

## Index

### **a**

ab initio wavefunction 86  
 ab initio periodic approaches 169  
 Abramov functional 432  
 Abramov energy density 432  
 absolute hardness 400  
 absorption intensity 79  
 accuracy of atomic integrations 17, 18  
 acenaphthylene 408  
 acetamide 333  
 acrolein 129, 135, 136  
 action integral 41  
 action principle 39, 40, 44  
 active site 511  
 additivity of the atomic energy 10  
 adenine 312  
 adenine binding site 305 ff., 308, 312, 313  
 adenine binding site of the protein hAR  
     302, 303, 310  
 adenosine 323  
 ADI 405, 406  
 agostic interaction 364, 366, 367, 512  
 agostic systems 365  
 AIM2000 27, 101, 103 ff.  
 AIMALL97 28  
 AIMDELOC 15, 28  
 AIMPAC 27, 29, 264  
 Al 216  
 $\text{Al}_2\text{C}_2\text{H}_{10}$  145  
 Al-Al bond 211  
 aliphatic hydrocarbons 379  
 alkali halides 214  
 alkali metal clusters 192  
 alkaline-earth metals 214  
 alkane 77, 91, 109, 116 f.  
*n*-alkanes 99  
*n*-alkenes 194  
 alkyne 114  
 amino acid 21, 22, 24, 301, 324, 325

amino acid residues 56, 285, 302, 303,  
     327  
 ammonia 276  
 analytical CPHF method 101  
 anharmonicity 98  
 anomeric effect 375, 386  
 anthracene 408  
 aromatic compounds 399  
 aromatic radicals 393  
 aromatic stabilization energy 400  
 aromatic transition state (TS) 418  
 aromatic  $\pi$ -sextets 416  
 aromaticity 394, 395, 399  
     – indices 394, 418 f.  
 asphericity shifts 334  
 atom types in proteins 26  
 atomic additivity schemes 82  
 atomic basin 6, 211, 428  
     – shape 209 ff.  
     – volume 16, 295  
 atomic charge 9, 16, 75, 328, 401  
     – derivatives 80, 81  
     – transfer derivatives 80  
     – transfer dipole contribution 75  
 atomic components 176  
 atomic continuity theorem 51  
 atomic contributions 50, 62, 65, 71, 73, 74,  
     76, 81, 90 ff., 108  
     – to  $\bar{\alpha}$  112  
     – to  $\Delta\bar{\alpha}/\Delta r_{\text{CH}}$  112  
     – to the electronic energy 18ff., 276  
     – to the magnetizability tensors 91  
     – to the polarizability tensors 77  
 atomic current theorem 51, 52  
 atomic dipolar polarization 20  
     – contribution 72  
     – gradient 75  
 atomic dipoles 109  
 atomic electric polarizability tensors 91

- atomic electron populations 16, 103, 175, 277, 401  
 atomic electronic energy 19, 84  
 atomic electronic kinetic energy 17, 82  
 atomic electronic virial theorem 19, 83  
 atomic electrostatic multipole moments 20–25, 126  
 atomic energy XXII, 20, 29, 84  
 atomic exchange matrices 138  
 atomic force  
   – microscope 54  
   – theorem 51  
 atomic fragments 317  
 atomic graph 348  
 atomic group source function 195  
 atomic interaction lines 8  
 atomic interactions 260, 347  
 atomic magnetic polarization contribution 88  
 atomic multipolar ED 296  
 atomic multipole moments 20–25, 126  
 atomic multipoles model 122  
 atomic net charges 16, 188, 295, 299  
 atomic net current contribution 88  
 atomic nuclear virial energy 82 ff., 85  
 atomic polarizability 77  
 atomic polarization 20–25, 78, 80  
 atomic populations *see* atomic electron population  
 atomic power theorem 51  
 atomic properties 15–25, 26, 194  
 atomic quadrupolar polarization 24  
 atomic quadrupole moment 24, 175, 352  
 atomic source contributions in  $Mn_2(CO)_{10}$  200  
 atomic surface derivative contributions 76  
 atomic theorems 51  
 atomic torque theorem 51  
 atomic virial theorem XXII, 19, 51  
 atomic volume 16, 277, 328, 352  
 attraction (repulsion) basin 210  
 Au (111) surface 240  
 $AX_4$  ( $CH_4$ ,  $CF_4$ ,  $SiCl_4$ ) 154  
 $AX_6E$  molecules 155 f.  
 $AX_7$  molecules 155 f.
- b**  
 $B_2H_6$  145  
 back bonds 180  
 back-bonding 363  
 back-donation 363, 364  
 $\pi$ -back-donation 352  
 basin populations 16, 154  
 basin volume 16, 297, 299  
 basins 142  
 basis set superposition error (BSSE) 460, 461  
 BCC *see* bonded charge concentration  
 BCP *see* bond critical point  
 Becke and Edgecombe 438  
 benzene 392, 393, 395, 403, 406, 408, 412  
 benzocyclobutadiene 408  
 $m$ -benzyne 392 ff.  
 $BF_3$  6 ff.  
 $BH_3$  368  
 bicyclo-[1.1.1]-pentane 98, 100, 101, 111, 116  
 bicyclo[3.3.1]nonane 115  
 bicycloalkane 99, 114, 116  
 binding energy 454  
 biphenylene 408  
 bond charges 72, 75, 80, 275  
 bond contribution 66 ff., 69 ff., 74, 92  
   – to the energy-gradient-based force 85  
 bond critical point (BCP) 4, 10, 25, 141, 168, 231, 260, 271, 375, 426, 431 ff., 477  
 bond current contribution 89  
 bond ellipticity 12, 184, 185  
 bond force 85  
 bond order 11, 13, 15, 25, 135  
 bond path 4, 11, 52, 141, 232, 260, 386  
   – connectivity 357  
 bond polarizability model 97  
 bond properties 11, 218  
 bonded charge concentration (BCCs) 182  
 bonded interactions 130  
 bonded radius 11  
 bond-length aberrations 334  
 bond-order model 425  
 borazine 407  
 Born–Oppenheimer energy surface 460  
 Born–Oppenheimer approximation 123  
 Born–Oppenheimer procedure 55  
 Bragg angle 285  
 branched alkane 114  
 BSSE *see* basis set superposition error  
 Buckingham-type potentials 437  
 buckminsterfullerene allotropes of carbon 208  
 buckybowls 409  
 bulk modulus 220, 221  
 1,3-butadiene 418  
 butane 111, 115, 129, 194  
 2-butanol 332
- c**  
 $C_2H_2$  156  
 $C_2H_2$  dimer 129

