

Index

A

- Ab-initio calculations, 83, 86, 92, 95, 118, 127–129, 132, 136, 142, 143
 - B and N-doped C-NT, 65
 - dielectric function, 67
 - dislocations, 74
 - hydrogen adsorption, 75–76
 - phonon dispersion relation, 72
- Arc discharge technique, 47–48
- Arc jet technique, 48
- Armchair nanotubes, 6
- Atomic transfer radical polymerization (ATRP), 256

B

- Bader analysis, 87
- B-C-N materials
 - bond hybridization and molecular packing, 1–3
 - boron, 13–14
 - boron carbide, 13
 - boron carbon-nitride (BCN)
 - cubic phase hybrid, 16–17
 - hexagonal phase hybrid, 15–16
 - nanostructures, 17–18
 - boron nitride
 - electronic configuration, 9
 - nanotubes, 11–12
 - phases, 9–11
 - carbon
 - carbon nanotubes, 5–9
 - C₆₀ fullerene, 5
 - diamond, 4
 - graphite and graphene, 3–4
 - carbon nitride, 14–15
 - doped CNTs, 18
- B–C–N ternary material system, 2
- Bethe–Salpeter equation, 67, 112, 115, 118

- Bond lengths, sp^2 and sp^3 hybridization, 2
- Boron allotropes
 - nanostructures
 - clusters, 274–276
 - nanotubes, 278–280
 - sheets, 276–278
 - solids
 - α - β_{12} electron density, 274
 - electron-deficiency, 272
 - icosahedral boron solids, 273
- Boron carbide allotropes
 - carbon solids, 280–281
 - hybrid structures
 - B_xC_y nanostructures, 285–287
 - B_xC_y solids, 281–284
- Boron carbonitride nanostructures
 - photoluminescence and electron field property, 207
 - properties and applications
 - field emission, 214–216
 - semiconducting property and photoluminescence, 213–214
 - structure and composition
 - bamboo like structure, 207–209
 - cactus like structure, 209
 - heterojunction, 210
 - phase separation, 209–210
 - single walled BCN
 - nanotubes, 210–213
- Boron carbon-nitride (BCN)
 - cubic phase hybrid, 16–17
 - hexagonal phase hybrid, 15–16
 - nanostructures, 17–18
- Boron clusters, 274–276
- Boron nanotubes (BNT)
 - crystalline bundles, 279
 - single-walled boron nanotubes (SWNT), 278
 - structural motifs, 278, 279

