

Index

- ACNTs *see* armchair carbon nanotubes
- acoustic modes 63–65, 71, 72, 151, 154, 173
- acoustic phonons 77, 96, 98, 155, 159, 171
 - long wavelength 73
 - low-frequency 130
- Anderson localization 60, 77, 78, 80
- anharmonic interactions 93, 100, 103–106
- anisotropy factor 119–121
- approaches 15, 16, 31, 110, 113, 114, 124, 125, 129, 144, 154, 173
 - chemical 113
 - decimation 104
 - double exponential fit 38
 - electrical 114
 - first-principles 111, 112, 147
 - frequency-domain 36, 40
 - many-body perturbation 105
 - mechanics-based 117
 - quantum-mechanical 14
 - single-particle scattering 152
 - statistical mechanics 3
 - thermal conductance curves 75
 - time-domain 36
- approximations 2, 112, 134, 179, 194
 - classical 2, 3
 - gradient 112
 - harmonic 66
 - local density 112, 127, 191
- armchair carbon nanotubes (ACNTs) 118–120
- ballistic phonon transport 72, 81, 153, 156, 176, 178, 183
- ballistic thermal conductance 125, 126, 128, 137, 142, 147, 149, 151, 153, 178, 185
- ballistic thermal rectification 177, 178, 186, 187
- ballistic thermal transport 94, 149, 150, 152, 154, 156, 158, 160, 162, 164, 166, 168, 170, 172, 178, 184–186
- ballistic transport 77, 94, 96
- BCs *see* boundary conditions
- behaviors 7, 113, 150, 172, 175, 178, 180, 197
 - low-temperature 75
 - microscopic 3
 - mode splitting 176
 - periodic transmission 150, 180
 - quantum thermal conductance 151
 - two-stage decaying 37
- boundary conditions
 - fixed 16, 18, 122
 - free 18, 45, 48
 - hard wall 159, 171, 174, 175, 178, 179
 - mixed 164

- periodic 45, 47, 48, 122
- stress-free 159, 160, 171, 173, 178
- boundary conditions (BCs) 4, 16, 18, 19, 45, 47, 48, 121, 122, 124, 149, 153, 155, 159, 160, 164, 171, 173–175, 178–180
- bulk materials 35, 60, 150, 151, 190
- bulk silicon 39, 44, 121, 130, 199, 203
- carbon nanotubes 24, 29, 53, 59, 60, 65, 70, 71, 73, 75–77, 79, 81, 82, 87, 88, 92, 146, 147, 184, 193
 - armchair 118
 - zigzag 118
- chemical vapour deposition (CVD) 113, 115
- conductance 126, 133, 134
- conductor 61, 63, 66, 67
 - central 61, 66–68
 - coherent phonon 60
 - isolated 67
- coupling 28, 31, 55, 83, 84, 93, 99
 - harmonic 100
 - resonant 172, 176
- CVD *see* chemical vapour deposition
- Debye temperature 3, 12, 14, 92, 117
- defects 2, 28, 52, 56, 72–75, 81, 147, 152, 173–175, 184, 199
 - extended 130, 147
 - isolated 130
 - local 73, 75
 - natural 28
 - structural 88, 149, 151, 171, 184
 - void 173, 174
- defect scattering 72, 73, 75, 82, 93, 130, 202
- density-functional theory (DFT) 2, 111, 112, 127, 191
- devices 65, 133, 150, 153
 - electronic 130, 176, 202
 - graphene-based QD 143
 - nanoelectronic 190
 - phononic/thermal 27
 - practical 82
 - silicon-based 130
 - thermal quantum 150
- DFT *see* density-functional theory
- dispersion 125, 127
 - linear 127
 - quadratic 127
- dynamical matrix 66–69, 71, 84
 - inter-layer 69
 - intra-layer 69
- edges 121, 123, 124, 135, 159, 164
 - armchair 122, 124, 135, 140
 - zigzag 124, 140
- edge shapes 117, 121–124, 133, 140–142, 144
- electron transport 171, 172, 176, 181
- EMD *see* equilibrium molecular dynamics
- EMD simulations 32, 36, 39, 41, 52, 194
- energy 6, 12, 17, 54, 83, 91, 93, 95, 96, 100, 127, 129
 - defect formation 130
 - electronic 154
 - potential 4, 9, 11, 71
 - total 11, 12, 66, 84, 195
 - zero-point 12, 13, 15
- equilibrium molecular dynamics (EMD) 15, 17, 19, 21, 23, 25–27, 29, 31–33, 35, 37, 39, 41, 43–45, 54, 189

