coupled impurities. This class of mechanisms is called extrinsic, as scattering events against impurities govern the spin Hall effect. In the second case, the anomalous velocity arises from the spin-orbit coupling present in the band structure itself. This class of mechanisms is called intrinsic, as the spin-charge conversion process does not require scattering to occur. Distinguishing between these different classes of effects is important from an experimental standpoint, as one might pertinent wonder "is it more favorable to increase or decrease the amount of impurities in order to obtain large spin-charge conversion efficiency?".

### 4.2.1. Impurity scattering driven spin Hall effect

In the limit of short range (delta-like) impurity potential, the extrinsic spin Hall effect is composed of two mechanisms: the Mott scattering (illustrated on Fig. 18(a)), also called skew scattering, and the side jump. The former was initially proposed by Smit in the context of anomalous Hall effect [164] and by Dyakonov in his pioneering work [138], while the latter was put forward by Berger [165], also in the context of anomalous Hall effect. To see explicitly how spin transport is affected by spin-orbit scattering, let us first consider the Hamiltonian of a spin-orbit coupled impurity (see for instance Ref. [166]). In real space, it reads

$$\hat{H}^{\text{imp}} = \sum_i V^{\text{imp}}(r - r_i) + (\lambda_{so}/\hbar)\hat{\sigma} \cdot [\nabla V^{\text{imp}}(r - r_i) \times \hat{p}],$$  \hspace{1cm} (14)

where $V^{\text{imp}}$ is the spin-independent impurity potential, and $\lambda_{so}$ is the spin-orbit coupling parameter of the impurity. In the reciprocal space, this impurity potential becomes

$$\hat{H}^{\text{imp}}_{kk'} = \sum_i V^{\text{imp}}_{kk'} e^{-i(k - k') \cdot (r - r_i)} [1 + i\lambda_{so}\hat{\sigma} \cdot (k' \times k)].$$  \hspace{1cm} (15)
It is clear that the spin-orbit coupled part of the impurity potential acts like a magnetic field $\mathbf{B}_{so} \propto \mathbf{k}' \times \mathbf{k}$ on the incoming electron spin $\hat{\sigma}$, where $\mathbf{k}$ is the momentum of the incoming electron and $\mathbf{k}'$ is the momentum of the outgoing electron. Therefore, in the case of an unpolarized charge current, this magnetic field defines a local quantization axis such that electrons with spins parallel and antiparallel to $\mathbf{B}_{so}$ experience a different $k$-dependent scattering rate, as illustrated on Fig. 18(a): electrons with a spin momentum pointing (anti)parallel to $\mathbf{k}' \times \mathbf{k}$ have the tendency to scatter towards the left (right).

Figure 18: (Color online) (a) Sketch of Mott scattering by a spin-orbit coupled impurity. Electrons with an out-of-plane spin polarization pointing up have a larger probability to scatter towards the right while electrons with an out-of-plane spin polarization pointing down have a larger probability to scatter towards the left. (b) Sketch of spin swapping mediated by a spin-orbit coupled impurity. When the spin of the carrier lies in the scattering plane $(\mathbf{k}, \mathbf{k}')$, it experiences a magnetic field $\mathbf{B}_{so} \propto \mathbf{k}' \times \mathbf{k}$ that depends on the direction towards which the spin is scattered. This induces a scattering-induced precession giving rise to the spin swapping. From [167].

In addition, the perturbed wave function in the presence of impurities reads

$$
\Psi_{s k}^s \sim e^{i \mathbf{k} \cdot \mathbf{r}} + \sum_{i} \sum_{k'} \frac{V_{\text{imp}}^{r i k k'}}{\epsilon_{s k}^i - \epsilon_{s k'}^j + i0^+} e^{-i (\mathbf{k} - \mathbf{k}') \cdot (\mathbf{r} - \mathbf{r}_i)} e^{i \mathbf{k}' \cdot \mathbf{r}_i} e^{is \lambda_{so} \mathbf{n} \cdot (\mathbf{k} \times \mathbf{k}')},
$$

where $s$ is the spin projection perpendicular to the scattering plane, defined by the unit vector $\mathbf{n}$. One can see that the scattering wave function acquires a spin-dependent phase $\sim s \lambda_{so} \mathbf{n} \cdot (\mathbf{k} \times \mathbf{k}')$ due to the local spin-orbit field. This phase can be rewritten in term of a spin-dependent spatial displacement

$$
\delta = s(\lambda_{so}/\hbar)(\mathbf{n} \times \mathbf{p}) [166],
$$

which is referred to as side-jump scattering. The skew scattering produces a spin Hall conductivity $\sigma_{\text{SH}}^{skew} \sim \sigma_{xz}$, namely the charge-to-spin conversion efficiency is independent on the scattering strength.

In contrast, the side-jump modifies directly the velocity operator of the electron and therefore it gives a spin Hall conductivity $\sigma_{\text{SH}}^{s-j} \sim O(\sigma_{xz})$, such that the spin Hall angle is inversely proportional to the scattering time: the stronger the scattering the larger the charge-to-spin conversion (see e.g., Ref. [145]).

These extrinsic contributions have been recently investigated using ab initio calculations. It was shown that even light impurities (such as Li, C and N) embedded in noble metals (such as Au or Cu) could lead to large extrinsic

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Figure 19: (Color online) (a) Extrinsic spin Hall effect induced by substitutional impurities in Au, computed by first principles calculations [159]. (b) Extrinsic spin Hall angle calculated using virtual bound state theory [168]. The filled symbols refer to skew scattering, while the open symbols refer to side-jump scattering. In this model, the metal is Cu and the 5d impurity possess \( Z_d \) electrons.

Spin Hall contributions (up to 10% in C-doped Au) [158, 159], as illustrated on Fig 19(a). The long-standing issue of the role of side-jump versus intrinsic contributions has been addressed by Lowitzer et al. [161], who demonstrated that side jump is general weak in alloys (except for the noticeable case of Au-doped Ag). Finally, the authors discovered that the sign of the spin Hall effect may also change as a function of the composition of the alloy.

Fert and Levy [168, 169] and Gu et al. [170] recently suggested that resonant scattering on \( d \) or \( p \) impurities could lead to large spin Hall angle, as illustrated on Fig 19(b). The spin Hall effect resulting from the scattering off the impurity spin-orbit coupled states close to the Fermi energy (such as \( j = 5/2 \) and \( j = 3/2 \) in the case of Ir-doped Cu, or \( j = 3/2 \) and \( j = 1/2 \) in the case of Bi-doped Cu) depends on the relative phase shifts acquired during scattering. Such phase shifts depend on the orbital filling of the impurities following Friedel’s law. This results in a different sign of the Hall angle when considering impurities with less than half-filled shells or more than half-filled shells [171]. Resonant scattering on magnetic impurities has also been investigated by Guo et al. [172] who suggested that orbital-dependent Kondo effect could lead to a large enhancement of the skew scattering and applied it to Fe-doped Au compounds [173]. Resonant scattering on Ce and Yb magnetic impurities has been addressed by Tanaka and Kontani [174]. Evidence of large Hall angles from resonant skew scattering was reported in Pt- [173, 170] and W-doped Au [175], as well as Ir- [176] and Bi-doped Cu [177].
4.2.2. Intrinsic spin Hall effect in transition metals

The prediction of the intrinsic spin Hall effect by Murakami et al. [178] and Sinova et al. [179] opened thrilling perspectives. The main idea is that the spin-orbit coupling present in the band structure gives a contribution to the velocity operator that depends on the spin projection, and can be directly related to the Berry curvature of the materials. Since intrinsic spin Hall effect arises from the distortion of the wave function in the presence of an electric field, it does not require the subtle treatment of impurity scattering beyond the relaxation time approximation and can be readily implemented in density functional theory. The spin Hall conductivity reads

\[
\sigma_{xy} = \frac{e^2}{\Omega} \sum_{n,m,k} 2 \Im \left[ \langle n | \hat{v}_y | m \rangle \langle n | \hat{v}_x | m \rangle \right] \left( \epsilon_{n,k} - \epsilon_{m,k} \right)^2 \left( f(\epsilon_{n,k}) - f(\epsilon_{m,k}) \right).
\]  

(17)

This term involves electric-field driven interband transitions and does not depend on the amount of disorder (at least in the limit of weak disorder). Guo et al. [157] and Kontani [152] predicted large intrinsic spin Hall effect in Pt and Sr$_2$MO$_4$ semiconductors, respectively. These studies were shortly followed by in-depth analysis of the origin of intrinsic spin Hall effect in metals, showing that the Berry curvature of the bands promotes a large orbital Hall effect, which induces spin Hall effect that is proportional to the spin-orbit coupling [153, 151]. Interestingly, the intrinsic orbital Hall effect is associated to "hot spots" in the band structure occurring at anti crossing points, which is a direct consequence of the denominator \( \sim (\epsilon_{n,k} - \epsilon_{m,k})^2 \) obtained from the first order perturbation theory given above. Note that intrinsic spin Hall effect in crystalline materials displays anisotropy [180].

Figure 20: (Color online) Intrinsic spin Hall effect computed using two different methods: (a) 9-orbital tight-binding model [151], and (b) using the full-potential linearized augmented-plane-wave code FLEUR [180].

An instructive aspect of the intrinsic spin Hall effect is the fact that the sign of the spin Hall angle is directly related to the band filling. Tanaka et al. [151]
observed that the intrinsic spin Hall effect is positive in noble metals with more than half filled $d$ band (Pt, Pd, Ir, Au, Ag, and Rh), while the spin Hall effect becomes negative in heavy metals with $d$ bands less than half filled (Ta, Nb, W and Mo) [see Fig. 20(a)]. Indeed, Hund’s third rule states that in a spin-orbit coupled system where the total angular momentum $J = L+S$ is a good quantum number, $J = |L - S|$ if the shell is less than half-filled and $J = |L + S|$ is the shell is more than half-filled. Therefore, while the orbital Hall current is set by the crystalline environment, the spin Hall current is opposite to the orbital Hall current in materials with less than half-filled shells and along the orbital Hall current in materials with more than half-filled shells. A similar trend has been obtained by Freimuth et al. [180] [see Fig. 20(b)]. Notice though that the two calculations reported on Fig. 20 show some quantitative differences, that could be attributed to the different computational methods. This trend is consistent with experimental observations [181]. Intrinsic spin Hall effect has also been recently investigated in transition metal antiferromagnets $XMn$ (X=Pt, Ir, Pd, Fe) [182]. The authors found sizable values of the spin Hall effect, together with large crystalline anisotropy.

