

## Index

### a

- ab initio* molecular dynamics (AIMD)
  - simulation tools 295, 532
- ab initio* nonadiabatic molecular dynamics 13
- action spectrum (AS) 142, 150–152, 459
- active species
  - generation at catalyst/water interface 486–490
  - in heterogeneous photocatalysis 494
- acyl imidazoles
  - with benzyl bromides 89
  - enantioselective alkylation of 89, 90
  - photoinduced enantioselective alkylation of 89
- adiabatic dynamics
  - quantum tunneling in 535–540
  - and reaction mechanisms 545
- adiabatic process
  - in photocatalysis 531–532
  - theory of 532
- advanced oxidation processes (AOPs) 27
- aerobic indole C-3 formylation reaction 402–404
- aerobic oxidation 12, 463
- Ag<sub>3</sub>PO<sub>4</sub>-glass nanocomposite 179–183
- air-saturated system
  - H<sub>2</sub>O<sub>2</sub> in 487
  - opposite effect 489
- alcohols to carbonyl derivatives
  - oxidation 413–414
- Al-doped zinc oxide (AZO) 200
- alizarin red (AR) 80, 266, 403
- alkyl halides
  - activation of 77–91
  - C–C bond forming reactions 78
  - photoreduction of 104
- alkynes
  - arylphosphine oxides with 397
  - 1,2-diketones synthesis from 399–400
- anatase
  - band structure 505
  - crystal structure 504–506
  - substitutional doping of 451
  - TiO<sub>2</sub> 505
- anatase-rich titania 451
- anchor-points reactive potential (APRP)
  - method 540
- anions
  - atomic p levels 454
  - doping with 425
  - hypophosphite (H<sub>2</sub>PO<sub>2</sub><sup>-</sup>) 428
  - role of 493–494
- apparent quantum efficiency (AQE) 10, 141, 142, 151
- apparent quantum yield (AQY) 9, 202, 238, 241, 347, 369, 431
- arenes
  - azolylations of 105
  - electronic effect of substituents 414
  - perfluoroarylation of 396–397
  - polyhalogenated 109
- artificial-force-induced reaction (AFIR) 531–532

- arylamidines oxidative annulation
    - 405–406
  - arylboronic acids, oxidative
    - hydroxylation 409–410
  - aryl halides
    - activation 91–108
    - carbon–halogen bond 108–109
    - C–H arylation reactions 99
    - photoredox catalysts and visible-light 92
  - atom transfer radical addition (ATRA)
    - reactions 84
  - Au–Cu nanoparticles 146–148
- b**
- band alignments 193–195, 205, 215, 255, 291, 293, 432, 433, 472
  - band bending
    - semiconductors 503
    - surface 506
  - band gap 5, 6, 54, 168, 196
    - energy 4, 504
    - engineering 174, 285–291
    - heterojunctions 468–470
    - modification for visible-light sensitization 452
    - semiconductor 255
  - benzimidazole synthesis 411–413
  - benzodithiophene (BDT) 240
  - benzo[b]phosphole oxides synthesis 397–398
  - benzothiazole synthesis 411–413
  - benzyl bromide 88, 89
  - Bethe–Salpeter equation (SBE) 529
  - bimetallic nanoparticles (NPs) 130, 131, 146–155
  - bimodal carbon modification effect 472
  - binding energy 7, 302, 351, 455
  - Bi<sub>2</sub>S<sub>3</sub>–glass nanocomposite 178
  - BiVO<sub>4</sub> 195–196
    - carbon-based materials 199
    - TiO<sub>2</sub> 199
    - WO<sub>3</sub> 197
    - ZnO 197–199
  - black TiO<sub>2</sub>
    - core-shell formation 121
    - designing 118–122
    - enhanced catalytic properties of 120
    - high thermal stability 123
    - nanomaterials 120, 121
    - nanotubes 120
    - photocatalyst 122, 123
    - synthesis strategies for 119
  - Bohr radius 177, 178, 231, 373
  - Born–Oppenheimer approximation 532
  - Born–Oppenheimer molecular dynamics (BOMD) 532, 544
  - 2-bromoacetophenone 77, 80
  - bulk modification 450
- c**
- C3-acylation of indoles 404
  - cadmium sulfide (CdS) 428
    - CdS-glass nanocomposite 174–178
    - nanospheres 469
  - calcium chloride (CaCl<sub>2</sub>) 169
  - cadmium selenide 9
  - capping agents 170, 171
  - carbon–bromine bonds 85, 86, 95, 104
  - carbon–carbon bond formation
    - reactions 80, 89
  - carbon dioxide (CO<sub>2</sub>) 283, 421
    - emissions 53
    - energy crisis and water splitting 14
    - harvest solar light and water splitting 587
    - mineralization of bacteria cells 138
    - photocatalytic conversion of 31
    - photoreduction into CH<sub>4</sub> 429
    - reduction 30–44
  - carbon–fluorine bonds 108
  - carbon–halogen bonds
    - activation of 76, 80, 91
    - arylated products 109
    - photoredox catalytic activation 75–110
  - carbon modified metal oxides 33–34
  - carbon nanotubes (CNTs) 33, 425, 519
  - carbon neutral cycle 6
  - carbon nitrides 332, 334, 336, 348–349, 430–434

