

## Index

### **a**

ABA stacking 170  
 ABC stacking 170, 171  
 activated carbonyl 85  
 activator molecules 89  
 adamantane 157, 158, 183, 184  
 addition reaction 85  
 adenosine triphosphate (ATP) 89  
 adsorbates 203–206, 230–231  
 adsorption isotherm 203–208, 231  
 aggregation 39–42, 87  
 Ag nanoparticles 8, 78, 227, 229, 230  
 alcohol 77, 78, 80, 84, 85  
 aldehyde functional group 84  
 alkoxide ( $\text{RO}^-$ ) 78  
 alkyl groups 76–78, 81  
 alkylthiols 78  
 amide functional group 87  
 amide solvents 87  
 amine groups ( $-\text{NR}_2$ ) 81–83, 87  
 amino acids 87–89  
 antibonding MO 60, 61, 63, 64, 66, 70, 73, 96, 127  
 archetypes 186  
     cesium chloride ( $\text{CsCl}$ ) 186–187  
     diamond cubic 188–189  
     rock salt ( $\text{NaCl}$ ) 187–188  
     zinc blende 188–189  
     wurtzite 188–189  
 aryl groups 76, 80, 81, 84  
 atomic basis 58, 59, 183–187

atomic orbitals 49–51, 55, 56, 58–64, 66, 67, 70, 96, 104–106, 110, 112–114, 133, 142, 210  
 Au nanoparticles 16, 17, 36, 79, 87, 164, 202, 203, 226, 230, 231

### **b**

back bonding 72, 73  
 back donation 73  
 ball-and-stick model 96  
 band, defined 97  
 band diagram 109, 111, 112, 114, 115, 117–119, 122–127, 142, 144, 152  
 band folding 121–123, 126  
 bandgap 98, 100–103, 114, 116, 118, 124, 127, 145, 153, 155, 158  
 band structure 104, 109–115, 143, 144, 152  
 bandwidth 110, 111, 114, 115, 145  
 base-centered unit cell 179  
 basis set 58, 59  
 BET model 206  
 binding energy 12, 14, 15, 22, 25, 32, 37, 38, 42, 73, 74, 118, 210, 212, 213, 217  
 Bloch function 105–109, 111, 116, 142, 143  
 body-centered cubic (bcc) surface 180, 215  
 body-centered unit cell 178  
 Boltzmann constant 100, 224  
 bond order 61, 66–68, 99, 118, 138  
 bond symmetry 54–55

- Bravais lattices 176–189  
 Buckyball 154–156  
 bulk vs. nanoscale gold 50
- c**
- capping agents 230, 231  
 carbon allotropes 134  
 carbon nanotubes (CNTs) 133  
     bonding and structure 146–149  
     electronic and optical properties 151–154  
     synthesis 150–151  
 carboxylate ion 86  
 carbonyl functional group ( $-C=O$ ) 83  
 carboxylic acid 85–87  
 carbonyl protonation 84  
 carboxyl functional group 86  
 cell membrane 32, 34, 35  
 cellulose molecules 21  
 cesium chloride (CsCl) 186–187  
 charge carriers 102  
 chemical exfoliation 140  
 chemical vapor deposition (CVD) 140  
 chemiluminescence 74  
 chemisorption 203, 204  
 cis-polyacetylene 121  
 cohesion energy 211  
 condensation reaction 89  
 conducting polymers 120  
     band folding 121–124  
     conductivity 124–127  
     structure 120–121  
 conduction bands 98–103, 120, 145, 153, 154  
 conductivity 95, 99–104, 117, 120, 121, 124–127, 136, 137, 155  
 conservation of orbitals 58–60  
 conservative forces 8  
 contact angle measurement 220–221  
 contour surface 50  
 coordination number 83, 167, 168, 171, 173–176, 188, 213  
 Coulomb's law 12, 18  
 crystal chemistry  
     archetypes 186  
     cesium chloride (CsCl) 186–187  
     diamond cubic 188–189  
     rock salt (NaCl) 187–188  
     zinc blende 188–189  
     wurtzite 188–189  
     atomic basis 183–187  
     bravais lattices 176–189  
     coordination geometries 173–176  
     hard-sphere packing  
         three-dimensions packing 169–172  
         two-dimensions packing 167–169  
     lattices and the unit cell 163–166  
     miller indices and crystal planes 190–194  
     crystalline solid 163, 213, 215  
     crystal momentum 106  
     crystal plane 190–194, 228, 229  
     crystal system 176–179, 191, 215  
     cubic close-packed (ccp) 171  
     cubic unit cell 165, 171, 172, 176–178, 180, 182–187, 190, 191, 215, 216, 218  
     curvature effects 222  
     Kelvin equation 224–226  
     Young–Laplace equation 222–224
- d**
- dangling bonds 212, 227  
 Debye force 23–25  
 Debye length 13–15  
 delocalization 58, 136, 155  
 delocalized electron motion 58  
 density of states (DOS) 97, 98, 116–120, 136, 144  
 diamond cubic archetype 188  
 diamondoids 157  
     electronic structure 158  
     structure and bonding 157  
 diamond unit cell 183, 184  
 diatomic transition metals 69–70, 115  
 dipole–dipole interaction 12, 20, 24, 25  
 dipole moment 18–20, 24, 25, 31, 53  
 dispersion force 23, 25, 31, 219  
 dopants 102, 103, 138

