
Subject Index

Computer programs are denoted in boldface, databases and journals are in italic

- 4d-Algorithm, 16
Ab initio molecular dynamics (AIMD),
101, 118
Abrasives, 119
Acceptance probability, 14
Actinide compounds, 249
Actinide-actinide bonds, 251, 270
Activation function, 369
Active orbitals, 252
Active space, 266
Adam-Gibbs relationship, 149
Adam-Gibbs theory, 26, 145
Adhesive interaction, 75
Adiabatic expansion, 163
Alpha-relaxation time, 3
AMBER, 9
Amorphous halo, 2, 32
Andersen barostat, 19
Angell plot, 4
Anionic clusters, 239
Annihilation operator, 200
ANO-RCC basis sets, 259
Antiferromagnetic clusters, 228
Antiferromagnetic spin ordering, 225
Anti-wear additives, 119
Anti-wear films, 117, 119
AO basis sets, 259
Apparent area of contact, 74, 110
Applications of SOMs, 384
Approximate preconditioner, 302
Arnoldi recursion, 319, 323
Arrhenius law, 4
Artificial neurons, 368
Artificial boundary inhomogeneity (ABI), 328
Artificial intelligence (AI), ix, 349
Artificial neural networks (ANNs), 367
Asperity, 74, 118
Atom clusters, 191, 364
Atomic force microscopy (AFM), 98
Atomic mean field integrals (AMFI), 258
Atomic natural orbital (ANO), 259
Atomic orbitals, 200
Atomic-scale roughness, 109
Atomistic modeling of friction, 68
Atomistic models, 9, 109, 160, 171
Atomistic simulations, 199
Autocorrelation function, 318
Automatic rule discovery, 374
Available volume, 138

Backpropagation, 373
Barostat, 18
Basis functions, 286
Basis set, 200
Basis set superposition error (BSSE), 278
Bead-spring model, 2, 6, 11, 19, 30, 34
Becker-Kistiakowski-Wilson (BKW) EOS, 164
Bessel functions, 325
Binary tournament selection, 355
Block copolymers, 95
Block Lanczos algorithm, 300
Bond-fluctuation lattice model, 11, 34, 22
Bond-orientational order, 128
Bound states, 326
Boundary conditions, 68, 92
Boundary lubricants, 73, 75

Reviews in Computational Chemistry, Volume 25
edited by Kenny B. Lipkowitz and Thomas R. Cundari
Copyright © 2007 Wiley-VCH, John Wiley & Sons, Inc.

- Brownian dynamics, 17
- Brownian motion, 5
- Bubbles, 181
- Building-block hypothesis, 358
- Bulk metals, 234
- Bulk-like atoms, 197, 240
- Byers Brown EOS, 164

- Canonical ensemble, 18
- Canonical partition function, 22
- Capillary electrophoresis, 376
- Carbon nanotubes, 113
- Car-Parrinello Molecular Dynamics (CPMD), 173
- Cascade-correlation learning, 378
- CASPT2, 254
- CASSCF state interaction (CASSI), 259
- Cavities, 138
- Cavity volumes, 138
- Centroid mapping, 384
- Cetane number, 375
- Chain connectivity, 11
- Chain stiffness, 22
- Chapman-Jouguet (C-J) state, 161
- Charge transfer, 202
- Charge-induced dipoles, 167
- CHARMM**, 9
- Chebyshev operator, 308
- Chebyshev polynomials, 164, 309
- Chebyshev propagation, 328
- Chebyshev recursion, ix, 308
- Cheetah**, 165, 170
- Chemical equilibrium, 161
- Chemical kinetic modeling, 167
- Chemically complex lubricant systems, 119
- Chemically realistic modeling, 7
- Chromium clusters, 225, 227
- Chromium-chromium multiple bond, 264
- Chromosome, 352
- CI expansion, 253
- C-J detonation theory, 163
- Classification, 377, 380
- Close lying electronic states, 250
- Cluster pivot algorithm, 147
- Cluster potential, 198
- Cluster surface, 203, 237, 240
- Clusters, 191, 192, 218, 364
- Clusters (“Magic”), 218
- Clusters of 4d elements, 234
- Coarse-grained models, 6, 11, 19, 103
- Coherent scattering function, 3
- Cold welding, 72, 74

