

Index

a

ab initio calculations 377, 411, 412
 aberration-corrected electron microscopy (AC-TEM) 345, 346, 349
 acid-catalysed dehydration 8
 – fructose 9, 10
 acid-catalysed esterification 17
 acrolein 690, 692
 acrylic acid 690
 acrylonitrile 688–690
 activation energy, chemisorption 101–104
 acyclic diene metathesis (ADMET) 413
 adiabatic reactors 516–518
 adipic acid 697, 698, 700
 adsorbate 67
 adsorption
 – clean solids 71–74
 – definition 67
 – energetics 113–126
 – heterogeneous reactions 132–140,
 142–147, 151
 – isotherms and isobars 79–88, 90–101
 – isotherms, kinetic principles 105–113
 – microkinetics 147, 148, 152–154
 – mobility 126, 127
 – ordered adlayers 74–76, 79
 – physical, chemisorptions and precursor
 states 67–70
 – surface reactions 127–129, 131, 132
 AES analysis *see* Auger electron spectroscopic (AES) analysis 573
 affinity coefficient 111
 agostic interactions 49, 51
 $\text{Al}_2\text{O}_3/\text{CeO}_2/\text{noble metal}$ 385
 algae biofuel challenge 13
 Algenol 13
 alkaline-earth oxides 430
 ALPO structure 384

ALPO-18 catalyst 188, 280
 aluminophosphate MeAPO-36 382
 aluminosilicates 382
 ammonia
 – absorption tower 585
 – adsorbed nitrogen 575, 576
 – Badische Anilin und Soda Fabrik (BASF)
 laboratories 569
 – BASF catalyst S6-10 570, 574
 – CO_2 removal 585
 – and copper catalyst 585
 – crystalline α -Fe phase 574
 – *ex situ* X-ray diffraction studies 574
 – Fe catalysts 570
 – high-temperature treatment 573
 – *in situ* X-ray powder diffractometric studies
 574
 – methanation 585
 – methane 585
 – N_2 fixation 568
 – natural gas 583
 – nitrogen-containing compounds 568
 – oxidation 588–592
 – potassium 582
 – potential-energy diagram 580
 – primary reforming furnace 583
 – process streams 585
 – production 569
 – promoted iron catalyst composition 573
 – promoters 570
 – reactor configurations 585–588
 – reforming reactions 583
 – Ru-based catalysts 570
 – shift converters 583
 – steam-reforming reactions 583
 – surface hydrogen 578–580
 – surface nitride 576–578
 – synthesis reactor 649

- ammonia (*continued*)
 - Temkin–Pyzhev description 571–573
 - typical arrangement, plant 584
 - world population 569, 570
 - X-ray photoelectron spectrum 573
 ammonia oxidation 527
 ammonia synthesis reactor 520
 ammonoxidation process 22
 ammonoxidation 22, 176, 589, 687
 argon adsorption isotherm 703
 aromatic alkylation 708
 artificial leaf 661, 662
 artificial photosynthesis systems 661
 atomic and ionic polarization 379
 atomic force microscopy (AFM) 229, 230, 239, 240
 atomistic studies 385, 389
 attenuated total reflection (ATR) IR spectroscopy 189
 Auger electron spectroscopy (AES) 40, 177, 190, 573, 575, 576
 auto-exhaust catalysts 23, 24, 46
 auto-thermal reactors (ATR) 493
 autocatalysis 133, 134, 144
 autothermal syngas production 492
 AVADA (advanced acetates by direct addition) 364
 Atzel cell 626
- b**
- Balandin volcano plot 35
 band bending 403–406, 408
 batch reactors 499, 500, 501, 510–512
 Belousov–Zhabotinskii (BZ) reaction 133
 benzene-free synthesis, catechol 7, 8
 BEP plot, *see* Brønsted–Evans–Polanyi (BEP) plot 562
 BET *see* Brunauer–Emmett–Teller 296
 bifunctional catalysts 42, 449–451
 bimetallic catalysts 721–723
 bimetallic cluster catalysts 206–209
 bimetallic nanoparticles 53
 bioinspired photosystems 659
 biomass 657
 biomass-derived carbon feedstocks 695
 biomass-derived polyols 8
 biorefineries 655
 bismuth molybdates 688, 689, 722
 bismuth molybdate catalysts 47, 688, 689, 722
 blue-coloured light 659
 body-centred cubic (bcc) metals
 - high-symmetry planes, 71, 72
 Boltzmann statistics 86, 380, 401
 Born model 379
 Brønsted catalysts 42, 43
 Brønsted-acid catalysed isomerization 720
 Brønsted–Evans–Polanyi (BEP) plot 562
 Brønsted–Evans–Polanyi (BEP) relation 52, 101–103, 415
 bridging hydroxyl groups 383
 BRIMTM 232, 237
 Brunauer classification 80
 Brunauer–Emmett–Teller (BET) isotherm 82, 110
 Brunauer–Emmett–Teller (BET) method
 - energetic heterogeneity 297
 - fractal analysis 297
 - nitrogen 297
 - principle 297
 - surface area 297
 - transformations 297
 butene isomer binding energies, ZSM-5 387
- c**
- catalytic reactors, coupling and decoupling 489
 C-hexene 423, 425, 426
 Caltech–Swiss solar reactor 726
 Cambridge–Tübingen–London (CTL) team 368
 capillary-microreactor 487
 caprolactam 646, 697, 698
 carbenium 637, 642
 carbohydrates starch and cellulose derived 7
 carbon nanotubes (CNT) 664, 683
 cascade catalytic reactions 700, 701
 catalysed hydrolysis of starch 16
 catalyst characterization methods 174, 175
 catalyst deactivation
 - models 455–457, 459–462
 - processes 452–454
 catalyst packing 515
 catalyst poisoning 37, 459, 460, 462
 catalysts design 719
 catalytic cracking 18, 19, 42
 - cycloparaffins 635
 - FCC catalyst 638–640
 - fluid catalytic cracking (FCC) 634
 - heavy gas oil or vacuum gas oil (HVGO) 634
 - high-activity robust catalysts 634
 - petroleum refineries 635
 - Shell middle distillate synthesis (SMDS) 636
 - ‘syn-gas’ 636
 catalytic cycle 148
 catalytic hydrogenation 17, 507

