

Index

A

- absorbers, switchable 324
- absorption
 - bulk 107–108
 - coating effects 105–107
 - hydrogen 94
- absorption curves 221
- activation energy
 - adsorption 117
 - decomposition of complex hydrides 223
- active components, fuel cells 346–348
- active layer, gas diffusion electrodes 347
- adsorbate, distance to substrate 176
- adsorbed hydrogen atoms, chemical potential 118
- adsorption
 - activation energy 117
 - coating effects 105–107
 - hydrogen 94, 173–188
- adsorption pressure 219
- AF *see* antiferromagnetic coupling
- air supply, fuel cells 351
- air/fuel ratio 374–375
- airships 14–16
- alkali metal alanates 234–236
- alkaline earth metal alanates 234–236
- alkaline electrolysis 158–159
 - manufacturers 158
- alkaline fuel cell (AFC) 344, 363–364, 369–371
- alkaline solutions, aqueous 245–246
- alloys
 - binary 100
 - enthalpy/entropy of formation 320–321
 - mischmetal nickel 137
- Allred-Rochow electronegativity 189
- all-solid-state switchable mirror 323
- aluminum hydrides, Ti-doped sodium aluminum hydrides 213–233
- ammonia, hydrogen storage 242–244
- anion structure, alanates 236
- antibonding orbital 110–111
- antiferromagnetic (AF) coupling 269, 272–273
- aqueous alkaline solutions 245–246
- Ariane 385
- Aristotle 7
- Arrhenius analysis 107–108
- Arrhenius equation 220
- Arrhenius plot 117, 222
- asymmetry ratios, magnetic 274
- atomic data, hydrogen isotopes 72
- atomic magnetic moment 273
- automotive applications
 - fuel cells 352, 355–358
 - hydrogen-ICE 379–381
- autothermal reforming, biomass 41–42

B

- back seeding 120
- bacteria, hydrogen storage 238–240
- band structure 307
 - calculated 292
 - local model 193
- batteries 337
 - metal hydride-based 326
 - nickel–hydrogen *see* nickel–hydrogen batteries
 - Ni–MH *see* NiMH batteries
- BETSCE sorption cryocooler 391
- binary alloys, surface segregation 100
- binary hydrides 188–189
- biomass
 - autothermal reforming 41–42
 - combustion 41–42
 - energy 39–40
 - hydrogasification 41–42
 - hydrogen production 40–42, 51
 - methanation 41–42

416 | Index

- biomass (*continued*)
 - renewable carbon resource 42–43
 - shift reaction 41–42
 - thermal conversion 41–42
- biomass gasification 155
- bionics 240
- biosphere cycles 47–48
- bipolar stacking, fuel cells 349
- bipropellant liquid propulsion systems 385
- black state 300–302, 309
- boil-off rate, hydrogen 172
- bond dissociation energies 88
- bonding, complex transition metal hydrides 200–201
- bonding orbital 110–111
- borohydride complex ion 245–246
- borohydride fuel cell *see* direct borohydride fuel cell
- borohydride solutions, crystallization 248
- Boudouard reaction 150–151
- Boyle, Robert 7
- brilliant eyes ten-kelvin sorption cryocooler experiment *see* BETSCE
- buffer layers, catalytic 316–318
- bulk absorption, relevance of surface reactions 107–108
- Bunsen, Robert 11
- Buran space shuttle 385
- C**
- calculated band structures 292
- calorific value of mixture 374
- Calvin–Benson cycle 239
- cap layers 278
 - catalytic 316–318
- capacity, storage *see* storage capacity
- carbon budget, global 44
- carbon cycle 37–39
 - replacement by hydrogen cycle 43–45
- carbon flows 39
- carbon hydrates, hydrogen storage 240–241
- carbon hydrides 240–242
- carbon materials, hydrogen storage 178–184
- carbon nanotubes 179–180
- carbon reservoirs 2
- carbon resources, renewable 42–43
- Carnot efficiency 340
- catalysis
 - borohydride fuel cells 369–370
 - deabsorption 220–223
 - hydrogen dissociation and recombination 108–125
 - hydrogen generation 130
 - hydrolysis 249
 - reabsorption 220–223
 - Sabatier reaction 406
- catalytic cap layers/buffer layers 316–318
- cation environments 195
- Cavendish, Henry 8, 13
- cell polarization, direct borohydride fuel cells 368
- cells
 - fuel cells *see* fuel cells
 - galvanic 337–339
- Challenger disaster 17–20, 400
- chemical elements *see* elements
- chemical loading 280
- chemical potential 99–100
 - adsorbed hydrogen atoms 118
- chemical reactions *see* reactions
- chemisorption 98–99, 175–177
 - heat of 99
 - metal oxides 102–104
 - metal surfaces 101–102
 - potential energy 96
- chloralkaline electrolysis 161
- climate 34–35
- CO₂ emissions 34–35
 - reduction 35–37
- coal
 - gasification 49
 - hydrogen production 149–155
 - reserves 30–31
- coating, thin film 105–107
- coexistence of Mg and MgH₂ 300–302
- combinatorial research 316–321
- combustion
 - air/fuel ratio 374–375
 - biomass 41–42
 - hydrogen 9, 91
 - internal combustion engines 371–373
 - methane, propane and gasoline 91
- common pressure vessel (CPV) 397, 400–401
- complex formation, “interstitial” hydrides 199–200
- complex hydrides 211–237
 - encapsulation 231–232
 - non-transition metal 203–213
 - safety aspects 231–232
 - thin films 283
 - transition metal *see* transition metal hydrides
- complexes
 - metal ammine 243–244
 - metal–hydrogen 195
 - mononuclear 196–198
 - polynuclear 198–199