- Combustion, 160
- Commensurability, 78
- Commensurate surfaces, 69, 78
- Commensurate systems, 106
- COMPASS**, 9
- Complete active space self-consistent field (CASSCF), viii, 251, 252
- Complex-symmetric matrices, 287, 322
- Compression, 117
- Compression rate, 132
- Computational bottleneck, 291
- Computational chemistry, v
- Computational convenience, 79
- Computational efficiency, 12
- Computational materials chemistry, vi
- Computer simulations, 2, 7
- Condensed-phase detonation simulations, 171
- Configuration functions (CFs), 252
- Configuration interaction (CI), 302
- Configuration space, 13
- Configurational entropy, 21, 22, 25, 145
- Confining walls, 91
- Conformational dynamics, 41, 45, 53
- Conformational rearrangements, 21
- Conformational transitions, 52
- Conjugate gradient (CG) method, 296
- Connection weight, 370
- Connectivity altering moves, 15
- Connectivity changing algorithm, 16
- Conservation of momentum, 89
- Continuous data, 376
- Continuous instabilities, 106
- Continuum models, 11, 109
- Continuum-mechanics-based models, 103
- Converged eigenvalues, 297
- Convergence dynamics, 297
- Cooling rate dependence, 18
- Cooperative motion algorithm, 15
- Copper-gold clusters, 365
- Cosine propagator, 308
- Coulomb correlation, 204
- Coulomb integrals, 201
- Coulomb’s law of friction, 76
- Coupled cluster (CC) theory, 251, 254
- CPU scaling law, 295
- Creation operator, 200
- Cross-correlation functions, 318
- Crossover operator, 357
- Crystal field potential, 202
- Crystal nucleation, 133
- Crystal structures, 364
- Crystal-independent metrics, 128

- Cullum-Willoughby test, 298, 305
Curie temperature, 194
Cut-off radius, 88
- d Electrons, 192, 198, 235
Darling-Dennison resonance, 321
Darwin term, 258
Data analysis, 349
Davidson method, 302
Decision-making process, 385
Delaunay tessellations, 138
Delta filter, 312, 317
Delta function, 314
Density fluctuations, 26, 136
Density functional theory (DFT), 100, 180, 203, 240, 251
Density of electronic states, 241
Density-of-states algorithm, 147
Detailed balance condition, 13
Determination of crystal structures, 364
Deterministic projection, 384
Detonation, 160
Detonation conditions, 160
Detonation tests, 161
Detonation velocity, 166, 170
Detonation wave, 161
Diagonalization, ix
Diamond anvil cell, 173, 181
Dielectric relaxation, 41
Dielectric screening, 167
Diffusion constant, 174
Diffusive motion, 5
Diffusivity, 136, 142
Dihedral barriers, 21, 46
Direct diagonalization, 289
Discrete energy representation (DER), 314
Discrete cosine propagator, 309
Discrete data, 376
Discrete variable representation (DVR), 288
Discretization, 286
Discretized Hamiltonian, 324
Dispersion interactions, 8
Dissipation mechanisms, 18
Dissipation of heat, 86
Dissipative particle dynamics (DPD), 88
Double-bridging algorithm, 15
Douglas-Kroll-Hess (DKH) Hamiltonian, 258
Drugs, 381, 384
Dual Lanczos algorithm, 323
Dynamic electron correlation, 251, 253, 254
Dynamic heterogeneity, 50, 53
Dynamic neutron scattering, 41
Dynamic scattering techniques, 3
Dynamics, 126
- Effective core potentials (ECPs), 259
Effective direct integrals, 201
Effective Kohn-Sham potential, 204
Effective Slater integrals, 221
Eigenpairs, 329
Eigenproblems, 285
Eigenvalues, 287
EISACK, 316
Elastic coupling, 72
Elastic instabilities, 72
18-Electron rule, 250
Electron correlation, 249, 254
Electron photodetachment spectroscopy, 239
Electron spin resonance (ESR) spectroscopy, 229
Electronic configurations, 192
Electronic nose, 377, 384
Electrostatic interactions, 167, 201
Empty lattice sites, 24
Entropy of glasses, 125
End-bridging algorithm, 15
Energetic materials, vii, 159
Energy content, 161
Energy dissipation, 71, 73, 85, 98, 105
Energy of detonation, 166
Entanglement, 14
Entanglement chain length, 5
Entropy, 7, 144
Entropy of liquids, 125
Epoch, 372
Equation of state (EOS), 163
Equations of motion, 89, 93
Equilibration in a polymer melt, 16
Equilibrium simulations, 68
Error cancellations, 205
Evolution operator, 324
Evolutionary algorithms, 350
Evolutionary operators, 353
Ewald summation, 100
Excess chemical potential, 24
Excess entropy, 130, 151
Exchange effects, 204
Exchange integrals, 201
Exchange interaction, 192
Exchange-correlation energy, 204
Exchange-correlation hole, 204
Exchange-correlation potential, 204
Excluded volume, 6, 11
Expectation values, 307

