

Index

a

- Abbe resolution limit 798–799
- aberrations 802, 803
- above threshold ionization (ATI) 52
- absorption edge 232–233
- absorption spectra
 - DRIFTS 450–453
 - EXAFS 233, 239, 245, 254
 - Infra-red 664, 667, 672, 676, 679–681
 - UV-VIS 262–263, 374–375
 - MBS 358, 367, 373–381
 - REMPI 34–35
 - THz 692–694, 696, 699–700, 704
 - transient 648
- absorption coefficient / module
 - DRIFTS 447–449, 451–453
 - EXAFS 232–233, 236–240
 - THz 692–697, 699, 700, 702–705, 708
 - X-ray 279
- adsorbates *see* substance and sample index
- adsorption
 - UPS, 503–505
 - STM 607–609, 613–614
 - SERS 438–439
 - DRIFTS 463–470
 - PEEM 526–537, 543–544
 - EQCM 593–594
 - LEED 634–640
 - surface stress 744
- adsorption layers 529, 639
- AFM *see* atomic force microscopy
- alignment of molecular ensembles 13–15
- alternating current (AC) method, SQUID magnetometers 778–780
- alternating-gradient deceleration 18
- alternating-gradient focusing 17
- analytical techniques 515–517, 548, 549, 751
- analyzer
 - electron energy 479–481, 484, 487, 507–509, 518, 519, 522–524, 530, 632
 - impedance 600
 - mass *see* mass spectrometer
 - multi channel 355, 359
 - polarization 659–660
- angular correlation 327–332
- angular motion, *see also* molecular motion
 - control 4
 - of molecules 13, 15, 102
- anisotropy *see* orientational anisotropy, *see* transient anisotropy
- anodic stripping 590–591
- anomalous dispersion 291, 292
- anti-bunching 721–723
- antiferromagnetism 774–775
- apodization 455, 460
- Arrhenius dependence 133, 135, 207, 218, 219, 788
- asymmetric double-well potential (ADWP) 220–222
- asymptotic Curie temperature 777
- atomic force microscopy (AFM) 603–605, 738–739
- atomic scale resolution 621
- atomic scattering factor 808, 809
- attosecond dynamics 4
- Auger process 236–237, 359, 394, 481–483, 494, 520, 799
- autocorrelation function
 - current density 193, 205–206
 - electric dipole 696, 697
 - photon-pair 723, 724
 - velocity 214
- automated diffraction tomography (ADT) 283

b

- band gap, HOMO-LUMO gap 398, 492–501, 536, 688
- band structure 393, 408
- Beer's law 693, 695
- binding forces and off-rates 746–749
- biomolecules *see* substance and sample index
- biosensors 752, 753
- bird navigation 169
- Bleaney–Bowers equation 771
- blocking temperature 175, 784, 788, 790
- Bohr magneton, μ_B 764
- Bragg
 - direction 659, 662,
 - law 236, 273–274, 277, 288, 298, 412, 627, 631, 810
 - peaks 284, 285, 631, 813
- Bravais lattices 276
- Brillouin function 767
- broadband conductivity spectroscopy 191–229
 - complex conductivities 197–204
 - first universality 212–213
 - Fourier transform infrared spectroscopy 202–204
 - frequency-dependence techniques 197–198
 - hopping 204, 206, 210–216, 223–224
 - linear response theory, current density and conductivity 204–207
 - mismatch generated relaxation for the accommodation and transport of ions
 - (MIGRATION) 213–216
 - nearly constant loss (NCL) effect 211
 - non-Arrhenius DC conductivities 217–218
 - random vs. correlated jump diffusion 193–194
 - second universality 211–227
 - side bottom time 210
 - self diffusion 208, 216
 - Summerfield scaling 207
 - time-dependent double-well potentials 221–223
 - waveguide spectroscopy 199–202
- c**
- calorimetry 744–745
- cantilever 605, 738–745
- carbon *see* substance and sample index
- CARS *see* coherent anti-stokes Raman scattering (CARS)
- catalysis
 - bio-catalysis 262–266
 - electro-catalysis 533–537
 - gas-phase models 79, 80
 - heterogeneous catalysis 250–258, 447, 463–470, 526–533
 - homogeneous catalysis 258–262
 - ion catalysis, mass spectrometry 68, 71, 79–81
- catalysts *see* substance and sample index
- CBED *see* convergent beam electron diffraction
- C-H bond activation 79
- characteristic decay length 581
- characteristic X-ray lines 277, 507
- charge flipping (CF) 281, 289–290
- charge-tagging methods 78–79
- chemical oscillations 592–593
- chemical shifts
 - anisotropic, solid state NMR 99, 101, 127, 145
 - core level binding energy shifts, XPS 493–495, 501–503
 - energy-loss near-edge structure, ELNES 406
 - g-factor, EPR 161
 - isotropic, solid state NMR 90, 96, 100–108, 113–119, 132–139
- chemical waves 526–533
- chromatic aberrations 802, 803
- classical pump–probe interactions 648, 649
- clusters *see* substance and sample index
- coherence
 - EPR 170, 185–187
 - solid state NMR 91, 100, 106, 109–118
 - vibrational 647–649, 653–657, 661
- coherence transfer techniques 109–110
- coherent anti-stokes Raman scattering (CARS) 653–657
 - Boxcars geometry 654, 658, 659
 - coherence (vibrational coherence) 648, 654
 - diagrammatic representation 648
 - free induction decay (FID) (Raman-FID) 91, 92, 654, 658
 - heterodyne detection 660
 - population (vibrational population) 651, 654
 - Stokes field 658
 - time-ordered diagram 653, 659
 - wave vector 655
- collision-induced dissociation (CID) 72–73
- commensurate 630
- composition analysis 272, 489–491
- conductivity 125, 175, 191–229, 605–607, 691–693, 779
- conductivity spectra 207–212
- confocal microscopy 434, 437, 657, 715–723

- conformers *see* isomers
 conformer selection 7, 19–21, 39–40
 constant analyzer energy (CAE) mode 508
 constructive interference 456, 457
 contact mode, SPM 740–741
 contrast mechanism, PEEM 525–526
 contrast variation, SAXS and SANS
 311–312, 321, 323
 continuous wave EMR 164–168
 convergent beam electron diffraction (CBED)
 807–808
 core-loss edges, EELS 402–407
 corrosion
 – EQCM 587–589
 – MBS 380–382
 corrosion studies 380–381, 586–589
 Coulomb explosion 16, 22
 critical points, electron density 281–282
 crystalline solids and symmetry 275–277
 crystal systems 274, 276
 Curie's law 767–773
 Curie paramagnetism 766
 Curie temperature, T_C 771
 Curie–Weiss' law 771, 775, 782
 current-density autocorrelation function 205
 cyclic voltammogram 592
 cyclotron resonance 68, 175, 184
- d**
- DQC *see* double-quantum coherences
 de Broglie wave length 309, 626, 798,
 Debye–Waller factor 235, 241–242, 249, 274,
 355
 Decelerator
 – alternating gradient 18
 – Stark 11, 12
 Deflector
 – electric 15, 16, 18, 19
 – magnetic 18, 19
 DEER *see* double electron electron resonance
 deflection technique 9
 degenerate four-wave mixing (DFWM)
 658, 659
 density functional theory (DFT) 88, 96,
 134–135, 137, 272, 348, 393, 408, 680
 density of states (DOS) 393, 402, 493
 – partial DOS 387, 403–407, 491–492
 – local DOS 623
 – vibrational 697–699
 deposits on electrodes 536
 destructive interference 456–457
 detectors
 – delay line detector (DLD) 539
 – electron detectors, photoelectron
 spectroscopy 509
 – charge-coupled devices 278, 309, 395, 431,
 433, 509, 524, 717, 719–720, 800, 816
 – image plate (IP) 278, 309
 – mercury cadmium telluride detectors,
 DRIFTS 455
 – multi-channel plate (MCP) 16–17, 509,
 524, 539, 633
 – neutron detection 277–278, 314
 – PAC detection 227, 229
 – Raman spectroscopy 431, 433–434
 – THz detection 690
 – X-ray detection 277–278, 308–309
 diamagnetic materials 781
 diagrammatic representation 648
 diamagnetism, SQUID magnetometers 766
 “Diesotto”-engines 463
 differential optical density (ΔOD) 650, 652
 differential thermogravimetry (DTG) 752
 diffraction aberrations 802
 diffraction limit 716
 diffraction methods 271–295, 806–813
 – automated diffraction tomography (ADT)
 283
 – Bragg's law 273–274
 – charge density analysis and chemical
 bonding 281–282
 – crystalline solids and symmetry 275–277
 – electron diffraction 213, 806–813
 – experimental set-up and data treatment
 278–279
 – Le Bail fit and structure solution 287–289
 – maximum entropy method (MEM) 290
 – micro- and nano-crystal structure
 determination 283
 – neutron powder diffraction (NPD) 291, 293
 – non-ambient diffraction and anomalous
 dispersion 291, 392
 – pair distribution function (PDF) analysis
 290–291
 – point groups/crystal classes 276
 – powder diffractometry 284–293
 – Rietveld structure refinement and phase
 fractions 285–287
 – scattering form factor 274
 – single crystal analysis 278–283
 – space groups 276
 – structure refinement residuals 280–281
 – structure solution, histogram matching and
 charge flipping (CF) 289–290
 diffuse reflectance infrared Fourier transform
 spectroscopy (DRIFTS) 445–475
 – adsorbate identification 464–467

- diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) (*contd.*)
 - adsorbate kinetics 466–467
 - experimental set-up 455
 - in situ measurements 466
 - interferometry and Fourier transformation 456–460
 - Kubelka–Munk model 449–453
 - Lambert–Beer’s law 449–450
 - NSR-technology 463–464
 - quantification of surface groups 470, 471
 - principles 448–449
 - reflectance 452, 453
 - transmission and scattering on thin layer 451
 - transmittance and reflectance spectrum 454
 - temperature programmed desorption (TPD) 471
 - reactor cell, heterogeneous catalysis 463–464
- diffusion
 - cation diffusion 562–566
 - depth profile 562, 563
 - diffusion equation 558, 571–573, 729–731
 - diffusive motion 249, 651
 - dissipation theorem 713
 - Fick’s law 572, 730
 - first universality 209–210, 212–220
 - ionic diffusion 194
 - mathematics of diffusion 571–573
 - mean square displacement 216–217
 - oxygen 557–561, 571
 - nuclear probes 345–347
 - second universality 210–212, 220–227
 - single-molecule tracking 729–732
 - tracer diffusion coefficients 564
- diffusion coefficient 216–217, 557, 562, 565, 571–573, 730
- dipolar couplings 101–102, 105, 109–128, 131, 147, 150
- direct current (DC) method, SQUID magnetometers 778–780
- direct methods, single crystal analysis 279
- disordered ionic materials 192–196
- distance measurement 170, 187
- double electron electron resonance (DEER) 170–172
- double-quantum coherences (DQC) 110–118
- double-quantum NMR 134, 139
- DRIFTS *see* diffuse reflectance infrared Fourier transform spectroscopy
- dynamical hydration shell 701, 705, 706
- dynamical vs. kinematic diffraction 812
- dynamic SIMS 555, 563
- e**
 - EDS *see* energy-dispersive X-ray spectroscopy
 - EELS *see* electron energy-loss spectroscopy
 - effective Bohr magneton number, μ_{eff} 768
 - effective dipole moment *see* Stark effect
 - elastic recoil detection analysis (ERDA) 548–549
 - ELDOR *see* electron double resonance
 - electric deflection 8, 9, 15–19
 - electric double layer 607–608
 - electric fields
 - ac 14, 19
 - dc (static) 13–15, 576–577
 - homogeneous 9, 10
 - induced forces 40
 - inhomogeneous 9, 10
 - laser 12–15, 43
 - electric field gradient (EFG) 97–99, 151, 334, 341–343, 362
 - electric permittivity 692
 - electric quadrupole moment 94, 97, 99, 123–124, 332 362
 - electrochemical cell 583
 - electrochemical interface 487
 - electrochemical nanostructuring 618
 - electrochemical polarization 533–536
 - electrochemical potential 543
 - electrochemical promotion of catalysis (EPOC) 534
 - electrochemical quartz crystal microbalance (EQCM) 575–601
 - electrocrystallization 614
 - electrode potential 592, 593, 609, 612, 613, 616
 - electrode surface 607
 - electroless deposition 590
 - electron density 181, 271–282, 293, 307, 311, 360–371, 394
 - electron diffraction 213, 806–811, 813
 - electron electron double resonance (ELDOR) 163, 164
 - electron energy-loss spectroscopy (EELS) 391–418, 798–799
 - composition determination 409
 - coordination fingerprint 405, 410–412
 - core-loss edge fine structure 402–407
 - core-loss region 398–399
 - density of states (DOS) 393, 394, 402–408
 - dipole approximation 406
 - dipole region 397
 - elastic scattering 394

- electronic transitions 399–400
- energy-loss near-edge structure (ELNES) 402–408
- elemental analysis 392, 401, 409
- experimental vs. calculated spectra 412–414
- generalized oscillator strength (GOS) 396
- high resolution electron energy loss spectroscopy (HREELS) 392
- inner-shell excitation 394
- instrumentation 395
- oxidation state 406, 410
- physical background 395–397
- solid state chemistry 393–394
- valence electron energy loss spectroscopy (VEELS) 398
- white lines 399–400
- zero-loss peak (ZLP) 397
- electron filtering transmission electron microscopy (EFTEM) 401
- electron magnetic resonance (EMR) 164–174
- electron paramagnetic resonance (EPR) 159–189
 - basic Principles 160–163
 - continuous wave EMR 164–168
 - cyclic electron motion 177
 - cyclotron resonance and Landau levels 184–185
 - double electron electron resonance (DEER) 170, 172
 - electron nuclear double resonance (ENDOR) 162, 172–173
 - electron electron double resonance (ELDOR) 164
 - effective spin Hamiltonian 183–184
 - electron spin echo envelope modulation (ESEEM) 185–186
 - frequency-domain zero field 175–176
 - hyperfine interactions 161
 - hyperfine sublevel correlation spectroscopy (HYSCORE) 170–171, 180, 187
 - periodic-orbit resonance 175
 - pulsed EMR 168–174
 - pulsed ENDOR 172–173
 - site-directed spin-labeling (SDSL) 180–181
 - van Hove singularities 167
 - Zeeman effect 182–183
 - zero-field-splitting (ZFS) 162, 167–168, 174–179
- electron nuclear double resonance (ENDOR) 162, 172–173
- electron spectroscopy for chemical analysis (ESCA) 480, 521
- electron spectroscopic imaging (ESI) 401
- electron spin echo envelope modulation (ESEEM) 185–186
- electron spin resonance *see* electron paramagnetic resonance
- electron-transfer
 - mass spectrometry 77–79
 - reactions 74, 77, 264, 535–536, 607–608, 709, 727–729
- electron tunneling 622–623
- electrospray ionization (ESI) 70–71
- electrostatic deflector 20, 21
- elemental analysis
 - EELS 401, 409
 - SIMS 556
 - XPS 488, 521
 - XRF 382, 568
- ELNES *see* energy-loss near-edge structure
- Emission
 - γ -rays 332
 - stimulated 649
- EMR *see* electron magnetic resonance
- ENDOR *see* electron nuclear double resonance
- energy band diagrams 393, 501, 502, 520, 622
- energy-dispersive X-ray spectroscopy (EDS) 797, 798
- energy level diagram 393, 660
 - CARS 655, 656
 - continuous wave EMR 167–168
 - ELNES 402
 - EPR 167–168
 - fluorescence 714
 - ion-dip spectroscopy 38
 - MBS 360
 - molecular magnets 174
 - PAC 334
 - Raman 423
 - structural isomers 7–8
 - solids 393
 - solid state NMR 150
 - spin crossover 371–372
 - STM 622
 - vibrational 670, 675
 - vibronic 371–372
 - XAS 236
 - XPS 483, 496, 520
 - Zeeman interaction 90, 182–183
- energy-loss near-edge structure (ELNES) 402–408
- energy shift analysis, XPS 493–495, 501–503

