

Index

a

acid fuel cells 36, 37, 219, 258, 260, 262–264
 acidic media 46, 61, 71, 121, 147, 199–201, 225, 236, 251, 260, 409
 activity principles 363–366
 adsorption energies 291, 349, 361–363, 366, 368, 380, 383, 397, 405, 411
 adsorption-structural evolution process 450
 advanced carbon-based electrocatalyst 339
 alkaline 201
 absorbents 13
 fuel cells 258–267
 alloy 54–55, 62, 64, 87, 92, 103, 108, 112, 114, 117–118, 121–123, 134, 138–139, 141, 144–145, 156–157, 170, 207, 214–215, 219, 237–238, 241–250, 301–306, 487
 ambient pressure X-ray photoelectron spectroscopy (AP-XPS) 430, 431, 454
 anion exchange membrane (AEM) 36, 118, 169, 170, 185, 204, 252, 253, 259, 260, 333, 334, 384, 394, 396, 490
 anthropogenic carbon cycle 11
 anthropogenic carbon emissions 12–13
 capture and recycle 13–14
 fixation and conversion 14–18

anthropogenic carbon conversion 17–18
 chemical/thermo reforming 16
 electrochemical reduction 15–16
 electrochemistry 17–18
 photochemical reduction 14–15
 physical fixation 16–17
 anthropogenic carbon emissions 12–13
 aqueous electrolyte 35, 45, 80, 160, 171, 176, 278, 279, 284, 293, 297, 298, 333, 334, 338, 339, 427, 471, 504
 artificial nature carbon cycle (ACC) 3
 artificial photosynthesis 14, 15
 atomic structure 56, 294, 313, 320, 355, 414, 423, 441, 442, 444–447, 457
 ATR-Fourier-transform (ATR-FTIR) 222, 426, 452
 attenuated total reflection (ATR) 426, 452
b
 band theory 359–361
 Basic Performance Index 499
 bicarbonate electrolyte 282, 461
 bifunctional mechanism 118, 205, 214, 483, 484, 487
 bilayer capacitance (Cdl) 58, 73, 104, 105, 141, 195, 196
 Born–Oppenheimer (BO) approximation 356

- Brönsted–Evans–Polanyi (BEP) 362, 363, 391
 relations 391
 bulk metals 276, 293–294, 298, 338, 504
- c**
- carbon cycle 3, 9–18, 465–466, 483–484, 499, 501–502
 carbon dioxide 11
 capture and fuel transport 500
 molecule 273
 carbon materials 4, 25, 64, 74, 86, 91, 149, 157–158, 175, 317, 322, 468, 473
 carbon-based materials 28, 73, 157, 339, 341, 471
 catalyst screening 310, 338, 345, 356
 Catalyst Stability/Decay 441, 457–459
 catalytic process
 electric double-layer 347–349
 electrode potential effects 350–352
 kinetics and thermodynamics 349–350
 CH₃CH₂OH oxidation 493, 501
 CH₃OH oxidation 491, 501
 chronoamperometry (CA) method 155, 189, 190, 445
 chronopotentiometry 28, 49, 58, 84
 C1 molecule oxidation
 formic acid oxidation 219–226
 methane oxidation
 reaction mechanism 199
 methanol oxidation 203–219
 C₂₊ molecule oxidation
 ethanol oxidation 235–250
 ethylene glycol oxidation 251
 glucose oxidase 250–251
 glycerol oxidation 251–253
 CO adsorption energy 208, 411, 484
 CO oxidation reaction 194, 400–402
 CO reduction, advances in 326–327
 CO₂ reduction reaction
 fundamental parameters
 current density 277
 electrode 283–285
 energetic efficiency 277–278
 experimental process and analysis
 methods 284–285
 factors affecting 278–283
 Faradaic efficiency 276–277
 overpotential 276
 Tafel slope 278
 cobalt phthalocyanine (CoPh) 145, 457, 473
 computational electrocatalysis
 calculation theories 356–358
 reactivity descriptors 358–361
 computational hydrogen electrode (CHE)
 approach 345, 366–368, 391
 computational screening 356–358
 concerted proton-coupled
 electron-transfer (CPET) 394
 β-CoOOH 447
 coordination numbers (CNs) 291, 311, 320, 361, 362, 380, 446
 copper (Cu) 54, 62, 71, 85, 92, 114, 116, 127, 299–301, 305, 314–316, 324, 326, 394, 395, 448, 455, 473
 covalent organic frameworks (COF) 321–322, 341, 504
 Cu-based catalysts 33, 122, 280, 299, 314, 324, 443, 473, 501
 Cu-free metal catalysts 473
 current density (j) 56, 276, 277
 cycle stability 58
- d**
- d-band model 359, 361, 377, 386, 387
 dehydration process 402, 487
 density functional theory (DFT) 356
 computational hydrogen electrode (CHE) approach 367–368
 electrocatalysis 413–414
 kinetic modelling 371–373
 microkinetic model 391
 solvation effects 406–409
 solvation models 368–371
 density of states (DOS) analysis 55, 357, 377, 386–388, 391, 413, 441