- Experimental magnetic moment, 222
Expert systems, ix, 374, 385
Explicit water molecules, 269
Explosives, 375
Extended symmetry-adapted discrete variable representation (ESADVR), 322
Extended X-ray absorption fine structure (EXAFS) spectroscopy, 269
External magnetic field, 194, 205
External orbitals, 252
Extreme conditions, 159
- Far from equilibrium, 68, 85, 180
Fast degrees of freedom, 17
Fast Fourier transform (FFT), 288
Fast-multipole methods, 100
Feature selection, 363
Feedforward network, 368
Fermi correlation, 204
Fermi energy, 197, 203
Fermi hole, 204
Fermi level, 204, 240
Ferromagnetic clusters, 193, 238
Fictitious forces, 101
Filter diagonalization, ix
Filter function, 314
Filter operator, 313
Filter-diagonalization (FD), 313, 316
Filters, 312, 319
Finitely extensible nonlinear elastic (FENE) potentials, 11
Finnis-Sinclair potential, 219
First principles simulations of high explosives, 179
First-order instabilities, 106, 108
Fitness, 352
Fitness function, 353
Fluctuation-dissipation theorem, 104
Force constants, 9
Force field, 7, 8, 99, 179
Force field parameterization, 9
Force field validation, 9
Four-component Dirac operator, 258
Fourier transform, 3, 43, 82
Fractal surface, 90
Fragile glass formers, 4, 19, 20
Free surface area, 137
Free volume, 125, 139
Free-volume autocorrelation function, 143
Frenkel-Kontorova (FK) model, 98
Friction, vi, 68, 73, 98
Friction coefficient, 5, 107
Friction mechanisms, 70
Friction-velocity dependence, 87
Friedel model, 197
Full CI, 252
Fully optimized reaction space (FORS), 252
- Gauss-Chebyshev quadrature points, 314
Gaussian filter, 315
Gaussian white noise processes, 17
Generalized gradient approximations (GGAs), 205, 229, 239
Generalized minimal residual (GMRES) method, 296, 301, 319
Generalized time representation (GTR), 314
Genetic algorithms, ix, 350
Geometric constraints, 94
Ghost particles, 16
Givens method, 289
Glass forming fluids, 19
Glass transition, v, 1, 2, 14, 126, 142
Glass-forming polymers, 1
Glassy freezing, 38
Glauber rates, 14
Global order, 133
Global orthogonality, 296, 300
Gram-Schmidt orthogonalization, 316
Grand canonical ensemble, 130
Graphical unitary group approach (GUGA), 252
Graphite, 113
Graphite sheets, 101
Green filter, 312, 319
Green operator, 327
Green's functions, 104, 203, 314
Growing cell structure (GCS), 384
Gupta potential, 212, 365
- Hamiltonian, 303
Hard-sphere chains, 34
Harmonic vibrations, 148
Hartree-Fock, 251
Heat capacity, 4
Heat-bath, 14
Hellmann-Feynman theorem, 308
Hermitian matrix, 287
Hermitian operators, 285
Hextuple bond, 265, 271, 274
Hidden layer, 370, 379
High explosive detonation, 162
High explosives, vii, 159
High spectral density, 327
High-pressure conditions, 99

