

## Index

### **a**

absorption coefficient 7–8  
 Acousto-optic Tunable Filter (AOTF)  
   infrared spectroscopy 425  
 AlInP 159–165  
 amines 309  
 ammonia detection 296–297  
 anion effect, aqueous electrolytes 249  
 anode reaction, hydrogen oxidation  
   reaction mechanism 324–326  
 anodic addition reactions 310–311  
 anodic oxidation 303, 305–309  
 anti-Stokes Raman scattering 428  
 applied bias photocurrent efficiency  
   (ABPE) 161, 213, 214, 221  
 APXPS 437  
 aqueous electrolytes 159, 183, 246  
   anion effect 249  
   cations effect 248–249  
   pH effect 247–248  
 artificial photosynthesis 207, 210, 397,  
   422  
 atmospheric pressure chemical vapor  
   deposition (APCVD) method  
   216  
 atom vacancy 277–278  
 atomic layer deposition (ALD) 149,  
   158, 160, 172, 213, 218, 221, 261,  
   326

ATP/Co-MoS<sub>x</sub> catalyst 19  
 attenuated total reflection FTIR  
   (ATR-FTIR) spectroscopy 425,  
   426

### **b**

band-edge emission 422, 423  
 benzothiadiazole (BTD) 10  
 BiVO<sub>4</sub> photoanode 146–148, 150, 176,  
   180–182, 185, 186, 210, 214–215,  
   222, 223, 410, 439  
 BODIPY-sensitized systems 7  
 Boltzman constant 411  
 Butler–Volmer equation 289

### **c**

cadmium selenide (CdSe) 41, 42, 80,  
   150–153  
 catalyst layer 161, 178, 259–263, 323  
 cathode oxygen reduction reaction  
   326  
   ORR mechanism 326–328  
   PGM-free catalysts 341–347  
   platinum-group-metal-based  
   catalysts 328–341  
 cation effect 248–249  
 cation vacancy 278  
 C–C coupling reactions 312  
 CdS 150–155

- CdS-based heterojunction photocatalyst  
cocatalytic material 40–67  
hetero/homojunction photocatalyst  
67–85
- CdS-based homojunction photocatalyst  
75–78
- CdTe 150, 153–154, 208
- cell configuration 295
- charge/carrier migration 16, 402
- charge-coupled device (CCD) 422
- chemical bath deposition 71, 73, 79,  
147
- C K-edge XANES analyses 376–378,  
382, 383
- C<sub>3</sub>N<sub>4</sub> 166, 256, 364, 369
- C–N coupling reactions 312, 314
- cocatalytic materials 40  
metal cocatalyst 40–56  
transition metal oxides and  
hydroxides cocatalyst 56–59  
transition metal phosphide and  
carbide cocatalyst 64–67  
transition metal sulphide cocatalyst  
60–64
- CO<sub>2</sub> electroreduction 242  
reaction pathways and mechanism  
242–244
- Co<sub>3</sub>N 170
- C–O oxygenation reactions 314–315
- copper-nickel mixed oxide (CuO:NiO)  
149
- covalent triazine frameworks (CTFs)  
147, 149, 150, 176, 223
- C–P coupling reactions 316
- C–S coupling reactions 315–316
- Cu-based single-atom/site  
electrocatalysts 256, 257
- CuGaSe<sub>2</sub> 150, 156–157, 177, 178
- CuInS<sub>2</sub> photocathode 150, 154–156,  
208
- CuIn<sub>x</sub>Ga<sub>1-x</sub>Se<sub>2</sub> solar cell-based PV-EC  
system 232
- Cu<sub>2</sub>O photocathode 148–150, 176,  
218–220, 223
- current density 158, 163, 182, 209,  
214, 228, 231, 244–247, 254, 266,  
282, 323, 326, 342, 345, 369, 418,  
420, 421
- cyanation reactions 310
- cyano electron-acceptor group 3
- cyclic voltammetry (CV) 289, 290,  
303, 418, 420
- d**
- data acquisition system 416
- differential electrochemical mass  
spectrometry (DEMS) 289–292
- diffuse reflectance infrared Fourier  
transform (DRIFT) 425, 426
- donor- $\pi$ -acceptor (D- $\pi$ -A) 3
- doping defect 273–277
- Doppler effect 438
- double atoms catalysis 279–280
- dye-sensitized photocatalysts 8, 20,  
172–174
- dye-sensitized solar cell (DSSC) 1, 2,  
4, 5, 10, 13, 27, 143, 172, 173, 232
- e**
- electrocatalysts 160, 178, 181, 217,  
229, 230, 242, 250, 253, 256, 262,  
285, 298–300, 307, 363, 386, 418
- IrO<sub>x</sub> 434
- NRR 274, 294
- Pt<sub>3</sub>Y 331
- electrochemical CO<sub>2</sub> reduction  
metal catalysts 250–253  
single-atom/site catalysts 253–259
- electrochemical in situ  
characterizations 286
- DEMS 289–292

