

Index

a

- ab initio molecular dynamics (AIMD) simulations 95
- absorption dehydration 147
- activated carbon 129, 147–150, 154–157, 362
- adsorption dehydration 147
- advanced process engineering co-simulator 48
- aliphatic polycarbonates CO₂/epoxide copolymerization 387–389
- mechanical properties 390–392
- monomer synthesis 386–387
- thermal stability and degradation pathways 389–390
- alkaline electrolysis cell (AEC) 71
- alkaline technology 241
- alkaline water electrolysis process 242
- amines 9, 10, 161, 212, 213, 413
- analytical system 257
- apparent quantum efficiency (AQE) 341
- artificial neuron networks 219
- artificial photosynthesis 337, 368, 442, 447–448
- Auger recombination 338

b

- BaFe-hexaaluminate catalysts 298, 318
- Beer's law 369
- benefit cost ratio (BCR) 242, 245, 246
- biodegradable polymers 367
- bioenergy 112

- biogas 163
 - composition and applications 127
 - production plants 125
 - upgrading processes
 - chemical scrubbing 129
 - cryogenic separation 130–131
 - membrane separation 129–130
 - organic physical scrubbing 129
 - pressure swing adsorption 129
 - water scrubbing 129
- biogas purification technologies
 - ammonia removal 156–157
 - contaminant treatability 146
 - hydrogen sulfide, removal of activated carbon adsorption 149–150
 - biological filters 152–153
 - iron oxide or hydroxide 152
 - organic solvent scrubbing 151
 - in situ precipitation 148–149
 - sodium hydroxide scrubbing 151–152
 - water scrubbing 150–151
 - zeolite based sieve 150
- oxygen and nitrogen removal 157
- siloxanes, removal of activated carbon, molecular sieves and silica gel adsorption 154–155
- biological filters 156
- cryogenic condensation 156
- membrane separation 155–156
- organic solvent scrubbing 154

- biogas purification technologies (*contd.*)
 - volatile organic compounds removal 156
 - water vapor, removal of 146–148
- biogas upgrading technologies
 - chemical scrubbing 160–162
 - organic solvent scrubbing 160
 - pressure swing adsorption (PSA) 162–163
 - water scrubbing 157–160
- biological filters 148, 152–153, 156
- biotrickling filter 152, 153, 156
- Bi-reforming of methane (BRM) 176, 367
- block copolymers 389
- body-centred cubic (BCC) arrangement 41
- boudouard reaction 75, 189, 437
- bulk defects 412
- b-butyrolactone 398

- C**
- calcium looping 6, 7, 21
- capture unit 17
- carbide support catalysts 187–188
- carbon capture and utilization (CCU)
 - technologies 127
 - algae production 133
 - chemicals 132
 - chemical scrubbing 134–135
 - cryogenic separation 136–138
 - enhanced oil recovery 133
 - fuels 133
 - membrane separation 135–136
 - mineral carbonation 132–133
 - supercritical CO₂ 131–132
- carbon capture combined with bioenergy (BECCS) 1
- carbon capture-conversion
 - electrochemical applications
 - electrolysis and co-electrolysis processes 69
 - methane dehydroaromatization 78
 - methane steam reforming 76
 - synthesis gas chemistry 75
- oxygen transport membranes
 - applications 63
 - development 63–65
 - mixed ionic-electronic conductivity (MIEC) 60
 - oxygen bulk diffusion 61
 - oxygen surface reactions 61
- polymer membranes 56–60
- protonic membranes
 - pressure gradient 65
 - proton conductivity 67, 68
 - proton defects in oxide ceramics 65–67
- carbon capture technologies
 - adsorption 3–6
 - chemical absorption 9–12
 - CO₂ capture deployment 2
 - fuel cells 13–17
 - high-temperature solids looping technologies 6–8
 - hybrid technologies 13
 - the industrial sector 21
 - membrane systems 8–9
 - oxyfuel process 3
 - post-combustion 3
 - in power plant and electricity grid 17–20
 - pre-combustion systems 2–3
 - process configurations 12
 - role of 1
- carbon capture, utilization and storage (CCU/CCUS) processes 207
- Carbon2Chem 118
- carbon deposition 188
- carbon dioxide catalytic conversion
 - DFT
 - calculations 87–89
 - high-throughput screening 92
 - machine learning 93–95
 - volcano plots and scaling relations 93
 - microkinetic modeling 89–92
 - theoretical catalysis research 85–87
- carbonic anhydrase (CA) 11
- carbon storage 41

