

Index

- 2₇ helix, 36
 3₁₀ helix, 36
 4₁₃ α helix, 36
 6₁₆ π helix, 36
 α domain, 42
 α helix, 36, 40
 dipole, 37
 α relaxation, 83, 85
 α -branch-and-bound, 286, 292, 349, 351
 α/β domain, 42
 barrel, 42
 horseshoe, 42
 open sheet, 42
 $\alpha + \beta$ domain, 42
 staphylococcus nuclease, 43
 $\alpha-\beta$ bifurcation temperature, 86
 β domain, 42
 β hairpin, 40, 41
 β sheet, 38, 40
 anti-parallel, 38, 39
 parallel, 38, 39
 β - α - β motif, 41, 42
 Φ value, 51, 64, 545
 fractional, 52
 Ac(ala)₃NHMe
 free energy disconnectivity graph, 270
 $G\ddot{o}$ potential
 BLN model, 560, 562
 ‘strange’ dynamics, 391
cis-butadiene, 132
Escherichia coli, 50
 o -terphenyl (OTP), 73, 95, 597, 625
 potential, 621
 superposition approximation, 633

 activated complex, 194
 activated dynamics, 618
 activation-relaxation method, 634
 Adam–Gibbs theory, 80, 599, 630, 632, 633
 adiabatic approximation, 126
 adiabatic switching, 309, 313
 aging, 102

 alkali halide clusters, 29, 247, 249, 492
 glide mechanism, 496, 497
 rearrangements, 496
 thermodynamics, 496
 allosteric interaction, 175
 amide hydrogen exchange, 46
 amino acid
 charged, 32
 enantiomers, 32
 hydrophobic, 32
 peptide bond, 32, 33
 polar, 32
 table, 31
 ammonia
 dipole moment, 188
 tunnelling, 188, 222
 amorphous material, 67
 amorphous silicon, *a*-Si, 74, 94, 621
 Anfinsen’s thermodynamic principle, 54
 anharmonicity, 124, 146, 295, 376
 perturbation approach, 377
 quasiclassical approach, 381
 anisotropy, 7
 anti-Mackay growth sequence, 15, 22, 182, 184
 architecture
 protein, 43
 Arrhenius law, 75
 atomic scattering factor, 88
 atomic units, 122

 bacteriorhodopsin, 133
 balanced geometry, 173
 banyan tree, 250, 252
 barnase, 38, 52
 barrier
 downhill, 210
 uphill, 210
 barstar, 38
 basin, 246
 basin of attraction, 290, 291, 365
 basin-hopping, 340, 579
 transformation, 340, 341
 biased sampling, 307, 317, 551

- bifurcation
 and catastrophe theory, 415
 bifurcation tunnelling
 water dimer, 224, 227
 binary mixture, 70, 71, 610, 616, 620, 627
 bioinformatics, 535
 BLN model, 559
 Gö potential, 560, 562
 disconnectivity graph, 560, 561, 564
 monotonic sequences, 560
 blue moon ensemble, 317
 blue tongue virus, 18
 bond-orientational order parameter, 473
 Born–Oppenheimer approximation, 119, 121, 192
 breakdown, 126
 boson peak, 93, 96, 621, 639
 bovine pancreatic polypeptide, 37
 bovine pancreatic trypsin inhibitor (BPTI), 48, 153, 531
 bovine spongiform encephalopathy, 54
 Bragg–Williams model, 452
 branch point, 192, 211, 212
 LJ₃₈, 408
 invariance to coordinate transformation, 233
 Brownian motion, 154, 319
 buckminsterfullerene, 17, 20, 29
 annealing, 501
 clusters, 491
 disconnectivity graph, 258, 260, 508
 formation, 501
 fullerene road, 502
 pentagon road, 502
 intermolecular potential, 480
 monotonic sequence, 505, 506
 Stone–Wales rearrangement, 258
- cage effect, 621
 cage-breaking process, 81, 640
 cage-preserving process, 640
 cage-rattling, 68
 caloric curve, 369, 436, 437, 447
 microcanonical, 446
 sodium cluster, 439
 canonical ensemble, 305, 306
 capillarity theory, 436
 CASP3, 335
 cat
 alive, 187
 dead, 187
 catalase-a, 43
 catastrophe
 cusp, 413, 414
 ratio, 415, 416
 fold, 412–413, 414
 ratio, 412, 415, 418
 catastrophe theory, 128, 202, 365, 410
 and acetal hydrolysis, 421
 and corannulene inversion, 422
 and electron transfer reactions, 420
 and Hammond’s postulate, 418
 and Landau free energy, 423
 and phase transitions, 424
 and two-level systems, 423
 catchment basin, 246, 345, 365
 central limit theorem, 72
 chalcogenide glass, 73
 chaos, 424
 and forecasting, 425
 chaperone, 54, 56
 chevron plot, 59
 Christoffel symbol, 232
 chymotrypsin inhibitor 2 (CI2), 52, 541
 Clausius inequality, 440
 cluster, 8, 434
 LJ₁₃, 255
 LJ₃₈, 338, 339, 344
 rearrangement rate, 406, 408, 409
 thermodynamics, 371, 474
 LJ₅₅
 fold ratio, 424
 thermodynamics, 377–379, 470, 471, 472
 LJ₇, 243
 dynamics, 453
 M₁₃
 master equation dynamics, 487
 (H₂O)₂₀
 relaxation, 521, 522
 alkali halide, 29, 247, 249, 492
 rearrangements, 496
 borane, 8
 boron suboxide, 18
 bulk limit, 8
 carborane, 8
 chaotic dynamics, 425
 definition, 8
 doped, 23
 electron diffraction, 11
 experiments, 9
 flow-reactor experiment, 11
 fullerene, 11, 29
 helium, 23
 Ino decahedron, 19
 ion, 10
 ion chromatography, 11, 29
 Lennard-Jones, 245, 370, 455
 global minima, 332, 333, 342
 magic numbers, 456
 small world properties, 279
 structure, 455
 magic number, 9, 17
 magnetic properties, 28
 Marks decahedron, 19
 mass selection, 11
 melting, 438
 met-car, 29, 30
 metal, 24
 metal–insulator transition, 28
 molecular, 23
 strain, 491
 Morse, 480
 anti-Mackay surface reconstruction, 450