- EPOC *see* electrochemical promotion of catalysis
- EPR *see* electron paramagnetic resonance
- ESR *see* electron magnetic resonance
- EQCM *see* electrochemical quartz crystal microbalance
- ergodic theorem 712, 732
- ESEEM *see* electron spin echo envelope modulation
- Ewald sphere 278, 284, 807, 810–811
- excited state absorption 671
- EXAFS *see* extended X-ray absorption fine structure
- exchange spectroscopy (EXSY) 105–106, 111
- EXELFS *see* extended energy-loss fine structure
- EXSY *see* exchange spectroscopy
- extended energy-loss fine structure (EXELFS) 407
- extended X-ray absorption fine structure (EXAFS) 121, 232–246
- extinction 277, 449–457, 692, 806, 810–812, 816
- extinction coefficient 449, 453, 692
- Eyring equation 746–747
- f**
- Faradaic current 609–610
- femtosecond laser mass spectrometry 48, 49
- femtosecond EELS 415
- femtosecond time-resolved vibrational spectroscopies 645–686
- applications 663–682
 - coherent anti-stokes Raman scattering (CARS) 653–657
 - infrared pump–probe spectroscopy 647–653
 - impulsive stimulated Raman scattering (ISRS) 657–662
 - optical Kerr effect (OKE) 667–669
 - Raman-induced optical Kerr effect (OKE) 657–662
 - vibrational dynamics 678–682
 - vibrational relaxation 669–677
- Fermi's golden rule 233, 402, 682
- Fermi level 95, 393–394, 403, 479–502, 520–521, 543–544, 609, 622, 688
- Fermi resonance 426, 669–670, 674
- Fermi surface 163, 175, 497–498
- ferrimagnetism 776–777
- ferroelectric material 177
- ferromagnetism 773–774
- Fick's law 572, 730
- fixed analyzer transmission (FAT) mode 508
- fluorescence 18, 236–237, 256, 263, 352–354, 382, 387, 422, 428–431, 711–735
- correlation spectroscopy 718
 - fluctuations 720
 - quantum yield 720
- fluorescence lifetime 713, 720–721, 723–725
- fluorescence microscopy 713, 717–721
- focuser
- AC 12
 - dynamic 17
- force spectroscopy 741–743, 746–749
- form factor 274–275, 302–305, 320, 396
- Förster resonance energy transfer (FRET) 726–727
- forth rank tensor 175
- Fourier transform infrared spectroscopy (FTIR) 202–204, 445–475
- Fourier transformation
- OHD-OKE 660–661, 668
 - DRIFTS 456–460
 - EPR 170, 186
 - EXAFS 237, 239–243
 - FTIR 203
 - NMR 91–92
 - PAC 333
 - XRD 281
- fragmentation 20, 33, 39–53, 59–60, 69, 557
- Franck–Condon transition 36, 41, 53, 72
- free electron laser 32, 267–268, 307, 537–538, 693
- free induction decay (FID) 91, 93, 106–107, 648, 654
- Fresnel reflection 448–449
- Fresnel zone plate 522, 542
- FRET *see* Förster resonance energy transfer
- FTIR *see* Fourier transform infrared spectroscopy
- g**
- galvanic deposition 589
- Galvani potential 543
- gas-phase molecules
- manipulation 8–13
 - rotation 13–15
 - translation 13, 14
- g-factor, g value 160–162, 166, 183, 765, 766
- Gibbs energy 65, 744, 746–747
- Gibbs-Helmholtz equation 65
- glasses *see* substance and sample index
- grain boundaries 492, 505, 540, 559–565
- gravimetry 575–601, 750–752
- ground-state bleach 649
- Guinier approximation 304–305, 323

h

hard ferromagnetic material 774
 hard ionization methods 67
 H-bond systems *see* substance and sample index
 Heisenberg uncertainty principle 30, 354
 Helmholtz plane (IHP, OHP) 487, 607–608
 hemispherical energy analyzer 522
 HETCOR *see* heteronuclear correlation
 hetero- and homonuclear decoupling 104–105
 heteronuclear correlation (HETCOR) spectra 110–111
 high-field-seeking states 11
 high resolution electron energy loss spectroscopy (HREELS) 392
 high resolution imaging, TEM 816–820
 high resolution transmission electron microscopy (HRTEM) 289, 816–820
 hole-burning spectroscopy 712
 homodyne detection 657
 homoenergy transfer 727
 hopping motion 193, 194, 204–216, 223–224, 347
 Howie Whelan equations 815, 816
 HREELS *see* high resolution electron energy loss spectroscopy
 HRTEM *see* high resolution transmission electron microscopy
 Hund's rules 371, 768
 hybrid materials 745
 hydrodynamic focusing 716, 717
 hyperfine (hf) interactions 161, 333, 357, 377–378
 hyperfine sublevel correlation spectroscopy (HYSCORE) 170–171, 180, 187
 HYSCORE *see* hyperfine sublevel correlation spectroscopy

i

image contrast, TEM 813–816
 impedance analysis, 597–599
 impedance spectroscopy 192, 197–198, 226–227
 impulsive stimulated Raman scattering (ISRS) 657–662
 indexing, powder diffractometry 287
 indirect magnetic dipolar interactions 94
 inelastic mean free path 480, 489
 inelastic scattering
 – SANS 310
 – MBS 353, 387
 – EELS 392–399, 799
 – Raman 423–425, 715

– XPS 481, 489, 495, 519
 – TEM 808
 infrared (IR) pump–probe spectroscopy 647–653
 infrared (IR) spectroscopy 202–204, 445–475
 IR spectroscopy of solid samples 446–447
 insulator-to-metal transition 338
 inter-band transition 394, 399
 intensity versus voltage (IV) curve 631
 interface analysis, XPS 501–503
 interfaces
 – metal/electrolyte 604, 607, 608, 623
 – metal/semiconductor 344, 499–502
 – semiconductor/electrolyte 487
 – semiconductor/semiconductor 501, 502
 – solid/liquid 487, 488
 – solid/solid 486, 487
 interference
 – FTIR 203, 456–458
 – EXAFS 243
 – X-ray 273–274
 – SAXS, SANS 298, 300, 301
 – EELS 407, 408
 – SIMS 558–560
 – LEED 626–627, 631–632
 – vibrational pump–probe spectroscopy 654, 660
 – THz 695
 – SQUID 763
 – TEM 810–812
 interferometry 202–204, 456–460
 intermolecular interactions 661, 670
 internal interactions, NMR 94
 intersystem crossing (ISC) 376, 714, 718
 inverse photoelectron spectroscopy (IPES) 520, 549
 ion-dip spectroscopy 38–40
 ion dynamics 192
 ion energetics, mass spectrometry 72–77
 ionic conductivity 193
 ionic liquids *see* substance and sample
 ionic solids *see* substance and sample
 ionization
 – above threshold ionization 42
 – anion photodetachment 72
 – electrospray (ES) 70–71
 – methods 64–65, 67, 71
 – multiphoton ionization 32–38
 – single-photon ionization 31–32
 – strong-field ionization 41–45
 – threshold ionization 30–31, 39–42, 72–75
 – tunneling ionization 43

