

Index

a

ab initio methodology 205, 461, 471
 activated carbons (AC)
 – micropores 333
 – thermo/electro-conductivity 333
 active pharmaceutical ingredients (APIs) 283
 adsorption sites, on crystal terraces 4
 agglomeration 137, 155, 176, 209, 216, 219, 231, 234, 255, 273, 379
 AgNPs, *see* silver nanoparticles (AgNPs)
 Ag-PVA film, reuse cycle 313
 alkali clusters, electronic properties 444
 alkali M_n clusters 445
 alkyl/arylphosphines 17
 alkylated polyethylenimine (PEI)
 – as protective agent 79
 – of palladium(0) NPs 79
 – Pd(0) NPs protection 79
 allyl alcohol 68, 82, 227, 231
 alumina 8, 19, 139, 204, 331, 436
 ammonia 285, 349
 – catalytic performance, correlations 351
 – decomposition 350–352, 434
 – synthesis of
 – B₅ step sites, necessary for N₂
 activation 462
 – confinement effects 429, 448
 – enhancement 429
 – Haber–Bosch process 350
 – rate-determining step of 462
 ammonium
 – derivatives, and predicted aggregate 61
 – surfactants, used as protective agents 60
 anatase (TiO₂) 377
 aqueous Knoevenagel condensation
 reaction 214
 Arrhenius plots, for rate of CO oxidation over
 Co₃O₄ 386
 artificial photosynthesis 36

asymmetric aldol reaction 389
 asymmetric Henry and Michael
 reactions 389
 – mechanism for 383
 atomic coordination reduction 6
 atomic emission spectroscopy (AES) 1
 atomic trapping potential 6
 Au/CeO₂ catalyst 401
 Au₂₄₆ cluster model 466
 Auger electron spectroscopy (AES) 157
 AuNPs, *see* gold nanoparticles (AuNPs)
 Au₅₅(PPh₃)₃C₁₆ isomers, optimized
 structures 464
 Au₅₅(PPh₃)₃(PH₃)₉C₁₆ model 463
 Au-supported CeO₂ nanoparticles 400

b

benzyl alcohol
 – aerobic oxidation 416
 – oxidation reaction 348, 382
 – microwave-assisted selective 394
 benzylic epoxides 65
 bimetallic catalysts 22, 168, 349
 bimetallic nanocrystals 17
 bimetallic systems 154
 – geometric and electronic structure
 168–173
 biphasic systems 56, 76, 88, 252, 314
 bis(cyclopentadienyl) iron (FeCp₂) 424
 bismuth oxyiodine (BiOI) 211
 block-copolymers 16
 bond formation, at transition-metal
 surface 453
 Bragg angle 160
p-bromoacetophenone 112, 224
 Brønsted–Evans–Polanyi (BEP) relations 455
 Brønsted hydroxyls 383
 Brunauer–Emmett–Teller (BET) surface
 areas 384

- 1-butyl-3-methylimidazolium hexafluorophosphate 203, 255
- 1-butyl-3-methylimidazolium tetrafluoroborate 255

C

- capillary effect 343
- capping agents 15, 16, 18, 20, 60, 125, 141, 164
 - dynamic organizations around NPs 73
- carbonaceous materials 356–360
- carbon–carbon cross-coupling reactions 346, 357
- carbon dioxide (CO₂) 124, 165, 284, 397
 - conversion, to isopropanol and other alcohols/hydrocarbons 435
 - CO₂-removal technology cells 350
 - energetic for CO₂ formation 437
 - gas-phase photoelectrocatalytic conversion 435
 - hydrogenation 150
 - monitoring 34
 - supercritical 104
- carbon materials, beneficial effects 36
- carbon monoxide (CO)
 - adsorption energies 459
 - detection 31
 - disproportionation 467
 - dissociation 466
 - molecular density 420
 - oxidation 5, 382
 - poisons 182
 - reactivity, at surface of small ruthenium NPs 18
- carbon nanofibers (CNFs) 12, 15, 113, 129, 269, 358–360
- carbon nanoparticles 12–14
 - arrangement 26
- carbon nanostructures 14, 15, 26
- carbon nanotubes (CNTs) 12, 19, 416
 - adsorption 419–421
 - advantage 333, 338
 - anchoring pre-formed nanoparticles 341, 342
 - application 334
 - carbonaceous structures 356–361
 - channels 430
 - CNF/graphene supported catalysts
 - catalytic reactions 361
 - confined PtRu catalyst 431
 - confinement effect (*see* confinement effects)
 - covalent functionalization 336
 - diffusion 421–423
 - durability 352
 - electrocatalysis 352–354
 - electron transport 355
 - encapsulated Eu nanowires 419
 - functionalization 335–339
 - by deprotonation-carbometalation 337
 - by gas-phase reactions 338, 339
 - schematic illustration 336
 - by wet chemical methods 336–338
 - gas-phase reactions 349–352
 - ammonia decomposition 350–352
 - catalytic reactions 432–435
 - Fischer–Tropsch synthesis 349, 350
 - graphene layers, interaction 423–428
 - herringbone 360, 394, 416
 - IL-coated 269
 - iron catalyst confined 433
 - Fischer–Tropsch synthesis activity 433
 - iron oxide nanoparticles 426
 - liquid-phase reactions 346–349
 - catalytic reactions 430–432
 - hydrogenation 346–348
 - oxidation 348, 349
 - localization, catalyst particles supported 345, 346
 - longitudinal cross section 343
 - metal catalyst-free chemical reactions 428–430
 - metal catalysts, selective place 343, 344
 - impregnation and selective washing 344
 - molecular recognition 344
 - two step biphasic impregnation 343, 344
 - metal-containing species synthesis 341
 - metallic nanoparticles selectively confined in inner cavity of 22
 - metal (Pt) particles, preparation 340
 - multiwalled carbon nanotubes (MWCNTs) 36, 228–231, 333, 336, 337, 353, 354, 416, 418, 431, 433, 435
 - as nanosupport 333, 334
 - noncovalent functionalization 337
 - oxidative treatment 336
 - oxide nanoparticles supported on 394, 395
 - photocatalysis 354–356
 - preparation of highly dispersed cobalt catalysts 175
 - purification 334, 335
 - quantitative description 361
 - Ru/CNTs-out 434
 - selective preparation of catalysts 342–344
 - spatial restriction 417–419
 - supported catalysts 229, 340
 - applications 346–356
 - preparation 340–346
 - surface