- descriptors 111, 345, 355, 356, 358–363, 377–380, 382–384, 386, 414, 441
 descriptors-guided screening 377–380
 device engineering 338, 340–342
 differential electrochemical mass spectrometry 38, 194, 331, 432, 455
 diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) mode 426
 direct dimethyl ether fuel cells (DDEFCS) 263
 direct ethanol fuel cell (DEFCs) 235, 241, 243, 244, 257, 258, 261, 265
 direct ethylene glycol fuel cells (DEGFCs) 261–262, 265
 direct formic acid fuel cells (DFAFCs) 219, 223, 262–265
 direct fuel cells (DFCs) 183, 185
 direct glycerol fuel cells (DGFCs) 262
 direct liquid fuel cell (DLFC) 258 operating principle 258 types 258–267
 direct methanol fuel cells (DMFCs) 203, 204, 235, 257–261, 263–265
 dominant reaction mechanism 358
- e**
 electric double-layer 105, 347–349
 electrocatalysts 503 advanced carbon-based electrocatalyst 339 next-generation electrocatalyst 341
 electrocatalytic carbon dioxide reduction (ECDR) 17, 18
 electrocatalytic mechanism CO oxidation reaction 400–402 ECR reaction 393–394 EOR reaction 404–406 FAOR reaction 402 HER reaction 397–398 HOR reaction 398–400 MOR reaction 402–404 OER reaction 394–396 O₂ reduction reaction (ORR) 396–397 pH effects 409–410 solvation effects 406–409
 electrocatalytic reaction parameters electric double layer capacitance method 105 electrochemically active surface area 104 half-wave potential 108 kinetic and exchange current density 105–106 overpotential HUPD 106–107 surface redox reaction 104–105 Tafel slope 108
 electrochemical carbon cycle (ECC) 3 Basic Performance Index 499 CO₂ capture and fuel transport 500 external management 500–502
 electrochemical carbon dioxide reduction reaction (ECDRR) catalysts for 473–474 cations and anions 281–282 CH₃CH₂OH 473, 477 CH₃OH 473, 475 CO 468–469 concentration 282 electrolytes/solvent 278–280 pH 280 temperature and pressure effect 282–283 theoretical reduction potential 467–468
 electrochemical catalysis processes ECO₂RR electrochemical cells 36 electrolytes 35–36 environmental impact and cost 35 faradaic efficiency 34 onset potential 34 parameters to evaluate 34–36 partial current density 34–35 possible reaction pathways 29–33 water splitting parameters to evaluate 27–28 reaction mechanism 23–26
 electrochemical cells 15, 21, 36, 76, 158

