SUBJECT INDEX

acceptor–donor (AD) reaction theory 803 active space 534 AD theory 798 adiabatic and non-adiabatic theory 224 adiabatic approximation 227	autocorrelation 306 automata, cellular 317 avoided crossing 256 Axilrod–Teller dispersion energy 741
adiabatic approximation 227 adiabatic approximation, vibrationally 785 adiabatic curve 253 adiabatic potential, vibrationally 786 affinity separation 881 Aharonov–Bohm effect 780 algebraic approximation 80 algorithm, Car–Parrinello 314 algorithm, Metropolis 312 amphiphilicity 748 amplitudes, Coupled Cluster 542 angular momenta addition 281 annealing, simulated 309 antibonding orbital 371, 387 anticommutation relation 114 antisymmetric function 33 apparent forces 93 approximants, Padé 721 approximation, adiabatic 227 approximation, Born–Oppenheimer 231 ASCW 374 ASDW 374 associated Laguerre polynomials 178 associated Legendre polynomials 176 ASW 374 asymptotic convergence 210 atom, hydrogen-like 178 atomic basis set 363 atomic orbital 363 atomic orbital dimension 357	B3LYP 591 Bader analysis 573 balance, kinetic 118 band, conduction 455 band, valence 455 band gap 455 band structure 454 band width 454 barrier as shell opening 803 barrier of dissociation 689 barriers of reaction 772 baryon number 64 basis, biorthogonal 436 basis set, atomic 363 basis set superposition error (BSSE) 690 Bell inequality 43 Berry phase 780 bifurcation 861 bilocation 40 binding energy 175,687 biorthogonal basis 436 bipolaron 459 bispinors 116 Bloch function 435 Bloch theorem 435 BOAS 373 bobsleigh effect 774 Bohr magneton 649 bond, chemical 371 bonding orbital 371 and 387
attractor 573, 858 autocatalysis 866	bonds, σ , π , δ 403 Boolean variables 317

Born-Oppenheimer approximation 231 conduction band 455 Born-von Kármán condition 446 configuration 526 bound state 73 configuration, electronic 381 box with ends 145 configuration interaction 526 Boys localization method 399 configuration mixing 526 Breit equation 131 conical intersection 262 Breit-Pauli Hamiltonian 131 constant, lattice 432 Brillouin theorem 527 contact term 131 Brillouin zone 438 contraction of length 100 Brillouin-Wigner perturbation theory 556 contraction of orbitals 128 Brueckner function 526 convergence, asymptotic 210 brusselator 869 cooling protocol 309 BSSE 690 cooperativity 854 coordinate, collective 836 Car-Parrinello algorithm 314 coordinate system, Jacobi 279 Cartesian multipole moments 624 coordinate system, skew 770 CAS SCF 538 coordinates, democratic 776 catalyzed muon fusion 268 coordinates, mass-weighted 781 catastrophe set 575, 862 coordinates, natural 784 catenans 689 Copenhagen interpretation 37 CC, coupled cluster 539 Coriolis coupling 785 and 791 CCD 547 corrections to energy 205 CCW 374 corrections to wave function 205 cell, unit 432 correlation, explicit 502 cell, Wigner–Seitz 438 correlation, spatial 306 cellular automata 317 correlation, time 306 channels of reaction 772 correlation energy 499 chaos 861 correlation factors 188 characteristic frequency 294 correlation hole 599 charge conjugation 68 Coulomb hole 515 chemical bond 371 Coulomb self-interaction 348 chemical reaction, acceptor-donor (AD) Coulombic operator 337 theory 803 counter-poise method 690 chemical shift 664 Coupled cluster amplitudes 542 CI method, full 531 coupling, Coriolis 785, 791 clamped nuclei Hamiltonian 223 coupling, curvature 785, 791 classes, Fukutome 372 coupling constant 659, 669 closed shell 330 covalent structure 521 cluster operator 540 creation particle-antiparticle 134 collapse, polarization 717 critical (stationary) points 573, 768 collective coordinate 836 cross section of reaction 779 collectivity 863 crossing, avoided 256 combinatorial chemistry 855 crystal orbitals 450 commutator expansion 537 complete set of functions 202 current 155 complex, encounter 174 curvature coupling 785, 791 complex, endohedral cusp condition 504

