

Index

a

- A tensor 16
- aberration 448
- absorbance 98 ff, 186
- absorption 51, 107
 - AEO 82
 - anhydrous oxides 111
 - EPR 19
 - TEM 453
 - UV-Vis-NIR 59 f
- absorption coefficient
 - EXAFS 304
 - IR spectroscopy 57, 67, 99
 - XAS 301
- acceptors 55
- accuracy 309, 454
- acetaldehyde production 548, 554
- acetone 600, 624, 828
- acetonitrile 155
 - base catalysis 834
 - surface basicity 166
 - titanium silicalite-1 742
 - vanadium phosphate catalysts 507
- acid–base properties
 - CuMgAl 321
 - IR spectra 167
 - metal oxides 617
 - mixed metal oxides 415 f
 - NMR 195
 - POMs 567, 578
 - surface 227
 - thermal analysis 392
 - vanadium pentoxides 431
 - vanadium phosphates 507
 - zeolites 311
- acid-catalyzed reactions 677
- acid probes 586
- acid sites
 - IR spectra 139, 156
 - superacidic metal oxides 675, 682
 - thermal analysis 404
- acid zeolites 310 ff
- acidic oxides 406
- acidic systems 496
- acidity
 - IR spectra 147
 - POMs 572
 - surface properties 227
 - thermal analysis 402 f
- acoustic modes 124
- acrylic acid oxidation 281 f
- acrylic fibre ammoxidation 771
- acrylonitrile–butadiene–styrene (ABS) 771
- acrylonitrile synthesis 771–818
- actinide elements 540
- activation
 - base catalysis 829
 - IR spectra 134, 156
 - thermal analysis 399, 405
 - vanadium phosphate catalysts 500
- active centers 69
- active sites
 - ammoxidation 776
 - EXAFS 314
 - thermal analysis 392
 - titanium silicalite-1 720, 740 f
 - uranium oxides 551
 - vanadium phosphate catalysts 529
- activity
 - base catalysis 820
 - chromium oxides 597
 - IR spectroscopy 107
 - photocatalytic 762
 - POMs 564
 - superacidic metal oxides 673
 - uranium oxides 545
 - vanadia catalysts 605

- vanadium oxides 210
- vanadium phosphate catalysts 504
- addenda atoms 561, 569, 581
- adiponitrile (ADN) 803
- adsorbate–adsorbate interactions 398
- adsorbed probe molecules 133 f
- adsorption 394
 - base catalysis 823
 - Lewis/Brønsted sites 146
 - metal oxide catalysts 645
 - microcalorimetry 393
 - photocatalysis 760
 - superacidic metal oxides 681
 - titanium silicalite-1 705, 740 f
- adsorption–desorption heats 401 f
- aerobic partial oxidation 642
- aggregation 477
- alcohols
 - dehydration 618
 - methoxide solutions 623
 - oxidation 570, 727
 - surface basicity 166
 - titanium silicalite-1 708
 - TS-1 catalyzed 316, 724
 - vanadium phosphate catalysts 510
- aldehydes 316, 724
- aldol condensation 554, 830
- aliphatic nitriles 154
- aliphatic oximes 733
- alkali-exchanged zeolites 428
- alkali halides 101
- alkaline earth oxides (AEO)
 - base catalysis 826 f, 830
 - IR spectra 61, 153
 - PL spectra 81 f
 - powder EPR 33
 - promoted vanadium phosphates 523
- alkaline earth salts 423
 - destruction 547
 - hydroxylation 707 ff
 - NMR 195
 - oxidation 499
 - oxygenation 641
- alkane–alkene conversion 605
- alkanes
 - olefins 178
 - oxidative 416
 - vanadium oxides 210
 - vanadium/chromium oxides 595–612
- alkenes
 - epoxidation 570, 576
 - metathesis 650
 - TS-1 catalyzed 316
- alkenyl mechanism 524
- alkoxide mechanism 527
- alkyl acid anhydride 693
- alkyl amines 147
- alkyl chains 480
- alkyl radicals 47
- alkylaromatic ammoxidation 791
- alkylaromatic side-chain alkylation 819
- alkylation 618
- alkylbenzene ammoxidation 791
- allyl alcohol oxidation 725
- allyl chloride epoxidation 726
- alumina supports
 - surface structure 228, 231
- vanadium catalysts 214, 177–196
- vanadium oxide 211, 433, 602
- aluminas 121
 - bulk structure 347 f
 - CP-MAS NMR 230
 - differential heats 406
 - electronic structures 347, 351
 - hydroxyl groups 141
 - IR spectroscopy 115, 159, 311
 - Lewis acid sites 159 f
 - metal oxide catalysts 614
 - MQMAS 202
 - NMR 195
 - SATRAS 203
 - surface oxo-anions 136
 - surfaces 356, 359 f
 - thermal analysis 408
 - XPS 260
- aluminosilicates 425
- aluminum containing systems 204, 208 f, 780
- aluminum hydroxides 209, 341 f, 347
- aluminum layers 355
- aluminum oxides 221 f, 348
- aluminum supports 177–196, 221 f
- aluminum zeolites 124, 300
- amide ammoxidation 793
- amines 316, 733, 793
- ammonia
 - adsorption 408, 418 f
 - POMs 567, 586
 - surface basicity 166, 402
- ammonium salts 565
- ammoxidation
 - hydrocarbons/mixed oxides 771–818
 - propane 281
 - titanium silicalite-1 730 f
- amorphous material 110 f, 129 f, 505
- amorphous silica/aluminas 228, 425
- amorphous structures 200
- amphoteric oxides 406

amplitude reduction factor (AFAC) 302
 amplitudes 446
 analcime 478
 anatase 118
 Anderson structures 562
 angular momentum 2, 7, 53, 197
 anharmonic oscillator 77
 anhydrides 693
 anhydrous oxides 111 f
 aniline oxidation 733
 anion–cation distance 65
 anion doping 760
 anisotropic fine term 14
 anthracene 13
 anthrahydroquinone autoxidation (AO) 736
 antiferromagnetic AF₂ state 372
 antimonate catalysts 786
 antimony 549
 antiphases 446 f
 antisymmetrized wavefunctions 326
 aperture 446
 applications
 – base catalysis 840
 – EXAFS 309 f
 – IR spectroscopy 96 f
 – metal oxide catalysts 641
 – oxide systems 32 f
 – partial oxidation reactions 568
 – POMs 566 ff
 – superacidic metal oxides 698
 – surface chemistry 96 f
 – UV-Vis-NIR spectroscopy 51–94
 – vanadium oxide 256 f
 aqueous routes 509
 aqueous solutions 628
 aquocomplexes 132
 aragonite 123
 argon probe molecule 147, 678 ff
 aromatic acids ammoxidation 793
 aromatic compounds hydroxylation 712
 aromatic nitriles synthesis 792
 aromatic oximes 733
 aromatics Friedel–Crafts acylation 692 f
 atomic displacements 99
 atomic layer deposition (ALD) 409, 431
 atomic layers 455
 atomic number effect 453
 atomistic models 34
 attenuated multiple total internal reflection
 technique (ATR) 103
 Auger electron process 249, 265, 305
 augmented-wave pseudopotentials 341
 Aurivillius phases 456
 aziridine synthesis 827

b
 background function 306
 backscattering 301
 Baeyer–Villiger oxidation 570
 band gaps 68, 756
 band structures 51 f, 344, 377, 762
 band theory 332 f, 613
 base-catalyzed Claisen–Schmidt
 condensation 652
 base indicators 666
 base metal oxide catalysis 819–844
 base properties 617, 822
 baseline correction 307
 basic oxide crystal structures 454 f
 basic oxides 406
 basic principles
 – electronic structure methods 336 f
 – EPR 2 f
 – EXAFS 299 f
 – heterogeneous photocatalysis 756 f
 – XAS 300 f
 – XPS 244 f
 basic probe molecules 160, 586
 basic strength method 152
 basic zeolites 837
 basicity 402 f
 bayerite 116, 341, 348
 beam damage 256
 Becke–Lee–Yang–Parr (BLYP) approach
 331, 346
 Beer–Lambert law 99
 Bellamy–Hallam–Williams relation 150
 bending magnets 304
 bending mode 120
 benzaldehyde production 544, 552
 benzene
 – ammoxidation 805
 – hydroxylation 716
 – oxidation 544 ff, 570
 – XPS 263
 benzoate-like intermediates 551
 benzoic anhydride 694
 benzylation 692
 benzylic derivative oxidation 571
 Bi–Mo mixtures 553
 bifunctional catalysis 567
 bimolecular intermediates 682
 binary mixed metal oxides 415 f
 binary oxides 135 f
 binary systems 418
 binary vanadium oxides 269
 binding energy 59
 – alumina 336
 – base catalysis 824 f