- $(C_2H_2)_2$  132  
 $C_2H_4$  156  
 $C_2H_6$  348  
 $CaF_2$  216  
 cage critical point 4, 5, 168, 388  
 calculus of variations 41  
 Carbo index of similarity 26, 487  
 carbon monoxide 20, 21, 348, 445  
 carbonyl supported metal–metal interactions 357  
 Cash–Karp Runge–Kutta (CRRK) method 232  
 catalytic activity 236  
 catastrophe point 357  
 CH bond 111  
 CH stretching modes 96  
 $CH_4$  103, 109  
 characteristic set 4  
 charge-assisted hydrogen bonds 199, 458  
 charge concentrations 141  
 charge-density refinement 308  
 charge transfer 78, 176, 188, 431
 - contribution 73, 80
 - dipole 21
 - moments 176
 chemical structure 52  
 chemical transferability 195  
 chiral invariants 330  
 chiral modules 336  
 chirality 336  
 chlorine 276  
 chrysene 408  
 $CIF_3$  155  
 cisplatin 510  
 Clar structure 417  
 Clar's aromatic sextet 395, 416f.  
 class I clathrates 189  
 clathrate type I structure 187  
 closed-shell bonding 8, 12  
 closed-shell character 355, 445  
 closed-shell interactions 11, 174, 260, 358, 427, 436, 441, 443  
 clustering procedure 313  
 CO *see* carbon monoxide  
 $CO(NH_2)_2$  264, 272  
 $CO_2$  82  
 $Co_2(CO)_6(ASH_3)_2$  352, 353  
 $Co_2(CO)_6(NH_3)_2$  353  
 $Co_2(CO)_6(PH_3)_2$  353  
 $Co_2(CO)_6(XH_3)_2$  352  
 $Co_2(CO)_6(\mu\text{-CO})(\mu\text{-}C_4H_2O_2)$  355  
 $Co_2(CO)_8$  201, 369  
 $[(CO)_5Cr\text{-}H\text{-}X]^-$  368  
 $(CO)_5M(H_2)$  364  
 commutator average 47  
 compensatory transferability 56  
 complementary ligands 488  
 $\pi$ -complexes 357 ff.  
 $\pi$ -complex–metallcycle 364  
 compressibility 220, 221  
 conditional pair density 10, 192  
 conformational space 357  
 connectivities 207  
 contergan/thalidomide scandal 336  
 CONTOR 29  
 coordination 351  
 coordinatively unsaturated sites (CUS) 236  
 core basin 142  
 core-valence bifurcation index 439  
 correlation energy 276, 277  
 correspondence rule 345  
 Coulomb
 - correlation 14, 377
 - energy 123, 125, 134, 139
 - expansion 131
 - hole density 402
 - interaction 125, 129, 133
 coupling constants 375  
 covalence degree (DC) 447  
 covalent bonds 216, 354, 455  
 CPHF method 80, 91, 106  
 CPU time 129  
 $Cr(CO)_5$  368  
 $Cr(CO)_5(C_2H_4)$  363  
 $Cr(CO)_5(H_2)$  364  
 $Cr(CO)_6$  351  
 $Cr(PH_3)_5(H_2)$  364  
 $Cr\text{-}Cr$  path 367  
 $[Cr_2(\mu_2\text{-}H)(CO)_{10}]^-$  367  
 crambin 288  
 creation energy 247, 250  
 critical points 2, 167, 209, 210  
 $CrOs(CO)_{10}$  M–M bonds 352  
 CRRK *see* Cash–Karp Runge–Kutta  
 CRYSTAL 27, 166, 167, 174, 223, 336
 - graphs 232
 - software 170
 - topologies 224
 CRYSTAL's LCAO 225  
 crystalline isostructural families 214 ff.  
 crystallization 175, 176, 179  
 crystallographic R-factors 334, 337  
 cubic perovskite  $SrTiO_3$  270  
 current density 64, 89, 93  
 curvatures 3, 443  
 cusp condition 262  
 cyclic delocalization 404  
 cycloalkane 99, 114, 116