- ionization energy 31–32, 40–43, 53–56, 64, 75–76, 399, 479
 - isomers
 - populations 371
 - selection 49
 - structural 7–8, 45–48
 - isomerization 75, 133–134, 262, 263
 - ion milling 803–805
 - ion sputtering 485, 550–551
 - ion structures, mass spectrometry 69–72
 - ion transfer reaction 607
 - IPES *see* inverse photoelectron spectroscopy
 - irreversible photobleaching 714
 - IR spectroscopy *see* Fourier transform infrared spectroscopy
 - isomer shift, MBS 359–362
 - ISRS *see* impulsive stimulated Raman scattering
- j**
- Jablonski diagram, fluorescence 713, 714
- k**
- Kikuchi lines 811
 - kinetic method 64–65
 - kinetic THz absorption spectroscopy (KITA) 706–708
 - KITA *see* kinetic THz absorption spectroscopy
 - Knight shift 95
 - Kossel-Möllenstedt diagrams 808
 - Kubelka–Munk model 449–453
- l**
- Lambert-Beer's law 232, 449–454, 693, 695, 702
 - Lamb-Mössbauer factor 355
 - Landau levels 163, 184–185
 - Landau-Teller theory 676, 677
 - Landau quantization 163
 - laser ionization spectroscopy
 - collisional and rotational energy effects 54
 - conformer selection 39–40
 - femtosecond and nanosecond pulses 46–47
 - femtosecond laser mass spectrometry 48–50
 - fragmentation pattern 47
 - ion-dip spectroscopy 38–39
 - principles 30–31
 - pulsed-field ionization 39–41
 - resonance enhanced multiphoton ionization (REMPI) 32–38
 - single-photon ionization 31–32
 - state-selected ions 51–54
 - strong-field ionization 41–45
 - trace analysis 50–51
 - zero electron kinetic energy (ZEKE) spectroscopy 41–42
 - laser induced fluorescence 18
 - lasers
 - femtosecond 30, 42, 46, 48–49, 691, 692
 - free electron laser 32, 267–268, 307, 537–538, 693
 - gas lasers 429
 - Nd:YAG laser 32, 429
 - p-Ge laser 689–690, 702
 - quantum cascade lasers 689
 - lattice vectors 275, 627–630, 634–637
 - Laue
 - classes 277, 279
 - equation 627–631, 810
 - zones 807
 - Laue condition 631
 - Le Bail method 287–290
 - LEEM 531
 - LEED *see* low-energy electron diffraction
 - lens aberrations 802–803
 - ligand field 371–379, 412–413, 769–770
 - ligand-field effects 769–771
 - light-induced excited spin state trapping (LIESST) 371, 376
 - light sources
 - femtosecond 30, 42, 46, 48–49, 691–692
 - free electron laser 32, 267–268, 307, 537–538, 693
 - gas lasers 429
 - p-Ge laser 689–690, 702
 - global 455
 - Nd:YAG laser 32, 429
 - quantum cascade lasers 689
 - Raman spectroscopy 429–430
 - γ radiation 356
 - synchrotron radiation 29, 74–75, 236, 256, 261–283, 291, 307–309, 323, 352, 387, 407, 413, 480–492, 500, 508, 522, 537–542
 - THz sources 688
 - X-ray sources 277–278, 308, 479, 506–507
 - linear response theory 204–207
 - Lippincott-Schroeder potential 664, 665
 - Lorentz contrast microscopy 526
 - low-energy electron diffraction (LEED) 625–642
 - adsorbates 634–636
 - disordered layers 639–640
 - energy conservation 629
 - Laue equation 627–631

- LEED-IV structure determination 637–639
 - instrumentation 632–633
 - intensity versus voltage (IV) curves 630–631
 - reciprocal lattice vectors 627–629
 - spot profile analysis 631–632, 636–637
 - superstructures 630
 - surface periodicity 627
 - unit cells 627, 628
 - low-field-seeking states 11
- m**
- magic angle
 - infrared pump–probe spectroscopy 651–652
 - solid state NMR 97, 99–101, 105–106, 117, 145, 148
 - spinning (MAS) 100–101, 117
 - magnetically condensed systems 771–773
 - magnetically dilute systems 768–771
 - magnetic dipole–dipole interactions 93–96, 100–104, 110–120, 123, 125, 128–131, 147–148
 - magnetic dipole moment 332, 363–364, 764–766
 - magnetic dipole splitting 364–366
 - magnetic materials *see* substance and sample index
 - magnetic quantities and units
 - magnetic dipole moment 764–766
 - magnetic field 766
 - magnetic susceptibility 766, 778–780
 - magnetization 766
 - magnetic screening 93–96, 145–146
 - magnetic shielding anisotropy 145
 - magnetism
 - antiferromagnetism 774–776
 - Curie paramagnetism 766
 - diamagnetism 766
 - ferrimagnetism 776–777
 - ferromagnetism 773–774
 - magnetically condensed systems 771–773
 - magnetically dilute systems 768–771
 - metamagnetism 781–783
 - nuclear 89
 - Pauli paramagnetism 767
 - paramagnetism 766–767
 - single-molecule magnets 173–175, 788–790
 - superparamagnetism 783–785
 - temperature-independent paramagnetism (TIP) 767
 - magnetometry 763–795
 - magnetron sputtering 484, 490, 498, 503
 - manipulating the molecular motion of
 - complex molecules 3–28
 - manipulation of polar molecules 9–10
 - mass analyzers 66
 - mass of monolayers 581
 - mass spectrometer 66–68
 - quadrupole 12, 68, 555, 556
 - time-of-flight (TOF) 16–17, 45, 58–59, 68, 75, 552, 555, 570–571
 - mass spectrometry (MS) 48–49, 63–84, 547–574
 - charge-tagging methods 78–79
 - collision induced dissociation (CID) 72–73
 - electrospray ionization (ESI) 70–71
 - electron-transfer reactions 77–78
 - femtosecond-laser mass spectrometry 48–49
 - gas-phase basicities 65
 - ion catalysis 79–80
 - ion chemistry 69
 - ion energetics 73–77
 - ionization methods 67, 71
 - ion structures 69–72
 - kinetic method 64–65
 - neutral molecular reactions
 - neutralization–reionization mass spectrometry (NRMS) 77–78
 - secondary ion mass spectrometry (SIMS) 547–574
 - thermochemistry of gaseous ions 76–77
 - threshold ionization 73–76
 - maximum entropy method (MEM) 290
 - MBS *see* Mössbauer spectroscopy (MBS)
 - mean square displacement 216–217, 274, 557, 729–731
 - mechanical shear impedance 598
 - MES *see* Mössbauer emission spectroscopy (MES)
 - metal deposition 582–583, 589–591, 614–620
 - metamagnetic materials 781–783
 - MFP *see* molecular force probe
 - Michelson interferometer 202, 456
 - microbalance 575–600
 - microcrystal structure 283
 - micro-electromechanical system (MEMS) 750, 752, 757
 - micro-LEED 641
 - micromechanical cantilever 605, 738–745
 - micro-Raman spectroscopy 434, 436–438
 - microscopy
 - confocal 434, 437

