# Index

#### а

ab initio molecular dynamics (AIMD) 259, 335, 336 air plasma spray (APS) technique 387, 393.394 alkaline fuel cell (AFC) 5 anisotropy oxygen transport 244–246 A-site ordered double perovskites 244 - 246Ruddlesden-Popper (RP) perovskites 244anode catalytic properties 115 development materials alternative anode materials 118 - 124Ni-YSZ cermet materials 117 - 118sulfur tolerant anode materials 124 - 126electrochemical oxidation 115 reaction mechanism basic operating principles 114-115 and kinetics 126-135 three-phase boundary 115–117 Arrhenius equation 51

# b

 $\begin{array}{l} BaBi_{0.05}Co_{0.8}Nb_{0.15}O_{3-\delta}\ (BBCN) & 88\\ BaBi_{0.05}Co_{0.8}Ta_{0.15}O_{3-\delta}\ (BBCT) & 88\\ BaCo_{0.7}Fe_{0.2}Nb_{0.1}O_{3-\delta}\ (BCFN) & 88\\ Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}\ (BSCF) & 9, 85,\\ & 88, 93, 94, 101, 199, 234, 340,\\ & 359, 436, 438 \end{array}$ 

bi-layered fuel cell device 200, 205, 350 bulk heterojunction (BHJ) effects 198–200, 205, 266, 276, 359–360

## С

cathode material 79 materials development double perovskite cathode materials 89-94 perovskite cathode materials 82 - 89microstructure optimization 94-102 composite cathodes 97–102 nanostructured cathodes 94-96 properties 79 reaction mechanism 80-82 cell's performance stability 59, 401 Ceria (CeO<sub>2</sub>) 213 intermediate temperature 214-216 low temperature non-doped 222-235 surface doping 216-221 mixed ionic and electronic conduction 234 research and development 214 structure diagram 215 Ceria-carbonate nanocomposite transport model 18 cermet 113, 115, 117-120, 123-124, 128, 135, 177-178 charge transport electrochemical aspects 320-321 ionic conduction 321–326

Solid Oxide Fuel Cells: From Electrolyte-Based to Electrolyte-Free Devices, First Edition. Edited by Bin Zhu, Rizwan Raza, Liangdong Fan, and Chunwen Sun. © 2020 Wiley-VCH Verlag GmbH & Co. KGaA. Published 2020 by Wiley-VCH Verlag GmbH & Co. KGaA. charge transport (contd.) ionic transport number measurements 331–332 mechanism and coupling effects 326-330 physical aspects 319–320 superionic conduction and transportation 330-331 Co-based perovskite cathodes 85–88 composite cathodes 81, 84, 87, 97–102 composite electrolytes oxide-carbonate composite 53-60 materials fabrication 54–57 performance and stability optimization 57-60 oxide-oxide electrolyte 52-53 oxide-salt composite electrolytes 60 - 62

# d

3D contact control design 156–163 vs. 2D interface contact 151–153, 169–171 quantitative effects cell transient performance 163–166 on the steady-state performance of a cell 166–168 dense electrolyte 52, 79, 321, 387, 393–394, 408, 415 double perovskite cathode materials 89–94

# е

electrochemical impedance spectroscopy (EIS) 119, 181, 191, 220, 229–230, 233, 283, 286–287, 296–298, 300, 303, 307, 310–312, 323–325, 327–328, 332–335, 339–340 electrolysis 3, 43, 45, 66–67, 352, 361, 369, 452–453, 462 electrolyte-free fuel cells (EFFCs) 20, 179 advantages 177

conventional ionic electrochemistry 348 EIS analysis 334-335 electron and ionic conductivities 332 extensive research and demonstrations 181 industrial-grade rare-earth 279–287 oxide LCP 280-281 semiconductor-ionic composite based on LCP 281-287 ionic conducting/electronic insulting layer 348 materials development 275-276 natural materials 276-279 operational principles 347 semiconductor band effects 335 - 339semiconductors and associated methodologies 352 simulations 339-343 stability operation and Schottky iunction in-situ effect 288-290 performance stability 288 electromotive force (EMF) method 27, 332, 371 enhanced ionic conductivity by band bending 264-266 by strain 259-264

