Appendix

A.1: Work function of BP_v^N, BP_v, and BP^N monolayers

The work function is calculated using the formula:

$$\phi = E_{vac} - E_F \qquad \ldots(A.1)$$

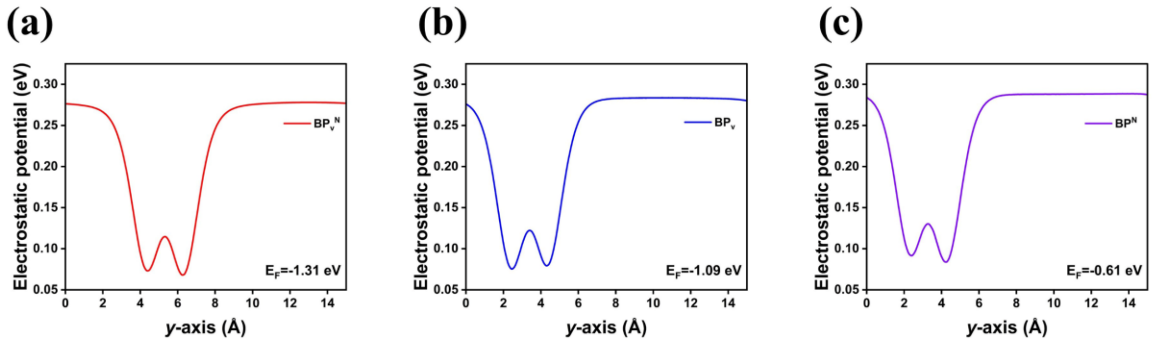

Figure A.1: *Electrostatic potential of* ***(a)*** *BP_v^N,* ***(b)*** *BP_v, and* ***(c)*** *BP^N monolayer, respectively.*

A.2: Schematic illustration of chemisorption and physisorption

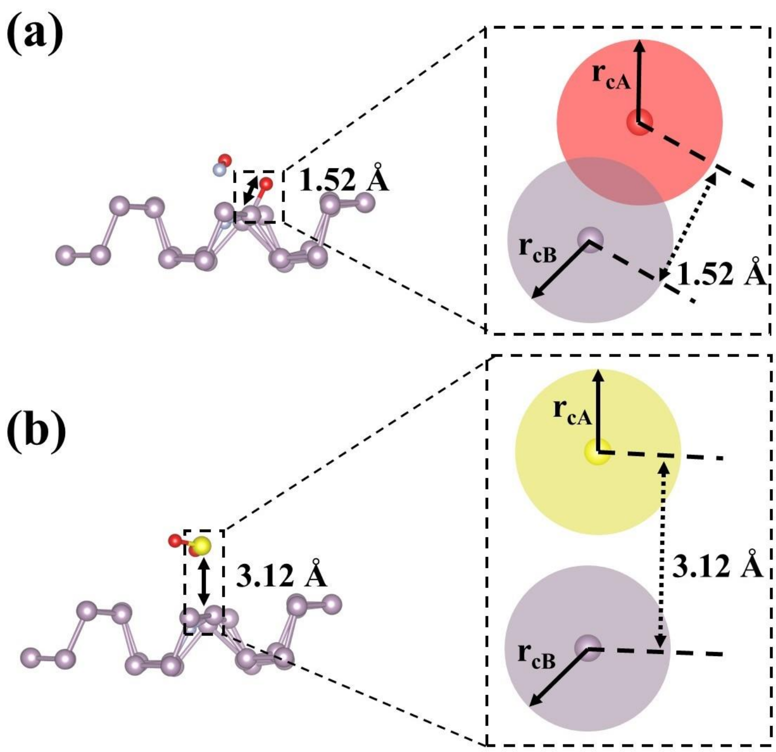

Figure A.2: *Schematic illustration of* ***(a)*** *chemisorption and* ***(b)*** *physisorption on BP_v^N surface.*

A.3: Surface adsorption of gas molecules with different orientations

Table A.3: Initial positions of molecules before atomic relaxation on BP_V^N monolayer and their respective adsorption energy after atomic relaxation.