- EC-STM 292
  - FTIR 289
  - in situ Raman measurement
    - 292–295
  - XAS 292–295
  - electrochemical in situ
    - Fourier-transformed infrared spectroscopy (FTIR) 258, 289
  - electrochemical scanning tunneling microscopy (EC-STM) 292, 293
  - electrochemical surface area (ECSA) 244, 245, 329, 340
  - electrode membrane assembly (MEA) 264–266, 323, 326, 342, 345, 347, 348
  - electrolytes 147, 148, 152, 153, 156, 157, 159, 160, 163, 164, 169, 173, 175, 176, 182–186, 210, 214, 215, 219–221, 227, 229, 242, 244, 246, 252, 260–262, 264–266, 287–292, 296–298, 300, 303, 304, 317, 322, 323, 325, 363, 385, 386, 429, 430
    - aqueous 247–249, 259
    - ionic liquids 250
    - sulfuric acid 329
  - electrolyte solution effect 281–282
    - molecular crowding 284–285
    - pH 282–283
  - electromagnetic spectrum 397–399, 438, 439
  - electromagnetic wave frequency 399
  - electron paramagnetic resonance (EPR) spectroscopy 314, 438, 439
  - electron spin resonance (ESR) spectroscopy 57, 439
  - electron transfer processes 2, 4, 12, 20, 24, 243, 288, 328, 399
  - electropolymerization 147, 149
  - energy conversion systems 16, 368–369
    - electrocatalysts 369–375
    - photocatalysts 375–383
    - photoelectrocatalysts 383–386
  - enzyme-like catalysis 280–281
  - extended X-ray absorption fine structure (EXAFS) 254, 255, 294, 370, 371, 374, 433
- f**
- Faradaic efficiency (FE) 182, 244, 245, 275, 279, 282, 288, 295, 300, 307
  - Fe<sub>2</sub>O<sub>3</sub> photoanode 182, 216–217
  - Fe-based single-atom/site electrocatalysts 253–254
  - FeMoPPc 279
  - ferroelectric materials 145
  - Fischer–Tropsch process (FTS) 367
  - flow cell 262–266, 290, 295, 316, 367
  - Forster resonance energy transfer (FRET) 378, 380, 381, 388
  - Fourier transform infrared (FTIR) spectroscopy 243, 258, 266, 289, 290, 425, 426
- g**
- GaAs 159–165, 208, 226, 227
  - GaInAs 159–165, 224
  - GaInAsP 165
  - GaInP 159–165, 224, 226
  - gallium indium phosphide 163
  - γ-ray-based spectroscopy 399
  - γ-ray source 438
  - GaN 159–165, 169–170, 175
  - GaON 172
  - gas chromatography 298, 300
  - gas collection subsystem 116

