

Index

a

abacus 3, 4
 7-alanine peptide 219
 alkyl diazonium salts 251
 amorphous carbon 353, 358
 anchor groups 141, 146, 240–245, 247, 249
 Anderson–Newns model 31
 anticrossing 393
 Arrhenius-type temperature dependence 204
 atomic force microscopy (AFM) 32, 57, 58, 108–113, 132, 144, 240, 262, 304, 347, 371
 atomic layer deposition (ALD) 326
 Au–benzenedithiol–Au junctions 49, 215, 250
 Aviram–Ratner model 253, 256–257
 Aviram–Ratner rectification 9, 259, 314

b

1,4-benzenedithiol (BDT) 208, 228, 284, 372, 379
 4,4'-bipyridine junction 241, 374
 Boolean computing 99
 Born approximation 30, 37, 38
 bottom electrodes 143, 149, 151, 155, 252, 314, 315, 317, 318, 321, 328–330, 332, 347, 352–355, 368
 bottom-up synthetic methods 2
 break-junction (BJ) method 31, 39, 58–68, 74, 79, 81, 82, 85, 86, 112, 193, 204, 206, 219, 240, 243, 251,

252, 255, 261, 265, 271, 272, 276, 279, 282, 283, 289, 347, 348, 371, 372, 375, 377, 389, 390

Brownian motion theory 395
 buffer interlayer-based junctions 316, 317

c

carbon nanotubes 91, 100, 103, 115–130, 287, 347, 359–363, 387, 389, 390, 391, 393–395
 carboxyl acid-terminated grapheme 242
 chemical vapor deposition (CVD) 64, 96, 137, 310, 367
 chemically derived graphene (CDG) 324
 chip fabrication process 62
 cleaved edge overgrowth technique 96
 coherent electronic transport 31
 complementary doping-free
 carbon-nanotube field-effect transistors (CNT-FETs) 91
 complementary metal oxide semiconductor (CMOS) 1, 79, 96, 239, 345
 composite electric field-guided assembly (CEGA) technique 101
 conductance switches
 chemical process 275–278
 light-induced switching 271–275
 spintronics-based switch 278–282
 voltage pulse induced switches 270–271

conducting atomic force microscopy (C-AFM) 32, 57, 196

conducting probe-atomic force microscopy (CP-AFM) 15, 108–113, 144, 193, 262, 304

π -conjugated molecular wires 13, 31

conjugated polymers (CPs) 326

contact geometry 123, 243, 245, 250, 265–266, 305

conventional device 8

conventional lithography methods 76

conventional microfabrication techniques 352

Coulomb blockade effects 45, 47

counter electrode (CE) 69, 70, 222, 276

crosswire junction 320–322

current-voltage analysis

- coherent tunneling transport 190–195
- incoherent transport 198–206
- transition voltage spectroscopy (TVS) 195–198

cyanide 155, 247, 379

d

D–A diblock molecular system 260–264

data-processing tool, in embryo 3, 4

Datta–Paulsson model 253, 257–259

density functional theory (DFT) 31, 68, 218, 228, 262, 385

destructive interference 31–33, 381–384, 386

device-electrode coupling 26, 29

device fabrication process 351, 352

dihydrobenzothiophene (BT) thioether linker 247

1,2-bis(4,4-dimethylthiochroman-6-yl) ethylene and 4,4-bipyridine 278

direct evaporation 302, 314–317, 319, 356

direct metal deposition 353, 355, 357

direct quantum tunneling process 393, 395

DNA hybridization sensor 361

double-angle evaporation 76

double-stranded DNA 15, 121

e

electrical rectifier

- anchoring groups 265
- asymmetric Schottky barriers 252
- Aviram–Ratner model 256–257
- contact geometry 265–266
- D– σ -A and D– π -A systems 259–260
- D–A diblock molecular system 260–264
- Datta–Paulsson model 258–259
- different electrodes 264–265
- interfacial distance 266–267
- Kornilovitch–Bratkovsky–Williams Model 257–258
- molecular rectification 256
- molecular rectifiers 267–269
- rectification ratio (RR) 252
- resonant tunneling mechanism 253
- self-assembled monolayers (SAM) 252

