Dedicated
to the loving memory of my
respected Mother and Father who passed
away in October 2006 and September 2014
respectively

May God rest their soul in eternal peace
To God we belong, and to Him we do return
They sacrificed their life’s best moments for
me and my sister. They always waited for this
day and wished to live to see and share this
moment with me, but, God did what He
ordained to do.
Declaration

I, hereby, affirm that the work presented in this thesis is exclusively my own and there are no collaborators. It does not contain any work for which a degree/diploma has been awarded by any other University/Institution.

A major part of thesis work has already been published/presented in international and national Journals/Conferences/Symposia.

Dinesh Kumar

26-06-2015
Day Month Year

Countersigned

Supervisor

(Dr. H.S. Bhatti)
Professor
Department of Physics
Punjabi University
Patiala-147002
Punjab (India)

Co-Supervisor

(Dr. Veena Verma)
Associate Professor
Department of Physics
Govt. Shivalik College
Naya Nangal Distt. Ropar
Punjab (India)-140126

26-06-2015
Day Month Year
Acknowledgements

Let me have the privilege of acknowledging the contribution of all who helped me in carrying out research work and submit my thesis.

At the very outset I owe profound gratitude to my esteemed supervisor Dr. (Prof.) H S Bhatti, Department of Physics, Punjabi University, Patiala with whose invaluable personal guidance it has been possible for me to accomplish this task. He is an excellent example of perfect physicist and professor. Of course I am also indebted to my co supervisor Dr. Veena Verma Department of Physics, Govt. Shivalik College, Naya Nangal Distt. Ropar for her kind cooperation and selfless help. Under the proficient and methodological approach and amiable nature, I was able to remove obstacles that came in my way during the course of research work. So, I felt my self lucky that I got the golden chance to work under kind guidance of such eminent personalities.

I am extremely thankful to Prof.(Mrs.) Keya Dharamvir, Department of Physics, Panjab University Chandigarh;, Prof. Kawaljeet Singh Director Punjabi University Computer Center; Dr. Sushil Kansal, Associate Professor, Department of Chemical Engineering, Panjab University Chandigarh; Dr. Kanchan Lal Singh, Associate Professor (Physics) & HOD M. Tech, Nanoscience and Technology, DAVIET, Jalandhar, Prof. Sanjeev Aggarwal, Department of Physics, Kurukshetra University, Kurukshetra and Dr. Karamjit Singh, Assistant Professor Department of Physics, Punjabi University, Patiala for their kind help and guidance throughout this research work. Suresh Mohan Soni (Sr. Techn.), Ravinder Singh (Sr. Techn.) Dr. Ankush Vig, NIT Hamirpur, Manjit Singh Dahyia, DCRUST Murthal. Balwinder kaur, Rampal, Dr. kavita, Sheilja Sharma, Dr. Rupinder kaur Saini, Inderpal
Singh, Mandeep Singh, Suresh Kumar, Anju Dogra, Narender Budhiraja, Sunil Sharma. Manjit Singh Kang, Gurpreet Singh, Savita Bhardwaj and Ritika deserve a special mention for their assistance throughout my work. I am thankful to former HODs of Physics which includes my own guide Prof. H S Bhatti, Prof. Darshan Singh, Prof. Bhajan Singh and Present HOD Prof. B. S. Sandhu for providing adequate facilities to work. Fruitful discussion during annual seminars with Prof. Raj Mittal. Prof. Gurmail Singh, Prof. Darshan Singh, Prof. B S Sandhu, Prof. V. K. Mittal, Prof Bhajan Singh, Prof. Parjit Shamsher Singh Sandhu and Dr. Vinayak Garg helped me to improve the quality of my research work.

Principal Inderjit Kaur of my School (G.S.S.S. Lang) must be thanked for her highly positive attitude and much needed support. I shall be failing in my duty if I don’t mention the names of my sister in law & brother in law Deep Shikha Behl and Hatinder Singh who became my timely teacher whenever I faced any crisis. I show gratefulness to my loving sister Indu Bala and wife Archana Behl to be at the back of my dreams.

I shall always remain indebted to my well wishers and friends for their affection and unvarying encouragement.

Above all I am always aware of the presence of Almighty by my side that has planned and shaped things for me including this task.

Dinesh Kumar
## Contents

<table>
<thead>
<tr>
<th>Contents</th>
<th>Page No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Details of contents (Index)</td>
<td>i-iv</td>
</tr>
<tr>
<td>List of figures and tables</td>
<td>v-xvi</td>
</tr>
<tr>
<td>Abbreviations</td>
<td>xvii-xviii</td>
</tr>
<tr>
<td>Preface</td>
<td>xix-xxiv</td>
</tr>
</tbody>
</table>

### Chapter 1: Introduction

1.1 Introduction ................................................................................. 1
1.2 Carbon Nanotubes ......................................................................... 3
  1.2.1 Single Walled Carbon Nanotubes ......................................... 4
  1.2.2 Double Walled Carbon Nanotubes ........................................ 5
  1.2.3 Multi Walled Carbon Nanotubes ......................................... 6
1.3 Optical Properties ....................................................................... 6
1.4 Mechanical Properties .................................................................. 6
1.5 Applications of Carbon Nanotubes ............................................. 7
1.6 Literature Review for Carbon Nanotubes .................................... 8
1.7 Carbon Nanohorns ......................................................................... 15
1.8 Graphene ..................................................................................... 18
  1.8.1 Structural Features of Graphene .......................................... 19
  1.8.2 Electronic Structure of Graphene ........................................ 20
  1.8.3 Physical Properties .......................................................... 20
  1.8.4 Mechanical Properties ........................................................ 20
1.9 Graphene Oxide ........................................................................... 20
  1.9.1 Structural Analysis of Graphene Oxide .................................... 22
1.10 Synthesis of Graphene ................................................................ 22
1.11 Metal Nanoparticles: .................................................................. 23
  1.11.1 Silver Nanoparticles .......................................................... 24
  1.11.2 Structure of Armchair (or Zigzag) Silver Nanotubes .............. 25
  1.11.3 Structure of Icosahedral Silver Nanowire ............................. 26
1.12 Gallium Nitride ................................................................. 27
   1.12.1 Crystalline structure of Gallium Nitride ............... 27
   1.12.2 Literature Review for Gallium Nitride Nanostructures ... 28
1.13 Motivation and Aim of the Present Thesis .......................... 39

Chapter 2: Model Potentials
2.1 Introduction........................................................................ 41
2.3 Potential Parameters for Carbon and III-Nitride Nanotubes ......... 47
2.4 Model Potential for Silver: The Gupta Potential ...................... 49

