

Index

- adatoms 179
- AFM, *see* atomic force microscopy
- ALD, *see* atomic layer deposition
- ambient conditions 25, 28, 33–35,
37, 39, 47, 49, 67, 72,
104–105, 220, 226, 228–231,
242–243, 249–252
- amorphous phosphorus 271, 275
- amorphous red phosphorus 4, 34,
73
- amorphous structures 72, 272
- anisotropic 88, 99, 103, 112, 121,
154, 179, 197, 261
- anisotropy 84, 112, 133, 154, 159,
162, 223, 225
 - ratio 132, 135
 - strong 84, 100, 121, 132, 144,
151
 - structural 110, 112
- anode materials 73, 255, 258,
267–268
- armchair direction 82, 84, 88,
98–101, 103, 110–112,
133–136, 143–145, 160–161,
168, 184, 197, 199, 202–205,
223–225
- armchair edge 97–98, 116
- atomic force microscopy (AFM)
17–18, 48–49, 101–102, 206,
226, 251
- atomic layer deposition (ALD) 13,
39, 175, 221, 235, 237
- atoms 2–3, 68–69, 73, 75–76,
81–82, 117, 119, 121,
163–164, 176–177, 179,
183–186, 191, 205, 268–270
- dangling 106, 109, 117
- edge 116–117
- pair of 117, 205
- rows of 20
- bandgap 32, 35, 39, 80–81,
115–116, 149–152, 155–157,
162–163, 166–169, 172,
176–177, 191–192, 203–204,
208, 216, 219–220, 231, 243
 - finite 149, 151, 238
 - indirect 151, 167–168
 - thickness-dependent 155–156
- band structures 60, 152, 163,
166–167, 179, 204, 240
 - electronic 118, 153, 170, 190
- barrier 37–39, 106–108, 110, 113,
117, 175, 222, 231, 252, 261
- binding energy 58, 173, 179,
182–186, 191, 265
- black phosphorene 165, 169, 194,
208
- black phosphorous 53, 251, 276
 - few-layer 144
- black phosphorus (BP) 1–9,
13–16, 23–28, 31–36, 68–71,
164–166, 169–171, 215–217,
219–220, 222–223, 225–228,
230–234, 236–244, 249–253,
259–261
- bandgap of 150, 169

- materials 33
- samples 89, 220
- surface 17, 36–37, 40, 251
- thicknesses 17–18, 219
- black phosphorus crystals 3, 6–7, 11, 16, 19, 22–23, 25, 28, 226
 - layered bulk 12–13
- black phosphorus devices 226, 242–244
- black phosphorus FETs 216–219, 221–223, 225, 227, 229–231, 235
- black phosphorus flake 97, 206, 250
 - exfoliated 206, 250
- BP, *see* black phosphorus
- BP channel 221, 224–225, 234–235, 237, 242
- BP coating layer 281–283
- BP films 15–17, 22, 37, 234, 285
- BP flakes 13–14, 16–17, 23–24, 34–37, 39, 217, 249–253, 277
 - degradation of 251
- BP nanoflakes 283, 285–286
 - liquid-exfoliated 285–286
- BP nanosheets 19, 21, 26, 30, 33, 36
 - few-layer 28
- bulk BP 13, 16, 20–21, 27, 29–32, 39, 267
 - exfoliation of 14, 40
- bulk modulus 88, 100
- bulk phosphorene 56, 74, 153, 202
- bulk phosphorene sample 56
- carbon nanotubes 79–81, 119, 122, 186, 221, 238, 271
- carrier mobility 133, 152, 215, 218, 220, 225, 228–229
- CB, *see* conduction band
- CBM, *see* conduction band minimum
- CCM, *see* collective compression mode
- channels 119–120, 194, 216, 225, 230–231, 236–237, 275
 - length 215, 217, 226, 228, 232
 - material 34, 233
- charge transfer 36, 179, 182, 185, 187, 190, 193–194, 239
- chemical vapor deposition (CVD) 8, 119, 238
- collective compression mode (CCM) 89
- compressive strains 168, 187, 194, 207
- conduction band (CB) 58, 157, 162–164, 168, 176, 179, 205, 208, 222, 231, 259
- conduction band minimum (CBM) 118, 157–159, 166, 168
- configurations, lowest energy 173, 182, 184, 186
- contact metals 14, 221–222
- Coulombic efficiency 255–256, 272, 278, 280, 282
- crystalline orientation 51–54, 60
- crystal orientation 223–225, 243
- crystals 8, 12, 17, 52, 270
- current densities 258, 266, 271, 273–274, 277–282
- curvature effect 79, 186–187, 205
- CVD, *see* chemical vapor deposition
- cycle performance 259–260, 276
- defects 67–68, 70, 72, 74, 76, 78, 80, 82, 90, 104–106, 112–116, 118, 120–122, 171–173, 251–252
 - complex 35, 251, 253
 - linear 113–115
 - site of 252
- degradation 33, 37