- gas diffusion electrode 259–260
    - catalyst layer 261–263
    - flow cell 262–264
    - gas diffusion layer 260–261
    - membrane electrode assembly (MEA) cell 264–265
  - gas diffusion layer 260–261
  - ground-state bleach (GSB) 408–409
  - ground state 4, 11–12
  - Group III–V semiconductor materials 162
- h**
- H<sub>2</sub> production 19
    - CdS-based heterojunction photocatalyst 40–85
    - chemical additives for 38–40
    - oxidative coupling reactions coupled with 312–317
  - Haber–Bosch process 279, 286–288
  - halogenation reactions 311
  - halogen reagents 311
  - hard template-based techniques 336
  - heteroatom doping 273, 274
  - hetero/homojunction photocatalyst
    - carbon-based materials–CdS 71–74
    - CdS-based homojunction photocatalyst 75–78
    - metal oxide–CdS 68–71
    - metal sulfide/selenide–CdS 78–83
  - highest occupied molecular orbital (HOMO) 2–5, 10, 18, 25, 83, 383
  - high temperature PEMFCs 322–323
  - hydrocarbons, oxidation 305–306
  - hydrofluoric acid (HF) 292, 293
  - hydrogen evolution reaction (HER)
    - 151, 158, 162, 176, 178, 182, 209, 210, 218, 224–226, 228–232, 241, 246–249, 251, 253, 259, 262, 273, 274, 277–285, 303, 304, 324, 363, 369, 374, 375, 402, 426, 439
  - hydrogen oxidation/evolution reaction (HOR/HER) 324
  - hydrogen oxidation reaction 324–326
  - hypsochromic shift 7, 10
- i**
- III–V solar cell based PV-EC system 226–227
  - incident photon-to-electron conversion efficiency (IPCE) 405
  - inelastic scattering 425, 430
  - infrared (IR) spectroscopy 425–428, 430
  - InN 169–170
  - inner shell, electron transition 406, 431–438
  - in situ Raman measurement 292–295, 431
  - in situ Raman spectroelectrochemistry 294
  - interferometric scattering microscopy (iSCAT) 424
  - ionic effect 282, 283
  - ionic liquids 246, 250, 252
- j**
- Jablonski-type diagram 420
- l**
- Lambert–Beer law 398, 413, 416, 418, 425
  - LaTiO<sub>2</sub>N 172
  - lattice oxygen-mediated mechanism (LOM) 426
  - layer-by-layer (LBL) assembly 14
  - life cycle assessment (LCA) 108, 122–124
    - goal and scope definition 124
    - life cycle inventory analysis 124–127
  - light absorbers 1–15, 18, 25, 162, 174, 218, 233, 398

- light absorption 10–12, 16, 25, 36, 37, 40, 48, 67, 70, 71, 73, 76, 81, 83, 84, 144–147, 151, 154–157, 161–163, 166, 167, 171–175, 178–180, 211, 213, 216, 379, 380, 397, 400
- localized surface plasmon resonance (LSPR) 48, 49, 179, 180, 377, 380, 381
- lowest unoccupied molecular orbital (LUMO) 2–5, 7, 10, 11, 18, 25, 383
- m**
- mass spectroscopy 298, 426
- membrane electrode assembly (MEA) cell 264–266, 323, 326, 342, 345, 347, 348
- metal catalysts for CO<sub>2</sub> reduction into CO 252 into formate 251–252 into hydrocarbons and alcohols 253
- metal cocatalyst 40–56
- metal-insulator-semiconductor (MIS) strategy 213
- metal organic chemical vapor deposition (MOCVD) 163, 164
- metal oxide–CdS heterojunction photocatalyst 68–71
- metal phospho-sulfides/-selenides 22
- metal selenide–CdS heterojunction photocatalyst 78–83
- metal sulfide–CdS heterojunction photocatalyst 78–83
- metal-to-ligand charge transfer (MLCT) 3
- Michelson interferometer 425, 426
- Mn-based catalysts 434, 435
- MOF-derived structures 345–347
- molecular crowding effect 284–285
- Mössbauer spectroscopy 438
- n**
- N749 5, 6, 21
- natural photosynthesis 397, 422, 434
- N-doped RGO (N-RGO) 21
- near-edge X-ray absorption fine structure spectroscopy (NEXAFS) 364, 433, 434
- Ni-based single-atom/site electrocatalysts 256
- NiFe-layered double hydroxide (NiFe LDH) catalyst 228
- nitrides and oxynitrides 165–166 C<sub>3</sub>N<sub>4</sub> 166 Co<sub>3</sub>N 170 GaN 169–170 GaON 172 InN 169–170 LaTiO<sub>2</sub>N 172 Ta<sub>3</sub>N<sub>5</sub> 166–169 TaON 170–171 TiN 170
- nitrogen defect-rich porous carbon nitride (CN) 364, 376, 377
- nitrogen reduction reaction (NRR) ammonia detection 296–297 atom vacancy 277–278 catalyst surface environment effect 285–286 detection method for 295–296 doping defect 273–277 electrolyte solution effect 281–285 enzyme-like catalysis 280–281 mechanism 286–289 NO<sub>x</sub> contaminations 297–300 process 291–295 single/double atoms catalysis 279–280
- N K-edge XANES analyses 376–378, 382, 383
- nonaqueous electrolyte 249–250
- nonradiative energy transfer 378
- nonradiative quenching 7
- NO<sub>x</sub> contaminations 297–300