Molecule	initial orientation (atom closest to the defect site)	E_{ad} (eV)
NO_2	N	-4.43
	O	-5.74
SO_2	S	-0.13
	O	-0.08
CO	C	-0.02
	O	-0.01
CO_2	C	-0.01
	O	-0.05
NH_3	N	-0.02
	H	-0.03

A.4: Electronic band structure after adsorption of NO_2, and SO_2

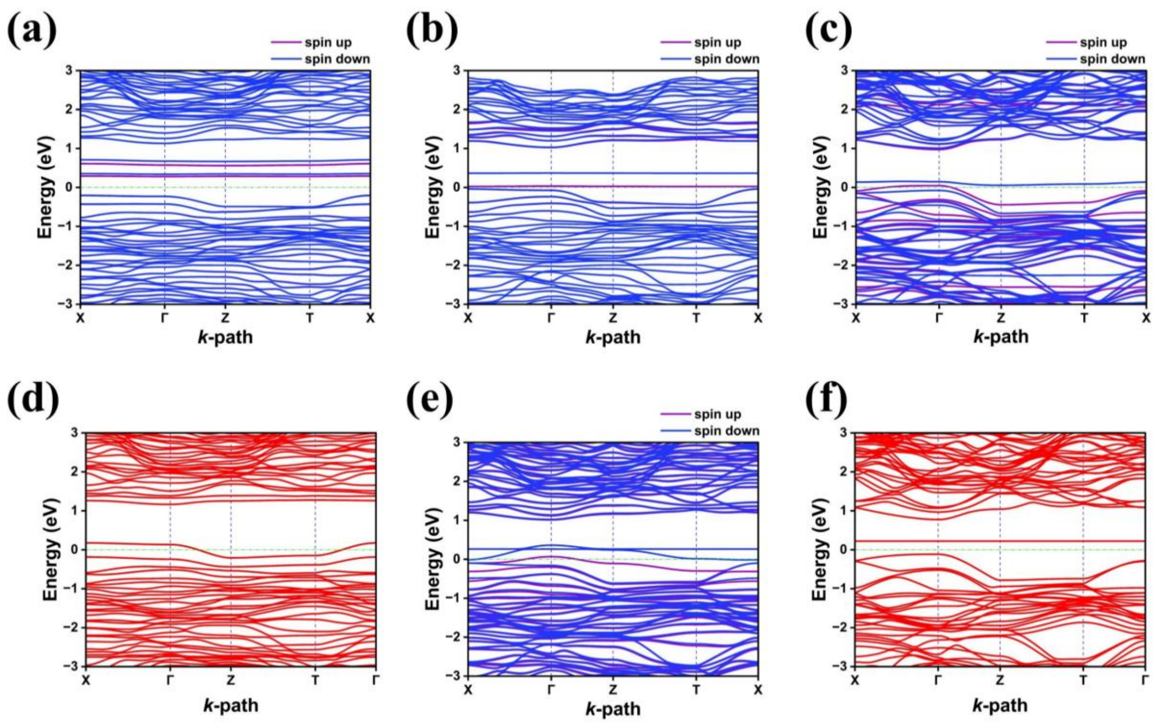

Figure A.4: *Electronic band structure of BP_v^N, BP_v, and BP^N sheet after adsorption of (a-c) NO_2, and (d-f) SO_2 molecules, respectively.*

