

Index

Note: Page numbers in *italics* refers to figures respectively.

a

ab initio calculation 89–90
acenaphthylene-imide (AI) 232
A–D–A conjugated molecules 223
adsorption-based self-assembly 48
AD-TPE compound 134–136, *136*
aggregation-caused quenching (ACQ)
effect 127
aggregation-induced delayed fluorescence
(AIDF) 6, 138–141
aggregation-induced emission (AIE) 3,
4, 44, 103, 127, 164, 322, 336
AIEgens 5–6
air-stable olympicenyl monoradical 354
all-polymer solar cells (all-PSCs) 259
anionic electrolytes 53
anthracene (AN) 114
aqueous zinc-ion batteries (AZIBs) 54
atom force microscope (AFM) 102
atom transfer radical polymerization
(ATRP) 62
azaacene-based small molecules as ETLs
in HPSCs 233–234, *234*
azo diisobutyronitrile (AIBN) 51
azo groups 46

b

band structure 96
4,4'-benzildiboronic acid (BZL) 106,
107, *338*
benzothiophene (BT) 250

benzoyl peroxide (BPO) 51
 β -cyclodextrin (β -CD) 58
bifluorene (BF) core 210
binding energy of exciton 100–101
bio-applications of organic luminescence
materials 3
bisphenaleno-thieno(3,2-b)
thiophene 357
1,2-bisthienylethene (BTE) 114
blade-coating process 269–270
Bloch function 97
Born–Oppenheimer approximation 89
borondipyrromethene (BODIPY)
248, 254
Bridgman–Stockbarger method
37, 38, 39
Broyden and Pulay density mixing
schemes 95
bulk heterojunction (BHJ) 246

c

calixarene based macrocyclic
octaradical 344
carbazole 178, *179*, 209
2-(9H-carbazol-9-yl)ethanol
(CZEO) 179, *179*
carboxymethyl chitosan (CMCS) 52
carrier effective mass 96–99
cetrimonium bromide (CTAB) 48
charged radical materials 358–360,
358–361

- chemical cross-linking 59–62
 - by chemical agents 59–60
 - by heat 60–61
 - by light 61
 - by radicals 61–62
 - chemical gels 50–53. *see also*
 - supramolecular gels
 - chemically doped small molecule
 - HTLs 205, 205–218, 207, 211, 214
 - chemical (molecular) doping 205
 - chemical stimuli 13
 - chemical substances 117–119
 - Chichibabin's hydrocarbon 358
 - chlorobenzene (CB) 251
 - chloroform (CF) 251
 - 1-chloronaphthalene (CN) 271
 - circular dichroism (CD) 181
 - circularly polarized luminescence (CPL) 183
 - "Click Chemistry" reaction 60
 - cocrystals 13
 - conduction band (CB) 203
 - conduction band minimum (CBM) 101
 - configurational polymorphism 317
 - controlled radical polymerization (CRP) 62
 - conventional Bridgman method 38
 - conventional linear polymers 64
 - coordination interactions 43
 - Coulombic attraction 7
 - Coulomb repulsion 89
 - covalent adaptive networks (CANs) 66
 - covalent cross-linked networks 64
 - covalently cross-linked polymers 66
 - covalent organic frameworks (COFs) 333. *see also* metal–organic frameworks (MOFs)
 - construction with different aggregation states 334–336, 335–336
 - optical properties of 336–339, 337, 338
 - properties with different aggregation states 336
 - semiconducting properties of 339–342, 340–342
 - cross-linking
 - advantages of 64–67
 - chemical 59–62
 - physical 62–63
 - radiation 52–53, 63–64
 - crucible descent method. *see* conventional Bridgman method
 - crystal engineering 33–34
 - melt growth 37–40
 - organic crystals grown from solution 34–37
 - vapor phase growth method 37, 38
 - crystal growth technology 34–37
 - crystallization 34, 55, 63
 - crystallization-induced emission
 - enhancement (CIEE) 105–106
 - crystallization-induced phosphorescence (CIP) 5, 106, 145
 - crystal pulling. *see* Czochralski process
 - crystal structure analysis 107, 313
 - cucurbiturils (CBs) 67
 - cyanoacetic acid (CAA) 150
 - cyano-substituted distyrylbenzene (CN-DBS) 36
 - 1-cyano-trans-1,2-bis-(4'-methylbiphenyl)-ethylene (CN-MBE) 114
 - cyclodextrins (CDs) 58, 67
 - Czochralski growth method 37, 40
- d**
- degree of branching (DB) 299
 - delayed fluorescence, generation of 137–138
 - dendrimers 6
 - density functional theory (DFT) 89, 91–92, 210
 - density of states (DOS) 95, 96
 - diamond anvil cell (DAC) 112
 - dibenzo(a,c)-carbazole (DBC) core 215
 - dibenzochrysenetetraamine (DBCTA) 336
 - di-block copolymers 45
 - dibutyltin dilaurate (DBTDL) 66
 - dichlorobenzene (DCB) 225