- Boron nitride(BN)
- clusters
 - arc-melting method, 151
 - atomic structure model, 153
 - discrete variational (DV)-X α method, 155
 - heat formation, 156
 - highest and lowest occupied molecular orbital, 155
 - high performance liquid chromatography, 157
 - isolated pentagon rule, 153
 - laser desorption time-of-flight (LD-TOF) mass spectra, 151
 - MacTempas software, 155
 - scherrer defocus, 155
 - cup-stacked structures, nanotubes
 - atomic structure model, 164
 - electron diffraction pattern, 164, 165
 - enlarged STM image, 168, 169
 - highly oriented, pyrolytic graphite (HOPG), 168
 - solubulization, 163
 - TEM image, 164
 - X-ray diffraction patterns, 164, 165
 - electronic configuration, 9
 - encaging Fe nanowires
 - EDX spectrum, 169, 170
 - Fourier transform, 170
 - gibb's energy, 172
 - HREM image, Fe-filled, 171
 - nanocapsules
 - electronic transport properties, 182
 - ellingham diagram, 183, 184
 - magnetic hysteresis loop, 184
 - Scherrer equation, 183
 - TEM images, 186
 - thermal annealing method, 183
 - X-ray diffraction patterns, 183
 - nanohorns
 - atomic structure model, 174
 - composition ratio, 173
 - energy level diagram, 175
 - formation enthalpy, 178
 - HREM images, 174, 176
 - nanoparticles
 - atomic structure model, 181
 - Debye-Scherrer rings, 179
 - electron diffraction pattern, 179, 180
 - filtered HREM image, 179, 181
 - role of van der Waal bondings, 181
 - TEM images, CVD-BN, 180
 - twin boundaries, 179
 - nanotubes, 11–12
 - armchair-type structure, 159
 - Fourier noise filtering, 158
 - HREM image, 159
 - inverse Fourier transform, 159
 - quadruple-walled, structure model, 162
 - phases, 9–11
 - Boron nitride nanotubes (BNNTs), 11–12
 - electronic properties
 - buckling distance, 86
 - chiral vector, 85, 86
 - electron energy loss spectroscopy analysis, 84
 - excitonic binding energy, 91, 92, 94
 - excitonic wavefunction, 94
 - fullerenes physics, 95–96
 - h-BN quasiparticle band structure, 88–89
 - interlayer state, 90–91
 - large ionicity band gap insulator, 87–88
 - optical properties, 91–94
 - polarization effects, 95
 - structure and stability, 85–87
 - total energy, eV/atom, 84
 - Boron sheets
 - buckled triangular sheet, 277
 - carbon nanotubes (CNT), 276
 - 2D pristine configurations, 277
 - Buckling effect, 86
 - Buckminsterfullerene, 5
 - B_xC_y hybrid nanostructures, 286–287
 - B_xC_y solids
 - amorphous boron carbide ($a-B_4C$), 283
 - BC_3 structure, 284
 - boron carbide (B_4C), 281
 - B_xC_{1-x} binary compounds, 283
 - electron-phonon coupling, 283
 - icosahedral B_4C atomic structure, 281, 282
- C**
- Carbon nanostructures, 285–286
 - Carbon nanotubes (CNTs), 5–9
 - Carbon nanotubes (CNTs), doped, 18
 - boron and nitrogen
 - Fermi level, 229, 230
 - Young's modulus, 230
 - covalent or non-covalent functionalization, 224, 228
 - doping types
 - arc discharge technique, 225
 - EDX elemental mapping, 231
 - electron-donating, 225
 - endohedral doping, 225
 - exohedral doping, 226
 - fullerene peapods, 225
 - structural configurations, 228

- electronic and transport characterization
 - densities of states (DOS), 242
 - electron spin resonance (ESR), 243
 - phosphorous and nitrogen
 - heterodoping process, 230
 - high resolution electron microscopy and microanalysis techniques, 231
 - plasma assisted CVD, 237
 - preparation of substitutional, 231–238
 - direct synthesis, 232
 - postsynthesis methods, 237–238
 - spray-pyrolysis technique, 236
 - transmission electron micrographs, 233
 - structural properties
 - atomic structure of b-doped mwnts, 240
 - electron energy loss spectroscopy (EELS), 239
 - scanning electron microscopy (SEM), 239
 - X-ray powder diffraction (XRD), 239
 - types, 225–228
 - vibrational properties, 244–245
 - B and N doping, 246–248
 - efficient metal surfaces, anchoring molecules, 256–262
 - nonsubstitutional doping, 248–252
 - wider applications, 252–256
 - Carbon nitride nanostructures
 - arc-discharge process, 7
 - chemical vapor deposition (CVD), 197
 - electron-conducting properties, 196
 - physical vapor deposition (PVD), 197
 - properties and application
 - conductance and field emission, 204–205
 - hydrogen storage, 205–206
 - lithium storage, 206
 - structure and composition
 - bamboo-like and polymerized nanobell, 197–198
 - formation mechanism, 200–201
 - heterojunction, 200
 - nitrogen concentration and chemical bonding, 202–203
 - separation, 198–200
 - Carbon nitride system, 14–15
 - Carbothermal synthesis approach, 51–52
 - Carbothermic reduction, 51
 - C₆₀ fullerene system, 5
 - Chemical reactivity, 74–75
 - Chemical vapor deposition (CVD), 7, 50–51, 197
 - Chirality, 56
 - Chiral nanotubes, 6
 - Composite boron-carbonitride nanotubes
 - C/BN hetero-junction properties, 98–99
 - h-BC₂N phase
 - electronic properties, 98
 - non-stoichiometric h-B_xC_yN_z structures, 99–100
 - structure and properties, 97–98
 - Coulomb electron-hole interactions, 67, 69
 - Coulomb interaction, 92, 93
 - CVD. *See* Chemical vapor deposition
- D**
- Densities of states (DOS), 155, 157, 175
 - Density-functional perturbation theory, 140
 - Density functional theory (DFT), 89, 98, 112
 - band structure, 66
 - dislocations, 74
 - hydrogen adsorption, 76
 - Density of states (DOS), 9, 65
 - Diamond system, 4
 - Doped carbon nanotubes. *See* Carbon nanotubes, doped
 - DOS. *See* Densities of states
- E**
- EELS. *See* Electron-energy loss spectroscopy (EELS)
 - Electro-mechanical properties, 74
 - Electron-deficiency, 272
 - Electron diffraction (ED), 239–241
 - Electron diffraction pattern (EDP), 56–57
 - Electron energy loss spectroscopy (EELS), 33, 202
 - chemical maps, 61–62
 - core loss region, 57–58
 - doping element composition, 60–61
 - elemental maps, 58, 63
 - spectrum-line (SPLI), 58–59
 - Electron-energy loss spectroscopy (EELS), 107, 116, 124, 125, 129
 - Electronic properties and transport, 64–66
 - Energy-filtered transmission electron microscopy (EFTEM), 58
 - Excimer laser, 28
 - Excitonic effects, 67
- F**
- Ferrocene:etabnol:bencylamine (FEB), 233, 234
 - Filtered Fourier transform, 158–161, 170
 - Fourier transformed infra-red (FTIR) spectroscopy, 33, 34
 - Fowler–Nordheim (FN) mechanism, 204

