Ph.D. Thesis

Interplay between non-relativistic spin-splitting and spin-orbit coupling in metallic systems

By

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Abstract in English

Non relativistic spin splitting is typically a characteristic phenomenon observed in systems with broken time-reversal symmetry. It is primarily influenced by the effect of magnetic exchange interaction J_{ex} between the spins causing an energy shift between spin-up and spin-down electrons. The occurrence of spin splitting cannot be observed in a system where the time-reversal symmetry (TRS) is preserved, as this symmetry leads to the Kramer's degeneracy. The spin-splitting occurs independently of spin-orbit coupling (SOC) effects though its presence can produce interesting effects through its interplay with the spin-splitting, such effects will be the main topic of this thesis. The property of non-relativistic spin-splitting has proved its importance in spintronics and has several effects on the materials' properties. For example, it can lead to the formation of spin-polarized currents and with SOC can lead to spin Hall (SHE) and anomalous Hall effects (AHE).

The presence or absence of symmetries has become one of the most important aspects in condensed matter physics as it leads to the description of robust phenomena, especially in magnetic and topological systems. The effect of broken space-inversion symmetry in large SOC systems, for instance, is necessary for the presence of the Dzyaloshinskii-Moriya interaction (DMI) which leads to the creation of chiral magnetic structures arising from spin dynamics. In addition, breaking time-reversal symmetry is essential for the emergence of transport responses, such as the AHE, which not only depends on SOC but can also be controlled by its effects. In the presence of spin-orbit coupling in systems with broken inversion symmetry, other significant effects such as the Rashba spin-orbit and the Dresselhaus effect can arise. Furthermore, in topological materials, the breaking of the time-reversal symmetry can give rise to topological Weyl semi-metals.

This thesis includes studies of a few systems characterized by the property of broken time-reversal symmetry exhibiting non-relativistic spin-splitting of energy bands visible in the band structure where its interplay with spin-orbit coupling can generate DMI and/or AHE. These systems with broken time-reversal symmetry can be classified into two categories:

1. **Ferromagnetic systems**: Magnetic thin films of Re/Co/Pt were studied in the first two papers; this system produces very high DMI values due to the availability of the vital conditions. Space-Inversion symmetry is broken due to the presence of interfaces, and the effect of SOC is relatively too strong stemming mainly from platinum. This work presented in Chapter 3, is purely theoretical, based on density functional theory calculations (DFT) in which we examine the effect of tuning the thickness of Co thin films and the effect of interface intermixing on the overall dynamics of the studied system. Chapter 4, is a collective experimental and theoretical study of the same system, it focuses mainly on the importance of interface type and quality on the DMI contribution. Chapter 5, the anomalous Hall effect in the Weyl semi-metal CeAlSi, specifically in its ferromagnetic phase in our DFT calculations, was studied using the Wannierization method. The Weyl points present

in this system originate from the breaking of the inversion symmetry as well as from the lack of TRS. In the presence of SOC, the positions of these Weyl points were monitored and associated with a sign change in the AHE results.

2. **Altermagnetic systems:** Recently, research was ignited with the concept of a new type of magnetism dubbed "altermagnetism" characterized by spin-splitting in the band structure regardless of its compensated magnetization constrained by symmetry. Breaking the time-reversal symmetry in altermagnetism has been an important feature in exploring macroscopic responses that were already seen in ferromagnets. In Chapter 6, CrAs, an altermagnetic candidate, is examined. The effect of SOC acts selectively on the band crossings/anticrossings producing an anomalous Hall effect.

Chapter 1 is an introduction to magnetism, spin-orbit coupling, and symmetries in condensed matter physics. Chapter 2 is devoted to the computational framework. Chapters 3 to 6 include the publications discussed, while Chapter 7 is dedicated to future outlooks and discussions.

Abstract in Polish

Nierelatywistyczne rozszczepienie spinów jest charakterystycznym zjawiskiem zazwyczaj obserwowanym w układach z naruszoną symetrią odwrócenia czasu. Jest ono przede wszystkim determinowane przez efekt magnetycznych oddziaływań wymiany Jex między spinami, które powodują różnicę energii elektronów o spinie skierowanym w górę i w dół. Rozszczepienie spinów nie może być zaobserwowane w układzie, w którym symetria odwrócenia czasu (TRS) jest zachowana, ponieważ symetria ta prowadzi do degeneracji Kramersa. Rozszczepienie spinów zachodzi niezależnie od efektów sprzężenia spin-orbita (SOC), jednak obecność tego sprzężenia może generować ciekawe efekty wynikające z interakcji ze zjawiskiem rozszczepienia spinów. Te efekty są głównym tematem niniejszej rozprawy doktorskiej. Właściwość nierelatywistycznego rozszczepienia spinów okazała się istotna w spintronice i wywiera istotny wpływ na właściwości materiałów. Na przykład może prowadzić do powstawania spinowo spolaryzowanych prądów, a wraz z SOC – do spinowego efektu Halla (SHE) i anomalnego efektu Halla (AHE). Obecność lub brak symetrii stały się jednym z najważniejszych aspektów fizyki materii skondensowanej, ponieważ stan ten pozwala na opisanie trwałych zjawisk, szczególnie w układach magnetycznych i topologicznych. Na przykład, efekt złamania symetrii inwersji przestrzennej w układach o silnym SOC jest główną przyczyną obecności oddziaływania Dzyaloshinskii-Moriya (DMI), które prowadzi do powstania chiralnych struktur magnetycznych wynikających z dynamiki spinowej. Ponadto złamanie symetrii odwrócenia czasu jest niezbędne do powstania reakcji transportowych, takich jak AHE, które nie tylko zależą od SOC, ale także mogą być kontrolowane przez jego efekty. W układach o naruszonej symetrii inwersji przestrzennej w obecności SOC występują także inne istotne efekty, takie jak efekt Rashby i Dresselhause'a. Co więcej, w materiałach topologicznych, złamanie symetrii odwrócenia czasu może prowadzić do powstawania topologicznych półmetali Weyla. Niniejsza praca obejmuje badania kilku układów, w których naruszona jest symetria odwrócenia czasu, co skutkuje nierelatywistycznym rozszczepieniem spinów widocznym w strukturze pasmowej, a poprzez oddziaływanie ze sprzężeniem spin-orbita może generować DMI i/lub AHE. Układy z naruszoną symetrią odwrócenia czasu można podzielić na dwie kategorie:

1. **Układy ferromagnetyczne:** Magnetyczne cienkie warstwy Re/Co/Pt zostały opisane w dwóch pierwszych artykułach. Układ ten generuje bardzo wysokie wartości DMI dzięki występowaniu kluczowych warunków. Symetria inwersji przestrzennej jest naruszona z powodu obecności interfejsów, a efekt SOC jest stosunkowo silny i głównie pochodzi od platyny. Artykuł przedstawiony w Rozdziale 3 jest czysto teoretyczny, oparty na obliczeniach z wykorzystaniem teorii funkcjonału gęstości (DFT), w których badany jest wpływ dostrajania grubości cienkich warstw Co i efektu wymieszania na interfejsie na ogólną dynamikę badanego układu warstwowego. Rozdział 4 zawiera opis zbiorczego badania eksperymentalnego i teoretycznego tego samego układu, które skupia się głównie na wpływie rodzaju i jakości interfejsu na wielkość DMI. Rozdział 5 omawia anomalny efekt Halla

w półmetalu Weyla CeAlSi, konkretnie w jego ferromagnetycznej fazie, z wykorzystaniem metody Wannieryzacji zastosowanej w naszych obliczeniach DFT. Punkty Weyla obecne w tym układzie wynikają z naruszenia symetrii inwersji oraz braku TRS. W obecności SOC monitorowano pozycje tych punktów Weyla, które powiązano ze zmianą znaku w wynikach AHE.

2. **Układy altermagnetyczne:** Niedawno badania wzbudziły zainteresowanie nowym rodzajem magnetyzmu, nazwanym „altermagnetyzmem," który charakteryzuje się rozszczepieniem spinów w strukturze pasmowej, niezależnie od skompensowanego namagnesowania ograniczonego przez symetrię. Naruszenie symetrii odwrócenia czasu w altermagnetyzmie było ważnym czynnikiem w badaniu makroskopowych reakcji, które były wcześniej obserwowane w ferromagnetykach. W Rozdziale 6 opisano badania CrAs, jako kandydata na altermagnetyk. Efekt SOC działa selektywnie na przecinanie/nieprzecinanie pasm, prowadząc do anomalnego efektu Halla.

Rozdział 1 jest wprowadzeniem do magnetyzmu, sprzężenia spin-orbita i symetrii w fizyce materii skondensowanej. Rozdział 2 poświęcony jest zastosowanej metodologii obliczeniowej. Rozdziały 3 do 6 zawierają omówione publikacje, natomiast w Rozdziale 7 dyskutowane są perspektywy przyszłych badań.

To the woman I have become,

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My thesis stands as a tribute to those who lifted me during moments of doubt, those who embraced me as I am.

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AUTHOR'S DECLARATION

I hereby certify that the work contained in this dissertation has not been submitted for consideration in any other academic awards and has been completed in accordance with the rules and guidelines of the Institute of Physics, Polish Academy of Science (IFPAN) and the Code of Practice for Research Degree Programs. Unless otherwise specified by a specific reference in the text, the work is the candidate's own contribution. Work accomplished with the assistance of or in collaboration with others is acknowledged as such. In the dissertation, only the author's viewpoints are given.

SIGNED: ..... DATE: .....

List of publications

The thesis incorporates the following papers to which I have contributed as either a primary or secondary author.

1. **Amar Fakhredine**, Andrzej Wawro, and Carmine Autieri. *"Huge Dzyaloshinskii–Moriya interactions in Pt/Co/Re thin films."* Journal of Applied Physics 135, no. 3 (2024)
2. Anuj Kumar Dhiman, **Amar Fakhredine**, Ryszard Gieniusz, Zbigniew Kurant, Iosif Sveklo, Piotr Dłużewski, Wojciech Dobrogowski, Sukanta Kumar Jena, Aleksiej Pietruczik, Carmine Autieri, Andrzej Wawro, and Andrzej Maziewski. *"Evolution of static and dynamic magnetic properties of Re/Co/Pt and Pt/Co/Re trilayers with enhanced Dzyaloshinskii-Moriya interaction"* Applied Surface Science, 679:161151, 2025
3. Alam, Md Shahin, **Amar Fakhredine**, Mujeeb Ahmad, P. K. Tanwar, Hung-Yu Yang, Fazel Tafti, Giuseppe Cuono et al. *"Sign change of anomalous Hall effect and anomalous Nernst effect in the Weyl semimetal CeAlSi."* Physical Review B 107, no. 8 (2023): 085102
4. **Amar Fakhredine**, Raghottam M. Sattigeri, Giuseppe Cuono, and Carmine Autieri. *"Interplay between altermagnetism and nonsymmorphic symmetries generating large anomalous Hall conductivity by semi-Dirac points induced anticrossings."* Physical Review B 108, no. 11 (2023): 115138

OTHER PUBLICATIONS CARRIED OUT DURING THE PH.D.

The below list includes publications that are not included in the thesis.

1. Hussain, Ghulam, **Amar Fakhredine**, Rajibul Islam, Raghottam M. Sattigeri, Carmine Autieri, and Giuseppe Cuono. *"Correlation-Driven Topological Transition in Janus Two-Dimensional Vanadates."* Materials 16, no. 4 (2023): 1649

2. Giuseppe Cuono, Ghulam Hussain, **Amar Fakhredine**, and Carmine Autieri. *"Topological Phase Diagram of $Pb_{1-x}Sn_xSe_{1-y}Te_y$ Quaternary Compound."* Acta Physica Polonica A 142, no. 4 (2022): 521-528

3. Sukanta K. Jena, Jan Kisielewski, Ryszard Gieniusz, Urszula Guzowska, **Amar Fakhredine**, Carmine Autieri, Artem Lynnyk, Aleks Pietruczik, Andrzej Maziewski, and Andrzej Wawro. *"Field angle-dependent bubble lattice formation in $Re/Co/Pt$ multilayers."* In 2023 IEEE International Magnetic Conference-Short Papers (INTERMAG Short Papers), pp. 1-2. IEEE, 2023

OTHER WORKS IN PROGRESS CARRIED OUT DURING THE PH.D.

These works were also conducted during the Ph.D. program and are currently in progress for publication.

1. Autieri, Carmine, Raghottam M. Sattigeri, Giuseppe Cuono, and **Amar Fakhredine**. *"Staggered Dzyaloshinskii-Moriya interaction inducing weak ferromagnetism in centrosymmetric altermagnets and weak ferrimagnetism in noncentrosymmetric altermagnets."* arXiv preprint arXiv:2312.07678 (2023)

2. Lim, Ji Soo, Carmine Autieri, **Amar Fakhredine**, Merit Spring, Martin Kamp, Louis Veyrat, Axel Lubk, Bernd Büchner, Michael Sing, and Ralph Claessen. *"Spontaneous Anomalous Hall Effect in $SrIrO_3$ (111) Thin Film."* Manuscript in preparation.

3. Cuono, Giuseppe, Carmine Autieri, **Amar Fakhredine**, Jan Skolimowski, Silvia Picozzi, Mario Cuoco, and Filomena Forte. *"Transition between Two Distinct Altermagnetic Phases under Modulation of the Electric Field in Orbital-Selective Altermagnet Ca_2RuO_4."* Manuscript in preparation.

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CHAPTER 1

INTRODUCTION

1.1 Magnetism

Magnetism stems from the intricate relationship between the orbital and spin properties of electrons and their interactions. Each electron carries an orbital angular momentum (l) and a spin angular momentum (s), both of which contribute to the electron's magnetic moment. The total orbital and spin angular momentum of a system with n electrons is written as:

$$L = \sum_{i}^{n} l_i \quad S = \sum_{i}^{n} s_i \tag{1.1}$$

To understand the electronic arrangement in a system of electrons such as atoms and molecules, one has to consider the Pauli exclusion principle which describes the behaviour of the half-integer particles. The principle simply states that no two electrons that share the same quantum numbers can be in the same electronic state, therefore they should at least have opposite spins. The second part of the rule is that in a single orbital, only two electrons can be accommodated. Following this rule, it is rather clear that if all the orbitals were to be completely filled, no net magnetic moment would result.

