Index

Note: Page numbers in *italics* and **bold** refers to figures and tables respectively.

a

ABC fast ionic conductor 26
advanced assembly technology
  preparation method 255–256
  solid-state batteries development 256–258
alloy-based anodes 181–182, *182*, *183*
alloys 155–156
all-solid-state lithium batteries (ASSLBs) 61, 70, 79, 80, 153, 255
anode materials research
  alloys 155–156
  dendrite formation 156
  graphite anodes 153–154
  Li–Ag alloying process 156
  metal fluoride 156
  silicon anodes 154–155
  three-dimensional (3D) current collectors 157
atomic force microscopy (AFM)
  applications 210–214
  constant force mode 208
  density functional theory (DFT) 211
  electrolyte additives 213
  functionalized **210**
  imaging 214, *214*
  imaging principle 207
  in-situ observation 212–213
  operating modes 209, **209**
  principle of 207–210
  representative images *211*
  solid electrolyte interphase (SEI) film 214
automatic-flow for materials discovery (AFLOW) 27

b

Bayesian learning 45, *46*
Born–Oppenheimer approximation 34

c

cathode materials
  additives and electronic percolation 62
  crystallographic and morphological engineering, CAMs 61–62
  development prospect 79–80
  high-Ni NCM cathodes 67–69
  high-voltage ternary cathodes 72–79
  interfacial engineering 62–63
  Li^+ percolation pathways 62–63
  Li-rich Mn-based cathodes and applications 70–72
  material development to device application 66–67
  research on 61–63
  in solid-state batteries 63–65
  spinel lithium manganate (LMO) 69–70
  types of 63–72
clustering (group analysis) 50–51, *51*
cobalt sulfide (CoS) 175
composite polymer electrolyte (CPE) 141
  characterization of 142, *143*
  electrochemical performance 144
  interfacial stability 143, *144*
  LFP/Li cells 144
  WAXD scattering angle 143
conductive AFM (C-AFM) 210
cyclic voltammetry
  applications 224–226
  BQ1-COF electrode 226, *226*
  curves 224, *224*
  data processing 223
  insufficient cycling 224
  overview 222–224
  rate performance 224
  single-phase $LiMnO_2$ stability 225, *225*

d
data-driven machine learning methods 42
dendrite formation 156
dendrite growth mechanism
  active sites 157
  chemical failures 158
  electric failures 158–159
  mechanical failures 159–160
  substantial volume expansion 157
density functional theory (DFT) 161
  generalized gradient approximation (GGA) 32
  Hohenberg–Kohn theory 32
  Kohn–Sham equations 31, 33–34
  theoretical basis of 30
  Thomas–Fermi (TF) theory 33
dry electrode manufacturing 255
dynamically adaptive interface (DAI) layer 14

e
elastic network model 44
electrochemical impedance spectroscopy (EIS)
  applications 227–229
  characterization 226
  electrochemical tests 227
  graphene–sulfur composite cathode 228
  overview 226–227
  plots 227, *227*
  shuttle effect 227
  sulfur host materials 229
electronic percolation 155
electron spectroscopy for chemical analysis (ESCA) 215
electrostatic force microscopy (EFM) 210
ensemble learning method 49–50

f
fabrication of thin SSEs 99–100, *100*, **101–102**
  cold/hot pressing 104
  extrusion forms 104
  hydrothermal synthesis controls 104
  solution impregnation 103
  solution/slurry casting 100, 103
  tape casting 103
  3D printing 104
  ultrathin SSE films 104–107, *105*
fuzzy logic methods 42

g
galvanostatic charge–discharge (GCD)
  applications 230–232
  charge–discharge diagrams *231*, *232*
  limited cycling performance 230–231
  overview 230
Gaussian process regression 49
GITT test
  applications 237, *237*
  overview 236–237
graphite anodes 153–154

h
high-throughput computing in lithium batteries
  Born–Oppenheimer approximation 20
  databases 51–53, *52*
  density functional theory (DFT) 30–34
  first-principles calculation method 19
  Hartree–Fock approximation 20–21
  machine learning 41–51
  material genome method 21–26, *21*, *23*, *25*
  molecular dynamics simulations 34–41
  Schrödinger equation 20
  solid electrolytes 26–30, *27*, *29*
high-voltage ternary cathodes
  crystal structure and degradation mechanisms 73
  degradation mechanisms 73–76
  modification strategies 77–79
  preparation methods 76–77
Hohenberg–Kohn theory 32

i
inorganic crystal structure database 161
inorganic solid-state electrolytes 185–187, *185*, *186*, *187*
in-situ AFM
  application 247–250, *248*, *249*
  overview 246–247
in-situ impedance electrochemical test (EIS)
  application 244–246, *245*
  electrochemical test 245
  high-entropy oxides (HEOs) 244
  overview 243–244
  sinusoidal AC voltage 243
  synergistic modification strategy 244
  three-dimensional data *246*
in-situ Raman spectroscopy
  application 242–243, *242*
  overview 240–242
  patterns *241*
in-situ XRD
  application 238–239, *240*
  Bragg's equation 238
  overview 238
  real-time capturing 238
  slow kinetics, anode materials 239
intercalation-type anodes 183–184

j
Jinshi Battery 11

k
Kelvin probe force microscopy (KPFM) 210

l
lasso regression model 44, *44*, 45
layered Ni-rich oxides 80
Li–Ag alloying process 156
linear model 43

lithium-ion batteries (LIBs) 153, 255
lithium metal anodes modification strategy
  buffer layer 162–163
  ex-situ SEI 161–162
  in situ SEI 162
lithium plating 161

