INVESTIGATING THE ROLE OF SULFUR VACANCY AND MORPHOLOGY IN MODULATING THE OPTOELECTRONIC, FERROELECTRIC, AND NANOTRIBOLOGICAL PROPERTIES OF CVD GROWN ReS_2

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DEPARTMENT OF PHYSICS

INDIAN INSTITUTE OF TECHNOLOGY DELHI

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by

SAKSHI

DEPARTMENT OF PHYSICS

Submitted

in fulfilment of requirements of degree of Doctor of Philosophy

to the



INDIAN INSTITUTE OF TECHNOLOGY DELHI

July 2026

Dedicated to my mother

DECLARATION

I hereby declare that:

1. The work presented in this thesis is original and has been carried out by me as a student of IIT Delhi.

2. To the best of my knowledge, the work presented in this thesis has not been submitted, either in whole or in part, to any other institution for the award of any degree or diploma.

3. I have adhered to the guidelines prescribed by the Institute for thesis preparation.

4. I have complied with the provisions of the Institute's Honor Code and have neither engaged in nor tolerated any form of academic dishonesty, including plagiarism, intentional data fabrication, data falsification, data misrepresentation, or unauthorized collaboration beyond that permitted by the Student Research Committee, as defined and approved by the Institute.

5. I take full responsibility for all data presented in this thesis and confirm that no data has been collected without appropriate permission. Where required, ethical approval has been obtained for the research, and all relevant approvals and documentation have been included as part of the thesis submission.

6. All sources of information, including data, ideas, and text, have been duly acknowledged and appropriately cited in the thesis.

7. The use of artificial intelligence (AI) tools (if any), including large language models, has been appropriately disclosed. All analysis interpretations, and conclusions presented in this thesis are my own. Alternatively, I declare that no AI tools, including large language models, have been used in the preparation of this thesis.

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Date: 14th July 2026

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This is to certify that the thesis entitled **"Investigating the Role of Sulfur Vacancy and Morphology in Modulating the Optoelectronic, Ferroelectric and Nanotribological Properties of CVD Grown ReS_2"** being submitted by **Ms. Sakshi** to the **Indian Institute of Technology Delhi, India** for the award of the degree of **Doctor of Philosophy** is a record of bonafide research work carried out by her. She has worked under my guidance and supervision and has fulfilled the requirements, which to my knowledge have reached the requisite standard for the submission of the thesis.

The results contained in this thesis have not been submitted in part or full to any other University or Institute for the award of any degree or diploma.

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Date:

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यत्र योगेश्वरः कृष्णो यत्र पार्थो धनुर्धरः ।

तत्र श्रीर्विजयो भूतिर्ध्रुवा नीतिर्मतिर्मम ॥ ७८ ॥

(Where wisdom guides and dedication persist, success inevitably follows)

Sakshi

Abstract

The increasing demand for high-performance, miniaturized optoelectronic devices has exposed fundamental limitations of bulk silicon at the nanoscale, including short-channel effects, quantum tunnelling, reduced gate controllability, elevated power consumption, and significant heat dissipation. These constraints challenge the continued scaling of semiconductor technologies in accordance with Moore's Law. Consequently, there is a need for alternative channel materials that offer ultrashort dimensions, low power consumption, reduced frictional losses, and cost-effective, large-area production. Two-dimensional (2D) transition metal dichalcogenides (TMDCs) have emerged as promising candidates due to their van der Waals layer structure, large surface-to-volume ratio, tunable direct bandgap, high carrier mobility, and strong light-matter interactions that surpass those of bulk materials. This thesis examines the synthesis, characterization, and device applications of rhenium disulfide (ReS_2), a group VII 2D material film synthesized via chemical vapour deposition (CVD).