- High-temperature kinetics, 363
HMX, 167, 180
HMX α -polymorph, 180
Hopping integrals, 201
Householder method, 290
Hund's rule, 192
Hurst roughness exponent, 82
Hydrodynamic interactions, 89
Hydrodynamic lubrication, 91
Hydrodynamic reaction zone, 161
Hydrogen bonding, 173
Hysteresis, 71, 74, 105, 108, 175
- Icosahedral growth, 212
Ideal randomness, 131
Implicitly restarted Lanczos algorithms, 300
Improper torsion, 8
Inactive orbitals, 252
Incommensurate surfaces, 69, 76, 92, 106
Individual, 352
Information content, 318
Infrared spectrum, 372
Insertion probability, 24
Instabilities, 87, 98, 105
Integration time step, 18
Interfacial symmetry, 77
Internal relaxation processes, 21
Interstitial space, 210
Intramolecular vibrational energy redistribution (IVR), 326
Intruder states, 257
Inverse iteration, 290
Iron clusters, 225, 227, 238
Irreversible tribological phenomena, 74
Isothermal compression, 134, 136
Isotropic liquid, 130
Itinerant exchange, 193
- Jacobi rotation, 289
Jacobs-Cowperthwaite-Zwissler (JCZ3) EOS, 164
Jellium model, 218
- Kauzmann paradox, 25
Kauzmann temperature, 21, 22, 48
Kinetic friction, 17, 107
Kinetic friction force, 68, 69, 116
Kinetic hindrance of ordering, 7
Kinetic modeling, 364
Kinetic studies, 363
Kohlrausch-Williams-Watts (KWW) law, 6, 37, 49
- Kohn-Sham equations, 203
Kohn-Sham Hamiltonian, 207
Kohonen network, 381
Kronecker delta, 288
Krylov subspace, 292, 304, 329
Kubo theory, 104
- Lamellar phase, 95
Lanczos algorithm, 294
Lanczos interpolation, 300
Lanczos phenomenon, 297
Lanczos recursion, ix, 293
Langevin dynamics, 105
Langevin thermostat, 85
Large eigenproblems, viii
Large matrices, 297
Large tensile stresses, 99
Lattice polymer models, 6, 11
Lattice potential, 198
LDA+U Method, 220
Learning, 349
Learning Genetic Algorithms, 361
Lees-Edwards periodic boundary conditions, 93
Legendre transformation, 22
Lennard-Jones (LJ) potentials, 99
Lennard-Jones system, 132
Ligand to metal charge transfer (LMCT), 262
Light scattering, 376
Linear response, 76
Linear response theory, 85, 88
Linear scaling, 288
Liouville equation, 26
Liouville super-operator, 325
Liouville-von Neumann equation, 325
Liquid water, 134
Load, 73, 83
Load-dependence of friction, 74
Local conformational flexibility, 12
Local coordination number, 224, 227
Local density approximation (LDA), 204
Local density of electronic states, 197, 240
Local Green's functions, 242
Local magnetic moments, 212
Local moments, 227
Local orbital moments, 222
Local order, 133
Local spin density approximation (LSDA), 208, 229
Local spin polarization, 224
Long-lives resonances, 328
Long-range ordered structure, 2

