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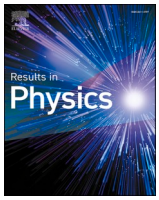

Designing ultrathin and long ferromagnetic nanowires array for Tunable-Range Majorana zero mode studies

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ABSTRACT

We have conducted a study that focuses on designing a quasi-1D ultrathin and long ferromagnetic nanowires array with excellent linearity. The purpose of this design is to test the presence of Majorana zero modes in pairs over a long distance and the influence of the lateral interaction. Specifically, we investigate the magnetic properties of a one-unit cell thick MoSX nanowire array, where dopant X (H, C, N, O, and F. etc) is utilized, to assess its suitability for our intended purposes. Our findings reveal that the edge magnetization of the optimized MoSX nanowires is comparable to that of 3d transition metals with the Curie transition temperature surpassing room temperature. Our study indicates that the ferromagnetism of the optimized MoSX nanowires is unlikely to be eliminated when placed on an s-wave superconductor due to lattice mismatch. By conducting comparative case studies of various dopants, we establish a connection between the source of magnetism in the nanowires and internal electric fields, charge perturbation, spin-orbital coupling and p-d hybridization. The strong exchange interaction, robust spin-orbital coupling and large local magnetic moment exhibited by long and ultrathin room-temperature ferromagnetic nanowires open up avenues for diverse topological applications.

Introduction

Quantum computing has the potential to revolutionize various fields, credited to its increased computational power compared to classical computers [1]. It can solve complex problems that are currently infeasible for conventional systems. It also enables fast simulation and insights into complex physical systems, leading to advancements in chemistry, physics, materials science, genetics, and other scientific disciplines [1,2]. In addition, optimization and machine learning benefit from the extraordinary computational power of quantum systems, allowing for more efficient solutions and improved data analysis [1,2]. Quantum computing can drive technological innovations by solving complex problems and providing deeper insights into fundamental scientific phenomena, leading to practical applications in industries such as material development, drug discovery, and energy efficiency [1,2].

However, one of the main challenges in building practical quantum computers is preserving the fragile quantum states, or qubits, from environmental noise and decoherence [1,2]. Quantum nanowires characterized by their length without width or height offer an ideal setting for the emergence and observation of a special particle called a Majorana zero mode [3]. Majorana zero modes (MZMs) have been theorized to enable long-distance communication without interference, which offers the possibility of creating highly stable qubits that are less susceptible to external disturbances and greatly enhance the efficiency and reliability of quantum information processing [4,5,6]. These exotic quasiparticles are predicted to occur at the ends of one-dimensional topological superconductors and possess unique properties that make them highly desirable for quantum computing applications [4,5,6].

Although MZMs hold great promise, their observation and manipulation have proven to be extremely challenging [7]. These elusive

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quasiparticles can emerge in specific systems, such as ultrathin ferromagnetic nanowires on top of a s-wave superconductor, triggered by spin–orbit coupling [8]. In order to investigate the one-dimensional (1D) limit of the Majorana Zero Mode (MZM) theory, it is necessary to use an ultrathin thin ferromagnetic nanowire, as opposed to a thick one which may trap the MZMs inside vortices. Although one of the rare systems where MZMs have been found in the monoatomic Fe nanowire on a Pb (1 1 0) substrate, the manufacturing process for long monoatomic Fe chains poses difficulties, leading to irregularities in atomic positions [8,9]. It remains an open question whether these irregularities affect the probability of MZMs emergence in such systems. Furthermore, monoatomic Fe nanowires are limited in length in the experiment, typically reaching a maximum of around 40 atoms only (~7nm) [9]. This limitation hinders the ability to demonstrate the existence of two MZMs at opposite ends of a sufficiently long separation, as predicted theoretically. Worse still, the monoatomic Fe chain is difficult to be fabricated in the form of a nanowires array which presents a hurdle to studying if the MZMs are affected by the lateral interaction across the nanowires.