- cyclohexa-1,3-diene 408  
 cyclohexa-1,4-diene 408  
 cyclohexane 98, 101, 111, 113, 115, 408  
 cyclohexene 408  
 cytosine 415
- d**
- Dalton's atomic hypothesis 39  
 dangling bonds (DBs) 180  
 database of protein fragment contents 313  
 dative bond 350 ff.  
 DB *see* dangling bonds  
 DC *see* covalence degree  
 DCBS *see* dimer-centered basis set  
 DCD *see* Dewar–Chatt–Duncanson  
 Debye–Waller factor 286  
 deformation density 172, 173  
   – maps 354  
 delocalization 9, 13–15, 351, 375  
 $\pi$ -delocalization 407  
 delocalization index 13–15, 135, 166, 167,  
   201, 347, 351, 355, 363, 375, 377, 378, 391,  
   395, 402, 405, 407, 460  
 density of states (DOS) 187  
 depletions 141  
 Dewar structure 403  
 Dewar–Chatt–Duncanson (DCD)  
   – donor–acceptor complexes 357, 361,  
   363  
   – ring complex 359  
   – mechanism 351  
   – model 364  
 DI *see* delocalization index  
 diagonalized quadrupole tensor 24  
 diamagnetic spin–orbit interactions 378  
 diamond 208, 216, 219  
 dielectric polarization 20  
 Diels–Adler reaction 409, 418 f.  
 1,12-difluoro[4]helicenes 5, 6  
 diffuseness  $D$  183  
 dihydrogen bond 426, 456  
 dihydrogen bonding 8  
 dihydrogen complexes 364  
 dimer-centered basis set (DCBS) 460  
 dimethylcyclobutane 115  
 dimethyl-phosphinoyl (methylsulfonyl)  
   methane 390  
 dipeptide L-phenylalanyl–L-proline H<sub>2</sub>O 318  
 dipole derivative 80  
 dipole moment 21, 22  
   – derivatives of CO<sub>2</sub> 81  
 dipole polarizability tensor 74  
 Dirac–Slater exchange density 272  
 diradicals 393
- dispersion energy 459  
 dissociation energy 436, 439, 440  
 disynaptic basins 145, 438  
 DL-serine 329, 334  
 DMACB 170, 171  
 DMSDA *see* mean-square displacement amplitudes  
 DNA bases 25  
 docking applications 314  
 domain-averaged Fermi hole 487  
 $\sigma$ -donation 352  
 donor–acceptor bond 350  
 donor–acceptor interaction 352  
 DOS *see* density of states  
 Drude model 215
- e**
- ECP *see* effective core potential  
 EF *see* eigenvector following  
 effective core potential (ECP) 27  
 Ehrenfest  
   – force 53, 64, 260, 381  
   – theorem 52  
 eigenvector following (EF) 168  
 electric dipole derivative 80  
 electric dipole moment 68, 71  
 electric dipole polarization 61  
 electric field 78, 109, 110  
   – derivative 73, 75  
   – flux 63  
 electric polarizability 68, 73 ff., 90  
   – tensor 76  
 electric susceptibility 50  
 electron delocalization 13–15, 376, 382, 385,  
   395, 399, 400–401  
 electron isodensity maps 391  
 electron localization 9, 14, 128, 143, 401,  
   440  
 electron localization function (ELF) 142 ff.,  
   191, 277, 438  
 electron pair localization 347  
 electron transfer 431  
 electron tunneling microscope 54  
 electronegativity 20, 150, 215, 294, 218, 313,  
   311, 484  
 electronic current density 90  
 electronic energy of an atom in a molecule 82  
 electronic pressure density 83  
 electronic structure of molecules 54  
 electrophile attack 249  
 electrostatic force 86  
   – on a nucleus 87  
 electrostatic interaction energies 312, 313

- electrostatic model 351
- electrostatic moments 20–25, 138, 139
- electrostatic potential 249, 311, 400, 475, 482
- electrostatic properties 287, 289, 305 ff.
  - of a protein site 313
- electrostatic–covalent hydrogen bond model 459
- ELF *see* electron localization function
  - ELF basins 149 ff.
  - ELF population analysis 147 ff.
  - ELF topology 144 ff.
  - ELF valence basin 166, 200
- ellipticity 12
- elpasolites 214
- energy density 12 ff., 272
- energy derivatives 84
- energy-gradient-based force 64, 65, 86
  - on the nucleus 83
- enzymes 511
- estrone hormone 15
- ethane 98, 109, 112, 113, 194, 379, 380, 418
- ethanol 332
- ethene 98, 111
- ethyne 98, 111
- Euler equation 41
- Euler's invariant formula 211
- exact exchange energies 133
- exact exchange force 127
- EXAFS *see* X-ray absorption fine structure
- exchange between electrons of the same spin 272
- exchange correlation 377
- exchange density 274
- exchange eigenvalues 138
- exchange energy 122, 124, 125, 127, 128, 130 ff., 136, 276, 277
- exchange force 136, 137
- exchange interaction 131
- exchange interaction energy 461
- exchange moments 126, 139
- exchange potential 278
- exchange-correlation density 401, 402
- exchange-correlation energy 271
- expectation value of an operator 9
- experimental electron density 261
- experimental H–O interactions 436
- external magnetic field 89
- external potential 474
- EXTREME 27
  