- global minima, 332
 - monotonic sequence, 486
- non-metal, 29
- packing schemes, 19
- passivated, 29
- phase coexistence, 436
- phase transition, 434
- polyhedral structure, 11
- polyicosahedral, 22
- polytetrahedral, 186
- rare gas, 19, 21
- SF₆, 438
- silicon, 29
- simulations, 452
- sodium, 26, 27
- solid–solid transition, 370, 372
- superparamagnetic model, 28
- supershell, 27
- surface melting, 450
- tellurium hexafluoride, 438
- thermodynamic properties
 - ensemble dependence, 438
- transition metal, 8
- water, 23, 24
- zero-point energy, 383
- clustering coefficient, 276
- coherence, 186
- coiled-coil, 42
- collocation method, 147
- common neighbour analysis, 178
- complete nuclear permutation-inversion (CNPI) group, 172, 218
- compression, 337–338, 339
- condition number, 298
- conical intersection, 128, 129
- conservation laws, 235
- continuous random network (CRN), 94
- convex intruder, 444
- coordinate transformation, 135, 229
 - operator, 140
- corannulene
 - inversion, 422
- coset, 162
- covariant derivative, 231
- Coxeter construction, 15
- Creutzfeld–Jakob disease, 54
- critical assessment of techniques for protein structure prediction (CASP), 539
- critical nucleus, 61
- critical point, 192
- crystallin, 41
- cuboctahedron, 16
 - transition state, 207, 208
- curved space, 615
- curvilinear coordinates, 231
- cyclobutene, 132
- cytochrome b₅₆₂, 44

- de Boer parameter, 380
- Debye–Waller factor, 91, 100
- Delaunay network, 180
- delocalised state, 186

- dense random packing (DRP), 94, 614
- density functional theory, 28, 612
- density of states
 - harmonic, 367
- density–density correlation function, 92
- detailed balance, 389
- deterministic methods
 - α -branch-and-bound, 286
- diabatic functions, 126
- diabolo, 128
- diatomic molecule, 123
- dielectric loss spectroscopy, 82–86, 592, 595
 - α relaxation, 83, 85, 608
 - excess wing, 83, 85
 - Johari–Goldstein slow β peak, 83, 85
- diffusion constant, 602
- diffusion Monte Carlo method, 153
 - for rigid bodies, 156
 - for water clusters, 156
- H-densities, 156
- dihedral angle, 7
 - improper, 7, 567
- disclination line, 178, 179, 614
- disconnectivity graph, 241, 250
 - (NaCl)₃₅Cl[−], 493
 - Ac(ala)₁₂NHMe, 579, 581, 583
 - Ac(ala)₁₆NHMe, 579, 582, 583
 - Ac(ala)₃NHMe, 263, 265
 - free energy, 269, 270, 271
 - Ac(ala)₈NHMe, 579, 580
 - LJ₁₃, 255, 256, 257, 460, 461
 - simplified, 468
 - LJ₁₉, 460, 463
 - simplified, 468
 - LJ₃₁, 460, 464
 - LJ₃₈, 460, 464
 - analysis, 470
 - simplified, 467, 468, 469
 - LJ₅₅, 460, 462
 - analysis, 469
 - simplified, 468
 - LJ₇₅, 460, 464
 - simplified, 467
- M₁₃, 485
- (H₂O)₂₀, 515, 518, 519, 520, 521
- alanine hexapeptides, 272–274, 576
- binary Lennard-Jones, 637
- BLN model, 560, 561, 564
- bulk Lennard-Jones, 637, 638
- bulk silicon, 637, 639, 640
- C₆₀, 258, 260, 508
- free energy, 251, 267, 270, 271
- isobutryl-(ala)₃-NH-methyl (IAN), 565, 569, 571
- Lennard-Jones polymer, 258, 262
- NATMA, 571, 573
- RGDS peptide, 272, 275
- simplification, 254, 264
- size evolution, 459
- spin system, 612, 613
- water hexamer, 512, 513, 514, 516

