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Theoretical Analysis of Physical Property Regulation and Quantum Effects in Two-Dimensional Altermagnetic Materials

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Abstract. This review carries out a comprehensive narration on the theory area which surrounds two-dimensional altermagnets, and it puts emphasis on their multi-function adjustment mechanisms. In the aspect of theory, a framework for "altermagnet (valley) electronics" has been constructed by us, and the physical origins of many effects—for example valley polarization and chiral magnons—have been made clear from the angle of material symmetries. As well as, from the practical perspective, the combination of these researches puts forward feasible roads for making next-generation, low-energy-consumption spintronic and topological quantum devices, and at the same time hence finds out key problems in material preparation and experiment measurement analysis. Future development in this hopeful domain depends on the cooperating progress in multiple core aspects: the credible synthesizing of high-grade materials, the creating of advanced detectors for directly measuring new quantum effects, and the successful combining of heterostructures for use in functional device applications.

Keywords: two-dimensional (2d) altermagnets, first-principles calculations, valleytronics

1. Introduction

One of the core propellers behind the continuous development of spintronics and valleytronics resides in the exploration of new material platforms which can with high efficiency produce, control and test the spin and valley degree freedoms of electrons. Although the conventional iron-containing magnets can give out obvious spin polarisation, their own existing stray magnetic fields heavily restrict the combination of high-density apparatus; On the opposite side, although traditional antiferromagnets do not have overall magnetization, the physical effects related to their spins are usually weak and extremely dependent on spin-orbit coupling. In the past years, exchange magnets have been built up as a new magnetic phase, which is characterised by net-zero magnetisation in real space, and at the same time it shows strong spin splitting in the momentum-space energy band that is decided by crystal symmetry, hence it hence provides an ideal answer to the above-mentioned problems. In this newly appeared field, one special top-level research direction includes researching how to use the effective coordinated control of a single outer physical field in two-dimensional layered exchange magnetic bodies. This kind of "one-to-many" controlling ability is considered by

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people to be the key physical base for realizing the next generation of highly gathered, low energy consumption, multi-function quantum equipment [1].

In relation to this direction, recent theoretical research, through first-principles calculations and model analysis, has achieved a series of significant conceptual breakthroughs and predicted several promising material systems. For example, in a single layer of Co_2MoSe_4, theory has revealed that strain can simultaneously induce energy valley polarisation, piezoelectric response and Berry curvature redistribution; this phenomenon has been summarised as the "multi-piezoelectric effect", and potential pathways for achieving magnetoelectric response via doping have been predicted. Research on the Fe_2MoX_4 family has further proposed a fully electrical 'strain-doping' synergistic scheme to regulate net magnetisation. Research concerning the β-MnO_2 system has made the prediction that chiral magnetons and their strain-adjustable property exist, this does not require the use of an outside magnetic field. Furthermore, the theoretical models which are built on exchange magnet/topological superconductor heterostructures have given prediction about topologically protected quantised transport platforms. More researches afterwards have put forward that people can actively bring out exchange magnetism in systems just like $MnPTe_3$ via the designing of interlayer magnetic order (spin symmetry engineering), which, when it is combined with ferroelectricity, therefore displays new magnetoelectric coupling mechanisms. These early research works completely prove the huge potential of two-dimensional exchange magnets as a highly adjustable, property-abundant quantum material platform.

Nevertheless, a combing through of existing research has found several clear common points and key shortcomings. First of all, the great majority of pioneering forecasts are still strictly limited within the domain of theoretical computation; the making of high-quality test pieces of the forecasted materials (such as Co_2MoSe_4 and Fe_2MoX_4) and the experiment checking of their relevant performances still have not been solved. Secondly, the predicted semiconducting two-dimensional exchange magnets all generally encounter the bottleneck of low magnetic ordering temperatures, which therefore severely limits their prospects for room-temperature applications. What is more important, current researches have on the whole concentrated on proving whether new effects "can be found under perfect conditions", however, there is an absence of deep-going research into the steadiness and strength of these effects in real not-good environments (for example, the being of flaws, boundary surfaces, charge carrier scatter, and temperature changes). Furthermore, current research up to now still has not given systematic responses to key questions about the microscopic mechanisms that govern how different order parameters compete or cooperate under the action of multiple physical fields—such as strain, electric fields and magnetic fields—and therefore how to realize independent and accurate decoupled control of specific functions on the device level.