Chapter 3: Synthesis and Characterization of Nanomaterials
3.1 Introduction: ................................................................. 53
3.2 Synthesis
   3.2.1 Combustion Route.................................................... 54
   3.2.2 Hydrothermal & Solvothermal Method ...................... 54
   3.2.3 Gas Phase Methods ................................................. 54
   3.2.4 Microwave Synthesis ............................................. 55
   3.2.5 Polyol Process: ...................................................... 55
   3.2.6 One dimensional Silver Nanoparticles: ....................... 57
   3.2.7 Sol-gel Method....................................................... 58
3.3 Experimental Details
   3.3.1 Synthesis and Functionalization of Single Walled Carbon Nanotubes .. 60
   3.3.2 Synthesis and Functionalization of Multi Walled Carbon Nanotubes ... 61
   3.3.3 Synthesis and Functionalization of Single Walled Carbon Nanohorns . 62
   3.3.4 Synthesis of Graphene Nanoplatelets by Microwave Technique ....... 63
   3.3.5 Synthesis of Graphene Oxide...................................... 63
   3.3.6 Synthesis of Reduced Graphene Oxide .......................... 63
   3.3.7 Synthesis of Carbon Quantum Dots from Orange juice........... 64
   3.3.8 Synthesis of Silver Nanowires by Polyol Process .................. 64
   3.3.9 Synthesis of Intrinsic and Extrinsic Gallium Nitride Nanocrystals .... 65
3.4 Crystallographic Characterization of Nanostructures
   3.4.1 X-ray Diffraction..................................................... 65
3.5 Morphological Characteristics
   3.5.1 Field Emission Scanning Electron Microscopy .................... 71
3.5.2 Transmission Electron Microscopy Analysis................................. 79
3.5.3 Atomic Force Microscopy................................................................. 85
3.6 Surface area analysis and Pore size determination.............................. 91

Chapter 4: Electronic and Optical Characterization of Nanomaterials
4.1 Introduction ..................................................................................... 94
4.2 Energy Dispersive X-ray Spectroscopy ............................................ 95
4.3 X-ray Photoelectron Spectroscopy of Carbon Nanostructures ............ 98
4.4 Absorption Studies ........................................................................ 108
4.5 Fourier Transform Infrared Spectroscopy ....................................... 113
4.6 Raman Spectroscopy ..................................................................... 118
4.7 Photoluminescence ....................................................................... 123
4.8 Time Resolved Fluorescence Spectroscopy .................................... 133

Chapter 5: Elastic Modulii of Nanostructures
5.1 Introduction ..................................................................................... 144
5.2 Generation of Coordinates ............................................................... 146
5.3 Cohesive Energy with Aspect Ratio ............................................... 146
5.4 Minimization of Energy ................................................................. 147
5.6 General Method to Obtain Elastic Modulii .................................... 147
  5.5.1 Bending Energy ........................................................................ 147
  5.5.2 Young’s Modulus ...................................................................... 148
  5.5.3 Cohesive Energy and Structural Parameters for Silver Nanostructures .............................................................................. 152
  5.5.4 Poisson Ratio: .......................................................................... 153
  5.5.5 Shear Modulus .......................................................................... 154
5.6 Mechanical Properties of Carbon Nanohorns .................................. 161
  5.6.1 Young’s Modulus ...................................................................... 161
  5.6.2 Poisson Ratio ............................................................................ 163
  5.6.3 Shear Modulus .......................................................................... 165
5.7 Nanoindentation ............................................................................. 166

Chapter 6: Phonons in Graphene Sheet and h-BN Sheet and Radial Breathing Modes in Boron Nitride Nanotubes and Carbon Nanotubes
6.1 Introduction: .................................................................................. 177
6.2 Acoustic and Optical Phonons ....................................................... 178
6.3 Method of Calculation.................................................................... 178
List of Figures