### 4.2.3. Interfacial spin Hall effect

The extrinsic and intrinsic contributions we discussed in the previous Sections have been computed in the bulk of heavy metals. However, the vast majority of the devices on which spin Hall effect is measured consists of thin heavy metals in contact with ferromagnets. As discussed in Section 2, such interfaces involve strong orbital hybridization such that the orbital character of the wave functions close to the interface may be very different from the one of the bulk Bloch states, resulting in enhanced orbital angular momentum (see Fig. 5) and Rashba-type spin-orbit coupling (see Fig. 6). As a result, one can reasonably expect the charge-to-spin conversion process to be dramatically modified at the interface. This effect has been uncovered very recently by Wang et al. [183]. Using tight-binding linear muffin-tin orbitals, the authors investigate the spin Hall effect occurring along the interface of a Pt/NiFe system and found a very large enhancement of the spin Hall angle ($\theta_{sh} \approx 0.87$ at the interface, compared to 0.03 in bulk Pt). This observation opens inspiring directions for a better understanding of spin-charge conversion processes at transition metal interfaces.

### 4.2.4. Spin swapping

Another effect occurs together with the extrinsic spin Hall effect. Let us consider again the spin-orbit coupled Hamiltonian given in Eq. 15. We already stressed out that the spin-orbit coupling acts like a $k$-dependent Zeeman field, normal to the scattering plane. In the case of unpolarized electrons, this Zeeman field is responsible for skew scattering [Fig. 18(a)]. Let us now consider an incoming spin-polarized current, whose spin polarization lies in the scattering plane. In this case, the incoming spin precesses around the effective magnetic field $B_{so}$. Since this magnetic field only exists upon scattering from $k$ to $k'$, the spin polarization of the outgoing current is re-oriented [184]. Lifshits and Dyakonov tagged this effect ”spin swapping” as the spin polarization and flow
direction of the incoming spin current are swapped during this process: an
incoming spin current $\mathcal{J}^i_{s,j}$, flowing along $e_j$ and polarized along $e_i$, gives rise
to a spin current $\mathcal{J}^{i'}_{s,j}$, flowing along $e_i$ and polarized along $e_j$, when $i \neq j$, as
illustrated on Fig. 18(b). Consistently, a spin current $\mathcal{J}^{x}_{s,x}$ produces two spin
currents $\mathcal{J}^{y}_{s,y}$ and $\mathcal{J}^{z}_{s,z}$.
Spin swapping has been derived by several authors within the diffusive limit
[185, 186, 187, 188]. For instance, Shchelushkin and Brataas obtained the ex-
pression of the charge and spin currents [185, 189]

$$\mathbf{J}_c/\sigma_0 = -\nabla \mu_c + \frac{\xi_{so}}{\lambda k_F} \mathbf{\nabla} \times \mathbf{\mu}_s,$$

$$\epsilon \mathbf{J}_{s,i}/\sigma_0 = -\nabla \mu_s - \frac{\xi_{so}}{\lambda k_F} \mathbf{e}_i \times \mathbf{\nabla} \mu_c + \frac{2\xi_{so}}{3} \mathbf{\nabla} \times (\mathbf{e}_i \times \mathbf{\mu}_s).$$

Here, $\mathcal{J}_{s,i}$ is the spin current density flowing along the direction $e_i$, $\mu_c$ and $\mu_s$
are the spin-independent and spin-dependent chemical potentials, $\sigma_0$ is Drude
conductivity and $\xi_{so} = \lambda_{so} k_F^2$ is the unitless spin-orbit parameter. The metallic
system is described in terms of its free electron Fermi wave vector $k_F$ and its
mean free path $\lambda$. The first terms in Eqs. (18) and (19) are the diffusion terms,
the second terms ($\propto \xi_{so}/\lambda k_F$) are the side jump contributions producing spin
Hall effect [Eq. (19)] and inverse spin Hall effect [Eq. (18)]. The third term in
Eq. (19) is the spin swapping effect. Note that since these equations are derived
within the first Born approximation (i.e. up to the second order in impurity
potential $|V_{k\k'}^{imp}|^2$ only), skew scattering is neglected.

In order to visualize what spin swapping does, let us consider a tight-binding
model that represents a magnetic electrode connected to a non-magnetic layer
that possesses spin-orbit coupling. The idea is to inject a spin-polarized current
from a ferromagnet into a non-magnetic, spin-orbit coupled channel and observe
the spin accumulation along the edges of the channel. The model is a simple
spin-polarized single-band, where impurity-driven spin-orbit coupling is mod-
eled as a spin-dependent second-nearest neighbor hopping [167]. The system is
a two-dimensional square lattice connected laterally to external leads. The full
Hamiltonian of the central system reads

$$\hat{\mathcal{H}} = \sum_{i,j} \left( \epsilon_{ij} \hat{c}_{i,j}^{\dagger} \hat{c}_{i,j} + \Delta_{ij} \hat{c}_{i,j}^{\dagger} \mathbf{\hat{\sigma}} \cdot \mathbf{m} \hat{c}_{i,j} - t_N \left( \hat{c}_{i+1,j}^{\dagger} \hat{c}_{i,j} + \hat{c}_{i,j+1}^{\dagger} \hat{c}_{i,j} + h.c. \right) \right)$$

$$- \sum_{i,j} \left( t_{i-1,j-1}^{ij} \hat{c}_{i,j}^{\dagger} \hat{\sigma}_z \hat{c}_{i-1,j-1} + t_{i-1,j-1}^{ij} \hat{c}_{i,j}^{\dagger} \hat{\sigma}_z \hat{c}_{i-1,j-1} + h.c. \right).$$

The operator $\hat{c}_{i,j}^{\dagger} = (\epsilon_{ij}^{+}, c_{i,j}^{\dagger})$ creates a particle at position $(i,j)$. Here
the first line at the right-hand side of Eq. (20) contains the energy on site
$(i,j)$ ($\sim \epsilon_{ij}$), the magnetic exchange ($\sim \Delta_{ij}$) and the nearest neighbor hopping
($\sim t_N$). The site energy is defined $\epsilon_{ij} = \epsilon_0 + \gamma_{ij}$, $\epsilon_0$ being the unperturbed onsite
energy and $\gamma_{ij} \in [-\Gamma/2, \Gamma/2]$ a random potential of strength $\Gamma$ that introduces
disorder in the system. The second line is the next-nearest neighbor hopping
that account for the disorder-driven spin-orbit coupled scattering. The next-
nearest neighbor hopping parameter reads $t_{i,j}^{ij} = it_N \alpha (\epsilon_{i,j'} - \epsilon_{i',j})$, where $\alpha$ is
the dimensionless spin-orbit coupling strength. This approach models extrinsic spin Hall effect and spin swapping on equal footing [167]. We emphasize that the calculations need to be performed over a very large (~10^5) number of disorder configurations to enable the buildup of the spin accumulation.

Figure 21 represents the ferromagnetic layer (green region with the black arrow) adjacent to the normal metal in which extrinsic spin-charge conversion processes occur. In this work, we apply a small potential gradient across the system along x, the magnetization of the ferromagnet is set transverse to the flowing current direction, i.e. along y, and we compute the two dimensional map of the spin density components, \( \delta S_x \) and \( \delta S_z \). The former is due to spin swapping, i.e. from the conversion of the injected spin current \( J_s^x \) (flowing along x and polarized along y) into \( J_s^y \) (flowing along y and polarized along x). The latter is due to the spin Hall effect that converts the current flowing along x into a spin current \( J_s^z \) (polarized along z). The spin swapping mechanism results in a spin accumulation \( \delta S_x \), that only survives close to the interface with the ferromagnet. Away from the interface, at a distance corresponding to the spin relaxation length, \( \delta S_x \) vanishes and \( \delta S_z \) builds up, due to spin Hall effect [167]. As discussed below, this effect leads to unexpected torques in ultrathin bilayers.

4.2.5. Spin Hall and swapping torques

Let us now consider a bilayer composed of a ferromagnet on top of a heavy metal. The spin Hall and spin swapping effects produce a spin accumulation at the interface with the ferromagnet, which results in two main effects: a spin torque on the magnetization [108, 132] and an associated magnetoresistance.
The diffusive model given above can be solved to obtain the torque exerted on the adjacent layer. Using the spin mixing conductance \([191]\) to represent the spin absorption at the magnetic interface, we obtain \([136]\)

\[
\tau_{\text{sh}} = \frac{\hbar}{2e} \frac{\theta_{\text{sh}}}{D_0} \eta_0 \left( -\tilde{g}_{r}^{\uparrow\downarrow} + |\tilde{g}_{r}^{\uparrow\downarrow}|^2 \right) \mathbf{m} \times \left( \mathbf{z} \times \mathbf{j}_e \right) + \tilde{g}_{t}^{\uparrow\downarrow} \mathbf{m} \times \left( \mathbf{z} \times \mathbf{j}_e \right)
\]

\[
\tau_{\text{sw}} = \frac{\hbar}{2e} \frac{\theta_{\text{sw}}}{D_0} \left( (|\tilde{g}_{r}^{\uparrow\downarrow}|^2 - \eta \tilde{g}_{r}^{\uparrow\downarrow}) \mathbf{m} \times \mathbf{j}_e + \eta \tilde{g}_{t}^{\uparrow\downarrow} \mathbf{m} \times \left( \mathbf{j}_e \times \mathbf{m} \right) \right), \tag{22}
\]

\[
D_0 \approx \eta_0 \left( \tilde{g}_{t}^{\uparrow\downarrow} \right)^2 + (1 + \tilde{g}_{r}^{\uparrow\downarrow}) (1 + \tilde{g}_{r}^{\uparrow\downarrow} + \theta_{\text{sw}})] \end{equation}

\[
- \theta_{\text{sw}} m_2^z (\tilde{g}_{t}^{\uparrow\downarrow} + (\tilde{g}_{r}^{\uparrow\downarrow} - \eta)(1 + \tilde{g}_{r}^{\uparrow\downarrow})
\]

Here \(\sigma_{\text{F},N}\) and \(\lambda_{e,f}^{\text{N}}\) are the conductivity and spin diffusion length of the ferromagnetic (normal metal) layer, and \(\mathbf{j}_e\) is the charge current density flowing in the normal metal. In order to keep the notation compact, we defined the effective spin Hall angle \(\theta_{\text{sh}} = \theta_{\text{sh}}(1 - \cosh^{-1} d_N/\lambda_{e,f}^{\text{N}})\) and normalized mixing conductances \(\tilde{g}_{r}^{\uparrow\downarrow} = 4\lambda_{e,f}^{\text{N}} g_{r}^{\uparrow\downarrow}/\sigma_{\text{F},N}\), where \(\tilde{\lambda}_{e,f}^{\text{N}} = \lambda_{e,f}^{\text{N}}/\tanh(d_N/\lambda_{e,f}^{\text{N}})\) is the effective spin diffusion length of the normal metal. Finally, \(\eta = \frac{4(1 - \gamma^2) g \lambda_{e,f}^{\text{N}}/\sigma_{\text{F}}}{1 + 4(1 - \gamma^2) g \lambda_{e,f}^{\text{N}}/\sigma_{\text{F}}}, \) and \(\eta_0 = 1 + \eta + \theta_{\text{sw}}, \) where \(g\) is the interfacial conductance. The spin Hall effect produces both a damping-like torque and a field-like torque. While the former is related to the interfacial absorption of the spin current via the real part of the mixing conductance \((\sim \tilde{g}_{t}^{\uparrow\downarrow})\), the latter is associated with spin precession at the interface via the imaginary part of the mixing conductance \((\sim \tilde{g}_{r}^{\uparrow\downarrow})\). In general, \(\tilde{g}_{t}^{\uparrow\downarrow} \ll \tilde{g}_{r}^{\uparrow\downarrow}\) \([192]\) and the spin Hall effect produces mainly a damping-like torque in the diffusive regime. Within this limit, the spin swapping torque emerges at the second order in spin-orbit coupling \((\sim \theta_{\text{sw}} \theta_{\text{sh}})\), and produces also both torques, the dominant one being the damping-like component. As we shall see below, the nature of the torque actually dramatically depends on the transport regime considered.