electrochemical deposition method 68, 74

electrochemical jump-to-contact scanning tunneling microscope break junction (ECSTM-BJ) 243

electroless gold plating (EGP) 71, 72

electromigration (EM) 58, 60, 68, 78–89, 115, 171, 200, 208, 240, 281–284, 287–291, 308, 328, 348, 377

electron beam lithography (EBL) 17, 58, 61, 64, 81, 85, 105, 118, 326, 359

electron transport

- coherent electronic transport 31
- electron–electron interaction
 - Coulomb blockade 43–45
 - Kondo effect 45–48
- electron-vibration interaction
 - strong-coupling regime 40–42
 - weak coupling regime 37–40
- hopping transport 32–35
- single molecular devices
 - Master equation method 29–30
 - Nonequilibrium Green’s function method 26–29
 - transport mechanisms 26
- thermoelectric transport 48–51

environmental polarization 200
 4-ethynyl-1-thioacetylbenzene 226
 e-vib interaction 34, 36–38, 41, 52
 ex situ electromigration technique 79
 extreme ultraviolet lithography (EUVL)

1

f

feedback-controlled electroburning 131, 132, 242
 Fermi distribution 50, 190, 202, 204, 376
 ferrocenyl alkanethiols 307, 331
 first generation of computers 5
 flip-chip lamination 160, 161, 323, 324
 focused ion beam 58, 79, 102–108
 fourth generation of computers 5
 Fowler–Nordheim (F–N) tunneling 104, 195, 196, 273
 Franck–Condon (FC) matrix elements 41, 42

g

gallium arsenide (GaAs) films 94, 309
 gate electrode 43, 60–63, 81, 82, 110, 123, 216, 251, 253, 270, 275, 279, 282, 286–289, 313
 gold thin films 303
 grain boundary (GB) junctions 104
 graphene-based molecular devices 141, 318
 graphene electrodes 131–133, 135, 137–141, 143, 146, 149, 150, 242, 287, 287, 330
 graphene nanogap electrodes 135, 138, 143, 147, 350, 361
 graphene transferring process 367, 368
 Green's function 27–29, 37–39, 41, 44, 45, 48, 193, 378

h

helium ion beam lithography 105
 highest occupied molecular orbital (HOMO) 13, 31, 145, 191, 244, 245, 304
 Hilbert transform 39

Hückel–model calculations 381
 hybrid devices 153, 265, 351, 393
 hybrid system 346, 350, 393
 hyperfine coupling 393, 394

i

inelastic electron tunneling spectroscopy (IETS) 36, 38, 60, 87, 284, 285, 334, 371
 inelastic tunneling spectroscopy (IETS) applications of 218–219
 charge transport pathway 219–222
 line shape of 214–218
 principle and measurement of 206–209
 selection rule and charge transport pathway 209
 STM imaging 222–225
 inorganic films 94–96
 intramolecular vibrational relaxation or redistribution (IVR) 230

k

Kirchhoff's circuit law 31
 Kondo correlations 89, 291
 Kondo effect 45–48, 78, 82, 88, 89, 279, 283, 286, 290, 291, 389
 Kornilovitch–Bratkovsky–Williams model 257–258
 Kuznetsov–Ulstrup (KU) model 276, 277

l

Landauer formula 28, 31, 49, 193, 245
 Landauer–Büttiker approach 26
 Landauer–Büttiker formalism 31
 Lang–Firsov (LF) transformation 40
 Langmuir–Blodgett method 19, 312–314, 368
 law of corresponding states (LCS) 198
 lift-and-float approach 319–320, 357
 light-induced attachment method 310
 liquid metal contact 302, 314, 326–329
 local chemical bonds 375
 Lorentz force 320, 321