The growth of ReS_2 film was optimized on SiO_2/Si, sapphire, and mica substrates. Variation in growth conditions enabled the formation of distinct morphologies, including planar, bulk, and flower-like films on SiO_2/Si substrates. The mica microreactor facilitated centimetre-scale growth of monolayer and bilayer films, while bulk growth was achieved on sapphire substrates. Characterization of the as-grown films using Raman spectroscopy, photoluminescence (PL), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), and high-resolution transmission electron microscopy (HRTEM) confirmed the formation of the distorted 1T' phase of ReS_2. This low-symmetry crystal structure challenges established paradigms for hexagonal TMDCs and gives rise to several unconventional physical properties, including layer-independent direct electronic band gaps, highly anisotropic charge transport, atypical excitonic behaviour, emergent ferroelectricity, and exceptional nanotribological performance.

A metal-semiconductor-metal photodetector device was fabricated on a ReS_2 film grown on a SiO_2/Si substrate. Typically, photocurrent increases upon illumination; however, in this case, the current decreases below the dark current, a phenomenon known as negative photoconductivity (NPC). This anomalous behaviour is attributed to charge entrapment induced by trion and sulfur vacancies. The charge imbalance caused by trions shifts the photocurrent toward negative bias, while sulfur vacancies act as traps, leading to a prolonged time response. Density functional theory (DFT) bandgap and density of states (DOS) calculations further support this explanation, indicating the formation of mid-gap states as sulfur vacancy concentration increases. Annealing the film in a sulfur environment passivates the sulfur vacancies, thus disrupting trion formation and eliminating the observed NPC.

The increasing use of 2D materials in space environments, where exposure to highly energetic radiation, such as γ-rays, electrons, and proton beams, is common, necessitates evaluating their stability under these conditions. To address this, ReS_2 films grown on sapphire were irradiated with high-energy electrons, and the effects were analyzed. Raman and XRD spectra indicate that the material's phase remains intact, although crystallinity is reduced. Electron beam exposure disrupts the Re-S bond, resulting in sulfur removal from lattice sites and subsequent accumulation on the surface. The introduction of sulfur vacancies induces n-type behaviour, as demonstrated by increased current following irradiation, while sulfur accumulation at the surface leads to an increased refractive index. Density functional theory (DFT) calculations of sulfur vacancy formation energy support the conclusion that sulfur vacancies are the most probable defects formed after irradiation.

The pursuit of ultra-low-power nonvolatile memory and ongoing device miniaturization has intensified research into 2D quantum materials that exhibit ferroelectricity. Vacancies not only influence carrier concentration and optical properties but also act as symmetry-breaking centers, potentially enabling polar distortions that are otherwise forbidden in the pristine lattice. A systematic investigation using piezo response force microscopy and DFT

calculations reveals defect-induced bistable states, confirming ferroelectricity. Additionally, friction in mechanical systems accounts for approximately 23% of global energy consumption. ReS_2, characterized by low interlayer binding energy due to its 1T' phase, exhibits a significantly lower coefficient of friction compared to 2H phase 2D materials. Analysis of the nanotribological properties of films with varying morphologies demonstrates that friction can be tuned by adjusting thickness and morphology. Experimental results, interpreted using an analytical model, elucidate the underlying friction mechanisms and provide fundamental insights into the nanotribological behaviour of ReS_2, supporting its potential applications in space tribology and in advanced NEMS and MEMS devices.

In summary, this thesis presents a comprehensive study of CVD-grown 1T' phase ReS_2 films, with particular emphasis on the effects of sulfur vacancy engineering on optoelectronic and ferroelectric properties, as well as the influence of growth morphology on nanotribological behaviour.