- vanadium oxides 257
 - VPO XPS 270
 - XAS 300
 - XPS 244, 248 ff, 285
 - binominal expansion 12
 - biodiesel production 643
 - bismuth molybdate 417, 775
 - bismuth oxide-based solid solutions 455, 460 f
 - bismuth promoted vanadium phosphate catalysts 523
 - bismuth uranates 551
 - Bloch function 336
 - boehmite, Al-NMR 222, 229, 347 ff
 - Bohr frequency condition 4
 - Boltzmann factor 234
 - Boltzmann law 98
 - Boltzmann–Maxwell law 5
 - bond lengths/angles 97
 - bonding 340
 - metal oxide catalysts 614, 631
 - oxidation reactions 487 ff
 - borated superacidic metal oxides 674
 - borated surface oxo-anions 136
 - boria 409, 420
 - boron trifluoride 166
 - bottom-up preparation 619
 - boundary conditions 354, 616
 - Bragg angles 305
 - Bragg reflections 446, 450
 - branched alkane hydroxylation 709
 - Bravais cell 108, 112, 122
 - bridging 139
 - bright-field image 511
 - broadening 262
 - bromothymol blue 821
 - Brønsted acid sites
 - IR spectra 139 f
 - oxidation reactions 495
 - silica-aluminas 145
 - solid-state NMR 229 f
 - superacidic metal oxides 666, 683, 689
 - thermal analysis 392, 398, 404
 - vanadium phosphate catalysts 507
 - zeolites 427
 - Brønsted acidity
 - metal oxides 146 f, 153 f
 - POMs 567, 578
 - protonic zeolites 153 f
 - Brønsted basic–OH surface groups 652
 - brucite-type layers 130, 133
 - buckling 372
 - building blocks 57, 619
 - bulk catalyst structure 229
 - bulk energy 335
 - bulk excitons 82
 - bulk heteropolyacids 422 f
 - bulk oxide catalysts 404 f
 - bulk phases 519
 - bulk properties 196, 614
 - bulk structures 200, 323, 347 f
 - bulk termination 357
 - bulk-type catalysis 564
 - bulk V–P–O ammoxidation 791
 - Burstein–Moss effect 69
 - butadiene ammoxidation 798
 - butane–butene fractions 568
 - butane conversion 643, 690
 - butane dehydrogenation 210, 260 f, 266 f, 598
 - butane desorption 609
 - butane isomerization 682, 685 f
 - butane oxidation 269 f, 499, 507, 511, 524
 - butane reaction profile 690
 - butanol oxidation 729, 742
 - butanone 42
 - butene 263
 - butylamine 233
- C**
- C₂ hydrocarbons ammoxidation 807
 - C₄/C₅ olefins epoxidation 719
 - C₄ hydrocarbons ammoxidation 797
 - C–H bond
 - activation 221
 - breaking 492
 - hydroxylation 708 ff
 - POMs 575
 - vanadium phosphate catalysts 499, 507
 - XPS 255
 - calcination
 - aluminas 115
 - base catalysis 834
 - ceramic acids 695
 - metal oxide catalysts 627, 638
 - spikelet echo spectra 219
 - superacidic metal oxides 668 ff
 - uranium oxides 556
 - vanadium phosphate catalysts 515
 - calcite 123
 - calibration
 - electronic structures 340
 - TEM 453
 - volumetric-calorimetric line 395
 - XPS 252, 256 f
 - calorimetric methods 391–442
 - capillary pressure 623
 - carbon–carbon bonds 265, 403

- carbon deposition 598
- carbon dioxide 166, 402, 624
- carbon disulfide 166
- carbon formation 264
- carbon monoxide
 - chemisorption 384
 - IR spectra 161 f
 - oxidation 547, 552
 - redox properties 403
 - surface acidity 147
 - surface basicity 166
- carbon monoxide adsorption 419
- carbon-supported heteropolyacid catalysts 423
- carbonates 133 ff, 629
- carbonyl compounds ammoximation 730
- carboxylic acids 511
- carcinogenic properties 649
- case studies
 - surface adsorbed NO₂ 30 f
 - vanadia catalysts 429 f
 - XPS 256 f
- catalyst precursors *see* precursors
- catalysts
 - anatase 121
 - base catalysis 825 f
 - IR spectra 52, 61, 132
 - metal oxide 613–664
 - NMR 195
 - oxidation reactions 487–498
 - partial oxidation 561–594
 - powder EPR 33
 - solid-state NMR 195–242
 - spin number 24
 - thermal behavior 393 f
 - uranium oxides 543
 - vanadium phosphate 499–538
 - XAS 299–322
- catalytic activity
 - MoO₃/ZrO₂ 695
 - superacidic metal oxides 665–704
 - vanadium oxides 210
 - WO₃/SnO₂/Al₂O₃ 696 f
- catalytic ammoxidation 771–818
- catalytic cracking 195
- catechol hydroxylation 734
- cation exchanged zeolites 165 f
- cation ordering 455 f
- cationic centers 161 f
- cationic radicals 759
- CATOFIN process 596
- cavities 24 ff, 158 ff
- CdSe/ZnS quantum dots 477
- ceramic acid 695
- ceria 384, 632 f
- ceria-based catalysts 420
- ceria–lanthana coprecipitated mixed oxides 415
- ceria–zirconia solid solutions 415
- cerium-promoted vanadium phosphate catalysts 519 ff
- character tables 107
- characterization *see* properties
- charge carrier lifetimes 761
- charge-coupled devices (CCD) 470
- charge density difference 373
- charge localization 378
- charge migration 756
- charge separation 458
- charge transfer transitions 54 f, 87, 573
- charge trapping 761
- charging contributions 252
- chemical feedstocks 260
- chemical properties
 - metal oxide catalysts 616, 620
 - POMs 566
 - UV-Vis-NIR spectroscopy 51
- chemical shift
 - CRAMPS 209
 - NMR 197, 203
 - vanadium oxides 212
 - XPS 250
- chemical vapor deposition (CVD) 409
- chemisorption 604
- chlorinated compound removal 755
- chloroaniline 821
- chlorocarbon adsorption 649
- chloroform 166
- chloro-substituted xylene 794
- chromia–alumina catalyst 596
- chromium oxides
 - alkane dehydrogenation 595–612
 - combustion methods 639
 - TEM 472
- chromium promoted vanadium phosphate catalysts 519, 523
- Claisen–Schmidt condensation 652
- clay catalysts 424 f
- cleaning method 256
- close-packed structures 465
- clusters
 - DFT calculations 34, 278
 - heteropolyoxometallate catalysts 561
 - photocatalysis 763
 - POMs 587
 - TEM 477
 - uranium oxides 542
 - vanadium phosphate catalysts 503

- coal conversion 546
 - coating 463
 - cobalt metal ions 413
 - cobalt promoted vanadium phosphate catalysts 519, 522
 - coherent electron waves 448
 - coke 265, 598–608
 - color centers 36
 - combination modes 99
 - combined rotation/multiple pulse spectroscopy (CRAMPS) 209 f
 - combustion methods 544, 638
 - complex interactions 165 f
 - complex precipitates 132
 - Compton scattering 306
 - concerted mechanism 529
 - condensation 128, 622 f
 - conduction band 344
 - heterogeneous photocatalysis 756
 - UV-Vis-NIR spectroscopy 57
 - XPS 255
 - confinement effects 153
 - conjugated polyenes 182
 - consecutive alkenyl/alkoxide mechanism 524 ff
 - contamination 247
 - continuous-flow microwave reactor 632
 - convergent beam electron diffraction (CBED) 452
 - conversion data 52, 552
 - coordinates 325
 - coordination number 70, 302
 - coordination sites 65, 820
 - copper addenda elements 572
 - copper-exchanged ETS-10 catalysts 428
 - copper metal ions 28, 413
 - copper oxides 74
 - coprecipitation 415, 627 ff
 - core levels
 - electronic structures 341
 - XAS 300
 - XPS 248, 259, 277
 - core polarization 245, 249
 - core-shell nanoparticles 637
 - core-shell quantum dots 464
 - core-shell structures 476
 - corners 562, 615
 - correlation methods 327 f
 - corundum sesquioxides 142
 - corundum structure 347
 - Coulomb interactions 244, 370, 480
 - Coulomb operator 324
 - counter-cations 422, 572
 - counter ions 561
 - covalent bonding 615
 - coverage profiles 396, 399
 - cracking 195, 435
 - critical points 624, 633
 - cross-polarization (CP) NMR 206
 - crotonaldehyde production 554
 - crystal defects *see* defects
 - crystal field 18, 53
 - crystal growth 475
 - crystal structures
 - aluminas 362
 - divalent elements 113
 - metal oxide catalysts 615
 - NMR 200
 - TEM 443
 - ternary oxides 123
 - uranium oxides 541
 - UV-Vis-NIR spectroscopy 62
 - vanadium oxides 211
 - XPS 249
 - crystalline aluminosilicates 310, 425
 - crystalline anhydrous oxides 111 f
 - crystalline complex 121 f
 - crystalline nanoparticles 488
 - crystalline phases 318
 - crystalline solids 108 f
 - crystallites 614
 - crystallization 511, 706
 - crystallographic cell vector 354
 - Cs-corrected HRTEM 449
 - Cs₂Cu_x reduction 572 f
 - Cu–Cu scattering 313
 - cubic close packing (ccp) structures 443
 - cubic fluorite structure 541
 - cubic phases 467
 - cubic unit cell 356
 - CuO (tenorite) 115
 - cyano-pyridine synthesis 795
 - cycle time 596
 - cyclic amines 147
 - cyclization 727
 - cycloalkane isomerization 686
 - cyclohexanol oxidation 729
 - cyclohexanol/hexane ammoxidation 800 ff
 - cyclohexanone ammoxidation 730 ff, 800
 - cyclohexene epoxidation 576
 - cylindrical internal reflection technique (CIR) 104
- d**
- d bands 53, 72 f, 370 f
 - D tensor 17
 - Dawson structure 561
 - dead time 453

