## **Table of Contents**

Chapter 1: Introduction		
1.1	Bioconjugated Nanomaterials	1
1.2	Low Dimensional Carbon and its Derivatives	3
1.3	Boron Nitride Nanostructure	5
1.4	Research Objectives	7
1.5	Structure of the Present Thesis	8
References		11
Chap	pter 2: Background of Density Functional Theory	15
2.1	Basic Origin	15
	2.1.1 Many Body Problem	16
2.2	Wave Function Based Method to Solve Many Body Problem	18

	2.1.1	Many Body Problem	16
2.2	Wave	Function Based Method to Solve Many Body Problem	18
	2.2.1	Born-Oppenheimer Approximation	18
	2.2.2	Hartree Approximation	19
	2.2.3	Hartree-Fock Approximation	20
2.3	Densit	y Based Method- Density Functional Theory	21
	2.3.1	Thomas-Fermi Theory	21
	2.3.2	Hohenberg and Kohn Theorems	23
	2.3.3	Kohn-Sham Density Functional Theory	25

2.4	Self-C	onsistency in Kohn-Sham Equation	28
2.5	Exchange and Correlation Functional		29
	2.5.1	Local Density Approximation (LDA)	30
	2.5.2	Generalized-Gradient Approximation (GGA)	32
	2.5.3	Pseudopotentials	32
2.6	Densit	y Functional Perturbation Theory	34
2.7	Disper	rsion Correction to Density Functional Theory	38
Refere	References		39

(	Chap	ter 3: Sensing Properties of Boron Nitride Nanostructures Towards Alkaloids	41
	3.1	Introduction	41
	3.2	Computational Details	43
	3.3	Results and Discussions	45
	3.4	Conclusions	58
	References		

Chap	ter 4: "Haeckelite", a New Low Dimensional Cousin of Boron Nitride for Biosensing	64
4.1	Introduction	64
4.2	Computational Details	66
4.3	Results and Discussions	68

	4.3.1	Structural and Electronic Properties	68
	4.3.2	Vibrational Properties	72
	4.3.3	Adsorption Mechanisms	75
	4.3.4	Recovery Time and Work function	89
4.4	Conclu	isions	92
References		93	

Chapter 5: Boron Nitride Nanoribbon Conjugated with	
Neurotransmitter	99

5.1	Introduction	99
5.2	Computational Details	102
5.3	Results and Discussions	104
5.4	Conclusions	119
References		119

Chapter 6: Summary and Future Scope	123
Curriculum Vitae and List of Publications	130