Another rule which governs the way that the orbitals should be filled is known as the first Hund's rule. It states that during the assignment of electrons, the same energy should be distributed on each orbital before the electrons start pairing up in the half-filled orbitals. In other words, all the singly occupied orbitals will have the same spin which maximizes S. The second point of the rule, is that the highest value of L results in the lowest in energy. The total angular momentum, J = L + S, has the lowest value when the electronic arrangement has less than half-filled shells, while it is maximized if it is more than half-filled. This explains the magnetic moment found in 3d and 5d transition metals with partially filled shells, which results from the spin and orbital

momentum components.
Faraday categorized all the substances under his study into paramagnetic and diamagnetic. Paramagnetic substances were those attracted by an electromagnet, while the term diamagnetic was used for those repelled by it. In paramagnets, the atomic dipoles point in randomized directions in the absence of a field, resulting in no magnetization in any direction. The spins tend to align parallel to the external magnetic field enhancing the overall magnetization in the same direction and lowering the energy of the system. At low temperatures, where the thermal agitation is less effective, the Curie law was discovered where the susceptibilities of many systems follow the equation $\chi = \frac{C}{T}$. In diamagnetism, on the other hand, the atomic spins align such that the magnetization points as opposed to the applied magnetic field. In both paramagnets and diamagnets, the total magnetic moment is absent in a zero-applied field. Diamagnetic materials generate a weak, opposing magnetic moment in response to an external magnetic field, in accordance with Lenz's rule, which states that the direction of an induced current will oppose the change in magnetic flux. This causes diamagnets to be repelled by an external magnetic field. Ferromagnetic materials, such as cobalt, nickel,iron, and gadolinium are also attracted by an electromagnet but with a much stronger coupling interaction where the atomic spins interact with one another trying to align in the same direction[4]. This strong interaction creates an order that persists even with no applied field and results in a permanent magnetic moment[5].

While parallel alignment of the spins is typical in ferromagnets, it is not the only present configuration in magnetic systems. In 1936, Louis Néel introduced the theory of antiferromagnetism. In antiferromagnets, the magnetic moments form two equal but opposite sublattices defined as M_A and M_B which cancels out the total magnetization. The phase transition of such systems occurs at a specific temperature known as the Néel temperature T_N where the spins start to order. In other systems, the sublattices M_A and M_B are unequal giving rise to a finite magnetization, and this is known as ferrimagnetism. In ferrimagnetic systems, a net magnetic moment is also expected stemming from the difference in the magnitude of the moments. What is mentioned so far about the ordered states are known as collinear magnetic configurations, however, some systems do not have collinear magnetic moments but are known as helical or spiral structures[6]. Some other noncollinear magnetic systems having random directions of the moments are known as "spin glass", in which the magnetic atoms create a frustrated interaction between the spins.

Researchers have been outraged recently by the emergence of a new type of magnetism in which the magnetization densities obey the non-relativistic spin symmetry making a combination of two-fold spin-space rotations and a real-space rotation. Unlike, say antiferromagnetism where the spin-up and spin-down sublattices are simply related by translation and inversion symmetry, in altermagnets they are connected only through proper or improper rotations and symmorphic or nonsymmorphic symmetries. Altermagnetism combines the properties of both ferromagnets and antiferromagnets in the sense that such systems have no net magnetization but still show a band

splitting in the absence of spin-orbit coupling (SOC) as a consequence of a broken time-reversal symmetry[7]. This non-relativistic spin-splitting is sizable and can even exceed that of a bulk crystal with a heavy element. In conventional antiferromagnets, the Kramer's degeneracy is protected even in the presence of SOC, however, in altermagnets it is lifted even when no SOC nor inversion-symmetry breaking is present[8]. The schematic diagram presented in Fig.1.1 shows how to differentiate altermagnets from conventional antiferromagnets. One common mistake in the search for an altermagnetic behavior is observing the non-relativistic spin splitting (NRSS) at the time-reversal invariant momenta (TRIM) points in the band structure which is not a property of an altermagnet. TRIM points in altermagnetic systems still preserve the identity of Kramer's degeneracy even in the presence of SOC as long as no ferromagnetism is generated. Some antiferromagnets show spin-splitting as in Fig.1.1, however, their sublattices are not connected by any crystal symmetry which classifies them differently than antiferromagnets.

1.2 Spin-orbit coupling

Spin-orbit coupling (SOC) interaction is an important phenomenon in magnetism and is responsible for many other aspects such as band topology, magnetocrystalline anisotropy and magnetostriction. It arises from relativistic effects which are described by the famous equation of Dirac, and it links the motion of a particle in a crystal to its spin, making the energy in the

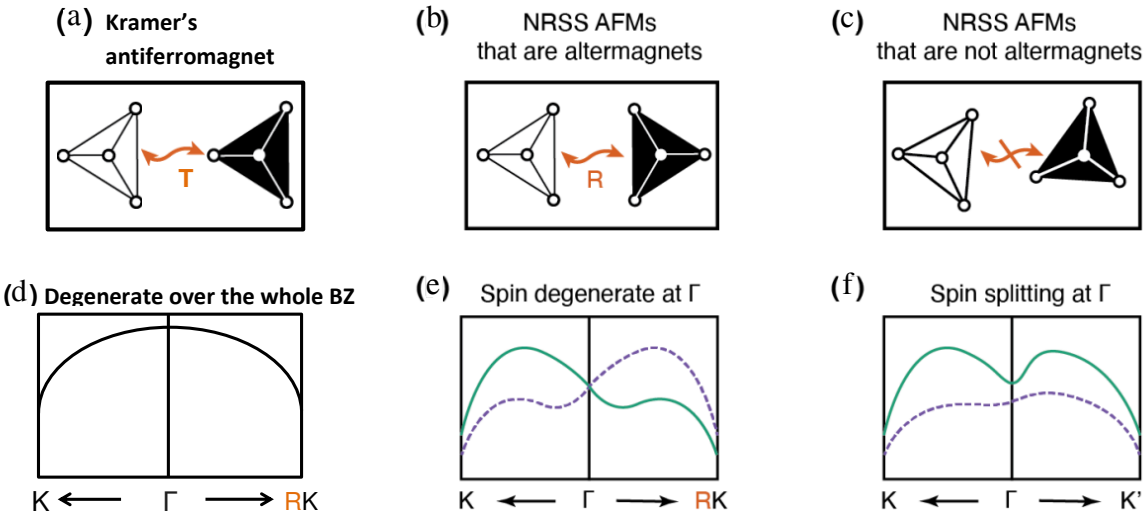

Figure 1.1: Schematic diagram of the behavior of the band structure in the case of a conventional Kramer's antiferromagnet (a,d), altermagnet (b,e), and neither an altermagnet nor an antiferromagnet (c,f). The figure is adapted from reference [1].

Hamiltonian as:

$$H_{SO} = \lambda \vec{L} \cdot \vec{S} \tag{1.2}$$

where λ is known as the SOC parameter.
The SOC causes a shift in the energy levels of an electron as it enters an electric field caused by the nucleus of an atom coupled by its spin to the effective magnetic field via the equation:

$$\hat{H} = -\hat{\vec{\mu}}_S \cdot \vec{B} \tag{1.3}$$

where $\hat{\vec{\mu}}_S = -\frac{g_s \mu_B}{\hbar} \hat{\vec{S}}$ is the spin magnetic dipole, where g_s is the spin-g-factor of the electron which is equal to 2, and $\mu_B = \frac{e\hbar}{2m}$ is the Bohr magneton[9].
The effect of SOC scales with the power four of the element's atomic number Z^4, therefore, when the nucleus of an atom gets bigger the SOC greatly increases[10]. Spin degenerate levels can be split by the effect of SOC into parallel and antiparallel. The degeneracy of states with the same orbital can be lifted with opposite spins in a free atom, but in solids, this splitting is not allowed due to the crystal symmetry. The time-reversal symmetry imposes that the Hamiltonian stays invariant under the reversal of the time's direction. This can also be reflected in the spin, an internal degree of freedom. Time reversal symmetry usually preserves Kramer's degeneracy in half-integer spin systems. Kramer's degeneracy is lifted only in the case where time-reversal symmetry is broken such as the application of external magnetic fields. At any energy E and point k satisfies the following equation:

$$E(k,\uparrow) = E(-k,\downarrow) \tag{1.4}$$

This degeneracy is unaffected by the inclusion of SOC in the Hamiltonian. If the system preserves inversion symmetry, meaning that the crystal lattice remains unchanged when $\vec{r} \rightarrow -\vec{r}$ we will get:

$$E(k,\uparrow) = E(-k,\uparrow) \;\; and \;\; E(k,\downarrow) = E(-k,\downarrow) \tag{1.5}$$

We can see that from the combination of both symmetries designated by equations 1.4 and 1.5 spin splitting is not possible since they yield the following constraint:

$$E(k,\uparrow) = E(k,\downarrow) \tag{1.6}$$

We can conclude that at least one of the symmetries should be broken to observe the spin-splitting caused by SOC.
The electric field generated by the positively charged nucleus results in the intrinsic spin-orbit coupling. However, other types of spin-orbit coupling can arise due to different electric field sources. The Dresselhaus spin-orbit coupling[11] occurs in systems with broken inversion symmetry while the Rashba[12] spin-orbit coupling arises in systems with broken time-reversal along a high symmetry axis symmetry. In systems where the time-reversal symmetry is broken, the SOC can induce several magnetic effects and interactions such as the Dzyaloshinskii-Moriya interaction (DMI) and the anomalous Hall effect (AHE).

1.3 Dzyaloshinskii-Moriya interaction

In 1958, Dzyaloshinskii demonstrated that in the thermodynamic theory of magnetic systems, spin-orbit coupling introduces both symmetric and antisymmetric terms in the spins[13]. While the symmetric terms contribute to magnetocrystalline anisotropy and can renormalize the magnetic exchange, the antisymmetric term enables a relativistic weak ferromagnetism (via spin canting) even in centrosymmetric systems with zero non-relativistic magnetization if time-reversal symmetry is broken. An elegant theory for those systems with zero non-relativistic magnetization and broken time-reversal symmetry were presented in 2022[7]. It was shown that these systems are non-conventional due to their even-parity wave in the k-space, these systems were named altermagnets to emphasize their difference from conventional antiferromagnets which preserve the time-reversal symmetry and consequently Kramers degeneracy. The Dzyaloshinskii-Moriya interaction is an antisymmetric exchange interaction that occurs between spins and may lead to non-collinear and/or chiral spin textures. It appeared as a consequence of adding the effect of SOC to the Heisenberg model. Unlike the collinear exchange interaction known as the *Heisenberg* interaction given as:

$$\hat{H} = -J_{ij} \ \ \vec{S}_i \cdot \vec{S}_j \tag{1.7}$$

which favors parallel spin alignments, the DMI favors a perpendicular one and is calculated from the product of two spins:

$$\hat{H}_{DMI} = \vec{D_{ij}} \cdot (\vec{S}_i \times \vec{S}_j) \tag{1.8}$$

The vector $\vec{D_{ij}}$ is the atomic DMI vector, while $\vec{J_{ij}}$ in the Heisenberg equation is the exchange constant. The origin of such an interaction is the absence of the inversion symmetry and the existence of SOC, typically occurring at the interface between a ferromagnetic material and a heavy metal. However, the DMI can also occur in bulk materials that inherently lack inversion symmetry, such as in chiral magnets like FeGe and MnSi[14, 15]. In these bulk materials, the crystallographic structure itself breaks inversion symmetry, allowing the DMI to emerge without the need for an interface.

The interfacial DMI was initially understood as weak ferromagnetism in antiferromagnetic insulators but later generalized to other systems[13, 16]. This interaction can stabilize the formation of skyrmions which has been verified experimentally, and these are magnetic textures which behave like particles having a size of a few nanometers. Their small size allows them to be easily manipulated which makes them very useful for abacus-type applications like information storage and logic functions[17]. There are two types of skyrmions depending on the direction of the rotation affected by different symmetries named as Bloch type and Néel type. Skyrmions are defined by the topological Skyrmion number S, which characterizes the emergent magnetism arising from the winding of the spins in the skyrmion configuration around the unit sphere. In

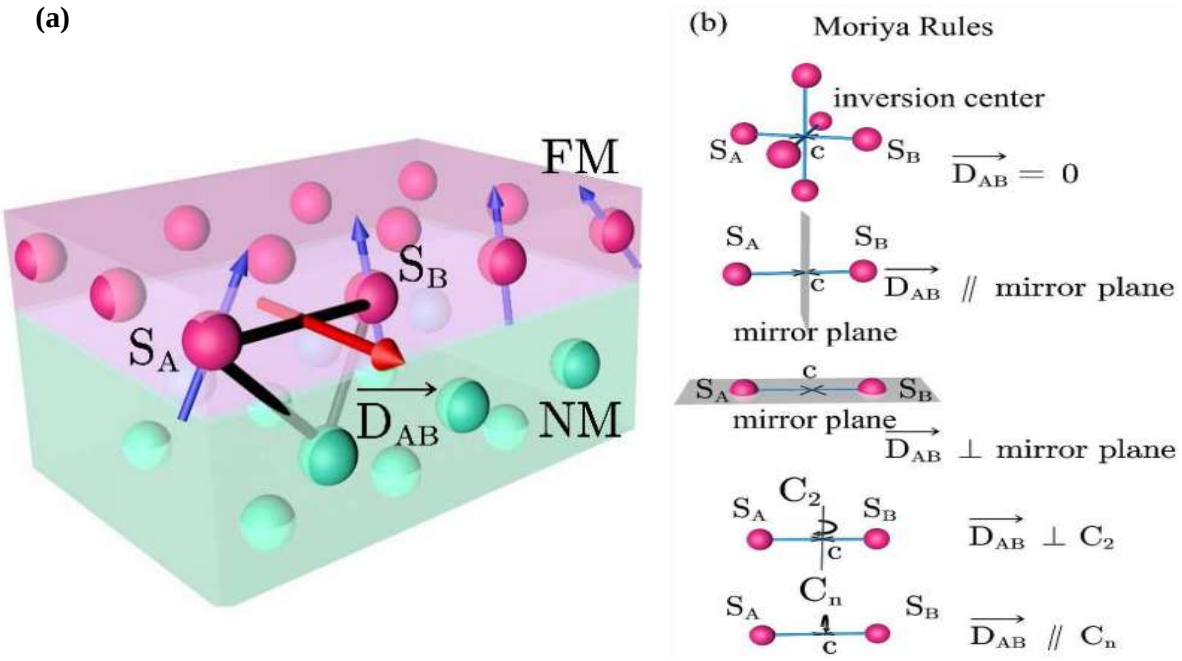

Figure 1.2: (a) Schematic diagram of the direction of the DMI vector in a layered structure of a nonmagnet (NM) and a ferromagnet (FM) (b) The Moriya rules. The figures are taken from reference [2].

the two-dimensional limit, this number is defined as :

$$S = \frac{1}{4\pi}\int \vec{m}\cdot(\partial_x\vec{m}\times\partial_y\vec{m})d_x d_y = \pm 1 \tag{1.9}$$

This number is zero for a ferromagnet or an antiferromagnet. The direction of the DMI vector $\vec{D_{ij}}$ is determined by the Moriya rules[16], but in the case of the interfacial DMI where a ferromagnetic material is placed on top of a non-magnetic material with strong spin-orbit coupling, then the direction of the vector is perpendicular to the triangle formed by the two spins and the third non-magnetic neighboring atom as shown in Fig.1.2.
Moriya has come up with five criteria that relate the crystal symmetry effect to the DMI[2]. Assuming that two magnetic ions have positions at points A and B, where the center is labeled by C then:

1. If the center C is also an inversion center, then $\vec{D}_{ij} = 0$.
2. If a mirror plane perpendicular to the line AB passes through the center C, then $\vec{D}_{ij} \parallel$ mirror plane or $\vec{D}_{ij} \perp$ AB.
3. If the mirror plane contains both the A and B points, then $\vec{D}_{ij}$ is $\perp$ to the mirror plane.
4. If there is a two-fold rotation axis $\perp$ to AB which passes through C then $\vec{D}_{ij} \perp$ to the two-fold rotation axis.