- equilibrium positions 3, 45, 71, 100, 111
- equilibrium states 102–104
- equipartition theorem 10, 11
- evanescent modes 155, 160, 185
- expansion coefficients 161, 163, 165

- fast Fourier transform (FFT) 50, 51
- FD *see* first dip
- Fermi–Dirac distribution function 126, 154
- FETs *see* field effect transistors
- FFT *see* fast Fourier transform
- field effect transistors (FETs) 130
- first dip (FD) 41–44
- fluctuation 42, 79, 80, 102
 - low-temperature 21
 - phonon transmission 80
 - universal 81
 - universal conductance 79, 88
- fluctuation–dissipation theorem 11, 32, 54, 102, 104, 206
- Fourier’s law 25, 27, 34, 59, 60, 64, 94
- Fourier transform 40, 50, 197
- frequency 12, 31, 51, 52, 61, 62, 77, 78, 80, 95, 96, 98, 107, 139, 154–156, 164, 171, 172
 - angular 63
 - oscillation 51
- function 62, 75, 77, 80, 96, 101, 108, 109, 139, 171, 172, 174, 175, 179, 195
 - anti-time-ordered Green’s 101
 - contour-ordered Green’s 100
 - correlation 41, 102
 - level width 66, 69
 - non-equilibrium Green’s 65, 93, 155, 172
 - partition 33
 - real-time Green’s 101
 - retarded Green’s 66
 - surface Green’s 70, 104, 105

- generalized gradient approximate (GGA) 191
- GGA *see* generalized gradient approximate
- GNRs *see* graphene nanoribbons
- GNRs
 - armchair 117
 - armchair metallic 131
 - patterned 130
 - rolled-up 118, 119
 - zigzag 117, 131
- graphene-based devices 130, 133, 135
- graphene-based nanodevices 116, 133, 135, 140, 143
- graphene junctions 130, 133, 135, 137, 139–141, 147, 183
- graphene nanoribbons (GNRs) 93, 116–119, 121–124, 128, 130, 133–137, 141, 144, 147, 183, 184, 186
- graphene quantum dots 130, 141, 143, 148
- graphene sheets 121, 133, 145, 147
- graphene structures 136–138, 140
- Green–Kubo formula 32, 56, 195
- Green’s functions 66, 68, 69, 83, 84, 101–106, 109, 110, 155

- HCACF *see* heat current autocorrelation function
- HCACF
 - longitudinal 51
 - steady state 34
 - truncated 41
- heat bath 4, 10, 11, 15, 16, 18–20, 22–26, 54
- heat bath layers 18–23, 25

- heat bath parameter 22–26
- heat conduction 15, 17, 35, 54, 56, 186
- heat current autocorrelation function (HCACF) 32, 36–38, 41–44, 46, 47, 50, 52
- heat dissipation 65, 117, 133, 143
- heat flux 13, 15–20, 23–25, 55, 88, 94, 150, 153, 154, 181
- heat reservoirs 61, 62, 65, 152
- heat transport 19, 20, 54, 86, 87, 182, 203, 204
- heterogeneous materials 18, 24, 25
- highly oriented pyrolytic graphite (HOPG) 115
- HOPG *see* highly oriented pyrolytic graphite

- interactions 4, 28, 52, 100, 103, 194
 - cell-to-cell 191
 - covalent 7
 - electron–phonon 118, 134
 - graphene–substrate 6
 - inter-layer 6
 - many body 129
 - nonlinear 100
 - phonon–phonon 105
 - spin-phonon 177
 - three-body 7
- interatomic interaction 3, 4, 8
- interface scattering 93, 130, 133, 136, 137, 139, 140, 151, 164, 172, 183

- junctions 131, 134, 140–142, 145, 186
 - metal-semiconductor 130, 131
 - molecular 152, 185

