Spin-Orbitronics at Transition Metal Interfaces

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Abstract

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 $3d^1 4s^2$ to Cu $3d^{10} 4s^1$ and Zn $3d^{10} 4s^2$ ($3d$ series), from Y $4d^1 5s^2$ to Ag $4d^{10} 5s^1$ and Cd $4d^{10} 5s^2$ ($4d$ series), and from La $5d^1 6s^2$ 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.

Figure 1: (a) Tight-binding parameters of transition metals and (b) Fermi energy, as parametrized in Ref. [17]. Notice that for Co, Fe and Ni, the hopping parameters duplicate due to spontaneous ferromagnetism.

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 ($nd^1 \rightarrow nd^{10}$) and correspondingly, the bandwidth

52 decreases with the electron filling. On the other hand, upon increasing the series
 53 index ($3d^n \rightarrow 5d^n$) the orbital gets more delocalized and as such more sensitive
 54 to the crystal field, resulting in d -orbital splitting and bandwidth broadening.
 55 This behavior is nicely represented by the evolution of the nearest neighbor
 56 hopping energies, as reported in Ref. [17] and collected in Fig. 1(a). It is clear
 57 that nearest neighbor hopping increases systematically from one series to an-
 58 other, $t_{5d} > t_{4d} > t_{3d}$, but decreases when increasing the orbital filling within
 59 one given series. Of course this rule is simply qualitative, as the bandwidth also
 60 depends on the coordination number (it is larger for fcc than for bcc crystals for
 61 instance) and is influenced by spd hybridization as well [18]. Fig. 1(b) shows
 62 the behavior of Fermi level throughout the three series, where the maximum is
 63 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.

64 The systematic increase of the hopping parameters when increasing the shell
 65 index has a direct consequence in terms of magnetism. Indeed, the exchange
 66 integral I is an intra-atomic interaction, and it should scale with the localization
 67 of the orbital considered. Hence, one would expect $I_{3d} > I_{4d} > I_{5d}$, as demon-
 68 strated in Fig. 2(a). Furthermore, since the density of states is roughly inversely
 69 proportional to the bandwidth, one expects $n_{3d}(\epsilon_F) > n_{4d}(\epsilon_F) > n_{5d}(\epsilon_F)$ and
 70 naturally, 3d elements are more likely to be magnetic than any other 4d and 5d
 71 elements. The calculated Stoner criterion for transition metals is reported in Fig.
 72 2(b) and one can see that the criterion is in fact only satisfied for Fe, Ni and Co.
 73 Other 3d elements such as Mn, Cr or V are not too far from fulfilling the Stoner
 74 criterion and indeed show enhanced susceptibility to magnetism. For instance,
 75 Mn and Cr (as well as γ -Fe) display antiferromagnetism. A phenomenological
 76 estimation can be obtained based on Bethe-Slater argument stating that anti-
 77 ferromagnetism occurs upon reducing the inter-atomic distance. This picture

78 is supported by *ab initio* calculation on 3*d* monolayers deposited on 4*d* and 5*d*
 79 substrates [19].

80 Interestingly, Rh, Pd, and Pt are fairly close to fulfilling the Stoner criterion
 81 so that a slight modification of their environment (say, reduction of coordination
 82 number due to the presence of an interface) can lead to the onset of magnetism,
 83 as discussed below. Finally, of most importance for our topic, the atomic spin-
 84 orbit coupling also dramatically depends on the transition metal series, see Fig.
 85 2(c). Indeed, the spin-orbit coupling parameter increases with Z , such that 5*d*
 86 transition metals possess a much larger spin-orbit coupling than their 4*d* and 3*d*
 87 counterparts. Combined with their high sensitivity to magnetism, this property
 88 makes 4*d* and 5*d* interfaces quite appealing for spin-orbitronics.

89 2.2. Magnetic properties of transition metal interfaces

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

Figure 3: Schematic evolution of the *d*-orbital density of states upon increasing the orbital occupation for selected 3*d* and 5*d* monolayers. The energy position of the 3*d* 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 5*d* 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.

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

99 density of states of selected $3d$ and $5d$ monolayers, as illustrated on Fig. 3.
 100 Because of their large bandwidth, $4d$ and $5d$ elements do not show exchange
 101 splitting as expected and increasing the electronic filling pushes the density of
 102 states below the Fermi energy. As a results, Ag and Au display a d -orbital
 103 density of states located below Fermi energy. In contrast, $3d$ monolayers show
 104 a slightly different behavior. The density of states is also pushed down through
 105 Fermi level when increasing the number of electrons, but at the same time its
 106 exchange splitting also depends on orbital filling. When increasing the number
 107 of electrons from V to Mn, the exchange splitting increases while it decreases
 108 when going from Mn to Ni. This behavior can be understood following Hund's
 109 third rule that governs magnetism in isolated ions [20, 21]: Mn ion has a high
 110 spin configuration with 5 unpaired electrons, while Ni and V ions have a low
 111 spin configuration. The consequence is that V and Ni, on both sides of the $3d$
 112 series show a weak spin splitting while a large amount on one spin species is
 113 present at the Fermi level. In contrast, Mn has a large spin splitting but Fermi
 114 energy lies in-between the two spin species, leading to a reduced amount of $3d$
 115 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].

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

127 An interesting consequence is that upon such an orbital hybridization, (i) the
 128 $4(5)d$ 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 $\hat{\mathcal{H}}_{\text{so}} = (\xi/\hbar)\hat{\sigma} \cdot (\nabla\Phi \times \hat{\mathbf{p}})$ (ξ 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

145 gradient is particularly strong close to the atom nucleus, such that one can adopt
 146 the spherical approximation, $\nabla\Phi = (\partial_r\Phi/r)\hat{\mathbf{r}}$. Hence, the spin-orbit coupling
 147 reduces to the well-known atomic Russel-Saunders form $\hat{\mathcal{H}}_{\text{so}} = (\xi/\hbar)\langle\partial_r\Phi/r\rangle\hat{\mathbf{L}}\cdot$
 148 $\hat{\boldsymbol{\sigma}}$, where $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$ is the orbital angular momentum. This form neglects the
 149 crystal contribution to the spin-orbit coupling but is usually sufficient to model
 150 spin-orbit physics.

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 $+\mathbf{x}$ (red) and $-\mathbf{x}$ (blue). From Ref. [22].

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

$$|\mathbf{k}, n, +\rangle = [u_{\mathbf{k},n}^{\uparrow}|\uparrow\rangle + u_{\mathbf{k},n}^{\downarrow}|\downarrow\rangle]e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (1)$$

$$|\mathbf{k}, n, -\rangle = [-u_{-\mathbf{k},n}^{\downarrow*}|\uparrow\rangle + u_{-\mathbf{k},n}^{\uparrow*}|\downarrow\rangle]e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (2)$$

157 As a consequence, neither the spin angular momentum nor the linear momentum
 158 are good quantum numbers anymore. The impact of spin-orbit coupling on the
 159 band structure of bulk Pt is reported in Fig. 7. The spin-orbit coupling removes
 160 the band degeneracy away from the Γ 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, $\mathbf{k} = 0$, 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, $\mathbf{z}$.
Spatial inversion symmetry breaking allows the spin-orbit coupling to develop
terms that are *odd* in momentum $\mathbf{k}$, 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 $\langle \xi \nabla V \rangle \approx -\alpha \mathbf{z}$ and the spin-orbit coupling Hamil-
tonian reduces to $\hat{H}_R \approx -\alpha \hat{\sigma} \cdot (\mathbf{z} \times \mathbf{k})$, where α 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 $+\mathbf{x}$ (red) or $-\mathbf{x}$ (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 Russel-Saunders form, $\hat{\mathcal{H}}_{\text{so}} = (\xi/\hbar)\langle\partial_r\Phi/r\rangle\hat{\mathbf{L}}\cdot\hat{\boldsymbol{\sigma}}$. 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.

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 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

204 in Fig. 8(b), as well as the Stoner criterion reported on Fig. 2(a,b). Indeed, the
205 k -asymmetric spin-splitting is driven by the $4d$ or $5d$ orbitals (which possess the
206 strongest spin-orbit coupling) and is therefore expected to be maximum with
207 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 co-operation 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 ($\sim J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$) and a so-called antisymmetric exchange ($\sim \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$) [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 $E_{\text{DM}} \sim \mathbf{m} \cdot [(\mathbf{z} \times \nabla) \times \mathbf{m}]$. In other words, at interfaces, one expects that DMI creates an effective magnetic field $\mathbf{H}_{\text{DM}} \sim \mathbf{m} \times (\mathbf{z} \times \mathbf{e}_i)$, 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 at 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 $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{m}} + \hat{\mathcal{H}}_{\text{hop}} + \hat{\mathcal{H}}_{\text{so}}$, where

$$\hat{\mathcal{H}}_0 = \epsilon_A \hat{c}_{xz,A}^\dagger \hat{c}_{xz,A} + \epsilon_B \hat{c}_{xz,B}^\dagger \hat{c}_{xz,B} + \epsilon_C (\hat{c}_{xz,C}^\dagger \hat{c}_{xz,C} + \hat{c}_{yz,C}^\dagger \hat{c}_{yz,C}) \quad (3)$$

$$\hat{\mathcal{H}}_{\text{m}} = -\frac{J}{2} (\hat{c}_{xz,A}^\dagger (\hat{\boldsymbol{\sigma}} \cdot \mathbf{m}_A) \hat{c}_{xz,A} + \hat{c}_{xz,B}^\dagger (\hat{\boldsymbol{\sigma}} \cdot \mathbf{m}_B) \hat{c}_{xz,B}), \quad (4)$$

$$\hat{\mathcal{H}}_{\text{hop}} = t_1 (\hat{c}_{xz,A}^\dagger \hat{c}_{xz,C} + \hat{c}_{xz,B}^\dagger \hat{c}_{xz,C}) + t_2 (\hat{c}_{xz,A}^\dagger \hat{c}_{yz,C} - \hat{c}_{xz,B}^\dagger \hat{c}_{yz,C}) + c.c. \quad (5)$$