- discrete path sampling (DPS), 317, 364, 397
 LJ₃₈, 406, 408, 409
 water octamer, 403–405
- discrete variable representation (DVR), 148
- dispersion forces, 19
- distinguished coordinate method, 293
- disulphide bridge, 34, 48
- DNA
 amplification, 50
 polymerase, 50
- donor tunnelling
 water dimer, 224, 227
- Doolittle relation, 604
- dynamic scattering function, 90, 92
- Dzugutov potential, 184, 185, 622, 623
- EF hand, 40
- effective activation energy, 478, 549
- effective medium approximation, 393
- Eigen cation, 151, 152
- eigenvector-following, 286, 287
 basin of attraction, 288
 for bulk models, 634
 for saddle points, 298
 hybrid methods, 292, 293
 large systems, 292
- electron correlation, 120
- electron transfer reaction, 420, 421
- electrospray ionisation, 49
- energy gap, 543
 Z parameter, 543
- energy lid, 253, 263
- energy threshold, 253
- enthalpy surface, 639
- entropic sampling, 312
- entropy
 Kolmogorov–Sinai, 425
- entropy–enthalpy compensation, 55
- epikernel principle, 174
- equilibrium
 associated time scale, 67
- erabutoxin, 41
- even–odd alternation, 25
- far-infrared vibration-rotation tunnelling
 spectroscopy, 11
- fast β relaxation, 83, 85
- feasible operation, 164, 305
- Feynman–Hibbs effective potential, 381
- fibril, 54
- fluctuation-dissipation theorem, 104
- fluorescence, 127
- fluoroethane, 209
- Fokker–Planck equation, 154
- fold recognition, 535
- folding funnel, 246
- folding temperature, 65
- foldon, 537, 542
- force field, 6
 Urey–Bradley, 6
- forecasting, 425
- form factor, 88
- four-helix bundle, 42
- fractured state, 628
- Frank–Kasper phase, 178–180, 185, 622
- free energy
 difference
 calculation, 308
 Landau, 309, 334
- free energy surface, 1
 Ac(ala)₁₂NHMe, 575, 576
 Ac(ala)₅NHMe, 575
 Ac(gly)₅NHMe, 575
- free volume theory, 69, 604
- frustration, 13, 184, 546, 611, 613
 geometric, 546
 minimal, 546
 topological, 546
- fullerene, 11, 17, 29
 coated, 29
 ion chromatography, 502
 mass spectrum, 20
 shrink-wrapping, 29
 Stone–Wales rearrangement, 258
- funnel, 62
 free energy, 62, 63, 547
 potential energy, 65, 332
- Gaussian distribution, 547
 local minima, 72
- gelsolin, 156
- gene cloning, 50
- genetic algorithm, 346, 347
 crossover operation, 346, 347
 genotype algorithm, 346
 Lamarckian, 346
 mutation operation, 346, 347
 phenotype algorithm, 346
- genetic engineering, 50
- genomics, 535
- geometric phase, 129
- geometric point group, 165
- geometrical symmetry selection rules, 197, 215
- geometry optimisation
 α -branch-and-bound, 286
 and coordinate system, 300
 BFGS method, 285
 conjugate gradient method, 293
 constrained, 300
 coordinate driving, 293
 direct inversion of the iterative subspace
 (GDIIS), 284
 eigenvector-following, 286, 287
 higher index saddles, 298
 L-BFGS method, 283
 local minimum, 283
 Newton–Raphson, 286, 290, 644
 quasi-Newton, 285
 transition state, 284
 trust radius, 290
- glass, 66, 592
 aging, 102
 barrier distribution, 72, 633, 642
 boson peak, 93, 96