- f**
- F<sub>2</sub> 445
- F-center in sodium electrosodalite 190
- F-center basins 192
- F-centers 186
- Fe–Fe bonding 369
- Fermi
  - contact 378
  - contact contribution 379
  - to  $J_{HH}^3$  378
  - correlation 14
  - hole 144, 167, 375, 377, 378, 402, 403, 487
  - level 189
- ferromagnetic phase of SES 191
- Feynman path–integral method 271
- Feynman
  - force 52, 381
  - theorem 52
- F–F coupling constants 380
- F…H hydrogen bonded complexes 441
- [F…H…F]<sup>-</sup> system 444
- F–H…π hydrogen bond path 456
- FH…ClH 146
- (FH)<sub>2</sub> 420, 437
- first atomic electrostatic moment 20
- first derivative of the electric dipole moment 78
- first-order reduced density matrix 123
- Fisher information 144
- fixed nucleus approximation 55
- flatness 354
- π-fluctuation aromaticity index (FLU<sub>π</sub>)
  - 406 ff., 415, 419, 420
- flux through a surface 47
- force fields 26, 121
- formamide 333
- formic acid–formate anion complex 199
- Fourier
  - difference synthesis 225
  - transformation 289
- fpLAPW *see* full potential linearized plane wave
- FRAGDIP 21
- fragment charges 312
- fragment deformation maps 354
- fragment electroneutrality 307
- fragment representations 313
- fragment transferability 338
- free electron gas 215
- Fukui
  - frontier orbital theory 54
  - functions 475
  - Nobel Lecture XXI
  - radical reactivity indices 484
- full potential linearized augmented plane wave (fpLAPW) formalism 223

- fullerenes 319, 409  
 Fulton bound index 391
- g**  
 GAMESS 27, 29, 128  
 gauche effect 383  
 Gauss's theorem 18  
 Gaussian 27, 29, 30, 106, 114 ff., 332  
 Gaussian 03 129  
 Gaussian 94 295  
 genetic code 22–24, 26  
 GFMLX 336  
 GIAO 413  
 globbic structure factors 289  
 glycine 124  
 goodness of fit 334  
 gradient kinetic energy 17  
 gradient path 242, 428, 474  
 gradient vector 6
  - field 6, 142, 259, 323
  - field lines 211
  - instability 210
 gradient-corrected correlation energy 275  
 gradient-corrected energy density 272  
 gradient-corrected exchange density 274  
 graphite 208, 219  
 GRDVEC 28, 29  
 Green's function 192, 263, 271  
 GRIDV 28, 29  
 group additivity schemes 82  
 group contribution 22, 50
  - to the polarizability tensors 77
 guanine 415, 416  
 guanine–cytosine base pair 415  
 guest atoms 188  
 guest–host binding energy 189  
 guest–host systems 165 ff.
  - binding energy 189

**h**  
 $\text{H}_2\text{N}-\text{C}_x\text{H}_x(\text{R})-\text{COOH}$  21–23, 295  
 $\text{H}_3\text{N}\cdots\text{HF}$  439  
 $\text{H}_2\text{O}$  dimer 129  
 Hamiltonian approach to quantum mechanics 38  
 Hammett substituent constants 412  
 Hansen–Coppens XXII
 
  - multipole model 261, 262, 318
 hAR *see* human aldose reductase  
 harmonic approximation 78  
 harmonic oscillator model of aromaticity (HOMA) 394, 400, 404, 406 ff., 410, 412 ff., 420  
 Hartree–Fock

– energy 123  
 – virial 29–30  
 – wave functions 127

Hattig's recurrence formulae 129  
 HB *see* hydrogen bond  
 HCCH···HF complex 456  
 HCN 445  
 HCH···O intermolecular interactions 170  
 HDN *see* hydrodenitrogenation  
 HDS *see* hydrodesulfurization  
 heats of formation 50  
 heavy main-group element 352  
 hedrane 114, 116  
 Heisenberg
 
  - equation of motion 37
  - representation of quantum mechanics 51
 Hellman–Feyman
 
  - electrostatic force 19, 65, 83
  - electrostatic theorem 83, 85, 87, 88
 Hermitian operator, linear 46  
 Hermiticity 47  
 Hessian matrix 3, 231, 427  
 hexaprismane 117  
 1,3,5-hexatriene 129, 134  
 HF dimer 129, 130  
 $\text{H}\cdots\text{F}$  hydrogen-bonding interactions 437  
 $\text{H}\cdots\text{H}$  bonding 8, 9, 11  
 $\text{H}\cdots\text{H}$  electrostatic interaction 445  
 hierarchical merging/clustering algorithm 292, 301  
 higher-order polarizability 104  
 high-pressure phosphorous boride 215  
 high-resolution
 
  - electrostatic potentials 306, 308, 309
  - protein model 287
 Hirshfeld
 
  - multipole model 262
  - test 318, 335 $\text{H}\cdots\text{N}$  hydrogen-bonding interactions 441  
 $(\text{H}_2\text{O})_2$  131, 132, 430  
 $\text{H}\cdots\text{O}$  hydrogen bonds 436  
 $\text{H}\cdots\text{O}$  interactions 437  
 Hohenberg–Kohn
 
  - formulation of DFT 261
  - theorem XX, 474, 475
 HOMA *see* harmonic oscillator model of aromaticity  
 homodesmotic reaction 400  
 homogeneous electron gas 263  
 homoleptic  $\text{M}_2(\text{CO})_n$  dimers 352  
 host–guest
 
  - chemistry 186
  - systems 186 ff.