A.5: Electronic band structure after adsorption of CO, CO_2, and NH_3

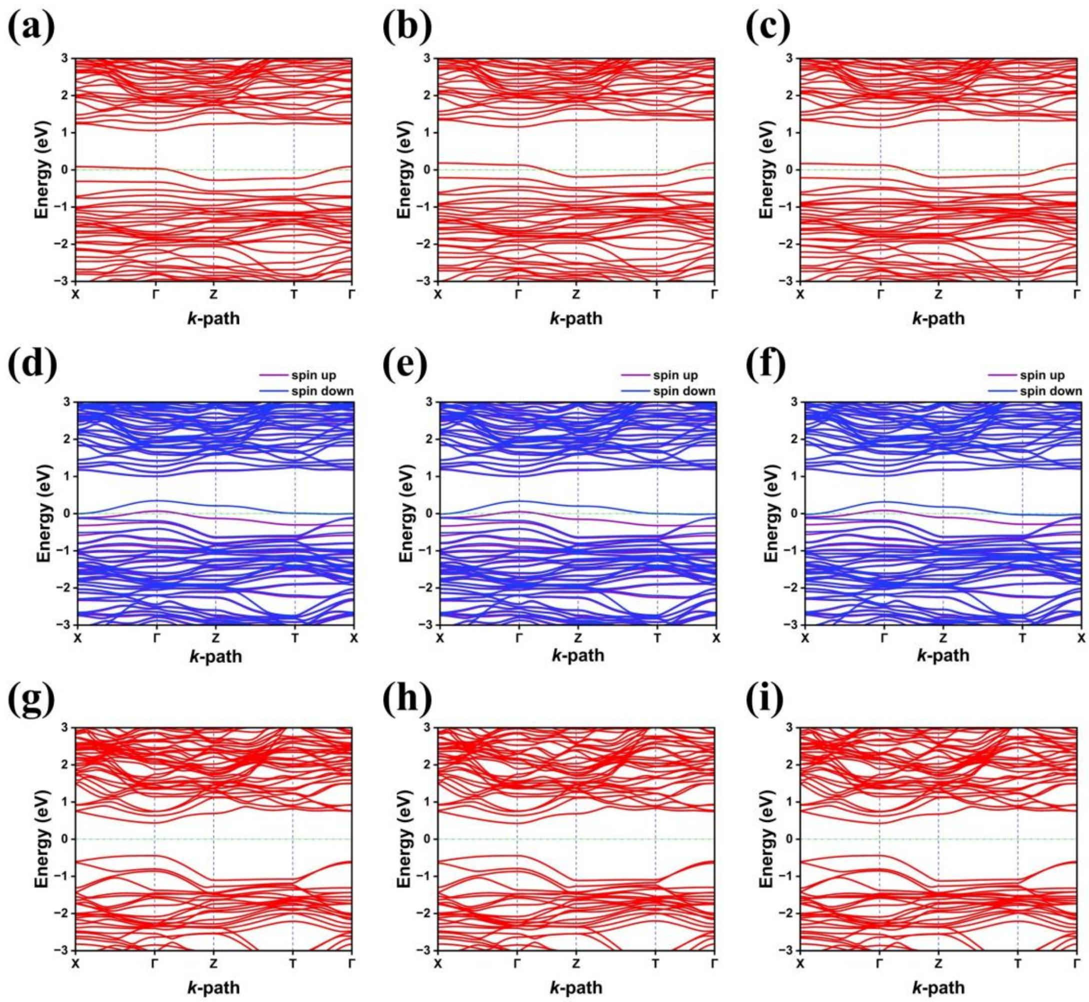

Figure A.5: *Electronic band structure of (a-c) BP_v^N, (d-f) BP_v, and (g-i) BP^N monolayer after the adsorption of CO, CO_2, and NH_3 molecule, respectively.*

A.6: Inert electronic and optical properties of *h*-BN

Before stacking SnS with *h*-BN, we first investigate the electronic and optical properties of the *h*-BN monolayer. DFT calculations indicate that pristine *h*-BN exhibits a direct band gap of 4.61 eV at the K point, though this value is underestimated. In contrast, GW calculations reveal that *h*-BN is actually an indirect band gap material, along the direction from K (VBM) to Γ (CBM) point. The indirect band gap is found to be 5.71 eV, while the direct band gap at the K point is 7.43 eV. Regarding optical absorption, the first excitonic peak appears at 5.73 eV, with an exciton binding energy of 1.7 eV. Given its wide and inert electronic states, *h*-BN is unlikely to strongly couple with the electronic states of SnS near the Fermi level, thereby preserving the pristine optical transitions of SnS.