- chemistry 349
- growing metal nanoparticles 340, 341
- properties 352
- titania composite materials based on MWCNTs 36
- types 341
- use 355
- catalytic applications, metallic nanoparticles 213
- bloc p 213
- early transition metals and bloc f metals 213, 214
- group 10
- carbon-carbon bond formation processes 223-227
- hydrogenation processes 227, 228
- nickel nanocatalysts 222
- palladium nanoparticles 223, 228, 229
- platinum nanocatalysts 229-231
- group 11
- copper nanoparticles 232, 233
- gold nanoparticles 233, 234
- zinc and cadmium nanoparticles 235
- groups 8, 9, 214
- cobalt nanoparticles (Co NPs) 218, 219
- iron nanoparticles 214, 215
- rhodium and iridium nanoparticles 219-222
- ruthenium nanoparticles 215-218
- C-C coupling reactions 5, 39, 57, 78
- catalysis by Pd DENs 104
- CDs, *see* cyclodextrins (CDs)
- centrifugation process 317, 318
- limitations 318
- CeO₂ nanorods 387
- Ce_{1-x}Cu_xO₂ nanocomposite catalysts 390
- Ce_{1-x}Zr_xO₂ systems 381
- charcoal 8
- charge transfer (CT) process 454
- chemical vapor deposition (CVD) 334, 335, 338, 339, 353, 358, 467
- 4-chloropropiophenone 316
- (-)-cinchonidine 65
- cinnamaldehyde (CALD) 346, 347
- Claisen-Schmidt condensation 389
- 'click'-ferrocenyl dendrimer-encapsulated PdNPs 108
- CNFs, *see* carbon nanofibers (CNFs)
- cobalt nano-objects 17
- cobalt nanoparticles (Co NPs) 129, 164, 176, 218, 219
- Co/CNF catalysts, performance 359
- colloids 2, 3
- chemistry 9
- metal 124, 141
- confinement effects 350, 352, 380
- in carbon nanotubes 416
- adsorption 419-421
- 'bamboo-like' morphology 416
- diffusion 421-423
- gas-phase catalytic reactions 432-435
- graphene layers, interaction 423-428
- liquid-phase catalytic reactions 430-432
- metal catalyst-free chemical reactions 428-430
- spatial restriction 417-419
- in nanosupports 415
- zeolite pores 415
- Co₃O₄ nanoparticles 386, 391, 400
- copper ceria doped nanoparticles 384
- copper nanoparticles (CuNPs) 207, 232, 233, 263, 292, 293
- COS hydrodesulfurization 386
- CO_x-free hydrogen 350
- cross-coupling reaction 74
- crystal binding intensity 6
- crystal face 4
- cubooctahedron 450
- CuNPs, *see* copper nanoparticles (CuNPs)
- Cu₂O-dominated nanowires 385
- CuO nanoparticles 435
- CVD, *see* chemical vapor deposition (CVD)
- cyclic voltammetry 107
- cyclodextrins (CDs) 55
- capped palladium(0) NPs 73
- carbon-carbon coupling reactions 73-77
- CD-capped nanocatalysts 67
- hydrogenation reactions 68-73
- perthiolated, as protective agents 73
- steric stabilization by 67
- used as protective agents, of metallic nanospecies 69
- cyclohexanol 21
- cyclohexanone 21
- d**
- d*-band model, *see* heterogeneous catalysis, electronic structure effect
- Debye-Waller factor 159
- dendrimer-encapsulated nanoparticles (DENs) 98
- characterization methods 99
- evidence for encapsulation 99
- generation from dendrimers, metal salts 98
- synthesis 98-102
- dendrimer-NP assemblies 102
- dendrimers 16, 22, 77, 82, 83, 97, 100, 102, 106, 141, 313