- dealumination 425
 - Debye–Waller factor 302
 - decay curves 79
 - decomposition
 - base catalysis 824, 831
 - IR spectra 133
 - metal oxides 645
 - defects 598
 - metal oxide catalysts 614 ff
 - oxides 465 f
 - transition metal oxides 375 f
 - UV-Vis-NIR spectroscopy 51
 - defocus 448
 - deformation modes 151
 - degeneracy 8, 197
 - deglitching 307
 - dehydrated state 178 f
 - dehydration 578, 672
 - dehydrogenation
 - base catalysis 825 f
 - NMR 195, 209
 - vanadia catalysts 604
 - vanadium/chromium oxides 595–612
 - XPS 260 ff
 - delocalization 344, 584
 - density functional theory (DFT)
 - electronic structures 323, 328 f, 371
 - oxidation reactions 494
 - vanadia catalysts 180
 - XPS 255, 278
 - density of states (DOS)
 - aluminas 364
 - electronic structures 342 f
 - NiO 374
 - TiO₂ surface 378
 - vanadyl pyrophosphate 278
 - desorption 394
 - thermal analysis 393
 - uranium oxides 548
 - vanadium phosphate catalysts 526
 - destructive adsorption 649
 - deuteroxyls 169
 - diaspore structures 130
 - dielectric properties 25, 59, 102
 - difference electronic charge density map 381
 - differential charging 253
 - differential heats 394 ff, 406
 - differential pumping 246
 - differential scanning calorimetry (DSC) 392
 - differential thermal analysis (DTA) 392, 586
 - differential thermogravimetry (DTG) 392, 586
 - diffraction techniques 443–486
 - diffuse reflectance Fourier transform (DRIFT) 105, 133, 647
 - diffuse reflectance spectroscopy (DRS) 59 f, 104 f, 134
 - oxidation reactions 490
 - polycrystalline AEO 63
 - diffusivity 156 f
 - dihydrofuran 526
 - diluted self-supporting disks 101
 - dimeric compounds 262
 - dimeric condensed tetrahedral anions 127
 - dimethyl amine probe molecules 155
 - dimethylcyclopentane hydroxylation 710
 - dinitrosyl species 46
 - diphenols 316
 - diphenylpropionitrile 155
 - dipolar coupling 197, 206
 - dipole interaction 32, 209
 - dipole operators 16
 - direct dehydrogenation 260 f
 - direct hydrogen peroxide synthesis 737
 - direct methanol fuel cell (DMFC) 646
 - direct propane oxidation 281 f
 - dislocations 617
 - disordered planes 507
 - dispersed metal oxide catalysts 487, 613–664
 - dispersion 69, 334
 - displacement 367
 - disproportionation 682
 - distortions 25, 462
 - divalent element oxides 112 f
 - domains 466
 - donors 55
 - doping 408 f, 525, 760
 - double bonds 135 f, 195
 - double resonance (DR) NMR 206 f
 - double rotation (DOR) 202
 - doublets 12
 - drying 620, 623, 673
 - dyes adsorption 760
 - dynamic angle spinning (DAS) 202
- e**
- edge X-ray absorption fine structure (EXAFS) 299 f
 - edges 562, 615
 - effective potentials 329
 - Eigen functions 8, 308
 - elastic scattering 306
 - elastic strain 479
 - electrochemistry 585
 - electron backdonation 162
 - electron delocalization 584

- electron diffraction 450 f
 - electron–electron interactions 18, 78, 323, 370
 - electron energy loss spectra (EELS) 371
 - electron–hole pairs 82, 756, 761
 - electron paramagnetic resonance (EPR) 1–50, 596
 - electron populations 370
 - electron–proton interactions 34
 - electron radiation 446
 - electron–solid interactions 445 f
 - electron spectroscopy–chemical analysis (ESCA) 249
 - electron spin resonance (ESR) 584
 - electron trapping 35
 - electron wavelength 445 f
 - electron Zeeman interaction 2 f
 - electronegativity
 - metal oxide catalysts 616
 - oxidation reactions 487
 - promoted vanadium phosphate catalysts 521
 - UV-Vis-NIR spectroscopy 56
 - electronic perturbation 157
 - electronic structures 324 f
 - heterogeneous photocatalysis 756
 - oxidation reactions 490
 - electronic transitions 52 f
 - electrostatic stability 355 f
 - emission IR spectroscopy (IRES) 105
 - emission technique 51, 82, 87, 105 f
 - emittance 105
 - energy dispersive X-ray spectroscopy (EDX) 445, 452 f
 - energy gap 56
 - energy levels 4, 197
 - energy state transitions 51
 - enthalpy diagram 398
 - environmental influences 367 f
 - epoxidation
 - olefins 717
 - POMs 576
 - titanium silicalite-1 316, 705
 - equilibrium constants 400, 665
 - Erythrosin B 760
 - escape depth 253
 - esterification 618
 - ethanol
 - critical point parameters 624
 - dimerization 839
 - oxidation 546, 549, 729
 - ethene oxidation 413
 - ethers 147
 - ethylbenzene dehydrogenation 555
 - ethylcyclopropane hydroxylation 711
 - ethylene polymerization 488
 - Ewald sphere 450
 - excess energy 306
 - exchange–correlation potential 329
 - exchange energy 324 f
 - exchange splitting 373
 - excitation
 - AEO 82
 - IR spectroscopy 51, 98
 - photocatalysis 760
 - PL spectroscopy 80
 - XPS 249, 274
 - excitonic surface states 59 ff
 - exfoliation 480, 511
 - exhaust gas removal 548
 - exothermic phenomenon 393
 - experimental techniques
 - EPR powder spectra 24 f
 - EXAFS 303 f
 - IR methods 97 f
 - thermal analysis 393 f
 - extended X-ray absorption fine structure (EXAFS) 490
 - external cationic sites 165 f
 - extra-framework aluminum (EFAL) 425
- f**
- F centers 615
 - factor group analysis 125
 - FAU 158, 307
 - faujasite (USY) 310, 425
 - FDU-12 470
 - feed composition, ammoxidation 777
 - feedstocks 260, 502–514
 - FER 154, 158
 - Fermi contact term 31, 40
 - Fermi energy 345
 - Fermi level 252, 290
 - Fermi–Dirac statistics 344
 - ferric oxides *see* iron oxides
 - field gradients 199
 - flame processes 638
 - flow adsorption microcalorimetry 399, 426
 - fluid catalytic cracking (FCC) 310
 - fluid solutions 10 ff
 - fluidized-bed reactor 774 ff
 - fluorescence
 - EXAFS 306
 - PL spectroscopy 77
 - TEM 453
 - UV-Vis-NIR spectroscopy 60
 - vanadia catalysts 179, 601
 - fluorite structure 461, 540, 554