Because of spin transfer torque, the amount of spin density accumulated against the magnetic interface through spin Hall effect can be tuned by the ferromagnet’s magnetization direction. Indeed, the spin current injection in the ferromagnet is more efficient when the magnetization lies perpendicular to the polarization of the injected spins, i.e. normal to \(\mathbf{z} \times \mathbf{j}_e\). The modulation of the spin absorption when varying the magnetization direction results in the so-called spin Hall magnetoresistance, which reads \([190, 193, 194]\),

\[
\frac{\Delta \sigma_{xx}}{\sigma_{xx}} = \frac{\tilde{\lambda}_e^{\text{N}} \sigma_N}{d_N \sigma_N + d_F \sigma_F} \frac{\tilde{\lambda}_f^{\text{F}} \sigma_F}{(1 + \tilde{\lambda}_e^{\text{N}} \sigma_N/\tilde{\lambda}_f^{\text{F}} \sigma_F)(1 + \sigma_N/(2 \tilde{\lambda}_e^{\text{N}} \sigma_N/\tilde{\lambda}_f^{\text{F}} \sigma_F))}, \tag{24}
\]

Remarkably, the spin Hall magnetoresistance displays an angular dependence that is quite different from it bulk counterpart. While bulk anisotropic magnetoresistance of polycrystalline materials is proportional to \((\mathbf{m} \cdot \mathbf{j}_e)^2\), the spin Hall magnetoresistance is proportional to \(\mathbf{m} \cdot (\mathbf{z} \times \mathbf{j}_e)\), see Fig. 22(a)-(c). This effect has been used recently as an alternative tool to extract the spin Hall angle
Figure 22: (Color online) Anomalous transport in three different rotation configurations of the magnetization for a bilayer composed of a ferromagnet (yellow layer) deposited on top of a heavy metal (gray layer). Depending on the magnetization rotation plane, the isolated ferromagnet exhibits bulk anomalous Hall effect (AHE), anisotropic magnetoresistance (AMR) or planar Hall effect (PHE). When adjacent to a heavy metal, spin Hall effect (SHE) induces additional effects as described below (a) When the magnetization lies in the \((y,z)\) plane, no bulk magnetoresistance is present and only spin Hall effect-induced magnetoresistance can be detected; (b) When the magnetization lies in the \((x,y)\) plane, both bulk and spin Hall effect-induced magnetoresistance are present; (c) When the magnetization lies in the \((z,x)\) plane, only bulk magnetoresistance is present. Bulk and spin Hall effect-induced anomalous and planar Hall effects have the same angular dependence and therefore cannot be distinguished by angle-dependent measurements. (d) Dependence of the magnetoresistance of the metallic bilayer as a function of the ferromagnetic thickness when the magnetization lies in the \((x,z)\) plane (black lines) and when it lies in the \((y,z)\) plane (red lines), for different noble metal spin diffusion length: \(\lambda_{N}^{S} = 1.5, 5 \text{ and } 10 \text{nm} \) (dotted, solid and dashes lines). The red and black symbols have been collected from Ref. [199].

in ultrathin bilayers [195, 196, 197, 194]. We also emphasize that the combination between spin Hall and inverse spin Hall effect produces an additional Hall voltage, the ”spin Hall-induced Hall effect” via the imaginary part of the mixing conductance. One can compute this effect within the drift-diffusion model (not shown), but in general it remains one to two orders of magnitude smaller than the spin Hall magnetoresistance [198]. Figure 22(d) shows an example of theoretical fit using Eq. (24) for a Pt/Co/Pt sample. It is however noteworthy to mention that several experimental and theoretical studies have suggested that other effects might lead to a very similar magnetoresistance phenomena [199, 200, 201], that can be attributed to Rashba spin-orbit coupling [202, 203] or semiclassical size effects [204]. The debate is not settled and we do not intend to further discuss it.
Figure 23: (Color online) Schematics of (a) spin Hall and (b) spin swapping effects in a bilayer composed of a normal metal (blue) and a ferromagnet (yellow) with magnetization \( \mathbf{m} \) in the diffusive and Knudsen regimes, respectively. The charge current \( \mathbf{j}_e \) is injected in the plane of the layers and results in a spin current \( \mathbf{J}_s \) flowing perpendicular to the interface. Depending on the regime, this spin current induces either (a) a damping-like torque \( \sim \mathbf{m} \times [(\mathbf{z} \times \mathbf{j}_e) \times \mathbf{m}] \), or (b) a field-like torque \( \sim \mathbf{m} \times (\mathbf{z} \times \mathbf{j}_e) \). From [136].

The drift-diffusion model presented above is very practical as it provides explicit analytical formulae for the spin torque and magnetoresistance. However, it is limited to diffusive systems, i.e. _bilayers whose thickness is much larger than the mean free path_, such that the linear momentum memory is lost. Such an assumption is invalid in most experimentally relevant transition metal bilayers. To model these systems properly, one needs to treat the momentum-resolved transport. One way is for instance to use a Boltzmann description that tracks the non-equilibrium momentum distribution in the system [132, 198]. Another approach is to use a tight-binding model [136].

Consider a metallic bilayer composed of a spin-orbit coupled normal metal and a ferromagnet without spin-orbit coupling [see Fig. 23]. In the limit where the thickness of the normal metal is comparable to the mean free path, the spin Hall effect and spin swapping give rise to two different torques. The former generates a spin current that flows along the normal to the interface \( \mathbf{z} \) with a spin polarization along \( \mathbf{z} \times \mathbf{j}_e \) and results in a damping-like torque on the form \( \sim \mathbf{m} \times [(\mathbf{z} \times \mathbf{j}_e) \times \mathbf{m}] \), see Fig. 23(a). In addition, electrons flowing in the ferromagnet acquire a spin polarization along \( \mathbf{m} \) and may scatter towards the normal metal. Once in the normal metal, these electrons experience spin swapping: upon scattering on spin-orbit coupled impurities, they experience a spin-orbit field oriented normal to the scattering plane [i.e. along \( (\mathbf{z} \times \mathbf{j}_e) \)] and about which their spin precess [184, 167, 136]. Upon this reorientation, a spin current polarized along \( \mathbf{m} \times (\mathbf{z} \times \mathbf{j}_e) \) is injected into the ferromagnet and induces a _field-like torque_, see Fig. 23(b), even in the absence of inverse spin galvanic effect. This effect only survives as long as the linear momentum is well defined, i.e. in a regime where the thickness of the normal metal is comparable to the mean free path. This regime is called the Knudsen regime. When the mean free path becomes much smaller than the normal metal thickness, the system enters the diffusive regime and Eqs. (21)-(22) apply.

So, in summary, as long as the thickness of the normal metal is comparable
to the mean free path, one should obtain a torque of the form

\[ \tau = \tau_{\text{sh}} \mathbf{m} \times [(\mathbf{z} \times \mathbf{j}_e) \times \mathbf{m}] + \tau_{\text{sw}} \mathbf{m} \times (\mathbf{z} \times \mathbf{j}_e), \]

which is quite different from the torques obtained in the diffusive regime [see Eqs. (21)-(22)]. These two effects dominate in distinct disorder regimes: spin Hall effect necessitates strong disorder, while spin swapping survives even for weak disorder. Hence, the nature of the torque should dramatically change from one regime to the other [136]. To confirm this phenomenological picture, we computed the spin transport in a magnetic bilayer using a tight-binding model similar to the one presented in the previous Section [205, 167]. In the present case, instead of injecting the current perpendicular to the interface (Fig. 21), the current is now injected along the interface. We calculate the non-equilibrium spin density in the ferromagnet \( \delta S \) and compute the torque \( \tau = (2\Delta/\hbar) \mathbf{m} \times \delta S \), which is then parsed between damping-like (\( \tau_{\text{DL}} \)) and field-like (\( \tau_{\text{FL}} \)) components. Figure 24 displays the ratio \( \tau_{\text{DL}}/\tau_{\text{FL}} \) as a function of disorder and spin-orbit coupling strengths. We find that the torque is dominated by the field-like component in the weak disorder/weak spin-orbit coupling regime, while it is dominated by the damping-like component in the strong disorder/strong spin-orbit coupling regime. When spin Hall effect dominates (strong disorder regime) the torque is mostly damping-like, \( \tau_{\text{DL}} > \tau_{\text{FL}} \), and when spin swapping dominates (weak disorder, Knudsen regime) the torque is mostly field-like, \( \tau_{\text{FL}} > \tau_{\text{DL}} \).

![Graph showing the ratio between the magnitude of the field-like torque and damping-like torque, \( \tau_{\text{DL}}/\tau_{\text{FL}} \), as a function of disorder strength and spin-orbit coupling strength. The graph is color-coded with red indicating higher values and blue indicating lower values. The dashed line indicates \( \tau_{\text{DL}}/\tau_{\text{FL}} = 1 \). From [136].

