

Index

a

ab-initio MD simulations 42
 absorption spectra 203
 acenes 135
 acoustic phonons 41
 acoustical-optical phonon upconversion 111
 all-inorganic halide perovskites 208, 213
 all-inorganic perovskites (AIP) 25–28, 218
 alternative divalent metal cation 175
 ambipolar semiconductor 131
 amplified spontaneous emission (ASE) 110, 111, 228
 anti-crossing energy splitting 68
 atomic layer deposition (ALD) technique 144
 Auger rates 110, 111, 227, 236
 Auger recombination process 227

b

Bader charge analysis 165
 bathocuproine diffusion barrier 191
 Bethe–Salpeter equation (BSE) 27, 47
 biexciton 72, 73, 228
 bifunctional alkylphosphonic cross-linking molecules 241
 bimolecular (BR) recombination 91, 103, 109–111, 127, 233, 257
 Block states 225
 Bloch-wave electrons 223
 Bohr equation 7
 Boltzmann distribution 111, 261, 262
 Bose–Einstein condensation (BEC) 68

bound excitons (BEs) 56, 119, 164, 227, 233
 Bragg-reflector cavities 234
 Brillouin zone (BZ) folding 26, 28–33, 102
 broadband visible emitters, structure of 57
 bulk inversion asymmetry (BIA) 36

c

carbon dioxide (CO₂), greenhouse gas 274, 275
 carrier diffusion lengths 104–107
 carrier-exciton scattering 254
 carrier lifetimes 104, 111, 120–122, 127
 Cauchy principal integral 123
 cesium lead halide based perovskite nanocrystals 233
 chalcogenide solar cells 189
 charge dynamics 107–108
 charge recombination layers (CRL) 192
 charge-transfer dynamics 115–117
 chemical vapour deposition (CVD) 190
 circular pump-probe technique 265
 collective vibrational excitations 41
 compact lasers 223
 conduction band (CB) 26, 108, 132, 148
 conduction band minimum (CBM) 30, 102, 140, 163, 169, 279
 corner-sharing octahedral network 162

- Coulomb interaction 72, 229
 Cu-In-Ga-S/Se (CIGS) chalcogenide layers 106
- d**
- Debye Waller factor measurements 41
 defect formation energy 164
 deformation potential mechanism 41
 density functional perturbation theory (DFPT) 41
 density-functional theory (DFT)
 method 26, 102, 161, 165
 MD simulations 42
 diamagnetic coefficient, e-h pairs 261
 dielectric confinement effects 45, 73
 diffusion coefficients 87, 111, 121–122
 diffusion lengths 87, 89, 93, 104, 105, 121–122, 126, 127, 172
 diode lasers 223, 225, 228, 229, 239–241
 diode-pumped solid-state (DPSS) 239
 distributed Bragg reflectors (DBR) 70, 236
 distributed feedback (DFB) 68, 234
 donor-acceptor (D-A) 12, 120, 135, 136, 146
 donor- π -acceptor (D- π -A) 135
 donor- π -donor (D- π -D) 135
 double perovskites 170
 Dresselhaus effect 36–40
 drift-diffusion models 89
 dual excited states model 108
 dye-sensitized solar cells (DSSCs) 85, 87, 90, 93, 94, 139, 174, 189, 282
- e**
- edge-sharing octahedral chain network 162
 e-h pair confinement 224, 229
 electrical injection, in perovskite 225–228, 239–241
 electrochemical-photovoltaic (EC-PV) configuration 277
 electrodeposition technique 144
- electroluminescence (EL) 15, 201, 206–209, 212, 214, 215, 217, 240, 252–260
 emission intensity 252, 255
 electroluminescent devices 202, 204, 209, 210, 215, 217, 224
 electron affinity 132, 226
 electron-hole (e-h) pairs 84, 103, 119, 120, 224, 227, 230, 240, 252, 255
 electronic band structure 28–33, 102–103
 electron-phonon coupling mechanisms 41, 62, 89, 240
 electron selective hole-blocking materials 139–147
 electron transfer process 115
 electron transport layer (ETL) 90, 104, 112, 206, 225
 energy dispersive X-ray analyser (EDX) 96, 140
 energy transfer mechanism 12, 59–60
 epitaxial single-crystal (SC) growth techniques 223
 exciton binding energy 45, 47, 56, 84–86, 94, 103–104, 119, 120, 127, 164, 170, 171, 203, 209, 227, 233, 241, 251, 263
 exciton vs. free carriers 103
 exciton-polariton 68
 extended Hückel tight-binding model 26
 extended Huckel theory (EHT) 162
 external quantum efficiency (EQE) 15, 118, 187
 external quantum efficiency for electroluminescence (EQE_{EL}) 201, 202
- f**
- fabrication processes 56
 Fabry-Perot (FP) cavity architecture 69
 Fabry-Perot type 236
 facile solution-processing 56
 Faraday configuration 261
 Fermi gas 233

