

Contents

Chapter 1: Introduction	1
1.1. Need for Toxic Gas Sensors	3
1.2. Two Dimensional (2D) Materials	5
1.3. Prediction of Novel 2D Materials	7
1.4. Single-layer hexagonal crystals of group IV and V elements	8
1.5. Definition and Approach to the problem	9
1.6. Specific Objectives	10
1.7. Structure of the Thesis	11
Bibliography	12
Chapter 2: Theoretical Framework	15
2.1. Theory of Electronic Structure	17
2.1.1. Many body problem	17
2.2. Wave function-based methods to solve many body problem	18
2.2.1. The Born-Oppenheimer approximation	18
2.2.2. Hartree approximation	19
2.2.3. Hartree-Fork (HF) approximation	20
2.3. Density based method: Density functional theory	21
2.3.1. Thomas-Fermi theory	22
2.3.2. Hohenberg and Kohn theorem	22
2.3.3. The Kohn-Sham equation	24
2.3.4. Self-consistent loop	26
2.4. Exchange and coorelation functionals	28
2.4.1. Local density approximation (LDA)	28

2.4.2. Generalized gradient approximation (GGA)	30
2.5. Boltzmann Transport Equation and BoltzTrap	31
2.5.1. Electrical Conductivity Calculation	32
2.5.2. Steps for BoltzTrap	33
Bibliography	34
Chapter 3: Interaction of Pristine and Defected α-CX (X = N, P)	36
3.1. Introduction	38
3.2. Computational Details	39
3.3. Results and Discussion	40
3.3.1. Structural and electronic properties of pristine and defect tuned α -CX (X = N, P) monolayers	40
3.3.2. Adsorption performance of CO gas molecule over pristine and C defected α -CX monolayers	42
3.3.3. Adsorption performance of NO gas molecule over pristine and C defected α -CX monolayers	45
3.3.4. Charge transfer analysis	47
3.3.5. Work Function	50
3.3.6. Recovery Time Analysis	51
3.4. Conclusion	52
Bibliography	53
Chapter 4: Enhanced Gas adsorption in Beryllium, Boron, and Aluminium doped α-CN	56
4.1. Introduction	57
4.2. Methodology	58
4.3. Results and Discussion	59
4.3.1. Physical and electronic characteristics of Beryllium, Boron and Aluminium doped α -CN monolayer	59

4.3.2. Adsorption performance of CO, NO and NH ₃ gas molecules on Be doped α -CN	61
4.3.3. Adsorption performance of CO, NO and NH ₃ gas molecules on B doped α -CN	65
4.3.4. Adsorption performance of CO, NO and NH ₃ gas molecules on Al doped α -CN	68
4.3.5. Work Function Analysis	71
4.3.6. Recovery Time Analysis	76
4.4. Conclusion	77
Bibliography	78
Chapter 5: Adsorption mechanism of Nickel decorated α-CN monolayer towards CO, NO and NH₃ gases	80
5.1. Introduction	82
5.2. Methodology	84
5.3. Results and Discussion	85
5.3.1. Structural and Electronic Properties of Ni decorated α -CN monolayer	85
5.3.2. Structural and electronic properties of gas adsorbed Ni decorated α -CN	86
5.3.3. Charge transfer analysis	88
5.3.4. Electrical Conductivity	89
5.3.5. Work Function Analysis	92
5.3.6. Recovery Time	93
5.3.7. Comparison with the Ni decorated α -CN and other nanomaterials	94
5.4. Conclusion	95
Bibliography	96
Chapter 6: Summary and Future Prospects	99
6.1. Thesis in a nutshell	101
6.2. Advanced Properties	105

6.2.1. Current-Voltage (I-V) Characteristics	105
6.2.2. Selectivity	105
6.3. 2D Materials Beyond α -CX and heterostructures	106
6.3.1. 2D Materials beyond α -CX monolayers	106
6.3.2. Heterostructure Formation	107
Bibliography	107

List of Publications and Curriculum Vitae