

Index

a

- acenes 136–137
 - and acene-like structures and self-organization motifs 137–141
 - application in organic electronic devices 141–142
- algorithms 2, 4–5, 6, 210–211
 - feasible 211–212, 213
 - unfeasible 212–213
- all-photonic multifunctional molecular logic device 75
- AND logic 14, 15, 18, 63, 64, 66, 67, 83, 90, 100, 101, 102, 108, 113, 115, 116, 194
 - consolidating 84–87
 - optimization 290–294
- arithmetic circuits, in subexcitable chemical media
 - awakening gates 175–176
 - Belousov–Zhabotinsky (BZ) medium
 - localizations in 176–180
 - memory cells with discs 201–203
 - regular and irregular disc networks 193–201
 - vesicles 180–181
 - binary ladder 186–188
 - carry out 191–193
 - sum 188–190
 - collision-based computing 176
 - interaction between wave fragments 181–183
 - universality and polymorphism 183–186
- artificial molecular machines 1
- artificial neural network (ANN) 328
- b**
- Belousov–Zhabotinsky (BZ) medium 1, 2
 - and chemical kinetics 240
 - localizations in 176–180
 - memory cells with discs 201–203
 - regular and irregular disc networks 193–201
 - proof-theoretic cellular automata for 268–271
 - vesicles 180–181
- bidirectional half subtractor and reversible logic device 28–32
- binary ladder 186–188
 - carry out 191–193
 - sum 188–190
- binary logic, with synthetic molecular and supramolecular species
 - chemical computers and 26–27
 - combinational logic gates and circuits
 - all-optical integrated logic operations based on communicating molecular switches 38–41
 - bidirectional half subtractor and reversible logic device 28–32
 - concepts 27–28
 - encoder/decoder based on ruthenium tris(bipyridine) 36–38
 - unimolecular multiplexer–demultiplexer 32–36
 - information processing 25–26
 - sequential logic circuits
 - concepts 41–42
 - memory effect in communicating molecular switches 42–43
 - molecular keypad lock 43–45
 - set–reset memory device based on a copper rotaxane 46–48
- biocomputing 281–283, 293, 294
- biomedical applications 281, 283
- biomimetics 327
- biomolecular systems. *See* biocomputing

Boolean operations 3, 4, 61–64
 Brotherston's cyclic proofs 267–268

c

carminic acid (CA) 157
 catechol 154
 cellular automaton 176, 180, 186–187,
 188, 189, 190, 191, 204
 chemical computers 26–27
 chemical computing 1, 2, 5–7
 chemical kinetics
 – Belousov–Zhabotinsky reaction 240
 – and chemical computing 237–238
 – – as theoretical challenge 238
 – discussion 244–245
 – dynamical systems 241
 – equations 239–240
 – external noise effect 245
 – limited accuracy 242
 – limited x_i values 242
 – natural hypothesis 240
 – need to consider auxiliary chemical
 substances 242–244
 – proof 246–256
 – time factor 241
 – until late 1950s 240
 – solving equations of 211–212
 chemically/biochemically switchable
 electrodes, and coupling with biomolecular
 computing systems 343–350
 collision-based computing 176
 combinational logic gates and circuits
 – all-optical integrated logic operations, based
 on communicating molecular switches
 38–41
 – bidirectional half subtractor and reversible
 logic device 28–32
 – concepts 27–28
 – encoder/decoder, based on ruthenium
 tris(bipyridine) 36–38
 – unimolecular multiplexer–demultiplexer
 32–36
 communicating molecular switches, all-optical
 integrated logic operations based on
 38–41
 cucurbiturils (CBs) 110–116
 cyclic voltammetry 91

d

Davydov splitting 155
 diagonal interaction 137
 digital information processing 281–285,
 287–289
 double-throw switches 60

e

electrochemical atomic layer deposition
 (ECALD) 131–132
 electrochemical atomic layer epitaxy (ECALE)
 126
 electrochemical deposition 125–133
 – nanoheterostructure preparation 133–135
 – nanoparticles directed self-assembly
 135–136
 electrochemistry 305
 – artificial cognitive materials 314–315
 – brain
 – – dynamics 323–324
 – – understanding of 321–323
 – electrochemical dynamics 324–325
 – experimental paradigms for information
 processing in complex systems 325–327
 – intelligent electrochemical platform
 315–321
 – intelligent response and pattern formation
 308–309
 – – emergent patterns and associative
 memory 312–314
 – – functional self-organizing systems
 310–312
 – – patterns in nature 310
 – – self-organization in systems removed
 from equilibrium state and 309–310
 – pattern formation in complex systems
 306–308
 electrode interfaces switchable by physical and
 chemical signals 333
 – chemically/biochemically switchable
 electrodes and coupling with biomolecular
 computing systems 343–350
 – light-switchable modified electrodes, based
 on photoisomerizable materials
 334–336
 – magnetoswitchable electrodes 336–339
 – potential-switchable modified electrodes
 339–343
 encoder/decoder, based on ruthenium
 tris(bipyridine) 36–38
 encoders and decoders 69–71
 engineering luminescent molecules 79–83
 – AND logic consolidation 84–87
 – lab-on-a-molecule systems 87–90
 – logic gates with the same modules in
 different arrangements 83–84
 – redox-fluorescent logic gates 90–95