double-walled CNTs 146, 149

Drude formula 101

## e

electric dipole moment 18

electronic transitions 61, 73–75, 95, 117

electron motion 50, 51, 53, 58, 104, 105

electron pair 49, 50, 81

electrophiles 84

electrostatic interactions 11–18, 26

elemental carbon 133

endohedral fullerenes 155

energy bands 95–99, 104, 107, 114, 122

entropy 33, 219

equilibrium, defined 10

equivalent hybrid orbitals 55–58, 90, 134

ether functional groups (ROR') 80

ether solvents 80

exohedral fullerenes 155

extended solids

conducting polymers

band folding 121–124

conductivity 124–127

structure 120–121

conductivity 99–103

density of states 116–120

energy bands 95–99

tight-binding approximation 104–115

extrinsic semiconductor 102

## f

face-centered cubic (fcc) 179, 183, 213,

215

face-centered unit cell 178

Fermi–Dirac distribution 100, 102, 103

Fermi energy 98, 144

Fermi level 99, 100

first responders, nanomaterials 199

frontier orbitals 71–73, 98

fullerenes

bonding and structure 154–155

electronic structure 155

synthesis 155

functional groups 15, 34, 49, 75–89, 140,

157, 230

## g

G–C base pairs 22, 23

Gibbs free energy 39, 210, 225

glycols 77

grain boundary 139

graphene 133, 137

bonding structure 137–139

electronic structure 142–145

hybrid orbitals of 137

synthesis and fabrication 139–142

graphene oxide 140

## h

Hamaker constant 29–32, 36

hard-sphere packing

three-dimensions packing 169–172

two-dimensions packing 167–169

hexagonal close-packing 170, 171, 185

hexagonal lattice 168–170

hexagonal unit cell 177, 178

homogeneous nucleation 225, 226

hybridization 21, 22, 55–58, 74, 83,  
133–138, 157, 210

hybrid orbitals 55–58, 67, 133, 134, 137,  
163

hybrid  $sp^3$  orbitals 56, 57

hydrogen acceptor 20

hydrogen bonding 7, 18–23, 32, 33, 78,  
84

hydrogen donor 20, 22

hydrogenic atomic orbitals 50, 51, 104

hydrophobic forces 32–36

hydroxyl functional group 21, 22, 75–80,  
86, 140, 221, 230

## i

inequivalent bonds 55

interatomic forces 7, 49, 210

interfacial energy 218–222

contact angle measurements 220–222

interlayer bond 138

intermolecular forces 3

electrostatic interactions 11–18

hydrogen bonding 18–23

hydrophobic forces 32–36

intermolecular forces (*contd.*)  
 pairwise potential 8–11  
 particle stability and aggregation  
   39–42  
 permanent dipole interactions  
   18–23  
 steric forces 36–39  
 van der Waals forces 23–32  
 interstitial sites 138, 168–170  
 intramolecular forces 20  
 ion–dipole interaction 19  
 ionic solid 14, 26, 163, 173  
 irreducible representation 164