- catalytic membrane reactor (CMR) 78
 cathodic exfoliation 353
 cetyl-trimethyl-ammonium bromide (CTAB) 373, 374
 chain-transfer agent 389, 397, 398
 chemical absorption-desorption process 17
 chemical-looping combustion 7
 chemical looping systems 8
 chemical-reaction equilibria 230
 chemical scrubbing 129, 134, 160
cis-2,3-epoxybutane 413
 CLEANER project 7, 21
 climbing-image NEB method (CI-NEB) 87
 CO_2 capture techniques 253, 274
 CO_2 catalytic conversion
 electro-reduction
 catalysts development 349–357
 electrode and electrolyte compositions 348
 parameters 348
 low-temperature electrocatalytic strategy 336
 photo reduction
 catalysts development for 339
 energy transfer efficiency 338
 gas-phase heterogeneous catalytic systems 338
 localized surface plasmon resonance effect 338
 reaction kinetics and energy efficiency 339
 CO_2 cycloadditions, MOFs 415–416
 defects in 416–419
 functional linkers 419–420
 Lewis acid and basic 416
 reaction mechanism 414–415
 CO_2 dissociation 443, 444
 CO_2 electrolysis 73
 CO_2 /epoxide copolymerization
 heterogeneous catalysts 393
 homogeneous catalytic systems 393–397
 limonene oxide 399–402
 terpolymerization pathways 398–399
 CO_2 hydrogenation reactions
 carbon capture and utilization (CCU)
 approach
 methane production 237–238
 methanol production 235–237
 techno-economic consideration 238–248
 equilibrium composition calculations 232–234
 thermodynamic aspects 229–231
 CO_2 methanation
 environmental protection industry and aerospace field 176
 fundamentals 177–178
 nickel-based catalysts 179–182
 rhodium and palladium-based catalysts 182
 ruthenium-based catalysts 178–179
 computational fluid dynamic (CFD)
 model 210, 215
 amine scrubbers 35
 of amine scrubbers 32
 biological utilization 46–47
 carbon storage and enhanced oil recovery 41–44
 carbon utilization, chemical conversion 44–46
 DEM 38
 experimental correlations 34
 F-factor 33
 oxy-fuel combustion technologies 41
 and process simulations 48
 reduced order models (ROM) 48
 representative elementary unit 33
 solid phase and gaseous phase 38
 VOF and Eulerian method 38
 volume-of-fluid (VOF) method 32
 computer-aided design (CAD) files 43
 confinement effect 363
 continuous liquid phase 209
 conventional gas-liquid contactors 213
 conventional reactors 205
 cooling dehydration 147

- C**
- CO₂ photoreduction with methane (CRM) 341
 - copolymerization process 387
 - copolymerization reaction 389
 - CO₂ recycling reactions
 - biodegradable polymers 367
 - carbon formation 367
 - CO₂ utilisation reactions 366–368
 - photochemical reactions 368–372
 - spatial and quantum confinement effects 366
 - supported metal nanoparticles 366
 - YS catalysts 367
 - CO₂ reforming reactions
 - catalytic supports 193–195
 - fundamental 190
 - Ni-based catalysts 191–193
 - noble metal-based catalysts 190–191
 - Core-shell (CS) and Yolk-Shell (YS)
 - hard templating techniques 375
 - metal oxide/carbide shells 375
 - soft templating techniques 373–374
 - Coulomb force 430
 - CO₂ utilization processes 175
 - cryogenic condensation 156
 - cryogenic separation 130
 - cryogenic treatment 157, 165–166
 - cyclohexene oxide (CHO) 386, 387
- d**
- dense discrete phase model (DDPM) 38
 - dense membranes 55
 - density functional theory (DFT) 86, 352, 448
 - deposition–precipitation method 283
 - dielectric barrier discharges (DBD) 436
 - dielectric materials 443
 - diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) measurement 307, 345
 - diffusion coefficients 57
 - dimethyl carbonate (DMC) 220
 - direct methanol conversion 255
 - direct power to gas process 271
- e**
- discrete element method (DEM) 38–40
 - dry reforming of methane (DRM) 90, 362, 367, 444
- f**
- electric swing adsorption (ESA) 6
 - electrification 431
 - electrochemical reduction 87, 317, 348, 351, 357
 - electroforming 207
 - electrolysis 112
 - encapsulated materials 362
 - energetic efficiency 351
 - energy efficiency 432, 440, 451
 - energy minimization multi-scale (EMMS) model 38
 - energy transfer 432
 - enhanced oil recovery 41
 - enthalpy change 229
 - equilibrium constants 67, 229–231, 255
 - etching 207
 - Euler-Euler method 34, 46, 47
 - Eulerian method 38, 39
- g**
- Fe-doping 327
 - FeN₄ sites 327
 - F-factor 33
 - first-principles approach 85
 - Fischer-Tropsch (F-T) 183
 - Fischer-Tropsch process 75, 76
 - Fischer-Tropsch reaction 76, 227
 - Fischer-Tropsch synthesis (FTS) 75, 188, 219, 319
 - flow-sheet simulations 276
 - flue gas line equipment 18
 - fouling 156
 - fractional free volume (FFV) parameter 57
 - Franck Condon principle 433
 - FReSME, 118
- g**
- galvanic replacement 375
 - gas hour space velocity (GHSV) 262