Fock operator 324
 formaldehyde oxidation 553
 Fourier filtering 307
 Fourier transform 208, 337
 framework silicates 128
 Franck–Condon principle 76 f
 free energies 350
 free fatty acids (FFA) 643
 freedom degrees 107, 327
 Freon 116 624
 frequencies 4, 27, 100
 Friedel–Crafts acylation 692 f
 F-test values 308
 FTIR spectra *see* IR spectra
 fuel oil oxidation, uranium oxides 543
 full width at half maximum (FWHM) 248, 256 f, 273
 fumaric acids 499
 functionality 554, 776
 functionalization agents 566
 fundamental transitions 99
 furan production 266 f, 526, 555

g

g factor 3
 g tensor 14
 gallium-containing catalysts 220
 gallium oxides
 – electronic structures 351
 – IR spectra 118, 135, 157 ff
 – NMR 225
 – polymorphs 142
 – TEM 635
 – thermal analysis 407 ff
 gaps 354
 gas flow thermal analysis 399 f
 gas-phase synthesis 513
 gas–solid interfaces 45
 gas–solid transformations 619
 gas/vapor manipulation 134
 Gaussian image plane 448
 Gaussian lineshape 24
 Gaussian smearing 381
 Gaussian target function 337
 gels 671
 geminal silanols 142
 generalized gradient approximation (GGA) 330, 341, 359
 germania 160
 gibbsite structures 222, 341, 347
 see also aluminas
 goethite structures 130
 gold-based catalysts 554
 gradient-corrected DFT technique 335

grain boundaries 446, 616
 graphitic paracrystals 599
 green catalytic processes 588
 group approximation 110
 group II oxides 33
 gyromagnetic ratio 197

h

H-FER zeolite 156
 H-method calculations 681
 Hamiltonians 1 ff, 197
 Hammett indicators 667–704, 820
 harmonic rejection 304
 harmonics 99
 Hartmann–Hahn condition 206
 Hartree–Fock (HF) approximation 323 ff
 heat diagram 398
 heat flow calorimetry 392 f
 heat treatment 620
 Heck reaction 840
 helium system 304
 hemihydrate precursors 508
 hemispherical analyzer (HSA) 245
 Henry constants 100, 714
 heterocyclic amines 147
 heterogeneous photocatalysis 42
 heterogroups, alkylaromatic 795
 heterolytic hydroxylation 715
 heteropolyacids (HPA) 422 f, 583, 791
 heteropolycompounds 416
 heteropolyoxometallate catalysts 561–594
 hexagonal close packing (hcp) 443
 hexagonal layered structure 541
 hexane ammoxidation 802
 Hf sulfated metal oxides 669
 hierarchical structures 562
 high T_c superconducting oxides 446, 463 ff
 high-order Laue zone (HOLZ) diffraction 450
 high-pressure setup 245 f
 high-resolution transmission electron microscopy (HRTEM) 443 f
 high-surface-area oxides 487
 highly dispersed metal oxide catalysts 613–664
 highly dispersed oxide materials 51
 highly dispersed supported oxo-species 69 f
 highly dispersed transition metal ions 85 f
 highly siliceous zeolites 128
 hindered basic probes 154
 hindered nitriles 165
 hindered rotations/translations 110
 Hohenberg–Kohn theorem 328
 hole trapping 43

- HOMO–LUMO structures 280
- homolytic hydroxylation 715
- host oxides 456
- hybrid functionals 376
- hybridization ratio 32
- hybridized orbitals 366
- hybrids 331
- hydrated compounds 132 f
- hydrazine 477
- hydrocarbons
 - catalytic ammoxidation 771–818
 - cracking 618
 - IR spectra 133
 - oxidative dehydrogenation 267 f
 - POMs 576
 - surface acidity 147
- hydrocarbon oxidation
 - EXAFS 315
 - selective 429
 - uranium oxides 544
 - vanadium phosphate catalysts 499
- hydrochloric acid 509
- hydrodesulfurization/denitrogenation 218
- hydrogen 82, 147
 - abstraction 526
 - bonding 147, 398, 405, 615
 - formation 260
 - reduction 182 f, 597
- hydrogen peroxide 569, 575 f, 588
 - hydroxylation 713
 - oxidation 575 ff
 - processing 705, 737
 - use problems 736
- hydrogen silicates 136
- hydrogenation 195, 829
- hydrolysis 620
- hydroquinone hydroxylation 734
- hydrotalcites 132, 420 f, 835
- hydrothermal processes 524, 633, 706
- hydroxide coprecipitation products 628
- hydroxides 132, 620 f
- hydroxy chloride paratacamite 130
- hydroxy silicoaluminum compounds 424
- hydroxyl coverage 406
- hydroxyl groups 61, 139 ff, 392, 377
- hydroxyl radicals 759
- hydroxylamines 316, 731
- hydroxylation 707 ff
- hyperfine parameters 7 f, 34, 39
- HYSCORE techniques 14
- i*
- ilmenites 122
- image contrast 445 f, 472
- image wave function 448
- imine ammoxidation 793
- impregnation 409, 826
- impurities 81, 133 f, 467
- incident electron wave 448
- incommensurate superstructures 460 f
- indicators 820
- indium oxide 411, 635
- indium promoted vanadium phosphate catalysts 523
- inelastic scattering 95, 579
- infrared reflection absorption spectroscopy (IRRAS) 103
- infrared spectroscopic methods 95–176
- inorganic dye adsorption 760
- inorganic radicals 38 f
- inorganic solids 107 f
- insulating oxides
 - AEO 81 f
 - electronic structures 345
 - UV-Vis-NIR spectroscopy 61
 - XPS 258
- integral heat 394 ff, 406
- intensity
 - Raman spectroscopy 186
 - TEM 448
 - XPS 247
- interband transitions 58
- intercalating compounds 511
- intercept 58
- interfaces 617
- interlayer coupling 480
- intermediates
 - epoxide solvolysis/rearrangement 726
 - propane ammoxidation 789 f, 793 ff
 - superacidic metal oxides 682, 687
 - titanium silicalite-1 743 f
 - uranium oxides 551
 - vanadium phosphate catalysts 507
- internal cationic sites 165 f
- internal vibrations 110
- interstitials 467, 616
- intersystem crossing (ISC) 79
- intravalence 56
- ion coordinations 113
- ion implantation 761
- ion–scattering spectroscopy 276
- ionization potential 56, 829
- IR spectra
 - gaseous CO₂, CO, NO, CH₄ 108
 - MgO monocrystal 103
 - POMs 581 f
 - superacidic metal oxides 672
- iron addenda elements 572

iron containing zeolite catalysts 313
 iron doped vanadium phosphate catalysts 519, 522
 iron hydroxides 670
 iron oxides 142, 308, 635
 – heterogeneous photocatalysis 757
 – nanoclusters 314
 – TEM 477
 iron sulfated metal oxides 669
 isobutyronitrile (IBN) 155 f
 isoelectric point 87
 isolated molecular species 107 f
 isolated surfaces 357
 isomerization 83, 682, 685 ff
 isopolyanions 561 ff
 isosteric heat 394
 isothermal measurements 401
 isotherms 396
 isotopic substitution 40
 isotopically labeled molecules 168 f
 isotropic hyperfine coupling 9 f
 isotropic spectra analysis 10 f

j

Jahn–Teller effect 53, 73

k

K-edge absorption 300, 318
k-point 335, 342, 355
 K–V–O catalysts 216
 Keggin-type
 – heteropolyoxometallates 561
 – heteropoly compounds 422
 – heteropolyacids 562
 – heteropolysalts 129
 – POMs 569, 585
 ketones 147, 316, 570, 708
 kinetic energy 244, 250, 300
 Kirchoff law 105
 KIT-6 471, 474
 Knoevenagel condensation 821, 840
 Kohn–Sham orbitals 329 ff, 338, 345
 Kubelka–Munk (KM) equation 60, 104

l

L-edge 262, 300
 L-method calculations 681
 labeled molecules 168 f
 Lambert–Beer law 248
 Langmuir adsorption 680
 lanthanides 225, 462
 Laporte (orbital) selection rule 54, 75
 lattice distortion 462
 lattice oxygen

– ammoxidation 776
 – DR UV-Vis spectra 71
 – POMs 568
 – thermal analysis 433
 – vanadium phosphate catalysts 526
 – VPO XPS 279
 lattice parameters 57, 362, 460
 lattice vacancies 542
 lattice vectors 332, 354
 lattice vibrations 110, 123
 layer silicates 128, 424 f
 layered defects 465 f
 layered double hydroxides (LDH) 132 f, 420, 834
 layered structures 541
 layers 60, 355 f, 455, 508
 Lewis acid sites
 – aluminas/SAs 159 f
 – base catalysis 820
 – CP-MAS NMR 233
 – superacidic metal oxides 682
 – thermal analysis 392, 405
 – vanadium phosphate catalysts 507
 – zeolites 427
 Lewis acid–base, metal oxide catalysts 613
 Lewis acidity
 – aluminas 364
 – highly covalent oxides 161 f
 – ionic oxides 160 f
 – metal oxide catalysts 617
 – protonic zeolites 161 f
 – thermal analysis 416
 Lewis-to-Brønsted acidity ratio (L/B ratio) 508
 ligand field theory 613
 ligand to metal charge-transfer transition (LMCT) 55, 69 f
 ligands 70
 Lindqvist structure 561
 line broadening 200, 208, 310
 linear alkane hydroxylation 708
 linear olefin epoxidation 718
 linewidths 24, 200
 linkages 70
 liquid–solid interface 25, 45
 liquid–solid transformations 619
 liquid superacids 667
 liquid–vapor interface 623
 lithium niobate structures 122
 local density approximation (LDA) 330, 341 ff, 346
 localized electron populations 370
 longitudinal optical mode 99, 102
 Lorentzian lineshape 24