- cage-breaking process, 81
 cage-rattling, 68
 chalcogenide, 73
 constraint theory, 593, 598
 continuous random network, 94
 definition, 68
 dense random packing, 94
 effect of pressure, 101
 entropy, 599
 eutectic point, 74
 examples, 73
 free volume theory, 69
 frustration-limited domain (FLD) model,
 614
 hypercube model, 645
 ideal, 81
 inherent structure, 70
 Kauzmann temperature, 80
 Kauzmann's paradox, 78
 landscape dominated regime, 71, 627
 landscape influenced regime, 71, 627
 low temperature heat capacity, 96, 97
 mechanical constraints, 74
 metallic, 69, 74
 microscopic process, 68
 model PES, 645, 646, 648
 nonergodicity, 103
 quenched disorder, 68
 random first-order transition, 612
 relaxation, 81, 83
 scattering experiments, 88
 simulation, 615
 stretched exponential relaxation, 70, 598
 strong/fragile classification, 75, 76, 78, 647,
 649
 tetrahedrally coordinated networks, 77
 time-temperature superposition principle,
 93
 transition, 592
 two-level systems, 96
 vibrational entropy, 626
 Vogel-Tammann-Fulcher equation, 75, 594
 Williams-Landel-Ferry equation, 76
 glass transition
 temperature, 65
 global minima
 effect of zero-point energy, 383
 Lennard-Jones clusters, 332, 333, 342
 Morse clusters, 332
 global optimisation, 280, 330
 basin-hopping, 340, 341, 579
 conformational space annealing, 335
 deformation methods, 335
 deterministic methods, 349
 α -branch-and-bound, 330, 349, 351
 TRUST, 350
 diffusion equation method (DEM), 335
 distance scaling method (DSM), 336
 effect of compression, 337, 338, 339
 genetic algorithm, 346, 347
 interval arithmetic, 330
 landscape paving, 330
 Lennard-Jones clusters, 332
 Monte Carlo plus energy minimisation, 342
 proteins, 535
 simulated annealing, 333
 smoothing transformation, 335
 taboo searches, 330
 travelling salesman problem, 330
 tunnelling methods, 330
 glutathione, 34
 Greek key motif, 41
 GroEL, 54
 GroES, 54
 Grotthus mechanism, 151, 152
 group
 coset, 162
 group theory, 161
 guanidinium chloride, 48, 55, 59
 Gō potential, 533

 H-density, 156
 Haarhoff model, 376
 haemoglobin, 36, 42
 space-filling representation, 175
 Hamiltonian replica exchange, 316
 Hammond's postulate, 418
 harmony principle, 62
 Hartree-Fock potential, 120
 HDEA, 336
 heat-shock protein, 54
 helium cluster, 23
 helix-turn-helix motif, 40
 Hessian eigenvalue
 and conservation laws, 235
 invariance to coordinate transformation, 232
 negative, 645
 shifting, 292
 zero, 202, 233
 heterogeneous dynamics, 596
 HF dimer, 210, 224
 HF molecule, 150
 histogram methods, 307, 551
 homology modelling, 535, 536
 Hsp60, 54
 Hsp70, 54
 hydrogen exchange reaction, 2
 hydronium ion, 23, 24
 hydrophobic collapse, 56
 hydrophobic effect
 iceberg model, 58
 hyperdynamics method, 326
 hypersphere
 volume, 368
 hypersurface deformation, 337

 iceberg model, 58
 icosahedral order
 in liquids, 178
 icospiral, 502
 ideal glass, 81, 599
 imino acid, 34
 implicit solvent, 533
 importance sampling, 304

incoherent scattering function, 92
 independent degrees of freedom, 119
 inherent structure, 70, 71, 246, 365, 624
 entropy, 624, 626
 equation of state, 627
 Ino decahedron, 15, 19
 instantaneous normal mode (INM) analysis,
 328, 618, 633
 intermediate scattering function, 93, 607
 intermolecular forces, 7, 23
 dispersion, 19
 electrostatic, 7
 internal conversion, 126, 131
 internal coordinates, 6, 301
 delocalised, 301
 extra-redundant, 301
 nonredundant, 301
 intersystem crossing, 127
 intrinsic reaction coordinate (IRC), 229
 Ioffe–Regel crossover, 99
 ion chromatography, 49, 492, 574
 fullerenes, 502
 isobutyryl-(ala)₃-NH-methyl (IAN), 250
 disconnectivity graph, 565, 569, 571
 isopotential ensemble, 448
 isotopic substitution, 125

Jahn–Teller effect, 126, 128, 130
 second-order, 219
 jellium model, 25
 Johari–Goldstein slow β peak, 83, 85
 jump-walking Monte Carlo, 314

Kasper polyhedra, 181, 182
 Kauzmann temperature, 80, 626
 Kauzmann’s paradox, 78, 599
 Kepler, 12
 keratin, 36
 kinetic Monte Carlo, 317, 395, 652
 kinetic trap, 2
 Knudsen cell, 10
 Kohlrausch–Williams–Watts (KWW)
 function, 82, 600
 Kolmogorov–Sinai (KS) entropy, 425, 603
 Kramers’ dynamics, 319, 384

lactate dehydrogenase, 45
 Landau free energy, 309, 334, 440, 441,
 472
 landscape dominated regime, 71, 627
 landscape influenced regime, 71, 627
 Langevin equation, 319
 lattice model, 65
 Leary tetrahedron, 17, 333, 457, 479
 Lee–Yang zeros, 438
 Legendre transformation, 451
 Lennard–Jones potential, 22, 243, 455
 binary, 70, 71, 607, 610, 616, 620, 627
 barrier distribution, 636
 crystal, 618
 frequencies, 641
 stationary points, 644

global minima, 16
 radial distribution function, 89
 reduced units, 456
 leucine zipper, 38
 Levinthal paradox, 53, 540
 and nucleation, 61
 resolution from the energy landscape,
 62
 Liapunov exponent, 425
 light-scattering spectra, 592
 Lindemann criterion, 612
 Liouville operator, 318
 liquid drop model, 25
 localised state, 186
 loop region, 40
 lysozyme, 2