- Look-ahead algorithm, 320
Lorentz-Berthelot combination rules, 165
Löwdin orbitals, 200
Low-storage filter-diagonalization (LFSF), 317
Lubricant, 73
- MacDonald's theorem, 289
Macroscopic properties, 125, 140
Magnetic anisotropy energy, 194
Magnetic moments of bulk metals, 193
Magnetic properties, 191, 192
Magnetism, 196, 240
Magnetism of small clusters, 192, 193, 202
Magnetization density, 207
Manganese clusters, 228, 229
Markov chain, 14
Material properties, 132
Mating operator, 357
Matrix isolation spectroscopy, 270
Matrix-vector multiplication, 288
Mean field approximation, 201
Mean interparticle distance, 2
Melt structure factor, 46
Melt viscosity, 6
Mesoscopic scales, 11
Mesoscopic time scale, 14
Metallic clusters, 212
Metallic fuels, 161
Metal-metal bond length, 274
4d Metals, 234
Metastable state, 97
Method of moments, 241
Metropolis rates, 14
Microcanonical ensemble, 18
Microcanonical partition function, 22
Microcanonical trajectory, 17
Microscopic points of contact, 73
Minimal residual (MINRES) method, 296, 301, 319
Mode coupling theory (MCT), 26, 46
Model building, 7
Molar excess entropy, 151
MOLCAS-6, 251
Molecular descriptors, 375
Molecular dynamics (MD), 10, 13, 17, 81, 147, 217, 270
Molecular orientational order, 128
Molecular shape, 167
Molecular-orbital methods, 100
Møller-Plesset second-order perturbation theory (MP2), 254
Monte Carlo (MC), 10, 13, 147, 164, 165
Moore's Law, 160
MoS₂, 113
MSINDO, 365
Multi time-step integrators, 17
Multiconfigurational quantum methods, 249
Multiconfigurational wave function, 251
Multilayer icosahedral (MIC) structures, 215
Multiple metal-metal bond, 259
Multi-reference CI (MRCI), 254
Mutation operator, 357
- Near IR (NIR) spectra, 363
Necking, 99
Neel temperature, 194
Network geometry, 370
Network-forming liquids, 148
Neural networks, ix, 363, 366
Neutron scattering, 29, 30, 41
Neutron spin echo experiment, 29
Newtonian mechanics, 70
Newton's equations of motion, 17, 96
Nickel clusters, 211, 219
Nitromethane, 161, 180
NMR, 29
NMR spin-lattice relaxation, 41
Noble metal clusters, 218
Noise, 374
Non-additive pair interactions, 165
Nonbonded interactions, 8
Noncollinear magnetic configurations, 209, 241
Noncollinear spin DFT, 209
Nonequilibrium conditions, 81
Nonequilibrium simulations, 68
Non-hermiticity, 257
Non-isotropic stresses, 96
Nonlinear dynamics, 98
Nonlinear functions, 369, 379
Non-molecular phases, 167, 179
Nonorthogonality effects, 202
Nonrelativistic quantum chemistry, 257
Normal load, 68, 101
Normal pressure, 75, 76
Nosé-Hoover method, 18
Nosé-Hoover thermostat, 19, 174
- Objective function, 353
Octet Rule, 250
Off-diagonal elements, 289
Off-lattice models, 11
Oligomers, 9

- OPLS-AA, 9
Optimum solutions, 358
Orbital magnetic moment, 222
Orbital magnetism, 241
Orbital polarization, 219, 220
Order, 125, 132
Order metrics, 127
Ordering map, 132
Organizing data, 383
Orientation autocorrelation function, 42
Origins of friction, 68
Oscillator strengths, 261
Out-of-equilibrium, 4, 20
Outliers, 374
Out-of-plane bending, 8
Overlap integrals, 198
Overlap matrix, 200
- p Electrons, 200, 217
Packing arrangements, 128
Packing effects, 46, 47
Padé approximation, 168
Paige test, 297
Palladium clusters, 234, 237
Parallel tempering, 47, 147
Parents, 353
Partition function, 14, 24
PCFF, 9
Penta-erythritol tetranitrate (PETN), 166, 170
Perceptron, 369
Perfect crystalline structure, 131
Periodic boundary conditions (PBCs), 92, 97, 99, 181
Persistence times, 143
Phase space volume, 17
Photodetachment spectroscopy, 239
Photoelectron spectrum, 239
Plane-wave basis sets, 101
Plastic deformation, 70, 72, 103, 111, 112
Plastic flow, 73
Plastic-bonded explosive (PBX), 159
Polarizable continuum medium, 269
Polarizable force field, 270
1,4-Polybutadiene, 40, 95
Polymer coil, 5
Polymer force fields, 8
Polymer melts, 1
Polymer properties, 377
Polymer repeat units, 9
Polymers, 1
Polymorph, 128, 180
Polystyrene, 40, 95
- Potential drug molecules, 384
Potential energy landscape (PEL), 145
Power method, 292
Prandtl-Tomlinson model, 71, 98
Preconditioned inexact spectra transform (PIST), 302
Preconditioned Lanczos algorithms, 302
Preconditioners, 320
Predictive material models, 160
Predictor-corrector methods, 86
Pressure-induced chemical reactions, 108
Principal components analysis, 377
Projection operator, 321
Propagation of wave packets, 324
Protein domain predictor, 377
Protein structure, 362
Proteins, 377
Pulay forces, 101
- QR factorization, 290
Quadruple bond, 263, 265, 271
Quantitative structure-activity relationship (QSAR), 375
Quantum chemical methods, 100, 117
Quantum chemistry, 249
Quantum mechanical methods, 179
Quantum mechanics, 285, 303
Quantum-based MD simulations, 173
Quasi-elastic neutron scattering (QENS), 41
Quasi-minimal residual (QMR) method, 296, 301, 319
Quasi-steady state, 364
Quintuple bond, 265, 274
- Radial distribution function, 30, 129, 152, 175
Radius of gyration, 5, 18
Raman spectra, 173
Random close-packed state, 132
Random coil-like configuration, 5
Random forces, 17, 86
Random projection, 384
Random walk (RW), 11
Randomness, 132
Rare gas matrices, 229, 268
Rate of crossover, 362
Rate of mutation, 362
Rayleigh line, 163
Rayleigh-Ritz variation, 289
RDX, 167
Reaction dynamics, 327
Reaction probability operator, 328