<table>
<thead>
<tr>
<th>Fig No</th>
<th>Title</th>
<th>Page No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fig 1.1</td>
<td>Illustrations of (a) SWCNTs, (b) DWCNTs and (c) MWCNTs.</td>
<td>3</td>
</tr>
<tr>
<td>Fig 1.2</td>
<td>Structures of (n, 0) and (n, n) nanotubes</td>
<td></td>
</tr>
<tr>
<td>Fig 1.3</td>
<td>Classification of SWCNTs according to chiral vector: zigzag, chiral and armchair CNTs</td>
<td>5</td>
</tr>
<tr>
<td>Fig 1.4</td>
<td>Construction of Cones</td>
<td>16</td>
</tr>
<tr>
<td>Fig 1.5</td>
<td>Formation of Carbon Nanohorns</td>
<td>17</td>
</tr>
<tr>
<td>Fig 1.6</td>
<td>Open CNHs and a (10, 10) CNT with the same heights but different apex angles. $R_T = R_{CNT} = 6.8 \text{ Å}, R_{b1} = 17.1 \text{ Å}, R_{b2} = 28.4 \text{ Å}, R_{b3} = 39.7 \text{ Å}, R_{b4} = 51 \text{ Å}, R_{b5} = 62.3 \text{ Å}, H = 61.0 \text{ Å}$</td>
<td>18</td>
</tr>
<tr>
<td>Fig 1.7</td>
<td>Graphene as a mother of all Graphitic forms</td>
<td>19</td>
</tr>
<tr>
<td>Fig 1.8</td>
<td>The schematic structure of graphene oxide (GO)</td>
<td>22</td>
</tr>
<tr>
<td>Fig 1.9</td>
<td>A (4, 4) AgNT</td>
<td>25</td>
</tr>
<tr>
<td>Fig 1.10</td>
<td>Two dimensional triangular lattice of Silver</td>
<td>26</td>
</tr>
<tr>
<td>Fig 1.11</td>
<td>Silver nanowire icosahedral structure</td>
<td>26</td>
</tr>
<tr>
<td>Fig 1.12</td>
<td>Crystal structure of (a) Wurzite GaN and (b) Zinc-blende GaN [159]</td>
<td>28</td>
</tr>
<tr>
<td>Fig 2.1</td>
<td>Plot of pair potentials using the parameters [223] as a function of interatomic distance</td>
<td>44</td>
</tr>
<tr>
<td>Fig 2.2</td>
<td>Plot of pair potentials obtained using the parameters [223] as a function of interatomic distance in comparison with Tersoff potential [220]</td>
<td>45</td>
</tr>
<tr>
<td>Fig 2.3</td>
<td>Plot of pair potentials obtained using the parameters [Present work Tab 2.1] as a function of interatomic distance in comparison with Tersoff potential [220]</td>
<td>46</td>
</tr>
<tr>
<td>Fig 2.4</td>
<td>Plot of pair potentials obtained using the modified parameters for BN system as a function of interatomic distance in comparison with Tersoff potential [229]</td>
<td>46</td>
</tr>
<tr>
<td>Fig 2.5</td>
<td>Plot of pair potentials obtained using the modified parameters for AlN system as a function of interatomic distance in comparison with Tersoff potential [229]</td>
<td>47</td>
</tr>
</tbody>
</table>
Fig 2.6  Plot of pair potentials obtained using the modified parameters for GaN system as a function of interatomic distance in comparison with Tersoff potential [229] ................. 47
Fig 2.7  Gupta potential for gold; dotted line is plotted with \( r_0 = 2.53 \, \text{Å} \) and solid line with \( r_0 = 2.89 \, \text{Å} \) ........................................................ 52
Fig 3.1  Reduction of Ag+ ions by EG leads to the formation of nuclei.[264] ..................................................................................... 56
Fig 3.2  Structure of Poly (vinylpyrrolidone) [272] ................................. 57
Fig 3.3  Schematic illustration of mechanism proposed to account for the growth of silver nanowires.[264] ........................................ 58
Fig 3.4  Mechanism of Sol-gel process .................................................. 59
Fig 3.5  CVD set up to synthesize SWCNTs ........................................... 60
Fig 3.6  DC Arc discharge in liquid nitrogen to synthesize SWCNHs ...... 62
Fig 3.7  XRD pattern of pristine SWCNTs (Red line) and functionalized SWCNTs (Blue line)....................................................... 66
Fig 3.8  XRD pattern of Pristine (I) and functionalized (II) MWCNTs ............................. 66
Fig 3.9  XRD Pattern of Pristine (Red) and water soluble (Blue) SWCNHs ....................................................................................... 67
Fig 3.10  XRD Pattern of GNPs (a) after acid treatment (Red colour) (b) after second microwave irradiation (blue colour) ............................... 68
Fig 3.11  XRD pattern of GO and rGO .................................................. 69
Fig 3.12  XRD pattern of Carbon quantum dots .................................... 69
Fig 3.13  XRD pattern of Silver nanowires .......................................... 70
Fig 3.14  (a) XRD pattern of pure (b) doped GaN nanocrystals ................. 71
Fig 3.15  (a) FESEM of Pristine SWCNTs (b) FESEM of functionalized SWCNTs ................................................................. 72
Fig 3.16  FESEM micrograph of (a) Pristine MWCNTs (b) functionalized MWCNTs................................................................. 72
Fig 3.17  FESEM micrograph of (a) SWCNHs (b) water soluble SWCNHs ..................................................................................... 72
Fig 3.18  FESEM micrographs of Microwave synthesized GNPs ............... 75
Fig 3.19  FESEM micrograph of Graphene Oxide (GO) ............................. 76
Fig 3.20  FESEM micrograph of reduced Graphene oxide (rGO) ............. 76
Fig 3.21  FESEM micrograph of Carbon quantum dots ........................................... 77
Fig 3.22  SEM micrograph of Silver nanowires ......................................................... 77
Fig 3.23  FESEM micrograph of Silver nanostructures at high concentration of NaCl (10mM) ................................................................. 78
Fig 3.24  FE-SEM micrograph of (a) pure (b) doped GaN nanocrystals ................................................................. 78
Fig 3.25  (a) HRTEM of SWCNTs (b) HRTEM of functionalized SWCNTs ................................................................. 79
Fig 3.26  HRTEM micrograph of (a) Pristine MWCNTs (b) functionalized MWCNTs ................................................................. 80
Fig 3.27  HRTEM micrograph of (a) SWCNHs (b) water soluble SWCNHs ................................................................. 81
Fig 3.28  HRTEM micrograph of microwave synthesized GNPs.............................. 81
Fig 3.29  HRTEM micrograph of GO ........................................................................ 82
Fig 3.30  HRTEM micrograph of rGO .................................................................. 83
Fig 3.31  HRTEM micrographs of Carbon quantum dots ........................................ 83
Fig 3.32  TEM micrograph of Silver nanowires .......................................................... 84
Fig 3.33  TEM micrograph of GaN nanoparticles ......................................................... 85
Fig 3.34  (a) 2D AFM topographic micrograph of SWCNTs and inset table showing topographic parameters (b) 3D AFM topographic micrograph of SWCNTs and inset table showing topographic parameters (c) AFM RMS roughness micrograph of SWCNTs and inset table showing roughness parameters calculated from inset graph (d) AFM analysis of SWCNTs to measure diameter, length and surface area and inset line profile graph used to calculate diameter and power spectrum graph used to calculate surface area ............................................. 86
Fig 3.35  (a) 2D AFM topographic micrograph of functionalized SWCNTs and inset table showing topographic parameters (b) 3D AFM topographic micrograph of functionalized SWCNTs and inset table showing topographic parameters (c) AFM RMS roughness micrograph of functionalized SWCNTs and inset table showing roughness parameters calculated from inset graph (d) AFM analysis of
functionalized SWCNTs to measure diameter, length and surface area ................................................................. 87

Fig 3.36  (a) 2D AFM topographic micrograph of MWCNTs and inset table showing topographic parameters (b) 3D AFM topographic micrograph of MWCNTs and inset table showing topographic parameters (c) AFM RMS roughness micrograph of MWCNTs and inset table showing roughness parameters calculated from inset graph (d) AFM analysis of MWCNTs to measure diameter, length and surface area and inset line profile graph used to calculate diameter and power spectrum graph used to calculate surface area ........................................... 88

Fig 3.37  (a) 2D AFM topographic micrograph of functionalized MWCNTs and inset table showing topographic parameters (b) 3D AFM topographic micrograph of functionalized MWCNTs and inset table showing topographic parameters (c) AFM RMS roughness micrograph of functionalized MWCNTs and inset table showing roughness parameters calculated from inset graph (d) AFM analysis of functionalized MWCNTs to measure diameter, length and surface area and inset line profile graph used to calculate diameter and power spectrum graph used to calculate surface area ........................................... 89

Fig 3.38  (a-c) AFM of SWCNHs (d-g) water soluble SWCNHs ............... 90

Fig 3.39  BET analyses of (a) SWCNTs and (b) functionalized SWCNTs ............................................................................................................. 92

Fig 3.40  BET analyses of (a) pristine MWCNTs and (b) functionalized MWCNTs ......................................................................................... 92

Fig 3.41  BET analyses of (a) SWCNHs and (b) water soluble SWCNHs .......................................................................................... 92

Fig 3.42  BET analysis of microwave synthesized GNP s ................................ 93

Fig 4.1  (a) EDS of pristine SWCNTs (b) EDS of functionalized SWCNTs .......................................................................................... 95