- electrochemical fuel oxidation
 catalyst poisoning 483
 CO electrooxidation 484
 CO/CH₄ electrooxidation 485, 487
 ethanol oxidation reaction (EOR) 490
 formic acid oxidation reaction (FAOR)
 487
 methanol oxidation reaction (MOR)
 reaction 487
 Pt-and Pd-based materials 483
 Pt-based catalysts 484
 electrochemical impedance (EIS) 57, 76,
 77, 81, 84, 105, 120, 197
 electrochemical reduction technology
 15
 electrochemical STM (EC-STM) 413,
 434, 435, 448, 450
 electrochemically active surface area
 (ECSA) 58, 67, 73, 76, 104, 105,
 120, 125, 130, 138–141, 144, 145,
 193–197, 208, 209, 212, 277, 355,
 456
 electrochemistry CO₂ reduction reaction
 (ECO₂RR)
 possible reaction pathways 29–30
 C₁ products formation 30–31
 C₂ products formation 31–32
 CH₃COOH and CH₃COO-formation
 33
 CO formation 30
 HCOO/HCOOH formation 29–30
 n-propanol formation 33
 electrode
 loading method 283–284
 preparation 284
 electrode design 342, 426, 503, 504
 electrode stability 206, 341–342
 electrode-electrolyte interface 168, 280,
 326, 336, 347
 electrolytes 35, 39
 aqueous electrolyte 35, 45, 80, 160,
 171, 176, 278, 279, 284, 293, 297,
 298, 333, 334, 338, 339, 427, 471,
 504
 bicarbonate electrolyte 282, 461
 selection 503
 non-aqueous electrolyte 279
 electron-based characterization
 techniques
 scanning probe microscopy (SPM)
 434–436
 TEM 434
 electrostatic perturbation 369
 energetic efficiency (EE) 276–278, 291,
 293, 334
 Environmental TEM (E-TEM) 317, 434
 ethanol oxidation 38, 185, 235–250, 261,
 404, 406, 490, 501
 ethanol oxidation reaction (EOR) 21, 40,
 203, 236, 237, 246, 247, 253,
 404–406, 461, 487, 490, 495
 ethanol production 14, 240, 473, 478
 ethylene glycol oxidation 251
 extended X-ray absorption fine structure
 (EXAFS) spectrum 113, 429, 430,
 442, 445–448, 451, 457, 458
- f**
- Faradaic efficiency (FE) 4, 33, 34, 49,
 276–277, 298, 300, 321, 331, 467,
 499
 flow-cell 314, 333, 430
 flow-type cells 299, 310, 331, 333, 336,
 338, 341, 504
 formic acid oxidation 219–226, 263, 402,
 487
 formic acid oxidation reaction (FAOR)
 402–404, 487, 495
 formic acid/formate generation 468
- g**
- gas diffuse electrode 478
 gas diffusion electrode (GDE) 35, 118,
 155, 158, 202, 299, 310, 333, 337,
 484, 504
 Generalization of the computational
 hydrogen electrode (GCHE) 368
 Generalized Gradient Approximation
 (GGA) 357, 391, 413