- dendrimer-stabilized metallic nanoparticles (DSNs) 98
- DENs, *see* dendrimer-encapsulated nanoparticles (DENs)
- density functional theory (DFT) methods 38, 209, 426, 443, 446
 - calculations 455
 - GGA calculations 463
 - modeling 451
 - optimization strategy 463
 - optimized Ru NP 450
 - Ru₅₅ cluster 458
- density of states (DOS) 161, 457
- designed nanocatalysts 123
- differential scanning calorimetry (DSC) 203
- diffusion ordered spectroscopy (DOSY) 208, 217
- 4-di(hydroxyethyl) aminobutyl tributylammonium bromide 224
- diisopropoxititanium bis(acetylacetonate) (DIPBAT) 291
- N,N*-dimethylacetamide 323
- N,N*-dimethylformamide 315, 323
- 2,2'-dipyridylamine 228
- direct methanol fuel cells 360
- dissociation
 - carbon monoxide 466–468
 - methane steam reforming 468, 469
- 3,3'-disulfanylbis(hexane-1,6-diyl)-bis(1-methylimidazol-3-ium) dichloride 206
- DLVO theory 206, 207, 211
- dodecanoic acid 103
- double-walled carbon nanotubes (DWCNTs) 416
- d*-type transition metals 7
- e**
 - (eco)toxicity 31
 - electrocatalysis 113, 352–354
 - electrodischarge machining (EDM) 299
 - electron levels 8
 - electron–phonon coupling 6
 - electron transport, through nanostructured TiO₂ particles 355
 - electrosteric stabilization
 - of nanospecies in neat water 65
 - by surfactants 59, 60
 - Eley–Rideal mechanism 464
 - enantioselective catalysis 16, 38–40
 - enzyme-like polymer folding 21
 - epoxidation 234
 - catalytic efficiency 394
 - ethylene epoxidation 456
 - olefins 389
 - propylene 124, 431
 - styrene
 - and alkenes 265
 - and cyclooctene 389
 - with H₂O₂ as oxidant 266
 - imidazolium ionic liquid for 234
 - task specific imidazolium ionic liquid 234
 - extended Hückel theory (EHT) 443
 - extended X-ray absorption fine structure (EXAFS) 157–159, 380
 - spectra 160
- f**
 - fcc crystal faces 4
 - Fenton-like reaction 390
 - Fe₂O₃ nanoparticles
 - agreement 427
 - in cyclohexane oxidation 389
 - Fe–Al effect 394
 - hydroxyapatite-encapsulated 214
 - porous structure 396
 - reduction 433
 - size-induced structural distortions 10
 - stabilized in 209
 - temperature-programmed desorption profiles 427
 - Fe₂O₃/ZrO₂ catalyst 400
 - ferromagnetism 7
 - filtration 322–324
 - Fischer–Tropsch (FT) reaction 78, 161, 349, 350, 432, 433, 447, 466
 - Ru catalysts on 350
 - fishbone nanofibers 359
 - fluorescence XAFS spectra 160, 161
 - Fourier-transform infrared (FTIR) analysis 210, 415
 - free energy 10, 210, 461
 - Friedel–Crafts reactions 392
 - acylation reaction 235
 - fuel cells 25–28
 - electrocatalysis 26
 - fuel oxidation reaction (FOR) 352
- g**
 - gas-phase reactions 338, 339, 349–352
 - advantage 338
 - ammonia decomposition 350–352
 - Fischer–Tropsch synthesis 349, 350
 - gas-sensors 31–34
 - based on semiconducting materials 33
 - electrochemical 31
 - G1-3 dihydroxybenzylalcohol-based dendrimers 104
 - geometric structure, of nanoparticles 154

- Gibbs free energy 463
- gold
- nanoclusters, *see* gold nanoparticles (AuNPs)
 - structures 452
- gold–ceria catalysts 401
- gold nanoparticles (AuNPs) 100, 106, 111, 204, 206, 207, 209, 227, 233, 234, 266, 268, 318, 320, 400, 401
- electrocatalytic activity 234
 - in epoxidation reactions 265
 - functionalized with iron(II) terpyridine complexes 215
 - model 466
 - stabilized by a water soluble functionalized phosphine 84
 - TEM images 356
- G2 polypropylene imine (PPI) dendrimers 100
- gradient corrected approximation (GGA) 456
- graphene 356–358
- based supported catalysts 357
 - oxides 356–358
 - walls, electron transfer 435
- graphene–TiO₂ composites 358
- green chemistry 56, 77
- h**
- Haber–Bosch process 350
- halogenoalkanes 60
- HDS, *see* hydrodesulfurization (HDS)
- Heck and Suzuki coupling reactions 80, 141
- Heck–Mizoroki reactions
- of aryl chlorides 224, 225
 - sulfonyl derivatives with alkenes 225
 - task-specific ionic liquid in 225
- Heck reactions 66, 67, 75, 76, 141
- aryl iodides and olefins 66
 - b/w iodobenzene 104, 288
 - b/w *n*-butyl acrylate 104
 - copper bronze catalyzed 232
 - of olefins with aryl halides 359
 - promoted by ultrasonic aqueous media 67
 - structure sensitivity 142
 - of *trans*-cinnamates in TBAB as solvent 224
- heterobimetallic nanoparticles 101, 104
- methods of synthesis 101
 - transition-metal nanoparticles 98
- heterogeneous catalysis 1, 3, 8, 15, 23, 41, 89, 111, 112, 389, 395
- electronic structure effect 452
- heterogeneous catalysts 28, 38, 78, 114, 125, 216, 251
- metal oxide nanoparticles as 381
 - problems encountered with 314
 - Rh/C catalyst 221
 - robust 396
 - *in situ* studies 161
- hexadecylamine 60
- hexafluorophosphate anion 204
- hexagonal mesoporous silica 394
- high-angle annular-dark field (HAADF) electron microscopy image 417
- Hoffmann's approach 454
- 'homeopathic' catalysis 108
- homogeneous catalysis 2, 39, 41, 84, 97, 314
- with DENs generated from dendrimers 102
- homogeneous catalysts 2, 16, 19, 39, 55, 56
- Ir-based 221
 - recycling of 19
- H₂O₂ pathway 466
- [HRh(CO)(PPh₃)₃] complex 430
- HRTEM image, two atom thick KI crystal 418
- hydrocinnamaldehyde (HCALD) 228, 346
- hydrodechlorination 106
- of chlorobenzene derivatives 64
- hydrodesulfurization (HDS) 289, 386, 387
- activity bulk catalyst 290
 - Co₃O₄ crystals with nanorods and nanopolyhedral morphology for 387
 - of sulfur compounds 302, 387
- hydrogenation 18, 57, 346–348
- acetophenone 87
 - alkene 19
 - allylic alcohol 69
 - arenes 220
 - aromatic ketones, asymmetric 217
 - benzene 63, 83
 - derivatives 72
 - biphasic 219
 - buta-1,3-diene 359
 - 1,3-butadiene 227
 - carbon monoxide 78
 - cinnamaldehyde (CALD) 346
 - citral and cinnamaldehyde 254
 - cyclohexene 218, 269, 315, 324
 - 1,3-cyclooctadiene 105
 - ethyl pyruvate 18
 - isophorone 70
 - methyl-9-octadecenoate 347
 - 2-methyl-2-pentenal 347
 - monosubstituted arene compounds 71
 - nickel nanocatalysts, process 222
 - nitroarene 102–104
 - nitrobenzene derivatives 228
 - 4-nitrophenol 112
 - olefin 81, 102–104, 215
 - within microreactor 80

