

CORRELATION BETWEEN ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF MoO₃ AND MoS₂

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Correlation between electronic structure and magnetic properties of MoO_3 and MoS_2

by

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Dedicated to....

.... My Parents & family....

who are a constant source of inspiration and encouragement

Certificate

*This is to certify that the thesis entitled, “**Correlation between electronic structure and magnetic properties of MoO_3 and MoS_2** ”, being submitted by **Ms. Sharmistha Dey** to the Indian Institute of Technology Delhi, for the award of the degree of ‘**Doctor of Philosophy**’ is a record of bonafide research work carried out by her under our supervision and guidance. She has partially fulfilled the requirements for the submission of the thesis, which to the best of our knowledge has reached the requisite standard.*

The material contained in the thesis has not been submitted in part or in full to any other university or institute for the award of any degree or diploma.

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Sharmistha Dey

Abstract

For optoelectronic and spintronic applications such as in spin valves, spin transistors, and spin light-emitting diodes, transparent magnetic semiconductors (TMS) and diluted magnetic semiconductor (DMS) materials have been the most promising options in the last decade due to their optical, semiconducting, and magnetic properties. However, the observation of room temperature ferromagnetism (RTFM) in non-transition metal-doped semiconductors, such as HfO_2 , ZnO , TiO_2 , GaN , and SnO_2 , has attracted the attention of the scientific community. It should be noted that these materials show magnetism; however, their anions and/or cations are non-magnetic. The main reason behind this induced magnetism is the different types of defects in the lattice, such as vacancies, interstitials, dislocations, strain, etc. The presence of a sufficient number of defects in solids can alter their electrical, optical, and magnetic properties due to lattice symmetry breaking. As a result, the name d^0 ferromagnetism is given to the ferromagnetism found in pure semiconducting materials. It is evident from the observed d^0 FM in numerous oxides and sulfides that FM ordering can be induced by numerous naturally occurring or intentionally produced lattice defects without transition metal doping.

Among transition metal oxides and sulfides, molybdenum trioxide (MoO_3) and molybdenum disulfide (MoS_2) have attracted tremendous attention due to their potential applications in optoelectronics. MoO_3 and bulk MoS_2 are semiconductors with band gaps of 3.2 and 1.2 eV, respectively, and show room temperature ferromagnetism with a high curie temperature due to intrinsic defects such as vacancies, interstitials, anti-site defects, etc. In the case of MoO_3 , the primary cause behind the induced magnetism is oxygen vacancies and vacancy clusters. After post-treatment of MoO_3 at hydrogen ambient formation of H_xMoO_3 is also another intriguing reason to induce ferromagnetism. In the case of MoS_2 , in addition to S-vacancies, the edge-terminated structure also plays an important role due to different coordination geometry than bulk in inducing ferromagnetism. The creation of S-H bonds in MoS_2 lattices following

hydrogen post-treatment also raises the saturation magnetisation value. The production of room-temperature ferromagnets using these materials will significantly influence the applications of spintronics.

Future optoelectronic, spintronic, and opto-spintronic devices may benefit from these semiconducting materials, which are substitutes for ferromagnetic metals and semiconductor junctions. Before using these materials in any kind of device, a few basic issues must be resolved. The main issues are: (i) the reported value of saturation magnetization value in MoO_3 and MoS_2 is too low for use in spintronics applications; (ii) due to hydrogen interaction with MoO_3 , the creation of a greater number of oxygen vacancies and vacancy clusters and H_xMoO_3 formation is expected and needs to be explored; (iii) CVD growth of different morphology MoS_2 thin films and corresponding tuning of room temperature ferromagnetism is needed to be examined; (iv) there is a need for tunable ferromagnetism in MoS_2 by controlling the number of S-vacancies and edge-terminated structure after different types of post-treatment such as low energy ion irradiation and annealing; (v) the role of edge-terminated structure and S-vacancies in nano-dimensional MoS_2 thin films to highly enhance the ferromagnetism is needed to be explored. The motivation to comprehend these basic issues via in-depth experimental and theoretical research is the source of the current thesis.