To address this limitation, it is necessary to explore alternative quasi-1D ultrathin and long ferromagnetic nanowires with good regularity and strong spin-orbital coupling. Magnetic modification of Transition metal dichalcogenides (TMD) nanowires has the potential to address this limitation. However, fabricating a TMD nanowire with a strong spin-orbital coupling that possesses good regularity, while also being one-unit-cell thick and long in length, presents a significant technological challenge. Moreover, achieving room-temperature ferromagnetism on these long and ultrathin TMD nanowires is another uphill struggle. Despite the challenges involved, there is reason for optimism due to the successful creation of a parallel array of over 200 nm long MoS_2 nanowires [10]. They are extremely thin, with a thickness of only one-unit-cell (diameter ~0.3 nm) [10]. This achievement provides a ray of hope for further advancements in the topological field. This MoS_2 nanowire exhibits excellent linearity and chemical stability. The next hurdle is figuring out how to induce ferromagnetism in the MoS_2 nanowire at room temperature. By doing so, it would be possible to demonstrate the potential for testing the probability of emerging MZMs in pairs as a function of a much longer distance (over 200 nm) if it is placed on top of a s-wave superconductor.

Although the next problem is how to make the MoS_2 nanowires ferromagnetic, achieving room-temperature ferromagnetism in MoS_2, even in thin-film conditions, is a difficult task. Previous attempts to make MoS_2 ferromagnetic have been unsuccessful, except when using a "conventional" approach, which involves doping with a strong ferromagnetic atom such as Fe. In this case, the Fe-doped monolayer of MoS_2 exhibits room-temperature magnetism due to the intrinsic ferromagnetism of Fe [11]. To ensure the stability of ultrathin nanowires, it is crucial to consider the potential destruction caused by internal chemical pressure. In contrast to two-dimensional systems with more neighboring atoms for stabilization, ultrathin nanowires are more susceptible to damage. Doping large Fe atoms may generate excessive internal pressure, leading to the breakage of the nanowires. To address this issue, we aim to investigate whether it is possible to introduce magnetic properties in MoS_2 nanowires by doping small atoms, though small atoms are usually non-magnetic. The proposed substituent dopant X is H, C, N, O, and F. etc, respectively. We will also examine the influence of strain on the magnetism induced in the MoSX nanowires, specifically for the scenario where the nanowires are deposited on an s-wave superconductor, resulting in a lattice mismatch that may eliminate the magnetism due to strain badly.

Computational methods

In this study, we employed the spin-unrestricted Generalized Gradient Approximation with the Perdew-Burke-Ernzerhof (GGA-PBE) functional under spin-orbital coupling to investigate the geometric optimization, electronic band diagram, and density of states (DOS) for various compounds [12,13]. Geometric optimization is a crucial step in understanding the structural properties of compounds. It involves finding the equilibrium positions of atoms by minimizing the total energy of the system. In our study, we utilized the spin-unrestricted GGA-PBE functional (unless otherwise specified) to perform geometric optimization for all compounds under investigation. The GGA-PBE functional is known for its good accuracy in describing the physical properties of materials [12,13]. The electronic band diagram and density of states provide valuable insights into the electronic properties of materials. The band diagram illustrates the allowed energy states (bands) for electrons in materials, while the DOS is directly proportional to electron concentration. In our calculations, we set the self-consistent field (SCF) tolerance to $1x10^{-5}$ eV/atom. The SCF method is an iterative procedure used to solve the electronic structure problem. Setting a low tolerance ensures that the SCF cycle converges to a sufficiently accurate solution [12,13]. Additionally, we employed a k-space interval of 0.025 (1/Å). K-space, or reciprocal space, is a mathematical representation used to describe the periodicity of crystals. The k-space interval determines the resolution of the calculations and is crucial for accurately capturing the electronic properties. To ensure convergence of the SCF calculations, we allowed a maximum of 1000 SCF cycles. This ensures that the data is sufficiently iterated. Density mixing is a crucial step in self-consistent calculations within density-functional theory (DFT). It involves updating the charge density at each iteration step to achieve convergence. In addition to the electronic properties, we also calculated phonon data for the compounds. Phonons are quantized lattice vibrations. To calculate phonon data, we utilized the finite displacement mode which can extract valuable information about the phonon modes and their frequencies. To accurately calculate phonon data [14], we defined a supercell using a cutoff radius of 5 Å. We employed a dispersion interval of 0.04 (1/Å). The dispersion interval determines the resolution of the phonon calculations and plays a crucial role in accurately determining the phonon frequencies.