- density functional theory (DFT)
 - 35, 40, 79, 161, 164, 171, 182, 261, 269
 - calculations 106–107, 110, 162, 203, 250–251, 264–265
- device fabrication 36, 94, 96, 186, 220, 225, 228, 232, 234
- device structure, cross-shape 133–134
- DFT, *see* density functional theory
- diffusion barriers 108, 110–111, 114, 261, 268
- Dirac cones 169–171, 191
- direct bandgap 80, 118, 151–153, 190–191, 204, 243
- dynamics, exciton and trion 57, 60
- edges 33, 71, 78, 96, 98, 113–118, 121, 162, 175, 252
 - band 158, 161–162, 176, 199, 205, 208
 - nanotube-terminated 117
- EDLCs, *see* electric double-layer capacitors
- effective mass 58, 84, 154, 159, 168, 219
- efficiency 205, 208, 272
- electrical properties 231, 243, 249
- electric double-layer capacitors (EDLCs) 283
- electric field 81, 150, 177, 180, 194, 202–203, 216
- electrochemical performance 256–259, 279–281
- electrode materials 254–255, 261, 264, 283, 285
 - phosphorene-based 265
- electrodes 30, 119–120, 155, 157, 194, 243, 259, 261, 273, 278–279, 283
 - flexible 285–286
 - pairs of 224
 - pure CNF 280–281
- electron diffraction pattern 259, 270–271
- electronic bandgap 55–56, 195
- electronic properties 35, 39, 71, 80, 113, 116, 154, 161, 163, 166–167, 169, 171, 177, 181, 203–206
- electronics 1, 30, 40, 208, 215–216, 244
 - flexible 9, 11, 18, 98, 208
- electronic states 69, 158, 160, 199, 202, 205
- electronic structures 23, 72, 81, 116, 139, 151, 153, 155, 157, 159, 161, 163–166, 176–177
- electron irradiation 107, 109
- electron–phonon coupling matrix 159
- electrons 58, 75–76, 84, 86, 88, 151–152, 154, 160–164, 168, 176–177, 179, 182–188, 193, 222, 231
 - transferred 185, 193–194
- electrons and holes 13, 58, 154, 156, 161–162, 202–203, 205, 231
- electron transport layer (ETL) 22
- energy barriers 175, 253, 264, 269–270
- energy difference 57, 79
- ETL, *see* electron transport layer
- Eucken model 143–144
- excitation power 57–58
- excitonic effect 195, 197
- excitons 56–60, 182, 195–198, 208
 - binding energy 55–56, 195, 197–198
 - charged 197–198
 - neutral 195, 197–199
- exfoliation 1–4, 6, 8, 10, 12, 14, 16, 18–20, 22, 24, 26–28, 30–34, 36, 38, 40