Consequently, the main objectives of this thesis are (i) to study the effect of hydrogen annealing and corresponding oxygen vacancies on the ferromagnetic behavior in MoO_3 flakes; (ii) to study the effect of morphology (nanoflowers, vertical nanosheets, horizontal nanosheets, and thin film) on the magnetic properties in MoS_2 ; (iii) to study the effect of irradiation of low energy comparatively heavy (Ar and Xe) and light (hydrogen) mass ions and hydrogen annealing on the ferromagnetic behaviour of vertically nanostructured MoS_2 ; (iv) to study the effect of low energy Ar ion irradiation on the ferromagnetic behaviour of nano-dimensional triangular flakes of MoS_2 . The samples are prepared by chemical vapor deposition technique

and characterized by X-ray diffraction (XRD), Raman spectroscopy, atomic force microscopy (AFM), photoluminescence (PL), field-emission scanning electron microscopy (FESEM), electron probe micro analyzer (EPMA), Rutherford backscattering spectrometry (RBS), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS). Magnetic property measurements are performed for all the samples by using an MPMS3 magnetometer. The correlation between magnetic properties, electronic structure, and DFT-based theoretical calculations is established here.

After the introduction and experimental details chapters, the third chapter of the thesis is the investigation of RTFM in H₂-annealed CVD-grown MoO₃ samples at different temperatures. The presence of oxygen vacancies has been analysed by EPMA and PL measurements. The increase in the saturation magnetisation value in the H₂-annealed samples is correlated broadly with its electronic structure and DFT-based theoretical calculations.

The next chapter of the present thesis includes morphology-controlled RTFM in MoS₂ thin films. MoS₂ thin films are grown by the CVD technique with four different morphologies, such as nanoflowers, vertical nanosheets, horizontal nanosheets, and thin film. The main reason behind the induced magnetism is mainly edge-terminated structure along with S-vacancies, as the highest saturation magnetisation value is observed in the sample, which contains the highest number of edge-terminated structures (vertical nanosheets here). The reason behind the induced magnetisation is correlated with the electronic structure of these samples.

The next chapter is divided into two parts. The synergetic effect of edge-terminated structures and S-vacancies in inducing ferromagnetism in vertical nanosheet-oriented MoS₂ thin films is elaborately explained in this chapter. In the first part, the vertical nanostructured MoS₂ is irradiated with low-energy Ar and Xe ions with different fluences (ions/cm²) to modify the structure and tune the magnetic properties. Vertical nanosheets with edge termination in the

pristine sample have been examined by field emission scanning electron microscopy (FESEM). Deterioration of vertical nanosheets is observed in low-energy Ar^+ and Xe^+ irradiated samples. An appreciably high magnetisation value of 1.7 emu/g was observed for edge-oriented nanostructured pristine MoS_2 thin films, and it decreased after ion irradiation. From X-ray photoelectron spectroscopy (XPS) data, it is evident that, due to oxygen incorporation in the sulfur vacancy sites, Mo 5+ and 6+ states increase after ion irradiation. The edge-oriented spins of the prismatic edges of the vertical nanosheets are primarily responsible for the high magnetic moment in the pristine film, and the edge degradation and reduction in sulfur vacancies by the incorporation of oxygen upon irradiation result in a decrease in the magnetic moment.

In the second part, the nanostructured MoS_2 thin films are irradiated with low-energy hydrogen ions with different fluences and annealed in a hydrogen environment at different temperatures independently to create defects and enhance ferromagnetism. The nanostructured pristine MoS_2 thin films show the formation of a pure 2-H MoS_2 phase, confirmed by X-ray diffraction (XRD) and Raman spectroscopy. Hydrogen annealing at a temperature of 200°C exhibits a maximum saturation magnetisation value of 2.7 emu/g at room temperature. The increase in ferromagnetism is attributed to an increment in sulfur vacancies, hydrogen adsorption with sulfur, and modification in edges, which is confirmed by the analysis of electron probe micro-analyzer (EPMA), X-ray photoelectron spectroscopy (XPS), and field emission scanning electron microscopy (FESEM) measurements. For both cases, DFT-based theoretical calculations are in agreement with the experimental findings.

In the last chapter, nano-dimensional triangular flakes-oriented CVD-grown MoS_2 thin films (20 nm) are irradiated with low-energy Ar ion irradiation. The pristine sample behaves as a diamagnetic sample as it does not contain a sufficient number of edge-terminated structures and S-vacancies. The irradiated sample shows enhancement in saturation magnetisation value. One of the most crucial factors behind it is the creation and modification of the edge-terminated

structure, which provides dangling bonds and free spin. Another factor is the increase in the number of sulfur vacancies, which is confirmed by the XPS and RBS analysis.