- Reaction time scales, 162
- Reactive force fields, 97, 100, 117
- Reactive scattering, 328
- Real area of contact, 73
- Realistic simulations, 81
- Real-symmetric matrices, 287, 308
- Reciprocal space, 82, 89, 104
- Recursive diagonalization methods, 288, 291
- Recursive linear equation solvers, 296, 301, 320
- Recursive methods, 319
- Recursive neural networks, 377
- Recursive residue generation method (RRGM), 303, 304
- Recursive solutions, 285
- Reference function, 257
- Relativistic AO basis sets, 259
- Relativistic corrections, 205
- Relativistic effects, 249, 251
- Relativity, 257
- Relaxation functions, 6
- Relaxation processes, 145
- Relaxation time, 2, 4, 14, 16
- Reptation moves, 16
- Reptation-like behavior, 5
- Resonance states, 323, 328
- Resonances, 330
- Restricted active space (RAS) SCF method, 253
- Rhodium clusters, 234, 235
- Rough surfaces, 81
- Roulette wheel selection, 355
- Round-off errors, 296
- Rouse mode, 6, 38
- Ro-vibrational Schrödinger equation, 326
- Rule-discovery by machine, 374
- Rules, 385
- Ruthenium clusters, 234, 237

- s Electrons, 200
- Scaling laws, 329
- Schema theorem, 361
- Shocked hydrocarbons, 162
- Schrödinger equation, 160, 173, 286
- Scraping, 74
- Second quantization, 200
- Second virial coefficients, 141
- Second-order Gear predictor-corrector method, 86
- Second-order perturbation theory, 266
- Segment length, 5
- Segmental friction, 38
- Segmental friction coefficient, 6
- Self-assembled monolayers (SAMs), 116
- Self-avoiding random walk (SAW), 11
- Self-consistent charge density-functional tight-binding (SCC-DFTB), 180
- Self-diffusion, 34, 136, 142, 144
- Self-diffusion coefficient, 6, 26, 34
- Self-diffusivity, 149
- Self-organizing maps (SOMs), ix, 380
- Self-similar surface, 82
- Semi-crystalline, 1
- Semi-empirical molecular orbital methods, 100
- Sensors, 377
- Sextuple bond, 225
- Shear, 83, 117
- Shear force, 73
- Shear rate, 93
- Shear stress, 75, 116
- Shock conditions, 160
- Shock Hugoniot, 163
- Shocked hydrocarbons, 180
- Short-iterative Lanczos (SIL) method, 325
- Short-range orientational correlations, 5
- Silicon clusters, 365
- Simulation methods, 13
- Simulations, 68
- Single Lanczos propagation (SLP) method, 305
- Single-chain structure factor, 30, 46
- Singular value diagonalization (SVD), 289, 316
- Sintering, 191
- Size-extensivity, 254
- Sliding velocity, 72, 76, 88
- Slip length, 79, 91
- Slow relaxation in polymers, 14
- Solid friction, 72
- Solvation shell, 270
- Solvent partitioning, 376
- Sparse data, 363
- Sparse Hamiltonian matrices, 319
- SPC/E Water, 135, 149
- Specific entropy, 18
- Specific heat, 7
- Specific volume, 18, 19
- Spectral density, 42, 43, 321
- Spectral density operator, 311
- Spectral method, 310, 313
- Spectral transform Lanczos algorithm, 301
- Spectral transforming filters, 301