- components, fuel cells 346–348
 - composition, fossil fuels 27–28
 - compounds
 - ammonia-based 242–244
 - intermetallic 190
 - compressed hydrogen gas,
 - volumetric/gravimetric density 169
 - compressibility 80
 - compression ratio 378
 - computational methods
 - force field calculations 229
 - Monte Carlo simulations 175
 - NaAlH₄ systems 225–231
 - concentration dependence
 - dielectric function 286
 - switchable mirror properties 281, 285
 - conductivity
 - specific 347
 - temperature dependence 287
 - conversion, energy *see* energy
 - cooling
 - efficiency 389
 - fuel cells 351
 - copper, hydrogen adsorption 115–116, 119–121
 - cost, fuel cells 361–363
 - coupled systems, exchange coupled 267–270
 - coupling
 - (anti-)ferromagnetic 269
 - interlayer exchange *see* interlayer exchange coupling
 - covalent bonds, hydrogen 88
 - coverage, atomic hydrogen on Cu(100) 120
 - CPV *see* common pressure vessel
 - cryocooler
 - BETSCE 391
 - Joule–Thomson 389
 - liquid hydrogen sorption 390
 - cryogenic tanks 404
 - cryogenic temperatures, hydrogen adsorption 181–183
 - cryogenics applications, hydrogen 388–394
 - cryostat, solid hydrogen 392
 - crystal structure
 - crystallization, borohydride solutions 248
 - cubic YH₃ 298–300
 - Curie temperature, ferromagnetic film 267
 - current–voltage characteristics, fuel cells 342
 - cycles
 - biosphere 47–48
 - carbon 37–39
 - geochemical 39
 - global water cycle 46
 - hydrogen *see* hydrogen cycle
 - 100 cycles test 224
 - cyclic stability, Ti-doped sodium aluminum hydrides 223–224
- ## D
- d-band 111
 - DBFC *see* direct borohydride fuel cell
 - deabsorption, catalyzed 220–223
 - decomposition
 - activation energy 223
 - Ti-doped sodium aluminum hydrides 223
 - decomposition temperature,
 - tetrahydroborates 207
 - defect, point 103
 - defect-free surface 104
 - dehydrogenation
 - reactions 129
 - reversible 236
 - density
 - compressed hydrogen gas 169, 173
 - energy *see* energy density
 - gravimetric 169
 - hydrogen in metallic hydrides 195
 - liquid hydrogen 173
 - p-hydrogen 76
 - power 368
 - solid hydrogen 173
 - volumetric 169
 - deposition, RE hydride thin films 279
 - deposition techniques, magnetic films 267
 - desorption, hydrogen 114–115
 - desorption enthalpy, complex transition metal hydrides 203
 - desorption pressure 219
 - detonability limits, hydrogen–air–water vapor 92
 - detonation 90–94
 - deuterium 12
 - diatomic hydrogen *see* molecular hydrogen
 - dielectric function
 - concentration dependence 286
 - magnesium hydride 297
 - Diesel-cycle gaseous-fuel engines 373
 - diffusion
 - gas diffusion electrodes 347–348
 - hydrogen 85–90
 - opaque materials 314–316
 - switchable mirrors 312–314
 - diffusion coefficients, hydrogen 85
 - dihydride state 281–282, 285
 - dihydrogen *see* molecular hydrogen