The thesis concludes with a summary of the work carried out and the future scope of work in the field.

सारांश

स्पिन वाल्व, स्पिन ट्रांजिस्टर और स्पिन लाइट-एमिटिंग डायोड जैसे ऑप्टोइलेक्ट्रॉनिक और स्पिनट्रॉनिक अनुप्रयोगों के लिए, पारदर्शी चुंबकीय अर्धचालक (TMS) और तनु चुंबकीय अर्धचालक (DMS) पदार्थ पिछले दशक में अपने प्रकाशिकी, अर्धचालक और चुंबकीय गुणों के कारण सबसे आशाजनक विकल्प रहे हैं। हालाँकि, गैर-संक्रमण धातु-डोपड अर्धचालकों, जैसे HfO_2 , ZnO , TiO_2 , GaN और SnO_2 में साधारण तापमान पर फेरोमैग्नेटिज्म (RTFM) के अवलोकन ने वैज्ञानिक समुदाय का ध्यान आकर्षित किया है। यह ध्यान दिया जाना चाहिए कि ये पदार्थ चुंबकत्व दिखाती हैं; हालाँकि, उनके ऋणायन और/या धनायन गैर-चुंबकीय हैं। इस प्रेरित चुंबकत्व के पीछे मुख्य कारण लैटिस में विभिन्न प्रकार के दोष हैं, जैसे रिक्तियाँ, अंतरालीय, अव्यवस्था, तनाव, आदि। ठोस पदार्थों में पर्याप्त संख्या में दोषों की उपस्थिति लैटिस समरूपता टूटने के कारण उनके विद्युत, ऑप्टिकल और चुंबकीय गुणों को बदल सकती है। परिणामस्वरूप, शुद्ध अर्धचालक पदार्थों में पाए जाने वाले फेरोमैग्नेटिज्म को d^0 फेरोमैग्नेटिज्म नाम दिया गया है। कई ऑक्साइड और सल्फाइड में देखे गए d^0 FM से यह स्पष्ट है कि FM व्यवस्था को संक्रमण धातु डोपिंग के बिना कई स्वाभाविक रूप से होने वाले या जानबूझकर उत्पादित लैटिस दोषों द्वारा प्रेरित किया जा सकता है। संक्रमण धातु ऑक्साइड और सल्फाइड में, मोलिब्डेनम ट्राइऑक्साइड (MoO_3) और मोलिब्डेनम डाइसल्फाइड (MoS_2) ने ऑप्टोइलेक्ट्रॉनिक्स में अपने संभावित अनुप्रयोगों के कारण बहुत ध्यान आकर्षित किया है। MoO_3 और बल्क MoS_2 क्रमशः 3.2 और 1.2 eV के बैंड गैप वाले अर्धचालक हैं, और रिक्तियों, अंतरालीय, एंटी-साइट दोष आदि जैसे आंतरिक दोषों के कारण उच्च क्यूरी तापमान के साथ साधारण तापमान पर फेरोमैग्नेटिज्म दिखाते हैं। MoO_3 के मामले में, प्रेरित चुंबकत्व के पीछे प्राथमिक कारण ऑक्सीजन रिक्तियाँ और रिक्ति समूह हैं। हाइड्रोजन परिवेश में MoO_3 के पोस्ट-ट्रीटमेंट के बाद H_xMoO_3 का निर्माण भी फेरोमैग्नेटिज्म को प्रेरित करने का एक और दिलचस्प कारण है। MoS_2 के मामले में, S-रिक्ति के अलावा, एज-टर्मिनेटेड संरचना भी फेरोमैग्नेटिज्म को प्रेरित करने में बल्क की तुलना में अलग समन्वय ज्यामिति के कारण एक महत्वपूर्ण भूमिका निभाती है। हाइड्रोजन पोस्ट-ट्रीटमेंट के बाद MoS_2 लैटिस में S-H बंध का निर्माण भी संतृप्ति चुंबकत्व मूल्य को बढ़ाता है। इन सामग्रियों का उपयोग करके साधारण तापमान पर फेरोमैग्नेट का उत्पादन स्पिनट्रॉनिक्स के अनुप्रयोगों को महत्वपूर्ण रूप से प्रभावित करेगा। भविष्य के ऑप्टोइलेक्ट्रॉनिक, स्पिनट्रॉनिक और ऑप्टो-स्पिनट्रॉनिक उपकरणों को इन अर्धचालक सामग्रियों से लाभ हो सकता है, जो फेरोमैग्नेटिक धातुओं और अर्धचालक जंक्शनों के विकल्प हैं। मुख्य मुद्दे हैं: (i) MoO_3 और MoS_2 में संतृप्ति चुंबकत्व मूल्य का रिपोर्ट किया गया मूल्य स्पिनट्रॉनिक्स अनुप्रयोगों में उपयोग के लिए बहुत कम है; (ii) MoO_3 के साथ हाइड्रोजन की परस्पर क्रिया के कारण, अधिक संख्या में ऑक्सीजन रिक्तियों और रिक्ति समूहों और H_xMoO_3 गठन का निर्माण