- catalytic hydrothermal reactor (Cat-HTR) 706
- catalytic monolith
 - applications 605
 - automobile exhaust applications 609
 - catalytic and homogeneous oxidation 611
 - catalytic combustion chamber 604
 - chemical and physical effects 610, 611
 - CO formation 607
 - combustion processes 606
 - computed temperature and concentration profiles 611
 - conjunction with combustion chambers 610
 - curve-fitting techniques 608
 - elementary surface reactions 608
 - exhaust-gas velocities 609
 - gaseous phase and catalytic combustion 607
 - initiation reaction 607
 - integral bundle, ceramic tubes 604
 - intraphase diffusion and mass transport 614
 - mass-transfer coefficient 610
 - metal oxide supports 608
 - open-mesh wire structures 605
 - Phang treatment 611
 - propane combustion 611
 - propane oxidation 613
 - shallow fixed-bed tubular reactor 604
 - steady-state energy balance 612
- catalytic oxidation 517
- catalytic RNAs 31, 32
- catalytic wall reactors 486
- CatApp
 - fcc and hcp surfaces 422
 - Haber–Bosch process 423
 - Quantum Materials Informatics Project 422
 - reaction and activation energies 421
- catechol 7, 8
- cellulose-to-ethanol conversion cycle 657
- chemical turbulence 146, 150
- chemisorbed species 118–122
- chromatographic analysis 259, 509
- classical stochastic diffusion theory 99
- Clausius–Clapeyron equation 81, 83
- CO molecules 77, 78, 83, 84
- CO structure, Pd(100) surface 78, 79
- CoALPO-18 188, 280
- cocatalysts 669
- coincidence structure 78
- combined oligomerization 708
- commodity chemicals 9
- computer modelling techniques 377
- concentration instabilities 139, 140
- continuous reactors 510, 513
- continuous stirred-tank reactor (CSTR) 504, 505
- conventional gas–liquid adsorbers 485
- conventional transportation fuels 707
- Core-Shell Co-Catalysts 669
- countercurrent flow 526
- cross-polarization (CP) 220
- crude feedstocks 712
- CSTR reactor *see* continuous stirred-tank reactor 505
- Cyclar process 22
- cyclohexane–benzene interconversions 38
- d**
- Davidson–Harrison model 523
- Deacon process 17
- De Donder relations 147, 154
- Debye's equation 182
- Debye–Waller factor 204
- degree of rate control 147, 154
- dehydrogenation of butane 22
- density functional theory (DFT) 3, 52, 102, 104, 152, 229, 302, 303, 343, 416, 417, 419
 - Brønsted–Evans–Polanyi (BEP) relations 419
 - macroscopic reaction rate 421
 - metal alloy catalysts 421
 - oxygen chemisorptions, energies 420
 - Pareto optimal catalysts 419, 421
 - structural schematics and coordination number 423
 - undoped TiO₂ surface 429
- desorption
 - precursor state 99, 101
 - rates 96–98
 - statistical mechanics 98, 99
- DFT, *see* density functional theory 302, 303
- diesel production vegetable oils 9
- differential anomalous X-ray scattering (DAXS) 280
- differential tubular reactor, *see* tubular reactors 502
- diffuse reflectance IR Fourier transform spectroscopy (DRIFTS) 273
- diffusion effects 504
- diffusional constant 389
- diffusive flux 444
- distortionless enhancement of polarization transfer (DEPT) 165
- docking method 386, 387
- donor–acceptor concentration 675