418 | Index

- direct borohydride fuel cell (DBFC) 125,
130, 134–135, 364–371
 - catalysts 369–370
 - electricity generation 367
 - electrochemistry 365
 - electrode kinetics 365–366
 - thermodynamics 365–366
- direct methanol fuel cell (DMFC) 241, 344,
364–365, 369
- disasters
 - Challenger 17–20, 400
 - Hindenburg 14–17, 66
- dissociation
 - catalyzed 108–125
 - hydrogen molecule 105–107
 - metal hydrides 218
- dissociation energies, covalent hydrogen
bonds 88
- dissociation reaction, hydrogen molecule
89
- distribution, hydrogen 56
- DMFC *see* Direct methanol fuel cells
- Döbereiner platinum lighter 10
- domain switching, optical 293
- doped NaAlH₄ systems, reversible
225–231
- dosing 122–123
- dual mode nuclear propulsion system 407
- dual-fuel vehicle 381
- dynamic hydriding/dehydriding process
253
- E**
- economic factors, hydrogen production 54
- effective medium approach 106
- efficiency
 - Carnot 340
 - cooling 389
 - electrochemical 341
 - fuel cells 340–343, 353–354
 - thermodynamic 378–379
- electric power train, hybrid 357–359
- electrical conductivity *see* conductivity
- electrical properties, switchable mirrors
286–288, 305–306
- electricity 155–163, 162
 - generation 367
- electrochemical efficiency 341
- electrochemical loading 266
- electrochemistry, borohydride fuel cells
365
- electrochromical devices 321–323
- electrode kinetics, borohydride fuel cells
365–366
- electrode potential, equilibrium 339
- electrode stack designs 398
- electrodes
 - gas diffusion 347–348
- electrolysis 5
 - alkaline 158–159
 - chloralkaline 161
 - hydrogen production 50–51, 155–163
 - solid-polymer 160
 - using renewable energy 161–163
 - water 155–157
- electrolytes
 - fuel cells 344–346
 - specific conductivity 347
- electrolytic loading 280
- electromigration, switchable mirrors
312–314
- electron correlation models 291
- electronegativity 87
 - Allred-Rochow 189
- electronic band structure 307
- elements
 - binary hydrides 189
 - hydrides 87
- empirical models, metal hydrides 192–195
- encapsulation, complex hydrides 231–232
- endothermic reactions, equilibrium
constants 152
- energy
 - activation *see* activation energy
 - conversion 41, 59–63
 - dissociation 88
 - Gibbs *see* Gibbs energy
 - potential *see* potential energy
 - production 49–63
 - renewable *see* renewable energy
- energy consumption, primary 25–26
- energy density, batteries and fuel cells 337
- engine torque 376
- enthalpy
 - desorption 203
 - hydrogen 78, 81–83
 - hydrogen production 150–151
- enthalpy diagram 209
- enthalpy of formation
 - alloys 320–321
 - hydrides 191–194
- enthalpy of segregation 100
- entropy
 - hydrogen 77–78
 - n-hydrogen 83
- entropy of formation
 - alloys 320–321
 - hydrides 191–194

- environmental effects
 - fossil fuels 33–35
 - hydrogen economy 65
 - hydrogen production 54
- environment, global 47–48
- epitaxial switchable mirrors 294–295
- epitaxial thin films, stress 282–283
- equation of state (EoS), hydrogen 77–81
- equations
 - first rocket equation 382
 - ideal gas law 119
 - Langmuir isotherm 174, 176
 - Lennard–Jones potential 175
 - Stirling approximation 119
 - Van der Waals 79, 167
 - Van’t Hoff equation 192
- equilibrium constants, exothermic and endothermic reactions 152
- equilibrium coverage, atomic hydrogen on Cu(100) 120
- equilibrium electrode potential
 - fuel cells 339
- ESA 392–394
- ex situ* hydrogen loading 279–281
- exchange coupled systems 267–270
- excrecence, vermicular 230
- exhaust water 244–256
- exothermic reactions, equilibrium constants 152
- explosion properties, hydrogen, methane, propane and gasoline 91
- explosive hazards 93
- F**
- F *see* ferromagnetic coupling
- Faraday efficiency 156
- Fe/V superlattices 270–271
 - ideal interfaces 275
 - magnetization 273
- ferromagnetic (F) coupling 269
- ferromagnetic film, Curie temperature 267
- fiber optic hydrogen sensors 325–326
- film deposition techniques 267
- films, thin *see* thin films
- fire hazards 92–93
- first rocket equation 382
- Fischer–Tropsch process 155
- flammability limits 91–92
- fluorinated surfaces 137–138
- force field calculations 229
- formation, fossil fuels 27–28
- fossil fuels 3
 - advantages and uses 25–27
 - consumption growth 23–25
 - environmental impact 33–35
 - formation and composition 27–28
 - future trends 35–37
 - global reserves and production 29–33
 - hydrogen production 149–154
 - proven reserves 30–31
 - replacement by hydrogen cycle 43–45
- free electron metals 121
- fuel cell power train 357–359
- fuel cell stacks 348–349
- fuel cell systems 348–354
 - low power 350
- fuel cells 14, 60–63
 - active components 346–348
 - AFC *see* alkaline fuel cell
 - air supply 351
 - alkaline
 - automotive applications 352, 355–358
 - bipolar stacking 349
 - cooling 351
 - cost 361–363
 - current–voltage characteristics 342
 - DBFC *see* direct borohydride fuel cell
 - DMFC *see* direct methanol fuel cell
 - efficiency 340–343, 353–354
 - electrolytes 344–346
 - equilibrium electrode potential 339
 - Gibbs energy 338–340
 - history 336–337
 - hydrogen as fuel 364–371
 - hydrogen/oxygen 339
 - lifetime 363
 - losses 342, 353
 - MCFC *see* molten carbonate fuel cell
 - micro-fuel cells 369
 - PAFC *see* phosphoric acid fuel cell
 - PEMFC *see* PEMFC
 - portable applications 354–355
 - power and heating 62–63
 - proton exchange membrane (PEM) 61
 - SOFC *see* solid oxide fuel cell
 - space applications 361
 - temperature range and reactants 343
 - thermodynamics 337
- fuels
 - air/fuel ratio 374–375
 - biomass energy 39–40
 - gasoline 91
 - fossil *see* fossil fuels
 - gaseous 373
 - hydrogen 16–20, 23–67, 127, 371–372
 - rocket fuel 382–388
 - space shuttle 16–20
- fugacity 81

