Index

a

acentric factor 167, 171, 335
acetaldehyde phenylhydrazone (APH) 440
acid-base (AB) interaction 73
activated complex 177–179, 392
activation energy 175, 179, 445, 447, 540, 545
activity coefficient 108, 121, 350, 353, 354, 361, 617
alloying 262, 296
amorphous solids 7, 260, 261, 403
analogous models 202
angle-averaged potentials 140
angular momentum 17, 22, 88, 283
anisotropic materials 92, 313, 316–319
Antoine constants 644
Antoine equation 386
Argand diagram 561, 587
Arrhenius equation 175, 179
Arrhenius-type behavior 178
Aufbau principle 283
auxiliary functions 101–102, 206
average absolute deviation (AAD) 163, 216
Axilrod–Teller three-body interaction 75
azimuthal quantum number 282

b

balance equations 83–85, 117, 118
Bartenev-Ritland relationship 534
basis set 49, 245, 280
Bayes' theorem 631, 633
Benedict–Webb–Rubin (BWR) equation 167
Berthelot's rule 71, 72, 168
binomial approximation 64
Bloch condition 271
Bloch's theorem 267, 277, 297
body-centered cubic (BCC) 268, 343, 411
Bohr atom 62, 500
Bohr frequency 36
Boltzmann
  approach
    recurrence 558
    time invariance 558–560
  constant 128, 155, 159, 298, 548
  entropy 132, 395
  factor 149, 193, 220, 351, 486
  probability (distribution) 131, 132, 202
  statistics 135
bond energy 284–286, 290–293
bond moments 190
bond valence model 289
Born–Mayer
  approach 290–294
  expression 291
  model 288–289
Born–Oppenheimer approximation 43, 57
Born repulsion 66
Born's theory 418
Born–von Karman boundary conditions 267
Bose–Einstein (BE)
  distribution 136
  particles 43
  statistics 136
bosons 43
Bravais lattice 265, 266, 275
Brillouin zone (BZ) 266, 273, 520
Buckingham potential 75
bulk modulus 103, 303–304, 314
Burgers vector 308, 309, 422, 434, 493

c

Cailletet–Mathias law 169
calculus of variations 26, 591–592
canonical energy 21
canonical equations 24, 560

Phases of Matter and their Transitions: Concepts and Principles for Chemists, Physicists, Engineers, and Materials Scientists, First Edition. Gijsbertus de With.
© 2024 WILEY-VCH GmbH. Published 2024 by WILEY-VCH GmbH.

capillary length 342
capillary wave theory (CWT) 341–343
Carnahan-Starling (CS)
  expression 163, 166, 216
  model 238
  thermodynamics 173
Cartesian coordinate system 482, 589
Cauchy–Riemann conditions 587
Cauchy's equations of motion 88–89
Cauchy stress tensor 87
Cayley tree 474
cell models 219–226
cellular automaton 542, 580
center of mass 22, 60, 79, 157
central-limit theorem 633–635
chain branching 264
change of variables 590–591
characteristic equation 595, 596
characteristic function (cf) 631
charge-dipole interaction 60, 61
chemical equilibrium 106–109, 228, 396
chemical isomerism 263
chemical potential 104, 107
Clapeyron–Clausius equation 235, 375–376, 386, 387
Clapeyron's equation 314, 375, 376
Clapeyron *vs.* Clapeyron-Clausius 375–376, 388
classical kinetic theory (CKT) 388–393
classical mechanics
  conservation laws 21–23
  frames, particles and coordinates 15–17
  Hamilton's equations 24–26
  Hamilton's principle 19–21
  Hamilton's principle for continuous systems 26–27
  Lagrange's equations 19–31
  virial theorem 27–28
classical nucleation theory (CNT) 397–399, 427
classical particle mechanics (PM) 11, 15, 125
classical thermodynamics
  auxiliary functions 101–102
  chemical content 103–106
  chemical equilibrium 106–109
  dissipative forces
  equation of state 100
  four laws 93–99
  mechanical equilibrium 101
  quasi-conservative forces 99–100
  thermal equilibrium 101
Clausius–Duhem inequality 98, 117
Clausius–Mossotti equation 182, 185, 189, 190, 250, 415, 503, 508
coarse graining model 557, 567, 576, 577
coherence length 467–470, 473
cohesive energy 72, 261, 291
coil-helix transformation 485–486
coincident site lattice (CSL) 310–311
Cole-Cole equation 188
Cole-Davidson equation 188
communal entropy 222–224
complex conjugate 31, 32, 67, 593
composite function 586
compressibility equation 203, 204, 215
condensation
  classical nucleation theory 397–399
  drops and bubbles 395–397
  modifications 401–404
  molecular aspects 404–408
  nucleation kinetics 399–401
conditional probability 631, 633
configuration interaction (CI) 47
conservation laws 21–23
conservation of energy 3, 115, 571, 652
conservation of mass 612
conservation of mechanical energy 95
continuity equation 84
continuous phase transitions 12, 372
continuous phase transitions L-G
  limiting behavior 458–461
  mean field theory, Landau theory 461–462
    fluid transitions 463–465
  renormalization 469–475
  scaling
    homogeneous function 465–466
    scaling lattices 467–469
    scaling potentials 466–467
continuous transformation theory (CTT) 536
continuum mechanics (CM) 11, 110
  balance equations 83–85
  kinematics 79
    general deformations 80–81
    material and spatial coordinates 79–80
    small displacement gradient approximation 81–83
  kinetics 85
    angular momentum 88