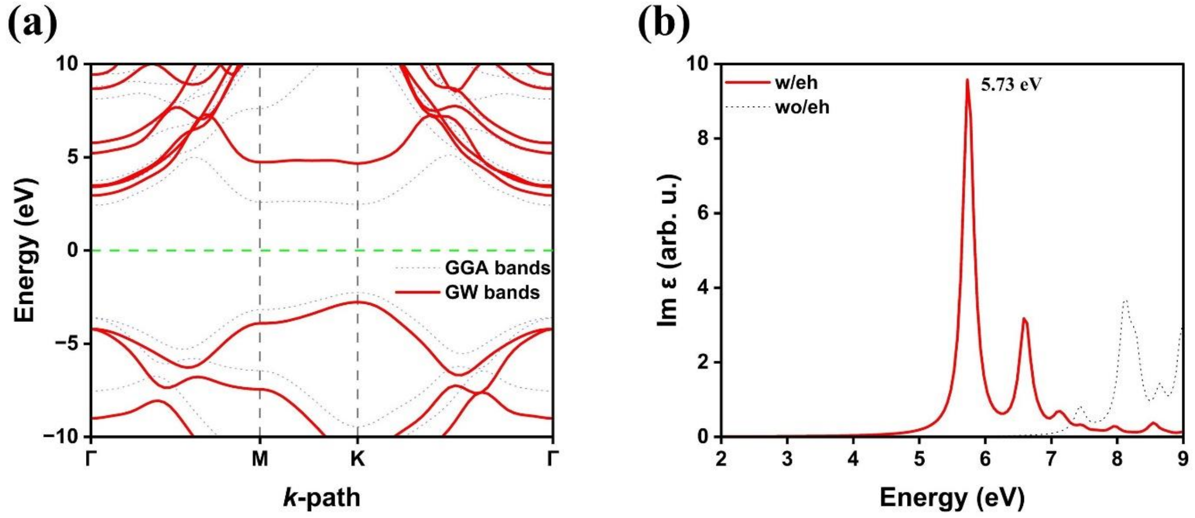

Figure A.6: *(a) Electronic band structure and (b) optical absorption spectra of h-BN monolayer, respectively.*

A.7: Electronic band structure of SnS/*h*-BN heterostructure without imposing any strain on SnS surface.

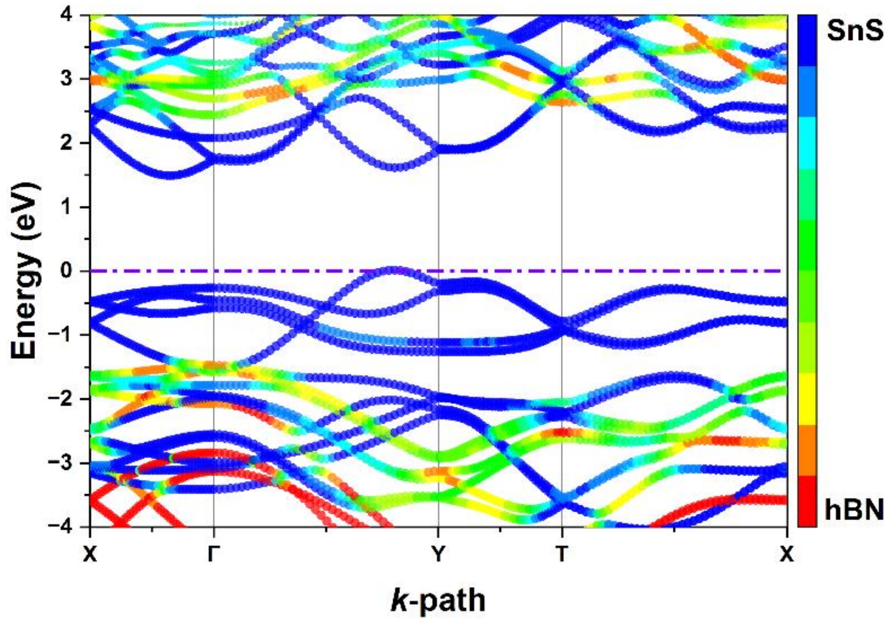

Figure A.7: *Layer projected electronic band structure of SnS/h-BN heterostructure with no strain on SnS layer, plotted along the X-Γ-Y-T-X high symmetric path (blue and red colour indicates the contribution from the SnS and h-BN monolayers, respectively).*