420 | *Index*

functionalized materials

- magnetic heterostructures 265–275
- switchable mirrors 275–327

fusion, inertial confinement 408

G

Gaia hypothesis 43

galvanic cells 337–339

gas chain 336

gas cylinders, high pressure 167–170

gas diffusion electrodes 347–348

gas loading/unloading 266, 279–280

gas reserves 30–31

gas turbines 59–60

gaseous hydrogen, physical properties 78

gaseous-fuel engines 373

gasification

- biomass 41–42

- coal 49,

gasoline, combustion and explosion properties 91

gas–solid surface interactions 132

geochemical cycle 39

Gibbs energy 77–78, 81

- fuel cells 338–340

- n-hydrogen 83

- water electrolysis 155–156

global carbon budget 44

global environment, biosphere cycles 47–48

global reserves, fossil fuels 29–33

global water cycle 46

graphene sheets 180

graphitic nanofibers 179–180

gravimetric density, compressed hydrogen gas 169

greenhouse effect 3

grid independent power 356

Grove, Sir William Robert 10–11, 336

GW approximation (GWA) 291, 293, 295

H

H *see* hydrogen

Haber, Fritz 11

halogens cycle 48

hazards

- explosive 93

- fire 92–93

- hydrogen economy 65–66

- preventive measures 93

heat

- specific heat ratio 378

heat engines, efficiency 341

heat of chemisorption 99

heat of solution 99

heat release rate 377

heating, fuel cells 62–63

Helmont, Jan Baptista van 7

heterostructures, magnetic 265–275

high pressure gas cylinders 167–170

high temperature, hydrogen adsorption 183–184

Hindenburg disaster 14–20, 66

history

- fuel cells 336–337

- hydrogen 7–20

homogeneous ternary hydride phase 229

homogenous water gas reaction 150

hybrid electric power train 357–359

hydride ion 129–131

hydride thin films 277–279

hydride-forming intermetallic compounds 190

hydrides 87

- binary 188–189

- carbon *see* carbon hydrides

- complex *see* complex hydrides

- formation *see* metal hydride formation

- homogeneous ternary hydride phase 229

- intermetallic 188–189

- metal *see* metal hydrides

- non-transition metal complex *see* non-transition metal complex hydrides

- organic *see* organic hydrides

- surface engineering 132–138

- transition metal complex *see* transition metal hydrides

hydrocarbons, hydrogen production 149–155

hydrogasification, biomass 41–42

hydrogen

- adsorption and absorption 94

- applications 127

- as a fuel 16–20, 23–67, 127, 371–372

- chemical properties 85–90

- combustion 9

- combustion and explosion properties 91

- conversion to energy 59–63

- cryocoolers 388–394

- density in metallic hydrides 195

- diffusion 85–90, 314–316

- diffusion coefficients 85

- dissociation 108–125, 134

- equation of state 77–81

- flammability limits 91–92

- four states 125–132

- fuel cells 364–371

- hazards 92–93
- history 7–20
- ignition and detonation 90–94
- interaction with solid surfaces 94–108
- o-hydrogen 73–74
- p-hydrogen 73–74
- present scenario 48–49
- primitive phase diagram 76, 166
- rocket fuel 382–388
- safety concepts 93
- space applications 381–410
- state transitions 126
- toxicology 93
- hydrogen adsorption 173–188
 - cryogenic temperatures 181–183
 - high temperature 183–184
 - measuring techniques 177–178
 - metal hydrides 189–192
- hydrogen as a fuel, internal combustion engines (ICE) 371–372
- hydrogen atoms, chemical potential 118
- hydrogen bomb 12
- hydrogen concentration dependence 281, 285
- hydrogen cryostat 392
- hydrogen cycle
 - energy production 49–63
 - implementation 63–67
 - key elements 45–46
 - replacement of fossil fuel 43–45
 - water 46–47
- hydrogen desorption
 - mass spectra 124
 - TPD spectra 115
- hydrogen distribution 56
- hydrogen functionalized materials *see* functionalized materials
- hydrogen gas 71–94
 - compressed 169
- hydrogen generation
 - hydrolysis 248–249
 - protide 130
 - systems and devices 250–252
- hydrogen in transportation 13–14
- hydrogen ion 128
- hydrogen isotopes 71–72
- hydrogen liquefaction 171
- hydrogen loading 266–267, 279–281
- hydrogen molecule 72–75
 - dissociation 89, 105–107
 - physical properties 75–77,
- hydrogen power train 380