According to the present research situation and the difficulties people have talked above, this paper has the goal to give a systematized literature summary and critical view on the newest developments in the control of physical characteristics and quantum effects in two-dimensional exchange magnets. This research is not only a simple listing of current theoretical results, but also is committed to reaching the following three goals: Firstly, to critically summary a number of latest representative studies, giving deep analysis on the universal physical image and the sources of symmetries which come from the coupling of multiple freedom degrees, such as 'lattice-charge-spin-energy valley-topology'; Second, for the purpose of systematically carrying out identification of the common difficulties that are met with in the whole research chain, from the exploring and preparing of new materials, through the experiment-based characterization of special order parameters, to the integration of functional heterogeneous structures; Thirdly, on the proactive side, people put forward potential breakthrough roads and future research key points, such as using high-throughput

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calculation screening to find new materials that have high Curie temperatures, developing advanced measuring methods for spin textures and chiral magnetic excitations in momentum space, and probing model devices on the basis of relatively simple heterostructures to prove core physical principles.

The theoretical significance of this work lies in the fact that, through systematic review and in-depth analysis, it helps to clarify the physical mechanisms, advantages and limitations of multifunctional control in two-dimensional exchange magnets, thereby driving the field's evolution from fragmented theoretical predictions towards a condensed matter physics research paradigm that is more closely aligned with real material systems and complex experimental conditions. Its practical significance lies in providing researchers in experimental physics, materials science and device engineering with clear, phased research guidance. It clearly points out the key scientific problems and technical difficulties which must be solved to confirm theoretical forecasts, get over material and making troubles, and finish sample equipments, hence helping the advance of these quantum materials from theoretical researches to experimental studies and possible utilizations.

2. Base natures and foundational physics of two-dimensional exchange magnetic materials

Two-dimensional exchange altermagnetic materials are the third kind of basic magnets that have been discovered, they come after ferromagnets and antiferromagnets. They are having the character of a net zero magnetisation in real space, meanwhile they show strong spin splitting in the momentum-space energy band, this is decided by the crystal symmetry [2]. This special electronic structure comes from the symmetry of the spin group, that is the combination of time-reversal symmetry breaking together with particular crystal rotations or mirror operations, it does not rely on net magnetic moments or strong spin-orbit coupling. The five front-edge researches summarized in this article take typical two-dimensional exchange-bonded magnetic systems, for instance Fe_2MoX_4, Co_2MoSe_4 and β-MnO_2, as special research objects, systematically investigating the abundant research orientations and functional adjustment paths that come from their kernel physical natures. These research works together concentrate on several key aspects: firstly, they have researched the inherent, spin-locked energy-valley degree and freedom, and how people realize synergistic control by using multiple physical fields like strain and electric fields; secondly, therefore, they carry out investigation on the unique chiral magneton excitation things and their responses to the external strain; in addition, they build heterostructure models on the basis of exchange magnetics, with the goal to achieve new quantum phenomena such as topological interface states and quantized transport; In the end, methods were put forward to bring out exchange magnetic states by means of the active design of interlayer magnetic coupling and symmetry, hence people explore the novel magnetoelectric coupling mechanisms that generate from this. These researches have made deep exploration into the possibility of two-dimensional exchange magnets as a platform for quantum materials from many different angles, therefore together drawing a full research picture which is marked by highly adjustable natural properties and the capacity to combine with many external freedom degrees to achieve a large number of functional uses.

3. Energy valley: the study of physics and multi-function electrical-mechanism control

In two-dimensional exchange magnets, the valley degree of freedom in momentum space is highly developed and is locked to the spin degree of freedom via crystal symmetry; this provides the theoretical basis for realising novel multifunctional devices that go beyond traditional valley electronics materials.