- carbon oxide redox reactions 546–547
- carbon-TiO<sub>2</sub> composites 518–520
- Car–Parrinello molecular dynamics (CPMD) method 532
- cascade radical cyclizations 80
- catalyst/water interface 486–490
- C atom tunneling 538, 539
- CB edge (CBE) 196, 197
- C–C coupling reaction 10, 542
- cetyltrimethyl ammonium bromide (CTAB) 170, 426
- CFO/WO<sub>3</sub> composites 469
- chalcogenide photocatalysts 170
- charge carrier 3
  - of BiVO<sub>4</sub> 197
  - charge transfer processes/chemical reactions 264
  - dynamics 13, 130, 156
  - mobility of 7, 150, 156
  - fast recombination of 142
  - formation 5
  - kinetics in heterojunction structure 209, 215
  - in photocatalyst 129
  - photogeneration of 28
  - recombination 134
  - separation 6
  - transfer 6
- charge transfer
  - mechanisms 437
  - resistance 212
- chemical reduction methods 119
- chemical vapor deposition (CVD) 119, 172
- chemiluminescence 488
- C–H functionalization 75–110, 407–408
- Chini clusters 133
- Claus process 166
- clean and renewable energy 329
- C:N ratio 335
- CO<sub>2</sub> capture, storage (CCS) 28
- codoping 455–456
- COFs, *see* covalent organic frameworks (COFs)
- coherent switching with
  - decay-of-mixing (CSDM) method 540
- colorless pollutants 265–268
- compound parabolic collectors (CPCs) 310
- compound parabolic concentrators (CPCs) 41, 311, 312, 573–574
- conducting polymers
  - applications of 233–245
  - hard templates 232
  - heterostructures 242–245
  - nanocomposites 231
  - nanoscale 231
  - nanostructured materials 231–233
  - organic semiconductor 228–230
  - for photocatalytic water splitting 237–242
  - soft templates 232–233
  - synthesis of 231, 233
  - template-free method 233
- conduction band (CB) 8, 10, 27, 54, 167, 191, 193, 452, 501, 503
- conduction band edge (CBE) 285, 289
- conduction band minimum (CBM) 330, 368, 451
- conjugated microporous polymers (CMPs) 10, 238, 351
- conjugated polymer nanostructures (CPNs) 6
- conjugated polymers, *see* conducting polymers
- consecutive photoinduced electron transfer (conPET) processes 92, 109
- constant phase element (CPE) 212
- constrained DFT (cDFT) 546
- contact angle 304
- contact potential difference (CPD) 213
- CoP/CdS hybrid catalyst 10
- core-shell metal-insulator nanoparticles 517
- core/shell nanocrystals 36
- core(gold)-shell(Ag) structure 463
- coupled reactions 386
- coupled semiconductors 518

- covalent organic frameworks (COFs)
  - 10, 331, 350–351, 435
- covalent triazine frameworks (CTFs)
  - 351, 436
- CPCs, *see* compound parabolic concentrators (CPCs)
- Creutz–Brunschwig–Sutin model 260
  - cross-dehydrogenative coupling reactions 407
  - of tertiary amines 406–407
- Cu<sub>2</sub>O-based junctions 204–207
- cyclic voltammetry (CV) method 234
  
- d**
- DDAT molecules 467
- decarboxylative/decarbonylative
  - C3-acylation, of indoles 404–405
- decoherence effects 533, 547
- degradation
  - organic pollutants 485
  - oxidative 490–492
  - oxidative photocatalytic 486
  - photocatalytic 492
- degree of transformation 263
- density functional theory (DFT) 13,
  - 287, 332, 372, 529
- deposited photocatalysts 569–570
- deposition precipitation method with urea (DPU) 146
- detoxification
  - graphene-TiO<sub>2</sub> composites for 299–303
  - metal doped photocatalysts for 296–299
  - photocatalysis applications of 303–312
- diazo compounds 406–407
- 2,4-dichlorophenol under visible-light irradiation 453
- dielectric constant 139
- diffuse reflectance spectroscopy (DRS)
  - 146, 150, 155
- 1,2-diketones synthesis, alkynes 399–400
- 1, 4-diphenylbutadiyne (DPB) monomer 234
- direct band gap 179
- direct C–H arylation of heteroarenes 398, 399
- direct photoexcitation 77
- 3,6-di(pyridin-2-yl)-1,2,4,5-tetrazine 411–414
- donor  $-\pi$  bridge-acceptor (D- $\pi$ -A) structures 261
- doped metal oxides 34–35
- doping 450, 451, 510
  - codoping 455–456
  - metal ion 451–453
  - of metal oxides 451
  - nonmetal ion 453–455
  - self-doping 450, 457–458
- doping-heterojunction nanostructure 472
- dual catalytic cycle 78
- dye, *see also* organic dyes
  - aggregation 260
  - photodegradation 263
  - sensitization 513
- dye modified TiO<sub>2</sub> photocatalysts 269–270, 586
- dye pollutants
  - mineralization of 264
  - self-sensitized degradation of 262–265
- dye radical cations 263, 266
- dye-SC electronic coupling 261
- dye sensitized
  - degradation process 264
  - heterogeneous photocatalytic process 586
  - mechanism of 513
  - mesoporous CN 347
  - photocatalytic hydrogen production 513
- dye sensitized solar cells (DSSCs) 466
  - development of 262
  - electron transfer in 465
  - energy conversion 260–262
  - photoelectrochemical 257
  - TiO<sub>2</sub> sensitizers for 262
- dye sensitization 513
- dye-TiO<sub>2</sub> photocatalytic system 265

**e**

electrochemical anodization method 308

electrochemical impedance spectroscopy (EIS) 202, 211–213

electrochemical reduction  
negative 29  
of oxidants 506  
process 120

electromagnetic energy 130

electromagnetic waves 5

electron and hole localisation 293–296

electron diffraction (ED) pattern 177

electron donor-acceptor (EDA) 398

electron/hole  
acceptors 4  
separation 14

electron–hole pair 5, 9, 10, 28, 63, 66, 136, 152, 153, 193, 212, 213, 227, 229, 284, 295, 299–301, 342, 366, 422, 436, 449, 455, 456, 461, 462, 499, 502, 515, 532, 545

electron–hole recombination 4, 122, 133, 138, 139, 146, 206, 208–210, 296, 307, 473, 514, 533, 546

electronic paramagnetic resonance (EPR) 266

electronic transitions 174, 457  
conduction band or from valence band 287  
HOMO to LUMO 467  
nonadiabatic 534, 548  
in photocatalytic systems 533  
RPMD methods 534  
uniform scaling of 533  
from VB of titania 471