Fig 4.2  (a) EDS of pristine MWCNTs (b) EDS of functionalized MWCNTs .......................................................................................... 95
Fig 4.3  EDS of (a) pristine SWCNHs & (b) water soluble SWCNHs........... 96
Fig 4.4  EDS of microwave synthesized GNPs ........................................ 96
Fig 4.5  EDS of (a) GO (b) r-GO .......................................................... 96
Fig 4.6  EDS of carbon quantum dots.................................................... 97
Fig 4.7  EDS of Silver nanostructures at high concentration of NaCl
(10mM) .......................................................................................... 97
Fig 4.8  EDS spectra of GaN nanocrystals (Inset table shows the
elemental composition)..................................................................... 98
Fig 4.9  EDS spectra of Ga$_{0.90}$Tb$_{0.10}$N nanocrystals (Inset table shows
the elemental composition) ................................................................ 98
Fig 4.10. (a) XPS survey (b) C1s and (c) O1s spectra of SWCNTs and
(d) O1s spectra of functionalized SWCNTs ....................................... 99
Fig 4.11  (a) XPS survey scans of pristine and functionalized
MWCNTs (b) XPS spectra of C1s pristine and functionalized
MWCNTs (c) XPS spectra of O1s functionalized MWCNTs...... 101
Fig 4.12  (a) XPS survey (b) C 1s and (c) O 1s spectra of SWCNHs
and water soluble SWCNHs ......................................................... 102
Fig 4.13  XPS of microwave synthesized GNPs..................................... 102
Fig 4.14  XPS spectra of GO (a) and rGO (b) survey scan & the C 1s
(c) and O 1s (d) core-level XPS spectra of GO and rGO . ............. 103
Fig 4.15  XPS survey and O 1s spectrum of carbon quantum dots........ 103
Fig 4.16  (a) XPS spectra of silver nanowires (b) XPS spectra of Ag3d
purified silver nanowires (c) XPS spectra of C 1s of purified
silver nanowires (d) XPS spectra of O 1s of purified silver
nanowires ...................................................................................... 104
Fig 4.17  (a) XPS wide survey scan for Pure and doped GaN
nanocrystals (b) high resolution binding energy spectra of
Ga$_{2p3/2}$ (c) N 1s (d) Tb 4d ions (e) Tb 3d ions ............................. 105
Fig 4.18  (a) XPS wide survey scan for Pure and doped GaN
nanocrystals (b) high resolution binding energy spectra of
Ga$_{2p3/2}$ (c) N 1s (d) Co 2p .......................................................... 106
Fig 4.19  (a) XPS wide survey scan for Pure and doped GaN
nanocrystals (b) high resolution binding energy spectra of
Ga$_{2p3/2}$(c) N 1s (d) Ni 2p .......................................................... 107
Fig 4.20  UV-Vis absorption spectra of SWCNTs and functionalized SWCNTs................................................................. 108

Fig 4.21 UV-Vis absorption spectra of pristine and Functionalized MWCNTs ..................................................................... 109

Fig 4.22 UV-Vis absorption spectra of SWCNHs and water soluble SWCNHs ................................................................. 109

Fig 4.23 UV-Vis absorption spectra of microwave synthesized GNPs ...... 110

Fig 4.24 UV-Vis absorption spectra of GO and rGO ........................................ 110

Fig 4.25 UV-Vis absorption spectra of Carbon quantum dots.............. 111

Fig 4.26 UV-visible absorption spectra of Silver nanowires............. 111

Fig 4.27 Absorption spectra of Ga$_{1-x}$Tb$_x$N (0\(\leq\)x\(\leq\)0.1) nanocrystals ............ 112

Fig 4.28 Absorption spectra of Ga$_{1-x}$Co$_x$N (0\(\leq\)x\(\leq\)0.1) nanocrystals ............ 112

Fig 4.29 Absorption spectra of Ga$_{1-x}$Ni$_x$N (0\(\leq\)x\(\leq\)0.1) nanocrystals ............ 113

Fig 4.30 FTIR spectra of pristine and functionalized SWCNTs ............... 114

Fig 4.31 FTIR spectra of pristine and functionalized MWCNTs ............. 115

Fig 4.32 FTIR spectra of SWCNHs and water soluble SWCNHs .............. 115

Fig 4.33 FTIR spectrum of microwave synthesized GNPs................. 115

Fig 4.34 FTIR spectra of GO and rGO ............................................. 116

Fig 4.35 FTIR spectra of Carbon quantum dots................................. 117

Fig 4.36 FTIR spectra of Silver nanowires .......................................... 118

Fig 4.37 FTIR spectra of Ga$_{1-x}$Tb$_x$N (0\(\leq\)x\(\leq\)0.1) nanocrystals ............ 118

Fig 4.38 Raman spectra of synthesized and functionalized SWCNTs ......... 119

Fig 4.39 Raman spectra of pristine and functionalized MWCNTs .......... 120

Fig 4.40 Raman spectra of SWCNHs and water soluble SWCNHs .......... 120

Fig 4.41 Raman spectra of GNPs (a) after acid treatment (Black colour) (b) after second microwave irradiation (red colour) ...... 121

Fig 4.42 Raman spectra of GO and rGO ............................................. 121

Fig 4.43 Raman spectra of carbon quantum dots .................................. 122

Fig 4.44 Raman spectra of silver nanowires ........................................ 123

Fig 4.45 Room Temperature PL spectra of Ga$_{1-x}$Ni$_x$N (0\(\leq\)x\(\leq\)0.1) nanocrystals ................................................................. 124

Fig 4.46 Room Temperature PL spectra of Ga$_{1-x}$Co$_x$N (0\(\leq\)x\(\leq\)0.1) nanocrystals ................................................................. 125
Fig 4.47  PL spectra of Ga$_{1-x}$Tb$_x$N (0≤x≤0.1) at excitation wavelength of 241nm ................................................................. 126
Fig 4.48  PL spectra of Ga$_{1-x}$Tb$_x$N (0≤x≤0.1) at excitation wavelength of 250nm ................................................................. 126
Fig 4.49  PL spectra of Ga$_{1-x}$Tb$_x$N (0≤x≤0.1) at excitation wavelength of 260nm ................................................................. 127
Fig 4.50  PL spectra of Ga$_{1-x}$Tb$_x$N (0≤x≤0.1) at excitation wavelength of 280nm ................................................................. 127
Fig 4.51  PL spectra of Ga$_{1-x}$Tb$_x$N (0≤x≤0.1) at excitation wavelength of 290nm ................................................................. 127
Fig 4.52  PL spectra of Ga$_{1-x}$Tb$_x$N (0≤x≤0.1) at excitation wavelength of 305nm ................................................................. 128
Fig 4.53  PL spectra of Ga$_{1-x}$Tb$_x$N (0≤x≤0.1) at excitation wavelength of 325nm ................................................................. 128
Fig 4.54  PL spectra of silver nanowires at excitation wavelength of 300 and 400nm ................................................................. 130
Fig 4.55  Room temperature PL spectra of microwave synthesized GNPs ................................................................. 130
Fig 4.56  PL spectra of Carbon quantum dots ................................................................. 131
Fig 4.57  PL spectra of Graphene Oxide ................................................................. 131
Fig 4.58  PL spectra of r-Graphene Oxide ................................................................. 131
Fig 4.59  PL spectra of SWCNHs ................................................................. 132
Fig 4.60  PL spectra of pristine MWCNTs (excitation wavelength 220nm) ................................................................. 132
Fig 4.61  PL spectra of functionalized MWCNTs (excitation wavelength 250nm) ................................................................. 133
Fig 4.62  Time resolved fluorescence spectra of Ga$_{1-x}$Tb$_x$N (a-c), Ga$_{1-x}$Ni$_x$N (d-f), Ga$_{1-x}$Co$_x$N (g-h) (0≤x≤0.1) nanocrystals ................................................................. 137
Fig 4.63  Time resolved decay curve for Silver nanowires at room temperature ................................................................. 138
Fig 4.64  Time resolved decay curve for Carbon quantum dots at room temperature ................................................................. 139
Fig 4.65  Time resolved decay curve for (a) GO (b) rGO ................................................................. 140
Fig 4.66  Time resolved decay curve for microwave synthesized GNPs .............................................................. 141