- low-dimensional oxide crystals 476 f
- low energy electron diffraction (LEED) 353
- low energy ion scattering spectroscopy (LEISS) 489
- low temperature coprecipitation 628
- lower valence band (LVB) 344
- lowest unoccupied molecular orbital (LUMO) 279
- Lowry–Brønsted acidity definition 146
- LPG dehydrogenation process 596 f
- luminescence center 81
- Lummus/Houdry CATOFIN process 596 f

- m**
- Madelung potential 65, 82, 617
- magic acids 666
- magic angle spinning (MAS) 200 f
- magnesia 408
 - active sites 645
 - differential heats 406
 - DOS plots 342
 - DR UV-Vis-NIR 61 ff, 81 ff
 - IR spectra 102, 112, 131
 - metal oxide catalysts 614
 - Miller planes 354
 - powder EPR 34
 - surface calculations 359 f
 - TEM 625, 832
- magnesium supports 231
- magnesium vanadates 434
- magnetic field 200
- magnetic moment 3, 197
- magnetization transfer 206
- magnetogyric ratio 7
- maleic anhydride conversion
 - metal oxide catalysts 643
 - selective oxidation/VPO 268 f
 - vanadium phosphate catalysts 499, 513, 524
- manganese polymorphs 119
- Mars–van Krevelen mechanism 196, 317, 375
- mass –thickness contrast 445, 470
- matrix isolation 42
- Maxwell–Boltzmann law 5
- MCM-41 materials 314, 472
- mean free path 302
- mechanical mixing 690
- mechanochemical activation 516, 526
- mesoporous materials 428
- mesoporous silica 470 f, 764
- mesoporous silica-aluminas 145 f
- metal–alkyl bonds 600
- metal antimonates 786
- metal catalysts 309
- metal-centered transitions 53 f
- metal–cupferron decomposition 635
- metal hydroxides 129 f
- metal ion doped zeolites 29
- metal ion implantation 761
- metal oxide catalysts 613–664
 - oxidation reactions 487–498
 - solid-state NMR 195–242
- metal oxide
 - base catalysis 819–844
 - supports 221 f
 - XPS 255
- metal–oxygen bonds 111, 132 f, 561
- metal–oxygen–metal bonding 443
- metal phosphates 791
- metal-to-insulator transition 460
- metal-to-ligand charge-transfer transition (MLCT) 55
- methacrolein oxidation 568
- methacrylic acid oxidation 568
- methane 33, 553
- methanol
 - adsorption/decomposition 645
 - base catalysis 834
 - critical point parameters 624
 - oxidation 493, 729
 - titanium silicalite-1 729, 742
 - transesterification 644
 - uranium oxides 553
- methyl-1-propanol oxidation 729
- methylamine 155
- MFI 154, 158, 310
- micelles 636
- Michael addition 821
- microcalorimetry 586
- microemulsion-mediated hydrothermal (MMH) method 634 f
- microheterogeneity 19
- microporous silica-aluminas 145 f
- microporous zeolites 468 f
- microtwin defects 466
- microwave-assisted coprecipitation 631
- microwave power 24, 29
- Mie theory 59
- Miller index 369
- Miller plane 354
- mirage effect 106, 121, 304
- mixed metal oxide catalysts 690
- mixed metal oxides 266 f
- mixed metallic insulating behavior 252
- mixed oxides 121 f, 771–818
- modified oxides 408 f
- modulation amplitudes 24
- molar integral heat 394

- molecular configurations 211
 - molecular oxygen oxidation 570
 - molecular probes 147, 166
 - molecular structure 487–498
 - molecular vibrational modes 107 f
 - Møller–Plesset perturbation methods 326
 - molybdate 137
 - molybdate catalysts 775
 - molybdated superacidic metal oxides 674
 - molybdenum addenda atoms 561, 572
 - molybdenum oxide catalysts 218, 379
 - molybdenum promoted vanadium phosphate catalysts 519
 - molybdenum trioxide 335, 379, 674
 - molybdenum–uranium oxide catalyst 553
 - momentum vector 57
 - monatomic non-absorbing gases 105
 - monoclinic fluorite structure 541
 - monolayer oxides 137, 488
 - monolayer surface coverage 490 f
 - monomeric compounds 262
 - monomolecular intermediate 682
 - mono-oxygen donors 707
 - monosulfate structure 688
 - Monte Carlo (QMC) simulations 330, 359
 - mordenite 426, 588, 680
 - Morse potential 76
 - Mott–Hubbard compounds 255
 - Mott–Hubbard model 371
 - MoV-based mixed metal oxides 281 f
 - Mo–V–Nb–Te–O system 780 ff
 - Mo–V–Te mixed-metal oxide catalysts 416
 - MO_x redox active systems 496
 - Mulliken analysis 339
 - Mulliken charges 255
 - multicomponent analysis 318
 - multicomponent catalysts 775 ff
 - multicomponent molybdate 791
 - multi-electron calculations 262
 - multi-electron wavefunction 325
 - multifrequency measurements 27 f
 - multimetal molybdates (MMM) 775
 - multiple adsorption sites 159
 - multiple product option 780
 - multiple quantum magic angle spinning (MQMAS) 202 f
 - multiple scattering 301 f, 312, 451
 - multiplet splitting 249, 256
 - multiwavelength excitation 177, 185
 - mutual exclusion rule 110
- n**
- N–H stretching 825
 - nanobelts/rods/wires 477 f
 - nanocrystallites 563, 626
 - nanomaterials 69, 614, 619
 - nanoparticles
 - metal oxide catalysts 614 f, 619, 625 ff
 - powder EPR 33
 - X-ray spectroscopy 476 f
 - naphtha steam reforming 557
 - near-edge X-ray absorption fine structure (NEXAFS) 301
 - negative differential resistance (NDR) 574
 - nephelauxetic support series 75
 - neutron diffraction 353, 582
 - Newton's laws 350
 - NH₃ adsorption 405
 - NH₃ probes 507
 - Ni/Co/Fe/Mg molybdates catalysts 775
 - nickel ions 413
 - nickel oxides 372
 - nickel–uranium oxide catalysts 555
 - NiMo/ASA catalyst 206
 - niobium oxides 413
 - nitrile–butadiene–rubber (NBR) 771
 - nitriles 147, 771
 - nitroaniline 821
 - nitrochlorobenzene indicators 666
 - nitrocompounds oxidation 732
 - nitrogen dioxide 30 f, 38
 - nitrogen monoxide 165 f, 403
 - nitrogen probe molecule 684
 - nitromethane 166
 - nitrotoluene indicators 666
 - nitrous oxide 624
 - nitroxide radical 27
 - NMR techniques
 - oxidation catalysts 195–242
 - POMs 579, 580 f
 - vanadia catalysts 601
 - normal modes 123 ff
 - NO_x reduction 555
 - nuclear magneton 8
 - nuclear spins 198
 - nuclear Zeeman interaction 6
 - nucleophilic reactions 280, 622
- o**
- O–H bonds 130, 139, 348, 526
 - occupancy 344
 - octanol oxidation 729
 - olefins 178 f
 - diffusion 742
 - epoxidation 717
 - isomerization 618
 - metathesis 488