अपेक्षित है और इसकी जांच की जानी चाहिए; (iii) विभिन्न आकारिकी MoS_2 पतली फिल्मों के CVD विकास और साधारण तापमान के फेरोमैग्नेटिज्म के संगत समंजन की जांच की जानी चाहिए; (iv) विभिन्न प्रकार के पोस्ट-ट्रीटमेंट जैसे कम ऊर्जा आयन विकिरण और एनीलिंग के बाद s-रिक्ति और एज-टर्मिनेटेड संरचना की संख्या को नियंत्रित करके MoS_2 में समंजस्य फेरोमैग्नेटिज्म की आवश्यकता है; (v) नैनो-आयामी MoS_2 पतली फिल्मों में फेरोमैग्नेटिज्म को अत्यधिक बढ़ाने के लिए एज-टर्मिनेटेड संरचना और s-रिक्ति की भूमिका की जांच की जानी चाहिए। गहन प्रयोगात्मक और सैद्धांतिक अनुसंधान के माध्यम से इन बुनियादी मुद्दों को समझने की प्रेरणा वर्तमान थीसिस का स्रोत है। परिणामस्वरूप, इस थीसिस के मुख्य उद्देश्य हैं (i) MoO_3 गुच्छों में फेरोमैग्नेटिक व्यवहार पर हाइड्रोजन एनीलिंग और संबंधित ऑक्सीजन रिक्तियों के प्रभाव का अध्ययन करना; (ii) MoS_2 में चुंबकीय गुणों पर आकृति विज्ञान (नैनोफ्लॉवर, ऊर्ध्वाधर नैनोशीट, क्षेत्रीय नैनोशीट और पतली फिल्म) के प्रभाव का अध्ययन करना; (iii) ऊर्ध्वाधर नैनो संरचना MoS_2 के फेरोमैग्नेटिक व्यवहार पर कम ऊर्जा वाले तुलनात्मक रूप से भारी (Ar और Xe) और हल्के (हाइड्रोजन) द्रव्यमान आयनों और हाइड्रोजन एनीलिंग के विकिरण के प्रभाव का अध्ययन करना; (iv) MoS_2 के नैनो-आयामी त्रिकोणीय गुच्छों के फेरोमैग्नेटिक व्यवहार पर कम ऊर्जा वाले Ar आयन विकिरण के प्रभाव का अध्ययन करना। नमूने रासायनिक वाष्प जमाव तकनीक द्वारा तैयार किए जाते हैं और एक्स-रे विवर्तन (XRD), रमन स्पेक्ट्रोस्कोपी, परमाणु बल माइक्रोस्कोपी (AFM), फोटोल्यूमिनेसेंस (PL), फील्ड-एमिशन स्कैनिंग इलेक्ट्रॉन माइक्रोस्कोपी (FESEM), इलेक्ट्रॉन जांच माइक्रो एनालाइजर (EPMA), रदरफोर्ड बैकस्कैटरिंग स्पेक्ट्रोमेट्री (RBS), ट्रांसमिशन इलेक्ट्रॉन माइक्रोस्कोपी (TEM), और एक्स-रे फोटोइलेक्ट्रॉन स्पेक्ट्रोस्कोपी (XPS) द्वारा उनकी विशेषताओं का पता लगाया जाता है। MPMS3 मैग्नेटोमीटर का उपयोग करके सभी नमूनों के लिए चुंबकीय गुण माप किए जाते हैं। चुंबकीय गुणों, इलेक्ट्रॉनिक संरचना और DFT-आधारित सैद्धांतिक गणनाओं के बीच संबंध यहाँ स्थापित किया गया है।