- Fermi level 113, 114, 121, 164, 165, 204, 276
- Fermi-plasma-type recombination 233
- field-effect transistors (FETs) 10, 15, 55, 87
- field-induced circular polarization (FICPO) effect 261
- field-induced circularly polarized emission 260, 262–263
- fill factor (FF) 83, 157, 186
- film fabrication techniques 90
- fluorene–dithiophene derivatives 194
- formamidineium (FA:[HC(NH₂)₂]⁺) 25
- formamidineium (HC(NH₂)₂⁺) 109, 126
- formamidineium tin iodide (FASnI₃) 164
- fossil fuels 273
- free exciton (FE) 6, 8, 55, 62, 63, 119, 164
- Frenkel excitons 225, 227
- Fröhlich electron–phonon interactions 112
- Fröhlich polar mechanism 41
- full width at half maximum (FWHM) 13, 62, 214
- g**
- GaAs pn-junction 282
- generalized gradient approximation (GGA) 162
- greenhouse gases 273
- guanidineium (GA:[C(NH₂)₃]⁺) 25
- h**
- half-width at half maximum (HWHM) 253, 258
- halide perovskite solar cells (PSCs) absorption and emission properties 118–120 carrier lifetimes 121–122 diffusion coefficients 121–122 diffusion lengths 121–122 perovskite tandem photovoltaic device research 188–194 recombination constants, surface and bulk regions 126–127 surface vs. bulk optical properties 120–121 tandem device type and performance limitation 184–188 transient spectral features 122–126
- high content (HC) region 6
- highest occupied molecular orbital (HOMO) 94, 114, 132, 157
- high magnetic field optical 260–263
- hole selective electron-blocking materials (HTM) 132–139
- hole transport layer (HTL) 89, 104, 112, 135, 206, 225
- hot carriers 111–112
- hot phonon effect 111, 112
- hybrid optoelectronic-spintronics (O-S) device 266, 267
- hybrid organic perovskites (HOP) 25
- hybrid perovskites excitons 202–205, 212, 217 free carriers 203 light-emitting diodes nanocrystals 209–218 n–i–p diodes 206, 208 p–i–n diodes 206 quantum dots 212, 215 quasi-2D structures 215, 217 transparent electrodes 205 low excitation intensity 205 photoluminescence 204, 205 solar cells 201 temporally fluctuating photoluminescence 204 trap states 204, 212
- hydrogen (H₂), photoelectrochemical generation 275, 276
- hyperfine interaction (HFI) 252
- i**
- impedance spectroscopy (IS) 95, 121
- InAs/GaAs material system 224, 240
- indium tin oxide (ITO) 16, 147, 188, 206
- ink-based coatings 191

- integrated PL intensity (IPL-IN) 6, 211
- intensity-modulated photocurrent spectroscopy (IMPS) 95
- intensity-modulated photovoltage spectroscopy (IMVS) 95
- interatomic forces 41
- interfacial polarization 93
- inverse photoelectron spectroscopy (IPES) 113
- ionization potential (IP) 132, 133
- irreducible representations (IR) 26, 29, 32, 35
- j**
- Jaynes–Cummings model 64–66
- k**
- Klemens relaxation pathway 112
- Kramers–Kronig relations 123
- l**
- Landau level transitions 263
- large polaron screening effect 111
- lattice strain 28–33
- lead halide perovskites 35, 64, 201, 203, 233, 252
- light-controlled magneto-resistance 266
- light-emitting devices (LEDs) 15, 251, 255
- all-inorganic halide perovskites 208, 213
- electrical injection in perovskite 225–228
- hybrid perovskites 201
- linearized augmented plane wave method (LAPW) 165
- load resistor 185
- local density approximation (LDA) 35, 162
- low-content (LC) region 6
- lower-dimensional perovskites 86, 159, 161
- lower polariton branch (LPB) 68
- lowest unoccupied molecular orbital (LUMO) 114, 139, 140, 146, 148, 157, 206
- m**
- magnetic field effect (MFE) 251–260
- magneto-absorption spectroscopy 263
- magneto-conductivity (MC) 252
- magneto-electroluminescence (MEL) 252
- magneto-photoconductivity (MPC) 252
- magneto-photoluminescence (MPL) 252
- metal–organic chemical vapor deposition (MOCVD) 223
- methylammonium (CH_3NH_3^+) 109, 126
- methylammonium (MA [CH_3NH_3] $^+$) 25
- methylammonium halide perovskites 203
- molecular beam epitaxy (MBE) 223
- molecular dynamics (MD) 27, 41–47
- molecular HTMs 132–135
- molecular relaxational processes, MA-based compounds 42
- monomolecular (MR) recombination 91, 110, 126
- multidimensional perovskites
- AMX₃ formula 155
- Goldschmidt tolerance 155
- HOMO–LUMO energy gap, organic ammonium cation 157
- layered structures, formation of 157
- mixed dimensional perovskites 157
- octahedral factors 155
- photovoltaics 157, 161
- Ruddlesden–Popper 156
- three-dimensional (3D) perovskites 155
- two-dimensional (2D) perovskites 156
- Pb-free halide perovskites
- ASnX₃ perovskites 161–164