gas-liquid catalytic hydrogenation reactions 209
 gas-liquid slug flow 209
 gas-supply 257
 Gaussian process 95
 generalized gradient approximations (GGA) 86
 Gibbs free energy 133, 229
 gliding arc discharge 437
 greenhouse gases (GHG) emissions 235
GrInHy, 118

h

Hartree-Fock (HF) method 86
 heat exchange and temperature control 210–212
 heat transfer coefficient 206
 high-throughput screening 92, 96
HiSarna 116
HiSarna, 117
 hot embossing 207
 hybrid technologies 13
 hydrogen-oxygen reaction 273
 hydrogen peroxide to propylene oxide (HPPO) process 386

i

in-plasma catalytic reactors 438
 industrial ozone generator 450
 injection molding 207
 ionic liquids (ILs) 11, 29, 213, 220, 324, 419

k

kernel ridge regression (KRR) 95
 kinetic Monte Carlo simulations 88

l

laser ablation 207
 Lattice-Boltzmann methods 31
 layered double hydroxide (LDH) 342–344, 372
 Le Chatelier principle 230–231, 256
 limonene oxide (LO) 386–388, 390, 397, 399–402

liquid-liquid reactions 206
 local density approximation (LDA) 86
 localized surface photothermal (LSPT) effect 339
 local/localized surface plasmonic resonance (LSPR) 338, 341, 345, 371–372

m

macrofluidics system 211
 mass spectrometry analysis 265, 268
 membrane separation 59, 129–130, 135–137, 139, 154–156
 membrane technology 55, 130
 MeOH synthesis 183
 metal-organic frameworks (MOF) 355
 CO₂ transformations 408
 Lewis acid sites
 bulk defects 412–413
 defect generation 411–412
 metal cluster 411
 OMS 410
 surface defect 412
 metallic membranes 56
 methanation 362
 methanation reaction 45–46, 49, 75, 105, 114–116, 136–137, 175–184, 195, 214–217, 237–238, 253–260, 262, 264–265, 267–274, 288–289, 294–295, 299–300, 318, 328, 340, 343–345, 362, 447
 methane dehydroaromatization 68–69, 78
 methane production 127–131, 237, 287
 methane steam reforming 76
 methane synthesis
 biogenic CO₂ sources 268–269
 CH₄ product gas mixtures, reuse of 270–273
 CO methanation 259
 coke oven gas 264–267
 combustion plant flue gas 260–264
 experimental setup 256–258
 industrial gas mixtures 258–260

- methane synthesis (*contd.*)
- oxyfuel operation, in gas engines 269–270
 - oxyhydrogen reaction 259
 - reversed water gas shift reaction (RWGS) 259
 - saline aquifers 267–268
 - thermodynamics of methane conversion 255–256
 - methanol 88, 114, 217–218, 227–228, 235–248, 253–277
 - methanol synthesis
 - catalysts performance 275
 - experimental setup 274
 - influence of N₂ admixture 275
 - Sabatier reaction 274 - microalgae cultivation 46–47, 134
 - microchannel reactor (MR) 205–221
 - microfluidics 208–211
 - and mixing flow 208–210
 - temperature control and pattern flow regulation 208
 - micromachining 207
 - microporous membranes 55, 155
 - microreactors 206
 - CO₂ capture and storage (CCS) 212–214
 - CO₂ methanation 214–217
 - CO₂-to-higher hydrocarbons and fuels 218–219
 - CO₂-to-methanol and dimethyl ether (DME) transformation 217–218
 - cyclic organic carbonates 219–220
 - microreaction technology 210, 220, 221
 - microwave discharges 432, 437
 - microwave plasmas 432, 436
 - microwave power generators 431
 - microwave swing adsorption (MSA) 6
 - mineral carbonation 38, 113, 131–133, 139, 212
 - mixed ionic-electronic conductivity (MIEC) 60–62
 - molecular organic frameworks (MOFs) 364
 - molecular sieves 129, 147–148, 150, 154–155, 157, 162, 212
 - molecular weight (MW) 320, 386, 389, 392–393, 397–398, 400
 - Molten carbonate fuel cells (MCFC) 13–17, 145
 - monodentate linker 412
 - monoethanolamine solutions (MEA) 9, 129, 161, 212, 241
 - MoSeS alloy monolayers 326
 - multi-phase flows 31–32, 206, 209
- n**
- N-bromosuccinimide (NBS) 387, 399–400
 - N-doped carbon nanofibers 327
 - N-doping 327
 - N-type semiconductors 369
 - nanocasting 207
 - nanosizing catalysts 351
 - nanostructuring strategies 339, 345
 - National Aeronautics Space Administration (NASA) 176, 215
 - Navier–Stokes equations 30–31, 34
 - neural networks (NN) 95–96
 - nickel-based catalysts 115, 179–182, 192, 258, 264, 268, 295
 - nitrogen functionalities 413
 - non-thermal ionization 430
 - non-thermal plasma (NTP) 430, 432–434, 436, 441
 - nudged elastic band (NEB) method 87
 - Nusselt number 211–212
- o**
- open metal sites 409, 411
 - organic physical scrubbing 129–130, 139
 - organic solvent scrubbing 148, 151, 154, 160
 - oxidative carboxylation 420
 - oxy-fuel combustion 41
 - oxyfuel process 3, 6, 267, 269