- Landauer formalism 94, 95, 110, 153
- Landauer formula 89, 96, 97, 125, 126, 128, 134, 153, 180
- Langevin heat bath 11, 15, 18, 20, 22–27
- LDA *see* local density approximation
- LDOS *see* local density of states
- LEM *see* localized edge mode
- local density approximation (LDA) 112, 127, 191
- local density of states (LDOS) 74, 107, 108, 134
- localized edge mode (LEM) 18–20, 22, 26
- log–log scale 27, 28

- MD *see* molecular dynamics
- MD
 - microcanonical ensemble 45
 - tight-binding 197
- MD simulation 2–4, 10–14, 28, 194, 195, 197, 200
- mechanisms 19, 77, 78, 82, 121, 129
 - diffusive scattering 78
 - resonance 52
- model 4, 6–8, 88, 149, 153, 178, 179, 193, 195
 - atomistic 152, 155
 - dielectric continuum 156
 - elastic 149, 153, 155, 156
 - elastic continuum 153, 180
 - gas 2
 - realistic 135, 141
 - theoretical 2, 27, 190
- modes 11, 12, 19, 20, 26, 52, 61, 62, 65, 71, 72, 138, 151, 152, 154, 159–161, 163, 164, 169, 171–177, 202
 - active 71
 - edge 18

- flexure 72
- high-frequency 12
- incident 172
- in-plane 157, 158
- longitudinal 28, 30, 52
- out-of-plane 157, 158
- transmitted 169
- transverse 28, 31, 51, 52
- molecular dynamics (MD) 1–4, 6, 8, 10–57, 75, 81, 89, 117, 152, 183, 189, 190, 203, 205
- nanostructures 2, 26, 31, 54, 70, 144, 150, 151, 180, 185, 190, 203
 - carbon 71
 - low-dimensional 82, 150, 180, 190
 - suspended insulating 98
- nanowires 17, 18, 23, 35, 63–65, 98, 114, 151, 152, 171, 184–186, 204, 205
 - defective 152
 - dielectric 152
 - double-bend 152
 - isotope-doping 191
 - superlatticed 191
 - surface-decorated 191
 - surface-disordered 191
 - vacancy-defected 191
- NEGF *see* non-equilibrium Green's function
- NEGF formalism 81, 84, 98, 100, 101, 105
- NEGF method 81, 98, 106, 110–112, 116, 117, 121, 133, 134, 144
- NEMD *see* non-equilibrium molecular dynamics
- NEMD simulation 16, 17, 29
- NH heat bath *see* Nosé–Hoover heat bath
- non-equilibrium Green's function (NEGF) 65, 93, 98, 103, 105–107
- non-equilibrium molecular dynamics (NEMD) 15, 17, 19, 21, 23, 25–27, 29, 31
- Nosé–Hoover heat bath (NH heat bath) 11, 18–20, 22–27
- optical phonons 37, 63, 98
 - high-frequency 130
- oscillation amplitude 50, 52
- PDOS *see* phonon density of state
- phonon branches 126, 172
- phonon channels 72, 155
- phonon density 73–75, 197
- phonon density of state (PDOS) 197, 201
- phonon dispersion 125, 126, 128
- phonon modes 63, 77, 78, 95–97, 118, 122, 134, 155
 - acoustic 77
 - ballistic 152
 - elastic 180
 - optical 65
 - vibrational 151
- phonons 60–63, 74–76, 78, 80, 91–96, 98–100, 117, 125–127, 129, 130, 134, 138–140, 149, 150, 152–154, 176–178, 182–184
 - ballistic 151
 - coherent 60, 76
 - coherent long-wavelength 51
 - diffusive 63
 - long-wavelength 38
 - short-wavelength 47
- phonon scatterings 93, 99, 103, 121, 122, 124, 134, 138, 139, 184, 193, 201