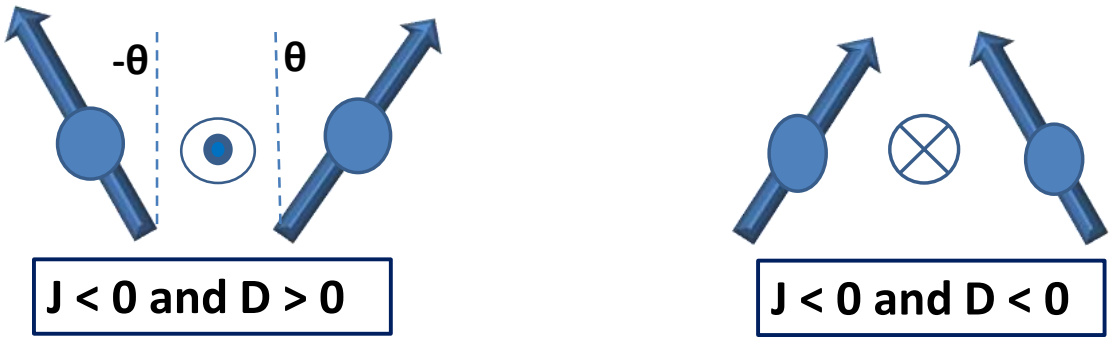

Figure 1.3: Competition between the DMI interaction D and the exchange interaction J.

5. If there is an n-fold rotation axis along the AB line, then $\vec{D}_{ij}$ is ∥ to AB.

1.4 Staggered Dzyaloshinskii-Moriya interaction

The staggered form of the Dzyaloshinskii-Moriya interaction occurs when the sign of the DMI alternates for instance along a chain of atoms. In this situation, the DMI interaction on different magnetic sublattices varies resulting in a modulated type of interaction. In the traditional form of the DMI discussed in Section 1.3, in a system with inversion symmetry the total DMI is null ($\sum_{i,j} D_{i,j} = 0$) and this makes any DMI interaction between two spins null as well ($D_{i,j} = 0$). In the case of staggered DMI, while the inversion symmetry remains unbroken, the DMI vector between sites can still be nonzero ($D_{i,j} \neq 0$). Depending on the sign of the DMI, we have different canting as depicted in Fig. 1.3. A uniform DMI in a ferromagnetic system can create chiral magnetic structures as illustrated in Fig. 1.4(a), while the uniform DMI is ineffective in antiferromagnets as seen in the top part of Fig. 1.4(b). This staggered DMI can induce a weak ferromagnetic/ferrimagnetic behavior in crystal systems in the presence or absence of inversion symmetry as can be seen in Fig.1.4 (b). The weak ferromagnetism (defined as ferromagnetism driven by spin-orbit coupling) can appear only in altermagnets since the spin-orbit needs a system with broken time-reversal symmetry to create ferromagnetism. In such systems, the weak ferromagnetism/ferrimagnetism appears as an interplay between the space group, magnetic order, and the direction of the Néel vector. As of the submission of this thesis, a preprint of our study on this topic is available on arXiv[18].

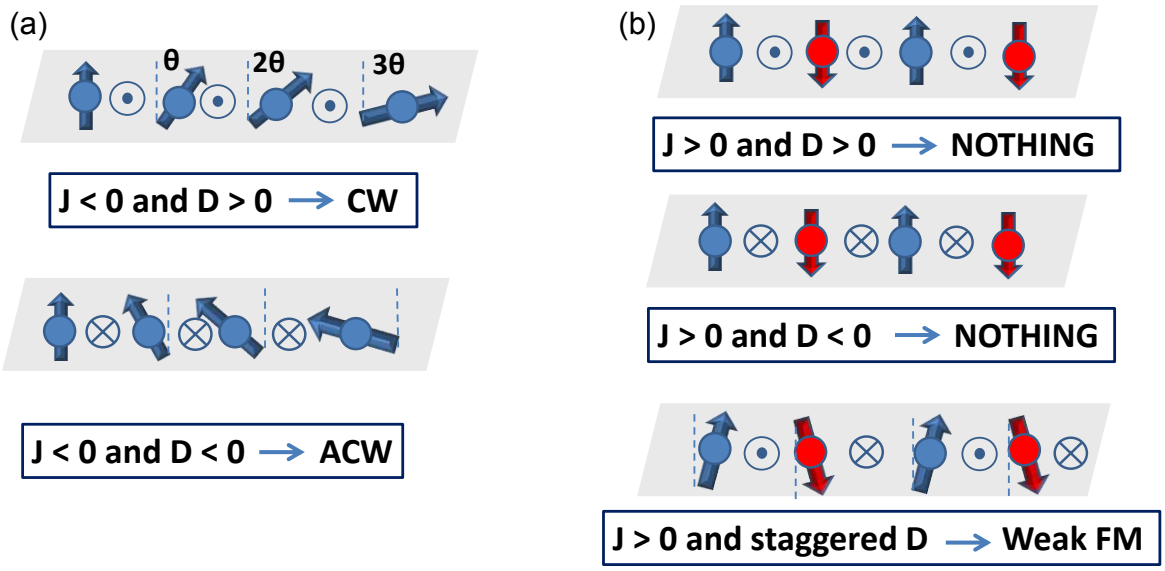

Figure 1.4: Competition between the DMI interaction D and the exchange interaction J in (a) ferromagnets and (b) altermagnets.

1.5 Anomalous Hall effect

The Hall effect, which was discovered in 1881 by Hall[19], and discussed that a conductor carrying a current under the effect of a magnetic field undergoes the effect of the Lorentz force which shifts the electrons to one side, was later overcome by a stronger effect found in ferromagnets [20]. This stronger effect is now known as the anomalous Hall effect (AHE) and it is related to the topology and to the geometry of the system, such as the Berry curvature. The AHE occurs in systems with broken time-reversal symmetry under the inclusion of SOC which results in intrinsic effects related to the band structure of the material and extrinsic effects related to the lattice impurity. The equation for the Hall's resistivity of ferromagnets is empirically known to follow the equation:

$$\rho_{xy} = R_0 B + R_s M_Z \tag{1.10}$$

where the second part $R_s M_z$ is related to the anomalous Hall coefficient originating from the fact that the current exists even in the absence of a magnetic field and is related to the magnetization M_z.

An observation made by Karplus and Luttinger in the 1950's[21] showed that spin splitting of the bands in the presence of spin-orbit coupling (SOC) can contribute to Hall conductivity. Another significant observation was made by Smit[22], who demonstrated that the anomalous Hall effect (AHE) can occur only through impurity scattering, where the skew scattering mechanism was introduced. In this mechanism, spin-up and spin-down electrons are scattered asymmetrically by the potential of the impurity under the influence of SOC. Another mechanism by Berger was

later introduced[23] called the side jump causing the spin-up and spin-down electrons to undergo a lateral shift where the wave vector is conserved.
The intrinsic contribution to the AHE is related to the Berry curvature[24] of the Bloch electrons which plays a similar role of an effective magnetic field in the real space. This field is derived from a vector potential in momentum space known as the Berry connection denoted as $\vec{A}_n$ representing the local phases of the wave function and is calculated using this equation:

$$\vec{A}_n = i\langle u_n|\nabla_k|u_n\rangle \tag{1.11}$$

where u_n is the lattice periodic part of the Bloch wave.
The Berry curvature is then related to the Berry connection through:

$$\vec{\mathscr{F}}_n = \vec{\nabla}_{\vec{k}} \times \vec{A}_n \tag{1.12}$$

One can think about the Berry curvature as a geometrical feature of an energy band that describes the evolution of the eigenstates of the system in response to variation to changes in the system's parameters such as the momentum. Lastly, the intrinsic AHE is related to the Berry curvature by the following equation:

$$\sigma_{xy} = -\frac{e^2}{h}\int \frac{d^2k}{2\pi}\sum_n f_{FD}^n \mathscr{F}_n \tag{1.13}$$

where f_{FD}^n is the Fermi-Dirac distribution function.

1.6 Weyl Semimetals

Weyl fermions discovered by Hermann Weyl, existed as massless particles in the Dirac equation in 1929 [25, 26]. A Weyl semimetal is a state that hosts Weyl fermions. A Weyl semimetal is a material in which the electronic bands touch at discrete points in momentum space, where the energy is cone-like, rather than being separated by an energy gap as in conventional insulators or semiconductors. The Weyl equation governs the energy excitations near the touching points. These points, known as Weyl points, arise in crystals that lack inversion symmetry and are characterized by low-energy excitations that behave like Weyl fermions. Such an observation was initially explained as "accidental" degeneracies, these band touchings are now understood to be topologically protected by recent advances in band theory, meaning they are robust against perturbations. In other words, at any generic point k in the BZ, a two-fold degenerate band crossing of non-degenerate bands occurs giving Weyl semimetals their distinct topological nature[27]. Weyl points act as sources and sinks to the Berry curvature as they are assigned to a topologically protected chiral charge of +C or -C, and they can occur in systems where either time-reversal symmetry or inversion symmetry is broken. The charge C is an integer number which is usually 1 or 2, this is also the Chern number of Hamiltonian projected from cutting the plane between the

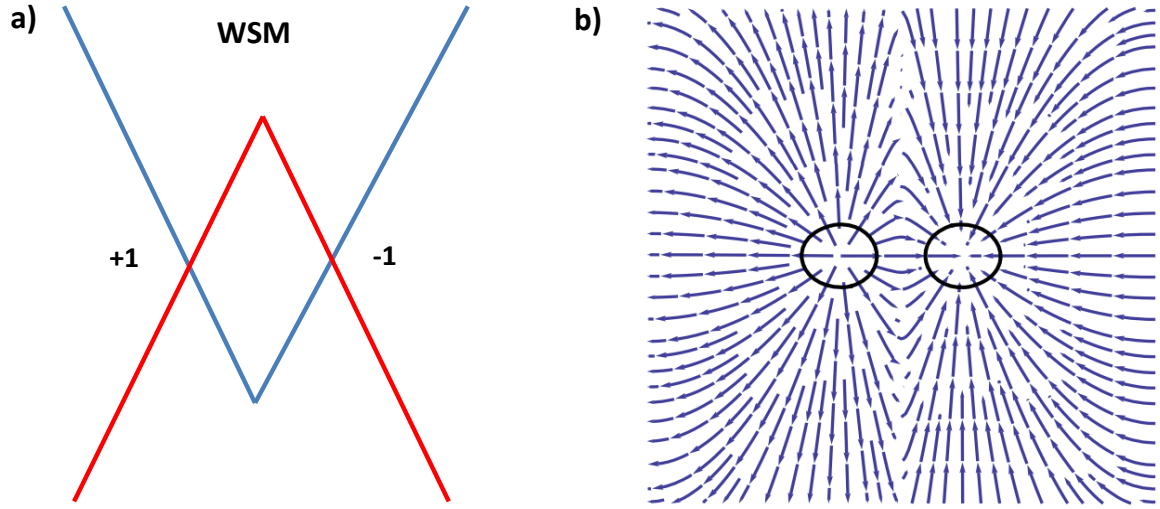

Figure 1.5: (a) Schematic diagram of two bands forming two Weyl points of chirality +1 and -1 (b) The field lines of the Berry curvature around the two Weyl points. The figure in b) is taken from reference [3].

Weyl fermions[28]. The energy around the Weyl point is characterized by the linear dispersion as:

$$H = v\ \vec{\sigma} \cdot \vec{k}. \tag{1.14}$$

where v is related to the chirality of the Weyl point, σ is the Pauli matrix and k is the crystal momentum. The realization of the Weyl semimetal with a pair of Weyl nodes exists only in the case where the time-reversal symmetry is broken, since the Berry curvature vanishes in a system where both time-reversal symmetry and inversion symmetry is preserved[29]. In systems where both symmetries are conserved, the situation will result in double degeneracy at all k which would generate Dirac fermions as a result of the superposition of two Weyl nodes. Weyl semimetals are widely known for giving rise to the anomalous Hall effect due to their distinct Berry curvature properties. The separation of two Weyl nodes having opposite chirality, which is analogous to monopoles in the momentum space, produces the Berry flux contributing to the AHE. This is similiar to a dipole's electric field with a non-zero defined value at a large distance [3, 30] as demonstrated in Fig.1.5.
Other types of protected nodal points that will be discussed are the semi-Dirac points. When the time-reversal symmetry (TRS) is broken, two pairs of Weyl points emerge from the semi-Dirac points[31].

1.7 Semi-Dirac Semimetals

A semi-Dirac cone was very recently observed in electron systems, where a point near the Fermi-surface in a 2D system has a linear dispersion relation along one momentum direction

but quadratic in the orthogonal direction near the band-touching points[32]. This property of a semi-Dirac point combines the characteristic of massless quasi-particles along one k direction and an effective mass-like along another direction[33, 34]. Such materials that exhibit the coexistence of massless and massive Dirac fermions are known as Semi-Dirac semi-metals. The semi-Dirac dispersion relation is given by:

$$\epsilon_k = \pm\sqrt{\left[\frac{k_x^2}{2m}\right]^2 + [v{k_y}^2]} \tag{1.15}$$

In this equation, to fulfill the property of a semi-Dirac point, the effective mass m applies along the k_x direction whereas the velocity applies to the k_y direction where the quasi-particles are massless[35]. The ± sign is related to the conduction band or to the valence band.
Semi-Dirac points are often protected by nonsymmorphic symmetries which are characterized by a rotational symmetry or a mirror reflection combined with a fractional lattice symmetry. This kind of symmetry protects the semi-Dirac points from being lifted upon the effect of spin-orbit coupling. As has been mentioned, the TRS breaking leads to two Weyl points emerging from a semi-Dirac point. In such a scenario, an additional breaking of the inversion symmetry can induce a gap opening which triggers the Berry curvature consequently leading to an enhanced anomalous Hall effect.