Here, $\hat{\mathcal{H}}_0$ is the unperturbed Hamiltonian of the three isolated atoms, $\hat{\mathcal{H}}_{\text{m}}$ de-

scribes the intrinsic magnetic coupling on atoms A and B, where $\mathbf{m}_{A,B} = (\cos \varphi, \pm \sin \varphi, 0)$ [70], and $\hat{\mathcal{H}}_{\text{hop}}$ describes the hopping between the three atoms. The hopping energies, t_1 and t_2 , are defined within Slater-Koster parametrization [71],

$$t_1 = \cos^2 \theta V_{dd\pi} + \sin^2 \theta V_{dd\delta}, \quad (6)$$

$$t_2 = \sin \theta \cos \theta (V_{dd\pi} - V_{dd\delta}), \quad (7)$$

where $V_{dd\pi}$ and $V_{dd\delta}$ are the Slater-Koster parameters and θ 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}^C and d_{yz}^C ,

$$\hat{\mathcal{H}}_{\text{so}} = \frac{i\xi}{2} ((\hat{c}_{xz,C}^\dagger)^\dagger \hat{c}_{yz,C}^\dagger - (\hat{c}_{yz,C}^\dagger)^\dagger \hat{c}_{xz,C}^\dagger) + c.c. \quad (8)$$

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

$$E_{\text{DM}} = \int_{-\infty}^{\epsilon_F} d\epsilon \text{Tr}[\hat{\rho}_0 \hat{\mathcal{H}}_{\text{so}}], \quad (9)$$

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_{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. [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 moment on the non-magnetic ion m_C

Figure 12: (a) Dependence of DMI energy E_{DM} , (b) induced magnetization m_C and (c) charge transfer Δn as a function of the relative energy shift between the magnetic and non-magnetic orbitals. The vertical dashed-dotted, dashed and dotted lines refer to $\epsilon_C - \epsilon_A = 0.75$ eV, $\epsilon_C - \epsilon_A = 0.93$ eV and $\epsilon_C - \epsilon_A = 1$ eV, respectively. (d) Dependence of DMI energy E_{DM} , (e) induced magnetization m_C and (f) charge transfer Δn as a function of the angle θ , as defined in Fig. 11. The vertical dashed-dotted, dashed and dotted lines refer to three noticeable situation discussed in the text.

and the charge transfer between the magnetic and non-magnetic ions Δn ,

$$m_C = \int_{-\infty}^{\epsilon_F} d\epsilon \text{Tr}[\hat{\rho}_0^C \hat{\sigma}_z], \quad (10)$$

$$\Delta n = \int_{-\infty}^{\epsilon_F} d\epsilon \text{Tr}[\hat{\rho}_0^A + \hat{\rho}_0^B - \hat{\rho}_0^C]. \quad (11)$$

These two quantities are reported on Fig. 12(b) and (c). We observe two remarkable features. First both positive maxima of E_{DM} at $\epsilon_C - \epsilon_A \approx 0.8$ eV and 1.08 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 Δn . 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 θ in the range $\pm\pi/3$, assuming that the overlap integrals,

331 $V_{dd\pi}$ and $V_{dd\delta}$ remain unmodified. The results for E_{DM} , m_C and Δn are re-
 332 ported on Fig. 12(d)-(f). The DMI is clearly antisymmetric, while the induced
 333 magnetism and charge imbalance remain symmetric. Again, a correlation be-
 334 tween these three quantities can be found for some specific points [denoted by
 335 the vertical lines in Fig. 12(d)-(f)], but no systematic rule of thumb can be
 336 determined, highlighting the complexity of the phenomena involved.

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

344 3.3. First principles methods

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

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

$$D_{ij} = \frac{\hbar}{2\pi\Omega} \Re \int d\epsilon f(\epsilon)(\epsilon - \epsilon_F) \text{Tr}[\mathcal{T}_i \hat{G}^R \hat{v}_j \partial_\epsilon \hat{G}^R - \mathcal{T}_i \partial_\epsilon \hat{G}^R \hat{v}_j \hat{G}^R], \quad (12)$$

367 where $\hat{v}$ is the velocity operator, $\hat{G}^R = (\epsilon - \hat{\mathcal{H}} - \hat{\Sigma}^R)^{-1}$ is the retarded perturbed
 368 Green's function of the system ($\hat{\Sigma}^R$ being the retarded self-energy including
 369 disorder etc.), $f(\epsilon)$ is Fermi-Dirac distribution, Ω is the volume of the unit
 370 cell, $\Re$ takes the real part and Tr denotes the trace. Here $\mathcal{T} = \mu_B \mathbf{B}^x \times \hat{\sigma}$,
 371 is the torque operator between the electron spin and the exchange field, μ_B is

Bohr's magneton. In this definition, D_{ij} is in $\text{eV}\cdot\text{m}^{-2}$. 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 $\hat{\mathbf{v}}$. 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 $\mathcal{J}_s$ that interacts with the magnetic texture through the DM energy term

$$\mathcal{H}_{\text{DM}} = (\hbar/2) \int_{\Omega} \mathbf{m} \cdot [(\mathcal{J}_s \cdot \nabla) \times \mathbf{m}] d^3\mathbf{r}, \quad (13)$$

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

3.4. DMI at 3d/5d interfaces

Figure 13: (a) Strength and sign of Dzyaloshinskii-Moriya interaction (DMI) D^{tot} in $3d$ transition metal monolayers on $5d$ substrates calculated around their magnetic ground state combining the relativistic spin-orbit coupling effect with spin spirals. A positive sign of D^{tot} indicates a left-rotational sense or "left chirality". (b) correlation between $E_{\text{DMI}} \sim D^{\text{tot}}/M^2_{3d/5d}$ averaged over $3d/5d$ interfaces (black line) versus the $3d$ overlayer, the magnetic moments in $3d$ transition metal unsupported monolayer (UML - dashed red line), and the local magnetic moment per atom averaged over $3d/5d$ interfaces (solid red line).

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

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^{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 $M_{3d/5d}^2$ 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 $3d/\text{Au}(111)$ 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-

440 pletely different chemical trend when moving along the $3d$ elements [18]. More
 441 specifically, although the magnetic anisotropy contributes to the magnetic ener-
 442 gies, it does not show a positive correlation with magnetic moment of $3d/5d$ thin
 443 films. For instance, Mn systems have the smallest magnetic anisotropies but the
 444 largest magnetic moment. In the same way, the Heisenberg-type exchange in-
 445 teraction parameter J is also independent of M , being smaller for Mn than for
 446 Co. Obviously, the nearest-neighbor exchange interaction (J_1) for $3d$ transition
 447 metals follows perfectly the Bethe-Slater curve and not Hund’s first rule [89].
 448 Further, this fact is also surprising as it is opposite to what is expected from the
 449 knowledge of magnetism in bulk and thin films. For instance, such uncorrelated
 450 behavior has also been recently observed in the skyrmion phase of $\text{Mn}_{1-x}\text{F}_x\text{Ge}$
 451 by Gayles et al. [83], where the strength of DMI does not show any correlation
 452 with the magnetic moment of the $3d$ transition metal. This provides additional
 453 evidence for a violation of direct relation of magnetic moment and DMI in alloy
 454 systems.

455 Since the relation between interfacial DMI and local magnetic moments of
 456 $5d$ substrate has been so controversially debated lately, we emphasize here that
 457 the DMI shows no direct correlation with the proximity induced magnetism
 458 in $5d$ across the $3d/5d$ interfaces [21]. Indeed, the $5d$ states are degenerate
 459 and partially occupied due the strong crystal-field splitting or large bandwidth,
 460 irrespective of deposited $3d$ overlayer on the top, in good agreement with the
 461 experimental observations [90] and previous theoretical studies [18, 73]. This
 462 result is in contrast, however, with recent experiment by Ryu et al. [91] who
 463 claim that DMI should scale with the induced magnetization of the heavy metal.

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

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

486 $3d$ - $5d$ interface states around the Fermi energy controls the magnetic coupling
 487 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. Δ_{CF} indicates the crystal-field splitting between the t_{2g} and e_g shells. From [21].

488 This fact is reflected, for instance, by the electronic configurations of the $3d$
 489 orbitals and their spin-split band positions with respect to $5d$ W states, see Fig.
 490 14. Inspecting this figure in more detail, one can see that the band lineups of
 491 $3d$ and $5d$ states reveal two interesting features, which are essentially similar
 492 to a first approximation. First, the W surface is weakly polarized where the
 493 $5d$ states are degenerate and partially filled, consistent with the fact that those
 494 configurations of the outer electrons shell are dominated by the significant large
 495 bandwidth or by the crystal-field splitting. Note that the number of available
 496 $5d$ states near the Fermi level and their bandwidth are fixed for a certain sub-
 497 strate depending on their filling. Second, the electron filling of the $3d$ orbitals,
 498 according to Hund's first rule, fits well the band alignment of $3d$ states around
 499 the Fermi level, as shown in Fig. 14. At this stage, it is important to stress out
 500 that the $3d$ - $5d$ majority and minority spin states and their exchange-splitting
 501 gap are energetically aligned according to their calculated band structure, as
 502 depicted on Fig. 14, right side. The latter is found to be consistent with the
 503 electronic occupation of $3d$ - $5d$ (in first approximation) spin channels (Fig. 14,
 504 left side) and thus obeying both crystal field splitting and Hund's first rule.

505 In this context, since the $5d$ bandwidth is significantly larger than the crystal-
 506 field splitting and the $5d$ states are weakly polarized (degenerate and partially
 507 filled), the overall physics of the predicted trend in Fig. 13 is mostly governed
 508 by the band lineup of $3d$ spin channels, themselves determined by Hund's first
 509 rule. Therefore, in a simple picture one can easily explain this fact for all $3d$
 510 elements.