परिचय और प्रायोगिक विवरण अध्यायों के बाद, थीसिस का तीसरा अध्याय विभिन्न तापमानों पर H_2 -एनीलड CVD-ग्रोन MoO_3 नमूनों में RTFM की जांच है। EPMA और PL मापों द्वारा ऑक्सीजन रिक्तियों की उपस्थिति का विश्लेषण किया गया है। H_2 -एनीलड नमूनों में संतृप्ति चुंबकत्व मूल्य में वृद्धि मोटे तौर पर इसकी इलेक्ट्रॉनिक संरचना और DFT-आधारित सैद्धांतिक गणनाओं के साथ सहसंबंधित है। वर्तमान थीसिस के अगले अध्याय में MoS_2 पतली फिल्मों में आकृति विज्ञान-नियंत्रित RTFM शामिल है। MoS_2 पतली फिल्मों को CVD तकनीक द्वारा चार अलग-अलग आकृति विज्ञानों, जैसे नैनोफ्लॉवर, ऊर्ध्वाधर नैनोशीट, क्षेत्रीय नैनोशीट और पतली फिल्म के साथ उगाया जाता है। प्रेरित चुंबकत्व के पीछे मुख्य कारण मुख्य रूप से s-रिक्ति के साथ एज-टर्मिनेटेड संरचना है, क्योंकि उच्चतम संतृप्ति चुंबकत्व मूल्य नमूने में

देखा जाता है, जिसमें एज-टर्मिनेटेड संरचनाओं (यहाँ ऊर्ध्वाधर नैनोशीट) की सबसे अधिक संख्या होती है। प्रेरित चुंबकत्व के पीछे का कारण इन नमूनों की इलेक्ट्रॉनिक संरचना के साथ सहसंबंधित है। अगला अध्याय दो भागों में विभाजित है। इस अध्याय में ऊर्ध्वाधर नैनोशीट-उन्मुख MoS_2 पतली फिल्मों में फेरोमैग्नेटिज्म को प्रेरित करने में एज-टर्मिनेटेड संरचनाओं और S-रिक्तियों के सहक्रियात्मक प्रभाव को विस्तार से समझाया गया है। पहले भाग में, ऊर्ध्वाधर नैनो संरचना MoS_2 की संरचना को संशोधित करने और चुंबकीय गुणों को समायोजित करने के लिए अलग-अलग प्रवाह (आयन/सेमी²) और कम ऊर्जा वाले Ar और Xe आयनों के साथ विकिरणित किया जाता है। शुद्ध नमूना नमूने में एज टर्मिनेशन वाली ऊर्ध्वाधर नैनोशीट की जांच फील्ड एमिशन स्कैनिंग इलेक्ट्रॉन माइक्रोस्कोपी (FESEM) द्वारा की गई है। कम ऊर्जा वाले Ar^+ और Xe^+ विकिरणित नमूनों में ऊर्ध्वाधर नैनोशीट की गिरावट देखी गई है। एज-ओरिएंटेड नैनो संरचनाशुद्ध नमूना MoS_2 पतली फिल्मों के लिए 1.7 emu/g का एक सराहनीय उच्च चुंबकत्व मूल्य देखा गया, और आयन विकिरण के बाद यह कम हो गया। एक्स-रे फोटोइलेक्ट्रॉन स्पेक्ट्रोस्कोपी (एक्सपीएस) आंकड़े से, यह स्पष्ट है कि, S रिक्ति साइटों में ऑक्सीजन के समावेश के कारण, आयन विकिरण के बाद Mo 5+ और 6+ अवस्थाएँ बढ़ जाती हैं। ऊर्ध्वाधर नैनोशीट के प्रिज्मीय किनारों के किनारे-उन्मुख स्पिन मुख्य रूप से शुद्ध नमूना फिल्म में उच्च चुंबकीय क्षण के लिए जिम्मेदार हैं, और विकिरण पर ऑक्सीजन के समावेश द्वारा सल्फर रिक्तियों में किनारे की गिरावट और कमी के परिणामस्वरूप चुंबकीय क्षण में कमी आती है।