Cauchy's equations of motion 88–89
linear momentum 86–88
principle of virtual power 86
mechanical energy 90–91
nature of continuum 78
stress tensor 89–90
continuum theory 79, 247
convolution theorem 604
coordination number (CN) 200, 226, 357
correlation energy 49, 274
correlation matrix 133
Coulomb energy 59, 273, 278, 287, 622
Coulomb hole 49, 281
Coulomb interaction 60, 61, 293
Coulomb's law 189, 622
coupling parameter 205, 210
Courtney distribution 400, 401
Courtney factor 400, 401
covalent crystals 269, 286
covalent energy 284
covalent radii 293, 649
covalent radius 284
Cramers's rule 594
critical micelle concentration (CMC) 361
critical opalescence 460
critical point (CP) 10, 168, 173, 340
crossover theories 476
crystalline solids 7–9, 260, 333, 478, 525
crystallization 270
crystallization of polymers 449
crystallized polymers 265
cumulants 634
cumulative distribution function 631
Curie principle 120

d

d'Alembert's principle 18
Dalton's law of partial pressures 107
Dawson's integral 484
d-dimensional (*d*D) complex vector 30
Debye
equation 183, 188, 190
frequency 299
interaction 62
model 242, 244, 250, 299, 302
relaxation 502
temperature 241, 300
Debye-Drude equations 188
Debye-Langevin equation 182–185
deep eutectic solutions 354
defects
Frenkel 305, 307
one-dimensional 308
other 310–312
Schottky 305, 307
zero-dimensional 305
degree of polymerization (DoP) 619
degrees of freedom (DoF) 16, 30, 105, 137, 219, 241
density-density correlation function 337
density functional theory (DFT) 278, 279, 336–341
density matrix 139
density of states 127, 271
density operator 53, 54
derived units 12
base 12
derived 12
Devonshire theory 518
dielectric matrix 624
dipole moment 58, 60
Dirac delta function 33, 127, 208, 297, 481, 603
direct correlation function 207
discontinuous phase transitions 12, 372
discontinuous phase transitions L-G
evaporation kinetics
classical kinetic theory 388–393
secondary effects 393–394
evaporation thermodynamics 385–387
inert gas presence 387–388
reverse transition, condensation
classical nucleation theory 397–399
drops and bubbles 395–397
modifications 401–404
molecular aspects 404–408
nucleation kinetics 399–401
discontinuous phase transitions S-L
freezing/solidification
nucleation and growth 444–445
polymers and metals 448–451
water 451–452
influence of pressure 436–440
mechanical/bulk melting
dislocations 422–424
interstitialcies 424–427
interstitials 419–422
lattice instability 418
melting/fusion 411–414
simulations 427–428

discontinuous phase transitions S-L (*contd.*)
vacancies 418–419
vibrational instability 414–417
perspective on melting 442–443
polymer melting 434–436
thermodynamic/surface mediated melting 428
dislocations revisited 432–434
nanoparticles melting 428–430
perspective on melting 442–443
vacancies revisited 430–432
dislocation
screw 308
edge 308
dislocation theories of melting (DTM) 422
dispersion energy 64, 68, 69
dispersion relations 297
divergence theorem 602
dividing surface 176
donor-acceptor interaction 73
Doolittle equation 537
doublet distribution function 199
double Yukawa potential 71
Drude atom 69
Drude model 63, 64, 74
Dulong-Petit law 301
dynamical matrix 297
dynamic compressive stress (DCS) 544
Dyson series 35