511 By comparing the early and late $3d$ overlayers, V and Ni respectively, one
 512 can observe that both spin channels are mostly either occupied or unoccupied;
 513 their band alignment with respect $5d$ states is energetically unfavorable and,
 514 consequently, the spin-flip excitation processes are not allowed. As a result,
 515 the DMI is weak in both cases since this mechanism requires the availability of
 516 $3d$ electrons, occupied and unoccupied, to facilitate the spin-flip process which
 517 is crucial for the appearance of the DMI. Proceeding from Ni to Co overlayer,
 518 the DMI remains relatively weak because of the small amount of unoccupied
 519 minority $3d$ states. Keep in mind that the degeneracy of $5d$ spin channels is
 520 not lifted by the presence of any $3d$ overlayer on the top, despite the overlap
 521 of the relatively more extended $5d$ wave function of the W substrate with the
 522 wave functions of $3d$ overlayers. In other words, since the $5d$ orbitals are more
 523 extended than $3d$ ones, these orbitals are only weakly perturbed by the ad-
 524 sorption of $3d$ elements. On the other hand, since the DMI is weaker it is more
 525 sensitive to the detail of the orbital hybridization between the substrate and the
 526 overlayer, resulting in a change of handedness of the magnetic structure. This
 527 actually happens for Ni/ $5d$ and V/ $5d$ interfaces on both sides of this trend, as
 528 well as for Co overlayer. This also holds true for Au substrate, because the $5d$
 529 states lie far below the Fermi level (the bonding character is less clear for the
 530 involved states) the DMI is weaker and therefore shows variations in the sign
 531 as a function of the $3d$ overlayer (Fig. 13, yellow line). Such an oscillation in
 532 sign has been analyzed extensively for $\text{Mn}_{1-x}\text{F}_x\text{Ge}$ by Gayles et al. [83] and
 533 has also been identified in the trimer model developed by Kashid et al. [70],
 534 where the sign and magnitude of DMI depend on the shifts of the single-particle
 535 energies with respect to the scalar-relativistic eigenvalues due to spin-orbit cou-
 536 pling ($\delta\epsilon_{k\nu} = \delta\epsilon_{k\nu}^{\text{SOC}} - \delta\epsilon_{k\nu}^{\text{SR}}$) in the energy range around the Fermi level [70].
 537 According to perturbation theory, the $5d$ orbitals "*spin-orbit active states*" are
 538 responsible for the spin-orbit coupling matrix elements $\mathcal{H}_{\text{so}}(\xi\mathbf{L})$ and make essen-
 539 tial contributions to DMI [see Fig. 6(a)]. However, despite the weak spin-orbit
 540 coupling in the $3d$ overlayer their intra-atomic exchange field can easily modify
 541 the electronic structure around the Fermi energy and consequently change the
 542 strength of the DMI. One may conclude that the spin-orbit-induced energy shift
 543 of the highest occupied orbital depends sensitively on the charge rearrangement
 544 between the $3d$ orbitals of opposite spin and, hence, Hund's first rule. In the
 545 following, we will demonstrate how the spin-flip excitations through spin-orbit
 546 coupling in half-filled or high spin $3d$ overlayer make the largest contribution to
 547 the DMI.

548 The situation is completely different when moving to half-filled $3d$ transition
 549 metals. In the case of Mn overlayer, the filling of the five Mn $3d$ orbitals adopts
 550 a stable "high spin state" due to the small crystal field splitting between the

t_{2g} and e_g shells and, hence, half-band filling occur (see Fig. 14). 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 Schweffinghaus 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: $\Delta\rho(\mathbf{r}) = \rho_{\text{tot}}(\mathbf{r}) - [\rho_{5d}(\mathbf{r}) + \rho_{3d}(\mathbf{r})]$, where $\rho_{\text{tot}}(\mathbf{r})$, $\rho_{5d}(\mathbf{r})$, and $\rho_{3d}(\mathbf{r})$ 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 $\mu(z) = \frac{1}{n} \int_{-c}^{-c+z/2} z' \Delta\bar{\rho}(z') dz'$, 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 $\Delta\bar{\rho}(z')$ is $\Delta\rho(\mathbf{r})$ integrated over lateral coordinates x and y for each z plane.

The DMI and the corresponding dipole moment values for $3d/\text{Au}(111)$ and $3d/\text{W}(001)$ 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

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 skyrmions 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*p* orbital affects the energetic ordering of Fe-3*d* spin channels with respect to the Fermi level and, consequently, controls the hybridization between Fe-3*d* and Ir-5*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*d* and 5*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*d* and 5*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 ϵ_F with respect to unperturbed one ϵ_F^0 for spin spiral of wave vector $q' = 0.25 \frac{2\pi}{a'} [see Fig. 16(c)]$. Note that the ϵ_F^0 and ϵ_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*d*/5*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 $\Delta\rho(\mathbf{r})$ 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 $1.2 \times 10^{-2} e/\text{\AA}^3$. From [84].

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

729 4. Spin-Orbit Torques

730 4.1. Overview

731 Let us now turn our attention towards the non-equilibrium properties of
 732 transition metal interfaces. In magnetic bilayers composed of a (metallic or in-
 733 sulating) magnet deposited on top of a heavy metal (W, Pt, Bi₂Se₃, WTe₂ etc.),
 734 the flowing charges experience spin-charge conversion mechanisms that produce
 735 a non-equilibrium spin accumulation at the interface with the ferromagnet, such
 736 that an overall torque is exerted on the magnetization. This effect, called spin-
 737 orbit torque, has been initially observed in transition metal bilayers [107, 108, 8,
 738 9, 109] and bulk non-centrosymmetric magnets [110, 111, 112], and recently ex-
 739 tended to a wide variety of transition metal bilayers [113, 109, 67, 114, 115, 116],
 740 oxide interfaces [117, 102, 118], thick multilayers [119, 120], magnetic insulators
 741 deposited on heavy metals [121, 122, 123], as well as ferromagnets deposited on
 742 topological insulators [124, 125, 126, 127], and Weyl semimetals [128].

743 Overall, the experiments confirm that the torque is of the form $\boldsymbol{\tau} = \tau_{\text{DL}}\mathbf{m} \times$
 744 $[(\mathbf{z} \times \mathbf{u}) \times \mathbf{m}] + \tau_{\text{FL}}\mathbf{m} \times (\mathbf{z} \times \mathbf{u})$, where $\mathbf{z}$ is the normal to the interface and
 745 $\mathbf{u}$ is the direction of injection of the flowing charges. The first term $\sim \tau_{\text{DL}}$
 746 is the damping-like torque while the second term $\sim \tau_{\text{FL}}$ is called the field-
 747 like torque. Both damping-like and field-like torques are present in most of
 748 the systems involving heavy metals. Uncovering the physical mechanisms that
 749 sustain the spin-orbit torque is quite challenging, as many effects are present in
 750 such ultrathin systems. In a nutshell, two main effects have been pointed out
 751 originally: the inverse spin-galvanic effect, localized at the interface between
 752 the heavy metal (or the oxide) and the ferromagnet, and the spin Hall effect
 753 present in the bulk of the heavy metal, as illustrated on Fig. 17. As explained
 754 in more details below, the former generates a field-like torque [129, 130, 131] $\sim$
 755 $\mathbf{m} \times (\mathbf{z} \times \mathbf{u})$, while the spin Hall effect generates a damping-like torque [108, 132]
 756 $\sim \mathbf{m} \times [(\mathbf{z} \times \mathbf{u}) \times \mathbf{m}]$. However, only a few systems, such as the Ti/NiFe/AlOx
 757 trilayers from Emori et al. [118], can be reasonably well explained by these
 758 two scenarii. In most cases, both torques are observed and their materials
 759 dependence raises many questions concerning the physical mechanism at their
 760 origin. More recently, two additional mechanisms have been proposed: the
 761 magnetoelectric effect and the spin swapping effect. The former is a correction
 762 to the inverse spin galvanic effect when inversion symmetry breaking, spin-orbit
 763 coupling and magnetic exchange are present on the same orbitals, and generates
 764 a damping-like torque [133, 134, 135]. The latter is a correction to the spin Hall
 765 effect and only survives in ultrathin multilayers as thin as the mean free path
 766 [136]. It creates a field-like torque.

767 Our objective is to present these various mechanisms, and discuss their phys-
 768 ical origin and their impact on the spin-orbit torque. We first address the physics
 769 of spin Hall and spin swapping in Section 4.2, and discuss the physics of inverse
 770 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, $\delta \mathbf{S} \sim \mathbf{z} \times \mathbf{u}$, 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.

771 4.2. Spin Hall and swapping effects

772 Spin Hall effect is the conversion of a unpolarized charge flow $\mathbf{j}_e$ into a
 773 chargeless spin current $\mathcal{J}_s$. In the bulk, it reads $e\mathcal{J}_s = \theta_{sh}\boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \times \mathbf{j}_e$, where $\boldsymbol{\sigma}$
 774 is the polarization of the spin current. We remind that the spin current $\mathcal{J}_s$ is a
 775 3×3 tensor in spin and real space. θ_{sh} is called the spin Hall angle and quantifies
 776 the charge-to-spin conversion efficiency. This effect was predicted originally by
 777 D'yakonov and Perel [137, 138] and revived about twenty years ago by Hirsch
 778 [139] and Zhang [140]. It has initially been observed optically in semiconductors
 779 [141, 142] and measured electrically in transition metals [143, 144]. Since then,
 780 spin Hall effect has drawn a massive amount of attention [145, 146, 147, 148, 149]
 781 as it offers a convenient way to generate pure spin currents, enabling non-local
 782 spin logic [150] as well as promoting spin-orbit torques [8, 108, 9].

783 Computing non-equilibrium properties of non-collinear magnetic systems in
 784 the presence of spin-orbit coupling is in itself a significant challenge since nei-
 785 ther the linear momentum nor the spin angular momentum are good quantum
 786 numbers in this case. Different approaches have been proposed to tackle this
 787 problem. The "simplest" microscopic multi-orbital approach is probably the one
 788 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 pertinently 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 D’yakonov 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

$$\hat{H}^{\text{imp}} = \sum_i V_{\text{imp}}(\mathbf{r} - \mathbf{r}_i) + (\lambda_{\text{so}}/\hbar) \hat{\boldsymbol{\sigma}} \cdot [\nabla V_{\text{imp}}(\mathbf{r} - \mathbf{r}_i) \times \hat{\mathbf{p}}], \quad (14)$$

where V_{imp} is the spin-independent impurity potential, and λ_{so} is the spin-orbit coupling parameter of the impurity. In the reciprocal space, this impurity potential becomes

$$\hat{H}_{\mathbf{k}\mathbf{k}'}^{\text{imp}} = \sum_i V_{\mathbf{k}\mathbf{k}'}^{\text{imp}} e^{-i(\mathbf{k}-\mathbf{k}') \cdot (\mathbf{r}-\mathbf{r}_i)} [1 + i\lambda_{\text{so}} \hat{\boldsymbol{\sigma}} \cdot (\mathbf{k}' \times \mathbf{k})]. \quad (15)$$

829 It is clear that the spin-orbit coupled part of the impurity potential acts like a
 830 magnetic field $\mathbf{B}_{\text{so}} \propto \mathbf{k}' \times \mathbf{k}$ on the incoming electron spin $\hat{\sigma}$, where $\mathbf{k}$ is the
 831 momentum of the incoming electron and $\mathbf{k}'$ is the momentum of the outgoing
 832 electron. Therefore, in the case of an unpolarized charge current, this magnetic
 833 field defines a local quantization axis such that electrons with spins parallel and
 834 antiparallel to $\mathbf{B}_{\text{so}}$ experience a different k -dependent scattering rate, as illus-
 835 trated on Fig. 18(a): electrons with a spin momentum pointing (anti)parallel
 836 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 $\mathbf{B}_{\text{so}} \propto \mathbf{k}' \times \mathbf{k}$ 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].