- human aldose reductase (hAR) 287 ff., 291 ff., 300  
   – crystal structure 299  
   – structure 307, 312, 313
- hybrid orbital-free energy functionals 271
- hydride bond 466
- hydride bridges 367 ff.
- hydrides 153
- hydrodenitrogenation (HDN) 236
- hydrodesulfurization (HDS) 236, 237
- hydrogen bond(ing) (HB) 170, 177, 197, 199, 217, 273, 331, 416, 425, 427, 429, 453  
   – Coulomb interaction 130  
   – donor 504  
   – energies 454  
   – exchange energy 132  
   – intermolecular 453  
   – molecular complexes 198
- hydrogen–hydrogen bonding 8
- hydroimidazo[4,5-*d*]imidazole 430
- hydrophilic regions 500
- hydrophobic effects 481
- hydrophobic regions 500
- hydrophobic–hydrophilic interaction tendency 483
- hydrophobicity 483
- hydroxy-2-aminopurine 508 (6-)
- hyperconjugation 386
- hyperpolarizability 61, 73
- hypervirial theorem 83, 86
- hyperwall mode 505
- i*
- I<sub>2</sub>O 216
- IAM *see* independent atom model
- ice VIII 436
- iceane *see* tetracyclo-[5.3.1.1<sup>2,6</sup>.0<sup>4,9</sup>]-dodecane
- independent atom model (IAM) 172, 174, 189, 286 f., 329, 334, 336
- independent transferability 113
- induced electronic magnetic dipole moments 88 f.
- influence function 192
- infrared intensity 50
- infrared spectrum 78
- infrared vibrational absorption intensity 68
- inhibitor–protein interactions 286
- inner-valence shell charge concentration (i-VSCC) 509 ff.
- inorganic clathrates 186
- integrated atomic electronic energy 277
- integration error 18, 276
- intensity of absorption 78
- interaction  
   – density 261  
   – energy 435  
   – energy-decomposition scheme 459  
   – potential 436  
   – tensor 127
- interatomic surface (IAS) 8, 11, 63, 244, 232, 377, 426, 477
- intermolecular interaction 131, 435
- invariom 317, 331, 334  
   – aspherical scattering factors 329  
   – database 330, 336  
   – pseudoatoms density 338
- inverse hydrogen bonding 466
- inverse moments 122
- ionic bonds 217
- ionic character 151
- ionic contributions 151
- ionicity 216
- isobutane 99
- isodensity envelope 17
- isopropanol 332
- isotropic polarizability 77
- k*
- Karplus-type behavior 379, 382  
   – of <sup>3</sup>J<sub>HH</sub> 395
- Kekulé  
   – resonance structure 416  
   – structures 403
- Kenichi Fukui XXI
- kinetic energy 43 f., 122, 123, 266  
   – density 12, 13, 18, 37, 259, 262 ff., 349, 354, 381, 391, 432, 482, 483  
   – operator 17  
   – per electron 192
- Kohn–Sham  
   – approximation 378  
   – density-functional theory 128  
   – exchange-correlation energy 128  
   – orbitals 128
- l*
- Lagrange polynominal interpolation 232
- Lagrangian  
   – action principle 37  
   – classical 41  
   – equation of motion 41  
   – representation of quantum mechanics 51
- L-alanine 208
- Laplacian of the electron density 3, 10, 17, 44, 141, 149 f., 177, 182, 192, 200, 215, 218,

- Laplacian of the electron density (cont.)  
   259, 262, 324, 346, 363, 427, 445, 458, 483,  
   488, 500 ff.
- LBHB** *see* low-barrier hydrogen bonds
- Le Chatelier principle** 56
- Leu-Enkephalin** 294
- Lewis, G. N.** 502  
   – acid 10, 252, 253, 466  
   – acidity VSCCs 367  
   – base 10, 466  
   – model 145, 345, 352, 378, 438  
   – structures 157
- LFT** *see* ligand-field theory
- Li** 216
- LiC=CLi···HF complex** 456
- LI-DICALC** 28
- LIF** 269, 270
- ligand–protein interactions** 286
- ligand-field theory (LFT)** 349, 352
- limits of transferability** 331
- local aromaticity criteria** 413
- local bulk moduli** 220, 221
- local dipole moment** 96
- local electron affinity** 484
- local electronic charge concentration** 10
- local energy densities** 443
- local exchange energy** 273
- local hardness** 484
- local polarizability** 484
- local source (LS)** 192, 194
- local statement of the virial theorem** XX, 13,  
   56, 346
- localization**  
   – domains 145 ff., 156  
   – function 142  
   – indices 14, 15, 167, 377  
   – nodes 146  
   – tree-diagram of H<sub>2</sub>CO 147  
   – tree-diagram of NaCl 147
- lock and key mechanism** 352
- lone pair** 145, 438  
   – electron concentrations 275
- Lorentzian form** 144
- low-barrier hydrogen bonds (LBHB)** 446
- low-electronegativity elements** 214
- low-pressure boron phosphide** 215
- LS** *see* local source
- m**
- M···CO interactions** 352
- M<sub>2</sub>(CO)<sub>n</sub>** 356
- macromolecular crystallography** 285
- magnetic dipole moment** 88
- magnetic susceptibility** 50
- magnetizability** 64, 68, 90  
   – tensor of naphthalene 92
- malonaldehyde** 199
- matrix of exchange moments** 136 ff.
- maximum entropy method (MEM)** 187, 188
- M–C interactions** 370
- mean molecular polarizability** 97, 98
- mean-path approximation** 271
- mean-square displacement amplitudes**  
   (DMSDA) 335
- measurable properties** 50
- medium-resolution electrostatic potential**  
   310
- MEM** *see* maximum entropy method
- metallacycles** 357
- metal–metal (M–M) bond(ing)** 199, 349, 352,  
   354 ff., 370  
   – bond path 354, 369  
   – contacts 352  
   – interactions 354, 370
- metal–olefin complexes** 361
- methane** 107, 109, 113
- methanol** 332
- methyl fluoride** 509
- methyl group** 77, 195
- N-methylacetamide** 333
- methylcycloalkanes** 99
- methylcyclobutane** 115
- N-methylformamide** 333
- methylcyclopropane** 115
- methylene group** 56, 109
- misdirected valence** 511
- Mn···(CO) intramolecular interactions** 356
- Mn<sub>2</sub>(CO)<sub>10</sub>** 201, 355
- Mn–Mn bond** 200, 201, 355
- molar volumes** 50
- molecular complexes** 196 ff.
- molecular crystals** 170 ff.
- molecular devices** 55
- molecular dipole** 170, 176
- molecular electrostatic potentials** 313
- molecular expectation value** 10
- molecular graph** 8, 52
- molecular orbital theory** 54
- molecular polarizability** 73, 77, 96 ff., 99,  
   109, 110, 113
- molecular potential** 122
- molecular quantum similarity measures**  
   (MQSM) 487
- molecular response properties** 61
- molecular similarity** 26
- molecular structure stability** 52
- molecular virial theorem** XX, 29, 86, 88
- molecular volume** 481