- DSC, *see* dye-sensitized cell
dual-function catalyst 21, 25
Dubinin–Kaganer–Radushkevich (DKR)
equation 82, 112, 113
DuPont strategy 57
dye-sensitized cell (DSC) 626, 628
- e**
4D electron microscopy 248, 249, 253
earth-abundant H₂-evolution photocatalysts
664
earth-abundant O₂-evolution photocatalysts
665
ecofining process flow-scheme 705, 706
Eddy diffusion coefficient 513
EFBMR *see* externally fluidized bed membrane
reactor 498, 596
electrocatalysts 663, 664, 666, 676, 683
electrochemical reduction of CO₂ 663
electron crystallography 245, 246
electron microscopy (EM) 240–242,
244–249, 251, 253
electron spin resonance (ESR) 40, 214–216
electron tomography (ET) 246, 247
electron-energy-loss spectroscopy (EELS)
40, 241–243, 249, 253, 275
Eley–Rideal (ER) mechanism 67, 68,
128–130
ellipsometry 250–252
ellipsomicroscopy for surface imaging (EMSI)
252
Elovich equation 93–96
endothermic chemisorption, hydrogen 86
energetics of adsorption 113
energy bands
– atomic arrays 393
– Brillouin zone 392
– crystal orbitals and wave functions 391,
392
– ID and 3D crystals 393–396
– density of states (DOS) plot 392, 393
– E(k) plot 392
– Fermi energy 392, 393
– ionic solids 395, 397
– transition-metal oxides 398, 399
energy minimization (EM) methods 53, 115,
117
energy-dispersive X-ray diffraction (EDXD)
technique 277
engineered *Escherichia coli* 712
environmental challenges 60
environmental TEM (ETEM) 248, 250
enzyme catalysis 43
enzymax analyser 31
- Escherichia coli* 12
ε-caprolactam 697, 698
ethylene catalytic polymerization 216
ethylene glycol production 58
European hydrogen and fuel platform (HFP)
679, 681
‘Ewald construction’ 196
exothermic adsorption 84, 85
exothermic and endothermic reactions
492–494
exothermic catalysed reactions 501
exothermic gas–solid catalytic reaction 504
extended X-ray absorption fine structure
(EXAFS) 200–202, 204, 207, 209
externally fluidized bed membrane reactor
498, 596
- f**
face-centred cubic (fcc) metals
high-symmetry planes, 71
Fe-based NH₃ synthesis catalyst 687
Fe nanoparticle 683
Fermi levels 399, 400, 402
Fermi–Dirac distribution function 400
field-ion microscopy 127
first-order rate coefficients vs. active sites
concentration, ZSM-5 34
Fischer–Tropsch catalysis
– C₂–C₄ olefins 548
– C₁₀–C₂₀ paraffins 548
– CO/H₂ ratio 547
– Fe₂O₃ 556
– fluidized-bed reactors 548, 558
– free energy, hydrocracking and methanol
547
– FT synthesis 559
– Haldo Topsøe technology 559
– hydroxymethylene intermediates 550–553
– Lurgi gasifiers 557
– methanation 548, 559, 560, 562
– multi-tubular shell assembly 557, 558
– naphthas 558
– nickel catalyst 548
– off-shore natural gas 559
– polymerization 549
– process conditions 555, 556
– SASOL plants 548, 558
– Schultz–Flory plot 549, 554
– steam reforming 563–568
– sulfur, nitrogen and aromatics 548
– syn-gas 546, 547, 558
– turbulent flow conditions 558
Fischer–Tropsch processes 18, 21, 48, 102,
660

- fixed-bed catalytic cracking 18
- fixed-bed-reactors 482–485
- flowing-solids reactors 507
- fluid-to-solid transport effects 504
- fluidized beds 523
- fluidized-bed reactors 522, 524
- fluidized catalytic cracking (FCC) 18, 20, 701
- fluorescence microscopy (FM) 239
- fossil fuels 656–658, 680
- free induction decay (FID) 219
- Frenkel's equation 87, 88
- Freundlich isotherm 82, 109, 110
- friction force microscopy (FFM) 240
- fuel cell 615

- g**
- γ-valerolactone (GVL) 714
- gas heated reformer (GHR) 494
- gas-to-liquid (GTL) technologies 492
- gas–solid catalytic reactions 504
- Gauze temperature 528
- General Utility Lattice Programme (GULP) 53
- genetic algorithm (GA) techniques 432, 433
- genuine water-splitting photocatalytic systems 660
- glossary of terms and processes
 - heterogeneous catalysis, 5, 6
- glucose isomerization 31
- gold, reconstructed surface 73, 74
- Grätzel cell and influence 626, 627
- green diesel production 705, 706
- green hydrocarbons and ethanol 716