837 In addition, the perturbed wave function in the presence of impurities reads
 838

$$\Psi_{\mathbf{k}}^s \sim e^{i\mathbf{k} \cdot \mathbf{r}} + \sum_i \sum_{\mathbf{k}'} \frac{V_{\mathbf{k}\mathbf{k}'}^{\text{imp}}}{\epsilon_{\mathbf{k}}^s - \epsilon_{\mathbf{k}'}^s + i0^+} e^{-i(\mathbf{k}-\mathbf{k}') \cdot (\mathbf{r}-\mathbf{r}_i)} e^{i\mathbf{k}' \cdot \mathbf{r}} e^{is\lambda_{\text{so}} \mathbf{k}' \cdot (\mathbf{n} \times \mathbf{k})}, \quad (16)$$

839 where s is the spin projection perpendicular to the scattering plane, defined
 840 by the unit vector $\mathbf{n}$. One can see that the scattering wave function acquires
 841 a spin-dependent phase $\sim s\lambda_{\text{so}} \mathbf{n} \cdot (\mathbf{k} \times \mathbf{k}')$ due to the local spin-orbit field.
 842 This phase can be rewritten in term of a spin-dependent spatial displacement
 843 $\boldsymbol{\delta} = s(\lambda_{\text{so}}/\hbar)(\mathbf{n} \times \mathbf{p})$ [166], which is referred to as side-jump scattering. The
 844 skew scattering produces a spin Hall conductivity $\sigma_{\text{SH}}^{\text{skew}} \sim \sigma_{xx}$, namely the
 845 charge-to-spin conversion efficiency is independent on the scattering strength.
 846 In contrast, the side-jump modifies directly the velocity operator of the electron
 847 and therefore it gives a spin Hall conductivity $\sigma_{\text{SH}}^{\text{s-j}} \sim O(\sigma_{xx})$, such that the
 848 spin Hall angle is inversely proportional to the scattering time: the stronger the
 849 scattering the larger the charge-to-spin conversion (see e.g., Ref. [145]).

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

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

$$\sigma_{xy} = \frac{e^2}{\Omega} \sum_{n,m,\mathbf{k}} \frac{2\Im[\langle n|\hat{v}_y|m\rangle\langle n|\hat{v}_x|m\rangle]}{(\epsilon_{n,\mathbf{k}} - \epsilon_{m,\mathbf{k}})^2} (f(\epsilon_{n,\mathbf{k}}) - f(\epsilon_{m,\mathbf{k}})). \quad (17)$$

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_2MO_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 $\sim (\epsilon_{n,\mathbf{k}} - \epsilon_{m,\mathbf{k}})^2$ 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]

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

916 4.2.3. Interfacial spin Hall effect

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

932 4.2.4. Spin swapping

933 Another effect occurs together with the extrinsic spin Hall effect. Let us
 934 consider again the spin-orbit coupled Hamiltonian given in Eq. 15. We already
 935 stressed out that the spin-orbit coupling acts like a k -dependent Zeeman field,
 936 normal to the scattering plane. In the case of unpolarized electrons, this Zeeman
 937 field is responsible for skew scattering [Fig. 18(a)]. Let us now consider an
 938 incoming *spin-polarized* current, whose spin polarization lies *in* the scattering
 939 plane. In this case, the incoming spin precesses around the effective magnetic
 940 field $\mathbf{B}_{\text{so}}$. Since this magnetic field only exists upon scattering from $\mathbf{k}$ to $\mathbf{k}'$,
 941 the spin polarization of the outgoing current is re-oriented [184]. Lifshits and
 942 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 $\mathcal{J}_{s,j}^i$, flowing along $\mathbf{e}_j$ and polarized along $\mathbf{e}_i$, gives rise to a spin current $\mathcal{J}_{s,i}^j$, flowing along $\mathbf{e}_i$ and polarized along $\mathbf{e}_j$, when $i \neq j$, as illustrated on Fig. 18(b). Consistently, a spin current $\mathcal{J}_{s,x}^x$ produces two spin currents $\mathcal{J}_{s,y}^y$ and $\mathcal{J}_{s,z}^z$.

Spin swapping has been derived by several authors within the diffusive limit [185, 186, 187, 188]. For instance, Shchelushkin and Brataas obtained the expression of the charge and spin currents [185, 189]

$$\mathbf{j}_e/\sigma_0 = -\nabla\mu_c + \frac{\xi_{\text{so}}}{\lambda k_F} \nabla \times \boldsymbol{\mu}_s, \quad (18)$$

$$e\mathcal{J}_{s,i}/\sigma_0 = -\nabla_i \boldsymbol{\mu}_s - \frac{\xi_{\text{so}}}{\lambda k_F} \mathbf{e}_i \times \nabla \mu_c + \frac{2\xi_{\text{so}}}{3} \nabla \times (\mathbf{e}_i \times \boldsymbol{\mu}_s). \quad (19)$$

Here, $\mathcal{J}_{s,i}$ is the spin current density flowing along the direction $\mathbf{e}_i$, μ_c and $\boldsymbol{\mu}_s$ are the spin-independent and spin-dependent chemical potentials, σ_0 is Drude conductivity and $\xi_{\text{so}} = \lambda_{\text{so}} k_F^2$ 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 λ . The first terms in Eqs. (18) and (19) are the diffusion terms, the second terms ($\propto \xi_{\text{so}}/\lambda k_F$) 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 $|V_{\mathbf{kk}'}^{\text{imp}}|^2$ 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 modeled 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

$$\begin{aligned} \hat{\mathcal{H}} = & \sum_{i,j} \left(\epsilon_{ij} \hat{c}_{i,j}^\dagger \hat{c}_{i,j} + \Delta_{ij} \hat{c}_{i,j}^\dagger \hat{\boldsymbol{\sigma}} \cdot \mathbf{m} \hat{c}_{i,j} - t_N \left(\hat{c}_{i+1,j}^\dagger \hat{c}_{i,j} + \hat{c}_{i,j+1}^\dagger \hat{c}_{i,j} \right) + h.c. \right) \\ & - \sum_{i,j} \left(t_{i-1,j-1}^{i,j} \hat{c}_{i,j}^\dagger \hat{\sigma}_z \hat{c}_{i-1,j-1} + t_{i-1,j}^{i,j-1} \hat{c}_{i,j-1}^\dagger \hat{\sigma}_z \hat{c}_{i-1,j} + h.c. \right). \end{aligned} \quad (20)$$

The operator $\hat{c}_{i,j}^\dagger = (c_{i,j}^\uparrow, c_{i,j}^\downarrow)^\dagger$ 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 $\epsilon_{ij} = \epsilon_0 + \gamma_{ij}$, ϵ_0 being the unperturbed onsite energy and $\gamma_{ij} \in [-\Gamma/2, \Gamma/2]$ a random potential of strength Γ 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 $t_{i',j'}^{i,j} = it_N \alpha(\epsilon_{i,j'} - \epsilon_{i',j})$, where α is

Figure 21: (Color online) Two dimensional mapping of the (a,c) x - and (b,d) z -components of the spin density (in unit of $10^{-3}\hbar/2$) demonstrating the crossover between extrinsic spin swapping and extrinsic spin Hall effect, for (a,b) $\alpha = 0.3$ and (c,d) $\alpha = 0.6$. The disorder strength is $\Gamma = 1\text{eV}$. The first 20 layers compose the ferromagnetic edge whose magnetization direction is indicated by the black arrow. From Ref. [167]

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 ($\sim 10^5$) 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, δS_x and δS_z . The former is due to spin swapping, i.e. from the conversion of the injected spin current $\mathcal{J}_{s,x}^y$ (flowing along x and polarized along y) into $\mathcal{J}_{s,y}^x$ (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 $\mathcal{J}_{s,y}^z$ (polarized along z). The spin swapping mechanism results in a spin accumulation δS_x , that only survives close to the interface with the ferromagnet. Away from the interface, at a distance corresponding to the spin relaxation length, δS_x vanishes and δS_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

effect [190]. 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]

$$\tau_{\text{sh}} = \frac{\hbar}{2e} \frac{\tilde{\theta}_{\text{sh}}}{D_{\theta}} \eta_0 \left[-(\tilde{g}_r^{\uparrow\downarrow} + |\tilde{g}^{\uparrow\downarrow}|^2) \mathbf{m} \times [(\mathbf{z} \times \mathbf{j}_e) \times \mathbf{m}] + \tilde{g}_i^{\uparrow\downarrow} \mathbf{m} \times (\mathbf{z} \times \mathbf{j}_e) \right] \quad (21)$$

$$\tau_{\text{sw}} = \frac{\hbar}{2e} \theta_{\text{sw}} \frac{\tilde{\theta}_{\text{sh}}}{D_{\theta}} \left[(|\tilde{g}^{\uparrow\downarrow}|^2 - \eta \tilde{g}_r^{\uparrow\downarrow}) m_z \mathbf{m} \times \mathbf{j}_e + \eta \tilde{g}_i^{\uparrow\downarrow} m_z \mathbf{m} \times (\mathbf{j}_e \times \mathbf{m}) \right], \quad (22)$$

$$D_{\theta} \approx \eta_0 [(\tilde{g}_i^{\uparrow\downarrow})^2 + (1 + \tilde{g}_r^{\uparrow\downarrow})(1 + \tilde{g}_r^{\uparrow\downarrow} + \theta_{\text{sw}})] - \theta_{\text{sw}} m_z^2 [(\tilde{g}_i^{\uparrow\downarrow})^2 + (\tilde{g}_r^{\uparrow\downarrow} - \eta)(1 + \tilde{g}_r^{\uparrow\downarrow})] \quad (23)$$