Mackay
 growth sequence, 15, 22
 icosahedron, 13, 17, 29, 332, 456, 469
 rearrangement, 207, 208, 412, 413,
 416
 strain, 14
 magic number, 9, 17
 mapping approach, 420
 Marcus–Hush theory, 420
 Markovian dynamics, 388
 Marks decahedron, 16, 19, 333, 457, 479
 mass-weighted coordinates, 229
 master equation dynamics, 364, 384, 387,
 634, 646
 (NaCl)₃₅Cl[−], 499
 LJ₃₈, 475, 477
 M₁₃, 487
 buckminsterfullerene, 508
 describing relaxation, 391
 net-flow index, 500
 simplified, 392
 Maxwell construction, 436, 445
 McIver–Stanton rules, 215, 217
 mean-field model, 436, 653
 megabasin, 637
 met-car, 29, 30
 met-enkephalin, 319
 metabasin, 637
 metal cluster, 24
 metal–insulator transition, 28
 metallic glass, 69, 74
 metastability, 67
 metric tensor, 231
 Metropolis algorithm, 304
 microcanonical ensemble, 305, 306
 microcanonical temperature, 449
 microscopic process, 68
 minimal frustration, 65
 minimum, 2
 dead-end, 266
 geometry optimisation, 283
 minimum cut, 271
 minimum energy path (MEP), 211, 230
 mode-coupling theory (MCT), 68, 70, 83, 85,
 603, 605, 621, 633, 643

- α -regime, 608
- β -regime, 606
- activated process, 606
- cage-rattling, 608
- caging, 606
- hopping process, 606
- localised process, 606
- memory kernel, 605
- microscopic process, 608
- nonergodicity parameter, 609
- molecular clusters, 23, 491
- molecular dynamics (MD), 304
 - longer time steps, 317
 - Verlet propagator, 304
- molecular point group, 165
- molecular symmetry group, 162, 163
 - nonrigid molecule, 170
 - ammonia, 170
 - water trimer, 170
 - rigid molecule, 165
 - ammonia, 169
 - ethene, 169
- molten globule, 57
- monkey saddle, 202, 203
- monotonic sequence, 246, 248, 249, 483, 486
 - BLN model, 560
 - buckminsterfullerene, 505, 506
- monotonic sequence basin (MSB), 247, 266
- Monte Carlo (MC) method, 304
 - jump-walking, 314
 - kinetic, 395
 - sampling configuration space, 453
 - smart-darting, 316
 - smart-walking, 316
- Monte Carlo plus energy minimisation, 342
- Morse potential, 124, 332, 411
 - for HF, 150
 - long range, 184
 - range, 411, 480
 - strain analysis, 482
- Morse rules, 245
- motif, 40
- multi-funnel landscape, 345, 370
- multicanonical sampling, 312
- Murrell–Laidler theorem, 193, 194, 216, 645, 651
- mutation, 50
- myoglobin, 36, 42, 44, 100, 392
- Müller–Brown potential, 298, 299, 300
- Møller–Plesset theory, 120

- N-acetyl tryptophan amide (NATA), 571
- N-acetyl tryptophan methyl amide (NATMA), 571
 - disconnectivity graph, 571, 573
- nanocrystal, 492
- near symmetry operation, 168
- network
 - random, 276, 277
 - regular, 276, 277
 - scale-free, 276, 277, 278
 - small world, 276
- neutron scattering, 90
- Newton–Raphson formula, 286
- Noether’s theorem, 233
- non-Boltzmann sampling, 307
- non-Morse point, 411
- nonadiabatic transition, 126
- noncrossing rule, 129
- nonergodicity, 67, 103, 305, 450
- nonradiative transition, 126
- normal mode, 140, 367
 - rotation, 235
 - translation, 145, 235
- NP-hard problem, 331
- nuclear dynamics, 135
 - collocation approach, 147
 - diffusion Monte Carlo approach, 153
 - discrete variable representation, 148
 - path integral approach, 150
 - pseudospectral approach, 148
 - semiclassical approaches, 150
 - time-dependent methods, 150
 - variational approach, 146, 147
 - vibrational self-consistent-field, 151
- nuclear Overhauser effect (NOE), 53
- nucleation, 61
 - and the Levinthal paradox, 61
 - critical nucleus, 61
- nucleation–condensation, 52
- nudged elastic band method, 297