Results and discussion

The MoS_2 nanowire, doped with substituent X, is abbreviated as MoSX. MoSN nanowire is the sample we study first. Fig. 1 includes an inset diagram that shows the schematic shape of MoSX nanowire. The

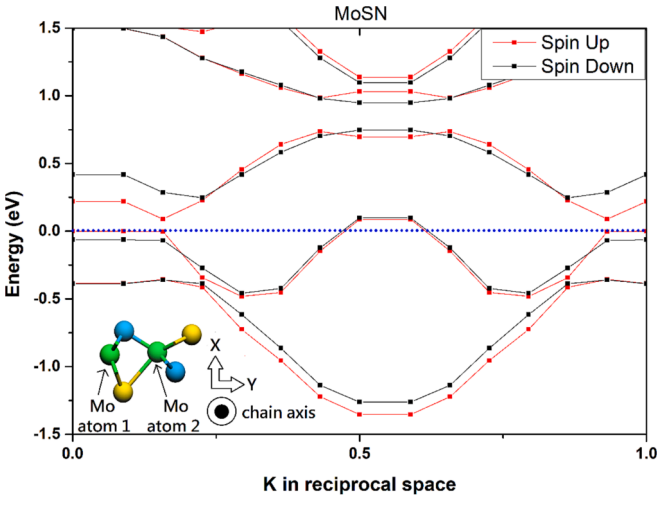

Fig. 1. An electronic band diagram of a one-unit-cell thick MoSN nanowire with a diameter of approximately 0.3 nm. The Fermi level has been shifted to 0 eV for convenience. The nanowire is composed of Mo (green), S (yellow), and N (blue) atoms, with two Mo atoms labeled as Mo 1 and Mo 2. The nanowires are laterally spaced by ~ 1.2 nm. The diagram also includes an inset showing the repeated unit of the MoSN nanowire. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

band structure of a one-unit-cell thick MoSN nanowire, as seen in Fig. 1, displays energy splitting [15] caused by magnetism. Based on Fig. 2, it can be confirmed that the MoSN nanowires exhibit a ferromagnetic nature with strong p-d hybridization [16], as evidenced by a partial spin density of states of approximately 0.3 electron/eV per atom at the Fermi level. The exchange–correlation energy of the MoSN nanowire is measured to be 447 K. In addition, as shown in Fig. 3, the phonon properties of the nanowires are also influenced by ferromagnetism [17]. The occurrence of negative phonon frequencies is rare, indicating that the sample is stable [18]. The average phonon frequency of the nanowire is decreased by approximately 5 % due to ferromagnetism.

The introduction of even a small strain at the interface due to lattice mismatch is unlikely to vanish the magnetic properties of MoSN nanowires, supported by our study of strain-modulated ferromagnetism in Fig. 4. Since MoS_2 has been extensively researched for its potential applications in flexible electronics, it is known that they can tolerate strains of up to approximately 10 % [19]. Thus, we have conducted an investigation to examine how strains up to 6 % affect the ferromagnetic properties of MoSN nanowires, where the strain value (6 %) matches the typical levels of strain observed in lattice mismatch on heterostructures. Fig. 4 displays the results, with the upper and lower panels referring to the magnetic moments of Mo atom 1 and Mo atom 2 (Fig. 1 – inset), respectively. We successfully adjusted the local magnetic moment of MoSN nanowires with mechanical strain, achieving a maximum moment of 1.6μB at 6 % strain, comparable to the magnetic moment of bulk Fe at 2.2uB. The 6 % strained MoSN nanowire holds an exchange energy of 394 K. If we compare a MoSN nanowire with a MoS_2 nanowire of the same scale (one-unit cell thick), the ground-state energy of the MoSN nanowire is more negative by ~12 %. Due to the experimental stability of the one-unit cell thick MoS2 nanowire, it is envisaged that the more negative ground state energy of the one-unit cell thick MoSN nanowire should exhibit a better chemical stability and potentially be fabricated over 200 nm in length.

Table 1 presents the distribution of the local magnetic moment in a MoSN nanowire at various lateral distances (d), where the magnetic moments align in a ferromagnetic configuration. Despite the reduction in lateral spacing from 1.2 nm to 0.6 nm, the impact of lateral interactions on the magnetism of the MoSN nanowires drops by ~3 % only. This is advantageous for creating densely packed arrays of magnetic nanowires, which can maintain high flux across the large area of the entire array regardless of the lateral spacing, while preserving their magnetic energy. We also investigate how changes in the concentration of nitrogen affect the magnetism of the one-unit cell thick MoSN nanowire. Specifically, when the concentration of N is halved resulting in Mo_2S_3N, we observe that the magnetic moment of Mo atom 1 decreases to 1.23 μB and the magnetic moment of Mo atom 2 decreases to 0.16 μB. However, the magnetic moments of the other atoms in the nanowire, including S and N, do not undergo noticeable changes.