cyclic box 149

cycloaddition reaction 823

complex systems 852

conditional extremum 336

Darwin solution 123	effect, funnel 266
decimation 863	effect, harpooning 258
decoherence 42	effect, hydrophobic 748
deexcitations 550	effect, Jahn-Teller 456
democratic coordinates 776	effect, paramagnetic 668
density matrix 531	effect, split nucleus 268
density matrix, one-particle 611	eigenfunction 16
determinant, secular 203	eigenvalue problem 22
determinant, Slater 332	Einstein equation 108
DFT 567	electron gas 567
diabatic and adiabatic states 828	electron pair distribution 592
diabatic curve 253	electron paramagnetic resonance 38
diagonal correction for the motion of the nu-	electronic configuration 381
clei 228	electronic density distribution 569
diagram of Jabłoński 391	electronic pair dimension 404
diamagnetic effect 668	electronic shells 381
diamagnetic spin–orbit contribution 669	electronic-vibrational-rotational spectrosco-
digonal hybridization 408	py 235
dilation of time 104	electrophilic attack 818
dimension of atomic orbital 357	electrostatic catastrophe 642
dimension of electronic pair 404	electrostatic energy 693
dipole, magnetic 649	electrostatic potential 798
dipole moment 283, 624, 630	enantiomers 67
Dirac electronic sea 112	encounter complex 174
Dirac equation 113	endohedral complexes 689
Dirac notation 19	energy, correlation 499
Dirac vacuum 112	energy, exchange–correlation 586
Dirac–Coulomb approximation 129	energy, free 292
Direct CI 533	energy, penetration 386
direct method 533	energy, self-interaction 585
direct spin–spin interaction 669	energy continuum 112
dispersion energy 694	energy corrections 205
dispersion energy, Axilrod–Teller 741	energy functional 335
dissipative structures 873	energy gap 454
dissociation barrier 689	energy of reorganization 841
dissociation energy 175,687	entangled states 38
DNA computing 878	entrance and exit channels 772
DNA hybridization 881	entropy 292
domino 863	EOM CC 548
donating mode 792	EPR effect 38
"drain-pipe" of reaction 772	equation, Hylleraas 210
DRC 768	equation, secular 203
dynamics, Langevin 310	"equation with many fathers" 109
dynamics, molecular 304	Equation-of-Motion Coupled Cluster meth-
dynamics, Monte Carlo 311	od (EOM-CC) 548
	evolution in time 20
effect, Aharonov–Bohm 780	exchange, polymers 485
effect, bobsleigh 774	exchange hole 516, 599
effect, diamagnetic 668	exchange operator 337
	- ·

exchange-correlation energy 586 fusion, muon catalyzed 268 exchange-correlation hole 598 fusion, nuclear 268 exchange-correlation potential 589 exchange-deformation interaction 722 Galilean transformation 97 exo- and endothermic reactions 787 gap of band 455 experiment of Aspect 46 Gauge Invariant Atomic Orbitals (GIAO) explicit correlation 502 exponentially correlated function 513 gauge symmetry 64 extremum, conditional 336 Gaussian-type orbital (GTO) 355 Gedankenexperiment 36 geminal 513 FBZ, First Brillouin Zone 438 feedback 866 General Hartree–Fock method (GHF) FEMO 147 GHF 341 femtosecond spectroscopy 768 Fermi contact contribution 670 ghosts 690 Fermi golden rule 84 global minimum 292 Fermi level 454 global optimization 292 field compensation method 492 golden rule of Fermi 84 finite field method 639 gradient approximation, NLDA (GEA) First Brillouin Zone 438 gyromagnetic factor 649 fixed point 858 Fock-Klein-Gordon equation 109 focus (stable and unstable) 872 Hadamard gate 48 force field 284 Hamilton graph 879 Hamiltonian, clamped nuclei 223 Forces, apparent 93 forcing of symmetry 710 Hamiltonian of reaction path 784 fractals 865 "hand-glove" interaction 744 Franck-Condon factors 840 harmonic generation, second/third 645 Franck-Condon rule 266 harmonic helium atom 507 free energy 292 harmonic oscillator 166 free particle 145 harmonics, spherical 176 frequency, characteristic 294 harpooning effect 258 frozen orbitals 534 Hartree–Fock method, general (GHF) 341 Fukutome classes 372 Hartree-Fock method, restricted (RHF) full CI method 531 function, antisymmetric 33 Hartree–Fock method, Unrestricted (UHF) function, Brueckner 526 341 function, Heitler-London 521 Hartree-Fock-Roothaan method 365 function, James-Coolidge 508 Heisenberg uncertainty principle 34 function, Kołos-Wolniewicz 508 Heitler–London function 521 function, molecular 875 helium harmonic atom 507 function, symmetric Hellman–Feynman theorem function, variational 196 Hermite polynomials 166 function, wave 16 HF, Hartree-Fock method 324 function with adapted symmetry 710 Hohenberg–Kohn functional 580 functional, energy 335 hole, correlation 599 functional, Hohenberg-Kohn 580 hole, Coulomb 515 functional, Hylleraas 209 hole, exchange 516, 599 funnel effect 266 hole, exchange-correlation 598