electronic tunneling 536, 537, 548

electron injection process 257

electron-nuclear back reaction 535, 543, 547

electron photogenerated 464

electron scavenger 61, 65, 137, 149, 210, 238, 298, 486, 487, 521, 546

electron spin resonance (ESR) spectroscopy 121, 259

electron transfer (ET) 460, 461, 463

in composite semiconductor 518

in DSSCs 465

feasibility of 271

reactions 257

processes 28, 193, 366

electron trapping  
energy evaluation 296  
NPs 149  
Pd-based nanoparticles 154  
process 268, 269  
rutile (100) surface 295  
in TiO<sub>2</sub> nanocrystals 295

electrospinning 232, 233

endergonic reaction 369

energy conversion efficiency 192, 204, 238, 349, 587

energy-dispersive X-ray (EDX) mapping 146

energy-dispersive X-ray spectroscopy (EDS) 147, 150

energy gap 54, 234, 261, 285, 287, 289, 293, 385, 437

energy relaxation pathways 13, 587

energy transfer 144, 243, 257, 394, 459–464, 473, 529, 532, 535, 542, 547, 548

enhanced NIR absorption 119

Eosin Y (EY) 80  
photocatalysis by 396–401  
redox potentials of 397

ethylene glycol 120, 426

**f**

fast dye regeneration 270

Fe<sub>2</sub>O<sub>3</sub>-based junctions 199–200

Fe<sub>2</sub>O<sub>3</sub>/OEC 207–209

Fermi level energy ( $E_F$ ) 29, 55–57, 130, 139, 193, 194, 197, 204, 210, 230, 376, 465, 472, 499, 505, 514, 515

Fisher–Tropsch synthesis 54

flat-band potential 57, 208, 213, 470

fluorescein 80, 400

Förster resonance energy transfer (FRET) 243

Fourier transform infra-red (FTIR) spectroscopy 121

**g**

gallium nitride (GaN) 37  
 gas phase and self-cleaning applications 570–571  
 gel combustion method 119  
 Gibbs free energy 62, 166, 167, 191, 366  
 glass–bandgap 174  
 glass transition temperature 174  
 glassy photocatalysts  
   glass by melt–quench technique 172–174  
   glasses preparation 172–174  
   semiconductor–glass  
     nanocomposites 171–172  
 gold nanoparticles 130, 132, 138–144  
 graphene  
   and CNT based nanocomposites 345  
   nitrogen doping in 382  
   TiO<sub>2</sub> composite via hydrothermal route 519  
   two-dimensional graphene sheets 170  
 graphene/semiconductor  
   nanocomposites (GSNs) 33  
 graphical processing unit (GPU)  
   computations 535  
 graphitic carbon nitrides (g-C<sub>3</sub>N<sub>4</sub>) 8, 10, 238, 331, 332, 334  
   halogens doping 344  
   hard templating 337–339  
   metal doping 341  
   metal oxides/g-CN nanocomposites 344, 345  
   nanosheets 340  
   nitrogen doping 342  
   nonmetal doping 342–344  
   oxygen doping 342  
   phosphorus doping 343  
   photocatalytic water splitting 331–349  
   precursor-derived 334–336  
   soft templating 339–340  
   sulfur doping 342, 343  
   template-free 340–341  
   templating methods 336

growing string method (GSM) 531, 532

GW approximation (GWA) 529

**h**

Haber–Bosch cycle 54  
 halogens doping 344  
 Hamiltonian model 537  
 Hammes-Schiffer group 540  
 heat exchanger 310  
 heavy atom tunneling 548  
 heptazine-based microporous polymers (HMPs) 349, 351  
 heteroarenes  
   applications 91  
   C–H arylation of 398–399  
   Eosin Y 105, 107  
 heteroatom doping 341–344  
 heterogeneous photocatalysis 485  
   active species in 494–495  
   degradation of phenolic pollutants 492  
   fundamental mechanisms of 587  
   TiO<sub>2</sub> 255, 283, 485  
 heterojunctions 468  
   band alignment in 193  
   band-gap 468–470  
   charge carrier kinetics in 209–215  
   Co–Pi/BiVO<sub>4</sub>/ZnO 198  
   excitation of one component 468–469  
   photoanodes 196  
   semiconductors 436–437  
 H<sub>2</sub> evolution reaction (HER) 10, 62, 65, 202–206, 346, 349, 375  
 high angle annular dark field scanning transmission electron microscopy (HAADF–STEM) 146  
 high concentrating/high temperature systems 42–43  
 high-energy radiation 131  
 high intensity LED-based photoreactor 266  
 high-resolution transmission electron microscopy (HRTEM) 121, 146, 148, 150, 153, 179, 181, 243