1.8 Non-symmorphic symmetries

The presence of non-symmorphic symmetries in a crystal structure plays an important role in protecting novel phases, which include insulating phases and semi-metallic phases[36]. Non-symmorphic symmetries include fractional translation symmetries, which could be either a glide reflection symmetry or a screw-axis rotation visualized as schemes in Fig.1.6. In such symmetries, the mirror reflection or the rotation changes the crystal where the role of the fractional translation is to keep the crystal invariant. The existence of non-symmorphic symmetries in a crystal structure leads to the emergence of non-trivial band structures designated by symmetry-protected non-trivial band crossings, such as Dirac points in semimetals.[37]. In such cases, in the presence of SOC, the degeneracy is lifted at all k except at some isolated points which form a nodal line[38].
Let us consider the two-fold unitary nonsymmorphic symmetry denoted by $G(k)$:

$$G(k) = \begin{pmatrix} 0 & e^{-ik} \\ 1 & 0 \end{pmatrix} \tag{1.16}$$

The Hamiltonian upon the action of $G(k)$ must satisfy:

$$G(k)H(k)G^{-1}(k) = H(k) \tag{1.17}$$

G(k) also anti-commutes with the Pauli matrix σ_3 which gives:

$$H(k) = \begin{pmatrix} 0 & q(k) \\ q^*(k) & 0 \end{pmatrix} \tag{1.18}$$

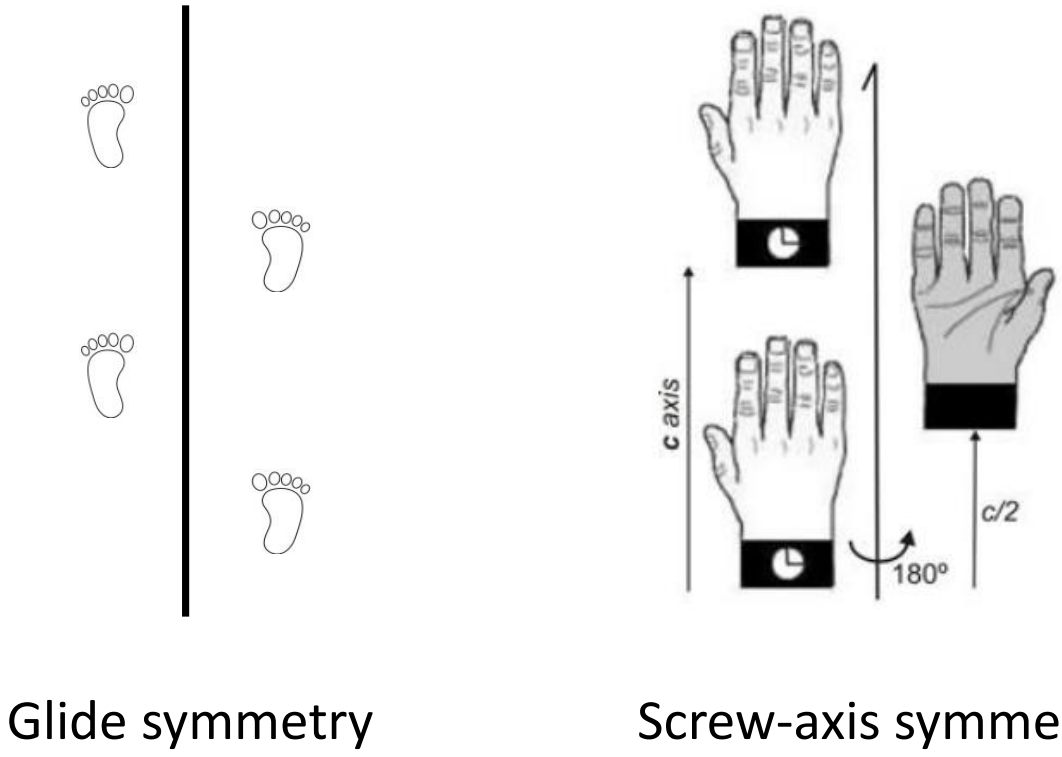

Figure 1.6: Schematic diagram of the nonsymmorphic symmetries. The glide symmetry is a mirror reflection followed by a translation, whereas the screw-axis symmetry is a rotation along an axis followed by translation.

To satisfy equation 1.17, then the following equation should apply:

$$q(k)e^{ik} = q^*(k) \tag{1.19}$$

Any function that satisfies equation 1.19 could be zero at any k in the Brillouin zone (BZ). Therefore, in such case any two-band Hamiltonian in the presence of a nonsymmorphic symmetry $G(k)$ must be gapless at a certain point. The presence of an inversion symmetry $\hat{P}$ in such a scenario assures pinning the band crossing at a certain position in the BZ which could be located at the origin or at the boundaries.

CHAPTER 2

METHODICAL APPROACH AND COMPUTATIONAL ASPECTS

All the results presented in this thesis are derived from ab initio calculations. The primary and most significant method used is Density Functional Theory (DFT), supported by Wannierization, a key technique based on the tight-binding approach and implemented through the Wannier90 code. The strength of DFT lies in its ability to predict and explain various atomic properties and behaviors without the reliability on experimental findings. Most importantly, it provides a rigorous approach to address any *interacting* problem by effectively converting it into a *non-interacting* problem which makes it easier to implement.

Chapter 2 is entirely devoted to the brief discussion of the fundamentals of DFT starting from a single electron aspect, followed by a more complex many-body problem. In the following section, the notable Kohn-Sham theory is presented along with various exchange-correlation functionals which are the the most formidable challenges within the realm of DFT. After that, we discuss the Wannierization technique and its construction starting from Bloch functions, an essential concept, which will be discussed beforehand.

2.1 Many body electron system

Any many-body electron system must be composed of a set of M atomic nuclei and N electrons where both sets occupy different positions in 3D Cartesian coordinates, let us assume that R_1,...,R_M represent those of the nuclei and r_1,...,r_k denote the position of each of the electrons at a fixed instant[39]. In such case, we should extract the eigenvalues (energies) and the eigenvectors (wave functions) from the Hamiltonian of the system, which encompasses the kinetic energies and the Coulomb interactions. Once the eigenvalues are obtained, it becomes simpler to calculate the system's total energy, forces, geometry, energy levels, charges, and other important properties

of the material being investigated. The equation below represents the total Hamiltonian of a system of electrons and nuclei:

$$\hat{H} = \hat{T}_n + \hat{T}_e + \hat{V}_{n-n} + \hat{V}_{e-e} + \hat{V}_{n-e} \tag{2.1}$$

where $\hat{T}_n$ and $\hat{T}_e$ represent the kinetic energies of the nuclei and electrons respectively, $\hat{V}_{n-n}$ is the Coulomb repulsion potential which is due to the nuclei, $\hat{V}_{e-e}$ is the potential due to the electrons, and finally $\hat{V}_{n-e}$ is the potential due to the interaction between the electrons and the nuclei.

These operators are defined by the mass of the respective particles and their positions, where m is the mass of an electron and M is that of a nucleus. Substituting each potential by its definition, the equation (2.1) will become :

$$\begin{aligned}\hat{H} = &\sum_{\alpha=1}^{K} \frac{(-i\hbar\nabla_{R\alpha})^2}{2M_\alpha} + \sum_{\alpha=1}^{N} \frac{(-i\hbar\nabla_i)^2}{2m} + \sum_{\alpha,\beta=1;\alpha<\beta}^{K} \frac{Z_\alpha Z_\beta e^2}{|\vec{R}_\alpha - \vec{R}_\beta|} \\ &+ \sum_{i,j=1;i<j}^{N} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \sum_{\alpha=1}^{K}\sum_{i=1}^{N} \frac{Z_\alpha e^2}{|\vec{R}_\alpha - \vec{r}_i|}\end{aligned} \tag{2.2}$$

where i,j and α,β run for electrons and nuclei respectively. In regular quantum mechanics, one must solve the presented Schrödinger equation in its simplest form as in (2.3) to understand the behavior of the quantum system and to calculate its energies and wavefunctions.

$$\hat{H}\Psi = E\Psi \tag{2.3}$$

In the latter equation, Ψ is a set ψ_n of eigenstates which are solutions for the Hamiltonian where each eigenstate has an associate energy E_n that satisfies the equation. To plug in the Hamiltonian written in (2.2) into equation (2.3), the situation becomes more challenging and requires certain approximations that allow us to solve the problem.

Born Oppenheimer

Electrons are at least three orders of magnitude lighter than protons and neutrons so they can move at much higher velocities than the nuclei. This brings us to the conclusion that at fixed positions, the kinetic energy of the nuclei can be neglected and their respective potential can be treated as a constant value. This is known as the *Born-Oppenheimer* (BO) approximation[40, 41] and it is the first simplification of our system where it allows us to separate the wave function into a product of ionic and electronic parts such as:

$$\Psi = \Psi^{\mathrm{n}}_{\mathrm{k}}(\vec{R}_\alpha)\Psi^{\mathrm{e}}_{\mathrm{k}}(\vec{r}_i,\vec{R}_\alpha) \tag{2.4}$$

where the $\Psi^{\mathrm{n}}_{\mathrm{ik}}$ is a nuclear wave function and $\Psi^{\mathrm{e}}_{\mathrm{k}}$ is the electronic wave function which also relies on the position of nuclei.

With this definition of the total wave function, we can now substitute it in the Schrödinger

equation only to find that the part related to the potential due to the attraction of electrons and nuclei would be more complicated because it should be applied on both of the separated wave functions.

$$[\hat{T}_e + \hat{V_{e-e}}] + \hat{V_{n-e}}]\Psi^{\mathrm{e}}_{\mathrm{k}}(\vec{r}_i, \vec{R}_\alpha) = E_k(R-\alpha)\Psi^{\mathrm{e}}_{\mathrm{k}}(\vec{r}_i, \vec{R}_\alpha) \tag{2.5}$$

Equation (2.5) is indeed now an electronic Schrödinger equation which depends also on the positions of the nuclei. This is the main point of the BO approximation where it allows us to calculate the electronic structure of a molecule without any interference of the quantum mechanics of the nuclei.

Hartree-Fock approximation

Although the BO approximation is sufficient for situations where the nuclear motion is slow, the difficulty to address the electron-electron effects remains. In such cases, the Hartree-Fock (HF) approximation is introduced to account for the correlation of electrons into the electronic wave functions[42]. HF basically defines an initial ansatz that the multi-electron wavefunction is a product of all wave functions of the electrons present in the system[43] . The ground state of the many body electron wave-function of the system assuming that we have i electrons can be described as:

$$\Psi^{\mathrm{e}}_0(\vec{r}_i\sigma_1, ...\vec{r}_N\sigma_N) \approx \phi_{1.....N}(\vec{r}_i\sigma_1, ...\vec{r}_N\sigma_N) \tag{2.6}$$

The set of ϕ_i represents the single wave-functions of electrons, where σ_i denotes their spins and $\phi_{1.....N}$ is the ground state that can be obtained using the variational principle. The most important part of the HF approximation is that the complex many-body wave function is given by a Slater determinant of the spin orbitals such as :

$$\Psi_{\mathrm{HF}} = \begin{vmatrix} \phi_1(x_1) & \phi_2(x_1) & \phi_3(x_1) & \cdots & \phi_N(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \phi_3(x_2) & \cdots & \phi_N(x_2) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \phi_1(x_N) & \phi_2(x_N) & \phi_3(x_N) & \cdots & \phi_N(x_N) \end{vmatrix} \tag{2.7}$$

here x denotes the space and spin coordinates of each single wave function. This approximation imposes that the electronic wave function must be antisymmetric for any exchange between two electron positions according to the Pauli exclusion principle.

$$\Psi^e(x_1, x_2, ...x_i, ..., x_j, ...x_N) = -\Psi^e(x_1, x_2, ...x_j, ..., x_i, ...x_N) \tag{2.8}$$

In order to evaluate the Hartree-Fock equations, the expectation value of the Hamiltonian should be considered for the wave functions $\phi_{1...N}$. The HF equations have a similar structure to the ordinary single-particle Schrödinger equation but instead, the total single particle potential in the HF equations is non-local and consists of two terms:

The Hartree (direct Coulomb) potential :

$$v_H(r) = \int \frac{d^3r'}{|\vec{r} - \vec{r'}|} \sum_{\sigma'=\uparrow,\downarrow} \sum_{j \neq i} |\phi_j(\vec{r'}, \sigma')|^2 \tag{2.9}$$

and the exchange potential :

$$V_x^{HF}(\vec{r}\sigma, \vec{r'}\sigma') = \frac{e^2}{|\vec{r} - \vec{r'}|} \sum_{j=1}^{N} \phi_j(\vec{r\sigma}) \phi_j^*(\vec{r'}\sigma') \tag{2.10}$$

The potentials and the states ϕ_i are treated through a self-consistent calculation starting from an initial guess of the total potential. They are improved consequently after each cycle when potentials are then calculated from ϕ_i states. This iterative process stops as soon as the required accuracy is achieved.

In the Hartree-Fock approach, each electron experiences an average field of the complete electron cloud, while the actual motion of electrons depends via the Coulomb repulsion on the positions of all electrons. To include this Coulomb correlation in the many body wave function, we have to realize a complete solution that incorporates both occupied and unoccupied states instead of the single Slater determinant. The developed wave function then could be written as such:

$$\psi_k(\vec{r}_1\sigma_1, ...\vec{r}_N\sigma_N) = \sum_{i_1,...,i_N} C^k_{i_1...i_N} \phi_{i_1}(\vec{r}_1\sigma_1)\phi_{i_2}(\vec{r}_2\sigma_2)\ldots\phi_{i_N}(\vec{r}_N\sigma_N) \tag{2.11}$$

Then, we expand the single-particle orbitals in terms of a finite set of basis functions, let's call it η_k such that:

$$\phi_i(\vec{r}\sigma) = \sum_{k=1}^{M} b_{i,k_\sigma} \eta_k(\vec{r}) \tag{2.12}$$

If we use the matrix elements $\langle \eta_k / \eta_l \rangle$, we could determine the expansion coefficients $b_{i,k\sigma}$ and $C^k_{i_1...i_N}$. For an effective single-electron problem, the equation looks like:

$$\sum_{l=1}^{M} \sum_{\sigma'} [\langle \eta_k \left| -\frac{(-i\hbar\nabla)^2}{2m} \delta_{\sigma,\sigma'} + v_{eff}\sigma,\sigma' \right| \eta_l \rangle - \epsilon_i \langle \eta_k | \eta_l \rangle] b_{i,l\sigma'} = 0 \tag{2.13}$$

where $v_{eff}\sigma\sigma'$ is the potential felt by the electrons of the system.