- low-energy electron diffraction (LEED) 306
- lowest order expansion (LOE) 37
- lowest unoccupied molecular orbital (LUMO) 13, 31, 145, 191, 244, 245, 304, 371
- low pressure chemical vapor deposition (LPCVD) technology 96
- m**
- magneto-crystalline anisotropy 280
- magnetoresistance 280, 350, 387–390
- mechanically controllable break junction (MCBJ) 286
- application of 64
- atomic-scale sharp and atomic-scale planar electrodes 65
- attenuation factor 61
- bending and relaxing process 59
- chip fabrication process 62
- clean face-to-face electrodes 60
- deposition method 74
- doped conductive silicon 62
- e-beam lithography technique 61, 64
- high coupling efficiency 60
- micro-fabrication 60
- microheater-embedded MCBJ 63
- noncontact side-gate electrode 62
- Raman intensity 68
- Raman scattering measurement system 65
- self-breaking method 64
- single-molecule junctions 68
- source-drain electrodes 62
- statistical analysis of 65
- stimuli-response and quantum interference 65
- surface plasmon polarizations (SPP) excitation efficiency 64
- thermopower measurements 63
- three-point adjustable bending mechanism 59
- three-terminal chip 60
- UV-vis absorption spectroscopy 65
- X-ray diffraction 65
- metal-ion recognition 361
- metallic liquid top electrodes 354–355
- metallic nanogap electrodes 27, 47, 113, 347–350, 359
- metal–molecule hybridization 250, 375
- molecular beam epitaxy (MBE) technology 94, 95
- molecular devices 8, 9, 13, 15, 17, 25–52, 65, 68, 81, 99, 102, 113, 114, 120, 123, 125, 130, 131, 135, 137, 140, 141, 143, 146, 149, 160, 163, 168, 169, 171, 174, 222, 258, 259, 275, 278, 282, 314, 318, 319, 322, 323, 332, 334, 335, 346–354, 359–368, 371, 386, 387, 389, 390, 395
- molecular electronics
- CMOS options 8–10
- computing, history of 3–6
- conventional semiconductor technology 2
- molecular scale electronics 13–16
- Moore's law 6–8
- organic electronics, molecular materials for 10–12
- molecular rectifiers 8, 16, 252, 255, 256, 259, 260, 265–269, 331
- molecule deformation 200
- molecule–electrode coupling 36, 44, 146, 193, 210, 215, 249, 273
- molecule–electrode interface 121, 146, 163, 189, 191, 210, 214, 223, 267, 272
- molecule–electrode interfacial bonds 219
- Mott formula 51
- multilayer graphene (MLG) films 149, 318, 364, 366, 367
- multiwalled carbon nanotubes (MWNTs) 100, 387
- n**
- nanogap electrodes 2, 352
- Brownian motion theory 395
- chemical deposition 74–75