- phonon transmission 69, 78, 79, 109, 110, 119, 122, 123, 134, 139, 140, 147, 172, 177, 179
- phonon transmission function 63, 65, 66, 72, 73, 82, 84, 96, 106, 110, 111, 138
- phonon transport 60–62, 65, 78, 81, 87, 88, 92, 95, 183, 184, 186, 187, 203
 - coherent 60, 76, 84
 - diffusive 151
 - fully-quantum 81
 - longitudinal 31
- properties 5–7, 111, 150, 170, 171, 191, 205
 - analytical 102
 - ballistic transmission 158
 - chemical 8
 - dynamic 102
 - electronic 29, 117, 145, 150, 193
 - intrinsic 27, 95, 152
 - lattice vibration 196
 - mechanical 113
 - optical 111
 - quantum-mechanical
 - microscopic 14
 - statistical 36
 - system-level 14
 - thermal-transfer 202
 - thermal-transport 133
- QDs *see* quantum dots
- QD structure 136–138, 142, 143
- quantum correction 11, 13, 14, 53
 - small 14, 15
- quantum dots (QDs) 130–133, 135, 137, 143, 147, 183
- quantum structures 150, 151, 153–156, 163, 170, 171, 178, 185
- quantum systems 12, 13, 150, 151, 158, 170
- quantum thermal transport 91, 93, 95, 97, 98, 106, 111, 112, 144, 183, 185
- quantum wires 64, 152, 170, 178, 184, 186, 187
- reactive empirical bond order (REBO) 54, 118, 134, 147
- REBO *see* reactive empirical bond order
- regions 19, 71, 75–78, 140, 158–162, 164, 165, 170, 176–178
 - diffusive 81, 94, 117, 125
 - high-frequency 122
 - hollow 44
 - low-energy 73
 - low-temperature 63, 92, 117, 127
 - shell 49
 - short-time 38, 42
 - transition 94
- reservoirs 4, 151, 154, 158, 170
 - cold 95, 153, 170
 - hot 95, 153
- scaled thermal conductance 118–124
- scaling factor 13–15, 21
- scattering matrix 162, 163, 169, 170
- scattering-matrix method 149, 152, 153, 155, 158, 180, 187
- scattering region 67, 76, 83, 84, 110, 172
- scatterings 61, 63, 74, 92, 94, 99, 138, 155
 - diffusive 77
 - elastic 158, 170
 - electron-phonon 61
 - geometric 93, 98

- isotope 80
- many-body 93
- silicon 3, 7, 8, 52, 54, 57, 130, 192, 194, 195, 200, 203, 206
 - crystalline 6, 40, 42
 - diamond-structured 3, 7
- silicon nanowires (SiNWs) 2, 13, 14, 16–18, 23, 44–49, 51, 53, 121, 129, 183, 189–194, 196–206
- simulations 2, 8, 15, 16, 18, 32, 44, 45, 146, 189, 190, 193, 196, 197, 199
 - finite time 41
 - molecular-dynamic 71
 - numerical 24, 190
 - practical 5
- single-interface junction 134–142
- single-walled carbon nanotubes (SWNTs) 27–29, 70–81, 85, 144
- SiNWs *see* silicon nanowires
- SiNWs
 - hydrogenated 193, 198, 201
 - naked surface 193, 196, 197
 - nitrogenated 193, 198, 199
- structures 27, 29, 50–52, 54, 130, 134, 136, 139–141, 150, 152, 158, 170, 171, 173, 176, 191
 - asymmetry 138
 - band 192
 - complex 133
 - geometric 153, 178
 - lattice 201
 - nanoscale 150, 183
 - stub 152, 178, 179, 185, 186
- superlattices 151, 182, 183, 186
- surface 2, 18, 45, 47, 48, 52, 87, 145, 191, 193, 197, 199, 201, 205
 - naked 197
- surface atoms 16, 202
- surface defects 199, 201, 206
- surface functionalization 189, 193
- surface layer 69, 197, 198
- surface nitrogenation 198–201
- surface nitrogenation ratio 194, 200, 201
- surface passivation 189, 193, 201, 202
- surface scattering 31, 199
- SWNTs *see* single-walled carbon nanotubes
- systems 2–6, 8, 10–12, 15–18, 32, 33, 60, 68–71, 93, 94, 98, 100–103, 116, 117, 124, 125, 129, 140, 141, 157, 158
 - carbon 92
 - electron 70
 - equilibrium 102
 - finite 19
 - finite-width 125
 - graphene-based 134
 - many-body 2, 112
 - mono-atomic 38
 - noninteracting 103
 - periodic 125
 - semi-infinite 69, 145
 - symmetric 61
 - three-terminal 176, 177
 - two-terminal 153, 176
- technique 66, 113, 145
 - fabrication 65
 - noncontact 129
 - numerical 65
 - optothermal Raman measurement 114
 - quantum correction 14
 - recursive Green's function 66, 67
 - thermal measurement 113
- temperature gradient 15, 17, 18, 22–24, 34, 91, 94
- temperature jump (TJ) 18, 20, 23, 26