- phenylacetylene 312
- propyne, heterogeneous 257
- selective, dienes to monoenes 107
- styrene 88
- toluene 359
- transition metal catalysts 4
- turnover numbers (TON)s 107
- hydrogen bonds 39, 203–205, 209, 210, 263, 285, 335, 383
- hydrogenolysis
 - asymmetric, ethylpyruvate 64, 65
 - styrene oxide 66
- hydrophobic-hydrophobic interactions 71
- 2-hydroxypropyl- α -cyclodextrin (α -HPCD) 74

i

- ILs, *see* ionic liquids (ILs)
- imidazolium rings 205, 212
- imidazolium sulfonate 84
- immobilization
 - functionalized MWCNTs 229
 - metallic nanoparticles
 - functionalized polymers 225
 - in ILs 223
 - molecular catalysts on nanostructured electrode surfaces 37
 - palladium catalysts applied in 215
 - peroxidases 260
 - Pt onto surfaces for electrocatalysis 113
 - on solid support 311–314
 - strategies to immobilize NPs on support 312
 - surface-grafted Au G2 PPI DSNs onto 112
- indium oxide nanoparticles, XRD pattern 378
- inelastic scattering 159
- infrared reflection absorption spectroscopy (IRAS) 207
- infrared (IR) spectroscopy 419
- in silico* nanocatalysis
 - multistep pathways, theoretical studies of
 - ammonia synthesis 462–463
 - dissociation 466–469
 - methods 460–462
 - oxidation 463–466
 - with transition metal particles 443
- in situ* HP ^{129}Xe MAS NMR spectra 422
- in situ* x-ray absorption spectroscopy 161
- intramolecular interactions 21
- intrinsic properties, of nanomaterials on catalysis 5–7
- ion diffusion coefficient 423
- ionic liquids (ILs) 65, 102, 131
 - act as reducing agents 204
 - compete with CO for 264

- effect on structures 210
- metallic nanoparticles, interactions with 204, 205
- nanoparticle catalysis with supported 254
- stabilization modes for 206
- supported ionic liquid phase (SILP) concept 252
- support interaction, on catalytic activity 203
- as surface modifier 253
- synthesis of nanoparticles
 - applied in cross-coupling reactions 316
- iridium nanoparticles (Ir NPs) 219
- iron nanoparticles (FeNPs) 212, 214, 432
- N-isopropyl acrylamide 82

j

- jellium approach 444

k

- K β emission spectroscopy 180
- normalized K β 1,3 emission spectrum of Co-foil and CoO 182
- KI crystal, HRTEM image of 418
- kinetically-controlled SFCD process (K-SFCD) 292, 293
- kinetic energy 14, 158
- Knudsen diffusion mechanism 421, 423
- Kohn–Sham orbitals 456

l

- laser ablation 299
- leaching 63, 104, 109, 110, 131, 231, 255, 273, 346
- Le Chatelier's principle 420
- ligands 16
 - poly-N-donor ligands 220
 - as stabilizing agents 449
 - steric stabilization by 83–88
 - synthesis of ligand-free PdNPs 223
- liquid-phase reactions 346–349
- liquid/solid interface energy 344
- localization 41, 102, 352
- catalyst particles supported on CNTs 345, 346
- iron 435
- N $_2$ 421
- low energy electron diffraction (LEED) 1

m

- Mackay transformation 451
- magnetite 377
- magic angle spinning (MAS) NMR spectra 422
- magic numbers 444