Fig 4.67  (a) Time resolved decay curve for pristine and (b) functionalized MWCNTs at room temperature ...................... 142

Fig 5.1  Variation of cohesive energy with aspect ratio for (10, 10) CNT ................................................................. 147

Fig 5.2  Strain energy per atom as a function of radius for (n, 0) and (n, n) tubes ............................................................... 148

Fig 5.3  Potential energy curve for a (10,10) SWCNTs ........................................ 150

Fig 5.4  Variation of Young’s modulus (Tpa) with radius (Å) for SWCNTs ................................................................. 151

Fig 5.5  Variation of Young’s modulus (GPa) with radius (Å) for III-V NNTs ................................................................. 151

Fig 5.6  Energy versus length of icosahedron NW (Ag 49)......................... 152

Fig 5.7  U verses length of AgNT (triangular lattice) ........................................ 153

Fig 5.8  Variation of Poisson’s ratio with radius (Å) for SWCNTs.............. 154

Fig 5.9  Variation of Poisson’s ratio with radius (Å) for III-V NNTs ...... 154

Fig 5.10  Potential energy of twisted (10,0) SWCNTs .............................. 155

Fig 5.11  Variation of Shear modulus (Gpa) and radius (Å) for SWCNTs ................................................................. 156

Fig 5.12  Variation of Shear modulus (GPa) with radius (Å) for III-V NNTs ................................................................. 156

Fig 5.13  U versus twist in radian for AgNT (triangular lattice) ............... 157

Fig 5.14  Variation of Y and G with radius of AgNT .............................. 157

Fig 5.15  Young’s modulus vs top radius apex angle 19.2° ....................... 162

Fig 5.16  Young’s modulus vs top radius apex angle of 38.9° ................. 162

Fig 5.17  Young’s modulus vs top radius apex angle of 60° ................. 163

Fig 5.18  Illustration of a single shell nanocone ........................................ 163

Fig 5.19  Shear modulus vs top radius, apex angle19.2° ........................... 165

Fig 5.20  Shear modulus vs top radius apex angle 38.9° ........................ 165

Fig 5.21  Shear modulus vs top radius apex angle 60° .......................... 166

Fig 5.22  Indentation with conical indenter .............................................. 168

Fig 5.23  AFM Micrograph of SWCNTs showing indents .......................... 172

Fig 5.24  AFM Micrograph of MWCNTs showing indents .......................... 172
Fig 5.25  AFM micrograph of SWCNHs showing various positions of indents ................................................................. 173
Fig 5.26  AFM micrographs of GNPs showing various positions of indents ................................................................. 173
Fig 5.27  AFM micrograph of AgNWs showing indents ................. 173
Fig 5.28  Load displacement curve at 200 µN for SWCNTs .............. 174
Fig 5.29  Load displacement curve at 700 µN for MWCNTs ............... 175
Fig 5.30  Load displacement curve at 1000 µN for SWCNHs ............. 175
Fig 5.31  Load displacement curve at 1000 µN for GNPs .................. 176
Fig 5.32  Load displacement curve at 1000 µN for AgNWs ............... 176
Fig 6.1  Bond angles .................................................................. 180
Fig 6.2  Unit cells in a hexagonal lattice containing (a) C-C atom (b) two types of atoms ...................................................... 181
Fig 6.3  Symmetry points in a single hexagon ................................. 188
Fig 6.4  Phonon dispersion of hexagonal Boron nitride and Graphene .... 189
Fig 6.5  Radial Breathing Mode .................................................... 190
Fig 6.6  Radial Breathing mode of (n,n) and (n,0) BNNTs (solid squares and open circles) and CNTs (open squares and solid circles) and from experiment (Stars) [401] ........................................ 190
Fig 7.1  Potential energy for two Graphitic sheets and Graphitic sheet – GaNNT system ......................................................... 194
Fig 7.2  Potential energy for two GaNNTs and Graphitic sheet – GaNNT system ................................................................. 195
Fig 7.3  U versus V for stack of h-GaN sheets under compression ....... 196
Fig 7.4  A GaNNT placed on h GaN surface showing various motions ............................................................................ 196
Fig 7.5  Spinning and in plane rotation of GaNNT on h-GaN sheet showing some of rotational barriers ................................. 197
Fig 7.6  Spinning of GaNNT on Graphitic sheet and on another GaNNT ........................................................................... 198
Fig 7.7  Seesaw motion of (10,10) GaNNT on Graphitic sheet ............... 199
Fig 7.8  Rolling of (10,10) GaNNT on h-GaN sheet ............................ 199
Fig 7.9  Some of translational barriers of (10,10) tube ......................... 200
Fig 7.10 Double walled GaNNT (5,5) @ (10,10) ................................ 202
Fig 7.11  Axial shift of inner (5,5) @ (10,10) GaNNT ................................. 202
Fig 7.12  Rotation barriers of (5,5) @ (10,10) GaNNT ............................... 203
Fig 7.13  Displacement of inner (5,5) @ (10,10) GaNNT along tube
           ig.axis ............................................................................................ 204
Fig 7.14  Extraction of inner tube (5,5) out of outer (10,10) GaNNT ........ 204
Fig 7.15  Oscillation of inner tube (5,5) @ (10,10) GaNNT ....................... 205
Fig 7.16  Translational barriers of (5,5) @ (10,10) GaNNT placed on
           h-GaN sheet .................................................................................. 205
### List of Tables