Here $\sigma_{\text{F,N}}$ and $\lambda_{\text{sf}}^{\text{F,N}}$ 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 $\tilde{\theta}_{\text{sh}} = \theta_{\text{sh}}(1 - \cosh^{-1} d_{\text{N}}/\lambda_{\text{sf}}^{\text{N}})$ and normalized mixing conductances $\tilde{g}_j^{\uparrow\downarrow} = 4\tilde{\lambda}_{\text{sf}}^{\text{N}} g_j^{\uparrow\downarrow}/\sigma_{\text{N}}$, where $\tilde{\lambda}_{\text{sf}}^{\text{N}} = \lambda_{\text{sf}}^{\text{N}}/\tanh(d_{\text{N}}/\lambda_{\text{sf}}^{\text{N}})$ is the effective spin diffusion length of the normal metal. Finally, $\eta = \frac{4(1-\gamma^2)g\tilde{\lambda}_{\text{sh}}^{\text{N}}/\sigma_{\text{N}}}{1+4(1-\gamma^2)g\lambda_{\text{sf}}^{\text{F}}/\sigma_{\text{F}}}$, 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 ($\sim g_r^{\uparrow\downarrow}$), the latter is associated with spin precession at the interface via the imaginary part of the mixing conductance ($\sim g_i^{\uparrow\downarrow}$). In general, $g_i^{\uparrow\downarrow} \ll g_r^{\uparrow\downarrow}$ [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 interfacial 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],

$$\frac{\Delta\sigma_{xx}}{\sigma_{xx}} = \tilde{\theta}_{\text{sh}}^2 \frac{\tilde{\lambda}_{\text{sf}}^{\text{N}}\sigma_{\text{N}}}{d_{\text{N}}\sigma_{\text{N}} + d_{\text{F}}\sigma_{\text{F}}} \frac{\tilde{\lambda}_{\text{sf}}^{\text{F}}\sigma_{\text{N}}/(\tilde{\lambda}_{\text{sf}}^{\text{N}}\sigma_{\text{F}}) - \sigma_{\text{N}}/(2\tilde{\lambda}_{\text{sf}}^{\text{N}}g_r^{\uparrow\downarrow})}{(1 + \tilde{\lambda}_{\text{sf}}^{\text{F}}\sigma_{\text{N}}/(\tilde{\lambda}_{\text{sf}}^{\text{N}}\sigma_{\text{F}}))(1 + \sigma_{\text{N}}/(2\tilde{\lambda}_{\text{sf}}^{\text{N}}g_r^{\uparrow\downarrow}))}. \quad (24)$$

Remarkably, the spin Hall magnetoresistance displays an angular dependence that is quite different from its 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 $[\mathbf{m} \cdot (\mathbf{z} \times \mathbf{j}_e)]^2$, 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 : $\lambda_{sf}^N = 1.5, 5$ and 10 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

$$\boldsymbol{\tau} = \tau_{\text{sh}} \mathbf{m} \times [(\mathbf{z} \times \mathbf{j}_e) \times \mathbf{m}] + \tau_{\text{sw}} \mathbf{m} \times (\mathbf{z} \times \mathbf{j}_e), \quad (25)$$

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 $\delta \mathbf{S}$ and compute the torque $\boldsymbol{\tau} = (2\Delta/\hbar) \mathbf{m} \times \delta \mathbf{S}$, which is then parsed between damping-like (τ_{DL}) and field-like (τ_{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, $\tau_{\text{FL}} > \tau_{\text{DL}}$.

Figure 24: (Color online) Ratio between the magnitude of the field-like torque and damping-like torque, $\tau_{\text{DL}}/\tau_{\text{FL}}$, as a function of Γ and α . The ratio is given in logarithmic scale and 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 convenient as they are analytically solvable. Several techniques can be used, such as semiclassical Boltzmann formula, quantum kinetics or Kubo formulae. For instance, in translationally invariant systems, the non-equilibrium spin density induced by an external electric field reads

$$\begin{aligned} \delta \mathbf{S} = & \frac{\hbar}{2\pi\Omega} \int d\epsilon \partial_\epsilon f(\epsilon) \text{Tr}[\hat{\zeta} \hat{G}_\epsilon^R (\hat{\mathbf{v}} \cdot e\mathbf{E}) (\hat{G}_\epsilon^A - \hat{G}_\epsilon^R)] \\ & + \frac{\hbar}{2\pi\Omega} \Re \int d\epsilon f(\epsilon) \text{Tr}[\hat{\zeta} \partial_\epsilon \hat{G}_\epsilon^R (\hat{\mathbf{v}} \cdot e\mathbf{E}) \hat{G}_\epsilon^R - \hat{\zeta} \hat{G}_\epsilon^R (\hat{\mathbf{v}} \cdot e\mathbf{E}) \partial_\epsilon \hat{G}_\epsilon^R]. \end{aligned} \quad (26)$$

Here, $\hat{G}_\epsilon^{R(A)}$ is the perturbed retarded (advanced) Green's function, $f(\epsilon)$ is Fermi-Dirac distribution, $\hat{\mathbf{v}}$ is the velocity operator, $\mathbf{E}$ the external electric field and $\hat{\zeta}$ 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, $\sim \text{Tr}[\hat{\zeta} \hat{G}_\epsilon^R (\hat{\mathbf{v}} \cdot e\mathbf{E}) \hat{G}_\epsilon^A]$, dominates in the weakly disordered metallic regime. In the limit of weak spin-independent constant energy broadening, $\Gamma \rightarrow 0$, one can parse this term into two main contributions [135]

$$\delta \mathbf{S}^{\text{intra}} = \frac{\hbar}{2\Gamma\Omega} \sum_{n,\mathbf{k}} \langle n, \mathbf{k} | \hat{\zeta} | n, \mathbf{k} \rangle \langle n, \mathbf{k} | \hat{\mathbf{v}} \cdot e\mathbf{E} | n, \mathbf{k} \rangle \delta(\epsilon_{n,\mathbf{k}} - \epsilon_F), \quad (27)$$

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

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 $\sim 1/(\epsilon_{n,\mathbf{k}} - \epsilon_{n',\mathbf{k}})^2$, 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,

$$\langle n, \mathbf{k} | \hat{\zeta} | n', \mathbf{k} \rangle \rightarrow -(\langle n, \mathbf{k} | \hat{\zeta} | n', \mathbf{k} \rangle)^*, \quad (29)$$

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

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

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

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]

$$\boldsymbol{\tau}_D = \tau_{\text{FL}}\mathbf{m} \times (\mathbf{z} \times e\mathbf{E}) + \tau_{\text{DL}}m_z\mathbf{m} \times e\mathbf{E}. \quad (34)$$

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 Ψ 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 *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

Figure 25: (Color online) (a) Layer-resolved field-like torque in Pt/Co(111) (black squares), when turning off the induced magnetization on Pt (open diamonds) and when turning off the spin-orbit coupling on Pt (open circles). The slab is composed of 2 Co monolayers (shaded region) deposited on 8 monolayers of Pt. From Ref. [30]. (b) Local density of states and (c) current-driven spin density profile in a Bi_2Se_3 slab composed of five quintuple layers. From [222].

Ref. [102]).

The inverse spin galvanic effect has also been investigated from first principles at the surface of Bi_2Se_3 using the ATK package [222]. Bi_2Se_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 L_{10} FePt/Pt. These calculations con-

1226 affirmed that spin-orbit torques are composed of both field-like and damping-like
 1227 torques, the latter being produced by interband transitions only. By calcu-
 1228 lating both spin-orbit torques and spin currents, the authors showed that in
 1229 the case of Pt/Co(111), both damping-like and field-like torques correlate fa-
 1230 vorably with absorption of spin current, as displayed in Fig. 26(a) and (b).
 1231 However, by capping the Co layer by either Al or O adatoms, the damping-like
 1232 torque is only slightly affected (its magnitude changes up to 50%, but it re-
 1233 mains correlated with the spin current - see Fig. 26), while the field-like torque
 1234 is dramatically altered: it does not correlate with the spin current anymore and
 1235 can even change its sign. This study emphasizes the different physical origin of
 1236 these two components, the field-like torque being much more sensitive to inter-
 1237 faces than the damping-like torque. Overall, these calculations seem to confirm,
 1238 although with a much higher level of complexity, the spin Hall and Rashba sce-
 1239 narii evoked above. Finally, let us mention that Ref. [224] also computed the
 1240 thermally-induced spin-orbit torque in L1₀ FePt/Pt, showing that reasonable
 1241 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].

1242 5. Unconventional dynamics

1243 In the previous Sections, we have seen that transition metal interfaces en-
 1244 compass several exotic effects enabled by spin-orbit coupling: Rashba-type spin
 1245 splitting, Dzyaloshinskii-Moriya antisymmetric exchange interaction, and spin-
 1246 orbit torques. As a result, the magnetic texture at these interfaces is likely to be
 1247 chiral and can be manipulated electrically. In this last Section, we are interested
 1248 in two aspects of the chiral magnetic textures: their energy dissipation and the
 1249 additional "topological" torque that flowing currents exert on these textures.