- magnetically recoverable nanocatalysts 402
 - magnetic memory 19
 - magnetic nanoparticles 402
 - magnetic separation, of nanoparticles 320, 321
 - magnetite-immobilized nano-Ru catalysts 396
 - MCM-41 silica, iron oxide supported on 394
 - Meerwein-Ponndorf-Verley reduction 389
 - mesoporous carbon 360
 - mesostructured SBA-15 material 392
 - metal-carbon interaction 352
 - metallic nanoparticles (MNPs) 6–9, 17, 19, 22, 30, 37, 59, 98, 124, 128, 132, 154, 161, 173, 340, 341
 - catalytic applications 213
 - effect of ionic liquids on structures 210
 - immobilization 225
 - interaction with ILs 204
 - ionized at surface 205
 - specific interaction, with coatings and supports 173–178
 - metallic surfaces 73, 206
 - cation-metallic surface interaction 208
 - H/D exchange 208
 - hydrophilic properties 207
 - hydrophobic nature 207
 - interaction of nitrile groups 227
 - by means of SO₂ group of anion 207
 - poisoning 228
 - of silver nanoparticles (AgNPs) 206
 - metal nanocrystals 16
 - metal-organic frameworks (MOFs) 20, 311, 378
 - metal oxide nanoparticles (MONPs) 9–12, 209, 375, 381
 - catalytic potential 395
 - precursors, crucial effect 377
 - unsupported nanoparticles 388
 - metal-support interaction 346
 - metal surfaces, electronic/geometric factors determining reactivity
 - bulk, surface and nanoparticles, theoretical point of view 457–460
 - density functional theory 456, 457
 - descriptors/predictive studies 455, 456
 - electronic structure effect, in heterogeneous catalysis 452–455
 - special sites 451, 452
 - methanation
 - Ni-Fe alloy 456
 - rate-limiting step 466
 - methylacrylate 66
 - methylene blue 235, 357, 358, 387, 391
 - N-methylimidazolium chloride 204
 - methylthiols 451
 - MgO nanoparticles 383
 - Michael addition reaction 112
 - microreactors 80, 81, 299–300
 - glass/glass 299
 - metal-based 299
 - supercritical 299
 - MNPs, *see* metallic nanoparticles (MNPs)
 - molecular orbital (MO) theory 443
 - molecular recognition 22
 - monodispersity 99, 124, 443
 - monometallic systems, electronic and geometric properties 161–168
 - Monte Carlo simulation 419
 - Moseley's law 156
 - Müller-Brown PES model, contour plot 460
 - multi-electron effects 158
 - multiphasic systems 314–317
 - multiwalled carbon nanotubes (MWCNTs) 36, 37, 228–231, 333, 336, 337, 353, 354, 416, 418, 431, 433, 435
- n**
- NaBH₄ reduction 449
 - N-alkyl-N-(2-hydroxyethyl) ammonium salts 60
 - nanoarchitecture 2
 - nanocatalysis 58
 - application in industry segments 24
 - catalyst market by end-use 24
 - expected benefits 24
 - objectives 23
 - nanocatalysts 2, 3, 8, 9, 19, 20, 41, 68, 78, 83, 85, 127
 - assembling strategies 20
 - for fuel cell devices 131–139
 - nickel nanocatalysts: hydrogenation 222
 - oxide nanocatalysts for green chemistry 395, 396
 - platinum nanocatalysts: hydrogenation 229
 - properties 15
 - for specific organic reactions 140, 141
 - synthesis of nanopowders as nanocatalysts in SCFs 286
 - nanocatalysis, basic features 124
 - nanocrystals synthesis, in SCmF 300–302
 - γ-nano-Fe₂O₃ catalysts 395
 - nano-oxides 375
 - as active phases 381–391
 - catalysis by supported oxide nanoparticles 391–396
 - on nanotubes 394, 395

- on ordered mesoporous/microporous materials 391–394
 - oxide nanocatalysts for green chemistry 395, 396
 - catalysis by unsupported oxide nanoparticles 388–391
 - hazardous compound abatement 389–391
 - organic reactions 388, 389
 - catalytic applications 381–402
 - catalytic performances 375, 376
 - metal oxide nanoparticles design 376–379
 - morphology 388
 - nanoparticles, catalytic behavior related characteristics 381–388
 - bulk materials compared with 381–383
 - effect of morphology 384–388
 - nanoparticles, effect of size 383, 384
 - size-dependent oxide properties 380, 381
 - as supports for active phases 396–402
 - synthesis and characterization 376–381
 - nanoparticles (NPs)
 - anchoring pre-formed 341, 342
 - body-centered cubic (bcc) lattice structure 450
 - bulk/surface, electronic structure of 457–460
 - catalysis with ionic liquids 254
 - SCILL systems 260–264
 - SILP systems 254–260
 - catalytic behaviors 383
 - diversity rationalization 448
 - morphology, effect of 384–388
 - oxide 331, 379, 391
 - ruthenium catalysts 462
 - shape-controlled 5
 - size, effect of 383
 - size/shape matter 446–448
 - structural/chemical bonding knowledge 448, 449
 - iron 450
 - platinum 450, 451
 - silver 449, 450
 - surface chemistry, density functional theory
 - limitations and challenges 456, 457
 - synthesis, in water 56–59
 - organometallic approach 58
 - salt approach for synthesis 59
 - strategies 57
 - synthesize colloidal 448
 - transition electron microscopy (TEM) 449
 - nanoparticles in IL surface modified systems 264, 265
 - carbon nanotubes 269, 270
 - IL-functionalized highly cross-linked polymers as support 267, 268
 - miscellaneous supports 270–272
 - natural clays with IL-functionalization 268, 269
 - surface modified nanocrystalline metal oxides 266, 267
 - surface-modified ordered meso-porous silica 265, 266
 - nanopowders as nanocatalysts in SCFs, synthesis 286–291
 - main routes, proposed 288
 - nanoscale systems, self-organization 22
 - nanoscience/catalysis studies 26
 - ruthenium models 444
 - nanosized NiO-doped cage cubic Pm3n mesoporous silica materials 392
 - nanostructured clusters, applications in energy-related processes 128
 - nanocatalysts for fuel cell devices 131–140
 - partial methane oxidation with NO 139, 140
 - size-selective Fischer–Tropsch nanocatalysts 128–131
 - nanostructured Co₃O₄ clusters 382
 - nanostructured exhaust catalysts 28–31
 - nanostructured materials, in energy-related processes
 - applications for energy and hydrogen storage 149–154
 - nanocomposites for batteries 145–148
 - nanomaterials for high-performance solar cells 142–145
 - nanostructured metallic catalyst precursors
 - characterization 154
 - interaction with coatings and supports 154
 - natural polymers 378
 - nickel nanocatalysts 222
 - nickel nanoparticles (NiNPs) 207, 222
 - nitrile-functionalized pyridinium 225
 - nitrogen oxides (NO_x) 139, 387
 - p*-nitrophenol 68
 - non-nano materials 2
 - NPs, *see* nanoparticles (NPs)
 - nudged elastic band (NEB)-derived methods 461
- o**
- one-pot synthesis 20, 30, 396
 - ordered mesoporous carbon (OMC) materials
 - properties 360
 - Ostwald ripening 124
 - oxidation 78, 348, 349, 396
 - anodic 132, 134