- hydrogen powered space launch vehicles 384
- hydrogen production
 - biomass 40–43, 51
 - coal gasification 49
 - cost 5
 - electrolysis 50–51, 155–163
 - environmental, economic and scaling factors 54
 - from carbon and water 154
 - from coal and hydrocarbons 149–155
 - natural gas reformation 49–50
 - non-renewable methods 49–55
 - nuclear power 49
 - photo-biological 53
 - photo-electrochemical 52–53
 - reactions 149–154
 - renewable methods 50–55
 - thermochemical 51–52
 - thermophysical 52
- hydrogen recombination, catalysis 108–125
- hydrogen sensors, fiber optic 325–326
- hydrogen sorption cryocooler 390
- hydrogen sources, water 246
- hydrogen spark ignition engine 373–379
- hydrogen storage 56–59, 95
 - alanates 234–236
 - ammonia and ammonia-based compounds 242–244
 - basic methods 168
 - carbon hydrides 240–242
 - carbon materials 178–184
 - complex transition metal hydrides 195–203
 - high pressure gas cylinders 167–170
 - in molecular form 165–172
 - indirect *see* indirect hydrogen storage
 - liquid hydrogen 170–172
 - lithium nitride and imide 236
 - metal hydrides 133, 188–195
 - metal–organic frameworks 186–187
 - non-transition metal complex hydrides 203–213
 - organic hydrides 237–244
 - reversible *see* reversible hydrogen storage
 - saturation capacity 183
 - silicate structures 184–186
 - space shuttle 387, 404–405
 - zeolites 184–186
- hydrogen storage materials
 - lightweight 318–320
 - reversible 212
- hydrogen transmission 55–56
- hydrogen/oxygen fuel cell, overall reaction 339

422 | Index

hydrogenation
– reactions 129
– reversible 236
hydrogen-ICE 372–373, 379–381
hydrogenography 320–321
hydrogen-to-carbon ratio 201
hydrolysis 248–250
hydroxonium ion 128
hysteresis, optical properties 288–290

I
ICE *see* internal combustion engines
ideal gas law 119
ideal interfaces, Fe/V superlattices 275
IEC *see* interlayer exchange coupling
ignition, hydrogen 90–94
image processing 356
imide, lithium 236
implementation, hydrogen cycle 63–67
in situ deposition, RE hydride thin films 279
indicator layers 311–316
indirect hydrogen storage 244–256
inertial confinement fusion 408
integrated thermal desorption spectra 208
Intensity map, reflection 310
interaction potential energy, hydrogen molecule 73
interfaces
– ideal 275
– solid–liquid 249–250
interlayer exchange coupling (IEC) 268–270, 272
intermetallic compounds, hydride-forming 190
intermetallic hydrides 188–189
internal combustion engines (ICE) 371–373
International Energy Agency (IEA) 35
International Space Station 399
“interstitial” hydrides, complex formation 199–200
inversion curve 84–85
ionization potential 89
Ising model 272
isorecticular MOFs 187
isotherm
– Langmuir 174, 176
– pressure–composition 216–217, 299–300, 304

J
Joule, James 81
Joule–Thomson coefficient 84

Joule–Thomson cryocooler 389
Joule–Thomson cycle 172
Joule–Thomson effect 81–84
Justi, Eduard 13

K

Kelvin, William Thomson, Lord of 81
kinetics, tetrahydroborates 208–211
Kirchhoff, Gustav 11

L

Langmuir isotherm 174, 176
laser deposition, pulsed 279
lattice defects, STM images 103
lattice planes 98
Lavoisier, Antoine Laurent 9
layering, self-organized 309
LDA *see* Local-density approximation
Lennard–Jones potential 96, 175, 190
lifetime
– fuel cells 363
– nickel–hydrogen batteries 403
ligands 196
lightweight hydrogen storage materials 318–320
Linde cycle 172
liquefaction, hydrogen 171
liquid electrolyte Gd–Mg switchable mirror 296
liquid hydrogen 170–172
– density 173
– physical properties 78
– storage vessels 171–172
liquid hydrogen sorption cryocooler 390
liquid propulsion systems, bipropellant 385
liquid–solid interface 249–250
liquid–solid surface interactions 133
lithium nitride and imide 236
loading, *ex situ* 279–281
loading technique 266–267
local band-structure model 193
Local-density approximation (LDA) 291–294
Long March vehicle 386
losses, fuel cells 342, 353
low power fuel cell systems 350
low temperature properties, p-hydrogen 76
Lurgi process 12

M

magnesium hydride, optical properties 295–296
magnesium–rare earth films, switchable mirrors 295–303