Fowler-Nordheim plot, 27
 Frenkel excitons, 91
 Fringe spacing, 53

G

Generalized-gradient approximation (GGA), 112
 GGA. *See* Generalized-gradient approximation
 Giant dc Stark effect, 95
 Graphite and graphene system, 3–4

H

HAADF-STEM. *See* High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM)
 Hartree-Fock approximation (HFA), 112, 113
 h-BN. *See* Hexagonal boron-nitride
 Heteroatomic single-wall nanotubes, 45–46
 nano-electro-mechanical systems (NEMS), 76–77
 physical and chemical properties
 chemical reactivity, 74–75
 electro-mechanical properties, 74
 electronic properties and transport, 64–66
 hydrogen storage, 75–76
 mechanical properties, 73–74
 optical properties, 66–69
 vibrational properties, 69–73
 structural and composition analysis, TEM
 electron energy loss spectroscopy, 57–63
 growth mechanism, 63–64
 HRTEM and electron diffraction, 52–57
 synthesis methods
 arc discharge, 47–48
 carbothermal synthesis approach, 51–52
 chemical vapor deposition, 50–51
 laser vaporization, 48–50
 Hexagonal boron-nitride
 ab initio calculations, 89
 contour plots, 90
 crystallographic structure, 85–87
 optical absorption spectra, 93
 quasiparticle band structure, 88–89
 sheet lattice structure, 85
 symbolic representation, 99
 HFA. *See* Hartree-Fock approximation
 High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM), 169
 Highest occupied molecular orbital (HOMO), 112, 117

High-resolution transmission electron (HRTEM), 106
 High resolution transmission electron microscopy (HRTEM), 209, 232, 234, 237, 239
 laser vaporization, 49
 structural and composition analysis
 B- and N-doped C-SWNT, 53–54
 BN-SWNT, 54–55
 boron nitride nanotubes, irradiation, 55–56
 HOMO. *See* Highest occupied molecular orbital
 Hot filament CVD method, 50, 51
 HRTEM. *See* High-resolution transmission electron microscopy
 HRTEM. *See* High-resolution transmission electron

I

Induction-heating furnace, 28
 Infrared (IR) absorption spectroscopy, 105
 Inverse Fourier transform, 159–161, 170, 171