- oxidation 549, 554, 717
 - polymerization 153
 - oligocations 424
 - operando spectroscopy 96, 169
 - optic axis 448
 - optical properties 51, 56 f, 109
 - orbitals 55, 244, 301, 324, 526
 - ordered mesoporous silicas 470
 - organic dyes adsorption 760
 - organic phosphates 233
 - organic solvents 510
 - organometallic derivatives 566
 - organoperoxy radicals 42
 - orthotoluonitrile 165
 - oscillations 302
 - outer shell electronic transitions 52
 - overlayer-type contamination 247
 - overoxidation 521
 - overtone modes 99, 151
 - oxalates 629
 - oxidation
 - hydrocarbons 773
 - IR spectra 164
 - NMR 195–245, 218
 - superacidic metal oxides 672
 - supported metal oxide catalysts 487–498
 - titanium silicalite-1 740 f
 - oxidation catalysts 299–322
 - oxidation states
 - cationic centers 161 f
 - chromium 597
 - heteropolyoxometallate catalysts 561
 - uranium oxides 540
 - vanadium phosphate catalysts 500 f
 - oxidative dehydrogenation 260–269, 416
 - oxide catalysts 613–664
 - cracking 196
 - IR spectra 52, 132
 - solid-state NMR 195 f
 - thermal analysis 404 f
 - XAS 299–322
 - X-ray spectroscopy 472 f
 - oxide materials 476 f, 755–770
 - oxide nanotubes 479 f
 - oxide supports 225 f
 - oxides/zeotype-systems 85 f
 - oximes oxidation 316, 733
 - oxoaluminum structure 62
 - oxoanions 561–594
 - oxo-salts 122 f
 - oxyfunctionalization 571
 - oxygen
 - binding energies 253, 275
 - defect structures 377
 - lattices 351
 - liberation 376
 - mobility 416
 - PL spectroscopy 82
 - removal 604
 - superstructures 459 f
 - vacancies 376 f, 383, 456, 466
 - vibrational modes 112
 - X-ray absorption 309, 312
 - oxygen-rebound mechanism 711
 - oxygenation 641, 727
- p**
- palladium catalysts 414
 - parabolic energy valley dependence 57
 - paraffin isomerization 668
 - paramagnetic centers 1
 - paratacamite 116
 - partial oxidation 403, 561–594
 - partial pressure 368
 - partially filled d bands 370 f
 - participating catalytic active site number 494
 - partition coefficients 740
 - patterns 11 f, 20, 452
 - Pauli's exclusion principle 57
 - pentane isomerization 682
 - pentanol oxidation 729
 - Perdew–Burke–Ernzerhof (PBE) approach 57, 330, 341, 346
 - Perdew–Wang (PW91) approach 331, 346
 - periodic electronic structures 323–390
 - periodic quantum chemistry 332 f
 - perovskites 122, 167, 455–467
 - peroxo intermediates 571
 - peroxyacyl radicals 42
 - perturbation methods 328
 - petroleum fractions 543
 - phase contrast 445
 - phase diagrams 370, 540
 - phase shifts 302, 307, 446 f
 - phenol
 - hydroxylation 712, 734
 - oxidation 544, 570
 - TS-1 catalyzed 316
 - phenylethylamine (PEA) 417
 - phonon absorption/emission 66
 - phosphine/-oxides 147, 233
 - phosphorescence 77 f
 - phosphorus enrichment 277
 - phosphorus-modified aluminas 224
 - phosphorus-to-vanadium ratio (P/V) 276, 504

- photoacoustic spectrometry (PAS) 106 f, 582 f
- photocatalysts 68, 225, 755–770
- photocatalytic processes
 - AEO 83
 - oxides 755–770
 - powder EPR 42
 - superacidic metal oxides 698
- photocurrent 244
- photoelectrochemical cell 768
- photoelectron process 302, 305
- photoelectron spectroscopy (PES) 243–298
- photoemission cross-sections 276
- photoionization cross-sections 287
- photoirradiation 42
- photoluminescence spectroscopy 60, 76 f, 80 f
- photonic sponges 763
- photons 57, 244, 300
- photothermal beam deflection spectroscopy (PBDS) 106 f
- physical mixtures 690
- physical photocatalytic activity enhancement 763
- physical properties 26 f, 392
 - metal oxide catalysts 613–620
 - POMs 566
- physical transformations 619
- physisorption 398, 406
- phytosterol esters synthesis 839
- picoline ammoxidation 795
- pillared clays (PILC) 424 f
- pitchblende 539
- Planck constant 98, 339, 445, 451
- plane wave basis set 338
- point defects 33, 467 f, 616
- point symmetry 36
- poisoning 260, 600
- polarization 100, 245
- polyatomic chemical species 97 f
- polymeric tetrahedral oxo-ions 128
- polyoxometallates (POMs) 561–594
- pore structure 156, 310, 564
- porous materials 468 f, 472 f
- potassium hexaniobate 480
- potassium modified uranium oxides 556
- potential-assisted photocatalysis 766
- powder spectra (EPR) 19 f, 24 ff
- powder X-ray diffraction 551
- precipitation 132, 627 f
- precursors
 - Al-NMR 222
 - base catalysis 831
 - IR spectra 51, 129 f, 132
 - metal oxide catalysts 617, 634
 - spin-echo mapping 205
 - uranium oxides 550, 556
 - vanadium phosphate catalysts 500–515
 - XPS 265
- pre-edges 309, 317
- preparation
 - EXAFS 314
 - photocatalysts 763
 - superacidic metal oxides 665–704
 - thermal analysis 415
 - uranium oxides 543
 - vanadia coverage 186
 - vanadium phosphate catalysts 500, 513
- pressure 396
- primary structures 563
- probing/probe molecules 160, 401 ff
- process integration 739
- product distribution 686 f
- promoted catalysts 519 f, 525, 689 f
- propane
 - ammoxidation 777 f
 - chemisorption 495
 - conversion 547, 691
 - dehydrogenation 213, 598
 - oxidation 281 f
- propanol oxidation 729, 742
- propene oxidation 718, 774 ff, 777
- propene oxide synthesis (HPPO) 735, 739
- properties
 - highly dispersed metal oxide catalysts 613–664
 - MoVTenb XPS 282
 - oxide catalysts 81 f
 - sulfated superacidic metal oxides 671
 - superacidic metal oxides 675
 - see also* chemical, physical properties
- propylene ammoxidation 549
- propylene oxidation 318
- proton affinity 402
- protonic acidity 435
- protonic zeolites
 - Brønsted acidity 153 f
 - IR spectra 158
 - Lewis acidity 161
 - surface hydroxyl groups 144 f
- pseudoboehmite 116
- pseudoliquid bulk type catalysis 564
- pseudopotentials 340 f
- pulsed flow calorimetry 399
- purification steps 777
- PW91 approach 360
- pyridine
 - POMs 586

- adsorption 84, 427
- CP-MAS NMR 233
- IR spectra 135, 153
- surface basicity 166, 402
- vanadium phosphate catalysts 507
- pyrolysis 640
- pyrophosphate groups 277
- pyrrole 166

q

- Q-size effect 68
- quadrupolar broadening 225
- quadrupolar interaction 14, 199
- quadrupolar phase adjusted spinning sideband (QPASS) 226
- quadrupolar vanadium isotopes 212
- quadrupole moment 198
- quantifications 24 f, 186 f, 247 f
- quantum chemistry calculations 323
- quantum dots 476
- quantum efficiency 79 f
- quantum mechanics 3, 197
- quantum mechanics/molecular mechanics (QM/MM) 323
- quaternary metal oxides 415 f
- quencher molecules 80

r

- Racah parameter 53
- radicals 12, 29, 38 f, 376
- radio frequencies 202
- Raman spectroscopy 95, 177–196
 - butane dehydrogenation 606
 - coke 599
 - CrO_x/alumina catalyst 597
 - polyatomic chemical species 97 f
 - skeletal 111
 - vanadia catalysts 489, 601
- rapid reduction 574
- rare earth oxides 836
- Rayleigh theory 100
- reactive intermediates 743
- real space 451
- reciprocal space 332, 451
- recombination 47, 756, 761
- recrystallization 463
- recycle processes 779
- redox properties 45
 - heterogeneous photocatalysis 756
 - metal oxide 613, 619 f, 227
 - oxidation reactions 495, 491
 - POMs 567, 578, 585
 - thermal analysis 392, 403 f
 - vanadium phosphate catalysts 516

- heterogeneous photocatalysis 756
- vanadia catalysts 178 f
- vanadium phosphate catalysts 530
- reduced states 183 f
- reducing agents 508, 707
- reduction 554 f, 585, 604
- refinery-based C₄ stream 650
- reflectance
 - divalent elements 112
 - IR spectroscopy 59, 98, 101
 - Raman spectroscopy 186
- reflection techniques 101 f
- refractive index 60, 102
- regeneration 596, 609, 745
- relativistic correction 445
- relaxation 5 f, 245, 251, 360, 366
- reoxidation 185, 260
- resolution 354, 448 f
- resonance absorption 21
- resonance enhancement 184, 189
- resonance line width 6
- resonance Raman spectroscopy 177–196
- resonant frequency 198
- restricted Hartree–Fock (RHF) 326, 346
- reststrahlen effect 102
- rhombic symmetry 21
- rock salt structure 63, 102, 143 f, 356
- rocking mode 120
- rosary pattern 472
- rotation effects 25 f, 107, 201
- rutile 118, 342 757, 786

s

- S-compound oxidation 734
- salt-free production 734
- sample preparation 100, 134, 309
- sample tumbling effects 25 f
- satellite transition magic angle spinning (SATRAS) 200 f, 256 f
- saturation effects 29
- SBA-15 472, 650
- scaling factor 203
- scanning electron microscopy (SEM) 445, 512
- scanning tunneling microscopy (STM) 462
- scattering 59
 - POMs 579
 - TEM 448, 451
 - XAS 302
- Scheelite-type structure 775
- Scherzer equation 449
- Schiff base amines 571
- Schottky pairs 616
- Schrödinger equation 244