e

edge dislocation 308
effective potential energy 44
Ehrenfest–Prigogine–Defay (EPD) 378, 380, 534
Ehrenfest ratio 379, 380
Ehrenfest relations 379
eigenvalue equation 32, 37, 594
Einstein
frequency 299
function 414–415
model 299, 300
elastic constants 492
elastic energy 314, 491
elastic solid 247
electric field strength 181
electron affinity (EA) 2, 284
electronegativity (EN) 284, 285
electronic polarization 501
electronic transitions 147
electrostatic interaction 59, 68
electrostatics elements
Coulomb, Gauss, Poisson and Laplace 622–624
dielectric matrix 624–626
spherical cavity 626–627
elementary reactions 174
embedded atom method (EAM) 296, 428
empirical entropy 97
energy barrier theory 394
energy density 110
energy equation 203
energy-momentum relation 611
energy of motion 4
Eötvös constant 334
Eötvös' rule 74, 332
equations of state (EoS) 100, 155, 164
equilibrium
Boltzmann approach 557
recurrence 560–561
time invariance 558–560
closure 578–580
constant 109, 175
distances 58
energy 58
formal approach 563–567
Gibbs approach 561–563
information theory approach 571
high and low probability manifolds 572–577
physical approach 567–571
equipartition theorem 151
equivalence principle 18
ergodic theorem 562
ergodic theory 557
Euclidean space 608
Euler condition 327, 592
Euler description 81
Euler's equation 100, 587
Euler's theorem 100, 104, 328, 587
Euler strain tensor 81
evaporation 385
evaporation kinetics
classical kinetic theory 388–393
secondary effects 393–394
exchange-correlation energy 280
exchange hole 49
excluded volume 135
extended defects 310
extent of reaction 106

f

face-centered cubic (FCC) 267
Fermi-Dirac (FD)
  distribution 136, 271
  particles 42, 43
  statistics 136
Fermi
  energy 271
  golden rule 53
  hole 49
  sphere 271
fermions 42
ferroelectric behavior
  microscopic approach 518–521
  thermodynamic approach 516–518
ferroelectric materials 512
ferroelectric transformation
  dielectric materials 500–501
  electronic polarization 501–503
  ferroelectric behavior
    microscopic approach 518–521
    thermodynamic approach 516–518
  ferroelectric materials 512–516
  orientational polarization 510–511
  preliminaries 498–501
  space-charge polarization 511–512
  vibrational polarization 503–507
    rigid ion model 507–510
first law 96, 115–116
Fisher's relation 460
Flory–Huggins (FH) entropy 352, 621
fluctuations 132, 136
Fock operator 48
force constant 58, 72
Fourier series 271, 563, 605
Fourier's law 391
Fourier transform 339, 604
Fox equation 528
Fox-Flory equation 528
Fox-Loshaek equation 528
Frank constants 492
Fréedericksz transformation 494
free volume theory (FVT) 536
freezing/solidification
  nucleation and growth 444–445
  polymers and metals 448–451
  water 451–452
Frenkel defects 305, 307
Frenkel frequency 240
frequency operator 547
functional derivative 592

g

Galilei's Principle of Relativity (PoR) 15
Galilei transformations 16, 608, 610
gamma function 603
gases
  corresponding states principle 168–171
    extended principle 171–174
  dielectric behavior
    basic aspects 180–182
    Debye-Langevin equation 182–185
    estimating μ and α 190–193
    frequency dependence 185–190
  equations of state 164–168
  kinetic theory of 155–158
  transition state theory 174
    activated complex 177–179
    chemical kinetics basics 174–175
    equilibrium constant 175–176
    link to experiment 179–180
    potential energy surfaces 176–177
  virial expansion 159–162
    systematic extension 162–164
Gauss' law 623
Gauss' theorem 88, 91, 602, 605, 656
Gauss-type orbital (GTO) 49
Gedankenexperiment 114
generalized force 20
generalized gradient approximation (GGA) 281
generalized Langevin equations 547
generalized van der Waals (GvdW)
  partition function 237
  theory 197
generic distribution function 198
geometric mean frequency 298
Gibbs adsorption equation (GAE) 329
Gibbs–Bogoliubov inequality 151, 152, 580
Gibbs–Duhem equation 104, 105, 121, 329, 396
Gibbs–Helmholtz equation 103, 205, 333
Gibbs–Thomson equation 450
Gibbs
  distribution 131
  energy 102, 105, 106, 329, 351, 353, 371, 374, 397, 418, 424, 425, 429, 444, 466, 469–471, 532, 533, 539
    of formation 398