- highest occupied molecular orbital (HOMO) 54, 261  
HOMO–LUMO 334, 380  
homolytic aromatic substitution (HAS) reaction 81, 85  
hot electrons 156, 460–462  
Hu’s reagent 86  
hybrid nanostructures 471–472  
hydrogenation, TiO<sub>2</sub> 118, 287, 289, 512  
hydrogen dissociation 463  
hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>)  
  in air-saturated system 487  
  decomposition 489  
  formation 257, 489  
  oxidative degradation of solutes 492–493  
  production 487  
hydrogen plasma 118, 119, 121, 123  
hydrogen sulfide (H<sub>2</sub>S) splitting  
  designing assembly 168–170  
  fundamentals of 166–168  
  photocatalyst and reagent system 169–170  
  photocatalyst, role of 167–168  
  standardization 168–169  
  thermodynamics of 166–167  
hydroperoxyl radical 27, 404, 487, 494  
hydroxylation  
  of arylboronic acids 240, 409–410  
  phenol 487  
hydroxyl radicals 492, 493, 506, 507  
  photocatalytic formation 488  
  surface bound 494  
3-hydroxyphthalic hydrazide 488
- i**  
imidazoheterocycles, thiocyanation of 401  
iminium cation 80  
impedance (Z) 211  
inclined plate collector (IPC) 39, 571–572  
inclined plate reactor (IPR) 571  
indirect bandgap 67, 179, 521  
indium-based oxides 427  
indoles  
  aerobic indole C-3 formylation reaction 402–404  
  coupling of bromopyrroloindoline with 87  
  decarboxylative/decarbonylative C3-acylation of 404–405  
inorganic semiconductors 229, 230, 245  
  metal oxides 424–428  
  oxynitrides 429–430  
  sulfides 428–429  
intensity-modulated photocurrent spectroscopy (IMPS) 213  
intensity-modulated photovoltage spectroscopy (IMVS) 213  
ion  
  doping 510  
  implantation 452, 510–513  
IPR, *see* inclined plate reactor (IPR)
- k**  
Kelvin Probe 213  
kinetic isotope effect (KIE) 537  
Kubelka–Munk function 335
- l**  
Langmuir–Hinshelwood kinetics 490  
large curvature tunneling (LCT) 537  
ligand-to-metal charge transfer (LMCT) 467  
light absorption 13, 14, 33, 34, 67, 117, 129, 153, 154, 168, 182, 195, 198, 200, 239, 260, 287, 291, 301, 340, 341, 347, 366, 462, 463, 469, 485, 499, 508, 514, 515, 520, 585, 586  
light-harvesting nanoheterojunction (LHNH) 242–245  
light harvesting units 366–369, 371, 378, 431  
light-induced electron transfer 453  
light irradiation sensitizer 368  
local electromagnetic field (LEMF) 462  
localized surface plasmon (LSP) 130  
localized surface plasmon resonance (LSPR) 5, 136, 138–140, 142–144, 156, 459–462

- lowest unoccupied molecular orbital (LUMO) 54, 203, 245, 258, 261, 334, 465, 467, 469
- lyotropic liquid crystal (LC) 233
- m**
- Marcus rate theory 546
- medium concentrating/medium temperature system 40–42
- melt-quench technique 172–174
- metal chalcogenides 10, 36–37
- metal complexes
- dyes 270, 460
  - photocatalytic reduction of 132
- metal-enhanced fluorescence (MEF) 136
- metal-free organic photocatalysts 587
- metal ion
- doping 451–453
  - implantation 452
- metal nanoparticles
- by photodeposition method 130–132
  - by radiolysis method 130–132
- metal organic frameworks (MOFs) 352, 434–435, 587
- metal oxides 424–428, 449
- band-gap structure 449
  - doping of 451
  - photocatalysts 14
  - semiconductors 567
- metal oxides/g-CN nanocomposites 344–345
- metal surface modification 458–467
- methanol photooxidation 541–544
- methylene blue (MB) 122, 301
- degradation of 10, 34
  - heteropolyaromatic 31
  - photocatalysis by 409–410
  - photophysical properties of 402
- methyl orange (MO) 31, 35, 122, 146, 234, 236, 266
- microwave irradiation 118, 119
- MOFs, *see* metal organic frameworks (MOFs)
- multiconfigurational time dependent Hartree (MCTDH) 534
- multielectron transfer processes 256, 269
- multiwalled carbon nanotubes (MWCNT) 299, 345
- n**
- NaBH<sub>4</sub> 119
- nanoarchitectures 14, 351, 466
- nanoclusters 139, 145, 148–150, 155, 289, 295, 464
- nano-Einstein (nano-ein) 133
- nanofibers 6, 120, 123, 231–234, 236, 243, 244, 521
- nanometer scale 3
- nanoparticles 29
- Au–Cu 146–148
  - Au–CuO 148–150
  - of controlled size and shape 131
  - core–shell metal-insulator 517
  - detecting and quantifying 574–575
  - Ni and Au 150–152
  - TiO<sub>2</sub> with Ag 136–138
  - TiO<sub>2</sub> with Au 138–144
  - TiO<sub>2</sub> with Bi clusters 144–145
  - TiO<sub>2</sub> with bimetallic 146–155
  - TiO<sub>2</sub> with Pd 135–136
  - toxicity 576–577
  - transformation of 575–576
- nanorod array electrodes 197
- nanoscale 5, 14, 228, 231, 245, 295, 568, 569, 574, 577, 587
- nanoseconds 209, 257, 270, 533, 549
- nanosheets 10, 340, 378
- nanosized
- crystals 502
  - photocatalysts 171
- nanospheres (NSPs) 6, 10, 32, 337, 469, 509
- nanostructures
- conducting polymers 227–246
  - designing black TiO<sub>2</sub> 118–122
  - effect of size 369–370
  - g-CN photocatalysts 336
  - hybrid 471–472
- nanotubes (NTs) 7, 10, 118–121, 123, 149, 150, 199, 231–233, 307, 308,