दूसरे भाग में, नैनो संरचना MoS_2 पतली फिल्मों को अलग-अलग प्रवाह के साथ कम ऊर्जा वाले हाइड्रोजन आयनों के साथ विकिरणित किया जाता है और दोष पैदा करने और फेरोमैग्नेटिज्म को बढ़ाने के लिए स्वतंत्र रूप से अलग-अलग तापमानों पर हाइड्रोजन वातावरण में एनील किया जाता है। नैनो संरचनाशुद्ध नमूना MoS_2 पतली फिल्में एक शुद्ध 2-H MoS_2 चरण का गठन दिखाती हैं, जिसकी पुष्टि एक्स-रे विवर्तन (XRD) और रमन स्पेक्ट्रोस्कोपी द्वारा की गई है। 200°C के तापमान पर हाइड्रोजन एनीलिंग साधारण तापमान पर 2.7 emu/g का अधिकतम संतृप्ति चुंबकत्व मूल्य प्रदर्शित करता है। फेरोमैग्नेटिज्म में वृद्धि सल्फर रिक्तियों में वृद्धि, सल्फर के साथ हाइड्रोजन सोखने और किनारों में संशोधन के कारण होती है, जिसकी पुष्टि इलेक्ट्रॉन जांच माइक्रो-विश्लेषक (EPMA), एक्स-रे फोटोइलेक्ट्रॉन स्पेक्ट्रोस्कोपी (XPS), और फील्ड एमिशन स्कैनिंग इलेक्ट्रॉन माइक्रोस्कोपी (FESEM) माप के विश्लेषण से होती है। दोनों मामलों के लिए, DFT-आधारित सैद्धांतिक गणना प्रयोगात्मक निष्कर्षों के अनुरूप है।

अंतिम अध्याय में, नैनो-आयामी त्रिकोणीय गुच्छे-उन्मुख CVD-उगाए गए MoS_2 पतली फिल्मों (20 एनएम) को कम ऊर्जा वाले Ar आयन विकिरण के साथ विकिरणित किया जाता है। इसके पीछे सबसे

महत्वपूर्ण कारकों में से एक एज-टर्मिनेटेड संरचना का निर्माण और संशोधन है, जो लटकते हुए बंधन और मुक्त स्पिन प्रदान करता है। एक अन्य कारक S रिक्तियों की संख्या में वृद्धि है, जिसकी पुष्टि XPS और RBS विश्लेषण द्वारा की जाती है। थीसिस किए गए कार्य के सारांश और क्षेत्र में काम के भविष्य के दायरे के साथ समाप्त होती है।

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NOMENCLATURE

Ar :	Argon
AFM :	Atomic force microscopy
B.E. :	Binding energy
BMP :	Bound magnetic polaron
CVD :	Chemical vapour deposition
CCD :	Charge coupled device
DOS :	Density of states
DMS :	Diluted magnetic semiconductor
DFT :	Density functional theory
EPMA :	Electron probe microanalyzer
ECR :	Electron cyclotron resonance
FWHM :	Full width at half maximum
FESEM :	Field emission scanning electron microscopy
GIXRD :	Glancing incidence x-ray diffraction
GMR :	Giant magneto-resistance
GGA :	Generalized gradient approximation
H :	Hydrogen
IC :	Integrated circuit
LEII :	Low energy ion irradiation
PBE :	Perdew-Burke-Ernzerhof
PAW :	Projected augmented wave
PVD :	Physical vapour deposition
PL :	Photoluminescence
RBS :	Rutherford backscattering spectrometry
RTFM :	Room temperature ferromagnetism
SQUID :	Super conducting quantum interference device
SAED :	Selected area electron diffraction
SRIM :	Stopping and range of ions in matter
TEM :	Transmission electron microscopy
TMS :	Transparent magnetic semiconductor
TMR :	Tunnelling magnetoresistance

2D :	Two dimensional
TMD :	Transition metal dichalcogenides
TRIM :	Transport of ions in matter
S _n :	Nuclear energy loss
V _s :	Sulfur vacancy
V _{Mo} :	Molybdenum vacancy
WDS :	Wavelength dispersive spectroscopy
Xe :	Xenon
XPS :	X-ray photoelectron spectroscopy
XRD :	X-ray diffraction
ZFC :	Zero field cooled
FC :	Field cooled