- orbit
 - of a point group, 209
- order parameter, 55, 92, 324, 334, 441, 547
 - bond-orientation, 473
 - radius of gyration, 551
- orthogonal transformation, 135

- pair correlation function, 88, 310
- pair distribution function, 88, 310
- palm tree, 250, 252
- parallel replica dynamics, 320
- parallel simulations, 314
 - dynamics, 320
- parallel tempering, 315
- parvalbumin, 40
- path integral approach, 150, 382
- pathway
 - calculation, 294
 - properties, 296
- Penrose tiling, 185, 187
- peptide bond, 32, 33
- percolation theory, 604
- permutation–inversion isomer, 221, 245, 255, 257, 365
- permutation–inversion operation, 164
- perturbation theory, 377
- Pesin’s theorem, 425
- phase diagram, 481
- phase transition
 - continuous, 595
 - Ehrenfest classification, 435
 - finite system, 434

- phase transition (*cont.*)
 first-order
 finite size, 424
 second-order, 595
 phosphorescence, 127
 photoabsorption spectrum, 373
 photochemistry, 127
 plasmon, 25
 Platonic solid, 11
 point group
 cyclic, 162
 generator, 162
 orbit, 209
 polyalanines, 573
 Ac(ala)₁₂NHMe, 575, 576
 disconnectivity graph, 579, 581, 583
 Ac(ala)₁₆NHMe
 disconnectivity graph, 579, 582, 583
 Ac(ala)₃NHMe, 263, 264
 disconnectivity graph, 263, 265
 Ac(ala)₈NHMe
 disconnectivity graph, 579, 580
 relaxation, 580
 global optimisation, 337
 helix to coil transition, 574
 hexapeptides
 disconnectivity graph, 272, 273, 274, 576, 578
 polyhedra, 11
 polymer
 collapse, 258
 disconnectivity graph, 258, 262
 polytetrahedral packing, 17, 178, 332, 614, 622
 polytope {3, 3, 5}, 183, 615
 porcine ribonuclease inhibitor, 45
 potential
o-terphenyl, 621
 anharmonic, 124
 Born–Mayer, 493
 diatomic molecule, 123
 Dzugutov, 184, 185, 622, 623
 G₅, 533
 Lennard–Jones, 16, 22, 243, 455
 Morse, 124, 332, 411
 range, 480
 Müller–Brown, 298, 299, 300
 of mean force, 310, 622
 range, 13, 332, 336, 411
 silica, 621
 silicon
 Stillinger–Weber, 618
 Sutton–Chen, 28
 truncation, 616, 617
 potential energy surface, 1
 and the range of the potential, 482
 biomolecules, 530
 branch point, 192
 calculation, 5
 critical point, 192
 crossings, 127, 131
 describing, 241
 exploration, 283
 features, 192
 global characteristics, 410
 golf course landscape, 543
 noncrossing rule, 129
 size evolution, 459
 stationary point, 192
 transition state, 194
 visualising, 241
 Potts model, 611
 power law
 scale-free property, 278
 Prigogine–Defay ratio, 595
 principal coordinate analysis, 254, 576
 prion, 54
 prion protein (PrP), 54
 proline
 isomerisation, 34, 49
 protein, 30
 Φ value, 51
 amide hydrogen exchange, 46
 architecture, 43
 BLN model, 559
 chevron plot, 59
 coiled-coil, 42
 denaturant, 48, 55, 59
 designability, 43, 173, 176
 dihedral angles, 33
 domain, 41, 42
 α , 42, 44
 α/β , 42, 45
 $\alpha + \beta$, 42, 46
 β , 42
 experimental techniques, 45
 family, 44
 fibrous, 41, 537
 fold, 43
 four-helix bundle, 42
 free energy surface, 551, 553
src-SH3, 551, 553, 554, 555
 betanova, 556
 cold shock protein A, 551, 553
 cytochrome *c*, 556, 557
 domain B of protein A, 551, 553
 protein GB1, 551, 553–555
 genetic engineering, 50
 geometry optimisation, 302
 globular, 41
 harmony principle, 62
 heat-shock, 54
 helix–turn–helix motif, 40
 homologous, 34
 hydrophobic collapse, 56
 hyperfamily, 44
 ion chromatography, 49, 492, 574
 lattice model, 65, 530, 531, 543
 marginal stability, 56
 molten globule, 57
 motif, 40
 principal coordinate analysis, 576
 simulations, 531
 unfolding, 534
 structure, 35, 43