- microscopy (*contd.*)
 - fluorescence 718, 720
 - optical resolution 713
 - microspectroscopy 516, 517
 - MIGRATION *see* mismatch generated
 - relaxation for the accommodation and transport of ions
 - mismatch generated relaxation for the accommodation and transport of ions (MIGRATION) 213–216
 - molecular alignment and orientation 13–15
 - molecular beams 4–8, 11, 15–21, 50, 484, 750, 754
 - molecular dynamics simulation 102, 249, 667, 680, 695
 - molecular ensemble alignment and orientation 13–15
 - molecular force probe (MFP) 741–743, 746–749
 - molecular-frame photoelectron angular spectroscopy 22–23
 - molecular motion of complex molecules 3–28
 - molecular motion
 - alignment and orientation, molecular ensembles 13–15
 - alternating-gradient deceleration 18
 - alternating-gradient focusing 17
 - cluster and biomolecules deflection 18–19
 - conformer selection 19–21
 - controlled molecules 4
 - deflection 15–17
 - large neutral molecules, gas phase 6–8
 - molecular beams 4–8
 - high-field-seeking quantum states 11–12
 - low-field-seeking quantum states 11
 - molecular-frame photoelectron angular distributions 22–23
 - three-dimensional orientation 20–22
 - monochromator 236, 256, 277–284, 307, 403, 432, 479, 506–507, 522, 542, 650, 658
 - Mössbauer emission spectroscopy (MES) 377–379
 - Mössbauer isotopes 353–354
 - Mössbauer spectrometer 355–356
 - transmission geometry 358
 - backscattering geometry 358
 - Mössbauer spectroscopy (MBS)
 - Doppler effect 357–358
 - electric monopole interaction 359–362
 - electric quadrupole interaction 362–363, 365–368, 375
 - high spin / low spin complexes 361–362, 371–373
 - hot atom chemistry 380
 - hyperfine interaction 357, 364, 377–378
 - isotopes and periodic table 353–354
 - industrial applications 380–381
 - ligand electronegativity effect 370
 - magnetic dipole interaction 364–366
 - nuclear decay-induced excited spin state trapping (NIESST) 379
 - nuclear decay scheme 356–357
 - portable miniaturization 382–387
 - principles 353–356
 - resonant excitation and de-excitation modes 358–359
 - switchable molecules, spin crossover 371–376
 - thermal spin transitions 377, 379
 - multi-color REMPI schemes 32
 - multi-dimensional NMR 105–109
 - multiplex FT EMR spectroscopy 169
 - multivariate curve resolution (MCR), Raman spectrum 440
- n**
- nano-diffraction 283, 807
 - nanosystems *see* substance and sample index
 - NCL *see* nearly constant loss
 - nearly constant loss (NCL) effect 211–212, 224–227
 - Néel temperature, T_N 771
 - NEMCA *see* non-Faradaic electrochemical modification of catalysis
 - Nernst potential 615
 - neutralization-reionization mass spectrometry (NRMS) 77–78
 - neutron diffraction 272, 291–293
 - neutron scattering 291, 293, 309–314
 - neutron sources 277–278, 313–314
 - NMR *see* nuclear magnetic resonance
 - non-ambient diffraction 291, 292
 - non-Arrhenius dependence 217–218, 669
 - non-classical light, SMFS 723–725
 - non-Faradaic electrochemical modification of catalysis (NEMCA) effect 534–535
 - nonlinear dynamics 527
 - NOx storage reduction (NSR) technology 463–464
 - NRMS *see* neutralization-reionization mass spectrometry
 - NSR *see* NOx storage reduction
 - nuclear decay-induced excited spin state trapping (NIESST) 379
 - nuclear electric quadrupolar interaction

- MBS 362–363, 365–368, 375
 - NMR 88, 94, 97–99, 149
 - PAC 333–334, 339–345
 - nuclear magnetic resonance (NMR) 87–158
 - basic principles 89–92
 - coherence transfer 109–110
 - decoupling 104–105
 - internal interactions 95–98
 - magic angle spinning 100–103
 - multi-dimensional NMR 105–109
 - recoupling 110–116
 - relaxation phenomena 92–94
 - spin echo 103–104
 - nuclear magnetic resonance (NMR) spectroscopy 87–158
 - nuclear magnetism 89
 - nuclear reaction analysis (NRA) 549
 - nuclear Zeeman effect 90, 94, 99, 148–149, 170, 185–186, 363–365
 - numerical aperture (NA) 434, 766, 798
- o**
- OHD-OKE *see* optically heterodyne detected optical Kerr effect
 - OKE *see* optical Kerr effect
 - optical Kerr effect (OKE) 658–662, 667–669
 - optical beam deflection 739–740
 - optical density 650–653
 - optical electronic rectifier 689
 - optically heterodyne detected optical Kerr effect (OHD-OKE) 660–662
 - orientation of molecular ensembles 13–15, 20–22
 - oscillating electrochemical reactions 592–593
 - oxidation state
 - ELNES 406, 410
 - MBS 359–361, 363
 - XANES 244–246
 - XAS 264–265
 - XPS 493–494, 506
- p**
- PAC *see* perturbed γ - γ angular correlation
 - pair distribution function (PDF) 290–291
 - paramagnetism 766–767
 - partial density of states 491–492
 - pass energy 507
 - Patterson method 279
 - Pauli paramagnetism 767
 - PEEM *see* photoelectron emission microscopy
 - PEM *see* photoelectron microscopy
 - periodic table
 - MBS 353–354
 - solid state NMR 98–99
 - permittivity 198–201, 210, 215–217, 597, 692
 - perturbed γ - γ angular correlation (PAC)
 - diffusion studies 345–347
 - γ ray emission 329–332
 - instrumentation 335–336
 - isotope selection 326, 328
 - local magnetic fields 337–338
 - magnetic interactions 334–335
 - nuclear decay 326–327
 - PAC isotopes 328
 - quadrupolar interactions 333–334
 - spin transitions 338–340
 - structural refinements 340–341
 - surface studies 341–342
 - thin film reactivity 343–344
 - phase matching 654, 655
 - phonon scattering 394
 - photoelectric effect 237, 479, 517, 543
 - photoelectron emission microscopy (PEEM) 523–526
 - photoelectron microscopy (PEM) 513–546
 - chemical waves 526–533
 - dark field imaging 533, 534
 - electrode reactions 534–538
 - electrochemical spill-over pumping 537, 538
 - electrochemical promotion of catalysis (EPOC) 534
 - free electron laser 537–538
 - low energy electron diffraction (LEED) 531, 532
 - instrumentation 522, 524
 - non-Faradaic electrochemical modification of catalysis (NEMCA) 534–535
 - photoelectron emission microscopy (PEEM) 523–526
 - potentials and work function 543–544
 - principles 515–517
 - scanning photoelectron microscopy (SPEM) 522–523
 - surface analysis 515, 516
 - synchrotron radiation 541, 542
 - time-of-flight (TOF) PEEM 538–539
 - ultraviolet photoelectron spectroscopy (UPS) 504–505, 519–520
 - X-ray photoelectron spectroscopy (XPS) 521
 - photoelectron spectroscopy 477–512, 515–521
 - adsorption, UPS, 503–505
 - Auger transitions 482, 483