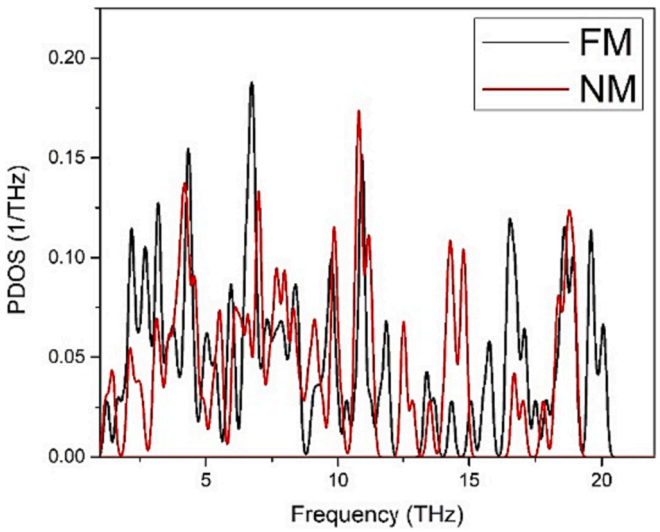

Fig. 3. Magnetic phonon exists in the one-unit-cell thick MoSN nanowire (FM ⇔spin-unrestricted mode; NM ⇔spin-restricted mode).

The synthesis of the one-unit-cell thick MoSN nanowire is not easy. Does ferromagnetism exist in a thicker MoSN nanowire? A positive outcome is expected. If the thickness of the MoSN nanowire is increased by a factor of three, the magnetic properties will persist, with a decrease in the magnetic moment of the Mo atoms to only 1.37μB and 0.41μB, while the magnetic moments of the S and N atoms are almost unaffected. The ground state energies of other MoSX nanowires, where X represents H, C, O, F, or Se, have not been successfully determined due to poor chemical stability. As a result, we have shifted our focus to study the role of ionic dopants in the localized magnetism of two Mo atoms in Mo_2S_3X nanowires, where X represents H, C, N, O, F, or Se, where each type of the Mo_2S_3X nanowire has been able to establish its own ground state energy. The optimized magnetism has been observed in the Mo_2S_3X nanowire with X being N. However, the Mo_2S_3B nanowire has not been able to reach the ground state owing to poor chemical stability, and consequently, no data has been reported for the B-doped case. Table 3 provides evidence for the potential source of the unexpected magnetism observed in Mo_2S_3X and MoSX nanowires. While one-unit cell thick MoS_2 nanowires do not exhibit any magnetic behavior, Mo_2S_3O and Mo_2S_3Se nanowires in the same diameter do exhibit magnetism surprisingly. It is worth noting that the introduction of dopants X = O, S, Se, does not generate any free radical electrons or lone pair electrons in the unit cell. The main difference between the three Group VI dopants is their size, which in turn creates an internal electric field owing to the difference in charge density. The magnetic moments arise from the

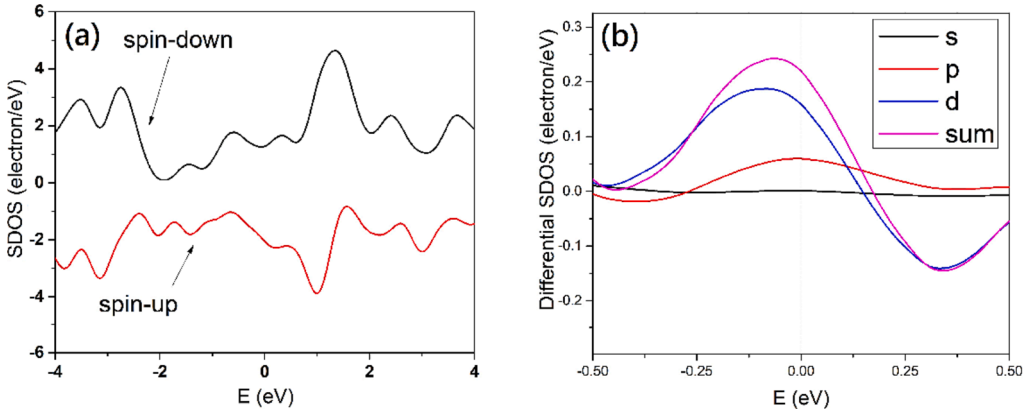

Fig. 2. A one-unit-cell thick MoSN nanowire (a) The spin density of states SDOS per unit cell. (b) The differential SDOS per atom on each orbital.