- magnesium–transition metal films, switchable mirrors 303–311
 - magnetic asymmetry ratio 274
 - magnetic heterostructures 265–275
 - magnetic saturation field 272
 - magnetization, Fe/V superlattices 273
 - magneto-optic Kerr effect 272
 - manufacturers
 - alkaline electrolysis 158
 - solid-polymer electrolysis 160
 - mass spectrometry 124
 - MCFC *see* molten carbonate fuel cell
 - melting point 247
 - metal ammine complexes 243–244
 - metal hydrides
 - batteries 326
 - dissociation 218
 - empirical models 192–195
 - formation 109, 121–124
 - hydrogen adsorption process 189–192
 - hydrogen density 195
 - hydrogen storage 133
 - hydrogen storage 188–195
 - NiMH batteries *see* NiMH batteries
 - non-transition metals 203–213
 - optical properties 275–327
 - space suit cooling 405
 - thin films 283
 - transition metals *see* transition metal hydrides
 - metal oxides, chemisorption 102–104
 - metal surfaces 101–102, 113
 - metal–hydrogen complexes 195
 - metal–insulator transition 286–288, 305–306
 - metallic RE films 277
 - metal–organic frameworks (MOFs), hydrogen storage 186–187
 - methane
 - biomass methanation 41–42
 - combustion and explosion properties 91
 - methanol, hydrogen storage 240–241
 - MI transition *see* metal–insulator transition
 - micro-fuel cells 369
 - microscopic shutter effect 296–298
 - military applications, portable fuel cells 356
 - mirrors, switchable 275–327
 - mischmetal nickel alloys 137
 - mobile communication 356
 - MOFs *see* metal–organic frameworks
 - molecular beam deposition 279
 - molecular hydrogen 126–128
 - storage 165–172,
 - molten carbonate fuel cell (MCFC) 345, 349, 359
 - monatomic hydrogen 128–129
 - mononuclear complexes 196–198
 - Monte Carlo simulations 175
 - multilayers, tailoring of optical properties 302–303
- N**
- NaAlH₄ *see* sodium aluminum hydrides
 - NaBH₄ *see* sodium borohydride
 - nanofibers, graphitic 179–180
 - nanosized surface structures 136–137
 - nanotubes 179–180
 - NASA 16–20, 361, 383, 401
 - natural gas 3, 27–28
 - reformation 49–50
 - NECAR 359
 - nickel alloys, mischmetal 137
 - nickel–hydrogen batteries
 - International Space Station 399
 - lifetime 403
 - pressure vessels 397, 400–401
 - reactions 395–396
 - space application 394–404
 - space performance characteristics 402
 - NiMH (nickel metal hydride) batteries, secondary 134
 - nitride, lithium 236
 - nitrogen cycle 48
 - NO_x-emissions, hydrogen spark ignition engine 373–375
 - non-renewable hydrogen production 49–55
 - non-transition metal complex hydrides 203–213
 - normal-hydrogen (n-hydrogen), triple point 77
 - nuclear power, hydrogen production 49
 - nuclear propulsion system, dual mode 407
- O**
- oil reserves 30–31
 - optical domain switching 293
 - optical properties
 - hysteresis 288–290
 - magnesium hydride 295–296
 - metal hydrides 275–327
 - switchable mirrors 284, 306–308
 - tailoring 302–303
 - orbitals, overlapping 110–111
 - organic hydrides 237–244
 - Organization of Petroleum Exporting Countries (OPEC) 24
 - ortho-hydrogen (o-hydrogen) 73–74