- A_2SnX_6 perovskites, metal deficient structures 165–166
 bismuth/antimony-based perovskites 168–169
 germanium-based perovskites 166–168
 Sn²⁺ and Ge²⁺ replacements for Pb²⁺ 172–174
 multi-quantum well (MQW) 62, 66
 multi-TCE/three terminal (3-T) mechanical stack 185–186
 multi-TCE/four-terminal (4-T) mechanical stack 186
 multi-TCE/four-terminal (4-T) spectrum split 186–188
- n**
- non-radiative recombination 94, 107, 147, 169, 184, 201, 204, 209, 217, 218, 230, 233
 n-type electron transport layer (ETL) 225
 n-type hole-blocking electron selective layer (ETM) 131
- o**
- ohmic contact 131, 202
 oleylamine 6
 open circuit voltage (VOC) limit 132
 optical resonators 234–239, 242
 optical phonons 41
 optical Stark effect (OSE) 65–66
 optical transitions 56, 102–103
 optoelectronic properties 55
 order–disorder mechanisms 42
 organic–inorganic hybrid perovskites 251
 magnetic field effect (MFE) 252–260
 optical 260–263
 spin-polarized carriers dynamics 263–265
 organic light-emitting diodes (OLEDs) 205, 206, 211, 223
 organic photovoltaic (OPV) materials 91
 organometallic complex HTMs 136–138
 oxygen evolution reaction (OER) 277
- p**
- (PEA)₂(MA)_{n-1}Pb_nI_{3n+1} perovskites energy transfer schemes 217
 unit cell structure 216
 PEC electrode materials 276–277
 PEC-PV tandem system 282–285
 perovskite/charge transport layer interfaces 112–115
 perovskite gain media 234–239
 perovskite laser
 electrical injection 239–241
 gain media 234–239
 light emitting diodes 225–228
 optical resonators 234–239
 thin film solid-state perovskites optical gain 228, 233
 perovskites
 non-saturated organic moiety BC 16–18
 saturated organic moiety
 bulk perovskites 5, 8
 conductivity measurements 15
 electroluminescence spectra 15
 field-effect transistors (FETs) 15
 low-dimensional (LD) perovskites 15
 photoconductivity measures 15
 3D and q-2D systems 13, 15
 structures 18
 perovskite solar cells (PSCs) 157
 hole selective electron-blocking materials 132–139
 electron selective hole-blocking materials 139–147
 perovskite tandem photovoltaic device research 188–194
 phonon spectroscopy techniques 41
 photoanode–photocathode strategy 278–281
 photobleaching (PB) 63, 108

- photoconductivity (PC) 15, 115
 photoconversion efficiency (PCE) 131
 photo/electrochemical CO₂ reduction 287
 photoelectrochemical generation 275, 276
 photoelectron spectroscopy (PES) 113, 204
 photoexcited species 103–104
 photoinduced absorption (PIA) 123
 photoluminescence (PL) 5, 58, 60, 91, 103, 159, 204, 227, 232, 252–260
 photoluminescence intensity (IPL-IN) 12
 photoluminescence quantum yield (PLQY) 202
 photophysical processes 108–111
 photovoltaic devices 40, 42, 189, 201, 255
 photovoltaic-electrocatalyst (PV-EC) 278, 285–287
 photovoltaic process 93
 picosecond pump–probe spectroscopy 260, 263–265
 PL band position (PL-BP) 6, 9, 14
 polariton bottleneck 68, 70
 polariton lasers 56, 64, 68, 74
 polarization mechanism 95
 polycrystalline thin films 102
 polyethylenimine hydriodide (PEI HI) 160
 polymeric HTMs 132, 135–136
 polymer solar cell 186
 polymethyl methacrylate (PMMA) 6
 post-annealing temperature 255
 power conversion efficiency (PCE) 108, 138, 157, 172, 184, 202, 251, 283
 proton exchange membrane (PEM) electrolyzer 286
 p-type electron-blocking hole selective layer (HTM) 131
 p-type hole transport layer (HTL) 225
 pump–probe correlation technique 101, 251
- q**
 quantum dots (QDs) 6, 58, 111, 147, 212–215, 224
 quantum tunneling process 94
 quantum wells (QW) 8, 11, 36, 55, 62, 72, 156, 223
 nanoplatelets 229
 quasiparticle self-consistent GW (QSGW) method 163
 quasi two dimensional (q-2D) 6, 10
 quasi-2D perovskite LEDs 215–217
- r**
 Rabi energy 64, 66, 67
 Rabi splitting 68, 70, 72
 Rashba–Dresselhaus effects 37, 39, 40, 251
 recombination constants 108–111
 Ruddlesden–Popper 25, 45, 156, 215
- s**
 self-trapped excitons (STE) 59, 61–63
 semiconductor light emitters 223
 semiconductor systems 64
 Shockley–Queisser limit 83, 117, 127, 183, 186
 Shockley–Read–Hall (SRH) 120
 single-junction photovoltaic devices 202
 single TCE/two-terminal (2-T) monolithic stack 184–185
 site inversion asymmetry (SIA) 36
 Sn-based materials 15, 267
 solar energy 183, 273, 274, 288
 solar to hydrogen (STH) conversion efficiency 277, 285
 space-charge-limited-current (SCLC) 121
 spin-coating technique 253
 spin-mixing process 258–260
 spin-mixing rates 252
 spin–orbit coupling (SOC) 27, 33–36, 162, 251, 252
 loss of inversion symmetry 36–40
 spin-polarized carrier carrier dynamics 263–265