- aqueous solution, aerobic phenylethanol oxidation 465, 466
 - Au/Co₃O₄ catalysts for 400, 401
 - benzyl alcohols 382
 - reaction scheme for 348
 - benzylic alcohols 78
 - cerium 30
 - CNTs 335
 - CO 28, 112, 168, 174, 267, 386, 387
 - cyclohexane 389
 - 1,2-diols 323
 - ethanol 213
 - ethylene 401
 - graphite 356
 - homogenous 394
 - hydrazine 113
 - 2-hydroxybenzyl alcohol 234
 - metal-catalyzed alcohol oxidation 348
 - methanol 136–138, 353, 360
 - partial methane oxidation with NO 139
 - phenylethanol 465–467
 - propane 359
 - propylene 464, 465
 - recyclable γ -nano-Fe₂O₃ catalysts in 395
 - selective propane 359
 - silver 465
 - styrene 463, 464
 - *o*-xylene 384
 - oxygen reduction reaction (ORR) 352
- P**
- palladium catalysts 79, 80, 84, 85, 110, 223, 261
 - CNF-supported 359
 - immobilization 215
 - modified 39
 - surface area activated charcoal supported 431
 - synthesis 80
 - TiO₂ supported 400
 - water soluble phosphine-stabilized 84
 - zeolite Y and AC-supported 430
 - palladium chelating complex 85
 - palladium nanoparticles (PdNPs) 22, 31, 73, 79, 84, 206, 223, 267
 - β -CDs, presence 68
 - capped with thiol/stabilized with ionic liquid 288
 - ‘click’-ferrocenyl dendrimer-encapsulated 108
 - dendrimer-stabilized 82
 - dual catalytic behavior of 228, 229
 - Heck–Mizoroki reaction catalyzed by 225
 - hydrogenation reaction of *trans*-stilbene derivatives using 228
 - immobilization 215
 - ionic liquid catalyst containing 255
 - on model oxide surface in presence of CO 264
 - PAMAM-dendrimer encapsulated 141
 - protected by alkylated polyethyleneimine 79
 - Sonogashira C–C couplings catalyzed by 226
 - stabilized by water soluble functionalized phosphine 84
 - supported on multiwalled carbon nanotubes in water 269
 - surrounded and stabilized by G0 nonaferrocenyl dendrimers 109
 - Suzuki coupling 141
 - synthesis of 108
 - biaryl derivatives, Suzuki cross-couplings reaction 224
 - presence of pyridine derivative ligand 230
 - XPS studies 206, 258
 - particles size 3, 8, 293, 298
 - Pauson–Khand reaction 319
 - Pd/AC catalyst 348
 - Pd–Au bimetallic catalyst 349
 - Pd/G catalyst 332, 357
 - PdNPs, *see* palladium nanoparticles (PdNPs)
 - Pd/TiO₂ catalyst 400
 - n*-pentane, temperature programmed desorption profiles 420
 - periodic-boundary methods, advantages 444
 - phenylazomethine dendrimer 18
 - phenylboronic acid 112
 - phosphinophosphonic acid-stabilized rhodium clusters 84
 - photocatalysis 11, 34–38, 150, 331, 354–356, 390, 391
 - basic steps 354
 - photocatalysts 35, 215, 321, 385, 390
 - photon energy 156
 - physical vapor deposition (PVD) 22
 - plate-like nanocrystals 386
 - platinum 7
 - based binary catalysts 25
 - carbon black catalyst 353
 - as catalysts, drawbacks 25
 - CNT catalysts 348
 - nanowires 25, 26
 - Pt/Al₂O₃ 179
 - platinum nanoparticles (PtNPs) 105, 206, 208, 229–231
 - average surface structure 259
 - CO poisoning 182
 - deposited on carbon aerogel 294