A.8: Electronic and optical properties of (5,0), (6,0), and (7,0) BNNTs

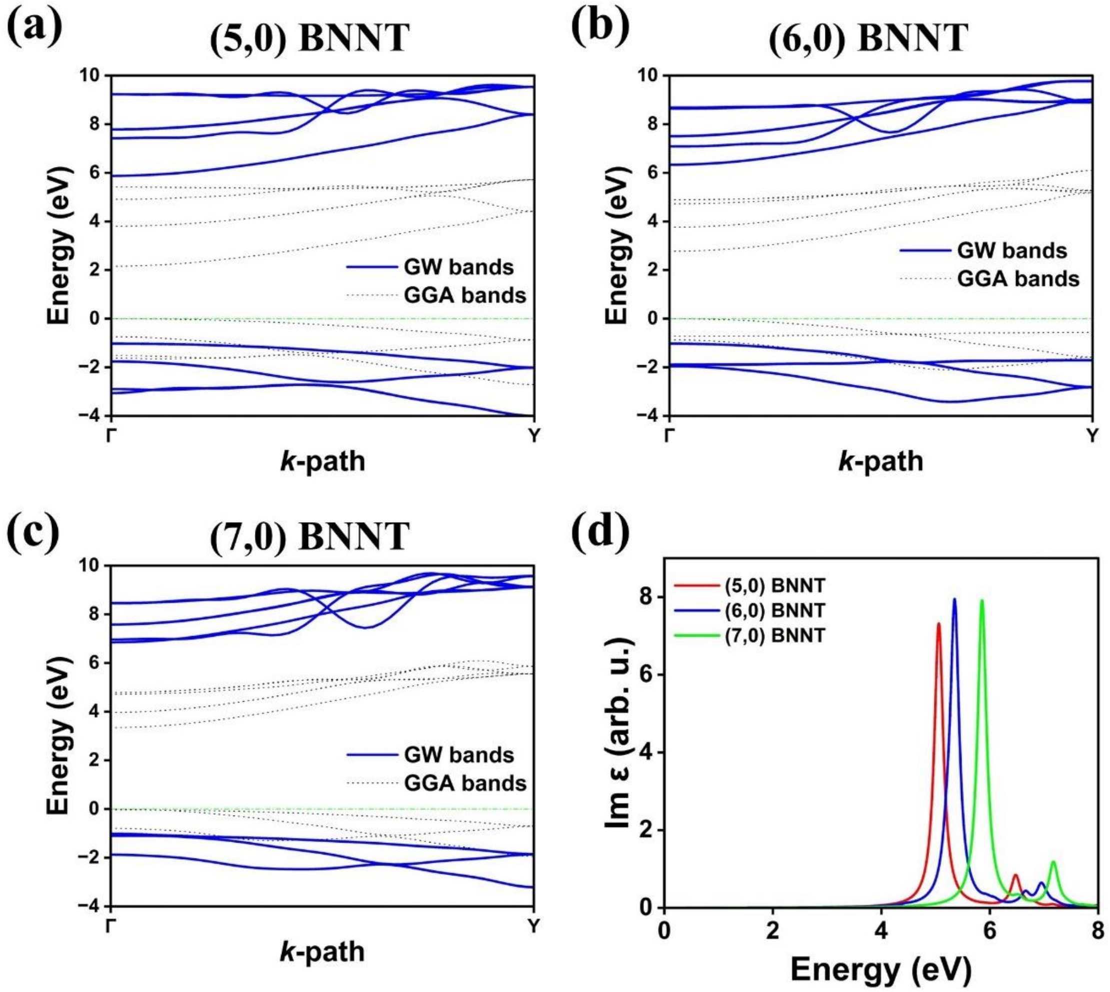

Figure A.8: *Band structure of (a) (5,0) (b) (6,0), and (c) (7,0) BNNTs; (d) optical absorption spectra of the BNNTs.*