These simulations demonstrate that in ultrathin bilayers field-like torques can emerge from spin-dependent scattering in the normal metal. A necessary
condition is that the thickness of the normal metal must be of the order of the
mean free path. This is in fact realized in most of the experiments on spin-orbit
torques (but also spin Seebeck effect and spin pumping) where the magnetic
multilayers have thicknesses from 10 nm down to less than 1 nm \[114, 206, 207,
208\]. Since the grain size ranges from 5 to 10 nm in sputtered thin films, the
transport is not expected to be diffusive and extrinsic spin swapping could lead
to sizable field-like torque (even in the absence of interfacial inverse spin galvanic
effect - see below). Magnetic bilayer involving a light metal doped with heavy
elements, such as Cu(Bi), Cu(Ir) or Ag(Au), could be an interesting candidate
to observe spin-swapping torque. These materials display large extrinsic spin-
orbit coupled scattering \[176, 177\], and hence extrinsic spin swapping, together
with ensuring the absence of inverse spin galvanic effect. Recent experiments
on Cu-Au alloys have reported unconventional temperature-dependence of both
damping-like and field-like torque components. This observation supports the
presence of extrinsic, disorder-driven spin-charge conversion mechanisms taking
place in the Cu-Au alloy and could be an indication of the presence of spin
swapping \[116\].

4.3. Inverse spin galvanic effect

The second class of mechanisms that leads to spin-orbit torques in magnetic
multilayers is the inverse spin galvanic effect at the interface with the ferromagnet.
This effect has been modeled by several authors using the toy model of
the magnetic Rashba gas \[129, 130, 209, 133, 210, 211, 202, 134, 135, 212\], and
magnetic Dirac gas \[213, 68, 214, 215, 216, 217\]. These models are quite con-
venient as they are analytically solvable. Several techniques can be used, such
as semiclassical Boltzmann formula, quantum kinetics or Kubo formulæ. For
instance, in translationally invariant systems, the non-equilibrium spin density
induced by an external electric field reads

\[
\delta S = \frac{\hbar}{2\pi \Omega} \int d\epsilon \partial_\epsilon f(\epsilon) \text{Tr} \left[ \xi \tilde{G}_e^{(R)}(\mathbf{v} \cdot \mathbf{E})(\tilde{G}_e^{(A)} - \tilde{G}_e^{(R)}) \right]
\]

(26)

Here, \(\tilde{G}_e^{(A)}\) is the perturbed retarded (advanced) Green’s function, \(f(\epsilon)\) is
Fermi-Dirac distribution, \(\mathbf{v}\) is the velocity operator, \(\mathbf{E}\) the external electric
field and \(\xi\) is the vertex-corrected spin operator. The non-equilibrium spin
density possesses three contributions that account for Fermi surface and Fermi
sea electrons. It turns out that the first term, \(\sim \text{Tr}[\xi \tilde{G}_e^{(R)}(\mathbf{v} \cdot \mathbf{E})\tilde{G}_e^{(A)}]\), dominates
in the weakly disordered metallic regime. In the limit of weak spin-independent
constant energy broadening, \(\Gamma \to 0\), one can parse this term into two main
contributions \[135\]
\[
\delta \mathbf{S}^\text{intra} = \frac{\hbar}{2\Gamma \Omega} \sum_{n,k} \langle n, k | \hat{\varsigma} | n, k \rangle \langle n, k | \hat{\mathbf{v}} \cdot e \mathbf{E} | n, k \rangle \delta (\epsilon_{n,k} - \epsilon_F), \quad (27)
\]

\[
\delta \mathbf{S}^\text{inter} = \frac{\hbar}{\Omega} \Im \sum_{n,n',k} \langle n, k | \hat{\varsigma} | n', k \rangle \langle n', k | \hat{\mathbf{v}} \cdot e \mathbf{E} | n, k \rangle \frac{f_{n,k} - f_{n',k}}{(\epsilon_{n,k} - \epsilon_{n',k})^2}. \quad (28)
\]

where \( n \) and \( n' \) refer to eigenstates of the unperturbed Hamiltonian, and \( \Im \) takes the imaginary part. The first term involves only transitions within a same band, while the second term involves transition between different bands [135, 218].

Since the latter arises from the perturbation of the eigenstates in the presence of electric field, it is inversely proportional to the energy difference between different bands \( \sim 1/\epsilon_{n,k} - \epsilon_{n',k} \), similarly to the intrinsic spin Hall effect given in Eq. (17). Furthermore, the intraband contribution is proportional to \( 1/\Gamma \), i.e. to the current density, while the interband contribution is independent of disorder in this limit and can be related to the Berry curvature in mixed spin-momentum space [112].

The distinction between these two terms is not purely technical, it has important implications in terms of spin-orbit torques. As a matter of fact, each contribution produces a different torque. If one applies time inversion,

\[
\langle n, k | \hat{\varsigma} | n', k \rangle \rightarrow - (\langle n, k | \hat{\varsigma} | n', k \rangle)^*, \quad (29)
\]

\[
\langle n', k | \hat{\mathbf{v}} \cdot e \mathbf{E} | n, k \rangle \rightarrow - (\langle n', k | \hat{\mathbf{v}} \cdot e \mathbf{E} | n, k \rangle)^*, \quad (30)
\]

we see that \( \delta \mathbf{S}^\text{intra} \) is even, while \( \delta \mathbf{S}^\text{inter} \) is odd [218]. In other words,

\[
\delta \mathbf{S}^\text{intra}(\mathbf{m}) = \delta \mathbf{S}^\text{intra}(-\mathbf{m}), \quad (31)
\]

\[
\delta \mathbf{S}^\text{inter}(\mathbf{m}) = -\delta \mathbf{S}^\text{inter}(-\mathbf{m}). \quad (32)
\]

As a result, the intraband contribution produces a torque that is odd as a function of the magnetization direction, while the interband contribution produces a torque that is even upon magnetization reversal. These two types of torques are referred to as field-like and damping-like, respectively. More specifically, in the case of a two dimensional electron gas with both magnetism and Rashba spin-orbit coupling, one obtains

\[
\tau_R = (2\Delta/\hbar) \mathbf{m} \times \delta \mathbf{S} = \tau_{FL} \mathbf{m} \times (\mathbf{z} \times e \mathbf{E}) + \tau_{DL} \mathbf{m} \times [(\mathbf{z} \times e \mathbf{E}) \times \mathbf{m}], \quad (33)
\]

the first term being attributed to intraband contribution, while the second is due to the interband contribution [133, 135, 134, 212]. The latter possesses exactly the same form as the damping-like torque coming from spin Hall effect and, as we shall see below, it is often hard to distinguish between them, even theoretically. Interestingly, in the case of the magnetic surface of topological insulators described by the massive Dirac Hamiltonian, the torque becomes [217]

\[
\tau_D = \tau_{FL} \mathbf{m} \times (\mathbf{z} \times e \mathbf{E}) + \tau_{DL} m_z \mathbf{m} \times e \mathbf{E}. \quad (34)
\]
While the field-like torque remains the same as in the Rashba gas, the damping-like torque now vanishes when the magnetization lies in the plane of the interface, a mechanism that is specific to topological insulators but can also be recovered in the strong Rashba limit for two-dimensional magnetic Rashba gases [135].

Unfortunately, the Rashba model used in many of the recent studies of spin-orbit torques presents major flaws that limit its quantitative predictive power. First, as already mentioned, it formally applies only to two-dimensional electron gases with sharp interfaces and completely miss the interfacial orbital physics. Second, its simplicity leads to pathological behaviors that have been put forward recently in the context of intrinsic spin Hall effect and Rashba torque. As a matter of fact, both intrinsic Rashba spin Hall effect [179, 219] and damping-like Rashba torque [212] vanish when taking into account vertex corrections, due to the unrealistically simple energy dispersion of the gas. To add to the confusion, Ado et al. [220, 221] recently demonstrated that the first Born approximation itself is insufficient to compute the intrinsic non-equilibrium properties, and that one should add higher order terms in the diagrammatic expansion (the authors specifically studied the $X$ and $\Psi$ diagrams). These studies emphasize the subtleties of the treatment of impurity self-averaging in these simple models. One way to circumvent these difficulties is to consider realistic systems, where the band dispersion is much more complicated than the simple free-electron parabolic dispersion (or than the infinite Dirac cone, in the case of topological insulator surfaces).

4.3.1. Inverse spin galvanic effect at realistic interfaces

Recently, Haney et al. [132] have computed the current-driven field-like torque in Pt/Co(111). The \textit{ab initio} method is based on a linear combination of spherical orbitals and the current and torque are calculated within the relaxation time approximation. This approach disregards the spin Hall effect or any intrinsic contributions to the inverse spin galvanic effect. These calculations, reported on Fig. 25(a), first show that in spite of the high complexity of the band structure [see Fig. 8(b,c)], sizable inverse spin galvanic effect emerges at the interface between Pt and Co. The magnitude of the Rashba field (about 100 Oe for $10^8$A/cm$^2$) is consistent with the experimental observations [223, 109]. Moreover, Fig. 25(a) displays the current-driven Rashba when the induced magnetism of the Pt is turned off (diamonds) and when the spin-orbit coupling on Pt is turned off (circles). It appears that while Pt magnetism has a negligible effect on the Rashba field, its spin-orbit coupling is the main driving force, confirming the simple Rashba scenario evoked previously. Nonetheless, even in the absence of Pt spin-orbit coupling, we emphasize that the Rashba field does not vanish since Co spin-orbit coupling is still present. This produces a Rashba field of the same sign but an order of magnitude smaller. Indeed, the sign of the Rashba field is associated with the distortion of the wave function at the interface, which is fixed by the Co/Pt slab ordering. Hence, one can speculate that such a torque exists at Co/MgO interfaces and can be controlled by oxygen and, by extension, gate voltage, in the same spirit as DMI (see Section 3 and
The inverse spin galvanic effect has also been investigated from first principles at the surface of Bi$_2$Se$_3$ using the ATK package [222]. Bi$_2$Se$_3$ is a topological insulator, namely it is insulating in its bulk and possesses highly conductive, spin-orbit coupled surface states. The spatial profile of the local density of states reported on Fig. 25(b) shows the extension of the surface states over 2 nm on each side of the slab. Although the system is not magnetic, one can clearly see the buildup of the spin accumulation across the slab, as displayed in Fig. 25(c).

We emphasize that the extension of "surface states" is actually very large (2 nm) and is comparable to the thicknesses of normal metals in magnetic bilayers (from 1 to 5 nm). Therefore, interfacial orbital hybridization and scattering against defects can severely impact the spin physics in this extended region. Considering the recent experimental interest for spin-orbit torques at the magnetic surface of topological insulators [124, 125, 126, 127, 128], more extensive and systematic investigations of such systems are highly desirable.