Kohn-Sham system 584 HOMO 343 Kołos–Wolniewicz function 508 Hund's rule 392 Huygens principle 41 Koopmans theorem 393 hybrid approximations, NLDA 591 KS, Kohn–Sham theory 584 hybridization, tetrahedral, trigonal, digonal 407 Lagrange multipliers 336, 997 hybrids 408 Laguerre polynomials 178 hydrogen bond 746 Laguerre polynomials, associated 178 hydrogen-like atom 178 Langevin dynamics 310 hydrophobic effect 748 lattice, inverse 436 Hylleraas CI 506 lattice, primitive 432 Hylleraas equation 210 lattice constant 432 Hylleraas function 506 LCAO CO 451 Hylleraas functional 209 LCAO MO 360 Hylleraas variational principle LDA 590 hypercycles 873 Legendre polynomials 176 hyperpolarizability, multipole 627 Legendre polynomials, associated 176 length contraction 100 induction energy 694 Lennard-Jones potential 287 inertial system 95 lepton number 64 instability 372 level, Fermi 454 insulators 455 limit cycle 859 interaction energy 684 linear response 627 interaction energy, van der Waals 742 local density approximation, LDA 590 interaction non-additivity 726 local magnetic field 659 interference of particles 42 localization of orbitals 396 intermediate spin–spin coupling 659 logical gate 47 intersection, conical 262 logistic equation 861 intrinsic reaction coordinate (IRC) 782 London orbitals 673 intrinsic semi-conductor 455 long-range interactions 475 invariance of theory 64 Lorentz transformation 100 invariance with respect to a unitary transfor-LUMO 343 mation 340 inverse lattice 436 magnetic dipole 649 inverse Marcus region 833 magnetic moment 649 inversion 65 magneton, Bohr 649 ionic structure 521 IRC 781 magneton, nuclear 649 many body perturbation theory (MBPT) isotope effect 172 551 many-body expansion 726 Jabłoński diagram 391 Jacobi coordinate system 279 mass relativistic 107 Jahn-Teller effect 456 mass-weighted coordinates James–Coolidge function 508 mathematical solution Jeziorski-Kołos perturbation theory 717 Maxwell equations 962 MBPT 551 MC SCF, classical 535 "key-lock" interaction 744

MC SCF unitary method 536

MD, molecular dynamics 304

kinetic balance 118

kinetic minimum 292

mean field 348	Morse oscillator 169
mean force potential 836	motif 432
mean value of an operator 24	MP2 558
measurement 22	MS-MA 715
measurement, wave function 251	multiconfigurational SCF methods 536
mechanics, molecular 290	multipliers, Lagrange 336, 997
Mendeleev Periodic Table 381	multipole expansion 480
metals 455	multipole hyperpolarizability 627
metastable states, non-bound 247	multipole moments, Cartesian 624, 698
method, direct 533	multipole polarizability 627
method, Equation-of-Motion Coupled Clus-	multipoles, permanent 701
ter (EOM-CC) 548	multireference methods 533
method, finite field 639	muon catalyzed fusion 268
method, General Hartree–Fock (GHF)	Murrell-Shaw and Musher-Amos (MS-
341	MA) perturbation theory 717
method, Hartree–Fock–Roothaan 365	7.1
method, MC SCF unitary 536	nanostructures 749
method, perturbational 203	natural coordinates 784
method, Restricted Hartree-Fock (RHF)	natural division 684
330, 342	natural orbitals 531
method, Ritz 202	NLDA 591
method, SCF multiconfigurational 536	NMR 659
method, sum over states 635	NMR shielding constants 659
method, Unrestricted Hartree-Fock (UHF)	NO, natural orbitals 531
341	noble gases 381
method, valence bond (VB) 520	nodes (stable and unstable) 872
Metropolis algorithm 312	non-additivity, interaction 726, 854
Michelson–Morley experiment 96	non-adiabatic theory 224
minimal model of a molecule 417	non-bound metastable states 247
minimum, global 292	non-bound states 247
minimum, kinetic 292	non-crossing rule 256
minimum, thermodynamic 292	non-linear response 628, 857
Minkowski space-time 104	non-nuclear attractor 573
MO and AD pictures 805	non-radiative transitions 266
mode, donating 792	normal modes 294
model, minimal of a molecule 417	NP-hard problem 879
modes, normal 294	nuclear fusion 268
molecular dynamics 304	Nuclear Magnetic Resonance 659
molecular electrostatic potential 798	nuclear magneton 649
molecular evolution 873	nuclear spin levels 665
molecular function 875	nucleophilic attack 816
molecular libraries 855	
molecular mechanics 290	occupied orbital 343
molecular orbital 330	octupole moments 624
molecular recognition 750	one-particle density matrix 611
molecular spinorbital 330, 330	operator, cluster 540
Møller–Plesset perturbation theory 558	operator, Coulombic 337
Moment, dipole 283	operator, exchange 337
Monte Carlo dynamics 311	operator, wave 540