Gibbs (*contd.*)
entropy 128, 571, 572
equation 100, 101, 110, 116, 181, 205
theorem 107
Ginzburg temperature 464
Girardi–Rimini–Weber interpretation 580
glass transition 12
glassy materials 528–529
lattice gas approach 541–543
mode-coupling theory (MCT) 546–549
phonon theory 543–546
property changes at T_g 529–530
structural approach 535
continuous transition theory 539–541
free volume theory 536–539
thermodynamic approach 530–535
glassy second phase 261
global part motion 79
Golden rule 570
grain boundary phase 260
grand partition function 130
grand potential 104
gravitation constant 18
Greek index 13
Grüneisen equation of state 302, 303
Grüneisen parameter 241, 298, 302, 303, 416, 423, 426
G-space 126
Guggenheim's formula 340
Guggenheim–Staverman entropy 352, 621

h

Hamaker constant 333
Hamaker–Israelachvili expression 333
Hamilton–Cayley equation 597
Hamilton
density 27
equations 24, 125, 556
function 126, 138, 141, 208, 471, 580, 611, 656
matrix elements 49
operator 37, 42, 44, 53, 266
principle 15, 19
principle for continuous systems 26
hard sphere (HS) 69, 225, 537
fluid 213
vs. Lennard-Jones 214
harmonic approximation (HA) 296
harmonic oscillator (HO) 21, 40, 137, 142, 561
Hartree–Fock self-consistent field (HF-SCF) equations 48
Hartree–Fock (HF) theory 47, 49, 245, 270
Havriliak–Negami equation 188
heat capacity 300–302
Heaviside function 214, 603
heavy water (D_2O) 2
Heisenberg
equation of motion 36
picture 36
uncertainty relations 39, 53
Helium atom 46
Hellmann–Feynman theorem 45
Helmholtz energy 61, 102, 104, 105, 131, 135, 140, 222, 226, 237, 241, 245, 247, 298, 302, 306, 320, 328, 330, 332, 337, 349, 357, 380, 382, 402, 403, 421, 423, 424, 428, 461, 480, 484, 488, 490, 509, 517, 543
density 482
of formation 398
Henderson's theorem 152
Henry's law 108
Hermite functions 40
Hermitian matrix 32
Hermitian operator 34
Hertz–Knudsen equation 389, 390
Hertz–Knudsen–Schrage equation 390
heterogeneity function 404, 446
heterogeneous nucleation 404, 446, 452
hexagonal close packed (HCP) 267
high-probability manifold (HPM) 573
Hilbert space 30, 563
Hildebrand's rule 387
Hohenberg–Kohn functional 279
hole model 226
hole theory 231
holonomic constraint 16
holonomic system 16
homogeneity of space 22
homogeneous function 465, 587
Hückel approximations 276
Hund's rules 283
hydrogen bond 72, 74, 264, 513
hydrostatic equilibrium 101
hydrostatic stress 314
Hyper–Netted Chain (HNC) approximation 211
hysteresis 312

i

ideal dipole moment 58
ideal solution 108
implicit function 586
induction interaction 62
inertial force 85
inertial frame 15
inexact differential 585
information theory 557, 563
information theory approach
  high and low probability manifolds 572–577
inorganics 261
integral equation method
  Ornstein-Zernike equation 206–209
  potential of mean force 212–214
  Yvon-Born-Green equation 209–210
interacting particles 141
interaction energy 60
interaction picture 37
interchange energy 227, 614
interfaces
  adsorption
    isotherms 360–365
    solutions 349–355
    statistics of 357–360
    thermodynamics 355–357
  semi-empirical considerations 331–336
  solid surface structure 343–345
    surface roughening 345–349
  theoretical considerations
    capillary wave theory 341–343
    density functional theory 336–341
  thermodynamics of 326–331
interfacial tension 327
intermolecular interactions 11
  model interactions 69–72
  quantum approach 66–69
  refinements
    accurate empirical potentials 74–75
    hydrogen bonding 72–74
    three-body interactions 74
  semi-classical approach 57–59
    dispersion interaction 63–64
    electrostatic interaction 59–61
    induction interaction 62–63
    total interaction 64–66
internal contributions
  electronic transitions 147–148
  rotations 145–147
  vibrations 142–145
internal energy 96
internal forces 85, 112
internal pressure 220
internal variables 111
interphase 326
interstitialcy theory 425
interstitial impurities 305
interventionism 557
ionic crystals 287, 290
ionic energy 284
ionic radii 287, 645
ionization potential (IP) 2, 284
isochoric process 96