- nuclear magnetic resonance (NMR) spectroscopy 438–439
- O**
- one-pot pyrolysis 343
- one-pot solvothermal approach 53, 54, 60, 337
- onset potential 149, 157, 159, 161, 164, 169, 171, 172, 182, 183, 185, 213–214, 216, 217, 220, 222, 223, 244, 245, 331, 342, 431
- open-circuit photovoltage 228
- open circuit potential (OCP) 186, 232, 289, 438
- operando/in situ spectroscopy techniques 397, 398, 406, 407
- optical-pump THz-probe (OPTP) spectroscopy 403
- organic solar cell-based PV-EC system 229–232
- organic solvents 10, 151, 246, 249, 250, 304, 307
- organofluorine compounds 310
- organophosphorus compounds 316
- ORR mechanism 323, 326–328
- outer shell, electron transition 406–408
  - PIAS 412–417
  - PL spectroscopy 420–424
  - SECAS 416–421
  - TAS/TDRS 408–412
  - TRPL 420–424
- outer shell, vibrational transition 424–425
  - infrared (IR) spectroscopy 425–428
  - Raman spectroscopy 428–431
- oxidative coupling reactions
  - C–C 312
  - C–N 312–314
  - C–O oxygenation 314–315
  - C–P 316
  - C–S 315–316
  - S–S 317
- oxide semiconductor 144–150
- oxygen evolution catalyst (OECs) 159, 160
- P**
- panchromatic dye (black dye) 5, 7
- perovskite solar cell-based PV-EC system 227–229
- PGM-free catalysts 341–342
  - MOF derived structures 345–347
  - one-pot pyrolysis 343
  - template derived structures 343–345
- pH effects 282–283
  - aqueous electrolytes 247, 248
- phosphoric-acid-doped membrane 323
- photoanodes 24, 148, 154, 160, 185, 207, 208, 210–211
  - BiVO<sub>4</sub> 146, 148, 181–183, 185, 186, 214–215
  - Fe<sub>2</sub>O<sub>3</sub> 216–217
  - silicon (Si) 159, 161, 167, 169–172, 213–214
  - TiO<sub>2</sub> 210–213
  - water-oxidation 23–25
- photocatalytic hydrogen production system 107–108
  - examples of 111–135
  - fundamentals of 108–109
- photocatalytic processes 406–439
- photocatalytic reaction subsystem 113–115
- photocathode 218
  - Cu<sub>2</sub>O 218–220
  - Sb<sub>2</sub>Se<sub>3</sub> 220–222
  - Si 220
- photochemical processes 109, 174, 398, 400, 403, 406–439