- temperature profile 17–19, 22–25, 114
- theory 52, 56, 59, 60, 115, 187
 - basic 60, 111, 116
 - classical kinetic gas 2
 - density-functional 2
 - elastic 156
 - elasticity 151
 - fluctuation–dissipation 15
 - functional 111, 127, 191
 - fundamental quantum 152
 - kinetic 93
 - linear response 32
 - Lippmann–Schwinger 84
 - mesoscopic transport 94
 - mode coupling 27
- thermal conductance 60, 61, 63–65, 72, 73, 75, 94–98, 109, 110, 118, 119, 121–126, 133–139, 141–143, 146, 147, 151–156, 172–175, 178–180, 183–186
 - anisotropic 119
 - ballistic 116, 125, 128, 129
 - electronic 126
 - lattice 152, 185
 - low temperature 151, 152, 178
 - phonon 152, 153, 185
 - quantum 174
 - suppressed 150
- thermal conductivity 13, 14, 17–19, 22–25, 27–32, 34, 35, 37–41, 44, 45, 47, 53, 54, 56, 57, 183, 184, 190, 191, 193, 195–199, 201–205
 - accumulative 41, 42, 44
 - longitudinal 196, 198
 - phonon 189, 193, 197, 201
 - room temperature 29, 115
 - spectral 40, 41
 - static 41
 - tailored 190
- thermal contact resistance 135, 137, 138, 140, 148
- thermal devices 82, 150, 176, 181
- thermal disturbance 33, 34, 56
- thermal equilibrium 32, 33, 61, 93
- thermal management 31, 133, 144, 180
- thermal memory 150, 181
- thermal phonons 151
- thermal properties 2, 18, 22, 23, 26, 150, 155, 176, 179
- thermal rectification 25, 55, 109, 176, 183
- thermal rectifier 82, 88, 150, 178, 181
- thermal reservoirs 154, 155
- thermal resistance 93, 138, 152
- thermal transistor 82, 88, 150, 181
- thermal transport 3, 19, 20, 57, 59, 60, 82, 91–94, 98, 100, 101, 115–117, 125, 128, 129, 133–136, 140, 141, 143–147, 183–186
 - nanoscale 64
 - non-Fourier 60
 - phonon-derived 60
- thermal transport carriers 91, 99, 117
- thermal transport properties 70, 81, 103, 106, 110, 112, 115–117, 125, 133, 141, 143, 144
- thermal transport systems 98, 99, 111
- thermoelectricity 143, 144, 152, 181, 185
- TJ *see* temperature jump
- transmission 62, 65, 72, 74, 151, 177, 186
 - perfect 65, 77, 173
 - resonant 179
 - zero 180
- transmission coefficient 89, 149, 155, 163, 164, 169, 171–173, 176, 177, 180

- transmission functions 95, 96, 111, 123
- transport 80, 89, 91, 94, 95, 130, 138, 141, 144, 176
 - diffusive 94
 - electrical current 64
- transport properties 116, 117, 133, 138, 140, 150, 153, 170, 176, 178, 180
- transport system 93, 99, 110, 117, 136, 138, 141
 - all-graphene 130
 - graphene-based 140
 - graphene-related 144
 - open thermal 103
 - realistic 144
 - thermal 95, 98, 99
- UCF *see* universal conductance fluctuation
- universal conductance fluctuation (UCF) 79–81, 88
- vector 156, 158, 163
 - chiral 71, 85
 - heat current 196
 - translation 85
 - translational 85, 86
- wave 156, 158, 162, 165, 169, 180
 - acoustic 51, 52
 - elastic 149, 153, 159, 173
 - elastic phonon 149