- liquid phase 21–22, 25–28, 30–31, 267, 283
- methods 3, 8–9, 11, 38
- exposure 16, 33–36, 39, 173, 188–189, 227–230, 238, 242, 249, 267
- long-time 226, 229
- faces, triangular 77–79
- Fermi level 151, 157, 164, 176, 179, 181, 185, 191–192, 222, 230
- Fermi pinning, weak 221–222
- Fermi surface 170–171
- FETs, *see* field-effect transistors
 - graphene RF 237
 - nanomaterial-based 218–221
- few-layer black phosphorus 94–96, 176, 215
- few-layer phosphorene 11, 13–14, 47–48, 51–52, 55–56, 59–60, 87–88, 131, 152–156, 158, 166, 171, 195, 198, 261
- few-layer phosphorene FETs 14
- field-effect transistors (FETs) 11, 15, 38, 71, 116, 149, 194, 215–221, 225, 228, 232–237, 239, 243
- flakes 8, 12, 14–16, 18, 21, 25, 27, 33, 35–36, 38, 49, 97, 154, 206, 250
 - thin 9, 12, 14–15
- frequencies 82, 86–87, 89–90, 94–95, 100, 136, 159, 237
 - maximum oscillation 236–237
- fullerenes 72, 78, 259
- gap, direct 167–168
- gate voltage 197–198, 203, 217–218, 231
- grain boundaries 113–115, 119, 122, 252
- graphene 8–10, 69, 71, 86–89, 101, 106–116, 119–120, 122, 141, 149, 169, 182–186, 190–194, 215–216, 236–239
 - single-layer 8, 40, 141–142
- graphene layers 191, 193, 276
- graphene nanoribbons 113
- graphene/phosphorene 190
- graphene sheet 137
- graphite 68–69, 184, 259, 261
- heterogeneous integration 233–234
- high mobility 71, 111, 121, 208, 215–216, 233, 240, 265
- Hittorf's phosphorus 73–74
- hopping parameters 162–164
- ICs, *see* integrated circuits
- integrated circuits (ICs) 233, 236, 243
- interaction, electron-hole 195–196
- interface 19, 25, 119, 158, 180, 190, 193–194
 - graphene–phosphorene 193
- interlayer coupling 69, 81, 88, 154, 156
 - strong 69, 89–90
- interlayer distance 9, 18, 191, 193
- kinetics 110, 117, 119, 121, 186, 268
- laser power 57, 59
- layer-dependent bandgaps 2, 60, 216
- layer number 24, 27–28, 48–51, 55–56, 60, 90, 141, 175, 195, 219–220, 244
 - characterization 48–49
 - function of 89

- layer thickness 18, 141, 252
- LF, *see* low-frequency
- LIB, *see* lithium-ion battery
- linear dichroism 190, 199, 202–203, 205
- liquid exfoliation 21, 23, 27, 31
- lithium-ion battery (LIB) 254–255, 261, 264–265, 267–268, 275–276
- low-dimensional materials 119, 122
- low-frequency (LF) 88–90, 141
- low-frequency rigid-layer mode 88–89

- Maxwell–Garnett model 143–144
- mechanical exfoliation 1, 8–9, 12, 15–16, 18, 36, 39
- mechanical properties 98–99, 101, 103, 119, 151
- metal oxide semiconductor field-effect transistor (MOSFET) 37, 221
- methods, top-down 8, 11
- modes 52–54, 81–82, 84–87, 89–98, 110, 158–159, 224, 243
 - breathing 86
 - flexural 141
- molecules 19, 71, 77, 79, 182–186, 189, 194, 238, 251–253, 268
 - environmental 182, 194, 252
 - oxygen/water 242–243
 - solvent 19–20, 283
- momentum 160–161
- monolayer graphene 132
- monolayer phosphorene 47, 49–50, 56–59, 132–133, 135, 137–139, 141, 154, 159, 162–163, 167, 172, 195–198, 268, 270
 - characteristics 50
 - free-standing 56
 - outperform 154
 - sample 57
 - sheet 179
- MOSFET, *see* metal oxide semiconductor field-effect transistor
- multilayer graphene 141
- multilayer phosphorene 16, 33, 86, 100, 131–132, 140–141, 155, 157, 162, 179, 195
 - samples 141
 - structures 86

- nanomaterials 9, 105, 221, 238
- nanoribbons 116, 118
- nanosheets 18, 29, 40, 283

- on-off ratio, current 217, 219–220, 228–230, 237
- OPL, *see* optical path length
- optical gap 55–57, 198
- optical path length (OPL) 49–50
- optoelectronic devices 94, 131, 133, 151
- oxygen atoms 173, 186, 251–252
- oxygen defects 35
- oxygen molecules 173, 186

- peak energies 54–55, 58, 198
- phase-shifting interferometry (PSI) 48–50
- phonon dispersion 81–82, 84, 144
- phononic crystal 144
- phonon modes 84, 91, 93, 141, 159
- phonons 67–68, 70–72, 74, 76, 78, 80–82, 84, 90, 94, 96, 120–122, 144, 151–152, 158–159, 161
 - optical 160–161
- phonon transmittances 135, 137