# f

fabrication 7, 35, 41, 44, 45, 52, 54–57, 59, 61, 63, 67–68, 95–96, 98–99, 102, 115, 118, 128, 182, 325–327, 384, 395, 398, 402, 408, 433, 439–441 fast oxygen migration 248 Fe-based perovskite cathodes 88–89 Fermi energy ( $E_{\rm F}$ ) 264–265, 336–337, 355, 366 fluorite anode materials 118–120 fuel battery 3 fuel cell (FC) 3 applications 213 definition 450 materials and technologies 5–10

new electrolyte developments 10 - 20principle 3-5 types 5 fuel cell semiconductor electrochemistry electrochemistry vs. semiconductor physics 355-356 extending applications by coupling devices 367-368 physics and electrochemistry at interfaces 353-355 working principle 356-366 fuel cell system biogas 454-458 biomass integration 453-454 efficiency 458-460 effect of different temperature 458 fuel utilization factor 458-460 operating pressure 460 integrated new clean energy system 460-462 solar cell 447-450 solar cell integration 450-452 solar-electrolysis 452-453

# g

gas-phase diffusion 82, 100

## h

heterostructure composite approach 17 high electronic conductivity 79, 122, 180, 257 hydrocarbon fuels 9, 39, 45, 113, 117–118, 120, 123, 133, 135 hydrogen-rich fuel 113

#### i

infiltration method 55, 60 internal manifold and external manifold 415–416 ion conduction/transportation 49–52 Arrhenius equation 51 general strategy 51 positive and negative charge 51 ionic conductivity 5, 35, 83, 114, 177, 213, 259, 275, 321, 347 iron 3, 9, 86, 89, 100, 278, 291–292, 305, 379

# k

Kröger–Vink Notation 80, 197, 330, 356

#### I

 $La_{0.33}Ce_{0.62}Pr_{0.05}O_{2-\delta}$  (LCP) 186–187, 200-201, 279-291, 295, 297-302, 406-408 La<sub>0.2</sub>Sr<sub>0.25</sub>Ca<sub>0.45</sub>TiO<sub>3</sub> (LSCT) 180–181, 185  $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$  (LSCF) 58, 85-86, 177, 185, 188-189, 199, 202, 234, 266, 276, 279-284, 295-297, 299-301, 309-313, 332-334, 395, 408, 436 La<sub>0.6</sub>Sr<sub>0.4</sub>Co<sub>0.2</sub>Fe<sub>0.8</sub>O<sub>3-δ</sub> (LSCF6428) 81, 86, 97, 100 La<sub>0.8</sub>Sr<sub>0.2</sub>Co<sub>0.17</sub>Mn<sub>0.83</sub>O<sub>3-6</sub> (LSMCo) 84-85  $La_{1-x}Sr_{x}CoO_{3-\delta}$  (LSC) 8, 85–86, 94-95,100 LaNi<sub>1-x</sub>Fe<sub>x</sub>O<sub>3</sub> (LNF) 89, 234, 381 LaNiO<sub>3</sub>-based perovskite oxides 89 lanthanum strontium cobalt ferrite (LSCF) 58, 85-86, 177, 185, 188-189, 199, 202, 234, 266, 276, 279-284, 295-297, 299-301, 309-313, 332-334, 395, 408, 436 laser cuter 396–397 LCP-LSCF 282-284, 286, 288-289, 291, 295, 297–301, 408 LCP-ZnO 192, 201, 284-288, 290-291 LiCo<sub>0.8</sub>Fe<sub>0.2</sub>O<sub>2</sub> (LCF) 185–186  $LnBaCo_2O_{5+\delta}$  double perovskites 91 Low Pressure Plasma Spray (LPPS) coating technology 388-395, 400 low temperature solid oxide fuel cell (LTSOFCs) 8–9, 11, 13, 21, 175, 178, 192, 214, 217, 221, 235, 329, 436

#### m

mathematical model 420-421 mechanical mixing method 54-55 membrane electrode assembly (MEA) 4-5, 7-8metal-to-insulator transitions (MITs) 256 - 257milling process 380, 382–383 mixed electronic and ionic conductor (MIEC) 185 mixed ionic and electronic conducting oxide (MIEC) 10, 80-82, 87, 90, 94-95, 97, 118, 184-185, 230, 232-233, 244, 275, 436 mixed ionic conducting electrolyte 42 - 44Mn-based perovskite cathodes 83-85 molten carbonate fuel cell (MCFC) 5, 13, 67, 308, 320