m

machine learning
  Bayesian learning 45, *46*
  clustering (group analysis) 50–51, *51*
  data-driven machine learning methods 42
  elastic network model 44
  ensemble learning method 49–50
  fuzzy logic methods 42
  Gaussian process regression 49
  lasso regression model 44, *44*, 45
  linear model 43
  neural network algorithm 46–49, *48*
magnesium-ion batteries
  alloy-based anodes 181–182, *182*, *183*
  inorganic solid-state electrolytes 185–187, *185*, *186*, *187*
  intercalation-type anodes 183–184
  metallic Mg anode 181
  organic compounds 180
  organic–inorganic composite solid-state electrolytes 189–190
  organic solid-state electrolytes 187–188, *188*, *189*
  overview 169–171, *170*
  polyanionic compounds 177–179, *178*
  Prussian blue analogs 179–180, *179*
  transition-metal oxides 172–174, *172*, *173*
  transition-metal sulfides/selenides 174–177, *174*, *177*
magnetic force microscopy (MFM) 210
metal fluoride 156
metallic Mg anode 181
Meyer–Neldel empirical rule 26
molecular dynamics simulations
  ab-initio molecular dynamics (AIMD) 34
  electrode–electrolyte interface 35, 38, *38*
  solid–solid contact problem 38–40
  space–charge layer (SCL) 35, 40–41, *41*
Monroe–Newman linear elasticity model 157

n

NASICON-type solids 111, *111*
neural network algorithm 46–49, *48*
Novel Materials Discovery (NOMAD) Laboratory 27

o

Open Quantum Materials Database (OQMD) 27
organic compounds 180
organic–inorganic composite solid-state electrolytes 189–190
organic solid-state electrolytes 187–188, *188*, *189*
oxide-based solid state electrolytes (SSEs)
  application of SSEs in gas sensor 110–111, *111*
  application of thin SSEs in LIBs 109–110
  ASSLMBs challenges 93
  design considerations 95, *96*
  development and challenges 91–107
  garnet-type LLTO electrolytes 99
  grain boundary and interface engineering 107–109, *108*
  LiPON-type electrolytes 97
  lithium-ion batteries (LIBs) 91, *92*
  NASICON-type electrolytes 97–98
  perovskite-type LLTO electrolytes 98–99
  production process 99–107
  study of 111–114, *112*, *113*

p

piezoresponse force microscopy (PFM) 210
polyanionic compounds 177–179, *178*
polyethylene oxide (PEO)–lithium salt system 141
polymer's crystalline state 112
polytetrafluoroethylene (PTFE) 256
polyvinylidene fluoride (PVDF) 255
position-sensitive photodiode detector (PSPD) 209
Prussian blue analogs 179–180, *179*

q

Qingtao Energy 15

r

rate performance test
  application 233–234
  capacity fade, Li–S batteries 233
  discharge capacities *233*
  overview 232–233
  poor cycling stability 234

s

scanning capacitance microscopy (SCM) 210
scanning electrochemical microscopy (SECM) 210
scanning electron microscopy (SEM)
  applications 201–204, *202*, *203*
  components of 201
  effective magnification 201
  imaging 199
  principle 199–201, **200**
  resolution 199
  signals interactions *200*
  TEM image analysis 207, *208*
  two-dimensional expanded vermiculite nanosheets 202
  volume expansion 206

scanning spreading resistance microscopy (SSRM) 210
silicon anodes 154–155
solid polymer electrolyte (SPE) membrane 257
solid-state electrolytes
  inorganic 185–187, *185*, *186*, *187*
  organic 187–188, *188*, *189*
  organic–inorganic composite 189–190
solid-state lithium-ion batteries
  carbonate solvents 1
  challenges and bottlenecks 13–14
  cutting-edge breakthroughs and solutions 14–15
  dendrites 1
  development history of 5–8
  domestic policies on 9
  electrochemical principles 4–5
  foreign policies on 9–10
  future development 15–16, *15*
  intrinsic properties 2
  overall development status 10–11
  R&D status 11–13
  working principles 3–4
sulfide solid electrolytes
  air stability 136–138
  calculation methods 129, *129*
  categories of 127–129
  electrochemical stability 132–133, *133*, **134**, 135–136
  electrochemical window 131–132, *132*
  intrinsic properties 133–141
  ion diffusion mechanism 130–131, *131*
  LISICON structure 128
  mechanical stability 140–141
  molecular dynamics (MD) simulations 129
  solvent stability 138–139
  study of 141–145, *143–145*
  synthesis methods 134–135
  thermal stability 139–140

t

Tafel test
  applications 235–236, *236*
  overview 235
Thomas–Fermi (TF) theory 33
three-dimensional (3D) current collectors 157
transition-metal oxides 172–174, *172*, *173*
transition-metal sulfides/selenides 174–177, *174*, *177*
transmission electron microscopy
  applications 205–207
  principle of 204–205

w

wet-chemical deposition 106
wet-processed electrodes 256

x

X-ray diffraction (XRD)
  applications 219–222
  monochromatic X-ray beam 219
  patterns 220, *220*
  powder patterns 221, *221*
  principle of 219
  spatial distribution and intensity 219
X-ray photoelectron spectroscopy
  application 215–219
  characterization data 216
  LiPS conversion electrochemistry 218, *219*
  lithium foil characterization 217, *217*
  overview 215
  photoelectric effect 215
  photoelectron intensity 215
  polysulfide shuttling 218
  XRD patterns 216, *216*
X-ray tomography 48, *48*