- Gibbs free energy 36, 94, 111, 349, 350, 385, 393, 396, 405
 glucose electro-oxidation 250, 251
 glucose oxidase 4, 183, 185, 250–251
 glycerol oxidation 251–253
 gold (Au) 39, 295–296
 Gouy–Chapman model 348
- h***
 H-Cell 159, 299, 314, 331–333, 426, 430
 H₂ fuel cell 167
 battery life 168
 charge and discharge curve 168–169
 charge and discharge rate 167–168
 electrode and device progress 170
 electrolyte 169–170
 impedance 168
 self-discharge rate 168
 separator 169
 theoretical specific capacities 167
 voltage 167
 H₂O oxidation
 catalysts 72–76
 noble metal catalysts 53–64
 photo-assisted 76–88
 transition metals 64–72
 H-shuttling model 369, 370, 408
 H-type cells 35, 36, 285, 310, 331–333, 336, 338, 340–342, 504
 half-wave potential 108, 136, 137, 141, 147, 149–152, 188
 HCOOH oxidation 36–37, 487, 488, 501
 Helmholtz model 348
 heteroatom doping strategy 471
 heterogeneous catalysis 347, 351, 359
 heterogeneous electrocatalysis 275
 heterogeneous electrochemical CO₂
 reduction reaction 289
 high-energy resolution fluorescence
 detected X-ray Absorption
 Spectroscopy (HERFD-XAS) 431
 homogeneous catalysis mechanism 274
 hybrid cluster-continuum 368, 369
 hydrogen binding energy (HBE) 92, 107, 111–114, 118, 121, 123
 hydrogen deposition under-potential
 (HUPD) 104–107, 112, 116, 130, 409
 hydrogen escape reaction (HER) 45, 394
 hydrogen evolution reaction (HER) 4, 10, 21, 26, 43, 67, 91, 107, 111, 168, 171, 278, 290, 310, 336, 377, 391, 445, 467, 468, 502
 hydrogen oxidation reaction (HOR) 101, 103, 398
 catalysts 112
 mechanism 111–112
 hydrogen binding energy 111–112
 underpotential deposition 112
 hydrogen peroxide (H₂O₂) 79, 80, 148, 154–160, 397
- i***
in situ characterizations
 active sites 441
 atomic structure 444–446
 catalyst phase transformation 446–449
 electronic structure 442–444
in situ techniques 99, 421, 429, 436, 444, 457, 462, 505
in situ X-ray diffraction 447
 infrared spectroscopy 236, 423–424, 426
 interfacial pH 460–461
 International Energy Agency 273
 ionic liquid 36, 80, 278–280, 297, 322, 339, 471, 473
 iridium-based materials 59
 iron (Fe) 49, 67, 69, 70, 137, 147, 149, 150, 209, 216, 260, 284, 311, 312
- k***
 kinetic and exchange current density 105–106
 Kinetic Monte Carlo (KMC) simulations 372, 373
- l***
 light-assisted electrochemical water
 oxidation 76

- linear sweep voltammetry (LSV) 48, 71, 77, 87, 92, 107, 152, 153, 155, 206, 207, 242, 250, 300, 455, 456
- liquid chromatography 38, 277, 285
- Liquid-Phase TEM (LP-TEM) 434, 435
- lithium-air battery 176
- Local Density Approximation (LDA) 357, 413
- local density of states (LDOSs) 360, 387
- m**
- mass spectrometric characterization techniques
- electron and chemical ionization (EI and CI) approaches 431–432
- membrane electrode assembly (MEA) 120, 139, 185, 267, 310, 333
- metal-air battery 167–180
- structure 171–180
- metal-free carbon-based catalyst 322–324
- metal-free carbon-based materials 471
- metal-free catalyst 149–153, 291, 322, 324, 341, 473, 478
- metal-free materials 72, 75, 103, 275, 322, 394, 468
- metal-organic frameworks (MOFs) 291, 312, 320, 341, 500
- methane oxidation 199–202
- reaction mechanism 199
- methanol crossover 207
- methanol oxidation 38, 40, 144, 203–219, 260, 263, 404, 461, 487, 490, 501
- reaction thermodynamics and mechanism 203–204
- methanol oxidation reaction (MOR)
- reaction 21, 40, 203–206, 208–210, 212, 214, 216, 217, 219, 402–405, 461, 487, 490, 495
- micro-flow cells 36
- microkinetic modeling 371, 392, 409, 410
- Monte Carlo simulations 371, 410
- n**
- nanoscale metals 294–295, 338
- natural carbon cycle (NCC) 3
- definition 9–10
 - from inorganic carbon to organic carbon 10–11
 - from organic carbon to inorganic carbon 11
- N-doped graphene quantum dots (NGQDs) 319, 323, 341, 504
- neutral media 69, 199, 201–202
- next-generation electrocatalyst 341
- nickel (Ni) 309
- Ni-incorporated sulfide 411
 - Ni-introduced sulfide 411
- nitrogen and sulfur co-doped
- hierarchically porous carbon nanofiber (NSHCF) 468
- nitrogen-doped carbon materials 149, 468
- noble metal catalysts 4, 46, 53–64, 185, 487, 490, 495
- non-aqueous electrolyte 279
- non-noble metal catalysts 4, 64, 93–95, 122, 147, 149
- o**
- online-electrochemical mass spectrometry (OLEMS) 432, 433, 454, 455
- onset potential 4, 21, 34, 72, 75, 77, 276, 301, 311, 408
- optical characterization techniques
- infrared spectroscopy 423–424
 - Raman Spectroscopy 424–426
 - UV–Vis spectroscopy 426–427
- optically transparent electrode (OTE) 426
- overpotential (η) 276
- overpotential HUPD 106–107
- oxidant metal catalysts 294–295
- oxidation charges 461
- oxide-derived nanocrystalline metals 468