1250 5.1. Chiral Damping

1251 5.1.1. Fundamentals of magnetic damping

1252 The magnetic damping arises from various mechanisms involving non-linear
 1253 spin waves processes [225, 226, 227] such as two- [228, 229, 230] and three-
 1254 magnon interactions [231] (dominant in magnetic insulators [232]) as well as
 1255 electronic processes driven by spin relaxation [233, 234, 235] (dominant in met-
 1256 als). The latter mechanisms are of primary interest for us because of the dom-
 1257 inant role of spin-orbit coupling. In the hydrodynamic limit, the magnetic
 1258 damping is a *non-local, anisotropic* 3×3 tensor of the form [236]

$$\partial_t \mathbf{m}(\mathbf{r}, t)|_{\text{diss}} = \mathbf{m}(\mathbf{r}, t) \times \int d\mathbf{r}' \underline{\alpha}(\mathbf{r}, \mathbf{r}') \cdot \partial_t \mathbf{m}(\mathbf{r}', t). \quad (35)$$

1259 In an isotropic magnetic material, the dissipation reduces to the well-known
 1260 Gilbert damping form, $\partial_t \mathbf{m}(\mathbf{r}, t)|_{\text{diss}} = \alpha \mathbf{m} \times \partial_t \mathbf{m}$. However, in magnetic metals
 1261 presenting a strong (bulk or interfacial) magnetic anisotropy, one can reasonably
 1262 expect that such anisotropy gets imprinted in the magnetic damping constant
 1263 [237, 3]. Mills and Rezende [3] showed that in a magnetic material with uniaxial
 1264 anisotropy axis $\mathbf{z}$, the damping reads

$$\partial_t \mathbf{m}|_{\text{diss}}^z = \epsilon_{\parallel} \mathbf{m} \times \mathbf{z} \partial_t m_z + \epsilon_{\perp} m_z \mathbf{z} \times \partial_t \mathbf{m}. \quad (36)$$

1265 This anisotropic damping is derived from general considerations and, in the
 1266 particular case considered here, only affects the components of the magnetiza-
 1267 tion *transverse* to the anisotropy direction $\mathbf{z}$. Although not observed yet, this
 1268 anisotropic damping should be quite large in systems with interfacial perpen-
 1269 dicular magnetic anisotropy.

1270 Physically, the mechanism responsible for the magnetic damping in met-
 1271 als can be summarized as follows: the precessing magnetization excites spin-
 1272 orbit coupled electron-hole pairs that relax their own spin angular momentum
 1273 through momentum relaxation processes via defects, impurities or phonon scat-
 1274 tering [234]. This process is usually modeled by the so-called breathing Fermi
 1275 surface model that relates the damping constant to the angular dependence of
 1276 the electronic energy, $\partial_{\theta} \epsilon_{n, \mathbf{k}}$, and to the momentum scattering time τ [238]

$$\lambda_{\text{BFS}} = \tau \frac{g^2 \mu_B^2}{\hbar^2 \Omega} \sum_{n, \mathbf{k}} (\partial_{\theta} \epsilon_{n, \mathbf{k}})^2 \delta(\epsilon_{n, \mathbf{k}} - \epsilon_F). \quad (37)$$

1277 The Gilbert damping is simply defined $\alpha = \lambda M_s / \gamma$, where M_s is the saturation
 1278 magnetization and γ is the gyromagnetic ratio. This formula is valid for $\tau \rightarrow$
 1279 $+\infty$ and only considers electrons close to the Fermi level. An equivalent picture
 1280 was also developed by Kambersky by considering the spin relaxation of long
 1281 wavelength magnons ($q \rightarrow 0$) [239, 240], yielding the so-called torque correlation
 1282 formula

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

1283 In the limit of weak scattering Eq. (38) reduces to Eq. (37) [234]. Equation
 1284 (38) is more general since it accounts for both intraband ($\propto \tau$) and interband
 1285 contributions ($\propto 1/\tau$), and therefore applies to a wider range of disorder regime
 1286 [241, 235]. When applied to realistic band structure, such as Co, Ni or Fe, the
 1287 magnetic damping adopts the symmetries of the crystal structure, resulting in
 1288 rotational and orientational anisotropic damping [242], as illustrated in Fig.
 1289 27. The damping anisotropy calculated in these systems can be as large as
 1290 50%. One has to recall that the magnetocrystalline anisotropy for these bulk
 1291 ferromagnets is of the order of a few $\mu\text{eV}/\text{atom}$. One can reasonably speculate
 1292 that damping anisotropy in ultrathin multilayers with interfacial perpendicular
 1293 magnetic anisotropy of the order of a few 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 ($\tau^{-1} \rightarrow +\infty$), this anisotropy vanishes. From Ref. [242].

1294 The two formulae presented above are quite popular but do not account for
 1295 non-locality. One way to circumvent this limitation is to derive the magnetic
 1296 damping within the linear response theory (see for instance [243, 244] or the

Supplementary material of [245]). Let us consider a general Hamiltonian, $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \Delta \hat{\boldsymbol{\sigma}} \cdot \mathbf{m}$, where the second term connects the itinerant electron spins $\hat{\boldsymbol{\sigma}}$ with the local magnetic moment $\mathbf{m}$. We now introduce a small perturbation to the magnetization $\mathbf{m} \rightarrow \mathbf{m} + \delta \mathbf{m}$ that is time-dependent, $\partial_t \delta \mathbf{m} \neq 0$. Hence, the moving magnetization pumps a non-equilibrium spin density $\delta \mathbf{S} = \underline{\underline{\chi}} \cdot \partial_t \mathbf{m}$, which in turn exerts a torque on the local magnetization, $\boldsymbol{\tau} = (2\Delta/\hbar) \mathbf{m} \times \delta \mathbf{S} \sim \mathbf{m} \times [\underline{\underline{\chi}} \cdot \partial_t \mathbf{m}]$. This torque modifies the dynamics of the magnetization, depending on the symmetry of the tensor $\underline{\underline{\chi}}$ upon magnetization reversal. Indeed, one can rewrite $\underline{\underline{\chi}}(\mathbf{m}) = \underline{\underline{\chi}}^{\text{odd}} + \underline{\underline{\chi}}^{\text{even}}$, where $\underline{\underline{\chi}}^{\text{odd}}(\mathbf{m}) = -\underline{\underline{\chi}}^{\text{odd}}(-\mathbf{m})$ and $\underline{\underline{\chi}}^{\text{even}}(\mathbf{m}) = \underline{\underline{\chi}}^{\text{even}}(-\mathbf{m})$. As a result, the torque possesses two components, $\boldsymbol{\tau} = \boldsymbol{\tau}_{\text{odd}} + \boldsymbol{\tau}_{\text{even}}$, renormalizing the magnetization precession rate, and inducing a magnetic damping, respectively. From Kubo formula, one obtains $\boldsymbol{\tau} = \mathbf{m} \times \int d^3 \mathbf{r}' (\underline{\underline{\alpha}} \cdot \partial_t \mathbf{m})$, where the tensor $\underline{\underline{\alpha}}(\mathbf{r}, \mathbf{r}')$ has the components [244, 245]

$$\begin{aligned} \alpha^{ij}(\mathbf{r}, \mathbf{r}') = & \frac{\Delta^2}{\pi \Omega} \Re \int d\epsilon \partial_\epsilon f(\epsilon) \text{Tr}[\hat{\xi}_i \hat{G}_\epsilon^R(\mathbf{r}, \mathbf{r}') \hat{\sigma}_j (\hat{G}_\epsilon^A(\mathbf{r}', \mathbf{r}) - \hat{G}_\epsilon^R(\mathbf{r}', \mathbf{r}))] \\ & + \frac{\Delta^2}{\pi \Omega} \Re \int d\epsilon f(\epsilon) \text{Tr}[\hat{\xi}_i \partial_\epsilon \hat{G}_\epsilon^R(\mathbf{r}, \mathbf{r}') \hat{\sigma}_j \hat{G}_\epsilon^R(\mathbf{r}', \mathbf{r}) - \hat{\xi}_i \hat{G}_\epsilon^R(\mathbf{r}, \mathbf{r}') \hat{\sigma}_j \partial_\epsilon \hat{G}_\epsilon^R(\mathbf{r}', \mathbf{r})]. \end{aligned} \quad (39)$$

The vertex correction included in $\hat{\xi}$ 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 $\hat{\mathcal{H}} = v \mathbf{p} \cdot (\mathbf{z} \times \hat{\boldsymbol{\sigma}})$, $\hat{\mathbf{v}} = \partial_{\mathbf{p}} \hat{\mathcal{H}} = v(\mathbf{z} \times \hat{\boldsymbol{\sigma}})$, 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, $\mathcal{J}_s|_{\text{interf}} = \hbar(g^{\uparrow\downarrow}/4\pi) \mathbf{m} \times \partial_t \mathbf{m}$, 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 $\alpha_{\text{sp}} = \mathcal{A} g^{\uparrow\downarrow}$, where $g^{\uparrow\downarrow}$ is the real part of the spin mixing conductance and $\mathcal{A}$ 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 [257]. In this case, the damping adopts a tensorial form, $\boldsymbol{\tau} = \mathbf{m} \times \mathcal{D} \cdot \partial_t \mathbf{m}$, where

$$\mathcal{D}_{ij} = \xi \sum_k (\mathbf{m} \times \partial_k \mathbf{m})_i (\mathbf{m} \times \partial_k \mathbf{m})_j, \quad (40)$$

and ξ 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 $1/\lambda_{\text{dw}}^2$, where λ_{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]

$$\alpha^{ij} = \alpha_0^{ij} + \sum_{lm} K_{lm}^{ij} m_l m_m + \sum_{klm} L_{klm}^{ij} m_k \partial_l m_m. \quad (41)$$

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, $L_{klm}^{ij} = L_{mlk}^{ij}$. However, where inversion symmetry is broken, $L_{klm}^{ij} = -L_{mlk}^{ij}$, and this term reduces to Lifshitz anti-symmetric 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

$$\alpha^{ij} = \alpha_0^{ij} + \alpha_{3d}^{ij} \lambda_{\text{dw}} \mathbf{m} \cdot (\nabla \times \mathbf{m}), \quad (42)$$

where λ_{dw} defines the characteristic exchange length. In a two-dimensional system with interfacial symmetry breaking along $\mathbf{z}$, i.e. invariant under $\mathcal{C}_{\infty z}$ rotation symmetry, the damping takes the form

$$\alpha^{ij} = \alpha_0^{ij} + \alpha_z^{ij} \lambda_{\text{dw}} \mathbf{m} \cdot [(\mathbf{z} \times \nabla) \times \mathbf{m}], \quad (43)$$