<table>
<thead>
<tr>
<th>Tab No</th>
<th>Title</th>
<th>Page No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tab 1.1</td>
<td>Classification of SWCNTs according to chiral index</td>
<td>5</td>
</tr>
<tr>
<td>Tab 1.2</td>
<td>Relationship between number of pentagons, angle of</td>
<td></td>
</tr>
<tr>
<td></td>
<td>disclination and angle of apex</td>
<td>17</td>
</tr>
<tr>
<td>Tab 1.3</td>
<td>Mechanical properties obtained by experimental method [89]</td>
<td>20</td>
</tr>
<tr>
<td>Tab 1.4</td>
<td>Physical properties of (a) wurzite GaN (b) zinc blende GaN</td>
<td>28</td>
</tr>
<tr>
<td>Tab 2.1</td>
<td>Second generation REBO potential parameters for C, BN,</td>
<td></td>
</tr>
<tr>
<td></td>
<td>AlN and GaN nanotubes</td>
<td>49</td>
</tr>
<tr>
<td>Tab 2.2</td>
<td>Bond length and cohesive energy</td>
<td></td>
</tr>
<tr>
<td>Tab 3.1</td>
<td>Surface area analysis, volume analysis and pore size</td>
<td></td>
</tr>
<tr>
<td></td>
<td>determination</td>
<td>93</td>
</tr>
<tr>
<td>Tab 4.1</td>
<td>Decay time and trap depth for Ga1-xTbxN, Ga1-xNixN,</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Ga1-xCoxN (0≤x≤0.1) nanocrystals</td>
<td>138</td>
</tr>
<tr>
<td>Tab 4.2</td>
<td>Transition probability, excited state life time, trap depth and</td>
<td></td>
</tr>
<tr>
<td></td>
<td>other important optical parameters of Silver nanowires (emission</td>
<td>139</td>
</tr>
<tr>
<td></td>
<td>wavelength 339.6nm) and μ=1.45)</td>
<td></td>
</tr>
<tr>
<td>Tab 4.3</td>
<td>Transition probability, excited state life time and trap depth and</td>
<td></td>
</tr>
<tr>
<td></td>
<td>other optical parameters of carbon quantum dots (emission</td>
<td>140</td>
</tr>
<tr>
<td></td>
<td>wavelength 452.6nm &amp; μ=1.5)</td>
<td></td>
</tr>
<tr>
<td>Tab 4.4</td>
<td>Transition probability, excited state life time and trap depth and</td>
<td></td>
</tr>
<tr>
<td></td>
<td>other optical parameters of optoelectronic</td>
<td></td>
</tr>
<tr>
<td></td>
<td>interest of GO (emission wavelength 489.3 nm &amp; μ=1.8)</td>
<td>141</td>
</tr>
<tr>
<td></td>
<td>and rGO (emission wavelength 466.9 nm &amp; μ=1.9)</td>
<td></td>
</tr>
<tr>
<td>Tab 4.5</td>
<td>Transition probability, excited state life time and trap depth and</td>
<td></td>
</tr>
<tr>
<td></td>
<td>other optical parameters of microwave synthesized GNPs (emission</td>
<td>142</td>
</tr>
<tr>
<td></td>
<td>wavelength 482 nm and μ=1.42)</td>
<td></td>
</tr>
<tr>
<td>Tab 4.6</td>
<td>Transition Probability, Excited state life time and trap depth and</td>
<td></td>
</tr>
<tr>
<td></td>
<td>other optical parameters of pristine and functionalized MWCNTs (emission wavelength 468 nm for MWCNTs whereas for functionalized MWCNTs emission wavelength 650 nm, μ=1.55 )</td>
<td>143</td>
</tr>
<tr>
<td>Tab 5.1</td>
<td>Elastic moduli of the armchair, zigzag and chiral CNTs</td>
<td>158</td>
</tr>
<tr>
<td>Tab 5.2</td>
<td>Elastic moduli of the armchair and zigzag BNNTs</td>
<td>159</td>
</tr>
</tbody>
</table>
Tab 5.3  Elastic moduli of the armchair and zigzag AlNNTs ................. 159
Tab 5.4  Elastic moduli of the armchair and zigzag GaNNTs ............... 160
Tab 5.5  Cohesive energy (U), b is the nearest neighbor distance within the ring, b’ between two adjacent rings in case of AgNT and for AgNW it represents distance between chain and ring atoms, Y, v and G for various AgNTs ......................... 161
Tab 5.6  Mechanical properties of SWCNTs ........................................ 169
Tab 5.7  Mechanical properties of MWCNTs ........................................ 169
Tab 5.8  Mechanical properties of SWCNHs ...................................... 170
Tab 5.9  Mechanical properties of GNPs ............................................. 170
Tab 5.10 Mechanical properties of AgNWs ....................................... 171
Tab 6.1  Indices of the site of some of atoms: ...................................... 181
Tab 6.2  Range of frequencies of all branches of Graphene (h-BN) ....... 189
Tab 6.3  RBMs for BNNTs and CNTs ................................................ 191
Tab 7.1  Minimum energy configuration for sheet-sheet, sheet–tube and tube–tube ................................................................. 195
Tab 7.2  Minimum energy configuration of (10, 10) GaNNT on graphitic sheet ................................................................. 200
Tab 7.3  Energy barriers and frequency modes of (10,10) GaNNT on h-GaN sheet ................................................................. 201
## List of Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Detail</th>
</tr>
</thead>
<tbody>
<tr>
<td>* 0D</td>
<td>Zero dimension</td>
</tr>
<tr>
<td>* 1D</td>
<td>One dimension</td>
</tr>
<tr>
<td>* 2D</td>
<td>Two dimension</td>
</tr>
<tr>
<td>* AFM</td>
<td>Atomic force microscope</td>
</tr>
<tr>
<td>* AgNTs</td>
<td>Silver nanotubes</td>
</tr>
<tr>
<td>* AgNWs</td>
<td>Silver nanowires</td>
</tr>
<tr>
<td>* AlN</td>
<td>Aluminium nitride</td>
</tr>
<tr>
<td>* AlN NTs</td>
<td>Aluminium nitride nanotubes</td>
</tr>
<tr>
<td>* B-C-N</td>
<td>Boron Carbon Nitride</td>
</tr>
<tr>
<td>* BET</td>
<td>Brunauer-Emmett-Teller</td>
</tr>
<tr>
<td>* BJH</td>
<td>Barrett-Joyner-Halenda</td>
</tr>
<tr>
<td>* BN</td>
<td>Boron Nitride</td>
</tr>
<tr>
<td>* BN NTs</td>
<td>Boron Nitride nanotubes</td>
</tr>
<tr>
<td>* ca.</td>
<td>Calculated approximately</td>
</tr>
<tr>
<td>* CNHs</td>
<td>Carbon nanohorns</td>
</tr>
<tr>
<td>* CNM</td>
<td>Carbon nanomaterials</td>
</tr>
<tr>
<td>* CNTs</td>
<td>Carbon nanotubes</td>
</tr>
<tr>
<td>* CQDs</td>
<td>Carbon quantum dots</td>
</tr>
<tr>
<td>* CVD</td>
<td>Chemical vapour deposition</td>
</tr>
<tr>
<td>* DFT</td>
<td>Density functional theory</td>
</tr>
<tr>
<td>* DOS</td>
<td>Density of states</td>
</tr>
<tr>
<td>* DWCNTs</td>
<td>Double walled carbon nanotubes</td>
</tr>
<tr>
<td>* EDS</td>
<td>Energy dispersive X-ray spectroscopy</td>
</tr>
<tr>
<td>* FESEM</td>
<td>Field emission scanning electron microscope</td>
</tr>
<tr>
<td>* FTIR</td>
<td>Fourier transform infrared spectroscopy</td>
</tr>
<tr>
<td>* GaN NTs</td>
<td>Gallium Nitride nanotubes</td>
</tr>
<tr>
<td>* GNP</td>
<td>Graphene nanoplatelets</td>
</tr>
<tr>
<td>* GO</td>
<td>Graphene Oxide</td>
</tr>
<tr>
<td>* h-GaN</td>
<td>Hexagonal Gallium Nitride</td>
</tr>
<tr>
<td>* HRTEM</td>
<td>High resolution transmission electron microscope</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Full Form</td>
</tr>
<tr>
<td>--------------</td>
<td>-----------</td>
</tr>
<tr>
<td>IPA</td>
<td>Isopropyl alcohol</td>
</tr>
<tr>
<td>LCAO</td>
<td>Linear combinational of atomic orbitals</td>
</tr>
<tr>
<td>MB</td>
<td>Methylene Blue</td>
</tr>
<tr>
<td>MD</td>
<td>Molecular dynamics</td>
</tr>
<tr>
<td>MoS2</td>
<td>Molybdenum Sulphide</td>
</tr>
<tr>
<td>MWCNTs</td>
<td>Multiwalled carbon nanotubes</td>
</tr>
<tr>
<td>NCs</td>
<td>Nanocrystals</td>
</tr>
<tr>
<td>NNTs</td>
<td>Nitride nanotubes</td>
</tr>
<tr>
<td>PDRs</td>
<td>Phonon dispersion relations</td>
</tr>
<tr>
<td>PEG</td>
<td>Polyethylene Glycol</td>
</tr>
<tr>
<td>PL</td>
<td>Photoluminescence</td>
</tr>
<tr>
<td>PVDF</td>
<td>Polyvinyl Difluoride</td>
</tr>
<tr>
<td>PVP</td>
<td>Poly (vinylpyrrolidone)</td>
</tr>
<tr>
<td>RBMs</td>
<td>Radial Breathing Modes</td>
</tr>
<tr>
<td>REBO</td>
<td>Reactive empirical bond order potential</td>
</tr>
<tr>
<td>rGO</td>
<td>Reduced Graphene Oxide</td>
</tr>
<tr>
<td>SAED</td>
<td>Scanned area electron diffraction</td>
</tr>
<tr>
<td>SEM</td>
<td>Scanning electron microscope</td>
</tr>
<tr>
<td>SERS</td>
<td>Surface enhanced Raman spectroscopy</td>
</tr>
<tr>
<td>SWCNHs</td>
<td>Single-walled carbon nanohorns</td>
</tr>
<tr>
<td>SWCNTs</td>
<td>Single-walled carbon nanotubes</td>
</tr>
<tr>
<td>TEM</td>
<td>Transmission electron microscope</td>
</tr>
<tr>
<td>TiO$_2$</td>
<td>Titanium Oxide</td>
</tr>
<tr>
<td>UV-vis.</td>
<td>UV visible</td>
</tr>
<tr>
<td>VdW</td>
<td>Vander waal</td>
</tr>
<tr>
<td>WS2</td>
<td>Tungsten Sulphide</td>
</tr>
<tr>
<td>XPS</td>
<td>X-ray photoelectron spectroscopy</td>
</tr>
<tr>
<td>XRD</td>
<td>X-ray powder diffractin</td>
</tr>
<tr>
<td>ZnO</td>
<td>Zinc Oxide</td>
</tr>
</tbody>
</table>
Nanotechnology is a field of applied science and technology, whose theme is to control the size of matter and fabrication of devices or materials on the atomic and molecular scale, generally between 1-100 nm. In other words, it is the design, characterization, production and application of structures, devices and systems by controlling shape and size at the nanometer scale. Nanotechnology is a highly multidisciplinary field, benefiting from the efforts and developments in many fields including applied physics, material science, interface & colloid science, supramolecular chemistry, chemical engineering, mechanical engineering, biological engineering, electrical engineering etc. Since the birth of cluster science and with the invention of scanning tunneling microscope (STM) in 1980’s, nanotechnology has been prosperously developed with ability to measure and visualize the novel phenomenon at nanoscale. It is also being used to manipulate and manufacture the materials & devices with nanostructures of 100 nm size or smaller.