- photoelectron spectroscopy (*contd.*)
 - core level binding energy shifts (chemical shift) 493–495, 501–503
 - composition analysis 488–491
 - binding energy 481
 - elemental analysis 488, 521
 - kinetic energy, of photoelectrons 481
 - inelastic mean free path, of electrons 480–481
 - instrumentation 479, 480, 506–508
 - interfaces analysis 486–488
 - sample preparation 483–488
 - surface potential changes 495–500
 - surface sensitivity 481
 - ultraviolet photoelectron spectroscopy (UPS) 504–505, 519–520
 - valence band spectra 504–505
 - X-ray photoelectron spectroscopy (XPS) 483–486, 492–501, 521
 - photo-excited radicals 169
 - photo-induced electron transfer (PET) 169, 727–728
 - photoionization *see* ionization
 - photon-pair autocorrelation function 723, 724
 - photon sources 506–507
 - photophysical processes 497, 499–501, 713–715, 721–722, 727
 - photostability/photobleaching 714, 720
 - photosynthetic reaction centers 169
 - photovoltage 497, 499–501
 - piezoelectricity 576–578
 - plasmon excitations 398, 439, 481, 489, 495
 - plasmon scattering 394
 - point spread function (PSF) 719, 817
 - Porod's law 306
 - population (vibrational population) 651, 654
 - potential energy surface 6–8, 65, 665, 747
 - powder diffractometry 278–280, 283–293
 - power-law 209, 213, 698–699
 - Praying Mantis system 460, 461
 - precession 89–96, 145, 163
 - precession electron diffraction technique 283, 813
 - pressure gap 539
 - principle component analysis (PCA), Raman spectrum 440
 - probe-pulse 652
 - proton induced gamma-ray emission (PIGE) 549
 - pulsed EMR 163, 168–172
 - pulsed-field ionization (PFI) 39–41
 - pulsed-field ionization-zero electron kinetic energy spectroscopy (PFI-ZEKE) 41
 - pump-induced absorption / emission 647–653, 681
 - pump-probe spectroscopy, *see also* infrared pump-probe spectroscopy; vibrational pump-probe spectroscopy, femtosecond (time-resolved) vibrational spectroscopy
 - anisotropy (orientational anisotropy, transient anisotropy) 652–653
 - coherence (vibrational coherence) 647, 648, 653, 654, 656, 659
 - diagrammatic representation 647
 - differential optical density (ΔOD) 650, 652
 - energy level diagram 654, 656
 - excited state absorption 671, 676
 - ground state bleach 649, 650, 653
 - magic angle 651, 652
 - optical density 651, 652
 - population (vibrational population) 651, 654
 - probe-pulse 652
 - pump-probe time trace 650
 - pump-pulse 652, 659
 - stimulated emission 649–650, 680–681
 - time-ordered diagram 647, 653, 659
 - transient absorption 648–640
 - transient spectrum 680
 - pump-probe time trace 650
 - pump-pulse 652, 659
- q**
- q-bit 182
 - quadrupole splitting
 - MBS 362–363, 365–368, 375
 - NMR 88, 94, 97–99, 149
 - PAC 333–334, 339–345
 - quantitative analysis 392, 401, 426–427, 453, 471, 488
 - quantum-level structure of large molecules 7–8
 - quantum numbers
 - electron spin 58, 160–161, 165, 169, 175, 182–183
 - electron orbital momentum 56, 58
 - Landau 177, 184, 185
 - nuclear spin 89, 113, 148, 162, 169, 326–328, 332, 356, 362–364
 - photon 332
 - principal 56
 - rotational 8–11, 35, 53–57
 - vibrational 36, 648
 - quantum states 8–10
 - electronic states 7
 - energy level structure 8–10
 - high-field-seeking 11–12

- low-field-seeking 11
- rotational states 8–13, 20
- vibrational states 8
- quartz crystal microbalance (QCM) 575, 581, 595
- quartz microbalance (QMB) 575–601
 - calibration 584
 - corrosion studies 587–589
 - (cyclic) voltammogram 591–592
 - electrochemical cell 583
 - metal deposition 589–592
 - metallization 582, 583
 - impedance analysis 598–599
 - oscillating electrochemical reactions 592–593
 - piezoelectricity of quartz 576–578
 - resonance frequency 578–581
 - self-assembled monolayers 593–594
 - selection 3–24
 - surface roughness 585–586
 - viscous media 581–582
- quartz oscillator 580–582

r

- radial distribution function (RDF) 239–243, 248–251, 260, 709, 807
- Raman-induced optical Kerr effect (OKE) 657–662
- Raman scattering 422–426, 715–716
- Raman scattering intensities 424–425
- Raman spectroscopy
 - applications 436–438
 - benefits of 435–436
 - lasers 429–430
 - inelastic scattering 423
 - instrumentation 427–434
 - quantitative analysis 426–427
 - principles 423–426
 - Raman microscopy 434–435
 - Raman scattering intensities 424–425
 - surface-enhanced Raman spectroscopy (SERS) 438–440
 - wavelength dependency 430
- random walk 193, 730–731
- rapid-scan technique, FTIR 646
- Rayleigh-wing scattering 658
- reaction coordinate 6–8, 65, 665, 747
- reaction-diffusion system 528
- reaction kinetics 71–79, 746–759
- reciprocal lattice 277, 627–630, 634–637, 806–807
- REDOR *see* rotational echo double resonance
- reflectance 452–454

- reflection / reflection condition 200–203, 273–288, 391–392, 447–451, 807, 812
- reflection factor, waveguide spectroscopy 200–203
- refractive index 659–660, 692, 697, 719, 798, 802
- relaxation
 - mismatch generated relaxation 213–216
 - spin relaxation, 91, 93, 169, 173, 698, 779, 784, 788
 - vibrational relaxation 666, 669–677, 713–714
- REMPI *see* resonance enhanced multiphoton ionization
- resonance enhanced multiphoton ionization (REMPI) 32–38, 56–58
- resonance frequency 89, 94, 170, 187, 424, 578–581, 595–599, 740, 743, 751
- resonance raman scattering (RRS) 438
- retarding field energy analyzer (RFA) 632, 633
- Rietveld structure refinement 285–292
- Rowland circle 507
- rotational echo double resonance (REDOR) 109, 116–119, 126–130, 150–152
- rotor-encoding 118, 119
- Rutherford back-scattering (RBS) 548, 549
- Rutherford formula 396, 808–809
- Rydberg states 32, 34, 35, 40, 41, 52, 55–56

s

- SAED *see* selected area electron diffraction
- sample preparation
 - ion milling 803–805
 - ion sputtering 485
 - magnetron sputtering 484, 490, 498, 503
 - XPS 483–487
- SANS *see* small-angle neutron scattering
- SAS *see* small-angle scattering
- Sauerbrey equation 575, 579, 584
- SAXS *see* small-angle X-ray scattering
- scanning electron microscopy (SEM) 517, 541, 566, 588, 739, 752, 797
- scanning force microscopy (SFM) 738, 745–746
- scanning near-field optical microscopy (SNOM) 713, 757
- scanning photoelectron microscopy (SPEM) 522–523
- scanning probe microscopy (SPM) 737–761
 - biosensors (nose) 752–754
 - calorimetry 744–745
 - force spectroscopy 741–743, 746–749
 - gravimetry 743, 750–752

- scanning probe microscopy (SPM) (*contd.*)
 - imaging in solution 745–746
 - micromechanical cantilever 738–745
 - resonance frequency 740, 743, 751
 - scanning force microscopy (SFM) 738, 745–746
 - surface stress 743–744
 - thermochemistry 754–756
 - (un)binding forces and off-rates 741–743, 746–749
 - working principle 739–740
- scanning tunneling microscope (STM) 603–624
 - adsorption 607–608
 - electrode potential 609
 - electron / ion transfer 607
 - electric double layer 607–608
 - electron tunneling 622–623
 - experimental methods 609–610
 - instrumentation 606
 - history 621–622
 - principles 605–606
 - ordered adlayers 613–614
 - reconstruction of surfaces 611–613
 - surface nanostructuring 618–620
 - underpotential deposition 615
- scattering
 - coherent anti-stokes raman scattering (CARS) 653–657
 - electron 625, 631, 637, 799, 820
 - impulsive stimulated raman scattering (ISRS) 657–662
 - multiple, EXAFS 243–244
 - neutron 291, 293, 309–314
 - nuclear, MBS 352, 387
 - phonon and plasmon scattering 394
 - resonant 291, 438
 - Raman 423, 715
 - Rayleigh-wing scattering 658
 - Rutherford back-scattering (RBS) 548, 549
 - X-ray 273–275
- scattering coefficient / module 449–453
- scattering length 274–275, 301–311, 319, 320, 323
- scattering form factor 274–275, 302–305, 320–321, 396
- scattering vector 279, 291, 299–305, 316, 396–397, 636, 809–810
- Scherzer defocus value 818–819
- Schottky barrier 498, 502
- secondary electron yield 523, 525, 536
- secondary ion intensity 552–555
- secondary ion mass spectrometry (SIMS)
 - capabilities 550–551
 - diffusion studies 556–565
 - depth profile analysis 558–560, 563–568
 - elemental distribution 568
 - instrumentation 554–556
 - ion sputtering 550–551
 - mathematics of diffusion 571–573
 - nuclear reaction analysis 549
 - principles 548–553
 - proton induced gamma-ray emission 549
 - Rutherford back-scattering 548–549
 - secondary ion mass spectrum 552, 557, 563
 - time-of-flight (TOF) mass spectrometer 570–571
 - vacuum conditions 569–570
- selected area electron diffraction (SAED) 801, 806–808, 813–814
- selection rules
 - magnetic dipole transitions 364
 - nuclear transitions 329, 332
 - optical transitions 33–36
 - parity allowed/forbidden transitions 245, 376
 - Raman scattering 426
 - spin transitions 165, 175, 185, 376
- self-assembled monolayers (SAMs) *see* substance and sample index
- semiconductors *see* substance and sample index
- SEM *see* scanning electron microscopy
- SERS *see* surface-enhanced Raman spectroscopy
- SFM *see* scanning force microscopy
- shear mode oscillator 578, 596, 597
- SIMS *see* secondary ion mass spectrometry
- single crystal analysis, diffraction 278–283, 806–808, 814, 818
- single crystals *see* substance and sample index
- single-molecule detection (SMD) 712, 713
- single-molecule fluorescence spectroscopy (SMFS) 711–735
 - background and noise 715–716
 - blinking 718
 - confocal microscopy 715–723
 - fluorescence lifetimes 720
 - fluorescence microscopy 713, 717–721
 - fluorophor and photophysical processes 713, 714
 - Fick's second law 729–730
 - Förster resonance energy transfer (FRET) 726–727
 - history 712–713
 - Jablonski diagram 713–715
 - instrumentation 716–721