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 $\mathcal{J}_s$. In the first case, the torque reads $\boldsymbol{\tau} = (2\Delta/\hbar) \mathbf{m} \times \delta \mathbf{S}$, while in the second case it is associated with the spatial gradient of the spin current $\boldsymbol{\tau} = -\nabla \cdot \mathcal{J}_s$. 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 $\boldsymbol{\tau} \sim \alpha_R \mathbf{m} \times (\mathbf{z} \times \mathbf{j}_e)$, where α_R is the Rashba parameter. A symmetric effect coexists: the precessing magnetization pumps a spin-polarized current through spin galvanic effect, $\mathcal{J}_s \sim \alpha_R \mathbf{m} \otimes \mathbf{z} \times \partial_t \mathbf{m}$ (we remind that the spin current is a tensor in the spin $\otimes$ real spaces). The corresponding spin current is then absorbed by the magnetic texture through $\boldsymbol{\tau} = -\nabla \cdot \mathcal{J}_s$. As a result, the total magnetic damping is linear in Rashba parameter, as well as in magnetization gradient, and [206, 202, 260]

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

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 $\mathbf{S}_i = \mathbf{S}_i^d + \hat{\mathbf{s}}_i^s$. The resulting DMI between sites *i* and *j* can be phenomenologically rewritten upto the linear order in $\hat{\mathbf{s}}^s$ as $\mathbf{D}_{ij} \cdot \mathbf{S}_i \times \mathbf{S}_j = \mathbf{D}_{ij}^{dd} \cdot \mathbf{S}_i^d \times \mathbf{S}_j^d + \mathbf{D}_{ij}^{sd} \cdot \mathbf{S}_i^d \times \hat{\mathbf{s}}_j^s$ (neglecting a higher order term $\sim \hat{\mathbf{s}}_i^s \times \hat{\mathbf{s}}_j^s$). 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

$$\hat{\mathcal{H}}_{\text{sd}} = \frac{\alpha_{\text{D}}}{\hbar} \hat{\boldsymbol{\sigma}} \cdot [(\mathbf{z} \times \hat{\mathbf{p}}) \times \mathbf{m}], \quad (45)$$

where $\alpha_{\text{D}} = D_{\text{sd}}a$ (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 $\sim (\mathbf{z} \times \boldsymbol{\nabla}) \times \mathbf{m}$. 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 [260]

$$\boldsymbol{\tau} \sim \{[(\mathbf{z} \times \boldsymbol{\nabla}) \times \mathbf{m}] \times (\mathbf{m} \times \partial_t \mathbf{m})\}_{\perp}, \quad (46)$$

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 $\mathbf{j}_e$ can be converted into a spin Hall current of the form $e\mathcal{J}_{s,i} = \theta_{\text{sh}} \mathbf{m} \otimes \mathbf{m} \times \mathbf{j}_e$, i.e. flowing along the direction $\mathbf{m} \times \mathbf{j}_e$ 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 $\mathbf{x}$ deposited on a normal metal with an interface normal to $\mathbf{z}$ [Fig. 28(c)], as long as the magnetization $\mathbf{m}$ has a non-zero component along $\mathbf{y}$, the spin Hall current that is injected in the adjacent metal along $\mathbf{z}$ is spin polarized along $\mathbf{y}$ and exerts the torque

$$\boldsymbol{\tau} \sim [(\partial_x \mathbf{m} \times \partial_t \mathbf{m}) \cdot \mathbf{y}] \mathbf{m} \times (\mathbf{y} \times \mathbf{m}). \quad (47)$$

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 $\mathcal{J}_{s,z}^{\text{pump}} \sim \mathbf{m} \times \partial_t \mathbf{m} \otimes \mathbf{z}$, 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 $\mathcal{J}_{s,z}^{\text{sw}} \sim \mathbf{y} \times (\mathbf{m} \times \partial_t \mathbf{m}) \otimes \mathbf{z}$ ($\mathbf{y}$ 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 $\tau \sim m_y \partial_t \mathbf{m}$. 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

1468 grain boundaries [13, 14, 15, 16, 275]. To learn how to control the motion of
 1469 such chiral textures, one needs to develop a precise understanding of the nature
 1470 of the torque exerted on these objects. In magnetic textures, the spin transfer
 1471 torque can be generally expressed as

$$\boldsymbol{\tau} = b_J(\mathbf{u} \cdot \nabla)\mathbf{m} - \beta b_J\mathbf{m} \times (\mathbf{u} \cdot \nabla)\mathbf{m}, \quad (48)$$

1472 where $\mathbf{u}$ is the direction of current injection, $\mathbf{m}$ is a unit vector in the direction
 1473 of the magnetization. The two terms on the right hand side of Eq. (48) are
 1474 called the adiabatic ($\sim b_J$) and non-adiabatic torques ($\sim \beta b_J$), respectively
 1475 [276, 277]. While the non-adiabatic parameter β in transverse walls is quite
 1476 small $\beta \approx \alpha$ (α being the magnetic damping of the homogeneous magnet), it
 1477 is much larger in magnetic vortices and reaches 8α to 10α [267, 268, 269, 278].
 1478 Several contributions to the non-adiabatic parameter have been identified: spin
 1479 relaxation [276] ($\beta \sim \lambda_{\text{ex}}^2/\lambda_{\text{sf}}^2$), spin mistracking [279, 280, 281] ($\beta \sim e^{-\lambda_{\text{dw}}/\lambda_{\text{ex}}}$),
 1480 anomalous Hall effect [282] ($\beta \sim \theta_H$), and more recently spin diffusion [283]
 1481 ($\beta \sim \lambda_{\text{ex}}^2/\lambda_{\text{dw}}^2$). Here λ_{dw} is the domain wall width, $\lambda_{\text{ex},\text{sf}}$ are the transverse
 1482 and longitudinal spin relaxation lengths and θ_H is the anomalous Hall angle.

1483 More recently, a few authors proposed that topological Hall effect, inherent
 1484 to both magnetic vortices and skyrmions, can lead to enhanced non-adiabaticity
 1485 [278, 284, 271, 285]. We believe this "topological torque" is of great importance
 1486 for current-driven skyrmion motion because it increases when reducing the size
 1487 of the skyrmion, and can therefore lead to improved dynamical properties upon
 1488 size reduction, as discussed at the end of this Section.

1489 5.2.1. Emergent Electrodynamics

1490 When conduction electrons flow in a smooth and slow magnetic texture,
 1491 $\mathbf{m}(\mathbf{r}, t)$, their spin adiabatically changes orientation so that these electrons ac-
 1492 quire a Berry phase [286, 287, 288]. This geometrical phase can be represented
 1493 by an emergent electromagnetic field ($\mathbf{E}_{\text{em}}, \mathbf{B}_{\text{em}}$) determined by the magnetic
 1494 texture gradients [289, 290, 253, 254, 280, 255, 291]. A useful way to see that
 1495 is to consider the simplest two dimensional s - d Hamiltonian (extension to three
 1496 dimensions is straightforward)

$$\hat{\mathcal{H}} = \frac{\hat{\mathbf{p}}^2}{2m} + J_{\text{sd}}\hat{\boldsymbol{\sigma}} \cdot \mathbf{m}(\mathbf{r}, t). \quad (49)$$

1497 The Schrödinger equation corresponding to Eq. (49) can be re-written in the
 1498 rotating frame of the magnetization, using the unitary transformation $\mathcal{U} =$
 1499 $e^{-i\frac{\theta}{2}\hat{\boldsymbol{\sigma}} \cdot \mathbf{n}}$ where $\mathbf{n} = \mathbf{z} \times \mathbf{m}/|\mathbf{z} \times \mathbf{m}|$ to obtain

$$\tilde{\mathcal{H}} = \frac{(\hat{\mathbf{p}} - e\hat{\mathcal{A}})^2}{2m} + J_{\text{sd}}\hat{\sigma}_z + e\hat{\mathcal{V}}, \quad (50)$$

1500 where the vector and scalar potentials are given respectively as $\hat{\mathcal{A}} = -\frac{\hbar}{2e}\hat{\boldsymbol{\sigma}} \cdot$
 1501 $(\mathbf{m} \times \partial_i \mathbf{m})\mathbf{e}_i$ and $\hat{\mathcal{V}} = \frac{\hbar}{2e}\hat{\boldsymbol{\sigma}} \cdot (\mathbf{m} \times \partial_t \mathbf{m})$. Hence, the electromagnetic field can be

1502 written the form [292, 290, 253, 254, 280, 255, 291, 293, 294, 257, 295]

$$\mathbf{E}_{\text{em}}^s = -\langle s | \partial_i \hat{\mathcal{V}} + \partial_t \hat{\mathcal{A}}_i | s \rangle = \frac{s\hbar}{2e} [\mathbf{m} \cdot (\partial_t \mathbf{m} \times \partial_i \mathbf{m})] \mathbf{e}_i, \quad (51)$$

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

1503 Here, $|s\rangle$ denotes the eigenstate of Eq. (50) in the absence of emergent electro-
1504 magnetic field. As a result, one can compute the charge current for spin s [278]

$$\mathbf{j}_e^s = \sigma_0^s \mathbf{E} + \sigma_0^s \mathbf{E}_{\text{em}}^s + \frac{\sigma_H^s}{B_H} \mathbf{E} \times \mathbf{B}_{\text{em}}^s + \frac{\sigma_H^s}{B_H} \mathbf{E}_{\text{em}}^s \times \mathbf{B}_{\text{em}}^s, \quad (53)$$

1506 where σ_0^s and σ_H^s are respectively the longitudinal and ordinary Hall conductiv-
1507 ities for spin s , $\mathbf{E} = E\mathbf{u}$ is the external electric field, and $B_H = |\mathbf{B}_{\text{em}}^s|$. From Eq.
1508 (53), we note that the spin-dependent current is driven by the external electric
1509 field $\mathbf{E}$ as well as by the emergent electric field governed by the time-variation
1510 of the magnetic texture, $\mathbf{E}_{\text{em}}^s$. We can obtain the expressions for the local spin
1511 current tensor, $\mathcal{J}_s = -\mathbf{m} \otimes (\mathbf{j}_e^\uparrow - \mathbf{j}_e^\downarrow)$, and charge current vector, $\mathbf{j}_e = \mathbf{j}_e^\uparrow + \mathbf{j}_e^\downarrow$,
1512 from Eq. (53). For a static texture ($\partial_t \mathbf{m} = 0$), we obtain

$$\mathcal{J}_s = -b_J \mathbf{m} \otimes \mathbf{u} + \frac{\mathcal{P}_H}{\mathcal{P}_0} \lambda_H^2 b_J [\mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m})] \mathbf{m} \otimes \mathbf{z} \times \mathbf{u}, \quad (54)$$

$$\mathbf{j}_e = \sigma_0 E \mathbf{u} - \sigma_0 \lambda_H^2 E [\mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m})] \mathbf{z} \times \mathbf{u}, \quad (55)$$

1513 where $\sigma_a = \sigma_a^\uparrow + \sigma_a^\downarrow$, $\mathcal{P}_a = (\sigma_a^\uparrow - \sigma_a^\downarrow)/\sigma_a$, ($a = 0, H$), $\lambda_H^2 = \hbar\sigma_H/2e\sigma_0 B_H$.
1514 In addition to the usual constant spin current moving along the direction of
1515 the applied electric field ($\sim \mathbf{u}$), the presence of a non-zero topological charge,
1516 $\mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m}) \neq 0$ (as it is the case for magnetic skyrmions and vortices),
1517 leads to a texture-induced emergent magnetic field that induces an additional
1518 spatially varying spin current along both the longitudinal ($\sim \mathbf{u}$) and transverse
1519 ($\sim \mathbf{z} \times \mathbf{u}$) directions to the electric field $\mathbf{E}$. This longitudinal spin current is
1520 responsible for (i) topological spin and charge Hall effects already observed in
1521 topological textures such as skyrmions [290, 270, 36, 296] and, (ii) enhanced
1522 non-adiabaticity already observed in vortices [278], as illustrated on Fig. 29.