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3.1. The 'multiple piezoelectric effect' induced by strain engineering

Zhang et al.'s systematic study of monolayer Co_2MoSe_4 revealed the 'multi-piezoelectric effect', whereby strain, as a single physical stimulus, can simultaneously trigger multiple responses [3]. Through first-principles calculations, this work first confirmed that Co_2MoSe_4 is an exchange-magnetic semiconductor with a direct bandgap of 0.97 eV, whose valence band top and conduction band bottom are located in the X and Y energy valleys of momentum space, respectively, and which exhibits significant spin splitting, with valence band splitting of approximately 0.53 eV and conduction band splitting of approximately 0.45 eV. The core new creation of this research lies in making clear that the using of in-plane single-axis stress can break the special crystal symmetry which guards the degeneracy of the energy valleys. At the same time, this strain causes an asymmetric change of the Baryon curvature distribution in the material, and therefore activates a quite big shear piezoelectric response, with a piezoelectric coefficient d_{16} that is about 3. 52 pm per V. This theory further gives prediction that, when strain is put together with hole doping, the energy valley occupation unbalance which strain causes will produce a net magnetisation, therefore realising the so-called piezo-magnetic effect. The meaning of this work is in its basic proving that exchange magnets can act as core materials for multifunctional strain-sensing devices, which have the ability to change one mechanical input into many physical outputs—including electrical, magnetic, and energy-valley effects—therefore hence giving a new model for the development of highly integrated sensing and information handling technologies. Its control mechanism, which is based on non-volatile lattice deformation, also shows potential advantages on reaching low static power consumption. Nevertheless, it is necessary to point out that all predictions of this study are constructed upon first-principles computation; Hence, thus there exists an urgent necessity to verify these points by means of experimentally manufacturing high-quality single-layer samples and utilizing controlled strain. In addition, the material's forecasted Néel temperature is around 84 Kelvin; This relatively low ordering temperature therefore limits its application prospects when at room temperature. Another point which is worthy of attention is that, although the strong interaction between many physical phenomena gives the device many functions, it also brings inherent complexity when people want to realize the independent and accurate control of each individual effect.

3.2. The synergetic mutual action between electric fields and strain makes possible a completely electrical piezoelectric reaction

In their study of the Fe_2MoX_4 (X = S, Se, Te) and Fe_2WTe_4 families of materials, Fan et al. proposed a fully electrical scheme combining strain and electrostatic doping to achieve a piezoelectric response [4]. This study first theoretically confirmed that these materials belong to the d-wave exchange magnetic semiconductors, with a pair of energy-degenerate but spin-locked energy valleys at points X and Y in momentum space. The core innovation of this work lies in the design of a two-step physical mechanism. The first step involves applying in-plane uniaxial strain to break the crystal symmetry that protects the degeneracy of the energy valleys, thereby creating an energy difference between the X and Y valleys—that is, achieving valley polarisation. The second step makes use of a gate voltage for adding holes into the material, thus making carriers selectively take up particular energy valleys the energy of which has been lowered by the strain. Because, in these exchange-coupled magnetic bodies, the energy valley freedom degrees have strong correlation with electron spin, this non-balance in energy valley occupation—which is caused together by strain and doping—is directly changed into the total net magnetisation of the whole system. In addition,

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theoretical computation results show that the size of this magnetisation holds an about linear connection with the applied strain. This principle provides a new technical road for the design of future extra-high-density, extra-low-power non-volatile magnetic random-access memory. A remarkable superiority of this method is that it wholly removes the dependence on overall outside magnetic fields or spin-polarized input currents, in theory showing bigger possibility for matching with current main-stream silicon-based CMOS craft procedures. But even so, the path that leads to real using faces very many obstacles. One basic difficult problem is in the situation that, to obtain high mobility and space-uniform electric field doping in two-dimensional material devices, it is still in itself very hard. In addition, the changes of magnetic moment which is modulated by strain that theory predicts are generally extremely feeble; the strength of their signals may get close to the detection boundaries of today's high-sensitivity magnetic sensing technologies, therefore bringing difficulties for experimental observation and device reading output. Moreover, this method needs the harmonious management of many physical domains, encompassing mechanical deformation, electric fields, charge distribution and magnetic sequence. This intense interaction among many physical domains causes the design of the final apparatus's working patterns and condition adjustment to be unusually complicated, hence it brings a serious threat to the dependability of apparatus engineering.