j

Jacobian matrix 590
Jordain's principle 19

k

KAM theorem 562
Kauzmann's paradox 532
Kauzmann temperature 532
Kechin equation 439
Keesom interaction 61, 65, 68
Kelvin equation 396
Kihara potential 70, 75
Kihara parameter 639
kinematics 79
  general deformations 80–81
  material and spatial coordinates 79–80
  small displacement gradient approximation 81–83
kinetic energy (KE) 4, 17, 20, 26, 27, 273
kinetic fragility index 550
kinetics 85
  angular momentum 88
  Cauchy's equations of motion 88–89
  linear momentum 86–88
  principle of virtual power 86
kinetic theory, gases 155
Kirchhoff equation 386
Kirkwood equation 210, 253, 254
Kirkwood factor 251, 252
Kirkwood–Fröhlich equation 253, 254
Knudsen layer 388
Kohlrausch–Williams–Watts equation 188
Kohn–Sham operator 279
Kohn–Sham orbital 281
Kosterlitz–Thouless class 346, 349

Kramers–Kronig transform 587
Kraus operator 565
Kraut–Kennedy relation 438
Kronecker delta 31, 297, 584

l

Lagrange density 26
Lagrange description 81
Lagrange function 18, 611
Lagrange multipliers 16, 571, 588
Lagrange's equations 19, 22
Lagrange technique 654
lamellae 265
Lamé's constants 313
Landau and Landau-like theory 380
Landau function 463
Landau theory 461–462, 482
  fluid transitions 463–465
Langevin equation 193, 519
Langevin function 183
Langmuir–Blodgett trough 360
Langmuir isotherm 363
Laplace operator 41
Laplace's equation 331, 587, 623
Laplace transform 604, 605
lattice dynamics 296
lattice energy 291
lattice gas model 226, 613
  athermal entropy for chain-like molecules 619
  first approximation or quasi-chemical solution 615–619
  zeroth approximation or mean field solution 613–615
law of mass action 176
Legendre
  equation 625
  operator 41
  polynomial 481
  transformation 24, 102, 104, 572, 588, 589
Lennard–Jones (LJ)
  parameters 636, 637
  potential 70, 75, 286
Lennard–Jones–Devonshire (LJD) 220, 413, 419
Lewis structures 292
Lifshitz theory 333
Lindemann's rule 415, 416, 423, 437
linear combination of atomic orbitals (LCAO) 48
linear irreversible thermodynamics 11, 120
linear momentum 20, 86–88, 89
Liouville's equation 25, 55
Liouville's theorem 25, 126, 202, 556, 558, 560, 656
liquid crystal elastomers 478
liquid crystal transformation
  coil-helix transformation 485–486
  discontinuous transformation 481–482
  elastic energy and defects 491–494
  Fréedericksz transformation 494–495
  Maier-Saupe theory 483–485
  nature and types 478–480
  nematic-isotropic transformation (NI) 480
  Onsager theory 486–488
  orientation as internal variable 480–481
liquids
  approaches to 197–198
  continuum aspects 245–248
  dielectric behavior 249–255
  distribution functions 198
    energetics 203–206
    structure 200–202
  Hard-Sphere *vs.* Lennard-Jones 214–217
  integral equation method 206
    integral equations 210–212
    Ornstein-Zernike Equation 206–209
    potential of mean force 212–214
    Yvon-Born-Green Equation 209–210
  phonon theory 240–244
  quantum cluster equilibrium model 244–245
  structural models 218
    cell models 220–226
    hole models 226–231
    hole theory 231–237
  van der Waals model 237–239
local density approximation (LDA) 280
local equilibrium 100, 110
local relaxation event (LRE) 240, 543, 545
London (dispersion) interaction 63, 64, 68
  binomial approximation 64
London theory 483
Lorentz-Berthelot (LB) rule 71
Lorentz
  contraction 610
  rule 71
  transformations 608, 610, 611

Lorenz-Lorentz expression 192
low-probability manifold (LPM) 573
Lyddane-Sachs-Teller (LST) relation 506, 507