- non-classical light 723–725
- photoelectron transfer (PET) 721, 727–728
- photophysics 725–729
- random walk, single molecules 731
- single-molecule tracking 729–732
- single quantum systems 721–723
- time-correlated single-photon counting (TCSPC) 720–721, 724
- single-molecule magnets *see* substance and sample index
- single-molecule microscopy 711
- single-molecule tracking, SMFS 729–732
- single quantum systems, SMFS 721–723
- site-directed spin-labeling (SDSL) 180–181
- small-angle neutron scattering (SANS) 298–306, 318–322
- small-angle scattering (SAS) 297–324
 - basic assumptions 300
 - contrast variation, SAXS and SANS 311–312, 321, 323
 - Guinier approximation 304–305, 323
 - interference pattern calculation 301–306
 - length scales, SANS and SAXS 298–299
 - microemulsions 317–322
 - nanopores 314–317
 - Porod's law 306
 - SAXS instrumentation 306–309
 - SANS instrumentation 309–314
 - scattering geometry 300
 - scattering length 306–307, 310–311
 - scattering vector 300–301
 - small-angle neutron scattering (SANS) 298–306, 318–322
 - small-angle X-ray scattering (SAXS) 298–306, 315–317
 - theory of small-angle scattering 300–306
 - Zimm approximation 305–306
- small-angle X-ray scattering (SAXS) 298–306, 315–317
- SMFS *see* single-molecule fluorescence spectroscopy
- Snell's law 719
- soft ferromagnetic material 774
- soft ionization methods 67
- solar cells 169, 478, 491, 492, 501, 805
- solid state chemistry 393–394
- solid state nuclear magnetic resonance (NMR) spectroscopy 87–158
 - chemical shift 90
 - coherence transfer techniques 109–110
 - cross-polarization 109
 - double-quantum coherences (DQC) 110–118
 - free induction decay 90–92
 - glasses 120–131
 - heteronuclear correlation (HETCOR) spectra 110
 - hetero- and homonuclear decoupling 104–105
 - internal interactions 94–99
 - Larmor frequency 89
 - Lee–Goldburg sequence 105–106
 - magic-angle spinning (MAS) 100–101
 - multi-dimensional NMR 105–99
 - multiple-quantum correlation (HMQC) 119–120
 - radio frequency driven recoupling (RFDR) sequence 112
 - reconversion rotor encoding (RRE) 115, 117
 - recoupled polarization transfer (REPT) 119–120
 - recoupling of magnetic dipole–dipole interactions 110–120
 - relaxation phenomena 92–94
 - rotational echo double resonance (REDOR) 116–119
 - sample spinning techniques 100–103
 - signal excitation and detection 90–92
 - spin echo decay methods 103–104
 - supramolecular systems 131–144
 - surfaces 142–144
 - two-dimensional exchange spectroscopy (EXSY) 105–106
 - Zeeman interaction 89
 - zero-quantum (ZQ) coherences 110
- solvation dynamics 702–706
- space focussing condition 59–60
- spallation sources 313–314
- specific anion adsorption 604
- spectromicroscopy, PEM 516, 517
- specular reflection, DRIFTS 448, 449
- SPEM *see* scanning photoelectron microscopy
- spin and charge recombination 169
- spin crossover, MBS 370–376
- spin echo 93, 99–107, 123–125, 145–148, 162, 172, 185–186
- spin echo double resonance (SEDOR) 124–126, 147, 148
- spin echo decay 103–104
- spin echo formation 93, 99
- spin Hamiltonian 94–100, 104, 117, 145–150, 163–167, 175–177, 182–184
- spin–orbit coupling 161–163, 376, 481–482, 766, 768

- spin transition 162, 170, 185, 338–340, 371–379
- SPM *see* scanning probe microscopy
- spot profile 631–632, 636–637
- spring constant 740, 747–748
- SQUID *see* superconducting quantum interference device
- Stark decelerator 11
- Stark effect 9–10
- electromagnetic high-frequency AC fields 12–13
 - electrostatic deflector 20, 21
 - high-field-seeking quantum states 11–12
 - low-field-seeking quantum states 11
- static SIMS 555–557
- sticking coefficient 483, 570
- stimulated emission 429, 649, 650, 680, 681, 689
- STM *see* scanning tunneling microscope
- Stoney's formula 744
- stroboscopic detection 647
- strong-field ionization 41–45
- structural disorder 192, 213
- structure factor 274–275, 280–281, 287–291, 303, 320, 809–810
- structure refinement residuals 280–281
- sublattice 174, 274, 347, 774–777
- Summerfield scaling 207, 211, 218
- superconducting quantum interference device (SQUID) 763
- superconducting quantum interference device (SQUID) magnetometers 763–795
- alternating current (AC) method 778–780
 - Brillouin function 767
 - Curie's law 768
 - description 763–764, 777
 - direct current (DC) method 777–778
 - magnetometry at high fields 780–781
 - magnetic materials 773–776
 - magnetic quantities and units 701–768
 - magnetic dipole moment 764–766
 - metamagnetic materials 780–783
 - single-molecule magnets 787–790
 - spin glasses 785–787
 - superparamagnets 783–785
- superconductivity 247–249, 293, 412, 764, 781
- superconductors *see* substance and sample index
- superparamagnets 783–785
- supersonic expansion *see* molecular beam
- superstructure matrix 630
- superstructures (commensurate or incommensurate) 630
- supramolecular organization 137, 139
- supramolecular systems *see* substrate and sample index
- surface analysis 341, 484, 515–516, 556, 626
- surface core level binding energy shifts 493
- surface crystallography 627, 640
- surface-enhanced Raman spectroscopy (SERS) 438–440
- surfaces and thin films *see* substance and sample index
- surface lattice 627, 630
- surface nanostructuring, STM 618–620
- surface periodicity and reciprocal lattice 627–629
- surface potential 495–503, 505, 543
- surface potential, XPS 495–503, 543
- surface reaction 462, 513–544
- surface reconstruction 493, 611–612
- surface roughness 316, 582, 585–586
- surface sensitivity 325, 478–481, 486, 490, 519, 547, 711
- surface stress 743–744, 752–753
- surface structure determination 638, 641
- surface topography contrast, UV-PEEM 525
- synchrotron induced X-ray photoelectron spectroscopy (SXPS) 487
- synchrotron radiation 29, 74–75, 236, 256, 261–283, 291, 307–309, 323, 354, 387, 407, 413, 480–492, 500, 508, 522, 537–542
- t**
- TCSPC *see* time-correlated single photon counting
- TEM *see* transmission electron microscopy
- temperature independent paramagnetism (TIP) 767
- temperature programmed desorption (TPD) 471
- terahertz radiation 169
- thermochemistry
- ion energetics, mass spectrometry 72–77
 - formation energies 754–755
 - solid–solid phase transitions 756
 - state selected ions 53
- three phase boundary 535–537
- THz-pump–THz-probe spectroscopy 658
- THz spectroscopy 687–710
- absorption coefficient 696–697, 702–705
 - applications 708–709
 - Beer's law 693, 695
 - biomolecule solvation 699–702
 - dipole moment autocorrelation function 696–697
 - dynamical reorientation 699–702