### n

nanocomposite approach 11–12 nanocomposite approach for advanced fuel cell technology (NANO COFC) 14, 37, 66-67, 330, 460 nanostructured cathodes 94–95, 100 - 102nanotechnology 12, 67, 94, 179 Nernst reversible voltage 457 Ni-YSZ cermet materials 117–118, 124, 135 Ni-based perovskite cathodes 89  $Ni_{0.8}Co_{0.15}Al_{0.05}LiO_{2-\delta}$  (NCAL) 185, 190, 199, 201, 234, 266, 276, 279, 286, 288-291, 296, 302-306, 308-310, 312, 352, 361, 363-366, 387, 391-393, 400, 404, 406-407  $Ni_{0.85}Co_{0.15}LiO_{2-\delta}$  (NCL) 185, 276

## 0

open circuit voltages (OCVs) 21, 25, 41, 44, 46, 53, 61, 115, 122–123, 158–159, 162–164, 166–167, 178, 180–181, 183, 185, 188, 190, 192, 196, 221, 230, 232, 235, 259, 276, 281–282, 284, 286, 288, 290, 294, 296–297, 300, 302–303, 305,

307, 310, 322, 325-326, 339-340, 356, 364, 367, 393, 398, 402, 408, 456-457 oxide-carbonate composite 53 - 60oxide-oxide composite 52 oxide-salt composite electrolytes 52, 60 - 62oxygen ionic conducting electrolyte doped ceria 39-41 SrO and MgO-doped lanthanum gallates 42 stabilized zirconia 37-39 oxygen reduction reaction (ORR) 5, 7, 10, 23-24, 40, 80-83, 85, 91-95, 97, 100-102, 177, 195, 207, 239, 303, 305, 312, 335, 348, 352, 367, 379 - 380

# р

perovskite anode materials 113, 115, 117-126, 133, 135, 137, 361, 380 perovskite cathode materials Co-based perovskite cathodes 85 - 88Fe-based perovskite cathodes 88-89 Mn-based perovskite cathodes 83-85 Ni-based perovskite cathodes 89 oxygen vacancy 82 perovskite oxides 184 oxygen diffusion 239-249 anisotropy oxygen transport 244 - 246diffusion coefficients 242-244 factors controlling oxygen migration barriers 248-249 oxygen ion diffusion at grain boundary 246-247 oxygen vacancy formation 239 - 241proton diffusion 249-253 hydrogen induced insulation 256-259 long-range proton conduction pathways 255-256 proton-dopant interaction 253 - 255

perovskite solar cell (PSC) 200, 202, 360 phosphoric acid fuel cell (PAFC) 3, 5 photo-enhanced fuel cell effect 367 photocatalytic fuel cell (PFC) 367-368 planar solid oxide fuel cell advantages 424-429 durability of sealing 428-429 thermal cycling of sealing 428 anti-oxidation coating 418–419 interconnect plate and control temperature distribution 419-424 crossflow and counter-flow 422-424 effect of co-flow 422-424 mathematical simulation 420 - 422interconnect plate and single cell 416-418 internal manifold and external manifold 415-416 life of stack 429–431 market products 431–442 plasma-cutting machine 396–397 plasma layer deposition (PLD) 6-7, 94 plasma spray 147, 150, 155, 157, 171, 387-395, 418 polymer electrolyte membrane fuel cell (PEMFC) 3, 5, 320, 405, 453 polyvinylidene fluoride (PVDF) 405-407 porosity 7, 80, 91, 94–95, 100, 102, 117, 206-207, 288, 387, 391, 438 proton conducting electrolyte 22, 42-45, 357 proton-conducting oxides 43-44, 249 proton transport frequency 251-252 proton-dopant interaction A site influence 253–254 B site influence 254–255 protonic conduction 249-250 r