- Schuster–Kubelka–Munk (SKM) model 59
- second generation TiO₂ photocatalysts 68
- secondary structures 563
- segregation 276, 617
- selected area electron diffraction (SAED) 450
- selection rules 98, 103
- selective n-butane dehydrogenation 260 f
- selective oxidation
 - EXAFS 315 f
 - maleic anhydride/VPO 268 f
 - uranium oxides 548
 - XPS 267 f
- selectivity
 - toluene oxidation 552
 - uranium oxides 556
 - vanadium phosphate catalysts 504, 519
- selectivity–activity relationships 487–498
- self-absorption 187
- self-interstitials 467
- semiconductors
 - electronic structures 345
 - photocatalysis 756, 760
 - transition metal oxide surfaces 381
 - UV absorption bands 66 f
- sensitivity
 - IR spectra 134
 - oxidation catalysts 198
 - photocatalysis 760
 - VPO 276
- sensors 698
- sesquioxides 121, 142 f, 836
- Shannon's tabulation 355
- shear planes 318
- shells 452
- shifting 182
- shrinkage 474, 623
- Si–(OH)–Al bridges 144
- Si–O–Si bridges 119, 160, 228
- side-chain alkylation 819
- signal-to-noise ratio 60, 134, 245
- silanol groups 141, 144
- silica
 - hydroxyl groups 141
 - optical absorption 62
 - polymorphs 119
 - supports 227, 433, 553
 - thermal analysis 408
 - X-ray spectroscopy 470 f
- silica-aluminas (SAs)
 - CP-MAS NMR 206, 229 f
 - Lewis acid sites 159 f
 - supports 206, 231
 - surface Brønsted acid sites 150
 - surface hydroxyl groups 145 f
 - thermal analysis 418
- silica-titania/zirconia 417
- silicalites 316, 428
- silicates 136, 424 f
- silicon 206, 757
- silicon sulfated metal oxides 669
- silver catalysts 413, 519
- single crystals 19, 26
- single-site active centers 69
- singlet state 77
- singularities 21
- site chains 383
- site symmetry 24
- skeletal IR spectra 111 f, 129 f
- skeletal isomerization 685
- slab models 353, 357 f
- Slater determinants 326
- smectites 424
- smoothing function 344
- Sn sulfated metal oxides 669
- SnO₂
 - heterogeneous photocatalysis 757
 - support 231
 - thermal analysis 407
- SO₂ adsorption 405
- SO₄/ZrO₂ preparation 672
- soft pseudopotentials 340
- SOHIO process 774 ff
- sol–gel precursors 634
- sol–gel processing 415, 620, 672
- solid acids 679
- solid solutions 121 f
- solid–gas interface 393, 404
- solid–liquid interface 400
- solid-state Hamiltonian 14
- solid-state NMR 195–242
- solid-state TEM 443
- solid superacids 667 f
- solids energy band transitions 56
- solvents 622 f, 741
- solvolysis/rearrangement 726
- solvothermal techniques 633
- sonochemical coprecipitation 630
- space group 454, 471
- space vector 332
- spacings 450
- spectral properties 13, 19, 51
- spectroscopic detection 97 f, 139–159
- spherical aberration 448
- spikelet-echo technique 208
- spin density 41, 384
- spin-echo mapping 204 f, 216
- spin Hamiltonian 1 ff, 44 ff

- spin–lattice relaxation 6
- spin–orbit coupling 79
- spin quantum number 197
- spin states 78, 325, 371
- spin–spin coupling Hamiltonian 18, 199
- spin–spin relaxation 6, 208
- spinel model 352
- spinel-type structure oxides 115 f, 121, 142 f
- spinning 209, 223
- splitting 372
 - EPR 10, 23, 27
 - IR spectroscopy 53, 110, 144
 - POMs 581
 - XPS 249
- spontaneous ionization 33
- spray pyrolysis 640
- structural defects 616
- stabilization 504, 633
- stacking faults 465, 617
- stacking sequence 349, 355, 469
- stannia gel 669
- state multiplicity 99
- static calorimetry–volumetry coupling 394 f
- steady-state kinetics 493
- steam cracker-based C_4 stream 650
- steam reforming 556 f
- Stefan's law 105
- Stern–Volmer equation 80
- stoichiometric range 276, 540
- Stokes shift 78
- strengths 147 f
- stretching
 - IR spectra 111, 123, 139, 161
 - POMs 581
 - vanadia catalysts 181
- structure–activity relationships 190, 195, 487–498
- structure calculations 323–390
- structural characterization 69 ff, 221
- structural transformations 517
- structures
 - Al_2O_3 -supported vanadia catalysts 178 f
 - boehmite 349
 - bulk oxides 209 f
 - heteropolyoxometallate catalysts 561 f
 - hydrotalcites 835
 - hydroxyl groups 140
 - M1 XPS 281
 - metal oxide catalysts 614
 - oxide crystals 454 f
 - sulfated zirconia 687
 - surface defects 35
 - surface properties 227
 - Ti–OOH species 742
 - Ti–zeolites 707
 - uranium oxides 540 f
 - USb_3O_{10} 550
- styrene–acrylonitrile (SAN) 771
- styrene dehydrogenation 607
- subshell photoionization 287
- substituted alkanes 709
- substituted alkylbenzenes 791
- substituted aromatic nitriles 793
- substituted benzenes 717
- substituted olefins 726
- sulfated metal oxide catalysts 669 ff
- sulfated oxides 143 f
- sulfated silicas 671
- sulfated titanias 408
- sulfated zirconias 234, 408, 673, 685 ff
- sulfates 133, 137
- sulfation 670
- sulfides/sulfoxides 316
- sulfur dioxide 166, 408, 432, 516
- sulfurous compound removal 755
- superacidic metal oxides 665–704
- superbase 824 ff, 837 ff
- supercells 336, 372
- superconducting oxides 455
- superhyperfine interactions 35
- superoxide radicals 759
- superoxo species 528
- superstructures 121, 455 f
- supported boria catalysts 409
- supported catalysts 252
- supported heteropolyacids 422 f, 791
- supported metal oxide catalysts 408 f, 487–498
- supported transition metal oxides 54 f, 496
- supported vanadium oxide catalysts 210 f
 - oxidation reactions 487–498
 - Raman spectroscopy 177–196
- supports 195 ff, 210, 221 f
- Suprasil 81
- surface acid–base properties 404
- surface acid sites 495
- surface acidity
 - IR spectra 147
 - NMR 196, 229 f
 - thermal analysis 402 f
- surface active sites 392
- surface adsorption 30 f, 323
- surface anion vacancies 35
- surface area 564, 617
- surface basicity 166
- surface calculations 359 f
- surface catalysis 564

surface chemistry 96 f, 133 f
 surface coverage 490 f
 surface defects 33 f
 surface density 180
 surface electromagnetic wave spectroscopy (SEWS) 104
 surface element–oxygen bonds 134 f
 surface energy 355, 368
 surface equilibration 401
 surface hydroxyl groups 142 ff
 surface M–O–M bridges 134 ff
 surface OH groups 142
 surface oxo-anions 136 f
 surface paramagnetic centers 1
 surface profile imaging 462 f
 surface properties
 – metal oxides 227 f, 614
 – NMR 196
 – oxides 402 ff
 surface reactivity 81, 492 f
 surface relaxation 112
 surface-sensitive techniques 244 f
 surface states 61
 surface structure 206 f, 227 f, 353 f
 surface tension 479
 surface-to-volume ratio 478
 surfactants 641
 symmetrical hydrogen bonding 150
 symmetry 157, 301
 symmetry point group 124, 136
 synchrotron 245
 synergistic interactions 433, 575
 synthesis, metal oxide catalysts 613–664, 706 f

t

Tanabe–Sugano diagrams 53
 tapered element oscillating microbalance (TEOM) 604
 tartaric acids 499
 tellurium cations capping 587
 tellurium dioxide, XPS 287
 temperature dependence 392 ff
 – adsorption–desorption heats 401 f
 – powder EPR 26 ff
 – reduced states 183
 temperature programmed desorption (TPD) 399
 – base catalysis 823
 – superacidic metal oxides 675 ff
 – uranium oxides 548
 – vanadium phosphate catalysts 526
 temperature programmed oxidation (TPO) 399, 619
 temperature programmed reduction (TPR)
 – chromia 596
 – metal oxide catalysts 619
 – superacidic metal oxides 678
 – vanadium phosphate catalysts 526
 temperature programmed surface reaction (TPSR) 489 ff
 templates 473, 640
 temporal analysis of products (TAP) 503, 548
 tensors 14 ff
 terminal planes 464
 terminating layer 253
 ternary phases 121 f
 ternary systems 418
 tertiary structures 563
 tetraethylorthosilicate (TEOS) 523
 tetravalent oxides 118 f, 143 f
 thermal analysis 391–442, 579
 thermal decomposition 46, 638
 thermal desorption 399
 – POMs 581
 – XPS 255
 thermal treatment 550, 567 f
 thermodynamic equilibrium constant 665
 thermogravimetric analysis (TGA) 391, 417, 579, 586
 thermokinetic parameters 398
 thermolysis 586
 thioethers oxidation 734
 thiols 166
 Ti-MCM 73
 Ti–OOH species 741 f
 time constants 398
 tin oxides 410
 titania
 – (110) surface 366
 – DOS plots 342
 – heterogeneous photocatalysis 757
 – metal oxide catalysts 614, 625, 634
 – nanotubular material 479
 – photocatalysis 757, 763
 – polymorphs 118, 143
 – supported vanadium oxide 433
 – surface calculations 359 f
 – surface oxo-anions 136
 – thermal analysis 408
 see also rutile
 titanium dioxide 42
 titanium oxide incorporation 764
 titanium promoted vanadium phosphate catalysts 521
 titanium silicalite-1 315, 705–754
 titanium sulfated metal oxides 669