- modification 320
 - one-pot preparation 21
 - pyrrole hydrogenation 447
 - stabilized by ILs 229
 - supported on magnetite nanoparticles 271
 - synthesis supported on ionic liquid functionalized Fe₃O₄ NPs 230
 - plug-flow reactor 127
 - Poiseuille flow 421
 - Poisson–Boltzmann equation, continuum solvation model 465
 - polarizable continuum model (PCM) 465
 - polarization 26, 208
 - effect at Au/Fe₃O₄ interface 400
 - parahydrogen-induced 256
 - polyacrylamide (PAM) 80
 - poly(amidoamine) (PAMAM) 16, 82, 97, 99
 - dendrimers using thiols as potential stabilizing ligands for 110
 - dendrimer synthesis 99
 - poly(diallyldimethylammonium chloride) 79
 - Pt NPs stabilization 82
 - poly(dimethyl)siloxane (PDMS) 299, 323
 - polyethylene glycol (PEG) 315
 - polyethyleneimine (PEI) 342
 - polymeric microreactors
 - for hydrogenation of olefins 79
 - TEM image 80
 - poly(methyl vinyl ether) (PMVE) 77
 - polyoxoanions 16
 - polypropyleneimine (PPI) dendrimers 100
 - poly[styrene-*co*-2-(acetoacetoxy)-ethylmethacrylate] (PS-*co*-PAEMA) 80
 - poly[styrene-*co*-2-(acetoacetoxy)ethyl methacrylate-*co*-methyl acrylic acid] (PS-*co*-PAEMA-*co*-PMAA) 80
 - microreactors, TEM image 80
 - polyvinyl alcohol (PVA) 16, 77
 - poly(*N*-vinyl-2-pyrrolidone) (PVP) 16, 77, 124, 259
 - catalytic investigations 77
 - potential energy surface (PES) 460
 - precipitation process 317
 - using photodestructible surfactants 319
 - preferential CO oxidation (PROX) process 390
 - propylene oxide 464
 - protective agents, dynamic organization 72
 - Pt₅₅ nanoclusters 451
 - PtNPs, *see* platinum nanoparticles (PtNPs)
 - Pt–Pt bond length 124
 - Pt-RGO-based fuel cell 357
 - PtRu/CNT 432
 - PtRu nanoagglomerates 340
 - Pt-SWCNT/Nafion catalyst 354
 - purification methods 334, 335
 - pyrogallol, biomimetic oxidative performance 357
 - pyrrole, hydrogenation of 447
- q**
- QEXAFS monochromator 161
 - quantum chemistry (QC) 443
 - quantum confinement effects 380
 - quasi-Newton algorithm 461
 - quaternary ammonium salts 204, 205
- r**
- Raman enhancement 357
 - Raman G-band 428
 - Raman spectroscopy 206, 209, 380, 427, 433
 - randomly methylated CDs (RAME-CDs) 70, 73
 - Rayleigh scattering (RRS) analyses 208
 - redispersion 317
 - reduced graphene oxide (RGO) sheets 356
 - resonant inelastic x-ray scattering (RIXS) 178–181
 - for *in situ* characterization 182
 - 1s3p RIXS plane of CoO 181
 - reverse microemulsion syntheses 378
 - Rh₅₅ cubooctahedron 468
 - rheological measurements 209
 - rhodamine B (RhB) 385
 - rhodium 28, 427, 468
 - rhodium(0) nanoclusters 66, 259, 268
 - rhodium nanoparticles (RhNPs) 219
 - Ru/CNT catalyst
 - electron tomography analysis 345
 - structure–function correlations 351
 - TEM image 345
 - Ru(III)/TiO₂ catalyst 395
 - RuNP, *see* ruthenium nanoparticles (RuNP)
 - RuO₂ nanoparticles 395, 416
 - Ru(0001) surface 457
 - DOS of naked and hydrogenated ruthenium 458
 - relative stability 459
 - ruthenium nanoparticles (RuNP) 84, 86, 88, 215–218
 - catalytic activity 360
 - stabilized by 87
 - synthesis 85
 - Wulff construction 450
- s**
- Sabatier principle 451, 455
 - scanning transmission X-ray microscope (STXM) 161
 - scanning tunneling microscopy (STM) 424

- SC μ F, *see* supercritical microfluidics (SC μ F)
- self-assembly of nanostructures 21
- SFCD, *see* supercritical fluids chemical deposition (SFCD) processes
- silica 8
- silver nanoparticles (AgNPs) 206, 207, 211, 312, 317, 319
- reshaping of 465
 - TEM images of 450
- single-site catalysts 21
- single-walled carbon nanotubes (SWCNTs) 333, 416
- *n*-heptane adsorption 421
 - temperature programmed desorption profiles 420
 - transmission electron microscopy images 332
- size-sensitivity 3
- small angle X-ray scattering (SAXS) 206
- SnO₂ sensors 33
- sodium bis(2-ethylhexyl)sulfosuccinate 319
- sodium clusters Nan photoionized, mass spectra of 445
- sol-gel process 376
- solid catalysts with ionic liquid layers (nano-SCILL) 253
- catalyzed reactions 272
- solid nuclear magnetic resonance (NMR) analyses 203
- solubility-controlled process 377
- Sonogashira reactions 73, 74, 76
- under ultrasound irradiation 226
- stabilization
- anionic mode 206, 207, 209
 - cationic mode 207–209
 - by [C₁C₂Im][BF₄] 206
 - conditions, adjustment 318–320
 - energy 454
 - ionic liquids
 - effect on structures 210–212
 - interactions of metal oxide nanoparticles 209, 209
 - metallic NPs 67
 - modes by ionic liquids 206
 - steric mode 207 (*see* steric stabilization)
- π - π -stacking interactions 205, 337
- static disorder 158
- steady-state isotropic transient kinetic analysis (SSITKA) 448
- steric stabilization
- cyclodextrins 67
 - ligands 83–89
 - mode 207
 - polymers and derivatives 77–83
- structural miniaturization 6
- structure sensitivity
- in catalysis 4
 - particle size relationship 449
- styrene oxide, hydrogenolysis with Pd(0) NPs 65
- supercritical fluids 281–286
- active pharmaceutical ingredients (APIs) 283
 - advantages over conventional processes 286
 - carbon dioxide, supercritical 284
 - chemical deposition processes 292
 - close to critical point (CP), characterized by 281
 - continuous process of nanomaterials synthesis using, flowsheet 287
 - critical coordinates and densities 284
 - fluid viscosity 283
 - supercritical antisolvent process 283
 - supercritical water (scH₂O) 283
 - supercritical water oxidation (SCWO) 283
 - thermophysical properties 284
- supercritical fluids chemical deposition (SFCD) processes 292
- kinetically-controlled 295
 - deposition 292
 - Ni nanoparticles 297
 - thermodynamically-controlled approach 293, 294
- supercritical microfluidics (SC μ F)
- motivations for, developing synthesis of nanocrystals using 298
 - nanocrystals, synthesis 297–302
- supercritical microreactors 299
- superparamagnetic nanosized crystals 394
- supported ionic liquid phase (nano-SILP) 203, 252
- benefits 272
 - possible reactor concepts 272
- supported nanoparticles, as nanocatalysts in SCFs
- applications 296
 - strategies, for synthesis 292
- surface atoms 9
- surface differential diffraction 386
- surfactants 16, 66, 137, 164, 214, 298, 317–319, 378, 390
- ammonium 60
 - electrosteric stabilization by 60–67
 - ionic 60
 - quantum dots surrounded with organic surfactants anchoring titania 144
- Suzuki–Miyaura coupling reaction 19, 39, 64, 73, 75, 77, 80, 82, 111