K

Kramers-Kronig analysis, 125

L

Laser vaporization technique, 48–50
 Lattice dynamics. *See* Vibrational properties
 LDA. *See* Local-density approximation
 LD-TOF mass spectrometry, 151, 155
 Local-density approximation (LDA), 109, 112–114, 118, 124, 127, 130
 Local density of electronic states (LDOS), 31
 Lowest unoccupied molecular orbital, 112, 117
 Luminescence, 67–69
 Luminescence spectroscopy
 bound and free exciton, 122
 cathodoluminescence spectrum, h-BN
 crystallite, 122
 electron-phonon coupling, 123
 photo-luminescence excitation (PLE), 122
 stark effect, 123
 LUMO. *See* Lowest unoccupied molecular orbital
 Lyddanne-Sachs Teller relation, 22

M

Many-body perturbation theory, 112, 113

Mechanical properties, 73–74

Meissner effect, 65

Molecular dynamics simulations, 63, 74

Mott–Wannier excitons, 91

Multiwalled boron nitride nanotubes

applications

electronic and chemical

applications, 37–39

hydrogen storage, 35–36

mechanical applications, 36–37

molecular biological

applications, 39–41

bank structure, 39

CL and UV-vis absorption spectra, 37

DNA-BNNT fabrication, 40

FTIR spectra, 34

functionlization

bandgap tuning, 37–39

biomaterials, 40

noncovalent interactions, 36

optimized structure, 38

properties

electron field emission

properties, 26–27

electronic properties, 25–26

mechanical properties, 24

piezoelectric properties, 26

thermal properties, 24–25

Raman spectra, 34

SEM image, 33

synthesis

arc discharge method, 27–28

ball-milling technique, 29

catalytic chemical vapor deposition
(CCVD), 29–30

electron beam in-situ

deposition, 30–31

experimental setup, 33

FeB nanoparticles liquid flow, 30

horizontal tube furnace

growth, 32–35

laser-based method, 28

low temperature growth, 31–32

phase selective growth, 32

plasma jet method, 31

substitution reaction, 28–29

TEM image, 41

thermogravimetric analysis curves, 25

Multiwalled carbon nanotubes

(MWCNTs), 5, 7

MW-BNNT. *See* Multiwalled boron nitride
nanotubes

N

Nanobeam electron diffraction (NB-ED), 56

Nano-electro-mechanical systems (NEMS),
76–77

Nanotube helicity, 53–55, 57

O

Optical absorption spectra

absorption spectrum, BN tubes

dimensionality effects, 121

exciton, wavefunction, 120

SWBNNT, 119

absorption spectrum, bulk h-BN

electron probability density, 117

GW + BS calculation, 116

phonon renormalization, 118

band gap problem

calculation, 113–114

definition, 112

density functional theory (DFT), 112, 113

electron–electron interaction, 114

generalized-gradient approximation
(GGA), 112

GW approximation, 113, 114

Hartree–Fock approximation (HFA), 112

excitonic effects, 114–115

independent-particle picture

band structure comparison, 108, 109

depolarization effect, 110

Lorentzian broadening, 111

random-phase approximation (RPA), 108

RPA absorption spectrum, 108, 110

zone-folding procedure, 108

luminescence in BN tubes, 5

Optical and vibrational properties

luminescence spectroscopy, 122–124

optical absorption spectra, 107–122

phonons and vibrational spectroscopy,
125–143

plasmons and electron-energy loss
spectroscopy, 124–125

Optical properties

dielectric properties, 67–68

emission properties, 66

excitonic effects, 66–67

optical excitations, 68–69

saturable absorption effect, 66

Oven-laser ablation method, 28

P

PE-PLD. *See* Plasma-enhanced pulsed-laser
deposition

- Phonons and vibrational spectroscopy
- diameter dependence, Raman and IR active modes
 - frequency types, 136–137
 - radial phonon modes, 138
 - scaling constants, determination, 138–139