Diels–Alder (D–A) reaction 51, 60
 4-(4-(*N,N*-dimethylamino)styryl)–
 1-methylpyridinium
 4-methylbenzenesulfonate
 (DAST) 285, 285
N,N-dimethylaniline (DMA) 153
 DINS-2 crystal 286–287, 287
 diphenyl ether (DPE) 271
 diphenylmaleimide derivatives 106, 106
 diphenylmethanofullerene (DPM)
 moiety 225
 dipole–dipole interactions 9
 diradicaloids 356
 DITMS crystal 286, 287
 dodecyl benzene sulfonic acid
 (DBSA) 218
 donor–acceptor–donor (D–A–D)
 molecules 220
 donor aggregates, effects of 248–258,
 248–272, 260–263, 265–271
 dopamine-grafted sodium alginate
 (DA-Alg) 55
 dopant-free small molecule HTLs 218
 undoped HTLs in *n*-*i*-*p* structure
 219–221, 220
 undoped HTMs in *p*-*i*-*n* structure
 221–223, 222
 doping system, mechanoluminescence
 from 188–190
 DOPOD compound 105, 105
 dumb-belled PCBM (D-PCBM) 227
 dye aggregation 3
 dye-doped polymer films 15
 dye-sensitized solar cells (DSSCs) 245
 dynamic covalent bond
 for adaptive materials 66–67
 -based polymer 66
 dynamic covalent cross-linking 51

e

electroluminescence (EL) 5, 140
 electron beams (EB) 52
 electron density distribution (EDD) 210
 electron-rich thiophene-containing
 segments 215

electron transport layer (ETL) 200
 azaacene-based small molecules in
 HPSCs 233–234, 234
 IDT-based small molecules in
 HPSCs 234–237, 235
 NDIs in HPSCs 231, 231–233
 perylene diimides in HPSCs 227–230,
 228–229
 small molecules as ETLs in
 HPSCs 227–238, 237
 electro-optic (EO) modulator 281
 electrostatic interactions 8–9, 10, 43,
 53–54, 54, 69
 emission mechanism of
 mechanoluminescence 163–169
 energy-transfer (ET) 114
 ethoxylated trimethylolpropane
 triacrylate (ETPTA) 53
 9-ethyl-3-vinylcarbazole (ECz) 178
 excimer 130–133
 exciplex-based TADF 143–145
 exciton 100–101
 external quantum efficiency (EQE) 6, 249

f

fill factor (FF) 205
 fluorenyl radicals 353
 fluorescence 125–130
 fluorescent
 mechanoluminescence 169–186
 fluorine-doped tin oxide (FTO) 202
 Förster resonance energy transfer
 (FRET) 117
 free radical polymerization (FRP)
 50–51, 61
 Frenkel excitons 100
 frontier orbital theory 88
 fullerene derivatives 223–227, 247
 fulleropyrrolidinium iodide (FPI) 226
 fused ring electron acceptors
 (FREAs) 247

g

Gaussian basis functions 94
 gel polymer electrolytes (GPEs) 54

gel system 49
 chemical gels 50–53
 strategies for fabricating aggregated structures 49
 supramolecular gels 53–58
 global antiaromatic all-benzenoid macrocycle 359
 glutaraldehyde (GA) 52
 grazing incidence wide-angle X-ray scattering (GIWAXS) 102
 Green's function 95