Raman spectroscopy 57, 65, 129, 222, 225

Ruddlesden-Popper (RP) perovskites 89, 93-94, 244

#### S

samarium doped ceria (SDC) 13, 40, 87, 117, 175, 215, 276, 319, 361, 379 Schottky junction (SJ) effects 198–202, 205, 234, 276, 279, 282, 288-291, 335, 359-361, 379 semiconducting-ionic two-phase materials 189 semiconductor band structure vs. lithium battery electrochemical cell 371 semiconductor electrochemistry 348, 351-357, 359-360, 367-369, 372 semiconductor-ionic fuel cells (SIFCs) 184-196, 198-200, 202-207, 334 - 335semiconductor-ionic layer 202 semiconductor-ionic materials 21, 184-185, 205, 321, 329 semiconductor-ionic membrane fuel cells (SIMFCs) 21, 365 short stack 147, 395-400, 405 sealing and sealant-free short stack 396 single layer fuel cells (SLFC) 175 basic requirement 380 cell degradation mechanism 400-404 continuous efforts and future developments 404-409 development 179-184 durability test 399-400 engineering materials 379–383 hot pressing 385–386 ionic conductor based electrolyte 177 - 179semiconductor-ionic fuel cells 184 - 196short stack 395-397 bipolar plate design 396 extreme efforts 395-396 sealing and sealant-free short stack 396-397

single layer fuel cells (SLFC) (contd.) tape casting 383-385, 386 tests and evaluations 397-399 thermal spray coating technology 386-395 working principle 196–204 single-phase electrolytes alternative new electrolytes and research interests 44-49 ionic conductivity 37, 38 oxygen ionic conducting electrolyte doped ceria 39-41 SrO and MgO-doped lanthanum gallates 42 stabilized zirconia 37-39 proton conducting electrolyte and mixed ionic conducting electrolyte 42-44 requirements 37 soft ceramic membranes 405, 407, 409 solar cell 447-450 electrolysis 452-453 integration 450-452 solid oxide fuel cells (SOFCs) 3, 35–69, 79-102, 113-137, 145-172, 175-207, 213, 239-267, 275, 320, 347, 379, 415-443, 450 solid-state electrolytes composite electrolytes 52-66 ceria-carbonate composite 62-66 oxide-carbonate composite 53 - 60oxide–oxide electrolyte 52–53 oxide-salt composite electrolytes 60 - 62electrode reactions 35 ion conduction/transportation 49 - 52ionic conductivity 36 NANOCOFC and material design principle 66–67 single-phase electrolytes 37-49

alternative new electrolytes and research interests 44-49 mixed ionic conducting electrolyte 42 - 44oxygen ionic conducting electrolyte 37 - 42proton conducting electrolyte 42 - 44strategies 36 SrCoO<sub>3-6</sub>-based perovskite oxides SrO and MgO-doped lanthanum gallates (LSGM) 42 stabilized zirconia 5, 36-42, 44, 46, 49-51, 67-68, 81, 113, 120, 131-132, 175, 239, 260, 347, 435 stacks 39, 133, 145-172, 243, 395-397, 415-443, 453 sulfur tolerant anode materials 124 - 126sun 447

#### t

thermal spray coating technology low pressure plasma spray coating technology 388-395 traditional plasma spray coating technology 387-388 three possible paths 80, 81 three-phase boundary (TPB) 23-24, 80-83, 94-95, 97, 100-101, 115-117, 127-131, 134, 177, 320 - 321traditional electrolyte 3, 20, 28, 276, 371 traditional plasma spray coating technology 387-388 triple ion transport mechanism 13 two-dimensional (2D) contact cell output performance 3D contact contributions 151-153

design 145–147 mechanism of performance enhancement 153–156 structure improvements and enhancement 149–151 variations 147–149 control design 156–158 quantitative effects steady-state output performance of cell 161–163 transient output performance of cell 158–161 structure 145 typical cathode 177

#### x

X-ray diffraction (XRD) 84, 86, 88, 123, 222–223, 279–280, 282–285, 288–289, 292, 295, 297–299, 302–303, 305–306, 309–310, 322–323, 325, 379–381, 387, 391, 393, 429–430 X-ray photoelectron spectroscopy (XPS) 217–219, 231, 337, 366, 402, 405

## у

yttrium stabilized zirconia (YSZ) 5, 36, 81, 113, 150, 175, 214, 239, 249, 298, 347, 436