- h**
- H⁺-ZSM-5 125
- Hartree–Fock equations 377
- heat fluxes 519
- heat-balance equations 513, 529
- heat-transfer coefficient 513, 520
- heats of adsorption
 - decline 123–125
 - thermodynamic data 121, 123
- Henry's adsorption isotherm 109
- Hertz–Knudsen formula 86, 91
- heterogeneous and homogeneous reactions
 - comparison, 131, 132
- heterogeneous catalysis 1, 4–6, 13, 14, 31, 33, 36–39, 41–45, 47–50, 52, 53, 163, 184, 187, 215, 225, 238, 249, 268, 274, 275, 281
 - auto-exhaust catalysis scene 601
 - caprolactam 646
 - catalytic distillation 592–596
 - catalytic membrane processes 596–601
 - CO, HC and NO_x conversion 602
 - ethyl benzene dehydrogenation 650, 651
 - European Union standards, automotive exhaust gases 602
 - *in situ* catalytic reaction and separation 592
 - industrial reactor 651
 - inorganic membrane reactors 645
 - Mars–van Krevelen mechanism 648
 - methanol 541–546
 - monochloronaphthalenes 646
 - motor vehicles 601
 - organonitrogen compounds 648
 - phenol–acetone condensation reaction 645
 - photocatalytic reduction 647
 - practical examples 650
 - prochiral alkene 645
 - shape-selective catalysis 647
 - shape-selective olefin hydroformylation 645
 - stoichiometric engine A/F 603
 - temperature-programmed desorption (TPD) 647
 - three-way catalyst (TWC) 601, 603, 604
- heterogeneous catalyst
 - platinum 349
 - theoretical treatments 415, 416
- high-angle annular dark field (HAADF)-mode 27
- high-resolution electron energy-loss spectroscopy (HREELS) 189, 190, 417
- high-resolution electron microscopy (HREM) 27, 125, 136, 241, 243–245, 248, 440, 645
- high resolution transmission electron micrographs (HRTEM) 645, 671
- high-temperature shift (HTS) reactor 493
- highest occupied molecular orbital (HOMO) 50, 120
- Hitachi Green Center 663
- Honda–Fujishima cell 624
- HRTEM micrographs for Cu/Pt/TiO_x-xh series
 - of catalyst 671
- hydrocarbon reforming 25
- hydrocarbons catalytic oxidation 45
- hydrocarbons oxidation 215
- hydrocracking 19, 20
- hydrodenitrification 20
- hydrodenitrogenation reactions 526
- hydrodeoxygenation 714, 716
- hydrodesulfurization 20, 44, 45
- hydrogen and fuel cell applications 680
- hydrogen economy 677

- hydrogenation reactions 507
 hydroxymethylfurfural ethers 694
- i**
 immobilized enzymes and cells 29–31
 immobilized metals 26, 27, 29
 immobilized organometallic compounds 27
in situ methods, catalyst study
 – categories 266
 – CO hydrogenation 270
 – combined X-ray absorption and X-ray diffraction 278, 280
 – gas-chromatographic procedures 271
 – heterogeneous catalysts 267
 – *in situ* X-ray, electron and neutron diffraction studies 275–278
 – infrared Raman, NMR, and x-ray absorption spectroscopy 273–275
 – isotopic labelling and transient response 269
 – mathematical analysis 272
 – methane synthesis 265
 – nickel- and platinum-catalysed methanation reaction 269
 – TAP to SSITKA 272, 273
 – temporal analysis 271
 – XAFS studies 268
in situ studies, XRD 181, 182
 incident photon to current conversion (IPCE) 626
 inductively coupled plasma mass spectrometry (ICPMS) 175, 177
 industrial chemical reactors 510
 industrial solid catalysts
 – heterogeneous catalysis 163
 – single-crystal model catalysts 164
 industrial-scale applications, immobilized biocatalysts 31
 industrial-style MoS₂ nanocatalysts
 – AC-TEM 363
 – two-dimensional S-Mo-S layers 363
 inelastic electron tunnelling spectroscopy (IETS) 238
 inelastic neutron scattering (INS) 257
 infrared spectroscopy (IR) 184–189, 225, 228
 interparticle (fluid-to-solid) transfer resistance 505
 IPCE, *see* incident photon to current conversion 626
 Ir₄ clusters 207, 209
 Ir(001), reconstructed surface 73
 iridium tin oxide (ITO) 666
 IrO₂ nanoclusters 665
 irreversible catalytic reactions 442, 443
- isobars, adsorption 80, 81, 108
 isobutene (2-methylpropylene) 387
 isopulegol epoxide production 707
 isothermal fixed-bed reactor 514, 519
 isotherms, adsorption 80, 82
 isotopic labelling 47, 48
 itaconic acid (IA) 714, 715
 IUPAC classification, adsorption isotherms 82
- k**
 Kaganer's isotherm 112, 113
 kinetic laws 503
 kinetic models 149, 151, 153
- l**
¹⁴C-labelling 47
 'lab-on-a-chip' concept 481
 Langmuir isotherm 82, 105–109
 Langmuir–Hinshelwood (LH) mechanism 37, 67, 68, 128–130, 132, 139
 lattice energy minimization techniques 53
 lattice gas model 75
 Lennard-Jones equation 114, 379
 levulinic acid (LA) 714, 715
 Lewis–Gray group 664
 lignocellulosic biomass 714
 limit cycle diagram 142–144
 liquid film interfacial concentration 526
 liquid-phase reactions 504
 local density approximation (LDA) 416
 local density functional (LDF) method 377
 longitudinal dispersion 514
 Lotka mechanism 134
 Lotka–Volterra model 134, 136
 low-energy electron diffraction (LEED) 38, 40, 71, 193–197, 232
- m**
 M1 phase 690
 MAFBR, *see* membrane-assisted fluidized bed reactors 497, 596
 magic-angle-spinning NMR (MASNMR) 177, 220
 magnetic resonance imaging (MRI) 165, 166, 216
 manufacture of methyl *t*-butyl ether (MTBE) 495
 Mars–van Krevelen mechanism 1, 46, 164, 344
 mass transfer
 – intraparticle diffusion 440–442
 – interparticle mass and heat transfer 448, 449