perturbation theory, Rayleigh-Schrödinger operator of a quantity 18 optimization, global 292 perturbational method orbital, antibonding 371, 387 perturbed system orbital, atomic 363 phase, Berry 780 orbital, bonding 371, 387 photochemical reaction 266 orbital, frozen 534 photons, virtual 134 orbital, Gaussian-type (GTO) 355 physical solutions 76 orbital, hybrid 408 polarizability, multipole 627 orbital, London 673 polarization amplifier 738 orbital, molecular 330 polarization approximation, symmetrized orbital, natural 531 717 orbital, occupied 343 polarization catastrophe 738 orbital, Slater 355 polarization collapse 717 orbital, Slater-type 355 polarization of spin 589 orbital, virtual 343 polarization of vacuum 134 orbital centring 355 polarization perturbation theory 692 orbital localization polymer chain reaction (PCR) 881 orbitals, crystal polynomials, associated Laguerre 178 orbitals σ , π , δ polynomials, associated Legendre 176 oscillating field 645 polynomials, Hermite 166 oscillator, harmonic 166 polynomials, Laguerre oscillator, Morse 169 polynomials, Legendre positron 112 Padé approximants 721 potential, electrostatic 798 pair distribution 592 potential, exchange-correlation 589 paramagnetic effect 668 potential, Lennard-Jones 287 paramagnetic resonance 38 potential, torsional 287 paramagnetic spin-orbit effect 670 potential energy curve 229 parameters, variational 196 potential energy (hyper)surface 229 particle in a box 145 potential of mean force 836 particle-antiparticle creation 134 primitive lattice 432 Pauli blockade 722 protocol, cooling 309 Pauli matrices 25 PW 591 Peierls transition 456 penetration energy 386 **OED** 132 periodic perturbation 84 quadrupole moments 624 Periodic Table, Mendeleev 381 quasi-harmonic approximation 240 permanent multipoles 701 qubit 47 perturbation 204 perturbation, periodic 84 radiative corrections

perturbation, time-independent 83

perturbation theory, first-order 82

perturbation theory, Brillouin-Wigner 556

perturbation theory, Jeziorski-Kołos 717

perturbation theory, Møller–Plesset 558 perturbation theory, Murrell–Shaw and

Musher-Amos (MS-MA) 717

perturbation theory, polarization 692

radiative corrections 133
radius, van der Waals 742
Ramsey theory 666
rate of reaction 779
Rayleigh–Schrödinger perturbation theory 557
reaction, cycloaddition 823
reaction, exo- and endothermic 787
reaction, photochemical 266