- conducting probe-atomic force microscopy (CP-AFM) 112–113
 - electrochemical processes 395
 - electromigration and electrical breakdown method
 - device fabrication 79–82
 - electromigration applications 84–89
 - feedback-control 83, 85
 - gate electrode 81, 82
 - gate metal–dielectric interface 82
 - Kondo effect 82
 - pulsed electrical breakdown technique 81
 - self-breaking method 83
 - standard lithographic technique 81
 - transmission electron microscopy (TEM) 82
 - electroplating and feedback system 68–74
 - focused ion beam 102–108
 - inorganic films 94–96
 - liquid flow rates, detection of 399
 - mechanically controllable break junction 59–68
 - molecular rulers
 - conventional photolithographic and molecular lithographic techniques 89
 - molecular scale field-effect transistors (MSFETs) 90
 - N*-hydroxysuccinimide ester (NHS) 90
 - phenylalanine 90
 - self-assembled monolayers (SAMs) 93
 - nanowire mask 100–102
 - on-wire lithography 96–99
 - Poisson-distributed dilute solute 399
 - redox cycling 395, 396, 398, 399
 - scanning probe lithography and conducting probe-atomic force microscopy
 - AFM local oxidation method 110, 111
 - aluminum and residual polymer film 109
 - CuPc molecule 112
 - dip-pen nanolithography (DPN) 111
 - mechanical scratch lithography 110
 - Pt nanogap electrodes 108
 - nanotransfer printing (nTP) method 96, 161, 322, 357
 - nanotube transistor 8
 - nanowire mask 100–102
 - noise spectroscopy 233
 - nonequilibrium Green's function (NEGF) method 25–29, 51, 262, 378
 - non-metallic electrodes 354, 358
- O**
- oblique angle shadow evaporation method 75–78
 - octadecylsilane (OTS) monolayers 310
 - 1,8-octanedithiol 145, 208, 284, 374
 - oligophenylethylene (OPE) 40
 - on-chip nanogap electrodes 396, 397
 - on-wire lithography 58, 96–99, 226, 352
 - optical adhesive (OA) 303, 321
 - optical and optoelectronic spectroscopy 226–232
 - organic field-effect transistors (OFETs) 10–12, 98, 101
 - organic light-emitting diodes (OLEDs) 10–12, 310
 - organic photovoltaics (OPVs) 10, 12
- P**
- parallel fabrication 367
 - phenyl-pyrimidinyl diblock co-oligomers 262
 - photoinduced patterning techniques 310
 - bis(phthalocyaninato)terbium(III) (TbPc2) 391, 392
 - pH sensing 360, 361
 - pH values 277
 - planar configuration 17, 58, 125
 - planar metallic nanogap electrodes 347–349

- polydimethylsiloxane (PDMS) 95, 321, 355
- polymethylmethacrylate (PMMA) 117, 359
- poly(*p*-phenylene ethynylene)s (PPEs) 15
- pulsed electrical breakdown technique 81
- pyridine 228, 247, 249, 374, 375, 378
- pyrolyzed photoresist films (PPF) 171, 316
- pyrrolotetrathiafulvalene (pTTF) 276, 277
- q**
- quantum computing 8, 279
- quantum interference 17, 31, 65, 277, 291, 381–386
- quantum tunneling of magnetization (QTM) 393, 394
- quasi-Ohmic behavior 34
- r**
- Raman scattering measurement system 65
- rectification ratio (RR) 169, 252–254, 263, 266, 268, 307
- reduced density matrix (RDM) 29
- reduced graphene oxide (rGO) films 151, 326, 367
- reference electrode (RE) 70, 275, 276, 289
- reliability and robustness
- mechanical methods 371–375
 - molecular device, on monolayer
 - bottom electrodes 353–354
 - carbon nanotube/graphene interconnection 359–363
 - cross bar architecture 368–371
 - insulating layer with holes 353–354
 - metallic liquid top electrodes 354–355
 - molecule monolayer formation 354
 - non-metallic electrodes 358
 - revised metal deposition 355–357
 - self-assembled monolayers 364–368
 - transferring techniques 357–358
 - quantum interference 381–386
 - single molecular device
 - planar metallic nanogap electrodes 347–349
 - SWNTs 349–350
 - spintronics 386
 - thermoelectronics 375–380
- resonance inelastic tunneling process (RIET) 217, 218
- revised metal deposition 354–357
- s**
- scanning probe microscopy (SPM) 16, 57, 347
- scanning tunneling microscopy (STM) 16, 31, 57, 198, 240, 243, 305, 347, 389
- scattering reduced deposition 355, 356
- second generation of computers 5
- Seebeck coefficients 48–51, 376–380
- self-assembled monolayers (SAMs) 32
- crosswire junction 320–322
 - deposited metal
 - direct evaporation 315–316
 - indirect evaporation 316
 - design flexibility 301
 - diazonium moiety 331
 - graphene possesses 323, 324
 - Langmuir–Blodgett method 312–314
 - layer-by-layer molecular p/n junction assemblies 333
 - lift-and-float approach 319–320
 - liquid metal contact 326–329
 - molecular electronics devices
 - adsorbates and substrates 302
 - Au—S bonding interactions 304
 - copper 309
 - depolarization effect 306
 - ferrocenyl alkanethiols 307
 - gold surface-coated hybrids 303