h

halogen substitution 227
 Hamiltonian operator 88
 helical chiral fluorenyl radicals 353
 hexaazatrinaphtho(2, 3-c)(1, 2, 5)thiadiazole (HATNT) 234
 hexahydroxytriphenylene (HHTP) 334
 hexamethoxyl substituted monoradical 345
 hexaphenylsilole (HPS) 105, 127, 127–128
 highest occupied molecular orbital (HOMO) 204
 HMQ-TMS crystal 285, 285–286
 hole-transporting layer (HTLs) 3, 200
 hole-transporting materials (HTMs) 3, 6
 hole transport layers in HPSCs, small molecules as 204–223
 host–guest system 67–70, 68
 HPSCs 199, 200, 202, 202
 azaacene-based small molecules as ETLs in 233–234, 234
 construction and work principle 202
 device structure 202–203, 203
 IDT-based small molecules as ETLs in 234–237, 235
 NDIs as ETLs in 231, 231–233
 perylene diimides as ETLs in 227–230, 228–229
 small molecules as ETLs in 227–238
 small molecules as hole transport layers in 204–223
 work principle 203–204, 204

hybridized local and charge-transfer (HLCT) 112, 164
 hybridized locally excited and charge-transfer state 112
 hydrogen-bonded organic framework (HOF) 8, 117
 hydrogen bonding 7–8, 10, 41, 55–56, 63, 68
 hydrogen evolution reaction (HER) 342
 hydrophobic interactions 9, 10, 42–43, 54–55, 68–69
 hydrostatic pressure method 112–114
 hyperbranched polymer 296–300, 299
 dendronized 300, 301–302

i

IDT-based small molecules as ETLs 234–237, 235
 imide derivatives 182, 182, 185
 imine-linked COFs 69–70, 334, 336
 in situ multilayered gel polymer electrolyte (ISMGPE) 53
 interactions, types of 9–10
 intermolecular interactions 13
 intersystem crossing (ISC) 126, 137
 ionic composite gels 53
 ionic interactions 63
 isocyanate reaction 60
 isolation chromophore 296
 isomeric arylazopyrazole photoswitches 46
 isomerization 12
 isopropyl (iPr) groups 128
 isostructural doping strategy 5

j

Jablonski diagram 125–126
 J/H/X aggregate 133–137

k

kinetic energy operator 88

l

laponite (LP) 58
 laser-heated pedestal growth 37
 laser heating base method 40

- ligand binding 56–57
- light 114–116
 - chemical cross-linking triggered by 61
 - emission process 125
- light-emitting diodes (LEDs) 41, 61, 64
- linear optical phenomenon 282
- liquid crystal displays (LCDs) 16
- liquid crystal elastomers (LCEs) 65
- liquid crystals (LCs) 64
- liquid–liquid diffusion method 35, 37
- long persistent luminescence (LPL) 152–155
- luminescent behaviors 126
- luminogens 126
- m**
- macroscopic nonlinearities 281–284, 283
- malic-acid-based materials 16
- mechanical grinding method 110–112
- mechanochromic luminescent molecules 109
- mechanochromism (MC) 3, 174
- mechanoluminescence (ML) 3, 128, 163
 - from doping system 188–190
 - emission mechanism of 163
 - from gas discharge of organic crystal 165–167
 - organic 163–165
 - from organic compounds 167–169
 - organic crystals with
 - fluorescent 169–186
 - organic crystals with
 - phosphorescent 186–188
 - special mechanoluminescence phenomena 191–192
- mechanoresponsive luminescence (MRL) 13
- mechano-stimulation 11
- melt growth 37
 - Bridgman–Stockbarger method 37, 38, 39
 - Czochralski growth method 40
 - laser heating base method 40
 - subcooled melt method 38–39
 - zone-melting recrystallization 39–40
- membranes 44–45
- merocyanine (MC) 115
- meso position nitrogen-bridged macrocycle 359
- metal–organic frameworks (MOFs) 322–332, 323. *see also* covalent organic frameworks (COFs)
- methoxydiphenylamine-substituted carbazole (MODPACz) 213–214
- methoxy-substituted triphenylamine (TPA) moiety 212–213
- 1-methyl-1,2,3,4,5-pentaphenylsilole (MPPS) 127, 127
- methylammonium iodide (MAI) 226
- micelles 44, 45, 68
- Michael additions 51
- microscopic nonlinearities 281–284, 283
- molecular aggregates 2, 14–17, 377, 378
 - crystal engineering for 33–40
 - driving force of 7–10
 - history of 4–7
 - molecular interactions in 10–13, 11. *see also specific interactions*
 - motivation 1–4
 - organic compounds in 7
 - role of 13
 - strategic design and control of 13, 14
- molecular exciton theory 134
- molecular magnetic materials 311–322, 312, 314–316, 318–321
- molecular orbital theory 88
- molecular packing 126
- Molecular Uniting Set Identified Characteristic (MUSIC) 13, 17, 107, 147–148, 151, 282, 378
- Müller’s hydrocarbon diradical 347
- multi-chlorinated monoradicals 345
- multi-chlorinated triphenylmethayl monoradicals 349, 351
- n**
- nanoparticle 15, 44
- naphthalene-1, 5-tetracarboxylic diimide (NDI-H) 4, 8, 232
- N-containing heterocyclic derivatives 178–186