सार

उच्च-प्रदर्शन, सूक्ष्मीकृत ऑप्टोइलेक्ट्रॉनिक उपकरणों की बढ़ती मांग ने नैनोस्तर पर बल्क सिलिकॉन की मूलभूत सीमाओं को उजागर किया है, जिनमें शॉर्ट-चैनल प्रभाव, क्वांटम टनलिंग, गेट नियंत्रण में कमी, अधिक विद्युत-शक्ति खपत तथा अत्यधिक ऊष्मा अपव्यय शामिल हैं। ये बाधाएँ मूर के नियम के अनुरूप अर्धचालक प्रौद्योगिकी के सतत लघुकरण को चुनौती देती हैं। अतः ऐसे वैकल्पिक चैनल पदार्थों की आवश्यकता है जो अति-सूक्ष्म आयाम, कम शक्ति खपत, कम घर्षण हानि तथा कम लागत पर बड़े क्षेत्र में निर्माण की सुविधा प्रदान करें। द्वि-आयामी (2D) ट्रांजिशन मेटल डाइचैल्कोजेनाइड्स (TMDCs) अपनी वैन डर वाल्स परतदार संरचना, उच्च सतह-से-आयतन अनुपात, समायोज्य प्रत्यक्ष बैंडगैप, उच्च वाहक गतिशीलता तथा बल्क पदार्थों की तुलना में अधिक प्रबल प्रकाश–पदार्थ अंतःक्रिया के कारण आशाजनक विकल्प के रूप में उभरे हैं। यह शोध-प्रबंध रासायनिक वाष्प निक्षेपण (CVD) द्वारा संश्लेषित समूह VII के द्वि-आयामी पदार्थ रेनियम डाइसल्फाइड (ReS_2) पतली परतों के संश्लेषण, अभिलक्षणन तथा उपकरण अनुप्रयोगों का अध्ययन प्रस्तुत करता है।

ReS_2 का विकास SiO_2/Si, नीलम (sapphire), और माइका सब्सट्रेट्स पर अनुकूलित किया गया। विकास स्थितियों में परिवर्तन ने SiO_2/Si सब्सट्रेट्स पर समतलीय, बल्क तथा पुष्पाकार संरचनाओं वाली विभिन्न आकृतियाँ प्राप्त हुईं। माइका माइक्रोरिएक्टर ने एकल-परत और द्वि-परत फिल्मों का सेंटीमीटर-स्केल विकास सुगम किया, जबकि नीलम सब्सट्रेट्स पर बल्क विकास प्राप्त किया गया। विकसित फिल्मों का रमन स्पेक्ट्रोस्कोपी, फोटोल्यूमिनेसेंस (PL), एक्स-रे फोटोइलेक्ट्रॉन स्पेक्ट्रोस्कोपी (XPS), एक्स-रे विवर्तन (XRD), फील्ड एमिशन स्कैनिंग इलेक्ट्रॉन माइक्रोस्कोपी (FESEM) तथा उच्च-रिज़ॉल्यूशन ट्रांसमिशन इलेक्ट्रॉन माइक्रोस्कोपी (HRTEM) द्वारा अभिलक्षणन किया गया, जिससे ReS_2 की विकृत 1T' अवस्था की पुष्टि हुई। यह निम्न-सममिति क्रिस्टलीय संरचना षट्कोणीय TMDCs के स्थापित प्रतिमानों को चुनौती देती है और कई असामान्य भौतिक गुण उत्पन्न करती है, जैसे परत-स्वतंत्र प्रत्यक्ष इलेक्ट्रॉनिक बैंडगैप, अत्यधिक अनैसोट्रॉपिक आवेश परिवहन, असामान्य एक्साइटॉन व्यवहार, उद्भूत फेरोइलेक्ट्रिसिटी तथा उत्कृष्ट नैनोट्राइबोलॉजिकल प्रदर्शन।

SiO_2/Si सब्सट्रेट पर उगाई गई ReS_2 फिल्म पर मेटल–सेमीकंडक्टर–मेटल फोटोडिटेक्टर उपकरण निर्मित किया गया। सामान्यतः प्रकाश पड़ने पर फोटोकरेन्ट बढ़ता है, किंतु यहाँ धारा अंधकार धारा से भी कम हो जाती है, जिसे ऋणात्मक फोटोकंडक्टिविटी (NPC) कहा जाता है। यह असामान्य व्यवहार ट्रायॉन तथा सल्फर रिक्तियों द्वारा उत्पन्न आवेश फँसाव के कारण है। ट्रायॉन से उत्पन्न आवेश असंतुलन