- non-isothermal conditions 445–447
- mass-transfer coefficient 527
- Maxwell–Boltzmann statistics 91
- MeALPO, *see* metal–aluminium–phosphate 368
- membrane-assisted fluidized bed reactors (MAFBR) 497, 596
- mesoporous silicas 370, 373, 423, 426
- mesostructured Y zeolite 701, 703, 704
- metal catalysts
 - advanced acetates by direct addition (AVADA) 364
 - Ag particles 345, 346
 - clay catalysts 365
 - Cu/ZnO/Al₂O₃ catalysts 347–349
 - hydrocarbons 364
 - inter lamellar chemistry 365
 - montmorillonite, beidellite and hectorite 364
 - oxomolybdenum catalyst anion 366
- metal gauze reactors 527
- metal–organic frameworks (MOFs) 244, 301, 303, 304, 675, 676
- metal-oxide catalysts
 - arbitrary unit cell 360
 - crystallographic structures 359
 - M1 type 360, 361
 - solid-state chemistry of complex 360
 - symmetry-breaking 359
 - Te-oxo groups 360
 - V₂O₃ (0001) 362
- metal-semiconductor junctions 403–406, 408
- metallic grid microstructured reactors 487
- metallo-enzymes 658
- METAPOCS program 383
- metathesis 413, 414
- methanol decomposition 148, 152
- methanol economy 682
- methanol synthesis 411, 412, 541–546
- methyl isocyanate (MIC) 54
- methyl *t*-butyl ether (MTBE) 72, 387, 593, 595, 596
- metropolis algorithm 381
- micro-channel reactors 481
- microalgae to bioethanol 718
- microalgae to diesel 717, 718
- microchannel reactors 485–489, 491
- microcrystalline catalysts 256, 257
- microcrystalline MeAPO-36 382
- microkinetics 147, 148, 152
- microstructured falling film reactor (μ -FFR) 490, 491
- microstructured reactors 485, 486
- microstructured string-reactor 487
- mixed-metal carbonylates 27
- Mn-doped aluminophosphate catalysts 424, 425, 427
- MOFs, *see* metal–organic-frameworks 303
- molecular beam technique 87, 88
- molecular dynamics (MD) methods 116, 117, 378
- molecular sieve catalysts 276
- Monte Carlo (MC) methods 75, 116, 117, 378
- Monte Carlo scheme 381
- MTBE, *see* methyl *t*-butyl ether 593
- multifunctional catalysis 41
- multifunctional reactors 480, 492–499

- n**
- Nafion® 9
- nanogold
 - adsorption energies and geometries 357
 - Au(111) and Pt(111) surfaces, H₂ molecule 354
 - Au-CO and Au-O bonds 355
 - binding energy, CO and O 357, 358
 - *in situ* conditions 355, 356
 - carbon monoxide 354
 - catalytic activity 356
 - density functional theory 355
 - ethanol, aqueous-phase oxidation 353
 - Fe₂O₃ and NiO 353
 - H₂-D₂ exchange reaction 356
 - Langmuir–Hinshelwood (LH) mechanism 355
 - nanoglobules 353
 - O₂ adsorbate on metal surfaces 357
- nanoporous catalysts 370–373, 375, 376
- nanoporous solids 343
- nanorod catalysts 658
- near-edge X-ray absorption fine structure (NEXAFS) 211, 213
- Nernst theory 36
- neutron scattering 252, 254–258
- nicotine, chromic acid oxidation 721
- Nocera’s artificial leaf 661
- non-dissociative adsorption 91, 105
- non-dissociative and associative adsorption 106–109
- non-enzymatic catalytic processing 655, 711, 712, 714, 716
- non-invasive methods, catalytic reactors
 - MRI 165, 167, 168
 - positron emission methods 170