- phosphorene 8–21, 23–29, 35–40, 47–56, 69–71, 84–88, 98–101, 103–107, 109–122, 149–166, 170–180, 182–200, 202–208, 252–254, 267–269
 - bilayer 12, 163, 179, 250
 - bulk black phosphorus and few-layer 152
 - fabrication 11
 - five-layer 54–55
 - four-layer 176
 - layer 18, 86
 - materials 71, 208
 - molecules to 183–184
 - mono-layer 141
 - perfect flat 204–205
 - phononic properties of 81, 83, 85, 87–89, 91, 93, 95, 97
 - pristine 143–144, 265
 - rippled 186, 204–206
 - samples 49–50, 55, 175, 199, 254
 - single-layer 40, 50, 81, 86, 132, 141–142, 162
 - thermal properties of 131–132, 134, 136, 138, 140, 142, 144–145
 - thick 27, 181, 189
 - thin-layer 48, 60
 - trilayer 196–197
 - very-few-layer 49
- phosphorene flake 49–51, 53–54, 101–102, 155
- phosphorene-graphene 265, 267, 277–278
- phosphorene layers 20, 79, 87, 90, 152, 154, 157, 175–177, 179, 184, 188, 190–191, 193–194, 196, 268, 275
- phosphorene monolayers 20, 78
- phosphorene nanomaterials 203
- phosphorene nanoribbons 116–117
- phosphorene nanosheets 29, 187, 279
 - few-layer 27, 279
- phosphorene phononic crystal 132, 142–144
- phosphorene sensor 188–189
 - thick 187–188
- phosphorene sheets 19, 69, 86–87, 115–116, 118, 137–139, 177, 194
- phosphorene strips 102–103
- phosphorene surface 173, 177, 264, 269
 - rippled 187
- phosphoric acid 33, 72
- phosphorous fullerene structures 77
- phosphorus 2, 39, 67–68, 72, 74–75, 77, 79–80, 104–105, 226, 254
 - adjacent interlayer 169
 - atoms 69, 71, 73, 75, 79, 104, 109, 115, 173, 179, 185, 187, 191, 193–194, 216
 - elemental 2–3, 67
 - fibrous 74
 - violet 2, 6, 72–73
- phosphorus allotropes 68, 77, 79–80
- phosphorus clusters 74–75, 77
 - cationic 75–76
- phosphorus fullerenes 77–79
- phosphorus nanorods 73, 79
- phosphorus nanotubes 79, 117
- phosphorus oxide layer 176
- phosphorus structures 79
 - large-sized 76
- phosphorus vacancies 172
- plasma treatment 16–18
- Poisson's ratio 98–100
- polarization angles 53–54, 203
- polarized light 195–197, 199, 202–203
- polymeric structures 72

- pore size 21, 143–144
- pressure 2–4, 16, 18, 68, 104, 121, 169–170, 226, 259
 - high 2, 4, 32, 68, 104–105, 169
- pristine phosphorene layer 39
- pristine phosphorene monolayer 143
- PSI, *see* phase-shifting interferometry

- quasiparticle bandgap 165, 195, 197, 208

- Raman-active modes 81–82, 91, 94–95
- Raman-active phonon modes 90–91
- Raman intensities 53, 92–93
- Raman modes 53–54, 252
- Raman spectra 39, 51–52, 54, 60, 89, 91, 94–96, 224–225, 227, 258, 281
- Raman spectroscopy 48–49, 51, 53, 60, 91
- Raman tensors 91–93, 98
- red phosphorus (RP) 2–7, 34, 68, 70, 72–77, 255–261, 268, 270–271, 273, 275
 - fibrous 72–74
- reversible capacity 255, 257, 271, 273, 277
- RP, *see* red phosphorus

- saturable absorbers 19, 27, 29, 71
- Schottky barrier 14, 157, 221–222, 230
- semiconductors 47, 79, 166, 195, 218, 221, 234, 237, 240, 243, 259
 - low-dimensional 221
- shear modes 87
- shear moduli 99–100
- simulations, molecular dynamics 19, 137, 141, 143–144
- single crystals 4–5
- solvent exfoliation 25–26, 39
- species, ionic 9, 11, 18–19
- strain effect 95–96
- strain energies 79
 - larger 79
- strain modulation 81, 84
- stress, breaking 102–103
- supercapacitors 71, 283, 285
- supernatant 24, 27–29, 31
- surface degradation 35–36, 39–40