424 | Index

Otto-cycle engine 376–378

oxides, metal 102–104

P

PAFC *see* phosphoric acid fuel cell

Paracelsus 7

para-hydrogen (p-hydrogen) 73–74

– low temperature properties 76

– triple point 77

paramagnetic layers 268, 270

partition functions, H₂ and H 118

PEFC *see* PEMFC

Peierls distortion models 290–291

PEM (proton exchange membrane) fuel cell 61

PEMFC 127–128, 344, 364, 366

– automobile applications 249

– hydrogen dissociation 134

– hydrogen storage device 250–251

– thermodynamics 365

periodic table of the elements 87, 189

phase diagram, hydrogen 76, 166

phosphoric acid fuel cell (PAFC) 344–345, 364

photo-biological hydrogen production 53

photo-electrochemical hydrogen production 52–53

photosynthesis 2–3, 237–238

– hydrogen storage 238–240

– overall chemical reaction 238

physisorption 98–99, 173–175

pixel-by-pixel switching 294

Planck spacecraft 393

p-metal hydrides 203–204

point defects, STM images 103

polarization, cell 368

polycrystalline thin films, stress 282–283

polymer electrolyte fuel cell (PEFC) *see* PEMFC

polymer electrolyte membrane fuel cell *see* PEMFC

polymeric hydrides 203–204

polynuclear complexes 198–199

portable applications, fuel cells 354–355

potential

– chemical *see* chemical potential

– fuel cell electrodes 339

– ionization 89

– Lennard-Jones *see* Lennard-Jones potential

potential energy

– chemisorption 96

– hydrogen approaching metal surfaces

113

– hydrogen molecule on metal surface 109

– interaction 73

powder patterns 225, 227

power and heating, fuel cells 62–63

power density 368, 372

power trains 357–359

– hydrogen 380

precoverage, surface 105–107

pressure, ad-/desorption 219

pressure vessels, nickel–hydrogen batteries 397, 400–401

pressure–composition isotherm 216–217, 299–300, 304

primary energy consumption 25–26

production

– fossil fuels 29–33

– hydrogen 40–43

projection, H₂ states 112

propane, combustion and explosion

properties 91

propulsion system

– dual mode nuclear 407

– spacecrafts 385

protide 129–131, 245

– NaBH₄ synthesis 133–134, 254

protium 128–129

proton 128

proton exchange membrane (PEM) fuel cell 61

proton–proton separation 73

pulsed laser deposition 279

Q

quaternary 3d transition metal hydrides 198

R

Raney-nickel 158

rare-earth (RE) hydride thin films 277–279

– *in situ* deposition 279

– switchable mirrors 283

reabsorption, catalyzed 220–223

reactants, fuel cells 343

reactions

– Boudouard reaction 150–151

– Calvin–Benson cycle 239

– dissociation of hydrogen molecule 89

– equilibrium constants 152

– Fischer–Tropsch process 155

– homogenous water gas reaction 150

– hydrogen production 149–154

– hydrogen/oxygen fuel cell 339

– hydrogenation and dehydrogenation 129

– nickel–hydrogen batteries 396

- photosynthesis 238
 - Sabatier 406
 - solid-state 196
 - soot reactions 150–151
 - yield 153
 - reactions, surface 107–108
 - reactivity, surfaces 136
 - recombination, catalyzed 108–125
 - reflection
 - hydrogen concentration dependence 285
 - Intensity map 310
 - reflection spectra, switchable mirrors 303, 308
 - reformation, natural gas 49–50
 - renewable carbon resources 42–43
 - renewable energy
 - electricity 162
 - electrolysis 161–163
 - renewable hydrogen production 4, 50–55
 - reprocessing, NaBH_4 253–255
 - reserves, fossil fuels 30–31
 - resources, renewable carbon 42–43
 - reversible doped NaAlH_4 systems 225–231
 - reversible hydrogen storage
 - carbon hydrides 241–242
 - materials 212
 - reversible hydrogenation/dehydrogenation 236
 - Rochow *see* Allred-Rochow electronegativity
 - rocket fuel 382–388
- S**
- Sabatier reaction 406
 - safety
 - complex hydrides 231–232
 - fire and explosive hazards 93
 - hydrogen economy 65–66
 - saturation capacity, hydrogen storage 183
 - saturation field, magnetic 272
 - scaling factors, hydrogen production 54
 - scanning tunnel microscopy (STM), point defect images 103
 - seasonal hydrogen system 242
 - secondary batteries, Ni–MH 134
 - segregation
 - enthalpy 100
 - surface 98–101
 - self-organized layering 309
 - sensors 357
 - hydrogen 325–326
 - shift reaction, biomass 41–42
 - shutter effect, microscopic 296–298
 - Sievert's method 177
 - silicate structures, hydrogen storage 184–186
 - single pressure vessel (SPV) 397, 400–401
 - smart windows 324
 - sodium aluminum hydrides 213–233, 225–231
 - sodium borohydride 133–134, 253–255
 - SOFC *see* solid oxide fuel cell
 - solid hydrogen, density 173
 - solid hydrogen cryostats 392
 - solid oxide fuel cell (SOFC) 345–346, 349, 359
 - solid polymer electrolyte fuel cell (SPEFC) *see* PEMFC
 - solid solutions 191
 - solid surfaces, interaction with hydrogen 94–108
 - solid–liquid interface 249–250
 - solid-polymer electrolysis (SPE) 160
 - solid-state reactions 196
 - solubility, borohydrides 246–247
 - solutions
 - alkaline 245–246
 - crystallization 248
 - heat of 99
 - soot reactions 150–151
 - sorption cryocoolers 390–391
 - sorption mechanism, tetrahydroborates 208–211
 - space applications
 - fuel cells 361
 - hydrogen 381–410
 - nickel–hydrogen batteries 394–404
 - space launch vehicles, hydrogen powered 384
 - space shuttle 16–20, 386
 - Buran 385
 - hydrogen and oxygen storage systems 387
 - hydrogen storage 404–405
 - main engine 388
 - space suit cooling, metal hydrides 405
 - spark ignition engine 373–379
 - sp-band 110–111
 - SPE *see* solid-polymer electrolysis
 - specific conductivity, fuel cell electrolytes 347
 - specific heat ratio 378
 - specific surface area 183
 - spectra
 - reflection 303, 308
 - thermal desorption 208
 - TPD 115, 119, 123
 - transmission 303, 308