reaction barriers 772	secular equation 203
reaction centre 872	self-interaction energy 585
reaction channels 772	self-organization 854
reaction coordinate 782	self-similarity 865
reaction cross section 779	semi-conductor, intrinsic, <i>n</i> -type, <i>p</i> -type
reaction "drain-pipe" 772	455
reaction path Hamiltonian 784	shells, electronic 381
reaction rate 779	SHG 646
reaction spectator 795	shielding constants 659
reaction stages 807	simulated annealing 309
reactive and non-reactive trajectories 770	single-exchange (SE) mechanism 733
reduced resolvent 554	singlet 31
relativistic mass 107	size consistency 532
relativity principle 104	skew coordinate system 770
renormalization 863	Slater determinant 332
reorganization energy 841	Slater orbital 355
repellers 858	Slater-type orbital (STO) 355
resonance state 155	soliton 459
resonance theory 521	space-time of Minkowski 104
resonance tunneling 158	spatial correlation 306
Restricted Hartree–Fock method (RHF)	spectator of reaction 795
330, 342	spectroscopic state 62
retarded potential 131	spectroscopy, electronic-vibrational
RHF, Restricted Hartree–Fock method	rotational 235
330	spectroscopy, femtosecond 768
rigid rotator 176	spectrum, rovibrational 283
Ritz method 202	spherical harmonics 176
rotational symmetry 63	spin 122
rotator, rigid 176	spin angular momentum 25
rotaxans 689	spin coordinate 25
rovibrational spectrum 283	spin magnetic moment 649
Ruedenberg localization method 398	spin polarization 589
rule, Franck-Condon 266	spin waves 374
rule, Hund's 392	spin–dipole contribution 670
rules, Woodward-Hoffmann 825	spin–orbit coupling 131
	spin–orbit effect, paramagnetic 670
σ -, π -, δ -molecular orbitals 403	spin–spin coupling 131, 672
saddle point 768	spinorbital, molecular 330, 330
saddle point of reaction 872	spinors 116
Sadlej relation 640	split nucleus effect 268
SAPT 710	state, non-bound 247
SCF 350	state, underground 199
SCF LCAO CO 452	stationary (critical) points 573
SCF multiconfigurational methods 536	stationary state 22
Schrödinger equation 70	steepest descent trajectory (SDP) 769
SDP 769	stellar nodes (stable and unstable) 872
SE mechanism 733	steric effect 799
second/third harmonic generation 645	structure, band 454
secular determinant 203	structure covalent 521

structure, ionic 521 sum of states 283 sum over states method 635 supermolecular method 690 supramolecular architecture 744 supramolecular chemistry 744 surface potential energy 229 symmetric function 33 triplet 31 symmetrized polarization approximation symmetry, rotational 63 symmetry, translational 61, 432 TSW 374 Symmetry Adapted Perturbation Theory (SAPT) 710 symmetry C 68 symmetry forcing 710 symmetry of division into subsystems 492 UHF 341 symmetry of Hamiltonian 57 symmetry of wave function 33 symmetry orbital 435 symmetry P 65 synthon 750 system, perturbed 204 system, unperturbed 204 341 TE mechanism 734 teleportation 47 template interaction 751 tetrahedral hybridization 408 theorem of Brillouin 527 theorem of Koopmans 393 theory of resonance 521 thermalization 307

thermodynamic minimum 292 THG 646 three-body polarization amplifier 738 TICS 374 time correlation 306 time dilation 104 time evolution equation 20 time-evolution operator 77 time-independent perturbation torsional potential 287 trajectories, reactive and non-reactive 770 trajectory, steepest descent (SDP) 769 "trajectory-in-molasses" transformation, Galilean 97 transformation, Lorentz 100 transition, non-radiative 266

transition, Peierls 456
translational symmetry 61
transmission coefficient 155
travelling salesman problem 879
trial function 196
trigonal hybridization 408
triple-exchange (TE) mechanism 734
triplet 31
triplet instability 374
TSCW 374
TSDW 374
TSDW 374
TSW 374
tunnelling effect 153
Turing machine 878
two-state model 81

UHF 341
uncertainty principle 36
underground states 199
unit cell 432
unitary MC SCF method 536
unitary transformation, invariance 340
unperturbed system 204
Unrestricted Hartree–Fock method (UHF)
341

v-representability 580 vacuum polarization 134 valence band 455 valence bond (VB) method 520 valence repulsion 718 Valence Shell Electron Pair Repulsion (VSEPR) 421 van der Waals interaction energy van der Waals radius 742 van der Waals surface 743 variable, Boolean 317 variation of a spinorbital 336 variational function 196 variational method 196 variational parameters 196 variational principle 196 variational principle, Hylleraas 209 variational principle for excited states VB, Valence Bond 520 velocity addition law 103 vibrationally adiabatic approximation vibrationally adiabatic potential virtual orbital 343

virtual photons 134 VSEPR, Valence Shell Electron Pair Repulsion 421

wave function 16
wave function evolution 76
wave function "matching" 73
wave function "measurement" 251
wave operator 540
wave vector 433

width of band 454 Wigner–Seitz cell 438 Woodward–Hoffmann rules 825

XOR gate 48

ZDO 635 Zero Differential Overlap (ZDO) 635 zero-vibration energy 303 Zone, Brillouin 438