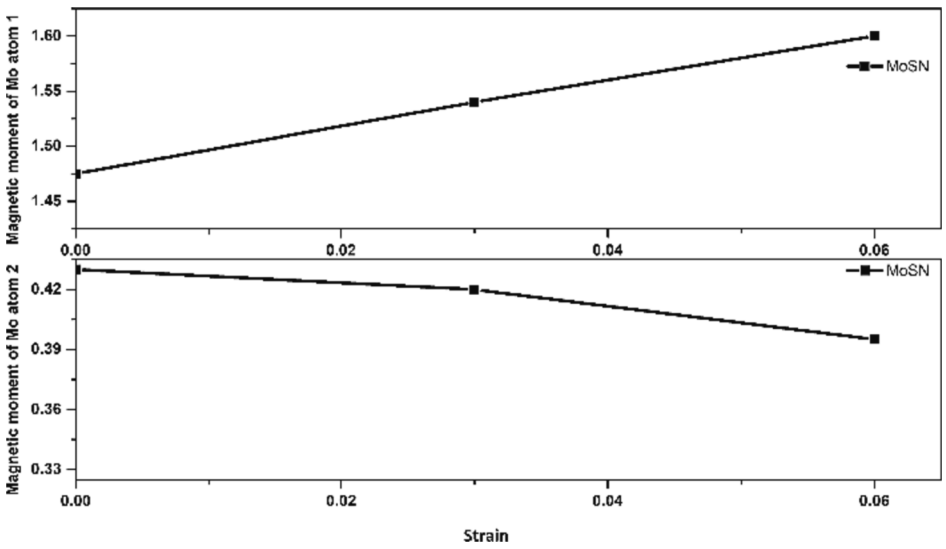

Fig. 4. The local magnetism of a MoSN nanowire is influenced by strain applied along its chain or longitudinal axis.

Table 1
The distribution of the magnetic moment in an unstrained MoSN nanowire.

	d (Å)	N (μ_B)	S (μ_B)	S (μ_B)	S (μ_B)	Mo atom 1 (μ_B)	Mo atom 2 (μ_B)
a	12	0.03	0.14	0.03	0.02	1.48	0.43
b	6	0.03	0.13	0.02	0.03	1.47	0.43
c	4	0.12	0.03	0.02	0.02	1.45	0.44

Table 2
The concentration of nitrogen has an impact on the magnetic properties of the nanowire.

	Mo atom 1 (μ_B)	Mo atom 2 (μ_B)
MoSN	1.48	0.43
Mo_2S_3N	1.23	0.16

Table 3
The magnetism of Mo_2S_3X (X: H, C, N, O, F, Se) nanowires across the first row of periodic table.

	Mo_2S_3H	Mo_2S_3C	Mo_2S_3N	Mo_2S_3O	Mo_2S_3F	Mo_2S_3Se
Mo atom 1 (μ_B)	0.48	0.91	1.23	1.19	0.42	1.05
Mo atom 2 (μ_B)	0.05	0.29	0.16	0.26	0.03	0.21

spinning motion of electrons within the atoms or ions. In an unmagnetized nanowire, these individual magnetic moments are randomly oriented and cancel each other out on average. In the presence of spin-orbital coupling, an electron passes through the nanowire, it interacts with the induced electric field present in the material due to dissimilar anions. This induced electric field causes the electron to experience a force due to the electric field. The magnitude and direction of this force depend on factors such as the charge of the electron and the strength and orientation of the electric field. As the electron moves through the nanowire, this force from the internal electric field may affect its spin orientation under a strong spin-orbital coupling. This induced electric field may be the cause of the observed magnetic behavior in the Mo_2S_3X and MoSX nanowires, where our optimized MoSN nanowire yields a strong spin-orbital coupling of ~43 meV. The existence of an internal electric field may generate orbitals that are more directional. With charge perturbations under the internal E-field, these more directional orbitals can result in an increased overlap of energy levels, ultimately promoting the hybridization of orbitals. Fig. 2b presents evidence for the presence of hybridized orbitals, where there is a significant p-d hybridization [16]. The increased overlap between the orbitals increases the likelihood of electron–electron interactions, which in turn leads to exchange coupling to generate magnetism [20].