- oxygen escape reaction (OER) 45, 394
 catalyst 53–55
 electrocatalytic mechanism 394–396
 oxygen reduction reaction (ORR) 103,
 133, 396, 461
 catalysis 461
 catalysts 134–153
 hydrogen peroxide synthesis 154–160
 catalysts advances 154–160
 mechanism 133–134
 oxygen-related electrocatalytic reactions
 503
- p**
- palladium (Pd) 206, 220–223, 235–238,
 297–298, 303, 447
 partial current density 4, 21, 34–35, 277,
 279, 283, 310, 323, 326
 Pd-based catalysts 120, 186, 204–207,
 220, 223, 235–239, 262, 303, 447,
 487, 495, 501
 permittivity parameter 369
 pH effects 80, 114, 121, 299, 409–410
 photo-assisted H₂O oxidation
 metal compound-based catalysts
 76–80
 metal–metal heterostructure catalysts
 80–86
 metal–nonmetal heterostructure
 catalysts 86–88
 photosynthesis 3, 7, 9–10, 14–15
 photovoltaic cell (PVC) 155
 platinum (Pt) 36, 38–39, 91–93, 116, 134,
 136, 138–145, 195, 208–219,
 225–226, 235–236, 240–244,
 246–249, 253, 260, 303, 397–398
 platinum-based nanocubes 215–217
 platinum-based nanotubes 210–212
 platinum-based nanowires 208–210
 porous coordination polymers (PCPs)
 320
 porous organic material
 covalent organic frameworks 321–322
 metal-free catalyst 322
- molecular organic frameworks
 320–321
 primary measurement methods 186–197
 primary parameter 193–197
 projected/partial density of states (PDOS)
 387
 Pt-Ru system 217–218, 239
- r**
- Raman in situ techniques 444
 Raman shift 453, 461
 Raman Spectroscopy 424–427, 442, 453
 reaction field concept 369
 reaction mechanism
 adsorption/activation 450–451
 in situ detections 454–457
 in situ probing 451–454
 reactivity descriptors 358, 359, 363, 377,
 380
 real-time analysis 432, 458
 reflection-absorption infrared
 spectroscopy (RAIRS) modes 426
 rotating ring-disk electrode (RRDE) 49,
 151–152, 155–156, 159
 Ru compounds 58
 ruthenium 92, 116, 121, 214, 219, 240,
 242, 250, 260
 ruthenium-based materials 59
- s**
- Sabatier principle 345, 363, 366, 413
 scaling relationships
 ECR, reactivity trends 380–382
 H-included reactions 385–386
 O-included reactions 382–384
 scanning electrochemical cell microscopy
 (SECCM) 436
 scanning electrochemical microscopy
 (SECM) 113, 156, 436, 454
 scanning probe microscopy (SPM)
 434–436
 scanning tunneling microscopy (STM)
 434, 436, 450
 surface enhanced infrared absorption
 (SEIRA) 426, 460–461