4. Hand magnetic excitation with rotation: a spin electron platform that has no outside magnetic field

Unlike traditional antiferromagnets, the spin waves (magnetons) excited in exchange magnetics possess intrinsic chirality, opening up the possibility of non-reciprocal spin information transfer (magnetronics) without the need for an external magnetic field [5].

In their study of β-MnO_2, Gauswami et al. systematically characterised its magnetic excitation spectrum by combining first-principles calculations with linear spin-wave theory [2]. The Heisenberg exchange parameters extracted from these calculations reveal a strong antiferromagnetic coupling of up to –14.19 meV between nearest-neighbour atoms, together with a comparatively weak ferromagnetic coupling which is about 0. 56 meV on the seventh-nearest-neighbor layer. The magneton spectrum which is calculated on the basis of these parameters indicates that along the specific directions in the momentum space, for example the M_1-Γ-M_2 path, there exists an energy separation which is approximately 3. 48 milli-electron volts that lie between the magneton branches, which namely is a chiral energy gap, and the sign of this gap will perform alternation along with the changes of the momentum point; This characteristic is an obvious marking symbol of chiral magnetons. This research further proves that the utilization of unidirectional strain can continuously adjust the size of this chiral energy gap; To be specific, compressive strain can bring about a growth of the energy gap, whilst tensile strain makes the gap become smaller or even totally eliminated, hence it is that people directly verify that it is feasible to adjust magnetic excitation properties by using the physical method of lattice strain. The meaning of this research is in its theoretical verification that exchange magnets can act as an ideal material platform for realizing internal, non-reciprocal magneton movement which does not need an outside magnetic field [6]. Furthermore, it thus defines strain as one effective in-situ controlling parameter, hence laying the theoretical basis for the future design of reconfigurable magnetonic logic devices, which are such as circulators and isolators. Nevertheless, the present research possesses certain restrictive aspects. Firstly, the β-MnO_2 which people research is basically a three-dimensional material, and its related properties under strict two-dimensional limits therefore still need to be further explained and verified. A more key challenge lies in the situation that accurately exciting and testing chiral magneton modes with

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particular wavevectors in nanoscale experiments still is a very big technical difficulty. Furthermore, the theoretical models that this study utilizes generally do not take into consideration magneton damping effects and defect scattering, these are factors which are frequently very important in real material systems and the running of devices [7].

5. Topological interface characters in heterojunctions and ideas for quantum devices

The combination of two-dimensional exchange magnets and other quantum materials, for example superconductors, therefore can induce new topologically protected quantum states at the interface, hence these states can be used by people for the topological quantum computing [8].

Wang and other persons the theoretical level, people have designed a sandwich junction of AM/AMTSC/AM (antiferromagnet/antiferromagnetic topological superconductor/antiferromagnet). The theoretical model of this research is built on a core supposition: that the antiferromagnetic topological superconductor which is in the middle area can enter a topological phase under suitable parameter conditions and hold chiral Majorana edge states [9]. Computations show that, because these topological edge states are existing, the transmission coefficient and cross-Andreev reflection coefficient of this heterojunction have quantized platforms near zero energy, for example $e^2/2h$ or $e^2/4h$. The numerical values of these quantised platforms are not invariant but can be toggled among multiple conditions through regulating the system's chemical potential, changing the magnetisation orientation of the exchange magnet electrodes, or choosing dissimilar superconducting pairing symmetries; This therefore constitutes the main prediction that this theory has. This work puts forward a new-style topological quantum device structure on the basis of physical principles, whose core superiority exists in using the characteristics of exchange magnets to realize electric control for topological transport; in addition, the theory gives prediction that this quantised electric conductance has strong resistance to a certain degree of disorder. Its meaning exists in the situation that this topologically protected quantized transportation provides a new theoretical framework and technical road for the future realization of addressable, controllable Majorana zero-energy modes. However, the movement of this scheme from theory to practice meets basic and very frightening difficulties in the field of materials science [10]. Up to now, there does not exist any credible two-dimensional topological superconductor that has obtained experimental confirmation, and the making of an atomically sharp heterojunction with another exchange-correlated magnet has gone far beyond current abilities in material synthesis and nano-processing. Moreover, the concerned quantum phenomena that are predicted by the theory can only be observed under the ultra-low-temperature condition which is in the millikelvin range, thus the computational outcomes are extremely sensitive to parameters like the heterojunction's interface transparency and band alignment. This indicates that all non-ideal situations which exist in actually made devices can therefore cause these subtle topology effects to completely disappear.