List of Publications

A. Journal articles

1. **Talukdar, D.**, Bora, S.S., Ahmed, G. A. Electronic, optical, and adsorption properties of Li-doped hexagonal boron nitride: a GW approach. *Physical Chemistry Chemical Physics*, 26(5): 4021-4028, 2024.

2. **Talukdar, D.**, Mohanta, D., Ahmed, G. A. Nitrogen doped compound defect in black phosphorene for enhanced gas sensing. *Surfaces and Interfaces*, 51: 104699, 2024.

3. **Talukdar, D.**, Mohanta, D., Ahmed, G. A. Enhancing optoelectronic properties of SnS via mixed phase heterostructure engineering. *Nanoscale*, 17(6): 3331-3340, 2025.

4. **Talukdar, D.**, Mohanta, D., Ahmed, G. A. Interfacial excitons across dimensional boundaries: mixed-dimensional SnS/BNNT heterostructure. *(under review).*

B. Book chapter

1. **Talukdar, D.**, Ahmed, G. A. Strain-tunable electronic nature of black phosphorene with compound defect. Chapter in the book "*Current Trends in Materials Science*", to be published by *Springer Nature*. (*under review*).

C. Other journal articles (not included in the thesis)

1. Deka, B., **Talukdar, D.**, Mohanta. D. Effect of 60 MeV nitrogen ion irradiation on few layer WSe_2 nanosystems. *Nuclear Inst. and methods in Physics Research, B* 554: 165438, 2024.
2. Deka, B., **Talukdar, D.**, Naik, V., Saha, A., Mohanta. D. Generating immiscible WC phase in layered WS_2 upon 15 keV C^{2+} irradiation. *Physica Scripta,* 100(2): 025931, 2025.
3. Boro, B., **Talukdar**, **D.**, Ahmed, G. A., Chowdhury, D. Deciphering amino acid-bivalent metal ion interactions: Experimental and Computational approach. (*under review*).

List of Conferences/Workshops attended

1. Presented **Poster** at the Seminar cum Workshop on Recent Trends in Quantum Materials, 3rd-4th March, 2025, organised by the Department of Electronics and Communication Engineering, Tezpur University.

2. **Oral** presentation at the XIV Biennial Conference of Physics Academy of North East (PANE 2024), 12th-14th November, 2024, organised by the Department of Physics, Tezpur University.

3. Presented **poster** at the Fourth International Conference on Material Science (ICMS 2024), 31st January-2nd February, 2024, organized by the Department of Physics, Tripura University.

4. Presented **poster** at 31st National Conference "Condensed Matter Days, CMDAYS 2023", held on 22nd-24th January, 2024, at Tezpur University, Assam.

5. **Oral** presentation at 2nd International Conference on Recent Trends in Materials Science & Devices 2023 (ICRTMD-2023), 29th-31st December, 2023 organized by Research Plateau Publishers & Sat Kabir Institute of Technology & Management, Bahadurgarh, Haryana, India.

6. Presented **poster** on 7th International Conference on Nanostructuring by Ion Beams "(ICNIB 2023)", 2nd-4th November, 2023, UPES, Dehradun, India.

7. **Oral** presentation at 30th National Conference on Condensed Matter Physics "**(**CMDAYS2022)", 14th-16th December, 2022, Department of science and humanities, National Institute of Technology, Nagaland, India.

8. **Oral** presentation at XIII Biennial National Conference of Physics Academy of North East "(PANE-2022)", November 8-10, 2022, Department of Physics, Manipur University, Imphal, Manipur, India.