- gold thin films 303
 - inorganic substrates 305
 - low-energy electron diffraction (LEED) 306
 - n*-alkanethiols 304
 - NHS-MUA 309
 - oligo(phenylene ethynylene)s (OPEs) 304
 - silver 306
 - non-metal substrates 309–312
 - radio frequency (RF) molecular diodes 331
 - self-organization 301
 - soft graphene electrodes 330
 - structure–property relationships 301
 - transfer printing 322–323
 - self-assembly 9, 15, 17, 19, 57, 58, 92, 94, 113, 129, 151, 155, 156, 161, 264, 290, 291, 304, 324, 326, 352
 - self-breaking method 64, 83
 - self-termination reaction 71
 - silicon p–n junction film 72, 73
 - simple tight-binding model 31
 - single-molecule electronic devices
 - anchor–bridge orbital overlap 245–250
 - anchor groups 240–245
 - π^* -antibonding orbitals 247
 - Coulomb blockade 249
 - diodes, transistors and memory elements 239
 - electrical rectifier 252–255
 - electrochemical gate control 288–290
 - electrostatic gate control 282–287
 - HOMO and LUMO conduction 247
 - in situ chemical reactions 250–252
 - ligands and transition metals 247
 - molecular quantum dots 290–291
 - molecule–electrode coupling 249
 - oligosilanes and oligogermanes 249
 - side gating 287–288
 - silicon complementary metal-oxide semiconductor (CMOS) technology 239
 - thermopower measurements 246
 - transport mechanisms 26
 - single-molecule magnet (SMM) compounds 279, 350
 - single-molecule quantum interference (QI) 291
 - single-walled carbon nanotubes (SWNTs) 85, 100, 347, 349–350, 387, 389
 - solution dipping method 310
 - sp² hybridization 58, 114
 - spin–orbit coupling 280, 386, 393
 - spin polarized scanning tunneling microscopy (SP-STM) 389
 - spintronics
 - molecule based hybrid spintronic devices 393–395
 - molecule based spin-valves or magnetic tunnel junctions 387–389
 - SAM-based magnetic tunnel junctions 386–387
 - single molecular nuclear spin transistor 391–393
 - single molecular spin transistor 389–391
 - steady-state approximation 202
 - stereoelectronic effects 138, 270, 271
 - suanpan 3
 - surface-diffusion-mediated deposition (SDMD) 316, 355, 356
 - surface-enhanced Raman spectroscopy (SERS) 65, 87, 226, 228, 395
 - surface plasmon polarizations (SPPs) 64
- t**
- temporary buffer layer during deposition 355
 - tetrabutylammonium fluoride 251
 - tetracyanoquinodimethane (TCNQ) 9, 128, 256
 - tetrathiafulvalene (TTF) 304
 - tetrathiofulvalene (TTF) 9, 256
 - thermoelectronics 17, 375–380
 - thermovoltage 376, 377
 - thiol-DNA-biotin template method 102

- thiol-terminated aromatic molecular junctions 379
 - third generation of computers 5
 - tip-enhanced Raman spectroscopy (TERS) 228
 - transfer printing 96, 302, 314, 319, 322–323, 357
 - transferring techniques 354, 357–358
 - transition voltage spectroscopy (TVS) 189, 195–198, 286, 334
 - transmission electron microscopy (TEM) 82, 92, 288
- U**
- ultraviolet photoelectron spectroscopy (UPS) 195, 233
- V**
- van der Waals (VdW) 152, 158, 324, 330, 349, 375
 - voltage pulse induced switches 270–271
- W**
- Wiedemann–Franz law 48
 - working electrodes (WE) 69, 275, 289