Materials having nanoscale dimensions show different properties compared to those exhibits on macroscale. As the size of the material decreases to nanoscale, the quantum confinement effects become pronounced due to which most of the properties of the solids are altered to great extent. On the other hand, the increase of surface area to volume ratio with decreasing size causes significant changes in physical, chemical, electrical, optical, mechanical, thermal and catalytic properties of nanomaterials. These distinct properties enable unique applications of nanomaterials. So for carbon nanotubes (CNTs), fullerenes, nanoparticles of silver, gold, silica, zinc (including ZnO and ZnS) and Ti (including titanium oxide) are being used in commercially available products. Till date there are already more than 1000 nanotechnological products existing in the world, with a number of new ones hitting the market at a pace of 3-4 per week. Nanotechnology is likely to have a profound impact on our economy and society in the 21st century comparable to that of semiconductor technology, information technology or cellular and molecular biology. It is widely felt that nanotechnology will bring the next industrial revolution.

The word "nanotube" is very often preceded by the word "carbon," but nanotubes made of other materials can be equally - or even more - interesting.
Carbon nanotubes claim the lion's share of high-profile journal articles, reports in the popular press, and presentations at major scientific meetings. But a number of inorganic chemists have also fallen under the nanotube's spell. Delving into the periodic table, these scientists are finding that nanotubes made from different yet equally interesting materials have intriguing properties quite different from those of their all-carbon cousins and a range of potential applications, e.g., boron nitride (BN) aluminium nitride (AlN), Gallium Nitride (Ga-N), silver, etc. Present thesis describes the structure, synthesis, photoluminescent and mechanical behaviour of carbon, silver and nitride nanostructures. Experimentally crystallography, topography and morphology of these nanostructures have been studied using X-ray diffraction (XRD), Field emission scanning electron microscopy (FESEM), Transmission electron microscopy (TEM) respectively. Topography of carbon nanostructures have also been studied using atomic force microscope (AFM). Electron spectroscopy of these three nanostructures have been studied by energy dispersive X-ray spectroscopy (EDS) and X-ray photoelectron spectroscopy (XPS). Surface studies of carbon nanomaterials have been done using Brunauer-Emmett-Teller surface area analysis, Barrett-Joyner-Halenda pore size and volume analysis (BET-BJH) technique. UV-vis absorption spectroscopy, fourier transmission infrared spectroscopy (FTIR), Raman spectroscopy, steady state energy resolved and time resolved photoluminescence (PL) spectroscopy studies have been opted for the investigation of quantitative, qualitative and optical behavior of synthesized nanomaterials. Mechanical behaviour of these nanomaterials have been studied using nanoindenter but as nanoindenter cannot calculate all mechanical properties so other mechanical properties have been studied using appropriate effective interatomic potentials. The energy barriers of nanotubes and the vibrational modes of hexagonal nanostructures form a part of this study.

Chapter 1 is aimed at providing a general overview of important concepts needed for understanding the present research work. It is by no means a complete overview, as many books are available that provide a comprehensive introduction to the field. The review of literature and motivation for the present research work has been given at the end of chapter.

In chapter 2, complete introduction of the model potentials used to study the nanostructures of carbon, silver and gallium nitride have been given. To describe covalent structures like gallium nitride details of the second generation reactive
empirical bond order potential and its parameters have been mentioned. Parameters have been modified for carbon and III-nitride systems. For silver nanostructures well known Gupta potential has been discussed in detail. The Gupta potential is a many body potential developed on the basis of second moment approximation of the tight binding or linear combination of atomic orbitals (LCAO) scheme. The mechanical behaviour of nanotubes has an important role in understanding nanostructures, and this subject connects with the strain range of nanotubes. The stiffness of nanotubes is important to both the scientist and engineer in various applications.