- NDIs as ETLs in HPSCs 231, 231–233
 N-hydroxysuccinimide (NHS) 60
 N-isopropyl carbazole (NIPCz) 191
 nitrogen heterocyclic derivatives 169
 nitroxide-mediated polymerization (NMP) 62
 non-aromatic polymers 55
 nonaromatic room-temperature phosphorescence 149–152
 nonconventional chromophores (NCCs) 55
 non-covalent interactions 53, 63, 68–70
 non-fullerene acceptors (NFAs) 247
 non-fullerene small molecules 227
 azaacene-based small molecules as ETLs in HPSCs 233–234, 234
 IDT-based small molecules as ETLs in HPSCs 234–237, 235
 NDIs as ETLs in HPSCs 231, 231–233
 perylene diimides as ETLs in HPSCs 227–230, 228–229
 small molecules as ETLs 237, 237–238
 nonlinear optical (NLO) 4, 33, 281
 norm-conserving pseudopotentials (NCPP) 95
 novel monoradical 345
 N-substituted aromatic groups 232
 nuclear magnetic resonance spectrum (NMR) 102
- O**
 o-dichlorobenzenes (ODCB) 251
 oligomer ether (OE) 225
 optical absorption spectrum 99–100
 optical frequency polarization 282
 opto-electronic MOFs
 other MOFs 328–330, 329–330
 properties of 330–333, 331–332
 structure of 323, 324
 TBAPy-based MOFs 324–325, 325
 TCBPE-based MOFs 325, 325
 TCPP-based MOFs 325–328, 327–328
 organic crystal 33
 with fluorescent mechanoluminescence 169–186
 grown from solution 34
 liquid–liquid diffusion method 35, 37
 ML derives from gas discharge of 165–167
 with phosphorescent mechanoluminescence 186–188
 slow cooling method 35, 36
 solvent evaporation method 34–35
 vapor diffusion method 35, 36
 organic field-effect transistors (OFETs) 33, 43, 51, 248, 356
 organic light-emitting diodes (OLEDs) 1, 5, 33, 345–346
 organic light-emitting transistors (OLETs) 1
 organic linkers 339
 organic luminescence materials, bio-applications of 3
 organic mechanoluminescence 163–165
 organic molecules 2, 284–287, 284–287
 organic open-shell materials. *see* organic radical materials
 organic photovoltaics (OPV) 4
 organic radical materials 341–362, 362
 organic RTP luminogens 107, 108
 organic semiconductors 6, 41
 organic small molecules 204
 organic solar cells (OSCs) 33, 245, 246
 effects of donor aggregates 248–258, 248–272, 260–263, 265–271
 organic systems, microscopic and macroscopic nonlinearities of 281–284, 283
 organic transport materials 201
- P**
 parallel-displaced (PD-shaped) stacking 8
 perovskite solar cells (PVSCs) 3, 245
 perturbation theory 95
 perylene diimides (PDIs) 227–230, 228–229, 260, 361
 phenanthroimidazole 183
 phenothiazine 180, 180–181
 phenyl-C₆₁-butyric acid methyl ester (PCBM) 201, 223–224
 phosphorescence 5, 126, 145–155