m

macroscopic thermodynamics (MT)
  classical thermodynamics
    auxiliary functions 101–102
    chemical content 103–106
    chemical equilibrium 106–109
    equation of state 100
    four laws 93–99
    mechanical and thermal equilibrium 101
    quasi-conservative and dissipative forces 99–100
  field formulation
    first law 115–116
    second law 116–118
  internal variables 111–113
  linear approximation 118–121
  local state 113–115
Madelung constant 287
magnetic quantum number 282
Maier-Saupe theory 483–485
majority rule 468
Margules equation 353
mass density 84
Massieu functions 102
master equation (ME) 565, 569, 576
mathematical concepts
  calculus of variations 591–592
  change of variables 590–591
  derivatives, differentials and variations 584–586
  Dirac function 603–604
  eigenvalue problem 594–597
  extremes and Lagrange multipliers 588
  Fourier transform 604–606
  gamma function 603–604
  Heaviside function 603–604
  Laplace transform 604–606
  Legendre transforms 588–589
  matrices and determinants 592–594
  matrix decompositions 597–598
  scalars, vectors and tensors 598–601
  symbols and conventions 584
  tensor analysis 601–603
  useful expressions 606–607
maximum-term method 149
Maxwell-Boltzmann (MB) distribution 136, 138, 155
Maxwell
  distribution 388, 390, 406–408, 566
  element 111, 242
  equal area rule 375
  equations 505
  relations 103, 303, 653
McLean isotherm 363
McMillan's model 485
Mean-field Kinetic Nucleation Theory (MKNT) 401
mean field solution 613
mean free path 157
mean normal stress 89
mean-spherical approximation (MSA) 209, 211
mechanical energy 21, 90–91
melting 411
memory function 547
mesogens 478
metal glasses 529
metallic bonding 270
metals 261
micro-canonical distribution 131
microconvection theory 394
microscopic theory 245
microscopic thermodynamics 11
  equipartition of energy 150–151
  fluctuations 149–150
  Gibbs-Bogoliubov inequality 151–152
  interacting particles 141
  internal contributions
    electronic transitions 147–148
    rotations 145–147
    vibrations 142–145
  mode or average 148–149
  non-interacting particles
    many particles 134–135
    pressure and energy 135–136
    single particle 134
  semi-classical approximation 136–140
  statistical thermodynamics
    entropy and partition functions 128–132
    fluctuations 132–134
    preliminaries 125–128
Miedema model 296, 343
Mie potential 70, 286

Miller indices 267
minimal basis set 49
Minkowski space 608
minus-first law 575
mode coupling theory (MCT) 546
  generalized (GMCT) 546
  inhomogeneous (IMCT) 548
molar density 106
molar polarization 182
molar surface energy 332
molecular crystals 261, 270, 286
molecular dynamics (MD) 197, 404, 427
molecular orbital (MO) 47
mole fraction 105, 108, 109
moment generating function 632
momentum density 27
monomers 263
Monte Carlo (MC) 197, 214, 469
Mori-Zwanzig formalism 549
Morse potential 71
multipole expansion 59, 61

n
nanoparticles melting 428
Navier-Stokes liquid 248
near equilibrium thermodynamics (NET) 394
nearly free electron (NFE) model 271
nematic-isotropic (NI) transformation 480
nematic potential 483
Neumann's principle 312
Newton
  equation 559
  First Law 20
  laws 17, 296
  liquid 248
  Second Law 20
  Third Law 22
N-(4-methoxybenzylidene)-4-butylaniline (MBBA) 479
non-interacting particles
  many particles 134–135
  pressure and energy 135–136
  single particle 134
normal boiling point 11
normal distribution 633
  central-limit theorem 634
normal water (H_2O) 2
nucleation kinetics 399
number representation 55

o
Onsager
  equation 190, 250
  model 487
  reciprocal relations 118
  theory 486
open system 130
orbital electronegativity model 290
order-disorder transformation 513
order parameter 458, 478
organic glasses 529
orientational polarization 510
orientation interaction 68
oriented amorphous 264
Ornstein-Zernike (OZ) equation 206, 207
orthogonalized plane wave (OPW) 273
orthogonal polynomials 354
orthonormal basis 600
oscillator strength 68, 503

p
Padé approximant 163
parachor 645
partial derivative 584
particle mechanics (PM) 11, 15, 125, 555
partition function 131, 576
Pauling's scale 284
Pauli's exclusion principle 42
Peng-Robinson (PR) equations 167
percolation 472, 473
Percus-Yevick (PY) approximation 211
perfect gas 107, 577
perfect solution 107
permeation theory 394
permittivity
  relative 181, 249, 498, 624
  vacuum 181, 498
permutation operator 42
perspective melting 442
perturbation theory 51
phase function 126
phase rule 105
phase space 125, 126
phase transitions 12
phenomenological equations 118
Philosophiæ Naturalis Principia Mathematica 17
phonon theory 197, 240–244, 543
Planck
  constant 34, 134, 139, 271