- of aryl bromides and chlorides 223
- of aryl chlorides and aryl bromides 84
- catalyzed by Fe₃O₄ nanoparticles-ionic liquid matrix 215
- with high TOF and TON value 110
- leaching mechanism 110
- between *p*-bromoacetophenone and phenylboronic acid 112
- synthesis of ligand-free PdNPs 223, 224
- using CD-capped Pd(0) NPs 75
- x-ray photoelectron spectroscopy 324
- SWCNTs, *see* single-walled carbon nanotubes (SWCNTs)

synergistic effect 354

syngas 447

t

task-specific ionic liquid (TSIL) 224

temperature programmed desorption (TPD) 419

tether gold colloidal nanoparticles, reaction scheme 341

tetrabutylammonium bromide (TBAB) 215, 314

tetradecyltrimethylammonium bromide (TTAB) 125, 207

tetraethylene glycol dodecyl ether 319

tetrahydrofuran (THF) 58, 315

tetra-*n*-butylammonium bromide 66

thermal stability 30

thermodynamically-controlled SFCD process (T-SFCD) 293–295

thio-functionalized CDs 68

three-way catalyst (TWC) 28

Ti-containing silicalite-1 (TS-1) 431

TiO₂ catalyst 35, 173, 290, 355, 358, 381, 391, 401

titanium tetraisopropoxide (TTIP) 290, 291

total turnover number (TTO) 66

transition metal (TM)

– clusters, prototypes 445

– co-catalysts 35

– nanoparticles 446

transition states (TSs) 460

transmission electron microscopy (TEM) 71, 72, 78, 99, 211, 217, 226, 265, 301, 345, 379, 401, 450

1,3,5-triaza-7-phosphaadamantane (PTA) 58, 84, 85

1,2,3-triazolyl dendrimers 106

1,2,3-triazolylsulphonate dendrimers 82

2,4,6-trichlorophenol (TCP) 382

– total removal, rate constant 382

trifluorotoluene 315

1-[*N,N',N''*-trimethyl-(4-butyl) ammonium]-2-(2-pyridyl) imidazole chloride 84

turnover frequency (TOF) 3, 4, 38, 105, 316, 334, 395, 430, 448

turnover number (TON) 66, 107, 270, 288, 290

u

Ullmann-type reductive homo-coupling 226, 227

ultraviolet-visible (UV-vis) spectroscopy 16, 206, 207, 298, 424

v

van der Waals interactions 337, 340, 457

volatile organic compounds (VOCs) 32

volcano plot 468, 469

Vulcan XC-72 352, 353

w

water-gas shift (WGS) reaction 387, 401

water-soluble nanoparticles 55

water-soluble nitrogen ligand 85

water-soluble platinum nanoclusters 37

water-soluble protective agents 59, 60

water-soluble ruthenium(0) nanoclusters 78

wave function approach (WFT) 457

wet chemical methods 336–338

Wulff construction 450, 451, 462, 463, 465

– large Ru particle 450

– Pd₂Ga nanoparticle 332

x

X-ray absorption near-edge spectroscopy (XANES) 29, 134, 156, 157, 162, 163, 165, 167, 170, 173, 262, 380, 427, 428

X-ray absorption spectroscopy (XAS) 29, 128, 156, 159, 166, 172, 174, 179, 182

X-ray diffraction (XRD) analysis 16, 135, 159, 169, 222, 289, 345, 380, 395, 418, 426, 433, 434

X-ray photoelectron spectroscopy (XPS) analysis 1, 16, 74, 206, 208, 262, 263, 339, 427, 467

y

Yamamoto's G4 phenylazomethine dendrimer 101

yolk shell catalysts 126

z

zeolite catalysts 20, 379, 394, 415, 416, 430

zero-valent nanoparticles 9

ZnFe₂O₄ nanoparticles 215

ZnO nanoparticles 210, 302, 396

– synthesis 378