- transient dynamics measurements 266
 - spin relaxation time, determination of 265
 - Spiro-OMeTAD 112, 113
 - hole selective contact materials 132
 - stimulated emission (SE) 64, 108, 230, 233, 234
 - stimulated scattering process 68
 - stochastic reorientations 41
 - strong exciton-photon coupling 55–74
 - structural instabilities 40
 - surface plasmon polariton (SPP) 72
 - surface recombination velocity (SRV) 120
 - symmetrized linear combinations of atomic orbitals (SLCAO) 26, 31
- t**
- tandem cell configurations 277, 285
 - PEC-PV tandem system 282–285
 - photoanode–photocathode strategy 278–281
 - photo/electrochemical CO₂ reduction reaction 287
 - photovoltaic-electrocatalyst (PV-EC) structure 285
 - thin film solid-state perovskites, optical gain 228–233
 - three-dimensional (3D) hybrid perovskites 202
 - three-dimensional organic–inorganic hybrid perovskites (3D-OIHPs) 55, 251, 252
 - time-dependent process 95
 - time-of-flight (ToF) 121
 - time-of-flight secondary ion mass spectrometry (ToF-SIMS) 96
 - transient absorption (TA) spectroscopy 101, 107, 217
 - transient absorption spectroscopy (TAS) 66
 - transient reflectivity (TR) spectra 123, 124
 - transparent conducting electrodes (TCE) 184, 185
 - transparent conducting oxide (TCO) 184
 - transverse electric (TE) mode 72
 - transverse magnetic (TM) mode 72
 - trapping mechanism 95
 - trivalent metal cations 175, 177
 - two-dimensional (2D) hybrid perovskites 209, 215
 - two-photon absorption (TPA) coefficients 123
- u**
- ultrafast optical spectroscopy (UOS) 108
 - ultraviolet photoelectron spectroscopy (UPS) 113, 204
 - universal plot 258–260
 - upper polariton branch (UPB) 68
 - Urbach energy 84
- v**
- vacuum Rabi frequency 64, 66
 - valence band (VB) 26, 35, 39, 56, 88, 92, 94, 107, 108, 111, 156, 162, 169, 170, 175, 207, 213, 260, 274, 276, 278
 - valence band maximum (VBM) 31, 34, 102, 163, 169, 204
 - variable stripe length (VSL) 230
 - vertical-cavity surface-emitting (VCSEL) 236
- w**
- Wannier–Mott exciton emission 86, 119, 225, 227
 - whispering gallery mode (WGM) 234, 236
 - white light emission (WLE), 2D-OIHPs 59
 - broadband defect emission 60–61
 - broadband visible emission 57–58
 - energy transfer mechanism 59–60
 - organic framework 63
 - self-trapped excitons 61–63
 - working mechanisms, PSCs

working mechanisms, PSCs (*contd.*)

- charge extraction/injection interfacial effects 93–95
- charge generation 84–86
- charge recombination 89–93
- charge transport 86–89
- fill factor 83
- ionic mechanisms 95–96
- open circuit potential 83
- perovskite photovoltaics 83
- recombination mechanisms 90
- short circuit current 83

x

- X-ray diffraction (XRD) analysis 159
- X-ray photoelectron spectroscopy (XPS) 113

y

- yellow non-perovskite phase 40

z

- Zeeman interaction 260
- Zeeman splitting 261