equation 385
formulation of the third law 99
Poincaré's recurrence theorem 560
point defects 260
Poisson bracket 24
Poisson's ratio 313, 318
polar covalence model 290
polarizability 62, 623
polarizable ion model 507
polycrystals 260
polymer crystallization 450
polymer melting 434
polymers 263–265
Porter's equation 350
potassium dihydrogen phosphate (KDP) 513
potential energy (PE) 608, 652
curve 57
density 27
landscape 57, 176
surface 57
potential of mean force 212
potentials
Born-Landé 291
Born-Mayer 291
Buckingham 75
Coulomb 59, 622
double Yukawa 71
exp-six 75
Kihara 75
Lennard-Jones 70, 75, 286
Mie 75
Morse 71
refinements
accurate empirical potentials 74–75
hydrogen bonding 72–74
three-body interactions 74
screened Coulomb 71
square-well (SW) 70, 163
Sutherland 70, 164
Yukawa 71
power density 111
Poynting equation 387, 396
preferential orientation 264
pressure equation 203
Prigogine-Defay equation 380
primitive lattice 265
principal axes 89, 596
principal quantum number 282
principal stresses 90
principal values 596
principle of corresponding states (PoCS) 169, 171–173, 234, 335
principle of indifference 630
principle of insufficient reason 630
principle of maximum entropy (PME) 557, 571, 630
principle of relativity (PoR) 608
principle of virtual power (PoVP) 19, 86
principle of virtual work (PoVW) 18
probability 629
probability amplitude 38
probability density function (pdf) 631
proper length 610
prototype phase 513
pseudo-vector component 314

q

quadrupole moment 58, 60
quantum cluster equilibrium (QCE) model 197, 244
quantum mechanics (QM) 11, 125
Born-Oppenheimer approximation 43–44
density functional theory 278–282
density operator 53–55
fundamental quantum kinematics 30–33
fundamental quantum kinetics 35–37
Hartree-Fock method 47–51
interpretation
exact solutions 37–39
harmonic oscillator 40–41
many particles 42–43
particle-in-a-box 39–40
rigid rotator 41–42
nearly free electron model 270–275
operators representation 33–35
perturbation theory 51–53
tight binding method 275–278
variation principle 44–47
quantum number 40
quasi-chemical approximation 228, 615
quasi-equilibrium assumption 177
quasi-ergodic theorem 562
quasi-harmonic approximation (QHA) 298
quasi-lattice models 218
quasi-static process 96

r

radial distribution function (RDF) 199
random close-packed (RCP) 526

random-phase approximation (RPA) 209
random variable 631
Raoult's law 108
rate of reaction 174
ratio rules 268
Rayleigh-Schrödinger perturbation equations 51
reaction coordinate 177
reaction principle 86
rectilinear diameter 169
Redlich–Kister expansion 353
Redlich–Kwong (RK) equation 166
  modified RK (mRK) 166
Redlich-Kwong-Soave (RKS) equation 167
reference coordinate system 79
regular solution (RS) model 349
renormalization group (RG) 469
reorganization energy 286
representative volume element (RVE) 78, 84, 100, 110, 112
Reststrahlen frequency 415, 507
reversible process 96
rheonomic system 16
rigid body motion 23, 79
rigid ion model 507
rigid rotator 41
root-mean-square speed 156
rotational isomerism 263
rotation matrix 589
Rydberg states 148

S

Sackur-Tetrode equation 136, 577
saturated liquid 247
scalar 598
scaled particle theory (SPT) 197, 217, 489
scaling lattices 467
Schmidt decomposition 564
Schmidt number 564
Schottky defects 305, 307
Schrödinger equation 35, 37, 40, 41, 43, 44, 52, 271, 275, 278, 569
  picture 36
  time-dependent 36
  time-independent 36
Schwartz inequality 31
scleronomic system 16
screw dislocation 308
second law 98, 116–118
semi-classical approach 57
  dispersion interaction 63–64
  electrostatic interaction 59–61
  induction interaction 62–63
  total interaction 64–66
semi-classical approximation 136
semi-classical partition function 138
Shannon-Prewitt radii 293
significant liquid structure (SLS) theory 231
Simon-Glatzel equation 436–439
single crystals 260
singlet distribution function 198
Slater determinant 43, 47
Slater's rules 284
small-angle grain boundary 310
small displacement gradient (SDG) 81
sodium dodecyl sulfate (SDS) 361
solid on solid (SoS) model 348
  absolute 348
solid surface roughening 345–349
solids
  crystalline structures 267–270
  defects
    extended defects 310–311
    one-dimensional defects 308–310
    zero-dimensional defects 305–308
  empirical approach
    atoms, ions and electronegativity 282–285
    covalent and molecular crystals 286–287
    metallic crystals 294–296
  inorganics and metals 260
  ionic crystals
    classical approach 287–289
    electronegativity approaches 290–294
  lattice concepts 265–267
  lattice dynamics 296–299
  polymers 263–265
  properties
    bulk modulus 303–304
    heat capacity 300–302
    thermal expansivity 302–303
  quantum-mechanics
    density functional theory 278–282
    nearly free electron model 270–275
    tight binding method 275–278
  thermo-elasticity 312
    anisotropic materials 316–319
    elastic behavior 312–313
    elastic energy 314–315