The challenge lies in handling the scaling of a many-body electron system, as the scaling factor M is directly proportional to the total number of electrons N. This implies that each additional electron requires an additional basis function to represent it. As a result, a method capable of efficiently addressing these complexities is needed—one that can reduce the many-body problem into an effective single-electron, non-interacting system, while also accounting for electron correlations and the Hartree-Fock approximation. A powerful approach that addresses this is Density Functional Theory (DFT), which replaces wave functions with the electron density n in real space.

2.2 Essentials of Density Functional Theory (DFT)

The concept of DFT is to reduce the complications of a given system and the scaling factors by simply introducing the idea of treating real-space electron densities instead of the k-dependent wave functions[44]. This means that instead of describing our ground state by an overlap of the electron orbitals, we define it as follows:

$$n(\vec{r}) = \langle \psi_0 | \hat{n}(\vec{r}) | \psi_0 \rangle = N \sum_{\sigma_1,.....\sigma_N} \int d^3_{r_2}.....d^3 r_N \left| (\vec{r}_1\sigma_1,.....\vec{r}_N\sigma_N)|\psi_0\rangle \right|^2 \tag{2.14}$$

Hohenberg-Kohn Theorem

The Hohenberg-Kohn theorem[45] is the heart of DFT since it determines uniquely all the properties of a system, in addition to the energy and the wave function of the ground state as a function of the electron density. The Hohenberg-Kohn idea is built upon two fundamental theorems:

- The ground-state energy, as derived from Schrödinger's equation, is a unique functional of the electron density. In other words, the electron density fully determines the energy and all other properties of the system.
- The true electron density is the one that minimizes the total energy functional. This minimizing electron density corresponds to the exact solution of the Schrödinger equation for the system's ground state.

The idea of a functional is basically to define a certain value from a function, such as the ground state energy E which would be *[E(n(r))]* where *n(r)* is the electron density. Applying this concept can grant us a solution by which instead of dealing with a 3N variables system, one could deal with 3 variables of the real space. To address the theorems, let us consider the total Hamiltonian of a system of interacting electrons:

$$\hat{H} = \hat{T} + \hat{V}_{ext} + \hat{V}_{ee} + \hat{V}_{ion} \tag{2.15}$$

Here $\hat{T}$ is the kinetic energy operator, $\hat{V}_{ext}$ is the external potential energy operator, $\hat{V}_{ee}$ is the potential energy operator of the electron-electron repulsion, and $\hat{V}_{ion}$ is the potential energy operator of the ions. The energy functional would result in a well-known analytical form as follows:

$$\begin{aligned} E[\psi_k] &= \langle \psi_k | \hat{H} | \psi_k \rangle \\ &= \frac{\hbar^2}{2m} \sum_{\sigma=\uparrow,\downarrow} \int d^3 r \hat{\psi}^\dagger(\vec{r}\sigma) \nabla^2 \hat{\psi}(\vec{r}\sigma) \\ &\quad + \int V(\vec{r}) n(\vec{r}) d^3 r + \frac{e^2}{2} \int \int \frac{n(\vec{r}) n(\vec{r'})}{|\vec{r} - \vec{r'}|} d^3 r d^3 r' + E_{ion} \end{aligned} \tag{2.16}$$

This energy functional includes the electronic kinetic energies, the Coulomb interactions between the electrons and the nuclei, the Coulomb energy between electrons themselves, and finally between the nuclei. This is one part of the energy functional, the other part is the exchange-correlation functional which remains unknown and includes the interactions of particles at a quantum scale. The picture of solving a problem using the DFT tool so far is still unclear, and this is where Kohn-Sham equations and its role appears.

Kohn Sham equations

The Kohn-Sham (KS) formalism was the first to make DFT an easily accessible tool for calculations starting from a simple fictitious system of non-interacting electrons[46]. The idea of Kohn-Sham was to introduce equations that involve only a single electron wave function, where the first equation looks somehow similar to Schrödinger's equation and has the form :

$$\left[\frac{h^2}{2m}\nabla^2 + V(\vec{r}) + V_H(\vec{r}) + V_{XC}(\vec{r})\right]\psi_i(\vec{r}) = \epsilon_i\psi_i(\vec{r}) \tag{2.17}$$

where $\psi_i(\vec{r})$ is the wave function of a single electron which depends on three spatial variables only.

The potential $V(\vec{r})$ here is the same potential that is responsible for the interactions between electrons and nuclei. The next potential $V_H(\vec{r})$ is the Hartree potential which has the following form:

$$v_H(\vec{r}) = e^2\int\frac{n(\vec{r'})}{|\vec{r}-\vec{r}'|}d^3r' \tag{2.18}$$

This potential is a self-consistent field arising from the interaction of a single electron with the total electron density of a whole system of electrons at a position r'. In other words, it describes the mean electrostatic interaction felt by an electron due to other electrons in the system where part of it should include the Coulomb interaction between the electron and itself but it remains unphysical. The last potential is the exchange-correlation potential $V_{XC}(\vec{r})$ which accounts for all the remaining electronic energy that is not included in the part of non-interacting terms. The exchange-correlation potential is described as a functional derivative of the electron density[47] :

$$V_{XC}(\vec{r}) = \frac{\delta E_{XC}(\vec{r})}{\delta n(\vec{r})} \tag{2.19}$$

The functional derivative δ is not a regular derivative, one can think about it as a derivative of a quantity that is a function as well. This energy due to the exchange-correlation effects is not known or straightforward, in fact, it requires some approximations to be evaluated. From equation 2.19, we can realize that the electron density must be calculated beforehand which indeed comes after initially calculating the single-electron wave functions. Up till now, the situation looks as if it's running in a loop, which is exactly what the whole idea of solving the Kohn-Sham equations requires. The problem is treated using an iterative procedure as follows:

1. Define an initial electron density which is usually calculated from the superposition of atomic orbitals.

2. Solve the Kohn-Sham equations using the trial density, which determines the single-wave functions $\psi_i(\vec{r})$.

3. Calculate the electron density again as a function of the new electron density as $n_{KS}(\vec{r}) = 2\sum_i \psi_i^*(\vec{r})\psi_i(\vec{r})$

4. Repeat the same cycle until the initial and the new electronic density become equal which is considered the ground state of the system.

Exchange-Correlation Functional

The exchange-correlation energy which was discussed in Eq.2.19, is an unknown quantity and requires a lot of approximations to be achieved. E_{XC} is divided into an exchange part E_X and a correlation part E_C. The exchange energy emerges from the exchange of electrons and is associated with the antisymmetrization of the electronic wave function. The correlation part, on the other hand, accounts for the interaction between electrons beyond the mean-field approximation.

Local Density Approximation (LDA)

The only case where this energy can be derived analytically is in the case of a *uniform electron gas* since the local electron density $n(\vec{r})$ is constant at all the spatial points in this case. Making use of this special condition, we can introduce the first approximation made to calculate $E_{XC}[\{\psi(r)\}]$ which is called the Local Density Approximation (LDA)[48, 49]. The general LDA approximation of a system yielding the exchange-correlation energy is calculated as:

$$E_{XC}(\vec{r}) = \int n(\vec{r})\epsilon_{xc}[n(\vec{r})]d^3r \tag{2.20}$$

where ϵ_{xc} is the exchange-correlation density per particle in a uniform electron gas having an electron density $n(\vec{r})$. The potential in this case is written as :

$$V_{XC}^{LDA}(\vec{r}) = V_{XC}^{electron\ gas}[n(\vec{r})] \tag{2.21}$$

Generalized Gradient Approximation (GGA)

An improvement to the LDA approximation is to include the gradient of the electron density of a homogeneous electron gas, since real systems are not really homogeneous and they have a varying electron density. This approach is called the Generalized Gradient Approximation (GGA)[50]. Among the most used XC functionals of this type are the Perdew-Burke-Ernzerhof (PBE) and the Becke exchange and Lee-Yang-Parr correlation (BLYP)[51]. The GGA functionals have shown in some cases to be superior over LDA, especially in predicting total energies and structural properties but it still underestimates the band gap of materials especially those with strong electronic correlation.

The general form of a GGA energy can be expressed as :

$$E_{XC}(\vec{r}) = \int n(\vec{r})\epsilon_{xc}[n(\vec{r}), \nabla(\vec{r})]d^3r \tag{2.22}$$

Other XC functionals

More advanced functionals exist beyond GGAs although they may increase the computational time of a calculation. Examples on these functionals are the meta-GGA, hyper-GGA, PBE0 and other hybrid functionals such as B3LYP which offer more accuracy of energies. Improvements done on GGA functionals include adding higher orders of the density gradient or mixing a certain amount of the nonlocal HF exchange energy.

The hybrid functionals are a GGA-type based functional in addition to a percentage of the accurate exchange energy from the HF method which usually does not take into account the correlation of electrons. It is expected that this type of mixing would bring better results and reduce errors if part of the HF exchange energy was added. Table 2.1 shows the most used XC functionals in DFT.

Classification	Example	Variables
Local	LDA	n(r)
Semi-Local	GGA	n(r), ∇n(r)
Semi-nonlocal	meta-GGA	n(r), ∇n(r),∇^2n(r)
Hybrid	B3LYP	GGA + HF

Table 2.1: XC functionals that are commonly used in DFT calculations

Plane Waves

All the DFT calculations that are included in this thesis are applied to arrangements of atoms that are periodic in space. These atoms can shape a cell, which is repeated periodically and is defined as a *supercell*. A supercell is designated by three lattice vectors $\vec{a_1}$, $\vec{a_2}$, and $\vec{a_3}$. Solving the Schrödinger equation for such a system to calculate the wave functions requires that the system should have a periodic Coulomb potential. In other words, the solution must satisfy a fundamental property known as **Bloch's theorem** which states that the solution must be expressed as a product of a plane wave and another function $u_{ik}(\vec{r})$.

$$\psi_{ik}(\vec{r}) = e^{i\vec{k}.\vec{r}}u_{ik}(\vec{r}), \qquad u_{ik}(\vec{r}+\vec{R}) = u_{ik}(\vec{r}) \tag{2.23}$$

The vector $\vec{R}$ is the translation vector of the crystallographic lattice. The function $u_{ik}(\vec{r})$ is periodic in space with the same periodicity of the supercell which means that $u_{ik}(\vec{r}+n_1\vec{a_1}+n_2\vec{a_2}+n_3\vec{a_3}) = u_{ik}(\vec{r})$ for any integer n_1, n_2 and n_3.

This theorem implies that we can solve the Schrödinger equation for each value of k, but it is equally applicable for quantities derived from the solutions, such as the electron density. Solutions based on this concept are much easier than in the real space, and since they are

calculated in terms of the plane waves $e^{i\vec{k}.\vec{r}}$, they are referred to as 'plane-wave calculations'[52]. The periodicity of $u_{ik}(\vec{r})$ means that they can be expanded in terms of a special set of plane waves such as :

$$u_{ik}(\vec{r}) = \sum_G c_G e^{i\vec{G}.\vec{r}} \tag{2.24}$$

where c_G is the expansion coefficient and the sum is over all the reciprocal lattice vectors defined by $\vec{G}$ such that $G = m_1\vec{b_1} + m_2\vec{b_2} + m_3\vec{b_3}$ with b_1, b_2, and b_3 being the reciprocal lattice vectors. The overall solution for the Schrödinger equation is as follows:

$$\psi_{i,k}(\vec{r}) = \sum_G C_{\vec{k}+\vec{G}} \quad e^{i(\vec{k}+\vec{G})\vec{r}} \tag{2.25}$$

This sum goes over an infinite number of possible values of G which is not very practical, so a simpler interpretation is used in which only the solutions with lower energies would be considered

$$E = \frac{\hbar^2}{2m}|\vec{k} + \vec{G}|^2 \tag{2.26}$$

such that the kinetic energy cut-off is

$$E_{cut} = \frac{\hbar^2}{2m}G_{cut}^2 \tag{2.27}$$

This cutoff energy must be wisely selected when performing a DFT calculation. The largest cutoff energy of the atoms in a supercell can be taken as the overall value.

Pseudopotentials

The burden in including a high energy cutoff parameter that includes plane waves that oscillate on a shorter wavelength is that these describe the electrons that are tightly bound to the core. These electrons are not necessarily important in describing chemical bonds and other physical properties that are governed by the less tightly bound valence electrons. In order to avoid computational costs, the use of pseudopotentials is essential where it replaces the core electrons and the true potential with a smoother one which produces the electronic wave functions with less oscillations[53]. This approach deals explicitly with the chemically active valence electrons while keeping the core electrons "frozen" so it is known as the "frozen core approximation". In frozen core calculations, the pseudopotential is achieved by considering a single atom of one element, but this pseudopotential is also reliable if used in a chemical environment which gives the pseudopotential a transferrable property. DFT codes provide a library of applicable pseudopotentials where each defines its minimum cutoff energy. One of the most used approaches to construct pseudopotentials is the projector augmented-wave (PAW) method which was introduced by Blöchl and later updated for plane-wave calculations by Joubert and Kresse. All the calculations presented in this thesis are applied using the PAW to extend the plane wave basis set through the implemented software VASP.

To obtain the smooth pseudo-wavefunction through solving the Kohn-Sham equations requires constructing a potential that satisfies certain conditions which are[54]:

(i) The modified potential should coincide with the original Kohn-Sham potential (obtained through an all-electron calculation) outside the pseudization region.

(ii) The modification is made in such a way that the solution of the KS equation yields precisely the pseudo-wavefunction inside of the pseudization region.