6. Symmetry engineering: new approaches to inducing exchange magnetism and parity-dependent magnetoelectric coupling

In addition to utilising existing magnetic exchange, another cutting-edge approach involves actively 'creating' or controlling this state through symmetrical design.

The authors Sun and other persons put forward a novel mechanism which is different from the traditional method of "breaking spatial symmetry", that is, through the modulation of spin-space symmetry to derive exchange magnetism from an antiferromagnetic ground state (this is defined as Route II). The core working principle of this research is proved by taking the $MnPTe_3$ double-layer

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structure as a theory model. Our research has the indication that changing the interlayer magnetic order from an antiparallel disposition (which people call the L1 type) to a parallel disposition (L2 type) can break a key spin-space symmetry operation [C_2||P], which in the beginning made spin degeneracy in the energy bands be enforced. This symmetry breaking lets the system directly produce the band spin splitting which is the feature of exchange magnetism, without changing its crystal lattice. By using tight-binding models and first-principle calculations, this research further confirms that the size of the spin splitting which is produced in this way rises along with the increase of interlayer coupling strength. One important expansion of this research work is the combination of the above-mentioned "spin symmetry engineering" with another method—"breaking spatial inversion symmetry" (Route I)—which is obtained by means of skimming ferroelectricity. This research discovered that in systems which possess L2-type exchange magnetic order, the reversal of ferroelectric polarisation can cause the full reversal of band spin splitting, and these two have an about linear functional relation—that is, it is an odd-function characteristic. This is equal to finishing a 180-degree turn of the magnetic moment through the use of only an electric field. This behaviour has a fundamental difference from the even-function relation—featured by a parabola-shaped curve—that is observed under L1-type magnetic order, therefore it reveals a new magnetoelectric coupling mechanism which is controlled by spin symmetry. The theoretical meaning of this research lies in that it opens a new direction for controlling exchange magnetism at a more basic level of symmetry, and hence exhibits a new physical picture which is different from traditional multiferroic materials on the aspect of coupling parity. This therefore gives an important theoretical frame for the design of new-type multifunctional devices which are based on symmetry engineering. But, this kind of effect until now has only been predicted in the special theoretical model of $MnPTe_3$. Whether that its basic physical rules are all world-shared, and whether that it can be achieved in a wider scope of material systems, is still to be researched and confirmed in the follow-up studies. Moreover, stably realizing the transformation of interlayer magnetic arrangement by means of externally applicable methods that are realizable in experiments (for example, the exertion of strain or an electric field) hence is the key to putting this theoretical plan into actual application.

7. Prospective difficulties

Through a systemic combing of theoretical researches on two-dimensional exchange magnetic materials, this review article expounds the physical mechanisms which lie under their multi-functional manipulation and their possible application prospects. Theoretical researches have already discovered the birthplaces of many new physical effects from the angle of symmetry, therefore they give a theoretical frame for the designing of new materials and the searching of new states of material. This research has moreover put forward conceptual methods for the making of new spintronic and quantum devices, meanwhile it has found out the key material and characterisation difficulties which must be solved in later experimental researches. The future progress of this research area hence will rely on continuous new findings in material making, performance testing and device combination, hence.

8. Conclusion

This review systematically gives a sum-up of theoretical studies on the multifunctional controlling of two-dimensional exchange-correlated magnetic materials, hence explaining their core physical mechanism and possible application uses. Through the establishment of the paradigm of "exchange-

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correlated magneto(valence)electronics", this theoretical work has given a unified explanation for the sources of many physical effects from the angle of symmetry, and thus has provided a theoretical framework for the designing of new materials and states of matter. On the practical aspect, these researches put forward usable idea frameworks for the growth of a new generation of low-power spin electronics and topological quantum apparatus, meanwhile they find out the key material and measurement difficulties which are contained in putting these ideas into practice. The development in the future therefore will be dependent on synergistic break-throughs in domains such as material preparation, experiment measurement and device physics.

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