matter of notation 315–316
stress states and associated elastic constants 313–314
temperature effect 319–320
two simple models 299–300
space-charge polarization 511
special relativity theory
Lagrange and Hamilton functions 611–612
Lorentz transformations 608–610
specific quantity 110
spherical harmonics 41, 282
spin angular momentum 39
spin quantum number 282
spontaneous polarization 501, 512
spreading coefficient 331
square gradient approximation (SGA) 339, 340
square-well (SW) potential 70, 163
stacking faults 310
intrinsic 310
extrinsic 310
Stanley's lemma 461
state function 95
statistical rate theory (SRT) 394
statistical thermodynamics (ST) 11, 125
entropy and partition functions 128–132
fluctuations 132–134
preliminaries 125–126
Stefan's ratio 333
steric isomerism 263
Stirling approximation 135
stoichiometric sum 174
stoichiometry 2
Stokes–Einstein relation 445, 550
Stokes' theorem 602
strain energy density 313, 314
strain tensor 81, 83
stress tensor 89–90
stress vector 85
structural models 218
substitutional impurities 305
substitution operator 584
substitution rule 586
superposition approximation 210
surface force 85
surface melting 428
surface roughening 345
surface tension 327
Sutherland potential 70, 164
Système International (SI) 12
Szigeti relation
first 508
second 508
Szyszkowski equation 365

t

Tait equation (TE) 247
Tait-Tammann equation (TTE) 247
Taylor series 59, 98, 585
tensor 599
terrace-ledge-kink (TLK) model 343, 344
thermal equilibration 114, 566
thermal equilibrium 101
thermal expansivity 302
thermodynamics (MT) 11, 94, 126
consistency 205
equilibrium 128, 458
first law 96
integration 206
of interfaces 326
limit 136, 149
linear approximation 118
minus-first law 575
potentials 102
second law 98
stability 375
state 93
system 578
third law 99
vapour pressure 637
thermo-elasticity
anisotropic materials 316–319
elastic behavior 312–313
elastic energy 314–315
matter of notation 315–316
stress states and associated elastic constants 313–314
temperature effect 319–320
thermoplastics 264
third law 99
Thomas-Fermi-Dirac model 278
three-body interaction 74
tight binding (TB) approximation 47, 275–278
time dilatation 610
time-evolution operator 35
time-temperature equivalence 535
Tolman length 336
total correlation function 206
total differential 585

trajectory 24, 126, 556
transitions general aspects
  Clapeyron equation 376–378
  Ehrenfest-Prigogine-Defay equations 378–380
  Gibbs energy 371
  Landau and Landau-like theory 380–383
transition state theory (TST) 174
  activated complex 177–179
  chemical kinetics basics 174–175
  equilibrium constant 175–176
  link to experiment 179–180
  potential energy surfaces 176–177
transport equation 557
transverse optic (TO) 506
tri-glycine sulphate (TGS) 513
triple product 599
Trouton constant 387, 638
Trouton's rule 387

u

uncertainty relations 39
universal bonding (UB) 296
Unsöld approximation 67, 68

v

vacuum permittivity 181, 498
van der Waals (vdW)
  adsorption isotherm 365
  constants 642
  critical exponent 464
  equation 165, 173
  interactions 65, 269, 480
  radius 284
  thermodynamics 173
van Hove singularity 298
van Laar expansion 354
van't Hoff equation 175
variation principle 44
variation theorem 45
vector 599
vibrational polarization 503–510
vibration-rotation interaction 146
vinyl polymers 263
virial theorem 27, 45
vitreous state 525
Vogel–Fulcher–Tammann (VFT) equation 242, 529
Voigt element 112
Volmer's equation 365
volume force 85
von Neumann equation 54
vulcanization 264

w

wave function 34, 37
wide-angle grain boundary 310
Wigner-Seitz cell 265
Wigner-Seitz radius 273, 275
Wigner variational theorem 176
Williams-Landel-Ferry (WLF) equation 535
Wulff plot 343

y

Young's equation 404
Young's modulus 313, 317
Yukawa potential 71
Yvon-Born-Green (YBG)
  equation 206, 210
  hierarchy 210

z

Zeldovich factor 401
zero-dimensional defects 305
zero-point energy 41, 300
zeroth approximation 613, 615