phosphorescence energy transfer
 (PET) 107
 phosphorescent
 mechanoluminescence 186–188
 photocatalytic hydrogen evolution 6–7
 photochromic molecules 12, 114
 photodimerization 12
 photo-induced charge transfer 12
 photoinduced organic radicals 360
 photoluminescence (PL) 4, 114,
 125–155, 167, 336
 photoluminescent quantum yield
 (PLQY) 346
 photomultiplier tube (PMT) 164
 photo-stimulation 12
 photovoltaic (PV) technologies 1, 3, 245
 physical cross-linking 62–63
 physical entanglement 62–63
 π - π interaction 8, 10, 14, 43
 Pillar(n)arenes 67
 planar conjugated systems 200–201
 PMB-T crystals 286
 polyacrylic acid (PAA) 50, 56
 polyaniline (PAN) 218
 polyarylmethyl radicals (PAMRs) 344
 polydimethylsiloxane (PDMS) 66
 polyelectrolyte complex (PEC) 53
 polyelectrolytes 63
 polymer encapsulation in
 nanoparticles 44
 polymers for second-order nonlinear
 optics 287–301, 289–295, 297–300
 polymorphic networks 317
 polymorphs 36
 polyphenylene derivatives 38
 polyradicals 345
 polyurethane (PU) 66
 polyvinyl alcohol (PVA) 50, 63
 polyvinylpyrrolidone (PVPON) 56
 porphyrin derivatives 248
 potential energy operator 89
 power conversion efficiency (PCE) 246
 pressure method 109–114
 projector augmented wave (PAW) 95
 pyrene-2, 7-diboronic acid (PDBA) 339

q

quadrilateral-like crystal CN-DBS-B 36
 quantum chemistry 87–93
 quantum dot solar cells (QDSCs) 245
 quantum mechanics 88
 quaternary ammonium halide
 moiety 227

r

radiation cross-linking 52–53, 63–64
 reactive oxygen species (ROS) 4
 rehybridization-induced emission
 enhancement (RIEE) 112
 research methodology
 calculation software 94–95
 chemical substances 117–119
 general methods 102–108
 light 114–116
 organic light harvesting PET
 system 109
 other methods 108
 pressure 109–114
 quantum chemistry calculation 88–93
 semiconductor optoelectronic
 materials, properties of 95–102
 temperature 116–117
 theoretical calculation 87
 restriction of intramolecular motion
 (RIM) 130
 restriction of intramolecular rotation
 (RIR) 128, 129
 restriction of intramolecular vibration
 (RIV) 129, 129
 reverse intersystem crossing
 (RISC) 137
 reversible addition–fragmentation chain
 transfer (RAFT) polymerization 62
 reversible cross-linked polymers 60
 reversible-deactivation radical
 polymerization (RDRP). *see* con-
 trolled radical polymerization (CRP)
 room-temperature ferromagnetic radical
 materials 361, 361–362
 room-temperature phosphorescence
 (RTP) 3, 43, 58, 106, 145–149, 164