फोटोकरेन्ट को ऋणात्मक बायस की ओर स्थानांतरित करता है, जबकि सल्फर रिक्तियाँ ट्रैप के रूप में कार्य कर समय प्रतिक्रिया को लंबा कर देती हैं। घनत्व क्रियात्मक सिद्धांत (DFT) द्वारा बैंडगैप एवं अवस्थाओं के घनत्व (DOS) की गणनाएँ इस व्याख्या का समर्थन करती हैं और दर्शाती हैं कि सल्फर रिक्तियों की सांद्रता बढ़ने पर मध्य-बैंड अवस्थाएँ निर्मित होती हैं। सल्फर वातावरण में फिल्म का एनीलिंग करने से ट्रायॉन निर्माण बाधित होता है और देखी गई NPC समाप्त हो जाती है।

अंतरिक्ष वातावरण में, जहाँ गामा किरणें, इलेक्ट्रॉन तथा प्रोटॉन किरण-पुंज जैसी उच्च-ऊर्जा विकिरण सामान्य हैं, 2D पदार्थों के बढ़ते उपयोग के कारण उनकी स्थिरता का मूल्यांकन आवश्यक हो गया है। इस उद्देश्य से सैफायर पर उगाई गई ReS_2 फिल्मों को उच्च-ऊर्जा इलेक्ट्रॉनों से विकिरणित किया गया तथा उसके प्रभावों का विश्लेषण किया गया। रमन और XRD स्पेक्ट्रा दर्शाते हैं कि पदार्थ की अवस्था यथावत रहती है, यद्यपि क्रिस्टलीयता में कमी आती है। इलेक्ट्रॉन किरण Re–S बंध को बाधित करती है, जिससे सल्फर जालिका स्थलों से हटकर सतह पर एकत्रित हो जाता है। सल्फर रिक्तियों के प्रवेश से n-प्रकार का व्यवहार उत्पन्न होता है, जो विकिरण के बाद धारा में वृद्धि से स्पष्ट है, जबकि सतह पर सल्फर संचय अपवर्तनांक में वृद्धि का कारण बनता है। DFT द्वारा सल्फर रिक्ति निर्माण ऊर्जा की गणनाएँ यह पुष्टि करती हैं कि विकिरण के पश्चात बनने वाले दोषों में सल्फर रिक्तियाँ सर्वाधिक संभावित हैं।

अत्यंत कम शक्ति वाली नॉन-वोलेटाइल मेमोरी तथा उपकरणों के निरंतर लघुकरण की दिशा में शोध ने उन 2D क्वांटम पदार्थों में रुचि बढ़ाई है जो फेरोइलेक्ट्रिसिटी प्रदर्शित करते हैं। रिक्तियाँ न केवल वाहक सांद्रता और प्रकाशीय गुणों को प्रभावित करती हैं, बल्कि सममिति-भंग केंद्र के रूप में कार्य कर ध्रुवीय विकृतियों को संभव बना सकती हैं, जो शुद्ध जालिका में वर्जित होती हैं। पीजो-रिस्पॉन्स फोर्स माइक्रोस्कोपी तथा DFT गणनाओं के माध्यम से व्यवस्थित अध्ययन ने दोष-प्रेरित द्विस्थिर अवस्थाओं का अनावरण किया, जिससे फेरोइलेक्ट्रिसिटी की पुष्टि हुई। इसके अतिरिक्त, यांत्रिक प्रणालियों में घर्षण वैश्विक ऊर्जा खपत का लगभग 23% भाग है। 1T' अवस्था के कारण कम अंतर-परत बंधन ऊर्जा वाले ReS_2 में 2H अवस्था वाले 2D पदार्थों की तुलना में घर्षण गुणांक उल्लेखनीय रूप से कम पाया गया। विभिन्न आकृतियों वाली फिल्मों के नैनोट्राइबोलॉजिकल गुणों के विश्लेषण से स्पष्ट हुआ कि मोटाई और संरचना में परिवर्तन द्वारा घर्षण को नियंत्रित किया जा सकता है। प्रायोगिक परिणामों को विश्लेषणात्मक मॉडल के माध्यम से समझाया गया, जिससे ReS_2 के नैनोट्राइबोलॉजिकल व्यवहार की मूलभूत समझ प्राप्त हुई और अंतरिक्ष ट्राइबोलॉजी तथा उन्नत NEMS और MEMS उपकरणों में इसके संभावित अनुप्रयोगों का समर्थन मिला।