- photoelectric conversion efficiency  
151–153, 162
- photoelectrocatalysts 363, 364, 368,  
369, 383–387
- photoelectrocatalytic water oxidation  
411, 413, 415
- photoelectrochemical (PEC) cell 144,  
149, 168, 171, 183, 208, 220, 223,  
224, 233
- photoelectrochemical (PEC)  
performance  
charge carrier separation 180  
heterojunction 176–178  
light absorption 178–180  
nanostructure 174–175  
oxygen evolution cocatalysts  
181–183  
surface passivation layer 184–186  
surface protection layer 183–184
- photoelectrochemical (PEC) water  
splitting  
dye-sensitized photocatalysts  
172–174  
GaAs, GaN, GaInAs/GaInP/AlInP  
159–165  
nitride and oxynitride semiconductor  
165–172  
oxide semiconductor 144–150  
sulfide semiconductor 150–158
- photoelectrosynthesis 25
- photoexcitation process 377
- photohole signal 410, 413
- photoinduced absorption (PIA) 408,  
409, 413, 414
- photoinduced absorption spectroscopy  
(PIAS) 412–417
- photoinduced charges/carriers 402,  
403, 409, 412
- photolithography 439
- photoluminescence (PL) spectroscopy  
408, 420–424
- photomultiplier (PMT) 422
- photosystem I (PSI) 422
- photosystem II (PSII) 422
- photovoltaic electrocatalysis (PV-EC)  
system 224  
CuIn<sub>x</sub>Ga<sub>1-x</sub>Se<sub>2</sub> solar cell-based 232  
dye-sensitized solar cell-based 232  
organic solar cell-based 229–232  
perovskite solar cell-based 227–229  
Si based 225–226  
III–V solar cell-based 226–227
- pilot plant 112  
gas collection subsystem 116  
life cycle assessment (LCA) 123–135  
photocatalytic reaction subsystem  
113–115  
solution-feeding subsystem 113  
waste liquid–discharging subsystem  
116
- plasmonic metal nanoparticles 377
- plasmon resonance energy transfer  
(PRET) 377, 378, 380, 381, 388
- platinum-group-metal-based catalysts  
atomic ordering 338–341  
composition control 331–335  
shape engineering 334–338  
size control 328–332
- poly(styrenesulfonate) 20
- polyoxometalates (POMs) 16
- proton-coupled electron transfer  
(PCET) 283, 286, 416
- proton-exchange membrane fuel cells  
(PEMFCs) 322–324  
anode hydrogen oxidation reaction  
324–326  
cathode oxygen reduction reaction  
326–347
- proton reduction reaction 1, 18–19
- pump-probe principle, for spectroscopy  
techniques 399–400

**r**

- Raman spectroscopy 425, 428–431, 438
- rate-determining step (RDS) 2, 243, 245, 249, 273, 279, 287, 406, 410, 413, 415, 416, 428
- Rayleigh scattering 428
- reduced graphene oxide 20–22, 73, 74, 146
- Ru complexes 5, 12
- Ru(II) trisdiimine 13, 15, 20, 25
- S**
- salting-out effect 283
- Sb<sub>2</sub>Se<sub>3</sub> 150, 151, 157–158, 174, 178, 183,
- Sb<sub>2</sub>Se<sub>3</sub> photocathode 151, 157, 158, 184, 220–222
- scanning near-field infrared microscopy (SNIRM) 428
- scanning transmission X-ray microscopy (STXM) 367, 385–388
- semiconductor materials 1, 15–16
- active-site molybdenum sulfide nanoparticles 18–19
  - covalent organic frameworks 16
  - metal phospho-sulfides/-selenides 22
  - reduced graphene oxide 21–22
  - solar energy conversion efficiency 19–21
- shape engineering 328
- SHINERS 431, 432
- Shockley–Queisser limit 227, 406
- Si based PV-EC system 225–226
- signal-to-noise ratio (SNR) 426
- SILAR method 147
- silicon and III–V group 159–165
- silicon (Si) photoanode 213–214
- silicon phthalocyanine dye (SiPc) 21
- single-atom alloy (SAA) 257–259
- single-atom catalysts (SACs) 279–280, 295, 330, 331, 342, 344, 374
- single-atom photocatalyst 381
- single atoms catalysis 279–280
- single-atom/site electrocatalysts
- Co-based 254–255
  - Cu-based 256, 257
  - Fe-based 253–254
  - Ni-based 256
  - other metal-based 257
  - single-atom alloy (SAA) 257–259
  - Sn-based 256, 258
- Si photocathode 214, 220, 221
- size control 328–331
- Sn-based single-atom electrocatalysts 256, 258
- solar energy 1–27, 35, 107, 133, 159, 162, 174, 187, 207, 209, 213, 218, 220, 375, 397
- solar-to-hydrogen (STH) 149, 185, 208, 209, 216, 223, 224, 231, 233, 375
- sol-gel process 378
- solution feeding subsystem 113
- spectroelectrochemical absorption spectroscopy (SECAS) 408, 415–421
- spectroelectrochemical spectroscopy techniques 416
- spin coating method 215
- sputtering method 161
- S–S coupling reactions 312, 317
- steady-state spectroscopy 399, 412
- sulfide semiconductor 78, 150
- CdS 150–152
  - CdSe 151–153
  - CdTe 153–154
  - CuGaSe<sub>2</sub> 156–157
  - CuInS<sub>2</sub> 154–156
  - Sb<sub>2</sub>Se<sub>3</sub> 157–158