- non-invasive methods, catalytic reactors
(continued)
 - spatially-resolved x-ray absorption 170–172
- non-invasive/*in situ* study, solid catalysts 1, 4
- non-isothermal catalytic reactors 520, 531
- non-reactive ‘cage’ 49, 51
- nuclear magnetic resonance (NMR) 216–222, 224, 225
- nylon 6, 697
- o**
- 1-octanol retrosynthetic analysis 716
- O₂-evolving catalysts (OEC) 661
- O–Si–O bonds 379
- olefin metathesis 411, 412
- oligomerization of lower olefins 19
- optical microscopy 250, 251, 254
- optimization procedures 381
- ordered adlayers 74–79
- ordered and reconstructed surfaces
 - bond distances 199
 - EXAFS 200–204, 206, 207, 209
 - LEED 193
 - NEXAFS 211, 212, 214
 - notations 198, 199
 - SEXAFS 209, 210
 - TPD 193
 - two- and three-dimensional surface crystallography 193, 194, 196, 197
 - XANES 210, 211
- oscillatory reactions 133–136
- oxidative dehydrogenation 22
- p**
- Péclet number 514, 516
- paraffin alkylation 19
- parametric sensitivity 532
- Pareto-optimal catalysts 104
- Patterson function 181
- periodic mesoporous organosilanes (PMO) 373, 375
- peripheral carbide clusters 49, 51
- perovskite-based oxide catalysts 430
- petroleum industry
 - atmospheric distillation column products 630
 - catalytic cracking 633, 635–640
 - catalytic reforming 631–633
 - commodity products 630
 - gas oil 630
 - hydrotreating 640–642, 644, 645
- lube oils and asphalt 631
- refinery production 629
- petroleum reforming reactions 444
- petroleum-derived jet fuel 709
- photo-electrochemical cells 431
- photo-emission electron microscopy (PEEM) 146, 147
- photoanodes 624–626, 662–664
- photocatalysts 655, 663, 667–669, 672, 673, 678
- photocatalytic decomposition 669, 678
- photocatalytic systems 667, 676
- photocatalytic water splitting 668
- photocorrosion 667
- photoelectrochemical (PEC)
 - splitting of water 674
 - hydrogen 664
- photoelectrochemistry 25, 26
- photoelectrolysis 25
- photosynthesis 25, 618, 657
- photosystem II (PSII) 615, 617, 666
- physically adsorbed species 114–117
- platinum
 - γ-Al₂O₃ 350
 - defect 349
 - hydrogen 350–352
 - MASNMR measurements 350
 - monoatomic Pt functions 350
 - reducible oxides 349
- platinum-group metals (PMG) catalysts 682
- plug and play’ process technology 480
- PMO, *see* periodic mesoporous organosilanes 373
- poisoned catalyst 457, 458
- poisoning and promotion 463
 - adatom electronegativity 470
 - adsorption complexes 464
 - butadiene, selective hydrogenation 463
 - catalytic hydrogenation 468
 - cis-2-butene, hydrogenation reaction rate 474
 - CO–metal interaction 468
 - factors responsible 471, 472
 - homogeneous catalysis 464
 - molecular adsorption and catalytic activity 466
 - Monte Carlo approach 463
 - *n*-alkanes, catalysed conversion 466
 - occupied and unoccupied spin orbitals 469
 - orbital contours 467, 470
 - Pt–Re alloy catalyst 467
 - sub-surface hydrogen 473

- sulfided catalyst 464
 - surface carbon and sub-surface hydrogen 473
 - poisoning of catalysts 16, 44
 - Polanyi's adsorption theory 110–112
 - Polanyi–Wigner equation 96
 - poly(ethylene furanoate) (PEF) 694
 - poly(ethylene terephthalate) (PET) 692, 694–696
 - poly-generation 481, 482
 - polymerization of alkenes 22
 - polyoxometalates 669
 - Porod's law 180
 - porous catalysts 344, 345
 - acid-catalysed hydration 339
 - advantages 301
 - aluminophosphates and comparable solids 293
 - Bessel functions 322
 - BET method 296
 - capillary condensation 294
 - catalyst material 294
 - catalytic gas reaction, packed tubular reactor 332–334
 - CO₂ removal 340
 - concentration gradient 319
 - cracking reactions 314
 - cylindrical catalyst pellet 322, 324
 - density functional theory 302, 303
 - diffusion coefficient 315
 - effective diffusivity measurement 315
 - experimental criterion, diffusion control 331
 - fractal approach 304
 - gas adsorption and permeation 295
 - geometric model 319
 - Hegedus' and Petersen's single catalyst pellet reactor 336
 - heterogeneous catalytic reaction 319, 339, 340
 - homogeneous media 315
 - hysteresis loops 294
 - internal pore surface area 319
 - intraparticle diffusion 319, 326–328
 - isotherm reconstruction methods 300
 - isothermal spherical pellet 340
 - Kelvin Equation and
 - Barrett–Joyner–Halenda method 300
 - kernel 301
 - kinetic diameter 296
 - Knudsen diffusion 317, 318, 339
 - krypton adsorption 337, 338
 - Maxwellian diffusion 316, 317
 - mercury porosimetry 306–308, 338
 - MOF nanoporous structure 293, 303
 - molecular/bulk diffusion 316, 317
 - non-local density functional theory 301
 - nonuniform cross-section 314
 - pore geometry 301
 - pore models 338
 - porosity 298, 299
 - practical considerations 305, 306
 - preparations 295
 - probe molecules 296
 - reaction rate 295
 - resistance to diffusion with pellet 321
 - scattering and diffraction methods 296
 - slab-shaped catalyst pellet 336
 - spherical catalyst pellet 323–326
 - surface area measurement 295
 - surface diffusion 314
 - Thiele modulus 321, 323
 - transition region of diffusion 318
 - transport mechanism 314
 - wafer/slab-shaped catalyst pellet 320
 - Wheeler's semi-empirical pore model, *see* Wheeler's semi-empirical pore model 308
 - positron-emission profiling (PEP) 170
 - positron-emission tomography (PET) 170
 - potential-energy diagrams 37 69, 70, 89, 90
 - precursor states 67–71, 99–101, 130, 131
 - precursor-mediated desorption process 100
 - 'probe' molecule dimensions, as adsorbates 173
 - probing surfaces
 - electron spectroscopy merits and limitations 190
 - HREELS 189
 - infrared spectroscopy (IR) 184–189
 - process intensification 479, 480
 - propylene 6, 11, 15, 19, 22, 46–48
 - proton-conducting membrane 664
 - proton-induced x-ray emission (PIXE) 175, 176
 - PROX (preferential oxidation) 676
 - PSII, *see* photosystem II (PSII) 615
 - PtOH_x species 352
 - PV-driven electrolysis 661
 - pyrolysis gas hydrogenation 488
- q**
- quantum chemical approaches 407
 - quantum mechanical cluster 378
 - quantum molecular dynamics methods 388