- loop region, 40
- prediction, 335, 535
- primary, 35
- quaternary, 41, 43
- secondary, 36
- secondary structure formation rates, 46
- sequence, 35
- tertiary, 41
- superfamily, 44
- supersecondary structure, 40
- symmetry, 174
- topology, 43
- turns, 40
- protein data bank (PDB), 535
- protein folding
 - all-or-none, 59
 - chaperone, 54, 56
 - cooperative, 59, 546
 - funnel, 62
 - intermediate, 49, 52
 - Levinthal paradox, 53
 - mechanism, 540
 - diffusion–collision model, 541
 - framework model, 541
 - hydrophobic collapse model, 541
 - hydrophobic zipper model, 541
 - jigsaw puzzle model, 540
 - nucleation–condensation model, 52, 541, 545
 - nucleation–growth model, 541
 - minimal frustration, 65
 - new view, 65, 544
 - old view, 65, 544
 - small world properties, 280
 - temperature, 65
 - two-state, 52
- proteomics, 535
- pseudospectral methods, 148
- quantum dot, 10
- quantum superposition approximation, 378
- quasicrystal, 75, 185, 598
 - dynamics, 598
- quasiperiodic function, 185
- radial distribution function, 88, 89, 179
- Ramachandran plot, 34, 35, 38
- random energy model (REM), 62, 546, 651
 - generalised, 550
- random graph, 276, 653
- rare event, 316
- rare gas cluster, 19, 21
- rate constant, 384
 - RRKM theory, 268, 386
- RATTLE algorithm, 317
- Rayleigh–Ritz variational principle, 146, 293
- reaction coordinate, 55, 324
- reactive flux, 321, 386
- rearrangement, 209
 - cage-breaking, 636
 - cage-preserving, 636
 - degenerate, 209
 - asymmetric, 209, 506
 - symmetric, 209, 218, 505
- geometrical symmetry selection rules, 215
- nondegenerate, 209
- of bulk glass formers, 635
- pyracylene, 502, 503, 505, 507
- Stone–Wales, 258, 502, 503, 505, 507
- Wooton–Winer–Weaire, 634
- rearrangement theorem, 162
- recombinant DNA techniques, 50
- reduced radial distribution function, 88
- relaxation, 81, 83
 - (NaCl)₃₅Cl[−], 499
 - Ac(ala)₈NHMe, 580
 - LJ₁₉, 247
 - LJ₃₈, 478
 - M₁₃, 487
 - (H₂O)₂₀, 521, 522
 - alkali halide cluster, 247
 - binary Lennard–Jones system, 627
 - buckminsterfullerene, 508
 - Debye, 82
 - from master equation dynamics, 391
 - hierarchical, 598
 - Kohlrausch–Williams–Watts function, 82
 - multi-exponential, 392
 - separation of time scales, 478
 - stretched exponential, 82
 - total energy, 488
- Renner effect, 126, 128
- replica exchange method, 315, 616
 - Hamiltonian, 316
- restricted free energy, 309
- restricted potential, 309, 436, 440
- restriction endonuclease, 50
- retinal, 133
- reverse turn, 40
- reversible reference system propagator
 - algorithm (RESPA), 317
- reversible scaling, 309, 313
- reweighting schemes, 312
- RGDS peptide
 - disconnectivity graph, 272, 275
- rhodopsin, 133, 134
- rhombic dodecahedron, 11
- rhombic triacontahedron, 11, 22, 182
- Riemann–Hugoniot catastrophe, 414
- rocksalt structure, 29, 493
- ROP, 44
- rotational predissociation, 221
- RRKM theory, 268, 386
- Rydberg state, 126, 129
- S-bend, 436, 437, 441, 442
 - and interfacial entropy, 449
 - necessary and sufficient conditions, 450
- saddle point
 - geometry optimisation, 298
- scattering experiments, 88
- separation of variables, 119
- SHAKE algorithm, 317
- shell structure, 27