- titanium(IV) oxide 755 f, 763 ff
 - titanosilicate ETS-10 428
 - TNU complex zeolites 468
 - tolerance factor 460
 - toluene 310, 544, 552, 692
 - top-down preparation 619
 - total electron yield (TEY) 247
 - total oxidation 547
 - toxic properties 649
 - transesterification 644, 839
 - transfer of population in double resonance (TRAPDOR) 207
 - transient radical intermediates 42
 - transition aluminas 221 f, 351, 404
 - transition metal ions (TMI) 45 f, 53, 69 f, 85 f
 - transition metal oxides 613
 - oxidation reactions 496
 - partially filled d bands 370 f
 - periodic electronic structures 323, 351
 - transition metal substituted polyoxometallates (TMSP) 568
 - transition metal zeolites 312 ff
 - transitions
 - energy bands 56 f
 - EPR 9
 - TEM 452
 - XAS 301
 - XPS 248
 - translations 107
 - transmission electron aberration-corrected microscope (TEAM) 450
 - transmission electron microscopy (TEM) 443–486
 - transmission/absorption IR technique 100 f, 133
 - transmittance 60, 98, 304
 - transverse optical mode 99, 102
 - trapping 761
 - triacetin transesterification 644
 - trialkyl-substituted phenols 571
 - triethylamine 402
 - triglycerides 643
 - trigonal-planar oxo-anions 123
 - trilayer units 363
 - trimer structural model 689
 - trimethylamine 155, 402
 - trimethylborate 166
 - triplet configurations 12, 78, 371
 - trivalent element oxides 115 f
 - tungstate 137
 - tungstated aluminas 697
 - tungstated oxides 143 f
 - tungstated stannia 696
 - tungstated superacidic metal oxides 674
 - tungsten addenda atoms 561
 - tungstic heteropolyacids 422
 - turnover frequency 493, 605
 - twin defects 466 f
 - twisting modes 132
 - two-spin Hamiltonian 9
- u**
- ultra-high vacuum (UHV) system 36, 245, 260
 - ultra-soft pseudopotentials 340
 - ultra-stable (USY) zeolites 310, 425
 - undulators 304
 - uniaxial symmetry 20
 - unit cell 332, 451, 563
 - unrestricted Hartree–Fock (UHF) 326
 - unsaturated alcohols epoxidation 724
 - upper valence band (UVB) 342
 - uranium oxides heterogeneous catalysis 539–560
 - UV absorption bands 61 f, 66 f
 - UV irradiation 43
 - UV photoemission spectroscopy (UPS) 376
 - UV-visible radiation 756
 - UV-visible spectroscopy 583
 - UV-vis-NIR spectroscopy 51–94
- v**
- V–Mg–O catalysts 216
 - V–Mo–Nb–Te oxide catalysts 779
 - V–Mo–O catalyst ammoxidation 804
 - V–O–M bonds 487 ff
 - V–O–S bonds 178
 - V–O-support bond 494
 - V–O–V bonds 267
 - V–P–Ti compound 214
 - V–Sb–O-based catalysts 789 f
 - vacancies
 - electronic structures 352, 376
 - metal oxide catalysts 614 ff
 - TEM 452, 466
 - transition metal oxide surfaces 376
 - uranium oxides 542
 - vacuum system 304
 - vacuum treatment 72
 - valence band 372
 - heterogeneous photocatalysis 756
 - UV-Vis-NIR spectroscopy 57
 - VPO 273
 - valence charges 255, 259, 286
 - valence electrons 244, 613
 - valence states 340
 - EPR 45
 - heteropolyoxometallates 561

- vanadia catalysts 178
- XPS 248 ff
- van der Waals interaction 405
- vanadates 137, 184, 216 f
- vanadia catalysts 429 f, 488–498, 601
- vanadia coverage 186
- vanadium 86
 - cation capping 587
 - heteropoly catalysts 578
 - impregnation 227
 - TiO₂ supported 791
- vanadium oxides
 - alkane dehydrogenation 595–612
 - oxidation reactions 487 ff
 - oxidative dehydrogenation 266 f
 - PL spectroscopy 86
 - Raman spectroscopy 177–196
 - solid-state NMR 210 f
 - XPS 255
- vanadium pentoxides 430
- vanadium phosphate catalysts 499–538
- vanadium phosphorus oxides (VPO) 499–538
 - selective dehydrogenation 268
 - solid-state NMR 216 f
 - spin-echo mapping 204
 - thermal analysis 416
- vanadyl groups 87, 259
- vanadyl phosphates 500, 508
- Vanderbilt potentials 340
- vapor condensation methods 639
- vegetable oils 643
- vibrational spectroscopies 76, 95–126
- visible light sensitization 760
- VO₂ P₂O₇, HREM 500
- VO_x/Al₂O₃ catalysts 230
- V₂O₅–Al₂O₃ catalysts 202, 489
- V_xO_y/alumina 260 f
- volatile organic compounds (VOCs) 547
- volumetric-calorimetric adsorption 394
- VPA route 509

W

- wagging modes 132
- water
 - addition 516, 547
 - adsorption 132 f, 139 f, 376
 - critical point 624
 - oil micro-emulsions 636
 - solvent 742
 - splitting 755
 - vapor adsorption 64
- wavefunctions 16, 332
- wavelengths 52, 445

- wavenumber 56, 98, 134, 521
- Weiss temperature 204
- wet chemical transformations 619
- wigglers 304
- WO₃ photocatalysis 757
- WO₃/ZrO₂ preparation 674
- work function 244
- wurtzite hexagonal-phases 477

X

- X-band frequency 4
- X-ray absorption fine structure spectroscopy (XAFS) 601
- X-ray absorption near-edge structure (XANES) 301, 308 f, 490
- X-ray absorption spectroscopy (XAS) 247, 299–322
- X-ray diffraction (XRD) 332, 353, 503, 512
- X-ray fluorescence process 305
- X-ray photoelectron spectroscopy (XPS) 248 f
 - chromia 596
 - monolayer surface coverage 489
 - superacidic metal oxides 672
 - surface sensitive technique 243 ff
 - vanadia catalysts 601
- X-ray transitions 248 f
- xylene ammoxidation 794

Y

- YBa₂Cu₃O₇₋₈ 463, 467
- YBaCo₂O_{5+x} 459
- YSrCo₂O₅ 448

Z

- ZAF calibration 453
- Zeeman interaction 2 ff
- Zeeman shift 197
- Zeeman states 207
- zeolite acid catalysis 154
- zeolites 29, 47, 62, 85 f
 - adsorption microcalorimetry 402
 - ammoxidation 810
 - analcime 478
 - base catalysis 837
 - cation exchanged 165 f
 - crystallites 469
 - EXAFS 310 ff
 - H-FER 300
 - IR spectra 121, 124, 143, 165
 - photocatalysis 763
 - POMs 588
 - surface Brønsted acid sites 150
 - thermal analysis 425 f

- titanium silicalite-1 707 ff
- X-ray spectroscopy 468 f
- ZSM-5 310 ff, 425
- zero field interactions 18, 27
- zero point of charge (PZC) 87
- zero valent state 47
- Ziegler–Natta catalysts 47
- zinc blende structure 333
- zinc oxides 635
- zinc promoted vanadium phosphate catalysts 519
- zirconia
 - IR spectra 143, 160
 - metal oxide catalysts 614
 - NMR 208, 234
 - polymorphs 118
 - precipitation methods 629
 - sulfated 669 ff
 - superacidic metal oxides 669
 - superbases 837
 - surface oxo-anions 139
 - thermal analysis 408
- zirconium promoted vanadium phosphate catalysts 519, 522
- ZnO 115, 334, 477
- ZnS photocatalysis 757