- sulfonyl hydrazines 305  
 surface-enhanced infrared absorption  
   spectrometry (SEIRAS) 291  
 surface plasmon resonance (SPR) effect  
   47, 48, 83, 85
- t**
- Tafel slope 226, 244, 245, 372, 420  
 tandem devices 149, 150, 165, 214,  
   220, 222–224, 230  
 tandem PEC water-splitting 209  
 tantalum nitride ( $\text{Ta}_3\text{N}_5$ ) 166–171  
 tantalum oxynitride ( $\text{TaON}$ ) 83, 166,  
   170–171, 210  
 tellurium nanowires 336  
 template derived structures 343–345  
 tetranitrophthalocyanine copper(II)  
   ( $\text{TNCuPc}$ ) 145  
 time-resolved microwave  
   photoconductivity (TRMC) 405  
 time-resolved photoluminescence  
   spectroscopy (TRPL) 408, 420,  
   422–424  
 time-resolved THz spectroscopy (TRTS)  
   403, 404  
 TiN 163, 170  
 $\text{TiO}_2$  photoanode 144, 181, 210–213,  
   364, 369, 384, 388, 416  
 $\text{TNCuPc/TiO}_2$  145  
 transient absorption/diffuse reflectance  
   spectroscopy (TAS/TDRS)  
   408–412, 438  
 transient absorption microscopy (TAM)  
   405, 406, 440  
 transition-metal doping 19, 212  
 transition-metal oxides 277, 295, 364,  
   369  
   and hydroxides cocatalyst 56–59  
 transition-metal phosphide, and carbide  
   cocatalyst 64–67
- transition-metal sulphide cocatalyst  
   60–64  
 tridentate terpyridine 5  
 trifluoromethylation reactions  
   310–311  
 triphenylamine 3, 4, 8–9, 11–13  
 tris(bipyridine)ruthenium(II) 3  
 turnover frequency (TOF) 55, 65,  
   244–246, 258, 348, 369, 421, 426,  
   434
- u**
- ultraviolet-visible-based spectroscopy  
   399  
 UV irradiation method 330
- w**
- waste liquid–discharging subsystem  
   112, 116  
 water nucleophilic attack mechanism  
   (WNRM) 426  
 water splitting 1, 16, 20, 23, 35–38, 41,  
   48, 49, 68, 86, 136, 278, 363, 364,  
   368, 369, 372, 374–381, 383–386,  
   388, 402, 403, 406, 410, 413, 439  
   dye-sensitized 24  
   photocatalytic 60, 83, 107–109,  
   111–135, 409  
   photoelectrochemical 143–187  
   photovoltaic electrocatalysis (PV-EC)  
   207, 209, 224–232  
   photovoltaic–electrochemical  
   207–233  
   solar 397–440  
   Z-scheme 20, 21  
 $\text{WO}_3$  photoelectrodes 148
- x**
- X-ray absorption near-edge structure  
   (XANES) 364, 375, 377,  
   433–435

- X-ray absorption spectroscopy (XAS)
    - 266, 363–388, 431, 433, 434, 436, 437
    - electrochemical in situ 292–295
    - in situ cells progress 366, 367, 369
  - X-ray-based spectroscopy 399
  - X-ray diffraction (XRD) 431, 437
  - X-ray emission (fluorescence) 433, 434
  - X-ray emission spectroscopy (XES)
    - 364, 365, 431
  - X-ray fluorescence (XRF) 431
  - X-ray photoelectron spectroscopy (XPS)
    - 57, 431, 433, 436, 437
- Z**
- ZnO nanorod array 154
  - Z-scheme process 20, 21

