- selected-ion flow tube mass spectrometry (SIFT-MS) 432–433, 455
- silicon oxide 87
- silver (Ag) 63, 213–214, 296–297, 305, 310, 334
- single-atom metal doped carbon catalysts (SACs) 309
- cobalt 311
- copper 314–316
- iron 311–314
- nickel 309–311
- zinc 314
- sluggish reaction kinetics 4, 490
- small organic molecules 67, 185, 251, 504
- primary measurement methods 186, 195–197
- small organic molecules oxidation
- electro-oxidation of alcohol 37–40
 - electrochemistry HCOOH oxidation 36–37
- solid-liquid-gas reaction system 199
- solid-state Zn-air batteries 175
- solvation conditions 392
- solvation effects 406–409
- solvation models 366, 368–371, 391
- SrTiO_3 59, 79
- standard hydrogen electrode (SHE) 47, 119, 280, 289–290, 322, 340, 368, 448, 467
- Stern model 348
- surface-enhanced infrared absorption spectroscopy (SEIRAS)
- measurements 426
- t**
- Tafel slope processes 26–27, 29, 45, 47–49, 57, 59, 62, 69, 71–73, 75–77, 91, 93, 95, 108, 144, 147, 193, 243, 278, 398
- thermodynamic relations 351, 363
- thermodynamic scaling 362
- titanium oxide 61, 87
- transition metal oxide (TMO) 63, 72, 74, 93, 178, 237, 377
- transition state (TS) 349, 358, 362–363, 366, 371–372, 381, 391, 393, 411–413
- transition state scaling (TSS) 362–364
- transmission electron microscopy (TEM) 28, 54, 55, 60, 64–66, 74, 87, 95, 146, 180, 210–212, 214–218, 317, 434, 435, 457, 509
- transparent conducting oxide (TCO) substrate 428
- two-dimensional transition metal dihalides (TMDs) 71
- two-step electrochemical reduction 339
- u**
- ultrahigh vacuum (UHV) 143, 429–431
- underpotential deposition (UPD) 104–105, 112, 130, 409
- universal reactivity descriptor 377, 380
- UV-Vis spectroscopy 423, 426–427
- v**
- valence band spectra 304, 451
- volcano plots 366, 380–381, 383–384
- voltage-dependent Raman spectra 461
- w**
- water splitting
- catalytic activity 47–50
 - Faradaic efficiency 49–50
 - overpotential 47–48
 - stability 49
 - tafel slope 48–49
 - turnover frequency 50
- composition and exact reactions 45–58
- electrocatalytic cell 96–99
- HER catalysts 91–92
- non-noble metal catalysts 93–95
- x**
- X-ray absorption near edge structure (XANES) spectrum 74–75, 95, 429, 445–446, 448, 451, 457–458

- X-ray absorption spectroscopy (XAS) 60, 65, 68, 99, 180, 429–431, 442, 444, 446–448, 450–451, 457–459, 490
- X-ray characterization techniques
- X-ray absorption spectroscopy (XAS) 429–431
 - X-ray diffraction (XRD) 429
 - X-ray photoelectron spectroscopy (XPS) 431
- X-ray diffraction (XRD) 28, 58, 60, 76, 87, 180, 216, 238, 241, 243, 248–250, 429, 447, 449, 457
- X-ray photoelectron spectroscopy (XPS) 28, 31, 53, 58, 60, 68, 75–76, 87, 114, 126, 180, 219, 242, 429, 431, 441, 450–451, 454

Z

- zero-point energy (ZPE) 350, 367
- Zigzag-edged graphene nanoribbons 152
- zinc (Zn) 13, 171, 298–299, 314
- zinc-air batteries 73, 149, 173–175