- silica
 superposition approximation, 633
- silicon, 618
- silicon cluster, 29
- simulated annealing, 333
- simulated tempering, 312
- small world, 276, 653
- smart-darting, 316
- smart-walking, 316
- sodium cluster, 26, 27, 373, 374, 375
 caloric curve, 439
 melting, 439
- soft-potential model, 99, 423
- spin glass, 68, 546, 611
 disconnectivity graph, 612, 613
 mean-field models, 611
- spin-orbit coupling, 127
- stability
 of phases, 440
- staphylococcus nuclease, 43, 46
- static structure factor, 92, 596
- stationary point, 192
 approach to, 205
 database
 creation, 394
 pruning, 391
 degenerate, 202
 higher index, 643
 how many?, 242
 minimum, 2
 non-Morse, 202, 411
 transition state, 194
- statistical honeycomb model, 183
- statistical rate theory, 385
- steepest-descent path, 192, 196
 approach to a stationary point, 205
 bifurcation point, 213
 calculation, 295
 connecting two transition states, 201
 from a transition state, 198
 invariance to coordinate transformation, 229, 233
 non-principal, 205
 principal, 205
 properties, 296
 symmetry, 197
 symmetry elements, 205
 uniqueness, 198
- stochastic differential equation, 319
- stochastic dynamics, 319
- Stokes–Einstein equation, 94, 622
- Stone–Wales rearrangement, 503, 505, 507
- strain energy, 13, 482
- stretched exponential relaxation, 70, 82, 598
- strong and fragile glass formers, 75, 76
- structural glass, 68
- subtilisin, 50
- super-Arrhenius behaviour, 75, 83, 652
- superbasin, 247, 250
- supercooled liquid, 66, 592
 Adam–Gibbs theory, 80, 599, 630
 barrier distributions, 633
 cage-breaking process, 81
- effect of pressure, 101
- entropy, 599
- free volume theory, 604
- frustration, 613
- heterogeneous dynamics, 596
- mode-coupling theory, 68, 70, 605
- relaxation, 81, 83
- simulation, 615
- time–temperature superposition principle, 608
 vibrational entropy, 626
- superparamagnetic model, 28
- superposition approximation, 365, 646
 (NaCl)₃₅Cl[−], 498
 o-terphenyl, 633
 anharmonic, 376
 binary Lennard–Jones systems, 627
 harmonic, 367
 perturbation theory, 377
 quantum, 378
 reweighted sum, 371
 sample incompleteness, 372
- silica, 633
- supercooled liquids and glasses, 624
- water, 632
- supersecondary structure, 40
- superselection rule, 187
- supershell, 27
- surface diffusion, 396
- surface melting, 450
- Sutton–Chen potential, 28
- symmetry, 161
 approximate, 161
 continuous, 172, 233
- temperature-accelerated dynamics (TAD), 326, 397
- tensor surface harmonic theory, 26
- tertiary motif, 43
- tetracene, 597
- thermodynamic integration, 310
- thermodynamic potential, 440
- thioredoxin, 42
- Thomson liquid drop model, 440
- threading, 535, 536
- threshold accepting, 342
- TIM barrel, 45
- time–temperature superposition principle, 93
- time-dependent methods, 150
- time-reversal symmetry, 163
- topological defect, 178
- transition path sampling, 317, 321
- transition state, 194
 dividing surface, 322
 double-ended search, 285
 geometry optimisation, 284
 recrossing, 195, 322
 separatrix, 195
 single-ended search, 285
- transition state theory, 195, 220, 322, 385
 thermodynamic formulation, 386
- transition vector, 216
- transmission coefficient, 322

- trap model, 104
 travelling salesman problem, 330
 tree
 banyan, 250, 252, 546
 graph, 251
 palm, 250, 252, 546
 willow, 250, 252, 508
 triosephosphate isomerase (TIM), 42, 45
 truncated octahedron, 16
 truncation schemes, 616, 617
 trust radius, 290
 tryptophan fluorescence, 48
 Tsallis statistics, 313
 tunnelling, 219
 ammonia, 222
 isotope effects, 220
 nondegenerate, 222
 water cluster, 23
 two-level systems, 96, 634, 639
 and catastrophe theory, 423
 two-state dynamics, 321, 391
 tyrosyl-tRNA synthetase, 50

 umbrella sampling, 309
 unimolecular rate theory, 194, 384, 385
 RRKM, 386
 united atom, 7
 urea, 48

 valence force field, 6
 valley-ridge inflection point, 211
 van der Waals loop, 436, 437, 441, 442
 van Hove space-time correlation function, 91
 distinct, 92
 self, 92
 van Hove theorem, 436
 variational transition state theory, 195
 Verlet propagator, 304
 vibration-rotation tunnelling spectroscopy, 225
 vibrational localisation, 99
 vibrational self-consistent-field (VSCF), 151
 villin headpiece subdomain, 533
 virus, 175
 vision, 133
 Vogel-Tammann-Fulcher (VTF) equation, 75,
 489, 594
 Voronoi construction, 180, 182

 waiting time
 Poisson processes, 321, 396
 Wang-Landau sampling, 313
 water, 57, 77
 (H₂O)₂₀, 515
 disconnectivity graph, 515, 518–521
 structures, 517
 cluster, 23, 511
 diffusion Monte Carlo, 156
 protonated, 23, 24
 rearrangement, 23
 dimer, 224–225, 226, 227, 228
 Eigen cation, 151, 152
 hexamer, 512
 disconnectivity graph, 512–514,
 516
 nonamer
 rearrangement rate, 404, 407
 octamer, 405
 rearrangement rate, 403, 405
 proton migration, 151, 152
 superposition approximation, 632
 trimer
 flip rearrangement, 171, 210, 211, 225,
 228, 419
 molecular symmetry group, 170
 tunnelling, 171
 Zundel cation, 151, 152
 watercourse, 247
 watershed, 247
 Werfelmeier growth sequence, 14
 Wien filter, 11
 Wigner-Kirkwood effective potential,
 381
 Williams-Landel-Ferry equation, 76
 willow tree, 250, 252
 Woods-Saxon potential, 25
 Woodward-Hoffmann rules, 197
 Wooton-Winer-Weaire rearrangement,
 634
 wurzite structure, 29, 182

 x-ray diffraction, 88

 zero Hessian eigenvalues, 202
 zinc blende structure, 29
 Zundel cation, 151, 152