- Spectroscopy, 326
Spherical harmonic, 131, 221
Spin magnetic moment, 222
Spin magnetism, 241
Spin polarization, 202, 205
Spin-density matrix, 206
Spin-dependent operators, 207
Spin-lattice relaxation time (T_1), 42, 45
Spin-orbit coupling (SOC), 251, 259, 268
Spin-orbit interaction, 222, 241
Spinors, 206
Spin-polarized DFT, 206, 208
Spurious eigenvalues, 323
Squashing function, 369
Starting population, 353
Static correlation effects, 254
Static defects, 181
Static friction force, 69, 107, 110
Statistical mechanics, 164
Stern-Gerlach deflection experiment, 231, 239
Stick condition, 91
Stick-slip motion, 79, 85, 107, 116
Stochastic dynamics, 13
String, 352
Strong glass formers, 4, 19, 20
Structural correlations, 126
Structural glass transition, 1
Structural metrics, 130
Structural order, 132
Structural order metrics, 127
Structural ordering maps, 132
Structure factor, 2, 3
Super-cooled Lennard-Jones fluid, 133
Super-cooled liquid, 7, 21, 127, 145
Super-cooled polymer melts, 26, 142
Supercritical phase, 181
Superionic solid, 172
Superionic water, 167, 172, 179
Superlubricity, 70, 74, 112
Super-paramagnetism, 194, 231
Supervised learning, 373
Surface area, 137
Surface asperities, 74
Surface atoms, 197, 220, 224
Surface roughness, 81
Survival of the fittest operator, 353
Swap Monte Carlo algorithm, 147
Symmetry adaptation, 320
Symmetry-adapted autocorrelation function, 321
Symmetry-adapted Lanczos algorithm, 322
Symplectic integrator, 17
Test set, 372
Tetrahedrality parameter, 134
Tetrahedral order, 134
Thermal expansion, 3
Thermal expansion coefficient, 3, 19
Thermal fluctuations, 76, 143, 175
Thermodynamic equilibrium, 194
Thermodynamic properties, 18
Thermostats, 19, 68, 85, 97, 134
Threshold force, 69
Tight binding calculations, 211, 241
Tight binding method, 198, 240
Tight-binding DFT, 100
Time propagator, 324, 327
Time scales, 184
Time-dependent Schrödinger equation, 324
Time-dependent friction, 18, 104
Time-temperature superposition principle, 6
Topological constraints, 94
Topology, 11
Torsional autocorrelation function, 52
Torsional correlation times, 45
Torsional transitions, 47
Toxicity, 376
Training set, 372, 379
Trajectory, 13, 86
Transfer function, 369
Transition amplitudes, 303
Transition elements, 191
Transition metal, 249
Transition metal clusters, vii
Transition rates, 13
Translational order, 128
Tribiochemical reactions, 108
Tribiochemistry, 100, 117
Tribological simulation, 97
Tribology, 68
Tribometer experiments, 84
Two-center integrals, 198
Ultra-low friction, 70, 74, 113
Uncertainty, 350
Uncertainty principle, 316
Union volume, 138
United atoms, 9, 30
Unrestricted Hartree-Fock approximation, 200
U-U bond, 274
van-Hove correlation functions, 51
Variable-cell AIMD simulations, 101
Velocity Verlet integrator, 17, 86
Velocity-dependence of friction, 76

- Vertical excitation energies, 261
- Vibrational entropy, 146
- Vibrational mode, 326
- Vibrational quantum numbers, 327
- Viscosimetric glass transition (T_g), 4
- Viscosity, 4, 91
- Vogel-Fulcher laws, 4, 19
- Vogel-Fulcher temperature, 5, 20, 22, 25, 48
- Voids, 181
- Volume relaxation, 21
- von Schweidler exponent, 28, 37
- von Schweidler law, 28, 49
- Vornoi tessellations, 138

- Wannier function, 178
- Water, 149

- Water environment, 270
- Water phase diagram, 172, 173
- Wave packet, 324
- Wavelets, 363
- Wear, 70, 74, 112, 119
- Winning node, 381

- X-ray diffraction, 173
- X-ray scattering, 30, 269

- Yield strength, 73, 75

- Zinc phosphates (ZPs), 117
- Zledovich-von Neumann-Doring (ZND) state, 172
- Zwanzig formalism, 104