Freimuth et al. [218, 80, 224] have recently developed an intensive effort towards the comprehensive computation of current-induced torques in magnetic thin films. Based on the full potential linear augmented plane wave method implemented in FLEUR and computing Kubo-Bastin formula, thereby accounting for intrinsic spin Hall torque as well as intrinsic and extrinsic inverse spin galvanic effect, the authors have investigated and characterized the spin-orbit torques in Pt/Co(111), W/Mn(001) and L1$_0$ FePt/Pt. These calculations con-
firmed that spin-orbit torques are composed of both field-like and damping-like
torques, the latter being produced by interband transitions only. By calcul-
ating both spin-orbit torques and spin currents, the authors showed that in
the case of Pt/Co(111), both damping-like and field-like torques correlate fa-
vorably with absorption of spin current, as displayed in Fig. 26(a) and (b).
However, by capping the Co layer by either Al or O adatoms, the damping-like
torque is only slightly affected (its magnitude changes up to 50%, but it re-
mains correlated with the spin current - see Fig. 26), while the field-like torque
is dramatically altered: it does not correlate with the spin current anymore and
can even change its sign. This study emphasizes the different physical origin of
these two components, the field-like torque being much more sensitive to inter-
faces than the damping-like torque. Overall, these calculations seem to confirm,
although with a much higher level of complexity, the spin Hall and Rashba sce-
narii evoked above. Finally, let us mention that Ref. [224] also computed the
thermally-induced spin-orbit torque in L1$_0$ FePt/Pt, showing that reasonable
thermal gradients (∼0.1 K/nm) are expected to generate detectable torques.

Figure 26: (Color online) Layer-resolved field-like (left panels) and damping-like torques (right
panels) in Pt/Co, Pt/Co/O and Pt/Co/Al stacks. The torques are represented by the filled
symbols, while the spin currents associated with them are represented by open symbols. The
Co region is denoted by the shaded area. From Ref. [218].
5. Unconventional dynamics

In the previous Sections, we have seen that transition metal interfaces encompass several exotic effects enabled by spin-orbit coupling: Rashba-type spin splitting, Dzyaloshinskii-Moriya antisymmetric exchange interaction, and spin-orbit torques. As a result, the magnetic texture at these interfaces is likely to be chiral and can be manipulated electrically. In this last Section, we are interested in two aspects of the chiral magnetic textures: their energy dissipation and the additional "topological" torque that flowing currents exert on these textures.

5.1. Chiral Damping

5.1.1. Fundamentals of magnetic damping

The magnetic damping arises from various mechanisms involving non-linear spin waves processes [225, 226, 227] such as two- [228, 229, 230] and three-magnon interactions [231] (dominant in magnetic insulators [232]) as well as electronic processes driven by spin relaxation [233, 234, 235] (dominant in metals). The latter mechanisms are of primary interest for us because of the dominant role of spin-orbit coupling. In the hydrodynamic limit, the magnetic damping is a non-local, anisotropic $3\times3$ tensor of the form [236]

$$\partial_t \mathbf{m}(\mathbf{r}, t)_{\text{diss}} = \mathbf{m}(\mathbf{r}, t) \times \int d\mathbf{r}' \alpha(\mathbf{r}, \mathbf{r}') \cdot \partial_t \mathbf{m}(\mathbf{r}', t).$$

(35)

In an isotropic magnetic material, the dissipation reduces to the well-known Gilbert damping form, $\partial_t \mathbf{m}(\mathbf{r}, t)_{\text{diss}} = \alpha \mathbf{m} \times \partial_t \mathbf{m}$. However, in magnetic metals presenting a strong (bulk or interfacial) magnetic anisotropy, one can reasonably expect that such anisotropy gets imprinted in the magnetic damping constant [237, 3]. Mills and Rezende [3] showed that in a magnetic material with uniaxial anisotropy axis $\mathbf{z}$, the damping reads

$$\partial_t \mathbf{m}^z_{\text{diss}} = \epsilon^z \mathbf{m} \times \mathbf{z} \partial_t m_z + \epsilon^\perp m_z \mathbf{z} \times \partial_t \mathbf{m}.$$  

(36)

This anisotropic damping is derived from general considerations and, in the particular case considered here, only affects the components of the magnetization transverse to the anisotropy direction $\mathbf{z}$. Although not observed yet, this anisotropic damping should be quite large in systems with interfacial perpendicular magnetic anisotropy.

Physically, the mechanism responsible for the magnetic damping in metals can be summarized as follows: the precessing magnetization excites spin-orbit coupled electron-hole pairs that relax their own spin angular momentum through momentum relaxation processes via defects, impurities or phonon scattering [234]. This process is usually modeled by the so-called breathing Fermi surface model that relates the damping constant to the angular dependence of the electronic energy, $\partial_\theta \epsilon_{n,k}$, and to the momentum scattering time $\tau$ [238]

$$\lambda_{\text{BFS}} = \frac{g^2 \mu^2}{\hbar^2 \Omega} \sum_{n,k} (\partial_\theta \epsilon_{n,k})^2 \delta(\epsilon_{n,k} - \epsilon_F).$$  

(37)
The Gilbert damping is simply defined \( \alpha = \lambda M_s / \gamma \), where \( M_s \) is the saturation magnetization and \( \gamma \) is the gyromagnetic ratio. This formula is valid for \( \tau \to +\infty \) and only considers electrons close to the Fermi level. An equivalent picture was also developed by Kambersky by considering the spin relaxation of long wavelength magnons \( (q \to 0) \) \([239, 240]\), yielding the so-called torque correlation formula

\[
\lambda_{\tau} = \frac{g^2 \mu_B^2}{\pi \hbar \Omega} \left( \frac{\hbar}{2\tau} \right)^2 \sum_{n,m,k} \frac{|\langle n, k | \hat{\sigma}^- , \hat{H}_{\text{so}} | m, k \rangle|^2}{[(\epsilon_F - \epsilon_{n,k})^2 + (\hbar/2\tau)^2][[(\epsilon_F - \epsilon_{m,k})^2 + (\hbar/2\tau)^2]}. \tag{38}
\]

In the limit of weak scattering Eq. (38) reduces to Eq. (37) \([234]\). Equation (38) is more general since it accounts for both intraband \( \propto \tau \) and interband contributions \( \propto 1/\tau \), and therefore applies to a wider range of disorder regime \([241, 235]\). When applied to realistic band structure, such as Co, Ni or Fe, the magnetic damping adopts the symmetries of the crystal structure, resulting in rotational and orientational anisotropic damping \([242]\), as illustrated in Fig. 27. The damping anisotropy calculated in these systems can be as large as 50%. One has to recall that the magnetocrystalline anisotropy for these bulk ferromagnets is of the order of a few \( \mu \text{eV/atom} \). One can reasonably speculate that damping anisotropy in ultrathin multilayers with interfacial perpendicular magnetic anisotropy of the order of a few \( \text{meV/atom} \) should be actually gigantic.

Figure 27: Magnetic damping in bulk Co from first principle calculations, using the effective field approach. The magnitude of the magnetic damping exhibits a significant anisotropy depending on the orientation of the precessing magnetization. In strongly disorder systems \( (\tau^{-1} \to +\infty) \), this anisotropy vanishes. From Ref. [242].

The two formulae presented above are quite popular but do not account for non-locality. One way to circumvent this limitation is to derive the magnetic damping within the linear response theory (see for instance \([243, 244]\) or the
Supplementary material of [245]). Let us consider a general Hamiltonian, $\hat{H} = \hat{H}_0 + \Delta \sigma \cdot \hat{m}$, where the second term connects the itinerant electron spins $\sigma$ with the local magnetic moment $\hat{m}$. We now introduce a small perturbation to the magnetization $\hat{m} \rightarrow \hat{m} + \delta \hat{m}$ that is time-dependent, $\partial_t \delta \hat{m} \neq 0$. Hence, the moving magnetization pumps a non-equilibrium spin density $\delta S = \chi \cdot \partial_t \hat{m}$, which is turns exerts a torque on the local magnetization, $\tau = (2\Delta/\hbar)\hat{m} \times \delta S \sim \hat{m} \times [\chi \cdot \partial_t \hat{m}]$. This torque modifies the dynamics of the magnetization, depending on the symmetry of the tensor $\chi$ upon magnetization reversal. Indeed, one can rewrite $\chi(\hat{m}) = \chi^{\text{odd}} + \chi^{\text{even}}$, where $\chi^{\text{odd}}(\hat{m}) = -\chi^{\text{odd}}(-\hat{m})$ and $\chi^{\text{even}}(\hat{m}) = \chi^{\text{even}}(-\hat{m})$. As a result, the torque possesses two components, $\tau = \tau^{\text{odd}} + \tau^{\text{even}}$, renormalizing the magnetization precession rate, and inducing a magnetic damping, respectively. From Kubo formula, one obtain $\tau = m \times \int d^3r' (\alpha \cdot \partial_t \hat{m})$, where the tensor $\alpha(r, r')$ has the components [244, 245]

$$
\alpha^{ij}(r, r') = \frac{\Delta^2}{\pi \Omega} \int d\epsilon f(\epsilon) \text{Tr}[\hat{\gamma}_i \hat{G}^R_{\epsilon}(r, r') \sigma_j (\hat{G}^A_{\epsilon}(r', r) - \hat{G}^R_{\epsilon}(r', r))] + \frac{\Delta^2}{\pi \Omega} \int d\epsilon f(\epsilon) \text{Tr}[\hat{\gamma}_i \partial_r \hat{G}^R_{\epsilon}(r, r') \sigma_j \hat{G}^A_{\epsilon}(r', r) - \hat{\gamma}_i \hat{G}^R_{\epsilon}(r, r') \sigma_j \partial_r \hat{G}^R_{\epsilon}(r', r)].
$$

The vertex correction included in $\hat{\gamma}$ is crucial to ensure the proper treatment of the 1st Born approximation [244]. Similarly to the spin-orbit torques discussed in the previous Section, Eq. (26), the non-local magnetic damping possesses a Fermi surface contribution as well as a Fermi sea contribution. This formula is quite convenient to compute the non-local magnetic damping, including its chiral contribution, although no such calculation has been performed yet, to the best of our knowledge. Notice finally that in the case of the magnetic surface of topological insulators, the magnetic damping is directly proportional to the conductivity tensor. Indeed, since $\hat{H} = v \hat{p} \cdot (\hat{z} \times \hat{\sigma})$, $\hat{v} = \partial_y \hat{H} = v(\hat{z} \times \hat{\sigma})$, establishing a direct equivalence between spin dynamics (spin-spin correlation) and charge dynamics (current-current correlation).

