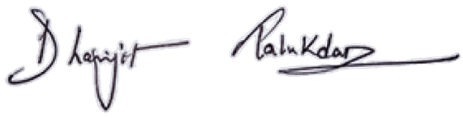
Dedicated to my
parents & my brother

Declaration by the Candidate

I, **Dhanjit Talukdar**, declare that the thesis entitled **"Investigation of electronic, optical, and surface adsorption properties in engineered black phosphorene and its isostructural tin sulfide systems"** is a record of my own work carried out under the supervision of **Prof. Gazi Ameen Ahmed** during the period from October, 2021 to May, 2025. I confirm that:

- This work was done wholly or mainly while in candidature for a research degree in Doctor of Philosophy at Tezpur University where no part of this thesis has previously been submitted for a degree or any other qualification at this university or any other institution.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work. I have acknowledged all main sources of help.
- Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself.



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Certificate by the Supervisor

This is to certify that the thesis entitled **"Investigation of electronic, optical, and surface adsorption properties in engineered black phosphorene and its isostructural tin sulfide systems"**, submitted to the School of Sciences, Tezpur University in partial fulfilment for the award of the degree of **Doctor of Philosophy** in Physics is a record of original research work carried out by **Mr. Dhanjit Talukdar** under my supervision and guidance.

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

Prof. Gazi Ameen Ahmed
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Date: 8th September, 2025
Place: Tezpur, Assam, India

Acknowledgements

I would like to express my heartfelt gratitude and deep appreciation to all those whose support and encouragement made my Ph.D. journey possible. First and foremost, I am profoundly thankful to my supervisor, Prof. Gazi Ameen Ahmed, for believing in me and giving me the opportunity to pursue my doctoral studies under his guidance. His trust and support have been instrumental in shaping my academic journey. I am especially grateful for the intellectual freedom he provided, which allowed me to explore, learn, and develop essential skills in the field.

I extend my sincere gratitude to my doctoral committee members, Prof. Pritam Deb and Prof. Dambarudhar Mohanta, for their valuable suggestions and insightful discussions, which greatly enriched my research. I am especially thankful to Prof. Mohanta for graciously allowing me to participate in his group meetings, which played a significant role in framing the direction of my research work. I also wish to express my appreciation to the former and present Heads of the Department, as well as all the faculty members, for their constant encouragement and support throughout my doctoral journey. I am grateful to Tezpur University for providing the fellowship that supported me during this time. I am also thankful to Prof. Nidhi S. Bhattacharyya for her consistent encouragement to take part in extracurricular activities, which contributed meaningfully to my personal growth. I extend my gratitude to the office staff of the department, especially Narayan da and Suman da, for their kind assistance and constant support in handling various administrative matters with patience and efficiency.

For a Ph.D. scholar in theoretical physics, computing facilities are the lifeline of research. I gratefully acknowledge the computational support that made my research work possible. I sincerely thank Tezpur University for providing access to the PARAM Tez high-performance computing system, as well as the Department of Physics, Tezpur University, for access to its dedicated HPC resources. I also acknowledge the support of the National Supercomputing Mission (NSM) for providing access to the 'PARAM Porul' supercomputing facility at NIT Trichy, implemented by C-DAC and supported by MeitY and DST, Government of India.

It gives me immense pleasure to thank my collaborators, Prof. Dambarudhar Mohanta and Ms. Bhupali Deka from the Department of Physics, Tezpur University, as well

as Prof. Devasish Chowdhury and Mr. Bitopan Boro from IASST, Guwahati, for their valuable contributions and support.

I would like to extend my heartfelt thanks to all the former and present research scholars in the department. While it is difficult to name everyone, I would like to thank Olag da, Hirak da, Sunny da, Sritam da, Hemanga da, Ritu da, Abinash da, Saransha da, Amrita ba, and Tanushree. A special word of thanks goes to Prankrishna da for bringing a joyful and creative dimension to my university life through our involvement in short films. I am truly fortunate to have some wonderful friends, especially Anil, Niranjan, Jubaraj, Debasish, and Hritwik. A special mention goes to Anil for always being there to help me with DFT discussions. I would also like to thank my former and present labmates Kabita ba, Nishant da, Kaushik, Janmejoy, Shahnaz, Debasish, Himakhi, Udipta, and Rahul. I am also grateful to the members of the NSL lab, Aftab da, Kakoli ba, Ankush da, Stuti, Susmita, Bikash, Anuj, Dipankar, Saddique, and Satyajit, for welcoming me as a member of their group. I am also deeply grateful to my friend-cum-mentors, Goutam, Bitopan, Jintu, Hirak, and Joseph, for their constant motivation, guidance, and belief in me, which have made a lasting impact on both my academic and personal journey.