p

p-block metals 326
 Paris Agreement 109, 366
 Pay Back Period (PBP) 246, 248
 Pd nanocrystals 344–345
 pentablocks 398
 perturbation Møller-Plesset (MP2) 86
 P2G technology 115–116
 photocatalysis 337, 368–369, 408
 photolithography 207
 photovoltaics (PV) 346
 plasma catalyst promoter (PCP) 442
 plasma-assisted CO₂ conversions
 catalyst development 440
 electrification 431
 experimental performance 442
 history 430–431
 homogeneous plasma-activation 432–433
 mechanism 433–435
 models 448
 mutual influence 439
 plasma reactors 435–437
 scale-up and process considerations 449–450
 thermodynamics 431–432
 poly(cyclohexene carbonate) (PCHC) 386, 392
 poly(limonene carbonate) (PLC) 386, 390, 392–393, 399–400, 402
 polymer alkaline electrolyser cell (PAEC) 71
 polymer membranes 56–59
 polymer poly(propylene carbonate) (PPC) 386, 389–390, 392–393, 398, 402
 polymeric membranes 9, 59, 71, 157, 163–165
 polyvinyl alcohol (PVA) 58, 374
 polyvinyl pyrrolidone (PVP) 374
 post-combustion 1–12, 14, 17–20, 58, 241, 254
 post-combustion capture 20
 post-synthetic approaches 412–413
 power plant steam turbine 19
 power supply technology 431

Power-to-Gas (P-t-G) concepts 115, 175–176, 237, 254, 260, 264
 pre-combustion systems 2, 7
 pressure swing adsorption (PSA) 5–6, 128–129, 139, 157, 162–163
 process engineering simulations 29–31
 process integration 17, 19, 116, 254, 267
 process intensification (PI) 65, 68, 78, 205–206, 217–218
 product separation 449
 propylene oxide (PO) 220, 386–387
 proton conductor solid oxide electrolyser cell (PC-SOEC) 71, 73
 proton exchange membrane electrolysis cell (PEM-EC) 71
 protonic membrane reformer (PMR) 77

q

quantum confinement effects 364–366, 371
 Quantum Mechanics and Molecular Dynamics 29–30

r

radiofrequency (RF) reactors 436
 rate determining step (RDS) 90–91, 177, 348–349, 395, 400, 447
 reaction kinetics 38, 41, 44–46, 70, 71, 256, 317, 339–340, 394, 395
 reaction parameters 229, 321, 327–328
 reduced order models (ROM) 48
 renewable energy development 125
 representative elementary unit 33
 repulsive van der Waals forces 364–365
 response surface methodology 219
 reverse water gas shift (RWGS) reaction 70, 88, 114–115, 175, 183, 216, 228, 259, 274, 281–307, 318, 328, 344, 362, 446
 Au-based catalysts 282–286
 Cu-based catalysts 290–294
 mechanism 306–307
 Ni-based catalysts 295–298
 oxide systems 298–300
 Pd and Ir-based catalysts 289–290