- molecular graph 5  
Møller–Plesset perturbation theory 29  
monopolar exchange moment 128  
monosynaptic basins 145, 438  
MORPHY 27, 332  
– 01 128, 129  
Morse equation (relationship) 4, 168, 172  
Morse-type potentials 437  
Mo–S  
– bond 242, 244, 246  
– inter-atomic surfaces 246  
MoS<sub>2</sub> 239, 245 ff.  
– bulk 241 ff., 244  
– unit cell 241  
MQSM *see* molecular quantum similarity measures  
mRNA codon 22–24  
muffin tins 223  
multiple bonds 156 ff.  
multiple-exchange energies 133  
multipolar database library 287, 306, 307, 309  
multipolar ED database fragment 287  
multipolar refinement technique XXII  
multipole expansion 130 ff., 137  
multipole model 264, 277, 336  
multipole moments 121
- n**
- N–N contacts 172  
N<sub>2</sub> 216  
N<sub>2</sub>–HF 439  
NaCl 146  
NADP<sup>+</sup> 293, 302, 312  
NaF 348  
nanotechnology 55  
naphthalene 91, 93, 392 ff., 408  
naphthacene 408  
natural bond orbital (NBO) 446  
natural coordinates 104  
natural orbitals 378  
NBM *see* non-bonded maxima  
NBO *see* natural bond orbital  
Ne<sub>2</sub> 348  
nearest-neighbor approximation (NNA) 333  
negative hyperconjugation 364  
net current vector 64  
neural networks 121  
Newton's equation of motion 41  
Newton–Raphson (NR) technique 168, 231, 236  
N–H hydrogen-bonding 433  
N–H–N hydrogen bonds 172, 446  
– complexes 441
- N–H–O hydrogen bonds 172, 448, 462  
NICS *see* nucleus-independent chemical shift  
NiMoS 239, 240  
Ni–Ni interaction 354  
NMR shielding tensors 90  
N–N  
– bond 217  
– contacts 171, 172  
NNA *see* non-nuclear attractors and nearest-neighbor approximation  
non-bonded charge concentration (NBCC) 182  
non-bonded interactions 130  
non-bonded maxima (NBM) 177, 178  
non-nuclear attractors (NNA) 6, 168, 191–193, 208, 314  
non-nuclear maxima (NNM) 6, 216, 218, 314, 225, 226  
non-stationary point geometry 62, 83, 84  
normal mode vibration 80  
normalized spherical harmonics 126  
normal-mode vibrational coordinates 79, 80  
NR *see* Newton–Raphson  
N-representability problem 378  
nuclear critical points 2, 4, 168  
nuclear momentum operator 86  
nuclear virial energy 62, 68, 83, 86  
nucleophilic attack 249, 250  
nucleus-independent chemical shift (NICS) 400–420  
null (zero value) molecular property 61, 62, 64, 66, 70  
numerical integration error 29
- o**
- observables 16  
occupation numbers 378  
octet rule 155  
OH fragment transferability 332  
O–H–O hydrogen bond 448, 462  
oligopeptide molecules 336 ff.  
one-electron density matrix 56, 123, 166, 260, 263  
open quantum system 44  
open-shell character 355  
orbital conservation 54  
orbital models 54  
ORCRIT 289, 290  
origin-dependent atomic charge-transfer dipole contribution 72  
origin-dependent atomic contributions 61, 68, 87  
origin-dependent atomic property 85