In chapter 3, various bottom up synthesis techniques to synthesize nanomaterials have been discussed in detail. Single-walled carbon nanotubes (SWCNTs) have been synthesized by chemical vapour deposition where as multiwalled carbon nanotubes (MWCNTs) have been synthesized by hydrothermal method. DC arc discharge method has been opted to synthesize single walled carbon nanohorns (SWCNHs). Microwave technique have been opted to synthesize graphene nanoplatelets (GNPs) and microwave polyl process have been opted for silver nanowires AgNWs). Hydrothermal method is used to synthesize carbon quantum dots (CQDs) with orange juice as precursor. Solvothermal approach have been used to synthesize gallium nitride nanostructures. In synthesized nanomaterials well controlled morphology in nano regime have been observed. Particle growth can be easily tuned with precursor type, precursor concentration, capping agent, pH value of the solution, temperature and reaction time along with other environmental conditions. XRD studies reveal that crystallography is directly related with particle morphology. Recorded diffraction patterns show that carbon and gallium nitride nanomaterials are having wurzite (hexagonal) crystal structure where as silver nanostructures are having face centered cubic structures. On the other hand amorphous structure has been observed for carbon quantum dots. For all synthesized nanomaterials average crystallite size is in nm range and the same is evident from electron microscopy. Moreover, comparison of XRD and electron microscope studies show that carbon and gallium nitride nanomaterials are single nanocrystals where as silver nanowires are multocrystalline.

In chapter 4, FTIR spectroscopy, UV-vis absorption spectroscopy, XPS and Raman spectroscopic studies have been performed for the functionalization confirmation. Optical, quantitative and qualitative analysis of the synthesized pristine and functionalized carbon nanostructures have been performed via energy
resolved, time resolved photoluminescence and EDS studies. Spectroscopic studies confirm the formation of good quality pristine and functionalized carbon nanomaterials with hydroxyl, carboxylic or both groups attached. All these characterizations were also performed for AgNWs and results reveals the formation of good quality AgNWs. The XPS investigation and Raman spectra in AgNWs further show that the PVP molecules are adsorbed on the surface of Ag nanowires through Ag-O coordination. A possible growth mechanism of the Ag nanowires has been proposed. It is implied that the PVP molecules are used as both a protecting agent and a structure-directing agent for the growth of Ag nanowires. For intrinsic and cobalt doped GaN nanocrystals, EDS confirm the formation of highly pure nanocrystals, as it shows the absence of side products or impurities. UV-vis absorption and energy resolved PL spectroscopic studies confirm the broad heterogeneous size distribution of synthesized nanoparticles. Synthesized nanocrystals show multi-chromatic emission spectra. PL emission intensity strongly depends on the doping concentration. Conventional luminescence quencher cobalt plays important role as an efficient luminescence killer in gallium nitride lattice. These nanomaterials seem good candidates for the fabrication of next generation smart opto-electronic devices. In nickel doped gallium nitride nanocrystals addition of dopant reduces the effective band gap of the material, but no dopant related PL emission peak has been observed. Synthesized nanoparticles show the multi-chromatic emission spectra, which indicate the possibility of synthesized nanomaterials as efficient nanophosphors for smart opto-electronic devices. Moreover, the traditional PL quencher nickel acts as luminescence promoter in the GaN nanocrystals. In Tb doped GaN nanocrystals synthesized samples are the ensemble of nanostructures bearing strong, weak and intermediate confinement potentials as confirmed by broad UV-vis. absorption spectra. Synthesized nanocrystals have tunable excitation spectra in the broad spectral width ranging from 241-325 nm. PL intensity and emission wavelength are strongly dependent on the excitation frequency. FWHM of major PL peaks decreases with increasing excitation wavelength between 241-290 nm, which confirm the narrow size distribution of nanocrystals having excitation tunability at lower excitation frequencies. At higher excitation wavelengths (~305 & 325 nm) emission intensity drastically decline due to lesser amount of weakly confined nanostructures. These nanomaterials seem potential candidates for next era smart opto-electronic industrial
applications. Further from time resolved florescence spectroscopy it is very clear that decays become faster with increase in dopant concentration. Also, lifetime values calculated from decay curve have been also used for the calculation of other important optical parameters of optoelectronic industrial interest like trap-depths, transition probabilities, oscillator strengths, Einstein’s coefficients, integrated cross-sections, etc., which will be beneficial for optical calibration curves and detailed phosphor characterization for twenty-first century industrial applications.

In chapter 5, basic definitions of Young’s modulus, poisson ratio, shear modulus, strain energy etc. and the method to calculate elastic modulii have been discussed. Mechanical properties of armchair, zigzag and chiral nanotubes for carbon, B-N, Al-N and Ga-N nanotubes, hypothetical silver nanowires under axial compression have been investigated. Minimization of energy is discussed and results have been compared with experimental as well as theoretical results. In addition to this elastic modulii of less explored structure i.e. carbon nanohorns have been investigated.

In chapter 6 the behaviour of gallium nitride nanotube (GaNNT) in Contact with h-GaN sheet and other GaNNT and also investigated double walled gallium nitride nanotubes (DW-GaNNT) as GHz oscillator In understanding the phenomenon of friction, bouncing, rolling, sliding and spinning of GaNNT on h-GaN surface is presented. The investigation have also been carried out for rotational and translational energy barriers. GaN nanotubes are predominantly double-walled. Seeing the possibility of existence of double walled GaNNTs, the dynamics of double walled GaNNT assembly has been studied. GaNNTs can also be applied as GHz nanotubes oscillators. In this work bulk modulus of h-GaN is computed and single walled (10, 10) GaNNT on a h-GaN surface is considered for bouncing, sliding and spinning. Double-walled GaNNT (5,5) @ (10,10) with a length of 513.5 nm was considered for translational, rotational as well as piston and cylinder motion. To understand the dynamics of GaNNTs, the method commonly used for molecular solids have been adopted; the rigid molecule approximation, assuming intermolecular potential energy to be provided by Vander waals interactions. The molecules in the present case are in the form of individual tubes or the graphitic sheets of gallium nitride. With the potential model the static and dynamic properties associated with various motions of h-GaN-h-GaN, GaNNT-h-GaN and GaNNT-
GaNNT have been studied in detail. In this work (10, 10) GaNNT have been considered.

In chapter 7 the phonons of graphene sheet and h-BN sheet have been described. A dynamical matrix using energy expression of second generation reactive empirical bond order potential for graphene and h-BN sheet have been constructed. Phonon dispersion relations have been calculated in symmetry directions and results are found to agree well with others work. Radial breathing modes of CNTs and BNNTs are also calculated and these are compared well with the experimental values.

Chapter 8 deals with conclusion of the present work along with a brief report of the future prospects like further progress on materials fabrication technologies, the understanding and design of devices, based on quantum mechanics, and importance of cooperative efforts from the basic science level up to system architecture level.