426 | Index

- SPEFC *see* PEMFC
sputtering 279, 319
SPV *see* single pressure vessel, 398
stacks, fuel cells 348–349
stationary applications, fuel cells 358–359
sticking coefficient 116–117
– molecular hydrogen on Cu(110) 120
sticking probability 116–117
Stirling approximation 119
STM *see* scanning tunnel microscopy
storage, hydrogen *see* hydrogen storage
storage capacity 183, 214
– Ti-doped sodium aluminum hydrides 223–224
storage vessels, liquid hydrogen 171–172
stress, in thin films 282–283
submarines, fuel cell propulsion system 360
substrate–adsorbate distance 176
sulfur cycle 48
superlattices, Fe/V *see* Fe/V superlattices
surface area, specific 183
surface engineering, hydrides 132–138
surface interactions 132–133
surface precoverage 105–107
surface reactions, relevance for bulk
absorption 107–108
surface reactivity 136
surface segregation 98–101
– binary alloys 100
surface structure 97–98
– nanosized 136–137
surfaces
– defect-free 104
– fluorinated 137–138
– interaction with hydrogen 94–108
– metal 101–102
switchable absorbers 324
switchable mirrors 275–327
– all-solid-state 323
– applications 311–321
– diffusion and electromigration 312–314
– electrical properties 286–288, 305–306
– epitaxial 294–295
– first-generation 283
– liquid electrolyte 296
– optical properties 306–308
– reflection and transmission spectra 303, 308
– second generation 295–303
– theoretical models 290–294
– thin film 277–283
– third generation 303–311
– transmission 281
syngas 154
- T**
T metal *see* transition metal . . .
tailoring
– optical properties 302–303
– thermodynamic 232–233
TDS *see* thermal desorption spectroscopy
temperature dependence, conductivity 287
temperature programmed desorption (TPD)
– hydrogen desorption 114–115
– spectra 114–115, 119, 123
temperature range, fuel cells 343
temperatures
– cryogenic *see* cryogenic temperatures
– decomposition 207
– high *see* high temperatures
– low *see* low temperatures
terminal hydrogen ligands 196
ternary hydride phase, homogeneous 229
ternary 3d transition metal hydrides 198
tetrahydroborates
– decomposition temperature 207
– sorption mechanism and kinetics 208–211
– stability 206–208
– structure 205–206
thermal conversion, biomass 41–42
thermal desorption spectroscopy (TDS) 178
thermochemical hydrogen production 51–52
thermochromic devices 323
thermodynamic efficiency 378–379
thermodynamic tailoring 232–233
thermodynamics
– adsorbed hydrogen 98–101
– borohydride fuel cells 365–366
– fuel cells 338–339
– hydrogen 77–81
– PEMFC 365
– Ti-doped sodium aluminum hydrides 215–220
thermogravimetry 178
thermophysical hydrogen production 52
thin film coating 105–107
thin films
– magnesium–rare earth 295–303
– magnesium–transition metal 303–311
– rare-earth hydride *see* rare-earth hydride thin films

- stress 282–283
- switchable mirrors 277–283
- thin films, complex metal hydrides 283
- Thomson, William *see* Kelvin
- titanium-doped sodium aluminum hydrides 213–233
 - decomposition 223
 - thermodynamic properties 215–220
- torque, engine 376
- toxicology, hydrogen 93
- TPD *see* temperature programmed desorption
- transition metal hydrides
 - bonding 200–201
 - complex 195–203, 237
 - hydrogen storage properties 202
 - ternary and quaternary 3d 198
- transmission
 - hydrogen 55–56
 - hydrogen concentration dependence 281, 285
 - hysteresis 289
- transmission spectra, switchable mirrors 303, 308
- trihydride state 281–282, 285
- triple point, p- and n-hydrogen 77
- tritium 12

U

unloading, hydrogen 266

V

Van der Waals equation 79, 167

- coefficients 80

Van der Waals force 79
Van't Hoff diagram, dissociation 218

Van't Hoff equation 192
Van't Hoff plot 194
vapor pressure, p-hydrogen 76
vermicular excrescence 230
vessels

- liquid hydrogen 171–172
- pressure 397, 400–401

viscosity, borohydrides 247
visualization, hydrogen diffusion 314–316
volumetric density, compressed hydrogen gas 169
volumetry 177

W

water

- electrolysis 155–157
- exhaust 244–256
- global cycle 46–47
- hydrogen source 246

water gas reaction, homogenous 150
wavefunction, hydrogen molecule 72, 74
windows, smart 324

X

yield 153

Y

yttria-stabilized zirconia (YSZ) 345–346

Z

zeolites, hydrogen storage 184–186
zeppelin 14–16
zero emission vehicles (ZEV) 61–62, 359

- historic 14

z-scheme, photosynthesis 239