- origin-dependent charge transfer term 62  
 origin-dependent polarization term 62  
 origin-independent atomic contribution 61  
 origin-independent property density 61  
 overlap function at a point 125
- p**  
 packing forces 368  
 PAH *see* polycyclic hydrocarbon  
 pair density 166, 376  
   – functions 376  
*para*-delocalization index (PDI) 404 ff., 410, 414, 415, 417  
 paramagnetic spin–orbit 378  
*para*-nitroaniline 71 ff., 74, 76 ff.  
 PASA *see* promolecular atom shell approximation  
 path integral approach 49  
 Pauli  
   – exclusion principle 377  
   – repulsion 144, 381, 438  
 PBH *see* polybenzenoid hydrocarbons  
 PCl<sub>5</sub> 155  
 PDI *see* para-delocalization index  
 penamycin 499, 504  
 penicillin 506, 507  
   – derivative 504  
*n*-pentacosane 114  
 pentadecane 114  
 pentane 111, 113, 115, 194  
 peptide  
   – bond 328  
   – crystals 297  
   – HN–H<sub>2</sub>C<sub>α</sub>–C=O group 299  
   – plane HN–H<sub>2</sub>C<sub>α</sub>–C=O 294  
 pericyclic concerted reaction 418  
 periodic systems 231  
 perovskites 214  
 pharmacophores 499  
 phenanthrene 8, 392 ff., 408, 416  
 phenol 332  
 pK<sub>a</sub> of weak acid 26  
 Poincaré–Hopf formula (relationship) 4, 6 f., 66, 209  
 point-charge models 122  
 polar bonds 215, 455  
 polarizability 64, 78, 80, 110, 111, 400, 483  
   – tensor 11103  
 polybenzenoid hydrocarbons (PBHs) 391, 393, 394  
   – aromatic dilution 394  
 polycyclic aromatic hydrocarbons (PAHs) 404, 409, 410, 416, 417  
 polymorphism 208
- polysynaptic basins 438  
 population analysis 145  
 porphyrin 288  
 post Hartree–Fock wave functions 27–30, 127  
 potential energy density 8, 12, 25, 56, 259, 262 ff., 349, 354, 381, 462  
 powerwall mode 505  
 primary bundle 211, 212  
 principle  
   – of least action 38  
   – of stationary action 47, 49  
 PROAIM 27, 29, 193, 477  
 procrystal 267  
 PROMEGA 193  
 promolecular atom shell approximation (PASA) 290  
 promolecular model 217, 222  
 promolecule maps 300  
 propane 98, 109 ff., 194  
 propellane 99, 114  
 proper open quantum system 7, 8, 50  
 proper operator 50  
 properties after molecular reconstruction 481  
 protein  
   – binding site 313  
   – crystal structures 285  
   – crystallography 285  
   – electrostatic properties 287  
   – main chain HN–C=O peptide plane 288  
   – molecules 336 ff.  
   – refinement 289  
   – retention time 26  
   – stability 26  
   – structure 289, 311  
 protein–DNA docking 290  
 protein–ligand interaction energies 289  
 protein–protein docking 290  
 protein–protein interaction energies 289  
 proton–proton vicinal coupling constants 380  
 pseudoatom 7, 275, 329  
   – fragments 317  
 pseudoatomic density 261  
 pseudopotential 169, 222  
 pyracelene 408  
 pyridine 406, 408  
 pyrimidine 408
- q**  
 QTAMC *see* quantum theory of atoms in molecules and crystals

- quadrupole moment 24  
 quality of an atomic integration 18  
 quantitative structure–activity/property relationship 473  
 quantum
  - observables 37
  - self-similarity measure 487
  - stress tensor density 51
  - vector current density 51
 quantum theory of atoms in molecules and crystals (QTAMC) 259, 272  
 quinoline 408
- r**  
 radial density functions 261  
 radius concept 207  
 Raman
  - scattering intensity 95, 97 ff., 103 ff.
  - spectroscopy 95
 rank 4  
 reciprocal space vectors 289  
 RECON 476 ff.  
 reduced density matrices 121  
 reference density 188  
 regularity in the genetic code 24  
 Reiss–Münch theorem 475  
 relative hardness 400  
 relativistic effects 55  
 relief map of the electron density 2  
 residual electron density 318, 337  
 resonance structures 416  
 resonance-assisted hydrogen bonds 457, 458  
 response properties 62  
 R-factor 336  
 ring
  - critical point (CP) 4, 5, 168, 388
  - currents 399
  - strain 5
  - surface 5
 rotational barriers 375
- s**  
 scanning tunneling microscopy (STM) 237  
 Schrock carbene 512  
 Schrödinger's
  - functional 46
  - kinetic energy 17
  - time dependent equation 41
 Schwinger's principle of stationary action 8, 46, 50, 476  
 scorpion toxin 288  
 SCVS *see* self-consistent virial scaling  
 SD *see* softening degree  
 second atomic electrostatic moment 24  
 second-order (pair) density 401  
 second-order density matrix 14  
 second-order Jahn–Teller symmetry rule 54  
 self-consistent virial scaling (SCVS) 30, 85, 86  
 self-interaction 124  
 separability 394 ( $\sigma$ – $\pi$ )  
 SES *see* sodium electrosodalite  
 SF<sub>4</sub> 155  
 SF<sub>6</sub> 155  
 shared-shell
  - character 445
  - interactions 174, 441, 443
 sharing of electrons 13  
 shell structure 346  
 SHELXL 336  
 short strong hydrogen bond (SSHb) 463  
 Si crystal 225, 226  
 Si(111)(1 × 1) 180 ff., 184  
 Si(111)(1 × 1)–H 181
  - surface 180
 Si(111)(2 × 1) 180
  - reconstructed surface 184 ff.
  - surface 185
 Si<sub>2</sub>Me<sub>2</sub> 157  
 Si<sub>2</sub>Me<sub>4</sub> 157  
 side-chain fragments 308  
 signature 4  
 silanes 114, 117 f.  
 silicon bulk 182  
 similarity index 26, 488  
 single-enantiomer drugs 336  
 singlet diradicals 393  
 Si–O bonds in silicates 436  
 Si–Si bond properties 180  
 slab model 180, 181  
 sodium electrosodalite (SES) 186, 190 ff.  
 softening degree (SD) 447  
 solid properties 207  
 source contribution 198, 201  
 source function 165, 192 ff., 196 ff., 201 f.  
 spherical harmonics 125  
 spin density 148, 190, 191  
 spin population 16, 143  
 spin–dipolar interactions 378  
 spin-independent electron correlation 272  
 spin-less pair density 401  
 S–S
  - bond 242, 251, 427
  - bond critical points 242, 245
  - bond paths 242
  - interatomic surface 253
 SSHb *see* short strong hydrogen bond  
 stability of gradient vector field 53