**k**

Keesom force 23  
 Kelvin equation 224–226  
 ketone functional group 84

**l**

Langmuir isotherm 205, 206  
 Laplace pressure 224  
 lattice parameter 164–167, 169–171, 174,  
   176, 178, 183, 185, 190, 191  
 lattice plane 190  
 lattice points 164, 168–170, 172, 173,  
   176, 178–192  
 Lennard-Jones potential 37  
 Lewis acids 84  
 Lewis dot structure 49, 53, 66, 68  
 ligand shell 230, 231  
 linear combination 52, 59, 63, 108  
 linear combinations of atomic orbitals  
   (LCAOs) 55, 58, 64, 67, 104, 105,  
   107, 109, 121  
 linear hydrogen chain 104  
 liposomes 8, 34, 35  
 liquid chromatography 155, 157  
 liquid-vapor (LV) 220  
 London dispersion forces 31, 219  
 London equation 25, 31  
 London force 23, 25  
 low-energy shapes 227–229  
 luminescence 74, 75, 154

**m**

macromolecules 120  
 mercaptans 78  
 mercapto (–SH) groups 77–80  
 metal, crystal structures 163  
 Miller indices 190–194  
 minimizes the total potential energy 8  
 molecular adsorbates 230  
 molecular bonds  
   atomic orbitals 49–51  
   electronic transitions 73–75  
   frontier orbitals and chemical reactions  
     71–73  
   molecular orbital theory 58–71  
   orbital overlap 61–63  
   valence bond theory 51–58  
 molecular orbital 49, 58–60  
   diagram 60–61, 95  
   theory 49, 58–71, 105, 155  
 molecule–surface interaction 26  
 monoclinic system 178  
 monolayer graphene 133, 139, 144,  
   145  
 monomers 120  
 multiply twinned particles 228, 229  
 multi-walled carbon nanotube (MWCNT)  
   146

**n**

nanocarbon  
   carbon nanotubes  
     bonding and structure 146–149  
     electronic and optical properties  
       151–154  
     synthesis 150–151  
   classes of 134  
   diamondoids  
     electronic structure 158  
     structure and bonding 157  
   fullerenes  
     bonding and structure 154  
     electronic structure 155  
     synthesis 155  
   graphene  
     bonding structure 137–139

- electronic structure 142–145  
 synthesis and fabrication 139–142  
 hybridization 133–137  
**nanoengineering**  
 atomic structure and bonding 3  
 chemical principles of 3–4  
 definition of 1  
 intermolecular forces 3  
 surface and interfacial phenomena 3–4  
**nanomaterials** 4, 8, 14, 28, 38, 49, 75, 78, 81, 87, 95, 98, 104, 133–136, 154, 157, 164, 166, 178, 194, 199, 215, 217, 222, 224, 226, 230  
**nanoscale systems** 7, 10, 11, 14, 30, 39, 40  
**nanostructures** 15, 34, 154, 199–202, 223, 226, 227  
**nearest-neighbor broken-bond model** 199, 212–218  
**nomenclature** 75–89  
**nonchemical exfoliation** 140  
**nonplanarity** 135  
**nucleophilic addition** 85  
**nucleophilic substitution reaction** 81
- o**  
**octahedral hole** 173, 187  
**O–H bonds** 75, 78  
**1D lattice** 164, 165  
**1D unit cell** 165  
**1s electron wavefunctions** 52  
**orbital mixing** 67–68  
**orbital overlap** 61–65, 67, 70, 96, 104, 109, 114, 115  
**orthonormality** 50  
**orthorhombic unit cell** 177  
**Ostwald ripening** 225
- p**  
**packing fraction** 168, 169, 171, 172, 201  
**pairwise potential** 8–11, 40–42  
**particle stability and aggregation** 39–42  
**passivation layers** 39, 230–232  
**PEGylation** 81
- Peierls distortion** 124, 125  
**peptide bond** 87, 89  
**permittivity** 12  
**phase equilibrium** 224  
**photoelectron spectroscopy (PES)** 73  
**photoemission spectroscopy** 73  
**photoluminescence** 74, 75, 154  
**physisorption** 204, 206, 232  
**planar density** 192, 193, 215–217  
**polar bonds** 18, 20, 53, 70–71  
**polarizability** 24, 25, 31  
**polycrystalline solids** 163  
**Polyethylene (PE)** 120  
**Polyethylene glycol (PEG)** 80  
**polymantanes** 157, 158  
**polymer-grafted nanoparticle** 39  
**potential well** 10, 37, 204  
**power-law potential** 37  
**p-type semiconductors** 102  
**pyramidalization** 135, 136
- q**  
**quantum mechanics** 25, 36, 49–51  
**quantum number** 50, 69, 152
- r**  
**radius ratio rules** 173, 176  
**rhombohedral unit cell** 178  
**rock salt (NaCl)** 187–188  
**rotational symmetry** 69, 168, 169, 176–178
- s**  
**Schrodinger equation** 110  
**self-assembled monolayers (SAM)** 34  
**semiconductors** 98, 100–103, 123, 126, 145, 155, 189  
**sigma ( $\sigma$ ) bond** 54, 60  
**Si lattice** 103  
**simple cubic (sc) surface** 172, 178, 180, 182, 187, 190, 215  
**single crystalline nanoparticles** 228  
**single-crystal solids** 163  
**single-walled carbon nanotubes (SWCNTs)** 118, 146, 147, 151, 154