S

- Schiff bases 117
- Schrödinger equation 88–89, 96
- second harmonic generation (SHG)
 - 6, 281
- second-order nonlinear optical effect,
 - molecular aggregates for 281–301
- selective solvents 13
- self-assembled monolayers (SAM) 48
- self-assembly 11, 41
 - adsorption-based self-assembly 48
 - aggregation types in 44–45
 - control methods of molecular 45–49
 - drivers of molecular 41–44, 42
 - stimuli-responsive 46, 47
 - supramolecular interactions and 63
 - template-guided 47, 48
- semiconductor optoelectronic materials
 - band structure and density of
 - states 96
 - carrier effective mass 96–99
 - exciton and binding energy of
 - exciton 100–101
 - optical absorption spectrum 99–100
 - properties of 95
 - rational design of optoelectronic
 - materials 101–102
 - structure optimization 95
 - thermodynamic stability and chemical
 - formation energy 96
- semi-crystalline polymers 63
- semiempirical molecular orbital
 - methods 92–93
- signal-to-background ratio
 - (SBR) 154–155
- single-crystal structure analysis 106
- single-crystal-to-single-crystal (SCSC)
 - transformation 311
- single-crystal X-ray diffraction (SCXRD)
 - method 103
- single-molecule magnet (SMM)
 - 311, 320
- site isolation principle 6, 289, 290
- slow cooling method 35, 36
- small molecules
 - chemically doped small molecule
 - HTLs 205, 205–218, 207, 211, 214, 216
 - dopant-free small molecule
 - HTLs 218–223
 - as ETLs in HPSCs 223, 237, 237–238
 - fullerene and derivatives
 - 223–227, 224
 - as hole transport layers in HPSCs 204
 - non-fullerene 227–238
- soft templates 48
- solvent evaporation 34–35, 35
 - self-assembly 46, 47
- solvent vapor annealing (SVA) 253
- spin-coating process 269–270
- spin crossover (SCO) materials
 - 311, 312, 320
- spin-orbit coupling (SOC) 126, 145, 164
- spiro-acridine-fluorene (SAF) core 210
- spirobifluorene-based bulky molecule
 - spiro-OMeTAD 206
- squaraines (SQs) 248
- S-shaped (sandwich) stacking 8
- stacking modes 8
- stimuli-responsive materials 108
- stimuli-responsive self-assembly 46, 47
- structure optimization 95
- subcooled melt method 37–39
- suitable isolation group, concept of
 - 6, 291, 295
- sulfone-locked Chichibabin's
 - diradicals 347
- supramolecular gels 53–59. *see also*
 - chemical gels
- supramolecular interactions,
 - self-assembly and 63
- switching mechanism 321

t

- tannic acid (TA) 56
- TCP-based MOFs 325–328, 327–328
- temperature-dependent aggregation
 - (TDA) 256
- template-guided self-assembly 47, 48

- 1,2,4,5-tetrahydroxybenzene (THB) 336
- tetrakis(4'-carboxy(1, 1'-biphenyl)-4-yl)ethylene (TCBPE) 322, 325, 325
- 1,3,6,8-tetrakis(4-benzoicacid)pyrene (TBAPy) 322, 323
- tetrakis(4-carboxyphenyl)ethylene (TCPE) 322, 323
- 2,2',7,7'-tetrakis(N, N-dimethoxyphenylamine)-9,9'-spirobifluorene (Spiro-OMeTAD) 200–201, 204, 207
- tetraphenylethylene (TPE) 114, 128, 169, 172–178, 228, 322, 336
- tetrathiafulvalene (TTF) 339
- tetrathiazolylthiophene 109, 110
- tetrathienylethene (TTE) 219
- thermal annealing (TA) 249, 268
- thermally activated delayed fluorescence (TADF) 6, 14, 137–145, 164
- thermochromism 116
- Thiele's hydrocarbon 347, 358
- through-space charge transfer (TSCT) 141
- through-space charge transfer based TADF 141–143
- through-space conjugation (TSC) 130
- time-resolved photoluminescence (TRPL) 215
- TPA-based borate ester derivative (TPA-B) 171
- TPE-cored boronic acids (TPEBA) 336
- transmission electron microscope (TEM) 102
- triarylmethyl-based fluorescent radical materials 343–352, 344–349, 351
- triboluminescence 163
- triformylphloroglucinol (TP) 342
- triphenylamine (TPA) 169–172, 210
- triphenylmethane (TPM) 130
- triphenylmethyl radicals 352
- triplet-triplet annihilation (TTA) 164
- triradical molecule 353
- Trux-OMeTAD 222
- “two-level” model 283
- U**
- ultra-soft pseudopotentials (USPP) 95
- ultrasonic wave induced ML (USML) 191
- undoped HTLs in n-i-p structure 219–221, 220
- V**
- valence band (VB) 203, 88
- valence band maximum (VBM) 101
- vapor diffusion method 35, 36
- vapor phase growth method 37, 38
- Virginia Academy of School Psychologists (VASP) 94–95
- W**
- Wannier function 96–97
- Wannier–Mott excitons 100–101
- wave function 88–90
- X**
- X-ray diffraction (XRD) 102
- X-ray single-crystal diffractometer 102
- X-type chromophore 294
- Z**
- zone-melting recrystallization 37, 39–40