Another source of magnetic damping in thin films is the spin pumping originally identified by Tserkovnyak et al. [246, 247]. In this mechanism, a precessing magnetization pumps a spin current out of the magnetic system, through an interface for instance. This spin current, $J_{\text{interf}} = \hbar (g^{\uparrow \downarrow} / 4 \pi) \hat{m} \times \partial_t \hat{m}$, is then absorbed by the adjacent layer through spin relaxation. As a reaction, the magnetic damping of the ferromagnet is enhanced [248, 249, 250, 251, 252].

Concretely, the spin pumping contribution to the magnetic damping reads $\alpha_{\text{sp}} = A g^{\uparrow \downarrow}$, where $g^{\uparrow \downarrow}$ is the real part of the spin mixing conductance and $A$ is a coefficient that accounts for the spin current backflow in the adjacent metals and that vanishes in the limit of infinite spin diffusion length. The concept of spin pumping has been recently extended to the case of time-dependent magnetic textures [253, 254, 255, 256, 36]. When a magnetic texture evolves in time, spin pumping acts locally so that itinerant electrons experience a spin-dependent emergent electromagnetic field induced by the texture. This emergent electromagnetic field is discussed in more details in Section 5.2. Zhang and Zhang
recently showed that this field contributes to energy dissipation in magnetic textures \cite{257}. In this case, the damping adopts a tensorial form, $\mathbf{\tau} = \mathbf{m} \times \mathbf{D} \cdot \partial \mathbf{m}$, where

$$D_{ij} = \xi \sum_k (\mathbf{m} \times \partial_k \mathbf{m})_i (\mathbf{m} \times \partial_k \mathbf{m})_j,$$  \hspace{1cm} (40)

and $\xi$ is a material dependent parameter ($\xi \sim 0.5 - 1 \text{ nm}^2$). This additional damping is second order in the spatial gradient of the magnetization and therefore expected to be only significant in sharp magnetic textures such as vortices or skyrmions.

5.1.2. Phenomenological theory of chiral damping

Most of the theories of magnetic damping developed to date assume the long wavelength limit ($q \rightarrow 0$). Since the energy relaxation rate of spin waves depends on their wave vector (the higher the spin wave energy, the stronger its dissipation), one expects that the energy dissipation of magnetic textures should depend on magnetization gradient \[see Eq. (40)\]. As discussed above, in magnets with inversion symmetry, the magnetic damping is enhanced by a corrective term of the order of $1/\lambda_{dw}^2$, where $\lambda_{dw}$ is the magnetic exchange length. However, in magnetic systems lacking inversion symmetry such as the systems in which Dzyaloshinskii-Moriya is observed, the energy dissipation becomes linear in the magnetization gradient and may depend on the chirality of the magnetic texture.

As a matter of fact, in the limit of smooth textures, the tensorial components of the damping is a function of the magnetization direction and of its spatial gradients, $\alpha^{ij} = \alpha^{ij}(\mathbf{m}, \nabla \mathbf{m})$, such that, to the first order in magnetization gradient \[258\]

$$\alpha^{ij} = \alpha^{ij}_0 + \sum_{lm} K^{ij}_{lm} m_l m_m + \sum_{klm} L^{ij}_{klm} m_k \partial_l m_m. \hspace{1cm} (41)$$

The first term is the isotropic damping, the second term amounts for the anisotropic contribution and the third term is the chiral damping. Only terms bilinear in magnetization direction $m_i$, i.e. even under time reversal symmetry, are retained in the expansion. In systems possessing inversion symmetry, the third term of Eq. (41) vanishes, $L^{ij}_{klm} = L^{ij}_{mlk}$. However, where inversion symmetry is broken, $L^{ij}_{klm} = -L^{ij}_{mlk}$, and this term reduces to Lifshitz antisymmetric invariants, $\propto m_k \partial_l m_m - m_m \partial_l m_k$. This functional dependence is similar to the Dzyaloshinskii-Moriya interaction: since both effects are bilinear in magnetization and fulfill Neumann’s principle, they adopt the same general form. In addition though, Onsager reciprocity imposes $\alpha^{ij} = \alpha^{ji}$, and hence, one can construct a chiral damping up to the linear order in magnetization gradient based on symmetry arguments. For instance, in a cubic system with bulk spatial inversion symmetry breaking, the chiral damping becomes

$$\alpha^{ij} = \alpha^{ij}_0 + \alpha^{ij}_{3d} \lambda_{dw} \mathbf{m} \cdot (\nabla \times \mathbf{m}), \hspace{1cm} (42)$$
where $\lambda_{dw}$ defines the characteristic exchange length. In a two-dimensional system with interfacial symmetry breaking along $z$, i.e., invariant under $C_{\infty z}$ rotation symmetry, the damping takes the form

$$\alpha^{ij} = \alpha_{0}^{ij} + \alpha_{2}^{ij} \lambda_{dw} \mathbf{m} \cdot [(\mathbf{z} \times \nabla) \times \mathbf{m}], \quad (43)$$

Other forms of Dzyaloshinskii-Moriya interaction have been derived in the case of magnetic interfaces for instance [259].

5.1.3. Microscopic origin of chiral damping

As discussed in Section 4, there are two manners to exert a torque on a magnetic order parameter: either by generating a non-equilibrium spin density $\delta \mathbf{S}$, or by injecting a spin current in the magnet $\mathbf{J}_s$. In the first case, the torque reads $\tau = (2\Delta / \hbar) \mathbf{m} \times \delta \mathbf{S}$, while in the second case it is associated with the spatial gradient of the spin current $\tau = -\nabla \cdot \mathbf{J}_s$. These two pictures are equivalent in the absence of spin-orbit coupling, but may lead to different torques when spin-orbit is present. We present below four phenomena that can lead to chiral magnetic damping.

Rashba spin-orbit coupling. In ferromagnets with interfacial Rashba spin-orbit coupling, it has been shown that the magnetic damping adopts the form of a tensor linear in both magnetization gradient and Rashba strength [206, 202] [see Fig. 28(a)]. Two distinct mechanisms can be identified. First, as already mentioned, a time-dependent magnetic texture generates an effective spin-dependent electric field on the itinerant electrons, producing a charge current $j_{e,i} \sim \mathbf{m} \cdot (\partial_i \mathbf{m} \times \partial_t \mathbf{m})$. Through inverse spin galvanic effect, this charge current induces a spin density that exerts a torque on the magnetization $\tau \sim \alpha_R \mathbf{m} \times (\mathbf{z} \times \mathbf{J}_s)$, where $\alpha_R$ is the Rashba parameter. A symmetric effect coexists: the precessing magnetization pumps a spin-polarized current through spin galvanic effect, $\mathbf{J}_s \sim \alpha_R \mathbf{m} \otimes \mathbf{z} \times \partial_t \mathbf{m}$ (we remind that the spin current is a tensor in the spin⊗real spaces). The corresponding spin current is then absorbed by the magnetic texture through $\tau = -\nabla \cdot \mathbf{J}_s$. As a result, the total magnetic damping is linear in Rashba parameter, as well as in magnetization gradient, and [206, 202, 260]

$$\tau \sim [(\mathbf{z} \times \partial_t \mathbf{m}) \cdot \nabla] \mathbf{m} - (\mathbf{z} \times \nabla) \times (\mathbf{m} \times \partial_t \mathbf{m}). \quad (44)$$

s-d antisymmetric interaction. As demonstrated in Ref. [70], in transition metal ferromagnets both localized ($pd$ hybridized) and delocalized electrons ($spd$ hybridized) contribute to DMI and therefore one can parse the total spin moment $\mathbf{S}_i$ into localized ($d$-dominated) and delocalized ($s$-dominated) contributions $\mathbf{S}_i = \mathbf{S}_i^d + \mathbf{s}_i^s$. The resulting DMI between sites $i$ and $j$ can be phenomenologically rewritten up to the linear order in $\mathbf{s}^s$ as $D_{ij} \cdot \mathbf{S}_i \times \mathbf{S}_j = D_{ij}^{dd} \cdot \mathbf{S}_i^d \times \mathbf{S}_j^d + D_{ij}^{sd} \cdot \mathbf{S}_i^d \times \mathbf{s}_j^s$ (neglecting a higher order term $\sim \mathbf{s}_i^s \times \mathbf{s}_j^s$). The first term only involves orbital overlap between localized states while the second term describes the chiral exchange between the local and itinerant spins. In the
continuous limit, the spin-orbit coupling Hamiltonian of the itinerant electrons can be written as

\[ \hat{H}_{\text{sd}} = \frac{\alpha_D}{\hbar} \sigma \cdot [(z \times \hat{p}) \times \mathbf{m}], \]  

(45)

where \( \alpha_D = D_{\text{sd}} a \) (\( a \) is the lattice parameter) is the strength of the \( s-d \) DM interaction. Equation (45) suggests that itinerant spins flowing through the magnetic texture illustrated on Fig. 28(b) experience both the inhomogeneous exchange field \( \sim \mathbf{m} \), and the inhomogeneous, texture-dependent \( s-d \) DM field \( \sim (z \times \nabla) \times \mathbf{m} \). The cooperation of these two terms introduces a distortion of the Fermi surface that depends on the magnetization gradient and therefore promotes chiral damping. Within the relaxation time approximation, one obtains a damping torque \[ \tau \sim \{[(z \times \nabla) \times \mathbf{m}] \times (\mathbf{m} \times \partial_t \mathbf{m}) \}_{\perp}, \]  

(46)

where the subscript \( \perp \) refers to the part that is transverse to the magnetization. Notice that the chiral damping arising from \( s-d \) DMI (\( \propto D_{\text{sd}} \)) does not necessarily scale with the DMI itself (\( \propto D_{\text{dd}} \)) as both effects, chiral damping and asymmetric exchange, involve different electron orbitals.

Anomalous spin pumping. This mechanism is illustrated in Fig. 28(c) and arises from the interplay between spin motive force and anomalous Hall effect. As mentioned above, time-dependent spin textures generate a local charge current \( j_{e,i} \sim \mathbf{m} \cdot (\partial_i \mathbf{m} \times \partial_t \mathbf{m}) \). When anomalous Hall effect is present in the ferromagnet, this charge current \( j_e \) can be converted into a spin Hall current of the form \( eJ_{s,i} = \theta_{\text{sh}} \mathbf{m} \otimes (\mathbf{m} \times j_e) \), i.e. flowing along the direction \( \mathbf{m} \times j_e \) and spin polarized along \( \mathbf{m} \). If this spin Hall current can be injected out of the ferromagnet into an adjacent spin sink, it exerts a dissipative torque on the magnetization, similarly to the well-known spin pumping mechanism [246]. Concretely, considering a domain wall along \( x \) deposited on a normal metal with an interface normal to \( z \) [Fig. 28(c)], as long as the magnetization \( \mathbf{m} \) has a non-zero component along \( y \), the spin Hall current that is injected in the adjacent metal along \( z \) is spin polarized along \( y \) and exerts the torque

\[ \tau \sim [(\partial_x \mathbf{m} \times \partial_t \mathbf{m}) \cdot \mathbf{y}] \mathbf{m} \times (\mathbf{y} \times \mathbf{m}). \]  

(47)

This damping torque vanishes when the wall is either in Bloch (\( \varphi = \pi/2 \)) or Néel configuration (\( \varphi = 0 \)) and is maximum in-between.