r

Raman spectroscopy 225, 254, 259, 273, 274
 Raschig process 698
 rates of adsorption 88–91
 reactor design, catalytic process engineering 479–482
 recycle reactors 506
 redox reaction 665
 renewable chemicals preparation 711
 renewable sources of energy 656
 renewable-jet fuel 709, 710
 Reppe IG Farben/BASF 687
 residence times 87, 88
 reverse flow catalytic membrane reactors (RFCMR) 496, 596
 reverse Monte Carlo technique 381
 Reynolds numbers 510, 513, 514
 RFCMR *see* reverse flow catalytic membrane reactors
 ribozymes 31, 32
 Rideal–Eley mechanism 37
 Rietveld neutron powder profile procedure 256
 ring-opening metathesis polymerization (ROMP) 413
 RiveTM mesoporous zeolite-Y 704
 the Russian ADAM–EVA cycle 58, 59

s

Sachtler–Fahrenfort plot 36
 scanning transmission electron microscopy (STEM) 244
 scanning tunnelling microscopy (STM) 4, 127, 229–240
 scanning tunnelling spectroscopy (STS) 238
 Schottky barrier theory 403–406, 408
 Schultz–Flory chain-length statistics 549
 selected-area Fourier diffractogram (SAFD) 245
 selective oxidation 16, 18, 19, 22, 28
 selective oxidation catalysts 46
 selectivity of catalysts 14–16
 self-cooled tubular reactors 521, 529
 semiconductor (SC)/liquid junctions 660
 semiconductor catalyst microcapsule 25, 26
 serial femtosecond crystallography (SFX) 275, 276
 Shell middle distillate synthesis (SMDS) 559, 636
 silicalite 431
 silicon-based T-shaped microreactor 488
 silicon-glass microreactor 488, 491
 single-site heterogeneous catalysts (SSHCs) 4, 125, 343, 700, 720–722

slurry reactors 507, 509
 Slygin–Frumkin isotherm 110
 small-angle scattering (SAXS) 179–181, 256
 SMDS, *see* Shell middle distillate synthesis (SMDS) 636
 solar energy
 – arctic ocean acts 615
 – artificial photosynthesis 615–618
 – curtail/eliminate emission 614
 – D₂¹⁸O 624
 – fuel cell 615
 – generation of H₂ and O₂ 618
 – genuine photocatalytic methods 615
 – Grätzel cell and influence 626, 627
 – Honda–Fujishima cell 624
 – hydrogen and oxygen by catalysed photolysis 621–623
 – hydrogen generation by photo-induced reduction 620, 621
 – light-induced water-splitting reactions 619
 – oxygen generation by photo-induced oxidation 619, 620
 – photoanode and platinum 624
 – photocatalytic processes 626
 – photodissociation of water 625
 – photoelectrosynthethis 625
 – photosynthesis 618
 – platinized TiO₂ 625
 – practical objectives 614
 – splitting water 615
 – SrTiO₃ 625
 – storable forms 614
 – tandem cells 628, 629
 – UV-laser excitation 625
 solar energy conversion 660
 solar fuel cell 658, 659, 662–664
 solar-driven catalytic reaction 658
 solar-fuel plants 659
 solid acid catalysts 11, 18
 Solid Fuel Centre for Chemical Innovation 658
 spatial variation, fixed-bed reactor 166, 167, 169
 spatially-resolved x-ray absorption 170, 172
 spatio-temporal behaviour and turbulence 145, 146, 149
 spin–echo double resonance (SEDR) 224
 spinning-basket catalytic reactor 505
 SSHCs *see* single-site heterogeneous catalysts 343
 statistical mechanics, adsorption 91, 92
 steady-state isotopic transient kinetic analysis (SSITKA) 272