- solid-liquid (SL) 220  
 solid-state nanoparticles 231  
 solid-vapor (SV) 220  
 space elevators 133  
 spatial representations 50, 51, 59, 60, 63, 67, 69, 72, 96, 97, 106–109, 111–113, 115, 123, 127, 143  
 spherical cluster approximation (SCA) 201  
 spherical fullerenes 136, 154, 155  
 $s\text{-}p$  mixing 67, 68, 71  
 steric forces 7, 36–39  
 steric hindrance 38  
 subbands 152  
 superhydrophobic surface 221  
 superlattices 174  
 supramolecular 3  
 surface atoms 201–203, 213–215, 227  
 surface energy 208–212, 214, 216, 218–220, 222, 224, 228–230  
 surface fraction 199  
 surface properties  
     adsorption 203–208  
     curvature effects  
         Kelvin equation 224–226  
         Young–Laplace equation 222–224  
     estimation 199–203  
     interfacial energy 218–221  
     nearest-neighbor broken-bond model 212–218  
     stabilize 226–232  
         surface energy 208–212  
     surface relaxation 227  
     surface–surface interaction 27  
     surface tension 211, 223  
     surface-to-volume (S/V) ratio 199, 203  
     symmetry pairing 63–67
- t**
- tetragonal unit cell 177, 178, 191  
 tetrahedral hole 173, 183, 184, 188, 189  
 thermal energy 40, 100, 101  
 thiolate 78
- tight-binding approximation 104–115  
*trans*-polyacetylene 121, 123–126  
 triclinic system 178  
 Turkevich method 230  
 two-dimensional atomic cluster 209
- u**
- unit cell 163–166  
 projection 182–183, 186, 189, 191–193, 215, 217, 218  
 types 178–179  
 unstable equilibrium 10
- v**
- valence band 98, 100, 102, 103, 145, 153, 154  
 valence bond (VB) method 51  
 valence bond (VB) theory 49  
 valence electrons 53, 57, 61, 63, 66, 73, 74, 79, 98, 103, 104, 113, 117, 120, 124, 126  
 van der Waals forces 7, 23–32, 138, 147, 174, 204  
 van der Waals interactions 23, 25, 28, 29, 32, 37, 42, 211, 231  
 van der Waals radius 37  
 Van Hove singularity 117
- w**
- Watson–Crick base pairs 22  
 wurtzite archetype 188–189
- x**
- X-ray photoelectron spectroscopy (XPS) 73
- y**
- Young–Laplace equation 222–224  
 Young’s equation 221
- z**
- zig-zag structure 121  
 zinc blende archetype 188, 189