Spin swapping. The last mechanism is spin swapping, discussed in Section 4 and illustrated in Fig. 28(d). A precessing magnetization pumps a spin current, polarized along \( J_{s,z}^{\text{amp}} \sim \mathbf{m} \times \partial_t \mathbf{m} \otimes \mathbf{z} \), into the normal metal [246]. Such a spin current can be converted into a charge current through inverse spin Hall effect [261], but also enhances the magnetic damping of the ferromagnet [246]. Upon spin swapping this pumped spin current is converted into another spin current \( J_{s,z}^{\text{sw}} \sim \mathbf{y} \times (\mathbf{m} \times \partial_t \mathbf{m}) \otimes \mathbf{z} \) (\( \mathbf{y} \) being the direction of the spin-orbit field perpendicular to the scattering plane). While this new spin current does
Figure 28: (Color online) Illustration of different microscopic mechanisms at the origin of chiral damping: (a) the interplay of inverse spin galvanic effect (ISGE) and spin transfer torque (STT) in the presence of Rashba spin-orbit coupling, (b) s-d Dzyaloshinskii-Moriya interaction, (c) spin pumping in the presence of anomalous Hall effect (AHE) and (d) the interplay between spin pumping and spin swapping. All these mechanisms give rise to a magnetic damping that is linear in spin-orbit coupling and magnetization gradient.

not contribute to additional electric signal, it produces an anisotropic damping on the form $\tau \sim m_\parallel m$. This effect vanishes by symmetry in homogeneous ferromagnets, but is expected to survive in magnetic domain walls resulting in unconventional magnetic damping.

5.2. Topological Torques

As discussed above, the presence of spin-orbit coupling at transition metal interfaces promotes the emergence of chiral textures, such as homochiral Néel walls [69, 262, 263, 50, 51, 52] that display very large velocities [264, 11, 262, 12] or magnetic skyrmions [13, 47, 45, 44, 14, 265]. The latter are topological magnetic defects [36] that present some similarities with the more traditional magnetic vortices [266, 267, 268, 269]. In both cases, the magnetic topology induces a Lorentz force on the flowing electrons, resulting in topological Hall effect [270, 36]. Both classes of magnetic textures also experience a Hall effect when driven by an electric flow, an effect sometimes referred to as skyrmion Hall effect, and recently observed in transition metal interfaces [15, 16].

The reason why magnetic skyrmions are currently attracting a massive amount of interest is because simulations suggest that they get very weakly pinned on defects, enabling motion at low critical current density and long data retention [271, 272, 273, 274]. That being said, the very recent observation of current-driven motion of skyrmions at transition metal interfaces suggests on contrary that in polycrystalline samples the motion is quite sensitive to disorder and
grain boundaries [13, 14, 15, 16, 275]. To learn how to control the motion of such chiral textures, one needs to develop a precise understanding of the nature of the torque exerted on these objects. In magnetic textures, the spin transfer torque can be generally expressed as

$$\tau = b_J (u \cdot \nabla) m - \beta b_J m \times (u \cdot \nabla) m,$$

(48)

where $u$ is the direction of current injection, $m$ is a unit vector in the direction of the magnetization. The two terms on the right hand side of Eq. (48) are called the adiabatic ($\sim b_J$) and non-adiabatic torques ($\sim \beta b_J$), respectively [276, 277]. While the non-adiabatic parameter $\beta$ in transverse walls is quite small $\beta \approx \alpha$ ($\alpha$ being the magnetic damping of the homogeneous magnet), it is much larger in magnetic vortices and reaches $8\alpha$ to $10\alpha$ [267, 268, 269, 278]. Several contributions to the non-adiabatic parameter have been identified: spin relaxation [276] ($\beta \sim \lambda_{ex}^2/\lambda_{sf}^2$), spin mistracking [279, 280, 281] ($\beta \sim e^{-\lambda_{dw}/\lambda_{ex}}$), anomalous Hall effect [282] ($\beta \sim \theta_H$), and more recently spin diffusion [283] ($\beta \sim \lambda_{ex}^2/\lambda_{dw}^2$). Here $\lambda_{dw}$ is the domain wall width, $\lambda_{ex}$, $\lambda_{sf}$ are the transverse and longitudinal spin relaxation lengths and $\theta_H$ is the anomalous Hall angle.

More recently, a few authors proposed that topological Hall effect, inherent to both magnetic vortices and skyrmions, can lead to enhanced non-adiabicity [278, 284, 271, 285]. We believe this "topological torque" is of great importance for current-driven skyrmion motion because it increases when reducing the size of the skyrmion, and can therefore lead to improved dynamical properties upon size reduction, as discussed at the end of this Section.

5.2.1. Emergent Electrodynamics

When conduction electrons flow in a smooth and slow magnetic texture, $m(r, t)$, their spin adiabatically changes orientation so that these electrons acquire a Berry phase [286, 287, 288]. This geometrical phase can be represented by an emergent electromagnetic field $(E_{em}, B_{em})$ determined by the magnetic texture gradients [289, 290, 253, 254, 280, 255, 291]. A useful way to see that is to consider the simplest two dimensional $s$-d Hamiltonian (extension to three dimensions is straightforward)

$$\hat{H} = \frac{\hat{p}^2}{2m} + J_{sd}\hat{\sigma} \cdot m(r, t).$$

(49)

The Schrödinger equation corresponding to Eq. (49) can be re-written in the rotating frame of the magnetization, using the unitary transformation $U = e^{-i\frac{\sigma \cdot m}{2m} \hat{m}}$ where $m = z \times m/|z \times m|$ to obtain

$$\hat{\mathcal{H}} = (\hat{p} - eA)\hat{\mathcal{H}} + J_{sd}\hat{\sigma}_z + e\hat{V},$$

(50)

where the vector and scalar potentials are given respectively as $\hat{\mathcal{A}} = -\frac{\hat{b}}{2e}\hat{\sigma} \cdot (m \times \partial_t m)e$, and $\hat{V} = \frac{n}{2e}\hat{\sigma} \cdot (m \times \partial_t m)$. Hence, the electromagnetic field can be
written the form [292, 290, 253, 254, 280, 255, 291, 293, 294, 257, 295]

\[ E_{em}^s = -(s|\partial_t \hat{\mathcal{V}} + \partial_r \hat{\mathcal{A}}_r|s) = \frac{\hbar}{2e}[\mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m})] e, \]  
\[ (51) \]

\[ B_{em}^s = \langle s|\nabla \cdot \hat{\mathcal{A}}|s\rangle = -\frac{\hbar}{2e}[\mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m})] z. \]  
\[ (52) \]

Here, \(|s\rangle\) denotes the eigenstate of Eq. (50) in the absence of emergent electromagnetic field. As a static texture \((\partial_t \mathbf{m} = 0)\), we note that the spin-dependent current is driven by the external electric field \(E\) and the presence of a non-zero topological charge, \(\mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m}) \neq 0\) (as it is the case for magnetic skyrmions and vortices), 

\[ J_s^e = \sigma_0^a E + \sigma_0^b E_{em}^s + \frac{\sigma_H^a}{B_H} E \times B_{em}^s + \frac{\sigma_H^b}{B_H} E_{em}^s \times B_{em}^s, \]  
\[ (53) \]

where \(\sigma_0^a\) and \(\sigma_0^b\) are respectively the longitudinal and ordinary Hall conductivities for spin \(s\), \(E = E_0 \mathbf{u}\) is the external electric field, and \(B_H = |B_{em}^s|\). From Eq. (53), we note that the spin-dependent current is driven by the external electric field \(E\) as well as by the emergent electric field governed by the time-variation of the magnetic texture, \(B_{em}^s\). We can obtain the expressions for the local spin current tensor, \(J_s = -\mathbf{m} \otimes (j^l_s \mathbf{j}^l_s - j^z_s \mathbf{j}^z_s)\), and charge current vector, \(j_c = j_c^l + j_c^z\), from Eq. (53). For a static texture \((\partial_t \mathbf{m} = 0)\), we obtain 

\[ J_s = -b_j \mathbf{m} \otimes \mathbf{u} + \frac{P_H}{\rho_0} \lambda_H^j b_j [\mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m})] \mathbf{m} \otimes \mathbf{z} \times \mathbf{u}, \]  
\[ (54) \]

\[ j_c = \sigma_0 E \mathbf{u} - \sigma_0 \lambda_H^j E [\mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m})] \mathbf{z} \times \mathbf{u}, \]  
\[ (55) \]

where \(\sigma_0 = \sigma_0^a + \sigma_0^b\), \(\rho_0 = (\sigma_0^a - \sigma_0^b)/\sigma_0\), \((a = 0, H)\), \(\lambda_H^j = h \sigma_0^a B_H/2e\). In addition to the usual constant spin current moving along the direction of the applied electric field \((\sim \mathbf{u})\), the presence of a non-zero topological charge, \(\mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m}) \neq 0\), leads to a texture-induced emergent magnetic field that induces an additional spatially varying spin current along both the longitudinal \((\sim \mathbf{u})\) and transverse \((\sim \mathbf{z} \times \mathbf{u})\) directions to the electric field \(E\). This longitudinal spin current is responsible for (i) topological spin and charge Hall effects already observed in topological textures such as skyrmions [290, 270, 36, 296] and, (ii) enhanced non-adiabaticity already observed in vortices [278], as illustrated on Fig. 29.