- reverse water gas shift (RWGS) reaction
(*contd.*)
- Pt-based catalysts 286
 - Rh-based catalysts 286–288
 - Ru-based catalysts 288–289
 - transition metal carbides 300–305
 - reverse water-gas shift reaction
 - carbide support catalysts 187–188
 - ceria-based support catalysts 186–187
 - copper-based catalysts 185–186
 - fundamentals 184
 - MeOH synthesis and downstream Fischer–Tropsch (F–T) 183
 - noble metal-based catalysts 185 - reverse water-gas shift reaction with
 - chemical looping cycles (RWGS-CL) 183 - reverse-Boudouard reaction 437
 - reversible hydrogen electrode (RHE) 321, 325–327, 349, 351–352, 355–356
 - Reynolds number 44, 208–209, 211–212
 - Reynolds stress model (RSM) 47, 219
 - room temperature ionic liquids (RTILs) 11
 - root mean squared error (RMSE) 96
 - ruthenium-based catalysts 178–179
- S**
- Sabatier reaction 114, 115, 176, 214, 271, 367
 - CO₂-methanation 254
 - direct methanation 253
 - direct methanol synthesis 255
 - SALCOS*, 118
 - semiconductor bandgap 339
 - Shockley–Read–Hall recombination 338
 - SIDERWIN*, 119
 - silica gel 147, 154–155, 269
 - single-crystal X-ray spectroscopy 393
 - single-phase flows 33, 209
 - slow-photon effect 371
 - sodium hydroxide scrubbing 151–152
 - soft lithography 207
 - soft templating techniques 373–374
 - Solid Oxide Electrolyser Cell (SOEC) 71, 73
 - Solid Oxide Fuel Cells (SOFCs) 15
 - solid-catalyzed gas-liquid 206
 - Sorption Enhanced Water-Gas Shift (SEWGS) technology 117
 - space-time yield (STY) 181, 220
 - Stöber process 361, 374
 - steady-state isotopic transient kinetic analysis (SSITKA) 307
 - steam extraction design 19
 - steam methane reforming (SMR) 21, 59, 68, 76
 - Steelanol, 117
 - steel industry
 - carbon-neutral production
 - basic oxygen furnace process (BF-BOF) 110
 - bioenergy 112
 - carbon capture and storage/use (CCS/U) 112
 - carbon monoxide 114
 - EAF-based technology 111
 - electrolysis 112
 - H₂ 112
 - methane 114
 - methanol and formic acid 114
 - steel recycling 111
 - urea 113 - CO₂ emissions 105
 - CO₂ methanation 114
 - corrosion resistance of material 108
 - emissions policies 109–110
 - energy investments 105
 - energy supply 108
 - non-renewable energy industries 108
 - regional share of production 107
 - strain-stress features 107
 - world crude steel production 106
 - supported metal nanoparticles (SMPs) 366
 - surface defect 287, 412, 413, 416
 - surface plasmon resonance (SPR) effect 339–341
 - syngas production

carbon-containing material 319
 $\text{CO}_2/\text{H}_2\text{O}$ mixtures
 cathode composition and structure
 324–327
 cell configuration and chemical
 environment 321–324
 EPOC for CO_2 hydrogenation
 328–329
 reaction parameters 327–328
 electrocatalysis 320
 electrochemical technologies 320
 H_2S , COS and mercaptans 320

t

Taylor flow 209, 213
 Technology Readiness Levels (TRL) 6–7,
 9–10, 12, 21, 23, 63, 64
 temperature swing adsorption (TSA)
 5–6, 163
 terpolymerization 392–393, 395,
 398–399, 402
 TGR-BF-Plasma 117
 thermal expansion coefficient (TEC) 74
 thermal swing adsorption (TSA) 5–6,
 163
 thermodynamics 31, 73, 78, 90, 93,
 229–231, 255, 431, 447
 thermogravimetric analysis 67, 354, 390
 total investment cost (TIC) 245
 transition metal carbides 187, 282,
 300–301, 318

transition state theory (TST) 87
 transition states (TS) 87, 89

u

urea 44, 113, 182

v

Van der Waals forces 364–365
 vibrationally-excited molecules 440–441
 volatile organic compounds 131, 145,
 156
 volume-of-fluid (VOF) method 32–34,
 38, 41, 44

w

Wagner's equation 61–62
 Wash coating 207
 water electrolysis 69–73, 116, 118, 176,
 183, 227, 238, 241, 242, 264, 269,
 337, 449
 water scrubbing 128–130, 139, 150–152,
 157–160
 Water-Gas Shift (WGS) reaction 15, 183,
 282, 291, 409
 wave function-based methods 86
 welding 207

z

zeolites 4, 76, 129, 148, 150, 220,
 286–288, 318, 364, 442, 445–446
 zero-emission strategy 131