- 345, 430, 457, 466, 507–509, 519, 568
- nanowire hybrid nanostructures 10
- NaTaO<sub>3</sub>, surface modification 464
- natural organic matter (NOM) 576
- N–B–TiO<sub>2</sub> (red anatase TiO<sub>2</sub>) 455
- negative electrochemical reduction 29
- Nernst's equation 60
- N*-ethoxy-2-methylpyridinium (EMP) 397, 398
- nitrates
- organic 306
  - photocatalytic reduction of 135
- nitrogen doping 342, 454
- N,N*-diisopropylethylamine (DIPEA) 78, 94
- noble metals (NM) 11, 459
- cocatalysts 235, 521
  - loading 514–518
  - NPs 129, 130, 136, 156, 256, 268
  - on semiconductor 267
- nonadiabatic dynamics
- of charge carriers 532
  - effects in photocatalysis 530
  - quantum tunneling in 535–540
- nonadiabatic effects
- on metal surfaces 530
  - in O<sub>2</sub> adsorption 546
  - in photocatalysis 532–535
- nonadiabatic molecular dynamics (NA-MD) 530
- nonadiabatic transition state theories (NA-TST) 534
- nonadiabatic tunneling
- effects 540
  - theories 540, 548
- non concentrating reactor (NCC) 39–40
- nonconcentrating solar collectors (NCCs) 310
- nonmetals
- ion doping 453–455
  - surface modification 464
- nonradiative transition 394
- normal hydrogen electrode (NHE) 61, 167, 191, 423, 503
- nuclear magnetic resonance (NMR) 121
- nudged elastic band (NEB) 531
- Nyquist plot 211, 212
- O**
- Ohm's Law 211
- one-electron reduction potentials 495
- one-step photocatalytic process 371–374
- optical antenna effect 5
- optical cut-off wavelength 174
- optical electron transfer (OET) 260, 467
- organic compounds
- colorless and color 464–467
  - mineralization of 33
  - oxidative decomposition of 460, 468
  - photocatalytic oxidation of 454
  - surface modification 464
- organic dyes
- electrochemical processes in 394
  - for organic synthesis 393–415
  - pollutants 262
  - photophysical processes in 394
  - photophysical properties of 393
  - visible-light photoredox catalysts 394, 396, 414
- organic pollutants 492
- conducting polymer nanostructures for 233–237
  - solar degradation of 38–44
- organic reactions
- catalyzed by semiconductor photocatalysts 541–547
  - photoinduced 538
- organic semiconductors
- carbon nitride and composite 430–434
  - conducting polymers 228–230
  - covalent organic frameworks (COFs) 435
  - donor–acceptor junction 245
  - metal organic frameworks (MOFs) 434–435
  - for photocatalytic water splitting 331–332

- organic transformations
    - nanostructures catalytic materials 585
    - photocatalysis for 11–12
  - organocatalytic cycle 79, 80
  - oxidation
    - of alcohols to carbonyl derivatives 413–414
    - reaction 503
  - oxidative annulation, of arylamidines 405–406
  - oxidative coupling, of primary amines 414
  - oxidative cross-coupling, of thiols 408–409
  - oxidative degradation, of solutes 490–492
  - oxidative hydroxylation, of arylboronic acids 409–410
  - oxidative photocatalytic degradation 486
  - oxide-based semiconductors 3, 4, 586
  - oxidized photosensitizer 466
  - oxygen doping 342
  - oxygen evolution catalysts (OECs) 195, 197, 207, 375
  - oxygen evolution reaction (OER) 8, 61, 195, 377
  - oxynitrides 6, 8, 11, 35, 36, 195, 379, 429–430, 437, 438, 469, 471, 586
- p**
- parabolic trough collector 40, 41, 309
  - parabolic trough concentrator (PTC) 572–573
  - Pd nanoparticles 135–136
  - perfluoroarylation, of arenes 105, 107, 108, 396–397, 415
  - perovskite 35–36, 44, 65
  - peroxyl radical 492
  - perylenediimide (PDI) 80, 92, 239, 240, 435
  - phenacyl bromides 77–79, 89
  - phenol
    - degradation of 134
    - hydroxylation 487
    - photodegradation 297
  - phenothiazine dyes 414
  - phenoxy radicals 491, 493
  - 10-phenylphenothiazine (PTH) 103
  - phosphorus doping 343
  - photoanodes 9, 58, 65–68, 165, 194, 196, 197, 200, 201, 206–208, 210, 260, 269
  - photo-Arbusov reactions 103
  - photocatalysis
    - computational approaches to model adiabatic processes in 531–532
    - computational approaches to model nonadiabatic effects in 532–535
    - computational modeling 529, 587
    - on C-modified NaTaO<sub>3</sub> 464
    - by 3,6-di(pyridin-2-yl)-1,2,4,5-tetrazine 411
    - efficiency of 502
    - by Eosin Y 396–401
    - heterogeneous 485
    - mechanism of 284, 450, 500
    - by methylene blue 409, 410
    - by phenothiazine dyes 414
    - plasmon-assisted 459
    - plasmonic 459
    - by Rose Bengal (RB) 402
    - slurry-style 569
    - in TiO<sub>2</sub>/water systems 486
  - photocatalysts
    - degradation 8, 122, 134, 135, 145, 227, 236, 244, 262, 264, 453, 486, 487, 492, 493, 570, 572
    - deposited 569–570
    - mono and bimetallic nanoparticles 155–156
    - organic reactions catalyzed by semiconductor 541–547
    - plasmonic 463
    - semiconductor 502
    - solar photochemical splitting of water 369
    - TiO<sub>2</sub> 255–271
  - photocatalytic CO<sub>2</sub> reduction
    - activity by MnCo<sub>2</sub>O<sub>4</sub> 427
    - advantages 421
    - inorganic semiconductors 424–430