सार रूप में, यह शोध-प्रबंध CVD द्वारा विकसित 1T' अवस्था की ReS_2 फिल्मों का व्यापक अध्ययन प्रस्तुत करता है, जिसमें विशेष रूप से सल्फर रिक्ति अभियांत्रिकी के ऑप्टोइलेक्ट्रॉनिक एवं फेरोइलेक्ट्रिक गुणों पर प्रभाव तथा वृद्धि आकृति-विज्ञान के नैनोट्राइबोलॉजिकल व्यवहार पर प्रभाव को रेखांकित किया गया है।

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List of Abbreviations

2D	Two-dimensional
3D	Three-dimensional
AFM	Atomic force microscopy
APCVD	Atmospheric Pressure Chemical Vapor Deposition
ASMD	Advance Semiconductor Material and Device Lab
BF	Bright Field
BG	Bulk Growth
BL	Bilayer
BN	Boron Nitride
BSE	Back Scattered Electron
CB	Conduction Band
CBM	Conduction Band Minima
CCD	Charge Coupled Device
COF	Coefficient of Friction
CPD	Contact Potential Difference
CRF	Central Research Facility
CVD	Chemical Vapor Deposition
DC	Direct Current
DF	Dark Field
DFT	Density Functional Theory
DOS	Density of Stated
EDX	Energy Dispersive X-ray
FESEM	Field Emission Secondary Electron Microscope
FET	Field Effect Transistor
FFM	Frictional Force Microscopy
FG	Flower Growth
FWHM	Full Width at Half Maxima

GGA	Generalized Gradient Approximation
HAADF	High Angle Annular Dark Field
HOPG	Highly Oriented Pyrolytic Graphite
HRTEM	High Resolution Transmission Electron Microscope
IBE	Interlayer Binding Energy
IDE	Inter Digitated Electrode
KOH	Potassium Hydroxide
KPFM	Kelvin Probe Force Microscopy
LFM	Lateral Force Microscopy
MBE	Molecular Beam Epitaxy
MEMS	Micro Electro Mechanical System
MFC	Mass Flow Controller
MSM	Metal Semiconductor Metal
NEMS	Nano Electro Mechanical System
NIR	Near Infra-red
NPC	Negative Photoconductivity
OM	Optical Microscope
PAW	Projector Augmented Wave
PBE	Perdew Burke Ernzerhof
PF	Planar Film
PFM	Piezo-response Force Microscopy
PID	Proportional Integral Derivative
PL	Photoluminescence
PLD	Pulsed Laser Deposition
PVD	Physical Vapor Deposition
RF	Radio Frequency
RMS	Root Mean Square
RPM	Revolution Per Minute
SAED	Selected Area Electron Diffraction

SCF	Self Consistent Field
SCS	Semiconductor Characterization System
SIMS	Secondary Ion Mass Spectroscopy
SPM	Scanning Probe Microscopy
STEM	Scanning Transmission Electron Microscopy
TMDC	Transition Metal Dichalcogenide
TOF	Time of Flight
UHV	Ultra High Vacuum
UV	Ultra Violet
VB	Valence Band
VBM	Valence Band Minima
XPS	X-ray Photoelectron Spectroscopy
XRD	X-ray Diffraction