1523 5.2.2. Topological spin torque

1524 Through spin transfer mechanism, the spin current given in Eq. (54) exerts
1525 a torque on the local magnetization, $\boldsymbol{\tau} = -\nabla \cdot \mathcal{J}_s$, which explicitly reads

$$\boldsymbol{\tau} = b_J (\mathbf{u} \cdot \nabla) \mathbf{m} - \frac{\mathcal{P}_H}{\mathcal{P}_0} \lambda_H^2 b_J [\mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m})] [(\mathbf{z} \times \mathbf{u}) \cdot \nabla] \mathbf{m}. \quad (56)$$

1526 A remarkable consequence of Eq. (56) is that since the second term is *even*
1527 upon magnetization reversal, it induces an *intrinsic topological* non-adiabatic
1528 spin transfer torque. This non-adiabatic torque is *intrinsic* as it does not rely
1529 on impurities or defects (in contrast with the non-adiabaticity studied in Refs.
1530 [276, 283]), and *topological* since its origin is associated to the topology of the
1531 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.

1532 To quantify the topological torque, we first study the current-driven dynam-
 1533 ics of an isolated magnetic skyrmion and vortex. To do so, we adopt the rigid
 1534 motion formalized developed by Thiele [297]. The equation of motion governing
 1535 the dynamics of these structures is given by the extended LLG equation

$$\partial_t \mathbf{m} = -\gamma \mathbf{m} \times \mathbf{H}_{\text{eff}} + \alpha \mathbf{m} \times \partial_t \mathbf{m} + \boldsymbol{\tau} - \beta b_J \mathbf{m} \times \partial_x \mathbf{m} \quad (57)$$

1536 where β is a constant non-adiabatic parameter introduced by hand [276, 277].
 1537 The magnetization profile in spherical coordinates is given by the polar angle θ
 1538 and the azimuthal angle φ . The polar angle is defined for an isolated skyrmion
 1539 as $\cos \theta = p(r_0^2 - r^2)/(r_0^2 + r^2)$, and for an isolated vortex as $\cos \theta = p(r_0^2 -$
 1540 $r^2)/(r_0^2 + r^2)$ for $r \leq r_0$, and $\theta = \pi/2$ for $r > r_0$. $p = \pm 1$ defines the skyrmion
 1541 (vortex core) polarity, r_0 is the radius of the skyrmion (vortex core). For both
 1542 textures, the azimuthal angle is defined $\Phi = q \text{Arg}(x + iy) + c\pi/2$, where $q = \pm 1$
 1543 is the vorticity and the $c = \pm 1$ defines the chirality. Using these profiles, we
 1544 obtain the analytical expressions of the velocity components as [284]

$$v_x = -\frac{1 + \alpha_{\text{eff}} \beta_{\text{eff}}}{1 + \alpha_{\text{eff}}^2} b_J, \quad (58)$$

$$v_y = pq \frac{\beta_{\text{eff}} - \alpha_{\text{eff}}}{1 + \alpha_{\text{eff}}^2} b_J, \quad (59)$$

1545 where $\mathcal{C} = 1 + \ln \sqrt{R/r_0}$, and β_{eff} and α_{eff} are the effective non-adiabatic param-
 1546 eter and enhanced magnetic damping, respectively. In the present discussion,
 1547 we neglect the effect of the enhanced damping, treated in Ref. [284], and focus
 1548 on the topological torque. The effective non-adiabatic parameter read,

$$\beta_{\text{eff}} = \begin{cases} \beta + \frac{4S_2}{3} \frac{\mathcal{P}_H}{\mathcal{P}_0} \frac{\lambda_H^2}{r_0^2}, & \text{for skyrmion} \\ \beta \mathcal{C} + \frac{7}{3} \frac{\mathcal{P}_H}{\mathcal{P}_0} \frac{\lambda_H^2}{r_0^2}, & \text{for vortex core,} \end{cases} \quad (60)$$

1549 where $\mathcal{S} = r_0^2/(r_0^2 + R^2)$, and $\mathcal{S}_k = \sum_{i=0}^{i=k} (\mathcal{S})^i$. Remarkably, in both cases
 1550 the topological non-adiabaticity scales with $1/r_0^2$. In other words, the sharper
 1551 the texture, the larger the non-adiabatic torque and the larger the skyrmion
 1552 Hall effect. Reducing the skyrmion (or vortex core) size by a factor of 2 en-
 1553 hances the non-adiabaticity by a factor of 4. Using realistic material param-
 1554 eters $r_0 = 30$ nm, $\theta_{\text{TH}} = \sigma_H/\sigma_0 = 0.01$, and $B_H = 2.5$ T [298], we obtain
 1555 $\lambda_H^2 = 1.32$ nm² and the corresponding topological contribution to the non-
 1556 adiabaticity parameter $\beta = 0.08$.

1557 5.2.3. Tight-binding model

1558 The analytical derivation proposed above relies on the assumption that spin
 1559 transport is adiabatic throughout the magnetic texture, i.e. the spin of the
 1560 conduction electrons remains aligned on the local magnetization direction and
 1561 no spin mistracking is considered [279]. To confirm the analytical results, we
 1562 computed the topological transport and torques in a magnetic skyrmions nu-
 1563 merically using the non-equilibrium wave function formalism implemented on a
 1564 tight-binding model in the KWANT package [205]. The system is composed of
 1565 a scattering region containing an isolated skyrmion or vortex core, attached to
 1566 two ferromagnetic leads. In the same spirit as the tight-binding models previ-
 1567 ously discussed, the system is a two dimensional square lattice described by the
 1568 Hamiltonian [296, 284]

$$\hat{\mathcal{H}} = \sum_i (\epsilon_i \hat{c}_i^\dagger \hat{c}_i + \Delta \hat{c}_i^\dagger \hat{\boldsymbol{\sigma}} \cdot \mathbf{m}_i \hat{c}_i) - t \sum_{\langle ij \rangle} \hat{c}_i^\dagger \hat{c}_j,$$

1569 where the sum $\langle ij \rangle$ is restricted to nearest neighbors, and the skyrmion
 1570 texture is encoded in the unit vector $\mathbf{m}_i$. The torque $\boldsymbol{\tau}_n$ at site $\mathbf{n}$ is computed
 1571 by using the local spin densities as

$$\boldsymbol{\tau}_n = \frac{2\Delta}{\hbar} \mathbf{m}_n \times \langle \mathbf{S}_n \rangle = \tau_n^{\text{ad}} \partial_x \mathbf{m}_n - \tau_n^{\text{na}} \mathbf{m}_n \times \partial_x \mathbf{m}_n, \quad (61)$$

1572 To investigate the total torque exerted on the magnetic skyrmion, we calculated
 1573 the normalized adiabatic and non-adiabatic torque components by integrating
 1574 the projections of the local torque on $\mathbf{m} \times \partial_y \mathbf{m}$ and $\mathbf{m} \times \partial_x \mathbf{m}$ respectively and
 1575 normalized accordingly i.e.

$$\tilde{\tau}_{\text{ad}} = \frac{\int \boldsymbol{\tau} \cdot (\mathbf{m} \times \partial_y \mathbf{m}) d^2 \mathbf{r}}{\int \mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m}) d^2 \mathbf{r}}, \quad (62)$$

$$\tilde{\tau}_{\text{na}} = \frac{\int \boldsymbol{\tau} \cdot (\mathbf{m} \times \partial_x \mathbf{m}) d^2 \mathbf{r}}{\int \mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m}) d^2 \mathbf{r}}. \quad (63)$$

1576 Figure 30 displays both torques as a function of the skyrmion radius r_0 . While
 1577 the adiabatic torque (open symbols) is almost constant, the non-adiabatic torque
 1578 (filled symbols) shows a substantial dependence on the skyrmion radius r_0 , in
 1579 agreement with the analytical results presented in Eq. (60). Besides providing
 1580 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 [284].

1581 magnetic vortices [278], this topological torque opens interesting perspectives
 1582 for the investigation of current-driven skyrmion dynamics. Since the topological
 1583 torque is an intrinsic property of the magnetic texture, one could continuously
 1584 deform this structure by applying, e.g., a perpendicular external magnetic field
 1585 [299, 300], and therefore influence the non-adiabaticity parameter. For instance,
 1586 Moreau-Luchaire *et. al.* [44] demonstrated a reduction of the skyrmion diam-
 1587 eter from 80 nm at 12 mT to 30 nm at 70 mT. Following our predictions, the
 1588 topological non-adiabaticity parameter should increase by a factor ~ 7 in this
 1589 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 *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.

1634 **Acknowledgments**

1635 The authors are grateful for the inspiring discussions with S. Blügel, G.
1636 Bihlmayer, P.M. Haney, S. Grytsyuk, G. Gaudin, M. Miron, V. Baltz, M. Kläui,
1637 H. Yang, J. Sinova, T. Jungwirth, X. Waintal, M. Chshiev, X.X. Zhang, J.
1638 Kosel, and B. Nikolić. This work is supported by the King Abdullah University
1639 of Science and Technology (KAUST).

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