f

fluorescence 100, 101, 102–108, 110,
 112–115

fluorophore-spacer-receptor modular configuration 81
 Fukui function 150
 functional integration 65

h

half adder 198–201
 – and half subtractors 65–68
 high-concentration chemical computing techniques, for hard-to-solve problems 209–210
 – algorithms 210–211
 – – feasible 211–212, 213
 – – unfeasible 212–213
 – problem significance 213–214
 – – class NP 215
 – – class P and P=NP problem 215–216
 – – description 214
 – – engineering 215
 – – exhaustive search 216
 – – NP-complete problems 216–217
 – – theoretical physics 215
 – propositional satisfiability 217–228
 – relation to optimization
 – – importance 228–229
 – – main idea 229–231
 – – relation to freedom of choice 233–234
 – – relation to neural computing 231–232
 – – relation to reasoning under uncertainty 232–233
 – – relational to numerical optimization 231
 Hilbert's inference rules 266
 hybrid semiconducting materials 121–122
 – digital devices based on PEPS effect 161–167
 – electrochemical deposition 125–133
 – – nanoheterostructure preparation 133–135
 – – nanoparticles directed self-assembly 135–136
 – organic semiconductors 136–137
 – – acenes application in organic electronic devices 141–142
 – – self-organization motifs exhibited by acenes and acene-like structures 137–141
 – photocurrent switching phenomena mechanisms 142–143
 – – composite semiconductor materials 144–148
 – – neat semiconductor 143–144
 – – optoelectronic devices based on organic molecules/semiconductors 160–161

– – semiconductor–absorbate interactions 148–152
 – – surface-modified semiconductor 152–159
 – semiconducting thin layers and nanoparticles 122–123
 – – chemical bath deposition 124–125
 – – nanoparticle microwave synthesis 123
 hydrogen-bonded supramolecular assemblies, as logic devices 102–103

i

information processing 1–7, 25–26. *See also individual entries*
 INHIBIT (INH) gate 62, 90, 106, 107, 108, 111, 113
 internal charge transfer (ICT) 81

k

Kabbalistic–Leibnizian automata, for universe simulation 259
 – historical background 259–264
 – proof-theoretic cellular automata 264–268
 – – for Belousov–Zhabotinsky reaction 268–271
 – – for *plasmodium of Physarum polycephalum* 271–276
 – unconventional computing, as novel paradigm in natural sciences 276–278
 Kröger's theory 127

l

lab-on-a-molecule systems 87–90, 95
 ligand, commonly used 124–125
 light-switchable modified electrodes, based on photoisomerizable materials 334–336
 logic. *See also individual entries*
 – expanding 16–17
 – generalizing 15–16
 – processing 4, 5
 – utilizing 17–19
 logic gates 15, 16, 19, 351
 – combinational, and circuits
 – – all-optical integrated logic operations based on communicating molecular switches 38–41
 – – bidirectional half subtractor and reversible logic device 28–32
 – – concepts 27–28
 – – encoder/decoder based on ruthenium tris(bipyridine) 36–38
 – – unimolecular multiplexer–demultiplexer 32–36
 – elementary 194–197

- logic gates (*contd.*)
 - with the same modules in different arrangements 83–84
- luminescence 29, 31, 32, 36–7, 39, 41, 42, 45. *See also* engineering luminescent molecules
- luminescent switching systems, designing 11–13

m

- magnetoswitchable electrodes 336–339
- Matiyasevich's chemical computer description 219–222
- medical diagnostics 80, 95
- memory effect, in communicating molecular switches 42–43
- metal ion inputs recognition, by crown ethers 100–102
- molecular computation 16, 19
- molecular computational identification (MCID) method 19
- molecular computer 26–27
- molecular keypad lock 43–45
- molecular logic gates 19
 - with [2]pseudorotaxane- and [2]rotaxane-based switches 103–110
- molecular sensors 12–13
- moleculators 68
- molecule-to-band charge transfer 155
- Moore neighborhood 264, 265
- multiplexer–demultiplexer 68–69
 - unimolecular 32–36
- multiplicity, of logic types 28

