"Knowing yourself is the beginning of all wisdom"

Aristotle

Declaration

I, *Mayuri Bora*, hereby declare that this thesis entitled "*Proximity induced spin related phenomena in 2D heterostructure*", in partial fulfillment of the requirements for the award of the degree of Doctor of Philosophy in Physics and submitted to School of Sciences, Tezpur University, Tezpur is an authentic record of my own work carried out during Ph.D. tenure under the supervision of Prof. Pritam Deb. The matter embodied in this thesis is an original work and have not been previously submitted for the award of any other degree of this or any other University/Institute.

Place: _____

(Mayuri Bora)

Date:

CERTIFICATE OF THE PRINCIPAL SUPERVISOR

TEZPUR UNIVERSITY

This is to certify that the thesis entitled ***"Proximity induced spin related phenomena in 2D heterostructure"*** submitted to the School of Sciences, Tezpur University in partial fulfillment for the award of the degree of Doctor of Philosophy in Physics, is a record of research work carried out by **Ms. Mayuri Bora** under my supervision and guidance.

All help received by her from various sources have been duly acknowledged. No part of this thesis has been submitted elsewhere for award of any other degree.

Date:

Place:

_____

(Principal Supervisor)

Pritam Deb

Professor, Department of Physics

School of Sciences, Tezpur University

CERTIFICATE OF THE EXTERNAL EXAMINER AND ODEC

TEZPUR UNIVERSITY

This is to certify that the thesis entitled ***"Proximity induced spin related phenomena in 2D heterostructure"*** submitted to the School of Sciences, Tezpur University in partial fulfillment for the award of the degree of Doctor of Philosophy in Physics, is a record of research work carried out by **Ms. Mayuri Bora** under my supervision and guidance.

The committee recommends for the award of the degree of Doctor of Philosophy.

Signatures:

Principal Supervisor **External Examiner**

Date: **Date:**

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Date:

Place: **(Mayuri Bora)**

Dedicated to my Beloved Parents

Bharat Chandra Bora

&

Dipali Bora

List of Figures

Nomenclatures

Parameters	Names
Å	Angstrom, atomic scale unit
DFT++	DFT Correction term
DFT+U	DFT correction term with potential parameter
E_X	Exchange energy
E_C	Correlation energy
$\hat{E}$	Total energy
E_{TF}	TF energy term
E_{XC}	Exchange-correlation energy
E^{GGA}	Energy term from GGA approach
E^{LDA}	LDA energy term
n(r)	Density of states
GW	Approximation to self-energy
Gr	Graphene
E^{nl}	Nonlocal correlation energy
E_F	Fermi energy
$\hat{T}$	Kinetic energy of the system
$\hat{U}_{en}$	Potential energy due to electron-nuclei interaction
$\hat{U}_{ee}$	Potential energy due to electron-electron interaction
X_C	Exchange-correlation
n_e	Number of electrons
n_h	Number of holes
vdW-DF	van der Waals correction by Grimme
C_v	Valley Chern number
$CrBr_3$	Chromium tribromide
$\hat{H}_{eff}$	Effective Hamiltonian
C_v	Valley Chern number
ZTe	Electronic Figure of merit
$NbSe_2$	Niobium Diselenide
WTe_2	Tungsten Ditelluride
σS^2	Power Factor
$\tau(E)$	Relaxation time
S_{xx}	Seebeck coefficient
S_{xy}	Anomalous Nernst thermopower
σ	Electrical conductivity
κ_e	Electronic thermal conductivity
T_C	Curie Temperature
P	Spin-polarization parameter
$\delta\rho$	Electrostatic Charge density
μ	Chemical potential

Abbreviations	Names
2D	Two-dimension
3D	Three-dimension
vdW	van der Waals
GQD	Graphene quantum dots
h-BN	Hexagonal Boron nitride
MPE	Magnetic proximity effect
QMC	Quantum Monte Carlo
DFT	Density Functional Theory
WTBH	Wannier tight binding Hamiltonian
SOI	Spin-orbit Interaction
TMDs	Transition metal Dichalcogenides
DOS	Density of states
SOC	Spin-orbit coupling
AHE	Anomalous Hall effect
YIG	Yttrium Iron garnet
BFO	Bismuth Ferrite ($BiFeO_3$)
QAHE	Quantum Anomalous Hall effect
HK	Hohenberg-Kohn
KS	Kohn-Sham
GGA	Generalized Gradient Approximation
LDA	Local Density Approximation
PAW	Projector Augmented Wave
QE	Quantum Espresso
PP	Pseudopotential
BOA	Born-Oppenheimer Approximation
TF	Thomas-Fermi
HEG	Homogeneous Electron Gas
GEA	Gradient expansion approximation
PBE	Perdew, Burke, Ernzerhof
NCPP	Norm-Conserving Pseudopotential
USPP	Ultrasoft Pseudopotential
HSC	Hamann, Schluter, Chiang
LAPW	Linear augmented plane wave
PS	Pseudo
DFPT	Density functional perturbation theory
RPA	Random Phase approximation
ACFDT	Adiabatic connection-fluctuation dissipation theorem
AIM	Anderson impurity model
TB	Tight-binding
WF	Wannier functions
MLWF	Maximally localized Wannier functions
NEGF	Non-equilibrium Green's function

BFGS	Broyden-Fletcher-Goldfarb-Shanno
PDOS	Partial density of states
SG-FET	Single-gate Field-effect transistor
TRS	Time reversal symmetry
QVH	Quantum Valley Hall
AFM	Antiferromagnetic
FM	Ferromagnetic
TI	Topological Insulator
HSE06	Hybrid functional
VASP	Vienna *ab initio* simulation package
CBM	Conduction band minimum
VBM	Valence band maximum
WCC	Wannier Charge Center
AHC	Anomalous Hall conductivity
SE	Seebeck effect
TE	Thermoelectric effect
TEG	Thermoelectric power generation
ANE	Anomalous Nernst effect
GNM	Graphene nanomesh
PF	Power factor
IDOS	Integrated density of states
BTE	Boltzmann Transport equation
CRTA	Constant relaxation time approximation
TDF	Transport distribution function
CDD	Charge density difference
WSM	Weyl Semimetal