 - equilibrium geometry, 127–128
 - experimental IR spectra, 143
 - experimental Raman spectra, 141–143
 - phonon calculations, 126–127
 - phonon dispersion relations, bulk h-BN
 - longitudinal and transverse optical, 128
 - Lyddanne–Sachs–Teller relation, 129
 - single sheet, h-BN, 130–131
 - tubes, 131
 - Raman intensities
 - cartesian component, 140
 - density-functional perturbation theory, 140
 - single sheet, h-BN, 130–131
 - symmetry analysis, 131–133
 - zone-folding method, 133–136
 - Photoemission and inverse photoemission spectroscopy, 112, 121
 - Photo luminescence excitation (PLE), 122
 - Physical vapor deposition (PVD), 197
 - Plasma enhanced CVD (PECVD), 15
 - Plasma-enhanced pulsed-laser deposition (PE-PLD), 31
 - Plasma torch. *See* Arc jet technique
 - Plasmons and electron-energy loss spectroscopy
 - continuum dielectric theory, 125
 - dielectric constant, 125
 - Kramers–Kronig analysis, 125
 - phonon dispersion relations, 125, 129
 - PLE. *See* Photo luminescence excitation
 - Point defects, 55
 - π - π tight-binding model, 88
- R**
- Radial breathing mode (RBM), 8, 107, 126, 132, 136–141, 144
 - Random-phase approximation (RPA), 109
 - Redox reaction, 29–30
 - Resonant raman spectroscopy, vibrational properties
 - B and N doping, 245
 - endohedral sites, 245
 - in-plane Raman-active mode, 244
 - non-substitutional doping
 - hybridization breaking, 248
 - resonant raman scattering data, 249
 - radial breathing mode (RBM), 244
 - Rydberg series, 92, 114
- S**
- Scanning electron micrographs, 233, 236
 - Scanning electron microscopy (SEM), 31, 32, 179, 180
 - Scanning transmission electron microscopy (STEM), 58
 - Scanning tunneling microscopy (STM), 168, 239
 - Scanning tunneling microscopy/spectroscopy (STM/STS), 106
 - Schottky junction, 200
 - Selected area electron diffraction (SAED), 56
 - SEM. *See* Scanning electron microscopy
 - Single-wall carbon nanotubes (SWCNTs)
 - density of electronic states, 8–9
 - structure, 5–7
 - synthesis techniques, 7
 - Single-walled boron nanotubes (SWBNTs), 278
 - Single-walled carbon nanotubes (SWCNTs), 285
 - Sommerfeld factors, 92
 - Spatially resolved electron energy loss spectroscopy (SR-EELS), 47, 58
 - Spectrum-imaging (SPIM), 58–59
 - Stark effects, 66
 - STM. *See* Scanning tunneling microscopy
 - SWBNTs. *See* Single-walled boron nanotubes
 - SWCNTs. *See* Single-walled carbon nanotubes
- T**
- TEM. *See* Transmission electron microscopy
 - TEP. *See* Thermoelectric power measurements
 - Thermoelectric power measurements (TEP), 243
 - Thermogravimetric analysis (TGA), 205
 - Tight-binding calculations, 65, 70, 74
 - Tight binding method, 24
 - Time-dependent density functional theory (TD-DFT), 91
 - Transmission electron microscopy (TEM), 24, 31
 - electron diffraction pattern (EDP), 56–57
 - electron energy loss spectroscopy (EELS)
 - chemical maps, 61–62
 - core loss region, 57–58
 - doping element composition, 60–61
 - elemental maps, 58, 63
 - spectrum-line (SPLI), 58–59
 - growth mechanism, nanotubes, 63–64

HRTEM

- B- and N-doped C-SWNT, 53–54
- BN-SWNT, 54–55
- boron nitride nanotubes, irradiation, 55–56

U

- UV-visible absorption spectroscopy, 34–35

V

- Van-der-Waals interactions, 143
- Vibrational properties
 - infrared spectrum, 70, 72
 - Raman spectra, 69–71
 - UV Raman spectra, 71–72

X

- X-ray photoelectron spectroscopy (XPS), 202, 239

Y

- Young's modulus, 24, 74

Z

- Zero-loss image, 63
- Zigzag nanotubes, 6
 - growth mechanism, 63–64
 - HRTEM imaging, 54–55, 57
 - hydrogen storage, 76
 - vibrational properties, 70