- NH<sub>2</sub>-MIL-101(Fe) 435  
 organic semiconductors 430, 435  
 principles 422–424  
 Ru/CN composite 432  
 semiconductor heterojunctions  
 436–437  
 photocatalytic degradation  
 of 2,4-dichlorophenol under  
 visible-light irradiation 453  
 photocatalytic detoxification 284, 585  
 photocatalytic hydrogen generation  
 61, 122, 123, 152, 380, 382  
 photocatalytic oxidation  
 of organic compounds 454  
 processes 235  
 reaction mechanism of 343  
 terbutylazine 265  
 photocatalytic reactions 5, 12, 13, 54,  
 60, 65, 136, 183, 415, 469, 470,  
 506–507, 510, 513, 532, 534, 538,  
 540, 548  
 photocatalytic reduction  
 of CO<sub>2</sub> 5, 6, 14, 422–425, 428–431,  
 433, 437, 438  
 of Cr(VI) 7, 268  
 in GO 300  
 of metal complexes 132  
 of nitrate 135  
 photocatalytic system  
 efficiency of 490  
 electronic transitions in 533  
 photocatalytic water splitting  
 conducting polymers 237, 240  
 crystalline carbon nitrides 347–348  
 development of 54–56  
 effect of light 58–62  
 electrolysis and photoelectrolysis  
 63–65  
 organic semiconductors for  
 331–332  
 process 329  
 semiconductors, electrochemistry of  
 56–58  
 soft templating, g-CN 339–340  
 solar photocatalysts for 65–66  
 structural modification with organic  
 groups 345–347  
 sulfur doping 342, 343  
 sunlight conversion and storage  
 62–63  
 template-free 340–341  
 templating methods, g-CN 336  
 visible-light absorbing metal oxides  
 66–67  
 photocathodes 65, 68, 204–206, 210  
 photochemical process 12, 39, 191,  
 585, 587  
 photoconductivity 130, 132, 151  
 photoconversion efficiency 65, 242,  
 499, 508, 509  
 photocorrosion 30, 32, 36, 54, 60, 65,  
 149, 168, 170, 174, 175, 179, 183,  
 192, 201, 203, 207, 330, 331  
 photocurrent efficiency 509  
 photodegradation 4, 31, 33, 35, 36,  
 122, 130, 146, 147, 234, 236, 245,  
 262–266, 297, 299–301, 511  
 photodissociation 463, 540, 541, 543,  
 547–549  
 photoelectrochemical (PEC) 9, 54, 66,  
 192, 215, 365  
 electrode 123  
 water reduction 65  
 photoelectrochemical impedance  
 spectroscopy (PEIS) 213  
 photoelectrodes 9, 62, 63, 65, 66, 68,  
 200, 207, 213, 214, 500  
 photogenerated charge mechanism,  
 (TiO<sub>2</sub>) 500  
 photogenerated electrons 5, 7–9, 28,  
 29, 34, 59, 62, 65, 66, 132, 156,  
 183, 202, 206, 214, 229, 237, 284,  
 285, 299, 300, 334, 384, 386, 424,  
 433, 449, 453, 455, 459, 464, 469,  
 471, 472, 499, 514  
 photoinduced charge transfer process  
 243, 457  
 photoinduced electron transfer (PET)  
 92, 258, 260, 393, 396  
 photoinduced oxidation 231, 541, 542  
 photoluminescence spectrometry (PL)  
 146, 155, 211  
 photooxidation, methanol 541–544  
 photoreactors 43, 309

- photoreactors (*contd.*)  
   for solar degradation 38–44  
   temperature 169  
 photoredox catalysis, *see* visible-light, photoredox catalysis  
 photoredox catalytic  
   activation of carbon–halogen bonds 75–110  
   approach 76  
 photoredox transformations 80, 91, 395  
 photosensitization 269, 270, 453  
 photosensitizers 9, 132, 261, 262, 266, 269, 368, 382, 402, 403, 409, 460, 465, 466, 519  
 photosynthesis, Z-scheme of 255  
 photosystem II (PSII) 193, 376  
 photovoltaic cells 53  
 phthalocyanines (Pc) 8, 259, 261, 267, 270, 347  
 plasma laser ablation techniques 118  
 plasmon-assisted catalysis 462  
 plasmon-assisted photocatalysis 459  
 plasmon-based photocatalysts 6  
 plasmon energy transfer (PRET) 461  
 plasmonic heating 459, 462, 463  
 plasmonic light harvesting 517  
 plasmonic nanostructures 4, 515  
 plasmonic photocatalysis 5, 156, 459, 462, 464  
 plasmonic photosensitizer 460  
 platinized SrTiO<sub>3</sub> 65  
 p–n heterojunctions 6, 255  
 poly(diphenylbutadiyne) (PDPB) 6, 234, 243  
 poly(3, 4 ethylene dioxythiophene) (PEDOT) 6, 228, 233, 235, 347  
 poly(3-hexylthiophene) (P3HT) 233, 237, 243  
 polychromatic and monochromatic light 150  
 polyethylene glycol (PEG) 426  
 polymer-based composites 4  
 polymeric graphitic carbon nitride 4, 12, 331, 431, 587  
 polyvinylpyrrolidone (PVP) 170  
 porous conjugated polymers (PCPs) 239, 350  
 potential energy surfaces (PES) 531  
 powder photocatalysts 38, 170–171  
 powder X-ray diffraction (PXRD) 121  
 primary amines, oxidative coupling 414  
 PROPHIS reactor 41, 309, 310  
 proton-coupled electron transfer (PCET) reactions 540  
 proton transfer 531, 537, 538, 545  
 proton tunneling 537, 545  
 PTC, *see* parabolic trough concentrator (PTC)  
 pulse radiolysis 488  
 pyrrole heterocycle 81, 85, 99  
 PYXAID program 534, 535
- q**  
 QDs, *see* quantum dots (QDs)  
 quantized Hamiltonian dynamics (QHD) 537  
 quantum-classical dynamics methods 547  
 quantum dots (QDs) 10, 171, 176, 262, 470  
 quantum effects 13  
 quantum tunneling  
   in adiabatic dynamics 535–540  
   in nonadiabatic dynamics 535–540  
 quantum yields 3, 9, 10, 30, 34, 110, 129, 141, 191, 202, 203, 207, 227, 238, 241, 331, 347, 350, 369, 402, 428, 431, 432, 449, 490, 529
- r**  
 radiative transition 394  
 radical trifluoromethylation 410–411  
 Raman spectroscopy 121  
 Randle circuit 212  
 reactive dioxygen species 402  
 reactive oxygen species (ROS) 27, 257, 262, 283, 451, 576, 587  
 receiver–reactor tubes 309  
 reduced graphene oxide (rGO) 199, 299, 303, 472, 519  
 resonant energy transfer (RET) 462