In examining the potential role of ionic radius in the magnetism of the X-doped MoS_2 nanowire, we analyze and compare its magnetism across various species, including X: H, C, N, O, or F in Table 3. Although an internal electric field is created when X = F, the presence of a lone pair of electrons causes strong repulsion, making it difficult for exchange interaction to occur effectively and resulting in weak magnetism [20]. Conversely, the small orbital radius of the H atom in combination with the lack of electrons means it cannot effectively interact with other electrons on S and Mo via exchange interaction, resulting in weak local magnetism [20]. The optimal choice of X = N strikes a balance between the internal E-field, electrostatic repulsion, and orbital radius which is believed to associate with the appearance of magnetism. The Mo_2S_3N nanowire exhibits a weaker internal E-field per unit cell compared to the MoSN nanowire because of the relatively lower concentration of N in the former, which pales the magnetic moments of the Mo atoms in the Mo_2S_3N nanowire (Table 2). The edge effect of Mo atom 1 is stronger than that of Mo atom 2 since Mo atom 1 connects to only two nearest neighbors, while Mo atom 2 connects to four nearest neighbors that could be a reason why the magnetic moment of Mo atom 1 is always stronger than that of Mo atom 2. Strong electron–electron interactions are induced along the edges of nanowires due to enhanced edge states. These interactions lead to a transition in the magnetic configuration of the nanowire from nonmagnetic to ferromagnetic [21]. Two Mo atoms 1 are magnetically coupled along the chain axis, with a short period of 3.24 Å. Each Mo atom 1 has a magnetic moment of approximately 1.5μB. The dipole moment per unit length along the edge formed by a series of Mo atoms 1 is strong, and its edge magnetism is similar to the magnetism of common transition metals. The magnetic properties of the MoSN nanowire array almost remain unaffected by its packing density, which simplifies the process of fabricating the desired nanowires array because the nanowires can be magnetic regardless of the lateral spacing, where precise alignment of the one-unit-cell thick nanowire is expected to offer a higher resolution study for MZMs [1]. The Dirac cone appears in the band structure of a monoatomic Fe nanowire only if the simulation includes Pb(1 1 0) substrate[9]. Hence, this is not surprise that the band diagram (Fig. 1) does not have a Dirac-like cone because the simulation does not include a superconducting substrate which will be our future

task.

Finally, we determine if the choice of DFT-functional affects the computed magnetic moment of Mo atoms in the unit cell. The simulation results are presented in Table 4. Interestingly, regardless of the DFT-functional used, Table 4 confirms that the Mo atoms consistently exhibit strong magnetic moments. This finding boosts our confidence in the existence of the strong magnetism associated with Mo atoms.

Table 4
The magnetic moments of Mo atoms in an isolated MoSN nanowire predicted by different DFT functional.

	LDA-CA-PZ	GGA-PBE	GGA-PW91	GGA-WC	GGA-RPBE	GGA-PBESOL
Mo atom 1(μ_B)	1.35	1.48	1.43	1.42	1.44	1.41
Mo atom 2(μ_B)	0.45	0.43	0.46	0.46	0.48	0.46

Conclusions

In our study, we focus on designing quasi-1D ultrathin and long ferromagnetic nanowires with excellent linearity. Our primary objective is to investigate the presence of Majorana zero modes in pairs over significant distances and explore their lateral interaction. To accomplish this, we examine the magnetic properties of a one-unit cell thick MoSX nanowire array, where various dopants X were utilized. Through our research, we discover that the edge magnetization of MoSN nanowire arrays is comparable to that of 3d transition metals. We established a connection between the source of magnetism in the nanowires and internal electric fields, charge perturbation, spin-orbital coupling and p-d hybridization. The MoSN nanowires array exhibits a strong exchange coupling that surpasses room temperature, making it a promising material for studying the physics of Majorana zero modes over long separations and lateral spacing. These findings open up new possibilities for advancing our understanding of topological phenomena and have potential applications in diverse fields.

Author contributions

C.H.W planned the project. C.H.W designed and supervised the project. C.H.W conducted the simulations. C.H.W and K.C.L conducted data analysis. C.H.W, L.Y.F.L, X.H and K.C.L, W.S.Y, S.T investigated the project. C.H.W and K.C.L contributed to writing the manuscript. W.S.Y provided funding for the project.

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Institutional review board statement

Not applicable.

Informed consent statement

Not applicable.

CRediT authorship contribution statement

Ka Chun Li: Formal analysis, Writing – original draft. **Leung Yuk Frank Lam:** . **Xijun Hu:** Investigation, Resources. **King Cheong Lam:** Investigation, Software. **Suet To:** Investigation. **Wai Sze Yip:** Funding acquisition, Investigation, Resources, Conceptualization. **Chi Ho Wong:** Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Project administration, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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