- $\pi$ - $\pi$  stacking interaction 25  
 STM *see* scanning tunneling microscopy  
 stress tensor 64  
 strong hydrogen bonds 455  
 strong van der Waal's covalent interactions 440  
 structural stability 52, 53  
 substituent effects 412  
 supramolecular chemistry 186  
 surface
  - contribution 46
  - derivatives 75
  - flux 47
  - layer 182
  - terms 46
 symmetry-stabilized agostic interaction 368  
 synaptic order 145, 166, 438  
 synchrotron radiation 318 ff.
- t**  
 TAE *see* transferable atom equivalent  
*tert*-butylcyclohexane 391  
 telalin 392  
 tetracyclene 99  
 tetracyclo-[5.3.1.1<sup>2,6</sup>.0<sup>4,9</sup>]-dodecane (iceane) 115  
 tetrahydroimidazol[4,5-*d*]imidazole 429  
 tetralin 395  
 thermodynamic property 208
  - of ice VIII 437
  - partitioning 220
 Thomas–Fermi
  - approximation 263
  - kinetic energy functional 438
 three-center (*3c*) systems 357  
 three-center bonding 356 ff.  
 $\text{TiCl}_3(\text{C}_2\text{H}_5)$  366  
 time-independent electric field 74  
 TMS *see* transition metal sulfides  
 topological atoms 123, 129  
 topological multipole expansion 122  
 topological polymorphism 215  
 topological polytypism 208, 214, 215  
 topological properties 376  
 TOPOND 27, 165 ff., 170  
 TOPXD 168 ff.  
 total energy 123  
 total energy density 346, 432  
 total molecular volume 178  
 total polarization contribution 73  
 transferability 55, 56, 82, 111, 194, 287, 294, 297 f., 317, 324, 327, 331, 332, 504  
 transferable atom equivalent (TAE) 474 ff., 513  
 transferable methylene contribution 77  
 transferable multipolar data 289  
 transition metal sulfides (TMS) 236  
 transition probability 26  
 transition metal
  - atoms 509 ff.
  - carbonyl complexes 351
  - ions 511
 triazine 408  
 triphenylene 408  
 trisynaptic basins 145, 438  
 TS *see* aromatic transition state  
 two-center bonding 349 ff.  
 two-center–two-electron ( $2c-2e$ ) bonds 349  
 two-electron density matrix 166, 260  
 tyrosine 22, 24, 294, 299  
 tyrosine–glycine peptide bond 294
- u**  
 uniform electron gas 272  
 unsaturated hydrocarbons 117 ff.  
 urea 171 ff., 264 ff.
  - crystal 171, 177
- v**  
 valence basin 142, 438
  - populations 149
 valence flatness 315  
 valence shell charge concentration (VSCC) 149, 177, 182, 347, 349, 350, 355, 502  
 valence shell charge depletion (VS<sub>D</sub>) 502, 508  
 valence shell electron pair repulsion (VSEPR) model 141, 149, 150, 153 ff., 157, 158, 378, 511
  - electron domains 149 ff.
 van der Waals
  - bonds in graphite 219
  - complexes 454
  - interactions 455
  - repulsion 383
 variation of the surface 45  
 vibrational frequency 84, 96  
 vibrational modes 96  
 vibrational spectra 79  
 virial 30  
 virial field 12, 56  
 virial graph 8  
 virial of the electronic Ehrenfest force 83  
 virial operator 83  
 virial path 8, 9, 260  
 virial ratio 20, 29  
 virial theorem XX, 20, 29, 37, 52, 85, 260, 271, 432

- virtual high-throughput screening 473  
 vitamin B<sub>12</sub> 320, 321, 323  
 VmoPro 307, 309, 311  
 volume rendering 500  
 volumes 150, 178  
 von Weizäcker kinetic energy functionals 438  
*VS<sub>CC</sub>* *see* valence shell charge concentrations  
*VSCD* *see* valence shell charge depletion  
*VSEPR* *see* valence shell electron pair repulsion
- w**  
 $\text{W}(\text{CO})_3(\text{PR}_3)_2(\text{H}_2)$  364  
 Walter Kohn XXII  
 water 276  
 water dimer 137, 138, 199  
 Watson–Crick base pair 415  
 wavefunction 27, 42, 85  
 weak hydrogen bonds 455  
 weak interactions 441
- weak van der Waal's covalent interactions 440  
 WIEN 223  
 WIEN's fpLAPW 225
- x**  
 XD 165, 168, 169  
 X–H…F–Y complexes 443, 444  
 X–H…O hydrogen-bonding interactions in crystals 436  
 X–H…Y hydrogen bonds 499  
 $(\text{XH}_3)(\text{CO})_3\text{Co–Co}(\text{CO})_3(\text{XH}_3)$  molecules 355  
 X-ray absorption fine structure (EXAFS) 236  
 XTAL 289, 290, 298, 300, 303
- z**  
 zero flux  
   – condition 6, 9, 17, 44, 46, 275  
   – surface 6, 9, 10, 44, 48, 323, 354, 426, 429