- rhodamine B (RB) 8, 35, 36, 80, 134, 135, 145, 206, 237, 245, 262–264, 400, 405, 407
- rhodamine 6G (Rh-6G) 94–96, 99–103, 296, 298
- ring polymer molecular dynamics (RPMD) 534, 536, 538
- Rose Bengal (RB) 8, 259, 400, 402–404
- Ru(bpy)<sub>3</sub><sup>2+</sup> 77, 79, 80, 82, 85, 368, 369, 382, 409, 410
- ruthenium-based dyes 368
- rutile 30, 31, 35, 65, 117–119, 123, 129, 133, 139, 152, 269, 295–297, 301, 308, 453, 458, 504–507, 521, 541–543, 546
- S**
- Sakata–Hashimoto–Hiramoto model 260
- scanning transmission electron microscopy (STEM) 155
- Schottky barrier 139, 194, 269
- S–C junctions 194
- self-cleaning
- glasses, principle of 305
  - materials 303–307
  - self-doping 450, 457–458
  - semiconductor liquid junction (SCLJ) 193
  - semiconductor photocatalysts 4
    - bandgap of 27
    - electron–hole pair in 422
    - organic reactions catalyzed by 541–547
    - photoexcitation of 28
- semiconductors 449
- band bending 503
  - coupled 518
  - doping 450
  - electron transfer mechanism in composite 518
  - heterojunctions 436, 450
  - inorganic 424–430
  - organic 430
  - oxides-based 586
  - photocatalysts 502
  - photo absorption 132
- semiconductor surfaces
- carbon oxide redox reactions on 546–547
  - methanol photooxidation on 541–544
  - water splitting reactions on 544–546
- sensitization dye 513
- SHARC 534, 535
- silica doped TiO<sub>2</sub> 296
- silver nanoparticles 130, 132, 136–138, 514
- silver phosphate 10, 179, 521
- single electron transfer (SET) 75–78, 80, 82, 84–86, 89, 91, 94, 99, 395
- slurry-style photocatalysis 569
- small curvature tunneling (SCT) 537
- sol–gel
- method 9
  - process 172, 452
  - technique 119
- solar degradation, photoreactors for 38–44
- solar emission spectrum 44
- solar energy
- chemical energy 269
  - fuels 365, 500
  - conversion 3, 4, 11, 62, 63, 65, 68, 227, 238, 349, 352, 366, 435, 449, 470, 529, 530, 585, 587
  - harvesting 231
  - overall efficiency ( $\eta_c$ ) of 366
  - renewable energy 585
- solar illumination 568, 571–573, 587
- solar irradiation 10, 38, 191, 206, 299, 306, 365, 372
- solar light induced photocatalysis 4, 228, 246
- solar photocatalytic
- applications 309, 568, 587
  - CPC plant 311
  - reactor/collector 38
  - reactor designs 13, 567–577
- solar photoreactors 29, 30, 38, 41, 312
- solar reactors
- parameters of 43–44
  - photocatalytic 40

- solar reactors (*contd.*)
    - thermal efficiency of 39
  - solar spectrum 4, 43, 61, 65, 67, 117, 129, 191, 227, 271, 284, 287–289, 313, 330, 449, 499, 504, 514, 568
  - solar-to-chemical energy conversion 365
  - solar-to-hydrogen (STH)
    - conversion 123, 192, 196
    - efficient 61
  - solar tracking devices 310
  - SOLARDETOX 311
  - SOLARIS reactor 309, 310
  - solvothermal-assisted method 122
  - solvothermal process 433
  - standard hydrogen electrode (SHE) 291, 345
  - stoichiometric ratio 335, 371, 372
  - substitutional doping 285, 451
  - sulphides 331
  - sulfur doping 342–343
  - superoxide radical anion 400, 402–404, 407, 486, 491, 494, 499
  - surface band bending 505, 506, 515
  - surface bound hydroxyl radicals 488, 489, 491, 493, 494
  - surface-enhanced Raman scattering (SERS) 136
  - surface modification 450, 458
    - heterojunctions 472
    - metals 458
    - NaTaO<sub>3</sub> 464
    - nonmetals 464
    - organic compounds 464
  - surface-modified semiconductor 450
  - surface photovoltage (SPV)
    - measurement 13
    - spectroscopy 199, 211, 213–215
  - surface plasmonic effect 54
  - surface plasmon resonance (SPR) 12, 143, 182, 499, 515
- t**
- template-free method 233, 340
  - terminal oxidant 402
  - tertiary amines
    - $\alpha$ -functionalization of 408
    - cross-dehydrogenative coupling of 406
  - tetrakis(hydroxymethyl) phosphonium chloride (THPC) 146
  - tetramethylethylenediamine (TMEDA) 402
  - thermodynamic energy 63
  - thermodynamic favourability of reactions 423–424
  - thermodynamic, H<sub>2</sub>S splitting 166–167
  - thiocyanation of imidazoheterocycles 401
  - thiols, oxidative cross-coupling 408–409
  - time-dependent density functional theory (TD-DFT) 13, 529
  - time dependent wave packet (TDWP) approach 534
  - time-resolved microwave conductivity (TRMC) method 13, 130, 132–138, 145, 146, 150, 266, 464
  - titania, *see also* titanium dioxide (TiO<sub>2</sub>)
    - band structure of 472
    - modification, urea-induced 467
    - with monometallic nanoparticles 133–138
    - with Pt clusters 133–135
    - sensitization 458
  - titaniananobelts (TNBs) 469
  - titanium butoxide 119, 120
  - titanium dioxide (TiO<sub>2</sub>) 8–11, 499, 568
    - alternatives to 520–521
    - anatase stability and photocatalytic activity 296
    - anion doped 512
    - antibacterial action of 307
    - band gap of 454
    - bactericidal 307–308
    - Bi clusters 144, 145
    - bimetallic nanoparticles 146–155
    - carbon-TiO<sub>2</sub> composites 518–520
    - catalytic effect 489
    - co-doping 290
    - coupled semiconductors 518
    - coupling of 255
    - crystal structure 505