- steam reforming
 - catalysts 687
 - of methane 15
 - reaction 426, 428
- steam–hydrocarbon reaction 21
- ‘structure-insensitive’ catalytic reaction 41
- ‘structure-sensitive’ catalytic reaction 41
- sum frequency generation (SFG) 225–228
- surface bonds strength determination 259
 - FDS 260
 - magnitude of heat and entropy of adsorption 263
 - TPD 260
 - TPRS 262
- surface crystallographic studies with EXAFS (SEXAFS) 200, 209, 210, 225
- surface defects 382
- surface electronic states 402, 403
- surface segregation 384
- surface-derivatized catalysts 207, 209
- sustainable methanol 683
- synthesis gas (syn-gas) 11, 15, 16, 18, 21, 64
 - ammonia synthesis 564
 - ATR 545
 - CO 544
 - CO/H₂ mixtures 547
 - Fischer–Tropsch synthesis 547, 548
 - methane production 559
 - methanol 541, 544
 - natural gas 545
 - purification 558
- synthetic cordierite (Mg₂Al₄Si₅O₁₈) 24
- synthetic zeolite catalysts 19

- t**
- Tanaka–Tamaru plot 36
- tandem cells 628, 629
- TAPO-5 700
- technological challenges 60
- Temkin isotherm 82, 110
- Temkin–Pyzhev description 93
- temperature-programmed desorption (TPD) 193
- temperature-programmed reaction
 - spectroscopy (TPRS) 262
- terephthalic acid 697
- thermal and mechanical stability 24
- thermal hysteresis 140–142
- thermal instabilities 138
- thermochemical cycles 59
- thermochemical reactions 724–726
- ‘tinderbox’ 16, 17
- thermophilic cyanobacterium 666
- thin films of TiO₂ 670

- thiophene (C₄H₄S) 233
- three-way catalyst (TWC) 603, 604
- Ti^{IV} ions 423, 425, 426
- time-resolved X-ray diffraction 277
- TiO₂-based photo-responsive solids 676
- TiO₄ species 678
- traditional methods, catalyst characterization 173
- transient phenomena 139, 141–144
- transition metals 389
 - band widths, DOS and Fermi levels 408, 409
 - CO chemisorption 410, 411
 - transition states (TS) 101, 154
 - transition-metal chalcogenides 44
- transmission EM (TEM) 241, 242
- trickle-bed reactors 482, 483, 488, 490, 525
- triglycerides transesterification 11
- tubular reactors 501, 502, 504
- turnover frequency (TOF) 33, 34, 665

- u**
- ultraviolet-visible and photoluminescence spectroscopy
 - adsorption of light 191
 - electronic transitions UV-vis-NIR 191
 - photoluminescent spectrum 191, 193
 - sensitive detectors 192
- uniform heterogeneous catalysts 124
- UV-vis spectra of TiO₂ thin films 672

- v**
- van der Waals adsorption 68
- van der Waals interactions 37, 389
- vibrational activation 90
- virial equation of state 82, 112, 113
- volcano plots 35, 36, 45, 46

- w**
- Wacker process 15
- wall-to-bed heat-transfer 522
- water gas shift (WGS) reactives 565
- water oxidation 666
- water oxidation photocatalysis 669
- water splitting 670
- Wheeler’s semi-empirical pore model
 - BET surface area 308
 - bidisperse systems 311
 - catalyst particle 309
 - dusty gas model 310
 - macro- and micro-voidages 311
 - pellet porosity 309
 - pore volume 309

- Wheeler's semi-empirical pore model (*continued*)
 - pore walls 309
 - porous media 308
 - statistical network theory 311
 - stochastic pore networks and fractals 311–313
 - work function 119
- x**
 - X-ray absorption near-edge spectroscopy (XANES) 170, 200, 210, 211
 - X-ray absorption spectroscopy 661
 - X-ray diffraction (XRD) 177–179, 181, 183, 184
 - X-ray emission (XRE) 175, 176
 - X-ray fluorescence (XRF) 175, 176
 - X-ray photoelectron spectra (XPS) 94
 - X-ray-induced photoelectron spectroscopy (XPS) 177, 191
 - xenon, adsorption 116
- z**
 - Z-scheme 667
 - ZeoFile anthology 431
- zeolites 80, 81, 83, 85, 110, 115, 117
 - zeolite framework crystal structures 431
 - zeolitic solid catalysts
 - aluminosilicates 366
 - Brønsted acid centres 366
 - Cambridge–Tübingen–London (CTL) team 368
 - framework density (FD) 369, 370
 - H-bonded H_3O^+ ions 367
 - metal–aluminium–phosphate (MeALPO) 368
 - microporous aluminosilicate catalysts 365
 - molecular sieves 366
 - petrochemicals production 365
 - probe molecules and intracrystalline cavities 367
 - siliceous ZSM-5 366
 - three-dimensional (3D) open-structure solids 368
 - three-dimensional (3D) surfaces 366
 - zero-field NMR 224
 - zero-point energy 92, 98
 - Ziegler–Natta catalyst 23
 - Ziegler–Natta conversions 23
 - ZSM-5 zeolites 708