n

- NAND logic 103, 195
- nanoparticles 336–339, 337, 339, 347, 349, 350
 - directed self-assembly 135–136
 - semiconducting thin layers and 122–123
 - – chemical bath deposition 124–125
 - – nanoparticle microwave synthesis 123
- nanotechnology 11
- nanowires 336, 338
- neural computing 231–232
- noise control approaches, in chemical and biochemical information and signal processing 281–282
 - AND gates optimization 290–294
 - gate level and beyond 286–290
 - gates and networks 283–286, 294–296
- NOR gate 90
- NOT logic gates 82

o

- optoelectronic devices, based on organic molecules/semiconductors 160–161
- organic semiconductors 136–137
 - acenes application in organic electronic devices 141–142
 - self-organization motifs exhibited by acenes and acene-like structures 137–141
- OR gate 195

p

- pentacene 136, 142
- 9-phenyl-benzol[1,2]quinolino[3,4,5,6-*fed*]phenanthridinium (PQP) 140
- photochemistry 11
- photochromic molecules 54–55
- photocurrent switching phenomena
 - mechanisms 142–143
 - composite semiconductor materials 144–148
 - neat semiconductor 143–144
 - optoelectronic devices based on organic molecules/semiconductors 160–161
 - semiconductor–absorbate interactions 148–152
 - surface-modified semiconductor 152–159
- photoelectrochemical photocurrent switching (PEPS) 122, 148
 - digital devices based on 161–167
- photoinduced electron transfer (PET) 11, 12, 80, 81
- phonically switched molecular logic devices 53
 - advanced logic functions 64–65
 - – all-photonic multifunctional molecular logic device 75
 - – encoders and decoders 69–71
 - – half-adders and half subtractors 65–68
 - – multiplexers and demultiplexers 68–69
 - – sequential logic devices 71–75
- Boolean logic gates 61–64
- photochromic molecules 54–55
- photonic control
 - – electron transfer 59–61
 - – energy transfer 55–58
- physical inputs 20
- physical integration 65
- polycyclic aromatic hydrocarbons (PAHs) 139, 140
- porphyrins 56–62, 68, 72
- potential-switchable modified electrodes 339–343

- propositional satisfiability 217
- chemical computing solving hard-to-solve problem of 218, 225–226
 - application 219
 - auxiliary result 226–228
 - discrete-time version of equations 225
 - high-concentration chemical reaction usage 223–224
 - history 218–219
 - Matiyasevich's chemical computer description 219–222
 - resulting equations 224
 - simplified equations 229
 - simplified version 222
- protein folding 213
- pseudorotaxane supramolecular complex 3
- r**
- reconfiguration 62, 71
- redox-fluorescent logic gates 90–95
- rubrene 141
- s**
- Schottky theory 151
- Schrödinger's equation 212
- sensing/switching conversion, into logic 13–14
- sensors 12, 283, 289, 294
- sequential logic circuits
- concepts 41–42
 - memory effect in communicating molecular switches 42–43
 - molecular keypad lock 43–45
 - set–reset memory device based on a copper rotaxane 46–48
- sequential logic devices 71–75
- sequential logic functions 28
- sequent inference rules 266–267
- set–reset memory device, based on a copper rotaxane 46–48
- signal passing problem 198
- signal-responsive electrodes 340, 343
- stimuli-responsive membrane 344
- sulfide ion precursors 124
- superposition, of logic types 28
- supramolecular assemblies, for information processing 99–100
- hydrogen-bonded supramolecular assemblies, as logic devices 102–103
 - metal ion inputs recognition, by crown ethers 100–102
 - molecular logic gates with [2]pseudorotaxane- and [2]rotaxane-based switches 103–110
 - supramolecular host-guest complexes with cyclodextrins and cucurbiturils 110–116
- supramolecular host-guest complexes, with cyclodextrins and cucurbiturils 110–116
- supramolecular systems 1
- surface potential 148
- switching systems 11–13
- conversion to logic 13–14
- t**
- titanium dioxide (TiO₂) 122, 133, 146, 147, 152, 153, 154, 157, 158–159, 162
- u**
- underpotential deposition 127
- universal characteristic 261–262, 263
- v**
- Von Neumann neighborhood 264, 265
- w**
- wave fragments, interaction between 181–183
- Weller equation 82–83
- wide-band-gap semiconductors 122, 133, 135, 148, 151, 153, 161, 162, 164, 167
- work function 149
- x**
- XNOR logic 105
- XOR gate 28, 29, 66, 67, 102, 104, 105, 108, 164, 196