5.2.2. Topological spin torque

Through spin transfer mechanism, the spin current given in Eq. (54) exerts a torque on the local magnetization, \(\mathbf{\tau} = -\nabla \cdot J_s\), which explicitly reads

\[ \mathbf{\tau} = b_j (\mathbf{u} \cdot \nabla) \mathbf{m} - \frac{P_H}{\rho_0} \lambda_H^j b_j [\mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m})] (\mathbf{z} \times \mathbf{u}) \cdot \nabla |\mathbf{m}|. \]  
\[ (56) \]

A remarkable consequence of Eq. (56) is that since the second term is even upon magnetization reversal, it induces an intrinsic topological non-adiabatic spin transfer torque. This non-adiabatic torque is intrinsic as it does not rely on impurities or defects (in contrast with the non-adiabaticity studied in Refs. [276, 283]), and topological since its origin is associated to the topology of the magnetic texture.
Figure 29: (Color online) The non-trivial topological texture of magnetic vortices and skyrmions distorts the trajectory of flowing electrons (left panel). This effect, called the topological Hall effect, can be clearly seen from tight-binding calculations (right panel), where the spin accumulation in the center of the magnetic vortex displays an antisymmetric distribution that is characteristic of spin Hall effect, although no spin-orbit coupling is present [278]. This asymmetric spin accumulation is a direct consequence of topological Hall effect and exerts a torque on the local texture, thereby inducing the so-called skyrmion Hall effect.

To quantify the topological torque, we first study the current-driven dynamics of an isolated magnetic skyrmion and vortex. To do so, we adopt the rigid motion formalized developed by Thiele [297]. The equation of motion governing the dynamics of these structures is given by the extended LLG equation

\[ \partial_t \mathbf{m} = -\gamma \mathbf{m} \times \mathbf{H}_{\text{eff}} + \alpha \mathbf{m} \times \partial_t \mathbf{m} + \beta \mathbf{J} \times \partial_x \mathbf{m} \]  

(57)

where \( \beta \) is a constant non-adiabatic parameter introduced by hand [276, 277]. The magnetization profile in spherical coordinates is given by the polar angle \( \theta \) and the azimuthal angle \( \varphi \). The polar angle is defined for an isolated skyrmion as \( \cos \theta = p(r_0^2 - r^2)/(r_0^2 + r^2) \) and for an isolated vortex as \( \cos \theta = p(r_0^2 - r^2)/(r_0^2 + r^2) \) for \( r \leq r_0 \), and \( \theta = \pi/2 \) for \( r > r_0 \). \( p = \pm 1 \) defines the skyrmion (vortex core) polarity, \( r_0 \) is the radius of the skyrmion (vortex core). For both textures, the azimuthal angle is defined \( \Phi = q \text{Arg}(x + iy) + c\pi/2 \), where \( q = \pm 1 \) is the vorticity and the \( c = \pm 1 \) defines the chirality. Using these profiles, we obtain the analytical expressions of the velocity components as [284]

\[ v_x = -\frac{1 + \alpha_{\text{eff}} \beta_{\text{eff}}}{1 + \alpha_{\text{eff}}^2} \mathbf{b}_J, \]

(58)

\[ v_y = pq\frac{\beta_{\text{eff}} - \alpha_{\text{eff}}}{1 + \alpha_{\text{eff}}^2} \mathbf{b}_J, \]

(59)

where \( C = 1 + \ln \sqrt{R/r_0} \), and \( \beta_{\text{eff}} \) and \( \alpha_{\text{eff}} \) are the effective non-adiabatic parameter and enhanced magnetic damping, respectively. In the present discussion, we neglect the effect of the enhanced damping, treated in Ref. [284], and focus on the topological torque. The effective non-adiabatic parameter read,

\[ \beta_{\text{eff}} = \begin{cases} 
\beta + \frac{4\lambda}{3} \frac{D_0}{r_0^2} \frac{\lambda^2}{r_0^2}, & \text{for skyrmion} \\
\beta C + \frac{7}{3} \frac{D_0}{r_0} \frac{\lambda^2}{r_0^2}, & \text{for vortex core},
\end{cases} \]

(60)
where $S = r_0^2 / (r_0^2 + R^2)$, and $S_k = \sum_{i=k}^{\infty} (S)_i$. Remarkably, in both cases the topological non-adiabaticity scales with $1/r_0^2$. In other words, the sharper the texture, the larger the non-adiabatic torque and the larger the skyrmion Hall effect. Reducing the skyrmion (or vortex core) size by a factor of 2 enhances the non-adiabaticity by a factor of 4. Using realistic material parameters $r_0 = 30$ nm, $\theta_{TH} = \sigma_H/\sigma_0 = 0.01$, and $B_H = 2.5$ T [298], we obtain $\lambda_H^2 = 1.32$ nm$^2$ and the corresponding topological contribution to the non-adiabaticity parameter $\beta = 0.08$.

5.2.3. Tight-binding model

The analytical derivation proposed above relies on the assumption that spin transport is adiabatic throughout the magnetic texture, i.e. the spin of the conduction electrons remains aligned on the local magnetization direction and no spin mistracking is considered [279]. To confirm the analytical results, we computed the topological transport and torques in a magnetic skyrmions numerically using the non-equilibrium wave function formalism implemented on a tight-binding model in the KWANT package [205]. The system is composed of a scattering region containing an isolated skyrmion or vortex core, attached to two ferromagnetic leads. In the same spirit as the tight-binding models previously discussed, the system is a two dimensional square lattice described by the Hamiltonian [296, 284]

$$\hat{H} = \sum_{i} (\epsilon_i \hat{c}_i^\dagger \hat{c}_i + \Delta \hat{c}_i^\dagger \hat{\sigma} \cdot \hat{m}_i \hat{c}_i) - t \sum_{<ij>} \hat{c}_i^\dagger \hat{c}_j,$$

where the sum $<ij>$ is restricted to nearest neighbors, and the skyrmion texture is encoded in the unit vector $\hat{m}_i$. The torque $\tau_n$ at site $\mathbf{n}$ is computed by using the local spin densities as

$$\tau_n = \frac{2\Delta}{\hbar} \hat{m}_n \times (\mathbf{S}_n) = \tau_{na} \partial_x \mathbf{m}_n - \tau_{na} \mathbf{m}_n \times \partial_x \mathbf{m}_n,$$  \hspace{1cm} (61)

To investigate the total torque exerted on the magnetic skyrmion, we calculated the normalized adiabatic and non-adiabatic torque components by integrating the projections of the local torque on $\hat{m}_n \times \partial_y \mathbf{m}_n$ and $\hat{m}_n \times \partial_x \mathbf{m}_n$ respectively and normalized accordingly i.e.

$$\tilde{\tau}_{ad} = \frac{\int \tau \cdot (\mathbf{m} \times \partial_y \mathbf{m}) d^2\mathbf{r}}{\int \mathbf{m} \cdot (\partial_y \mathbf{m} \times \partial_y \mathbf{m}) d^2\mathbf{r}},$$ \hspace{1cm} (62)

$$\tilde{\tau}_{na} = \frac{\int \tau \cdot (\mathbf{m} \times \partial_x \mathbf{m}) d^2\mathbf{r}}{\int \mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_x \mathbf{m}) d^2\mathbf{r}}.$$ \hspace{1cm} (63)

Figure 30 displays both torques as a function of the skyrmion radius $r_0$. While the adiabatic torque (open symbols) is almost constant, the non-adiabatic torque (filled symbols) shows a substantial dependence on the skyrmion radius $r_0$, in agreement with the analytical results presented in Eq. (60). Besides providing a reasonable explanation for the enhanced non-adiabaticity in skyrmions and
Figure 30: (Color online) Effective adiabatic and non-adiabatic torque dependence on the skyrmion radius. The adiabatic torque (open symbols) is almost non-dependent on the radius of the skyrmion while the non-adiabatic torque (filled symbols) shows substantial dependence on the skyrmion radius $r_0$. From [234].

Magnetic vortices [278], this topological torque opens interesting perspectives for the investigation of current-driven skyrmion dynamics. Since the topological torque is an intrinsic property of the magnetic texture, one could continuously deform this structure by applying, e.g., a perpendicular external magnetic field [299, 300], and therefore influence the non-adiabaticity parameter. For instance, Moreau-Luchaire et. al. [44] demonstrated a reduction of the skyrmion diameter from 80 nm at 12 mT to 30 nm at 70 mT. Following our predictions, the topological non-adiabaticity parameter should increase by a factor $\sim 7$ in this specific case.
6. Conclusion

The simultaneous presence of spin-orbit coupling, magnetism and interfacial symmetry breaking offers a vast playground for spintronics and modern magnetism, enabling the efficient electrical control of exotic magnetic textures. Although most of the physics at stake can be accounted for through phenomenological models (free electron model, Rashba spin-orbit coupling, adiabatic spin transport, micromagnetics etc.), the recent systematic investigation of spin-orbit coupled transition metal interfaces using first principles methods has nurtured major progress in the field. For instance, spin Hall effect [151], spin-orbit splitting [22] and DMI [21] have been investigated for a wide range of 3d/5d(4d) interfaces and systematic trends, well understood in terms of d-orbital hybridizations, have emerged. Yet, there are still several significant challenges that remain to be tackled. Offering a coherent description of the interplay between inverse spin galvanic effect, interfacial and bulk spin Hall effects at these interfaces is highly desirable to foster the realization of efficient spin-orbit torque devices. The concept of chiral damping, recently introduced [301, 260] needs to be rigorously treated using both linear response theory and \textit{ab initio} approaches. The correlation between all these effects and their dependence as a function of the nature of the orbital hybridization remain to be thoroughly understood.

Besides ferromagnetic interfaces, two large classes of systems are currently drawing an increasing amount of attention. The first class concerns the interfaces between heavy metals and antiferromagnets [302, 303]. As a matter of fact, the prediction of spin transfer torque in antiferromagnetic spin-valves ten years ago [304] has opened thrilling perspectives in the field of spintronics and beyond. These materials possess thought-provoking dynamical behavior, and, most importantly, can be manipulated electrically using spin-orbit torques [305, 306, 307, 308]. Spin Hall effect has been the object of a recent study [182], but the field is still at its infancy and all the effects discussed in the present chapter, such as antiferromagnetic skyrmions [309, 310], should also emerge in antiferromagnetic multilayers.

The second class of materials that could entirely renew this already fascinating field concerns the so-called topological materials, i.e. materials whose band structures are topologically non-trivial. We already briefly mentioned the topological insulators [311, 312, 313], which possess spin-orbit coupled surface states and remained to be understood in the context of spin-orbit torques. Other materials such as crystalline [314], Anderson [315, 316] or Kondo topological insulators [317], but also Weyl semimetals [318, 319] and Dirac semimetals [320] all possess very large spin-orbit coupling and display exotic surface states. For instance, Weyl semimetals are characterized by their surface Fermi arcs, i.e. disrupted Fermi surfaces that connect two opposite surfaces through bulk states [318]. In this ever-growing class of materials, spin-charge conversion processes (spin Hall, spin swapping, inverse spin galvanic effects) are yet to be explored theoretically and experimentally and the interplay between electric currents and magnetism holds promises for even more thrilling adventures.
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