Let us remember the Kohn-Sham equation which fulfills the property of a real wave function:

$$\left[-\frac{(\hbar\nabla_i)^2}{2m}+V_{eff}^{[\rho]}(\vec{r})\right]\Psi_i^{KS}(\vec{r})=E_i\Psi_i^{KS}(\vec{r}) \tag{2.28}$$

To construct the pseudo wave function, a projection operator $\hat{P}$ should be applied to the KS wave function as follows:

$$\Psi_i^{KS}(\vec{r})=(1-\hat{P})\phi_i(\vec{r}) \tag{2.29}$$

such that

$$\hat{P}=\sum_i|k_j\rangle\langle k_j| \tag{2.30}$$

where $|k_j\rangle$ are the core states. Substituting Eq.2.29 into the KS equation, the following equation will be yielded giving the pseudopotential $V_{ps}(\hat{r})$:

$$V_{ps}(\hat{r})=V_{eff}^{[\rho]}(\vec{r})-\left[-\frac{(\hbar\nabla_i)^2}{2m}+V_{eff}^{[\rho]}(\vec{r})\right]\hat{P}+E_i\hat{P} \tag{2.31}$$

2.3 Wannier functions

We have seen that the electronic ground state has been described so far through the extended Bloch functions, however, another approach using localized orbitals was established by Gregory Wannier in 1937[55] that of the Wannier functions (WF). The localized orbitals are described by a lattice vector $\vec{R}$ and a band-like index n. WF are potent in the study of materials' electronic and dielectric properties and offer valuable information about the nature of the chemical bonding[56]. The Wannier functions are represented as the Fourier transformation of the periodic Bloch states [57], and they are denoted as $W_n(\vec{r}-\vec{R})$ or $|\vec{R}_n\rangle$:

$$|W_n(\vec{r}-\vec{R})\rangle=\frac{V_{cell}}{(2\pi)^3}\int_{BZ}\sum_{m=1}^{N}U_{mn}^{(k)}|\psi_{m,\vec{k}}\rangle e^{-i\vec{k}.\vec{R}}d\vec{k}, \tag{2.32}$$

$U_{mn}^{(k)}$ is a unitary matrix which transforms a system of N bands at each wave vector k, and the Bloch functions are therefore:

$$|\psi_{m,\vec{k}}\rangle=\sum_{\vec{R}}e^{i\vec{k}.\vec{R}}|\vec{R}_n\rangle \tag{2.33}$$

where V_{cell} is the unit cell's volume. WFs are not eigenfunctions of the single-electron Hamiltonian but they form a complete and orthogonal basis set, where two WFs $|\vec{R}_n\rangle$ and $|\vec{R}'_m\rangle$ transform to each other through a translation vector $\vec{R} - \vec{R}'$.

$$\langle \vec{R}_n | \vec{R}'_m \rangle = \delta_{RR'} \delta mn \tag{2.34}$$

The phase indeterminacy $e^{i\phi_n(k)}$ makes the Wannier functions non-unique and the problem becomes even bigger if we consider a system of isolated bands as in the case of valence states in an insulator since each band will undergo a unitary transformation. This issue has caused impracticality to the use of Wannier functions which was later addressed by Nicola Marzari and David Vanderbilt in 1997 [58] in which they developed a method leading to well-defined and centrally localized functions known as the maximally localized Wannier functions (MLWFs) through the Marzari-Vanderbilt scheme (MV). The MV method is also effective in the case where one is interested in the partially filled band in a certain metal close to the Fermi level that is present at a specific energy range but happens to cross other bands. These kinds of bands are expressed as *entangled* bands, and in such a situation, the number of bands in the energy range would be greater than the number of necessary Wannier functions. This obstacle was further resolved by determining the MLWF through a *disentanglement* identified as the Souza-Marzari-Vanderbilt (SMV) strategy. The mappings from Bloch functions to *maximally localized* Wannier functions (MLWFs)[59] are through a family of transformations in a continuous space of unitary matrices. MLWFs are a very efficient tool for the construction of effective Hamiltonians for the study of ballistic transport, systems with strongly correlated electrons, and self-interaction corrections. Wannier90 is a tool used to implement these methods after obtaining an electronic structure calculation and calculating the overlap matrix between the periodic part $|u_{n\vec{k}}\rangle$ of the Bloch states.
Different approaches have been introduced to reduce the arbitrariness in $U^{(k)}_{mn}$ [60]. The most important was to define a "*localization criterion*" in which a functional measures the spread of the Wannier functions:

$$\Omega = \sum_n \left[\langle \vec{0}n | r^2 | \vec{0}n \rangle - \langle \vec{0}n | \vec{r} | \vec{0}n \rangle^2 \right] = \sum_n \left[\langle r^2 \rangle_n - \vec{\bar{r}}^2_n \right] \tag{2.35}$$

The spread runs over n functions $|\vec{0}n\rangle$ and $\vec{\bar{r}}^2_n = \langle r \rangle_n$. To aim for a maximized localization of the Wannier functions, we should find the choice of the matrices $U_{mn}(k)$ which minimizes the spread Ω.

2.4 Anomalous Hall effect

After obtaining a tight-binding model with the Wannier functions used as a basis set, the anomalous Hall conductivity (AHC) can be calculated [61] through the following equation:

$$\sigma_{xy} = -\frac{e^2}{\hbar}\sum_n \int_{BZ} \frac{d\vec{k}}{(2\pi)^3} f_n(\vec{k}) \mathscr{F}_{n,z}(\vec{k}) \tag{2.36}$$

where $f_n(\vec{k})$ is the Fermi-Dirac distribution function and $\mathscr{F}_{n,z}$ is the Berry curvature which is the main component in the theory of the anomalous Hall effect (AHE) and it is defined as:

$$\mathscr{F}_n(\vec{k}) = \vec{\nabla} \times A_n(\vec{k}) \tag{2.37}$$

where $A_n(\vec{k})$ is the Berry connection which is a vector potential calculated from the eigenstates $|u_{n\vec{k}}\rangle$ as:

$$A_n(\vec{k}) = i\langle u_{n,\vec{k}} | \vec{\nabla}_k | u_{n,\vec{k}} \rangle \tag{2.38}$$

The Berry curvature summed over all the occupied bands leads to the “sum over states equation" written as :

$$\mathscr{F}^{tot}_{\alpha\beta} = i\sum_{n,m}(f_n - f_m)\frac{\langle \psi_n | \hbar v_\alpha | \psi_m \rangle \langle \psi_m | \hbar v_\beta | \psi_n \rangle}{(\epsilon_m - \epsilon_n)^2} \tag{2.39}$$

where v_m and v_n are the velocities obtained from the band derivatives. This approach was used in the theoretical part of the calculation of the anomalous Hall conductivity in the paper [62] presented in Chapter 4.

CHAPTER 3

DZYALOSHINSKII-MORIYA INTERACTIONS IN INTERFACIAL MAGNETIC SYSTEMS WITH STRONG SPIN-ORBIT COUPLING

3.1 Overview of the results

The Dzyaloshinskii-Moriya interaction (DMI) is an antisymmetric exchange interaction [16, 63, 64] which pushes two spins to align perpendicular to each other and provokes a chirality of clockwise or anticlockwise rotation. DMI arises in systems where the time-reversal symmetry is broken and there is a strong spin-orbit coupling. DMI proved to be an important ingredient for the formation of numerous topological textures where it is mostly significant in metallic systems with surfaces and interfaces; especially since it can induce chiral magnetic properties such as domain walls, spin spirals, and skyrmions[65]. Skyrmions are very promising in many applications such as racetrack devices, logic devices, and spintronics[2]. First-principles calculations has emerged as a powerful tool to investigate the strength of the DMI and provide an in-depth understanding of its physical origin in different systems. A lot of research works using density functional theory (DFT) calculations have been done on magnetic bilayers based on the combination of heavy metal (HM)/Ferromagnet(FM) thin films where the band hybridization is a primary factor in controlling the strength of the DMI[66, 67]. In such systems, the arrangement of different multilayers, layer thickness, stacking sequence, and growth conditions allows for a widespread tuning of different magnetic parameters such as the DMI.

The motivation for this chapter comes from a joint experimental-theoretical research done previously by my group on Pt/Co/W thin films where the DMI reached higher values than $2mJ/m^2$ [68]. It was shown that sandwiching Cobalt with two transition metals possessing strong spin-orbit coupling can lead to a remarkable enhancement of the DMI.

The system studied in this paper is Re/Co/Pt where we show that although W is a good candidate

for strengthening the DMI in Co/Pt systems, rhenium can surpass it and contribute to a twofold enhancement. The system was also studied experimentally in my research group at IFPAN by S. K. Jena et al. [69] and by the experimental group in Białystok with which I collaborated[70].
The calculations are based on a practical method introduced by [71] using the Vienna ab initio simulation package (VASP) for calculating the DMI in Co/Pt thin films which are determined based on the energy difference between two different chiralities of the spin textures in the Co atoms in the presence of spin-orbit coupling (SOC). The DMI was calculated as a function of increasing the number of layers of cobalt, as well as of Re to demonstrate the dependence of the system on the thickness of the FM material discussed before [72, 73]. We prove that the DMI has an additive and interfacial property supported by the results of the layer-resolved DMI which shows the highest contributions at both interfaces.
The missing key in DFT calculations regarding multilayered systems and the reason behind our overestimated results is the intermixing at the interfaces which affects the DMI since it is highly sensitive to the quality of the interfaces[74, 75]. Considering this problem, we have established an intermixing scheme between Co and Pt atoms on one hand and Co and Re on the other hand. The results show that the Co/Pt interface is easily affected by the disorder and causes a noticeable reduction of the DMI which is quantitatively in excellent agreement with the experimental observations.
It was shown in early studies that the DMI can compete with other exchange interactions and lead to chiral spin-spiral ground states and magnetic skyrmions [76, 77]. This type of spiral magnetism was also recognized in a family of Weyl semimetals (WSMs) RAlSi [78–80]. For example, in the WSM NdAlSi, the chiral spin texture suggests significant DMI interactions as predicted by the Weyl-mediated RKKY coupling. In the next chapter, we study a WSM which belongs to the mentioned family where we study its AHE in different magnetic configurations. All the calculations and the figures in this paper were done and generated by me, including disscusions and writing.

3.2 PAPER I: Huge Dzyaloshinskii-Moriya interactions in Pt/Co/Re thin films

Dostęp do artykułu „Huge Dzyaloshinskii–Moriya interactions in Pt/Co/Re thin films”

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CHAPTER 4

EXPERIMENTAL AND THEORETICAL OBSERVATION OF THE DZYALOSHINSKII-MORIYA INTERACTION IN PT/CO/RE THIN FILMS

4.1 Overview of the results

In this chapter, we present the common work done between authors from the Institute of Physics (IFPAN) and the University of Białystok (UwB). The work combines experimental and theoretical studies using density functional theory (DFT) calculations on the investigation of the magnetic properties of Pt/Co/Re thin films. The results recorded in Chapter 3 which include the DMI values achieved from DFT calculations before and after the inclusion of disorder at both interfaces of the system were used as a confirmation for the high value of the Dzyaloshinskii-Moriya interaction (DMI) found in the studied Pt/Co/Re system.

Adding the effect of intermixing has proved the importance of the interface quality on the value of this magnetic parameter. This was revealed by a better agreement with the experimental results where the DMI revealed lower values ranging between 1 and 2 mJ/m^2, closer to the values achieved experimentally. A similar study on the effect of the crystallinity on the value of DMI was done before by Chen et al.[74] upon gradually mixing the interfacial atoms. This theoretical study was motivated by the observed discrepancy upon the deposition of Pt and [Co/Pd] multilayers using e-beam evaporation versus when the same multilayers were grown by magnetron sputtering. The level of atom mixing at the interface led the value of DMI to decrease gradually which was explained through the effect of layer-resolved SOC. Another theoretical study showed the robustness of the DMI value against the intermixing in Co/Pt thin films where it was found that the DMI reduces as an effect of interface disorder[75].

Moreover, it was made clear in other studies that introducing intermixing hinders the achievement of a strong interfacial DMI. It has been shown that in magnetic multilayers of heavy metal

(HM)/ ferromagnet (FM), the sign and the strength of the DMI can be highly affected by structural factors such as material composition, stacking order, and interface quality. Thus, tuning these parameters provides a way to control the DMI strength[81].
In symmetric systems like Pt/Co/Pt, the DMI at each interface are ideally equal and opposite which does not contribute to a DMI value. However, experimentally grown thin films can be deposited by tuning the temperature which increases the level of intermixing. This introduces a discrepancy in the strength of the DMI between the upper and the lower interface by breaking the inversion symmetry of the system contributing to a nonzero DMI value. This again highlights the sensitivity of interface conditions on the interfacial DMI effect[82].
In this paper, theoretical data were used as support for the experimental findings. The theoretical part, including the paragraph about the DFT calculation setup and details, the DFT data points in Figure 6, and the related data and data points in the supplementary materials were provided from my side.

4.2 PAPER II: Evolution of static and dynamic magnetic properties of Re/Co/Pt and Pt/Co/Re trilayers with enhanced Dzyaloshinskii-Moriya interaction

Dostęp do artykułu „Evolution of static and dynamic magnetic properties of Re/Co/Pt and Pt/Co/Re trilayers with enhanced Dzyaloshinskii-Moriya interaction”

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CHAPTER 5

ANOMALOUS HALL EFFECT IN WEYL SEMIMETALS

5.1 Overview of the results

The anomalous Hall effect (AHE) is observed in solids without time-reversal symmetry, typically in ferromagnets. It is proportional to the spin-orbit coupling (SOC), therefore, to be sizeable, heavy atom electrons are essential at the Fermi level. In this chapter, we study the anomalous Hall effect in the CeAlSi Weyl semimetal (WSM), however, the AHE can also be induced in other systems exhibiting a non-zero magnetization such as altermagnets which will be discussed in Chapter 6. CeAlSi combines two properties that can lead to the recognition of Weyl nodes, the broken inversion symmetry and the broken time-reversal symmetry which makes it capable of controlling the AHE. The f moments from the Ce^{3+} ion interact with the non-centrosymmetric lattice of this WSM and results in a non-collinear ferromagnetic order [83].
Studying the AHE in a solid requires a deeper understanding of its underlying topology and geometry such as the concept of the Berry curvature[24] which was earlier known as the “anomalous velocity". Electronic structure calculations serve as a very useful tool, especially for establishing a band structure that shows the band crossings and anticrossings near the Fermi level which has been proven capable of inducing a huge AHE[84].
Weyl nodes are topological points that appear as a result of a crossing between two bands with a lifted Kramer’s degeneracy, while they also act as sinks and sources of the Berry curvature. Detecting Weyl nodes specifically close to the Fermi level is known to affect the transverse electronic response such as the AHE by manipulating the direction of the magnetization[85]. We obtained the band structures of CeAlSi for three different configurations depending on the direction of the magnetization using DFT calculations and Wannierization techniques. The band structures showed discrepancies in the position of the Fermi level and the positions of the Weyl points as

well as the band anticrossings at the vicinity of the Fermi level. From the AHE calculations done by a tight-binding approach using Wannier functions, we detected the sign change which is impacted by changing the orientation of the magnetization. In agreement with the experimental findings, the results show an inverted sign of the anomalous Hall conductivity (AHC) between the magnetic system with the magnetization along the a-axis and that along the c-axis. Moreover, a shift detected between the two spikes of the AHC for both systems at the Fermi level was associated with the shift of the Weyl nodes observed in the band structures.
The appearance of Weyl points is magnetically promising for exhibiting complex magnetic structures such as spin spirals[86]. From the three studied magnetic orderings of CeAlSi, we found that the system with non-collinear magnetization displaying spins perpendicular to each other is the ground state. We suspect that in such a case, due to the presence of strong spin-orbit coupling and the broken inversion symmetry, the Dzyaloshinskii Moriya interaction (DMI) must be necessary to stabilize the structure. The DMI was not calculated in this work since it is out of the scope of the experimental observations presented in the paper.
Recently ab-initio calculations have revealed a newly studied WSM, GdAlSi which like CeAlSi, has both properties of broken time-reversal symmetry and broken inversion symmetry[87]. Interestingly enough, this WSM belongs to the family of the *altermagnets*, being a collinear antiferromagnet that exhibits relativistic spin-splitting in the momentum space. Along the paths where GdAlSi indicates a spin splitting, the avoided crossings have large but opposite contributions to the Berry curvature which contributes to the anomalous Hall effect.
My contribution to this paper involved performing DFT calculations to generate the band structure figures and to obtain results for the anomalous Hall effect across the three distinct magnetic configurations of CeAlSi.