- hydration shell 701, 705, 706
 - kinetic THz absorption spectroscopy (KITA) 706–708
 - instrumentation and technology 687–691, 702
 - solvated proteins 705–706
 - THz gap 688
 - THz time domain spectroscopy 669, 691–694
 - vibrational density of states 697–699
 - time-correlated single photon counting (TCSPC) 720–721, 724
 - time differential perturbed angular correlation (TDPAC) 331
 - time-of-flight mass spectrometry (TOF-MS) 16–17, 45, 58–59, 68, 75, 552, 555, 570–571
 - time-of-flight photoelectron emission microscopy (TOF-PEEM) 538–539
 - time-ordered diagram 647, 653, 659
 - time correlation functions 192, 213
 - time-resolved ion dynamics 192
 - TIP *see* temperature independent paramagnetism
 - TOF-MS *see* time-of-flight mass spectrometry
 - TOF-PEEM *see* time-of-flight photoelectron emission microscopy
 - trace analysis 30, 46, 50–51
 - tracer diffusion 556–559, 562–564, 571–572
 - transient absorption 648–650
 - transient spectrum 680 *see also* pump-induced (femtosecond) infrared spectra
 - transition state *see* potential energy surface
 - transmission electron microscopy (TEM) 797–821
 - Abbe resolution limit 798–799
 - atomic scattering factor 808–809
 - Bragg’s law 810
 - bright field (BF)/dark field (DF) imaging 814–815
 - components 799–802
 - convergent beam electron diffraction (CBED) 807–808
 - dynamical theory 812
 - electron diffraction 806–813
 - high resolution transmission electron microscopy (HRTEM) 816–820
 - history 798
 - Howie Whelan equations 815, 816
 - Laue criterion 810
 - lens aberrations 802–803
 - intensity distribution 811–812
 - image contrast 813–816
 - numerical aperture (NA) 798
 - Scherzer defocus value 818–819
 - selected area electron diffraction (SAED) 801, 806–808, 813–814
 - specimen Preparation 803–806
 - scanning electron microscopy (SEM) 797–798
 - structure factor 809–810
 - transmission spectra
 - DRIFTS 447–451
 - EMR 175–176
 - MBS 358, 368, 367, 373–381
 - THz 695
 - tunnel current 605–606, 610, 623
 - tunneling 43, 174–175, 606–612, 622–623, 788–790
 - turnover number (TON) 80
- u**
- ultra-high vacuum (UHV) conditions 483, 569–570
 - ultraviolet photoelectron spectroscopy (UPS) 479, 504–505, 518–520
 - ultraviolet-visible (UV-VIS) spectroscopy 261–263, 374–375
 - unbinding force 741–743, 746–749
 - underpotential deposition 615–616, 621
 - undulator 307, 522, 542
 - unimolecular dissociation reaction 75, 78–79, 746–747
 - unit cell 178, 274–279, 289, 415, 529, 532, 576, 611, 627–641, 774, 798, 809–811
 - universalities in diffusion
 - first 209–210, 212–220
 - second 210–212, 220–227
 - UPS *see* Ultraviolet photoelectron spectroscopy
 - UV-VIS *see* ultraviolet-visible
- v**
- vacuum level 497, 502, 518, 543
 - valence electron energy loss spectroscopy (VEELS) 398, 409
 - van Hove singularity 167, 177
 - van Vleck equation (NMR) 147–148
 - valence electron energy loss spectroscopy (VEELS) 398
 - van’t Hoff isotherm 744
 - van Vleck paramagnetism 767
 - van Vleck formula 104, 147, 151–152
 - VEELS *see* valence electron energy loss spectroscopy
 - velocity correlation function 193, 207, 213–214
 - vibrational density of states 697–699
 - vibrational dynamics 678–682

- vibrational energy relaxation (VER) 666, 669–677, 713–714
- vibrational pump–probe spectroscopy
 - coherence 647–649, 653–654, 656–657, 661
 - coherent anti-stokes raman scattering (CARS) 653–657
 - degenerate four-wave mixing 654, 658, 659
 - diffusive motion 651
 - homodyne detection 654–655, 657, 659
 - hydrogen bonding 663–667
 - impulsive stimulated raman scattering (ISRS) 657–662
 - infrared (IR) pump–probe spectroscopy 648–653
 - phase matching 654, 655
 - optical Kerr effect (OKE) 667–669
 - optically heterodyne detected Kerr effect (OHD-OKE) 660–662
 - Raman-induced optical Kerr effect (OKE) 657–662
 - Rayleigh-wing scattering 658
 - time-ordered diagrams 647, 653–654, 659
 - vibrational dynamics 678–682
 - vibrational energy relaxation (VER) 666, 669–677
- voltammogram 591–592
- volta potential 543

- w**
- water *see* substance and sample index
- waveguide spectroscopy 199–202
- weak phase object approximation (WPOA) 817
- Weiss constant 772
- Wood notation 634
- work function 31, 481, 487, 497, 502–506, 517–518, 525–527, 543–544, 609, 622
- work function contrast, PEEM 525, 544
- Wyckoff symbol 277

- x**
- XANES *see* X-ray absorption near edge structure
- X-ray absorption near edge structure (XANES) 238, 244–246, 253–254, 258–259, 526
- XAS *see* X-ray absorption spectroscopy
- XPS *see* X-ray photoelectron spectroscopy
- X-Ray absorption spectroscopy (XAS) 231–269
 - extended X-ray absorption fine structure (EXAFS) 232–246
 - absorption edge 232
 - absorption coefficient 233
 - X-ray absorption fine structure (XAFS) 231
 - catalysis 253–262
 - energy level diagrams 236
 - experimental design 236–237
 - Fourier transformation 239–241
 - initial and final state 234
 - multiple scattering 243–244
 - oxidation state 244–246, 264–265
 - radial distribution function (RDF) 239
 - schematic representation 232, 234
 - structural parameters 235
 - X-ray absorption near edge structure (XANES) 238, 244–246, 253–254, 258–259
- X-ray diffraction (XRD) 271–295
- X-ray magnetic circular dichroism (XMCD) 526
- X-ray photoelectron spectroscopy (XPS) 22–23, 483–486, 492–501, 518, 521
- X-ray scattering 137, 247, 274, 298–306, 315–317, 707
- X-ray fluorescence (XRF) 236–237, 382
- X-ray sources 277–278, 308, 479, 506–507
- XRD *see* X-ray diffraction
- XRF *see* X-ray fluorescence

- z**
- Zeeman effect 182–183, 769
 - electronic 163–165, 175, 178, 182–183, 769, 791
 - nuclear 90, 94, 99, 148–149, 170, 185, 186, 363–365
- ZEKE *see* zero electron kinetic energy
- zero electron kinetic energy (ZEKE) spectroscopy 41–42
- zero-field-splitting (ZFS) 162, 167–168, 174–179
- zero order Laue zone 807
- Zimm approximation 305–306