- from DFT simulations 287
  - doping and surface modification of
    - 285–291
  - DSSCs, sensitizers for 262
  - dye adsorption on 263
  - dye-modified 256–259
  - dye sensitization 513
  - electronic structure 513
  - electron transfer (ET) mechanism
    - 268, 514
  - energy gap 293
  - energy levels alignment 293
  - gold nanoparticles 138–144
  - high temperature stable anatase
    - 296
  - ion doping and ion implantation
    - 510
  - light absorption of silver supported in
    - 515
  - in limitation 129
  - materials for energy conversion
    - 260–262
  - metal-free organic dye 267
  - mono- and bimetallic nanoparticles
    - 155, 156
  - nanocluster 289
  - nanomaterials 118, 119
  - nanoparticles 516
  - nanowire system 291
  - noble metals loading 514–518
  - particles 488
  - Pd nanoparticles 135, 136
  - photoanode 269
  - photocatalyst system 312
  - photocatalytic activity of 129, 456
  - photocatalytic mechanisms in
    - TiO<sub>2</sub>-CNT composites 520
  - photocatalytic reactions 506–507
  - photo-generated charge mechanism
    - 500
  - physical architectures 507–509
  - physical structure 509
  - rare earth metal ions, effect of
    - 297–299
  - silver nanoparticles 136–138
  - structure 504
  - transition metals, effect of 296–297
  - undoped metal oxides different from
    - 30–33
  - valence band (VB) of 453
  - for visible-light assisted degradation
    - 265–268
  - visible-light photocatalysis 509
  - water systems, photocatalysis in 486
  - Togni reagents 86
  - total organic carbon (TOC) 237, 573
  - total sun energy 3, 372
  - toxicity, of nanoparticles 576
  - trajectory surface hopping (TSH) 533
  - transient absorption spectroscopy
    - (TAS) 7, 206, 209–211, 460
  - transition state theories (TST) 531,
    - 534
  - transmission electron microscopy
    - (TEM) 177, 243, 343
  - triazine and heptazine based organic
    - polymers 349–350
  - tri-doped titania 455
  - triethylamine (TEA) 105, 237, 240,
    - 396, 428
  - trifluoromethylation
    - of aromatic heterocycles 84, 85
    - radical 410–411
  - Tris 491, 493
  - tunneling-controlled reaction 537
  - turnover frequency (TOF) 369, 376
  - turnover number (TON)/turnover
    - frequency (TOF) 369
  - two-step photoexcitation process
    - 374–376
- U**
- ultrasonication 118, 120
  - ultrathin Bi<sub>2</sub>WO<sub>6</sub> nanoplates 425
  - ultraviolet (UV)
    - irradiation 3, 129, 134, 135, 139,
      - 191, 203, 236, 258, 451
    - light 330
    - photocatalysis 284
    - radiation 165
  - undoped TiO<sub>2</sub> 30–32
  - urea-induced titania modification
    - 467

**V**

valence band (VB) 8, 10, 27, 54, 121, 142, 165, 167, 191, 193, 235, 256, 257, 283, 287, 289, 291, 293, 329, 332, 342–344, 346, 423, 451, 453, 456, 501, 503

valence band maximum (VBM) 330, 342, 366, 368, 380, 451–454

vanadium 67, 298, 472

variational TST (VTST) 538

VB edge (VBE) 196

visible-light

- absorption in metal oxides 66
- active photocatalytic materials 4
- active photocatalytic water splitting 329, 352
- alcohols, induced oxidation of 11
- assisted degradation of colorless pollutants 258
- band gap modifications for 452
- benzene, induced hydroxylation of 12
- cross-dehydrogenative coupling 406
- degradation processes 227
- development of 11
- by dye photosensitization 269
- electron donating compounds 266
- environmental protection, photocatalysis for 4–8
- Eosin Y 105
- general mechanism 396
- harvesting capability 4
- harvesting efficiencies 6
- heterojunction for 4
- high surface area anatase 11
- illumination 199
- induced organic synthesis 12
- induced photocatalysts 6
- induced photocatalytic activity 5, 7
- irradiation 9, 10, 61, 91, 139, 237, 258
- mechanistic studies of 13–14
- organic dye as 396, 414
- photocatalyst/OEC junctions 207, 209
- photoactivity of small metal clusters 133

photoredox catalysis 393

range 8

responsive junctions 195–207

of TiO<sub>2</sub> materials 4

wavelengths of 94

**W**

wastewater

- detoxification 228, 308–312
- pollutants 5, 8, 262
- purification 4
- treatment 29, 38, 303, 310, 311

water oxidation

- and CBE 291–293
- oxygen 376–380
- valence 291–293

water oxidizing complex (WOC) 376

water purification

- applications 571
- heterogeneous photocatalysis 485
- photocatalysts for 33

water reduction

- C<sub>3</sub>N<sub>4</sub> 380–382
- multicomponent heterostructures 383–386
- semiconductors 382–383

water splitting 8–11

- band gap 284
- fundamentals of 366–367
- one-step photocatalytic process 371–373
- photocatalysis with oxygen evolution 500
- reactions on semiconductor surfaces 544–546
- thermodynamic requirements of 368
- Z-scheme photocatalysis/two-step photoexcitation process 374–376

wavefunction (WF)-based methods 529

Wentzel–Kramers–Brillouin (WKB) approximation 537

WO<sub>3</sub>-based junctions 201–202

WO<sub>3</sub>/OEC 208, 209



**X**

- X-ray fluorescence spectrometry (XRF) 155
- X-ray photoelectron spectroscopy (XPS) 121, 146, 150, 266, 335
- X-ray powder diffraction (XRD) 153, 155, 175, 334

**Z**

- zero-point energy 13, 534, 538, 545
- zinc gallium oxynitride (ZnGaNO)
  - nanorods 429
- Z-scheme photocatalysis 11, 374, 376, 470–471