5.2 PAPER III: Sign change of anomalous Hall effect and anomalous Nernst effect in the Weyl semimetal CeAlSi

Dostęp do artykułu „Sign change of anomalous Hall effect and anomalous Nernst effect in the Weyl semimetal CeAlSi”

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CHAPTER 6

ALTERMAGNETISM

6.1 Overview of the results

Altermagnetic compounds have been the subject of attention recently due to the emerging properties they exhibit. They incorporate characteristics of a spin-split band structure due to a broken time-reversal symmetry which occurs typically in ferromagnets, and a zero net magnetization due to anti-parallel spin ordering which is an aspect of antiferromagnetism[7, 8]. Research on altermagnets showing the lifting of Kramer's degeneracy has proved the advantage of compounds with compensated magnetization over ferromagnets, especially in spintronics after they have been excluded from the field for a long time. The disadvantage in ferromagnets, demonstrated in their weak resistance to external magnetic fields, is no longer a challenge in the case of zero-magnetization compounds showing alternating spin polarization with a broken time-reversal symmetry. In antiferromagnetic systems, where Kramer's degeneracy is preserved even in the presence of spin-orbit coupling (SOC), it was believed that responses to the time-reversal symmetry breaking such as the anomalous Hall effect (AHE), due to zero net magnetization, would not occur. This was contradicted by the unfolding phenomenon of altermagnetism (AM). Several studies were done on antiferromagnets such as RuO_2 and MnTe [88, 89] where the AHE effect was observed in the absence of an external field and the presence of a vanishing net magnetization and where the time-reversal symmetry is broken in a specific unconventional phase that arises due to the crystal environment of the magnetic atoms. Altermagnets have magnetization densities that obey the non-relativistic spin symmetry combining a two-fold spin-space rotation with a real-space rotation which are known by proper or improper and symmorphic or non-symmorphic symmetries. In addition to the absence of the non-relativistic global dipole magnetization, these magnetization densities do not have to contain even the local

dipole moments.
The combinations of point group operations with nonprimitive lattice translations, that are dubbed nonsymmorphic symmetries, can lead to new topological phases[90]. These kinds of symmetries impose global topological constraints on the band structure of a system which leads to additional crossings/anticrossings of bands near the Fermi level. There the Berry curvature has the highest contributions and may reveal novel topological response phenomena and unique magnetotransport properties[91].
CrAs belongs to the Pnma family and hosts nonsymmorphic symmetries[92] which results in many special band structure characteristics, such as the emergence of semi-Dirac points which are points having a linear dispersion along only one direction in the k-space[93, 94]. The presence of the non-magnetic atoms (As) in the crystal structure of CrAs is involved in breaking the inversion symmetry and the translation symmetry which connects the two sublattices of opposite directions. Consequently, the time-reversal symmetry was broken which was revealed by the spin splitting in the band structure of the C-type CrAs. The interplay between these two properties appearing at certain time-reversal invariant momenta (TRIM) points reveals interesting changes demonstrated by degeneracies at the edges of the Brillouin zone and the appearance of semi-Dirac points. In the non-magnetic phase, where the Kramer's degeneracy is protected, we show the network of the bands crossing and others avoiding each other in the band structure of the C-type CrAs. Upon the inclusion of SOC, we show that the magnetic space group can change depending on the direction of the Néel vector which causes a selective removal of the spin degeneracy. The band crossings and anti-crossings are generally further split by the effect of SOC when the orientation of the Néel vector is modified except at one point which could be a nodal line protected by the glide operator upon directing the Néel vector along x. The appearance of semi-Dirac points leads to several avoided band crossings which contribute to the Berry curvature and in turn enhance electronic transport properties such as the AHE which was confirmed and calculated using the Wannierization technique.
My contribution to this work has been related to performing and analyzing the theoretical calculations and producing all the figures except those related to the anomalous Hall conductivity.

6.2 PAPER IV: Interplay between altermagnetism and nonsymmorphic symmetries generating large anomalous Hall conductivity by semi-Dirac points induced anticrossings

Dostęp do artykułu „Interplay between altermagnetism and nonsymmorphic symmetries generating large anomalous Hall conductivity by semi-Dirac points induced anticrossings”

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CHAPTER 7

OUTLOOK

The field of spintronics has developed over the past decades where the manufacture of devices is mainly focused on manipulating both the charge and the spin degree of freedom[95]. The lack of time-reversal symmetry (TRS) in certain systems plays a huge role in enabling and stabilizing spin-polarized currents due to the lifted degeneracy between spin-up and spin-down states. In systems with large spin-orbit coupling, the breaking of TRS is necessary to generate topologically protected phases in both real and reciprocal space. In the reciprocal space, the spin-orbit and the breaking of the TRS can generate Weyl semimetal and quantum anomalous Hall phases, while in the real space, the main key focuses today shifts toward experimental spintronic devices that can exploit spin-textured topological states[96]. In many studies, it has been shown that systems with both a broken TRS and the absence of inversion symmetry are among the most promising for some applications such as the generation of spin-textured skyrmions and their variants.
In ferromagnetic systems, the presence of spin-orbit coupling (SOC) effects has been of growing importance remarkably in heterostructures where the SOC strength has shown comparable energy scales and therefore is promising for new spin-based applications. The emergence of the net Dzyaloshinskii-Moriya interaction (DMI), which requires the breaking of the inversion symmetry, has been shown essential to stabilize spin textures in ferromagnetic ultra-thin films[97]. DMI enables controlled, deterministic switching of magnetic states via spin-orbit torque (SOT), reducing critical current thresholds in certain materials and supporting advanced functionalities like multilevel storage and programmable spin logic gates, making it pivotal for efficient spintronic devices[98]. The existence of the DMI is also important for understanding the emergence of skyrmions which are also very promising candidates in applications concerning memory devices, skyrmion racetrack, transistors, and many other functions[99]. These topological objects have been realized experimentally in thin films and future advances in this field are essential and

prosperous as they offer great potential as systematic information carriers although certain limitations should be taken into consideration which might reduce their utility in spintronic devices[100].

In materials that combine both broken TRS and inversion symmetry, SOC can have a substantial impact on their electronic properties and topological phenomena in the reciprocal space, as demonstrated in our study of CeAlSi. Specifically, the presence of SOC in this system, alongside the dual symmetry-breaking properties, enables the formation of Weyl points, which act as sources and sinks of the Berry curvature. This non-trivial Berry curvature distribution induced by SOC gives rise to the tunable anomalous Hall effect (AHE) in CeAlSi. The exotic properties exhibited by Weyl semimetals (WSMs) hold great potential for high-speed electronics and spintronic applications. Their gapless nature enables high mobility with minimal resistance, and they also exhibit large magnetoresistance due to the chiral anomaly[25, 101, 102]. WSMs can also demonstrate a strong spin Hall effect due to their large Berry curvature and SOC. This characteristic is anticipated to play a crucial role in spin Hall effect devices capable of efficiently converting charge current into spin current.

The emergence of the anomalous Hall effect (AHE) has been recently extended to the newly discovered field dubbed "altermagnetism" upon the inclusion of SOC in which the lack of TRS is a built-in property. The altermagnets exhibit faster spin dynamics and lower sensitivity to stray magnetic fields compared to ferromagnetic materials. Many compounds including CrAs which have been studied in this thesis have opened new perspectives of what is named "spin-split antiferromagnetic spintronics"[103]. The AHE offers the potential for developing innovative spintronic devices, such as the Hall balance, which can significantly boost magnetoelectronic ratios. In other altermagnetic compounds like RuO_2 and MnTe, research has also confirmed that the AHE can be measured and that it explicitly depends on the orientation of the Néel vector. The Néel vector of RuO_2 has been predicted to be tunable by spin transfer torques, and possibly by spin-orbit torques paving the way to antiferromagnetic spintronic devices[104]. The field of altermagnetism has shown very promising physical properties that can revolutionize fields such as data storage, spintronics, spin-to-charge conversion, faster spin-caloritronic devices, and magnetic sensing by providing more efficient and long-lasting alternatives to conventional ferromagnetic and antiferromagnetic materials[105].

We believe that future research should prioritize the realization of protected magnetic structures in real space, such as skyrmions, within systems exhibiting an interplay between ferromagnetism and SOC. Progress in this area, alongside theoretical predictions using mesoscopic-scale approaches like atomistic spin dynamics and micromagnetic simulations, holds great promise. Regarding altermagnetic systems, research is still open for investigation theoretically and experimentally towards combining altermagnetism and topology in real and reciprocal space. Another aspect to investigate is the robustness of the weak ferromagnetism in real materials where domains and other defects are present. Experimentally, one of the main challenges would be the

control of the magnetic domains with different Néel vectors which is relevant for the realization of possible devices based on altermagnetism.

INSTYTUT FIZYKI
POLSKIEJ AKADEMII NAUK

Date: 04 November 2024

STATEMENT

I declare that my contribution to the paper **Amar Fakhredine**, Andrzej Wawro, and Carmine Autieri. "Huge Dzyaloshinskii–Moriya interactions in Pt/Co/Re thin films." *Journal of Applied Physics* 135, no. 3 (2024) is related to:

i. Performing all the density functional theory calculations and collecting the data.

ii. Analyzing the results and producing all the figures.

iii. Writing the draft.

iv. Discussion of the scientific results.

Amar Fakhredine

PhD student of ON-3.4 at the Institute of Physics, Polish Academy of Science IFPAN
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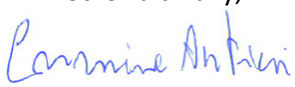
INSTYTUT FIZYKI
POLSKIEJ AKADEMII NAUK

Date: 6 September 2024

STATEMENT

I declare that my contribution to the paper **A. Fakhredine,** A. Wawro, C. Autieri, "Huge Dzyaloshinskii–Moriya interactions in Pt/Co/Re thin films" published in J. Appl. Phys. **135**, 035303 (2024) has been related to the discussion on the scientific project and the supervision of the project.

Yours Faithfully,



Carmine Autieri

Dr. hab. Carmine Autieri, IFPAN professor at the International Centre for Interfacing Magnetism and Superconductivity with Topological Matter (MagTop),
E-mail: autieri@MagTop.ifpan.edu.pl
Website: https://www.magtop.ifpan.edu.pl/resources/teams/
Google Scholar profile: https://scholar.google.it/citations?user=83pF0ywAAAA
ResearchGate profile: https://www.researchgate.net/profile/Carmine_Autieri

Warsaw, Nov. 6th, 2024

prof. dr hab. Andrzej Wawro
Institute of Physics Polish Academy of Sciences

Declaration of contribution

Hereby, I declare that my contribution to the research article as below included in the doctoral thesis by Amar Fakhredine entitled: "*Interplay between non-relativistic spin-splitting and spin-orbit coupling in metallic systems*" is the following:

Amar Fakhredine, Andrzej Wawro, and Carmine Autieri; "Huge Dzyaloshinskii–Moriya interactions in Pt/Co/Re thin films"; *Journal of Applied Physics* ***135****, 035303 (2024).*

> Suggestion of the investigated system and the interface structure

> Discussion of the obtained results

> Participation in the preparation of the paper final version.

I am a head of the project financed by the National Science Centre in Poland (no.: 2020/37/B/ST5/02299) from which this research was supported and Amar Fakhredine's PhD scholarship was paid.

Andrzej Waldemar Wawro

Elektronicznie podpisany przez Andrzej Waldemar Wawro
Data: 2024.11.06 19:38:18 +01'00'

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IM. ADAMA MICKIEWICZA
W POZNANIU

Dated – 02nd October 2024

Statement

I declare that my contribution to the paper with authors Anuj Kumar Dhiman, **Amar Fakhredine**, Ryszard Gieniusz, Zbigniew Kurant, Iosif Sveklo, Piotr Dłużewski, Wojciech Dobrogowski, Sukanta Kumar Jena, Aleksiej Pietruczik, Carmine Autieri, Andrzej Wawro, and Andrzej Maziewski with title ”Evolution of static and dynamic magnetic properties of Re/Co/Pt and Pt/Co/Re trilayers with enhanced Dzyaloshinskii-Moriya interaction” published on **Applied Surface Science** vol. 679, 161151 (2024). I have contributed in this work through experimental measurements, scientific results discussion and manuscript writing & editing.

Yours Faithfully,

Anuj Kumar Dhiman

Postdoctoral scholar, Faculty of Physics,

Adam Mickiewicz University, Poznan, Poland

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INSTYTUT FIZYKI
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Date: 04 November 2024

STATEMENT

I declare that my contribution to the paper Anuj Kumar Dhiman, **Amar Fakhredine**, Ryszard Gieniusz, Zbigniew Kurant, Iosif Sveklo, Piotr Dłużewski, Wojciech Dobrogowski et al. "Evolution of static and dynamic magnetic properties of Re/Co/Pt and Pt/Co/Re trilayers with enhanced Dzyaloshinskii-Moriya interaction." *Applied Surface Science* 679 (2025): 161151 is related to:

i. Performing the density functional theory calculations related to the theoretical part.

ii. Analyzing and providing the data for figure 6 in the main text and figure S4 in the supplementary material.

iii. Writing the theoretical part.

Amar Fakhredine

PhD student of ON-3.4 at the Institute of Physics, Polish Academy of Science IFPAN
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WYDZIAŁ FIZYKI
UNIWERSYTET W BIAŁYMSTOKU
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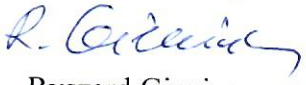
Date: 08 October 2024

STATEMENT

I declare that my contribution to the paper with authors Anuj Kumar Dhiman, **Amar Fakhredine**, Ryszard Gieniusz, Zbigniew Kurant, Iosif Sveklo, Piotr Dłużewski, Wojciech Dobrogowski, Sukanta Kumar Jena, Aleksiej Pietruczik, Carmine Autieri, Andrzej Wawro, Andrzej Maziewski and with title "Evolution of static and dynamic magnetic properties of Re/Co/Pt and Pt/Co/Re trilayers with enhanced Dzyaloshinskii-Moriya interaction" published on Applied Surface Science 679, 161151, (2025) https://doi.org/10.1016/j.apsusc.2024.161151 has been related to the made BLS measurements and analysis.