My deepest gratitude goes to Bhupali, my constant support, my companion through both happiness and sorrow. Her unwavering presence, patience, and encouragement have been a source of strength throughout this journey, and I am truly fortunate to have her by my side.

Finally, I am truly indebted to my Maa, Papa, and Moni. It is because of their constant support that I am standing where I am today. Their immense love, sacrifices, and enduring strength have shaped me, given me the courage to persevere through every challenge, and continue to inspire me to pursue my dreams.

Above all, I thank the Almighty for giving me the strength, clarity, and patience to navigate this journey and for guiding me every step of the way.

Dhanjit Talukdar

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List of Abbreviations

0D	Zero-Dimensional
1D	One-Dimensional
2D	Two-Dimensional
ac	armchair
AIMD	Ab-Initio Molecular Dynamics
BNNT	Boron Nitride Nanotube
BP	Black Phosphorene
BSE	Bethe-Salpeter Equation
BZ	Brillouin Zone
CB	Conduction Band
CBM	Conduction Band Minimum
CDD	Charge Density Difference
CNT	Carbon Nanotube
DFT	Density Functional Theory
EBE	Exciton Binding Energy
GGA	Generalized-Gradient-Approximation
GW	Green's function 'G' with screened Coulomb potential 'W'
h-BN	Hexagonal Boron Nitride
HF	Hartree-Fock
HVB	Highest Valence Band
IDE	Interdimensional Exciton
IFE	Interfacial Exciton
KS	Kohn-Sham
LCB	Lowest Conduction Band
LDA	Local Density Approximation
MBPT	Many-Body Perturbation Theory
ONCPPSP	Optimized Norm-Conserving Vanderbilt Pseudopotential
PAW	Projector Augmented-Wave
PDOS	Projected Density of States
PPA	Plasmon-Pole Approximation
PV	Photovoltaics
QP	Quasiparticle

RPA	Random Phase Approximation
SCF	Self-Consistent Field
SnS	Tin(II) Sulfide
TMDC	Transition Metal Dichalcogenide
TMMC	Transition Metal Monochalcogenide
VB	Valence Band
VBM	Valence Band Maximum
vdW	Van der Waals
zz	zigzag

List of Symbols

h	Planck's constant
U_{ei}	electron-ion interaction
W^H	Hartree potential
T	kinetic energy operator
H	Hamiltonian
e	electron
N	number of electrons
U_{ee}	electron-electron interaction
$T_{\mathrm{TF}}[n]$.	Thomas-Fermi kinetic energy functional
$n(r)$	electron density
Ψ	wavefunction
E_{el}	electronic energy
$F[n]$	universal functional
V_{ext}	external potential
$E_{xc}[n]$	exchange-correlation energy
$v_{KS}(r)$	Kohn-Sham potential
$V_{xc}(r)$	exchange-correlation potential
$\mathrm{V}_{pseudo}(r)$	potential mimicking the bare nuclear Coulomb potential and the effects of the core electrons
k	point in Brillouin Zone
$G^0_{nk}(\omega)$	non-interacting Green's function
f_{nk}	occupation factor
$G_{nk}(\omega)$	exact Green's function
$\Sigma_{nk}(\omega)$	GW self-energy
χ	response function
$\Omega_{GG'}$	plasmon frequencies
E^{QP}_{nk}	quasiparticle energy
Z_{nk}	renormalization factor
E_{ck}	quasiparticle energies of conduction band
E_{vk}	quasiparticle energies of valence band
A^S_{vck}	exciton amplitude

Ω^S	exciton eigenvalue
K^{eh}	electron-hole interaction kernal