Yours Faithfully,



Ryszard Gieniusz

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Date: 18 October 2024

STATEMENT

I declare that my contribution to the paper with authors Anuj Kumar Dhiman, **Amar Fakhredine**, Ryszard Gieniusz, Zbigniew Kurant, Iosif Sveklo, Piotr Dłużewski, Wojciech Dobrogowski, Sukanta Kumar Jena, Aleksiej Pietruczik, Carmine Autieri, Andrzej Wawro, Andrzej Maziewski and with title "Evolution of static and dynamic magnetic properties of Re/Co/Pt and Pt/Co/Re trilayers with enhanced Dzyaloshinskii-Moriya interaction" published on Applied Surface Science 679, 161151, (2025) has been related to writing – original draft and magneto-optics investigation and data analysis.

Zbigniew Kurant

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Date: 01 October 2024

STATEMENT

I declare that my contribution to the paper with authors Anuj Kumar Dhiman, **Amar Fakhredine**, Ryszard Gieniusz,Zbigniew Kurant, Iosif Sveklo, Piotr Dłużewski, Wojciech Dobrogowski, Sukanta Kumar Jena, Aleksiej Pietruczik, Carmine Autieri, Andrzej Wawro, Andrzej Maziewski and with title "Evolution of static and dynamic magnetic properties of Re/Co/Pt and Pt/Co/Re trilayers with enhanced Dzyaloshinskii-Moriya interaction" published on **Applied Surface Science, Volume 679, 15 January 2025, 161151**, has been related to the discussion on the scientific results.

Yours Faithfully,

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STATEMENT

I declare that my contribution to the paper with authors Anuj Kumar Dhiman, **Amar Fakhredine**, Ryszard Gieniusz,Zbigniew Kurant, Iosif Sveklo, Piotr Dłużewski, Wojciech Dobrogowski, Sukanta Kumar Jena, Aleksiej Pietruczik, Carmine Autieri, Andrzej Wawro, Andrzej Maziewski and with title ”Evolution of static and dynamic magnetic properties of Re/Co/Pt and Pt/Co/Re trilayers with enhanced Dzyaloshinskii-Moriya interaction” published on Applied Surface Science 679 (2025): 161151 has been related to the discussion on the scientific results.

Yours Faithfully,

Carmine Autieri

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Google Scholar profile: https://scholar.google.it/citations?user=83pF0ywAAAA
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Warsaw, Nov. 6th, 2024

prof. dr hab. Andrzej Wawro
Institute of Physics Polish Academy of Sciences

Declaration of contribution

Hereby, I declare that my contribution to the research article as below included in the doctoral thesis by Amar Fakhredine entitled: "*Interplay between non-relativistic spin-splitting and spin-orbit coupling in metallic systems*" is the following:

Anuj Kumar Dhiman, Amar Fakhredine, Ryszard Gieniusz, Zbigniew Kurant, Iosif Sveklo, Piotr Dłużewski, Wojciech Dobrogowski, Sukanta Kumar Jena, Aleksiej Pietruczik, Carmine Autieri, Andrzej Wawro, and Andrzej Maziewski;"Evolution of static and dynamic magnetic properties of Re/Co/Pt and Pt/Co/Re trilayers with enhanced Dzyaloshinskii-Moriya interaction"; *Applied Surface Science* ***679****, 161151 (2025).*

> Suggestion of the investigated system

> Responsibility for the samples fabrication

> Responsibility for sample structural investigations

> Discussion of the obtained results

> Participation in the preparation of the paper final version.

I am a head of the project financed by the National Science Centre in Poland (no.: 2020/37/B/ST5/02299) from which this research was supported and Amar Fakhredine's PhD scholarship was paid.

Andrzej Waldemar Wawro

Elektronicznie podpisany przez Andrzej Waldemar Wawro
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Department of Physics of Magnetism
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STATEMENT

I declare that my contribution to the paper with authors Anuj Kumar Dhiman, **Amar Fakhredine**, Ryszard Gieniusz, Zbigniew Kurant, Iosif Sveklo, Piotr Dłużewski, Wojciech Dobrogowski, Sukanta Kumar Jena, Aleksiej Pietruczik, Carmine Autieri, Andrzej Wawro, Andrzej Maziewski and with title "Evolution of static and dynamic magnetic properties of Re/Co/Pt and Pt/Co/Re trilayers with enhanced Dzyaloshinskii-Moriya interaction" published on Applied Surface Science 679 (2025) 161151 has been related to the discussion on the scientific results.

UNIVERSITAS BIALOSTOCENSIS 1997

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Date: 30 October 2024

STATEMENT

I declare that my contribution to the paper Md Shahin Alam, **Amar Fakhredine**, Mujeeb Ahmed, P.K. Tanwar, Hung-Yu Yang, Fazel Tafti, Giuseppe Cuono, Rajibul Islam, Bahadur Singh, Artem Lynnyk, Carmine Autieri, Marcin Matusiak, Sign change of anomalous Hall effect and anomalous Nernst effect in the Weyl semimetal CeAlSi, Phys. Rev. B **107**, 085102 (2023) is as follows,

Measurements: I did the measurements
Data Analysis: I analyzed the collected data and discuss with Amar Fakhredine for theoretical support
Figures: I made the figures (except for the DFT figures).
Manuscript: I prepared the draft (except for the DFT part).

Yours Faithfully,

Md. Shahin Alam.

Md Shahin Alam

Institute of Physics, Polish Academy of Sciences, Aleja Lotników 32/46, 02-668 Warsaw, Poland

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Date: 04 November 2024

STATEMENT

I declare that my contribution to the paper Md Shahin Alam, **Amar Fakhredine**, Mujeeb Ahmed, P.K. Tanwar, Hung-Yu Yang, Fazel Tafti, Giuseppe Cuono, Rajibul Islam, Bahadur Singh, Artem Lynnyk, Carmine Autieri, Marcin Matusiak, Sign change of anomalous Hall effect and anomalous Nernst effect in the Weyl semimetal CeAlSi, Phys. Rev. B **107**, 085102 (2023) is related to performing and analyzing the density functional theory (DFT) calculations and results, and making the related figures. In addition, I participated in the scientific discussion of the results and in proofreading the manuscript.

Amar Fakhredine

PhD student of ON-3.4 at the Institute of Physics, Polish Academy of Science IFPAN
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INSTYTUT FIZYKI
POLSKIEJ AKADEMII NAUK

Date: 10 July 2024

STATEMENT

I declare that my contribution to the paper Md Shahin Alam, **Amar Fakhredine**, Mujeeb Ahmed, P.K. Tanwar, Hung-Yu Yang, Fazel Tafti, Giuseppe Cuono, Rajibul Islam, Bahadur Singh, Artem Lynnyk, Carmine Autieri, Marcin Matusiak, Sign change of anomalous Hall effect and anomalous Nernst effect in the Weyl semimetal CeAlSi, Phys. Rev. B **107**, 085102 (2023) is as follows,

(i) Participated in the measurements

(ii) Provided the python code and analysed the electrical measurements data

(iii) Participated in conceptualizing the study

(iv) Review and edit the manucript

(v) Participated in addressing the critism raised by reviewers during review process

Yours Faithfully,

Pardeep Kumar
MagTop (6.2)

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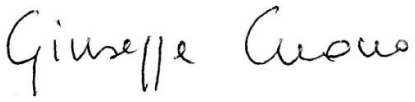
Date: 6 September 2024

STATEMENT

I declare that my contribution to the paper Md. S. Alam**, A. Fakhredine,** M. Ahmed, P. K. Tanwar, H.-Y. Yang, F. Tafti, G. Cuono, R. Islam, B. Singh, A. Lynnyk, C. Autieri, M. Matusiak, "Sign change of the anomalous Hall effect and the anomalous Nernst effect in Weyl semimetal CeAlSi", published in Phys. Rev. B **107,** 085102 (2023) has been related to participation to the scientific discussion.

Yours Faithfully,



Giuseppe Cuono

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Date: 6 September 2024

STATEMENT

I declare that my contribution to the paper Md. S. Alam**, A. Fakhredine,** M. Ahmed, P. K. Tanwar, H.-Y. Yang, F. Tafti, G. Cuono, R. Islam, B. Singh, A. Lynnyk, C. Autieri, M. Matusiak, "Sign change of the anomalous Hall effect and the anomalous Nernst effect in Weyl semimetal CeAlSi", published in Phys. Rev. B **107,** 085102 (2023) has been related to participation to the scientific discussion.

Yours Faithfully,

Rajibul Islam
Postdoctoral researcher,
Physics department, University of of Alabama at Birmingham,
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INSTYTUT FIZYKI
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Date: 16 July 2024

STATEMENT

I declare that my contribution to the paper Md Shahin Alam, **Amar Fakhredine**, Mujeeb Ahmed, P.K. Tanwar, Hung-Yu Yang, Fazel Tafti, Giuseppe Cuono, Rajibul Islam, Bahadur Singh, Artem Lynnyk, Carmine Autieri, Marcin Matusiak, Sign change of anomalous Hall effect and anomalous Nernst effect in the Weyl semimetal CeAlSi, Phys. Rev. B **107**, 085102 (2023) is as follows:

- The measurements of magnetic moment values along with ac susceptibility of Weyl semimetal CeAlSi by means of SQUID magnetometer.

Yours Faithfully,

Artem Lynnyk

Institute of Physics, Polish Academy of Sciences, Aleja Lotników 32/46, 02-668 Warsaw, Poland

INSTYTUT FIZYKI
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Date: 6 September 2024

STATEMENT

I declare that my contribution to the paper Md. S. Alam**, A. Fakhredine,** M. Ahmed, P. K. Tanwar, H.-Y. Yang, F. Tafti, G. Cuono, R. Islam, B. Singh, A. Lynnyk, C. Autieri, M. Matusiak, "Sign change of the anomalous Hall effect and the anomalous Nernst effect in Weyl semimetal CeAlSi", published in Phys. Rev. B **107,** 085102 (2023) has been related to the discussion on the scientific project and the supervision of the theoretical part of the project.

Yours Faithfully,

Carmine Autieri

Dr. hab. Carmine Autieri, IFPAN professor at the International Centre for Interfacing Magnetism and Superconductivity with Topological Matter (MagTop),
E-mail: autieri@MagTop.ifpan.edu.pl
Website: https://www.magtop.ifpan.edu.pl/resources/teams/
Google Scholar profile: https://scholar.google.it/citations?user=83pF0ywAAAA
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Wrocław, 10 July 2024

Dr hab. Marcin Matusiak
Institute of Low Temperature and Structure Research
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ul. Okólna 2, 50-422 Wrocław, Poland

STATEMENT

I declare that my contribution to the publication "Sign change of anomalous Hall effect and anomalous Nernst effect in the Weyl semimetal CeAlSi" by Md Shahin Alam, Amar Fakhredine, Mujeeb Ahmad, P.K. Tanwar, Hung-Yu Yang, Fazel Tafti, Giuseppe Cuono, Rajibul Islam, Bahadur Singh, Artem Lynnyk, Carmine Autieri, and Marcin Matusiak, Phys. Rev. B 107, 085102 (2023) dealt mainly with the experimental aspect of the research and was as follows:

I conceived the study as well as supervised the measurements, analysis, writing and reviewing the article.

INSTYTUT FIZYKI
POLSKIEJ AKADEMII NAUK

Date: 04 November 2024

STATEMENT

I declare that my contribution to the paper **Amar Fakhredine**, Raghottam M. Sattigeri, Giuseppe Cuono, and Carmine Autieri. "Interplay between altermagnetism and nonsymmorphic symmetries generating large anomalous Hall conductivity by semi-Dirac points induced anticrossings." *Physical Review B* 108, no. 11 (2023): 115138 is related to:

i. Performing the density functional theory calculations.

ii. Analyzing and collecting the data and discussing with the co-authors.

iii. Produced the figures aside from those related to the AHE.

iv. Writing the draft with the help of the co-authors.

Amar Fakhredine

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Institute of Physics, Polish Academy of Sciences, Aleja Lotników 32/46, 02-668 Warsaw, Poland

Date: 6 September 2024

STATEMENT

I declare that my contribution to the paper **Amar Fakhredine,** Raghottam M. Sattigeri, Giuseppe Cuono, and Carmine Autieri "Interplay between altermagnetism and nonsymmorphic symmetries generating large anomalous Hall conductivity by semi-Dirac points induced anticrossings" published in Phys. Rev. B **108**, 115138 (2023) has been related to the discussion on the scientific project and the plot of the results reported in Figure 8.

Yours Faithfully,

Raghottam Sattigeri

Affiliation:

Physics Department, Università degli Studi di Milano, Via Celoria 16, 20133 Milan, Italy

Date: 6 September 2024

STATEMENT

I declare that my contribution to the paper **Amar Fakhredine,** Raghottam M. Sattigeri, Giuseppe Cuono, and Carmine Autieri “Interplay between altermagnetism and nonsymmorphic symmetries generating large anomalous Hall conductivity by semi-Dirac points induced anticrossings” published in Phys. Rev. B **108**, 115138 (2023) has been related to the discussion on the scientific project and the plot of the results in Figure 1.

Yours Faithfully,

Giuseppe Cuono

Consiglio Nazionale delle Ricerche (CNR-SPIN),
Unità di Ricerca presso Terzi c/o Università “G. D'Annunzio", 66100 Chieti, Italy

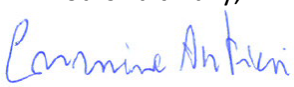
INSTYTUT FIZYKI
POLSKIEJ AKADEMII NAUK

Date: 6 September 2024

STATEMENT

I declare that my contribution to the paper **Amar Fakhredine,** Raghottam M. Sattigeri, Giuseppe Cuono, and Carmine Autieri "Interplay between altermagnetism and nonsymmorphic symmetries generating large anomalous Hall conductivity by semi-Dirac points induced anticrossings" published in Phys. Rev. B **108**, 115138 (2023) has been related to the discussion on the scientific project and the supervision of the project.

Yours Faithfully,



Carmine Autieri

Dr. hab. Carmine Autieri, IFPAN professor at the International Centre for Interfacing Magnetism and Superconductivity with Topological Matter (MagTop),
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Website: https://www.magtop.ifpan.edu.pl/resources/teams/
Google Scholar profile: https://scholar.google.it/citations?user=83pF0ywAAAA
ResearchGate profile: https://www.researchgate.net/profile/Carmine_Autieri

BIBLIOGRAPHY

[1] Lin-Ding Yuan, Alexandru B Georgescu, and James M Rondinelli. Non-relativistic spin splitting in compensated magnets that are not altermagnets. *arXiv preprint arXiv:2402.14321*, 2024.

[2] Albert Fert, Mairbek Chshiev, André Thiaville, and Hongxin Yang. From early theories of dzyaloshinskii–moriya interactions in metallic systems to today's novel roads. *Journal of the Physical Society of Japan*, 92(8):081001, 2023.

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