- TB, *see* tight-binding
- tensile strain 81, 96, 98, 132, 135, 166, 168
- thermal conductivity 51, 94, 131, 137–139, 141, 143–145, 158
- thermal expansion 51–52, 94–95
- threshold voltage 34, 36, 176, 234–236
- tight-binding (TB) 77, 161–166
 - model 162, 164–166
- TMDs, *see* transition metal dichalcogenides
- TMD semiconductors 48–49
- transconductance 154, 217–218
- transfer characteristics 220, 224–226, 230–232, 235
- transition metal dichalcogenides (TMDs) 8–12, 18, 26, 40, 47, 81, 116, 149, 151, 198, 208, 215–216, 237, 243, 285
- transitions 2, 104, 106, 108, 113, 167, 202, 279
- transition state (TS) 106–108
- trion binding energy 58, 60, 198
- trion dynamics 57, 59–60, 198
- trions 56–60, 197–198

- TS, *see* transition state
- uniaxial strain 85, 96, 98, 100,
103, 166–167
values of 134–136
- valence band 58, 157, 162,
164, 168–169, 172, 205,
222
- valence band maximum (VBM)
118, 157–159, 167
- VBM, *see* valence band maximum
- vibration directions 53–54
- voltage range 259, 271
- volume change 100, 255,
257–258, 264
- water absorption 34, 251
- water molecules 121, 173, 185,
226, 232, 242, 250–251
- white phosphorus (WP) 2, 4, 7, 67,
71–72, 226, 255, 268, 275
- work function 71, 156–158, 184,
188, 190, 221–222, 236
high 221–222
values of 157
- WP, *see* white phosphorus
- X-ray diffraction (XRD) 48, 105,
257–258, 260, 276
- XRD, *see* X-ray diffraction
- Young's modulus 98–101, 103
- zigzag 79–80, 84, 87, 96–97, 101,
111–112, 116, 118, 132–136,
166–167, 170, 195–196, 199,
204–206, 225
- zigzag direction 84–85, 91, 99,
103, 110–112, 116, 133–135,
137, 144–145, 154, 160–161,
168–169, 202–207, 223–225,
264
- zigzag edges 69, 97–98, 116

“As an emerging 2D material, black phosphorus (or phosphorene) has recently attracted extensive attention after graphene. The unique physical and chemical properties endow it with potential optoelectronic applications. This book showcases many aspects of the synthesis, fabrication, and integration of these materials.”

Prof. Zhen Zhou
Nankai University, China

“This timely book illustrates the intrinsic properties of a new star, black phosphorus, a layered 2D material beyond graphene. It not only covers the detailed mechanisms of the electronic and phononic properties of black phosphorus, but also illustrates real issues related to its applications such as growth and device fabrication.”

Prof. Junfeng Gao
Dalian University of Technology, China

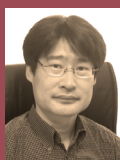
This book is the first attempt to systematically present the progress in the research of phosphorene, an elemental 2D material that, like the intensively studied graphene, can be exfoliated by mechanical or liquid methods. It provides a comprehensive overview of the synthesis, growth, characterization, and applications of phosphorene. It also compiles cutting-edge research in the field with respect to thermal conduction, transistors, and electrochemical applications and encompasses the intrinsic properties (structural, electronic, defective, and phononic) of phosphorene. Edited by three prominent theoretical researchers, the book provides details various phenomena observed for phosphorene. It will benefit graduate students of physics, chemistry, electrical and electronics engineering, and materials science and engineering; researchers in nanoscience working on phosphorene and similar 2D materials; and anyone involved in nanotechnology, nanoelectronics, materials preparation, and device fabrication based on layered materials.



Yongqing Cai is a theoretical scientist specializing in computational physics and condensed matter. He obtained his bachelor's (2004) and master's (2007) in materials science and engineering from Northwestern Polytechnical University, China. Thereafter, he attended the National University of Singapore and completed his PhD in 2012 in quantum simulation of electronic transport processes for spintronics applications. His research is focused on quantum first-principles simulations on electronic and phononic properties of nanomaterials.



Gang Zhang did his BSc and PhD in physics from Tsinghua University, China, in 1998 and 2002, respectively. He is currently a senior scientist and capability group manager at IHPC, A*STAR, Singapore, which he joined in February 2013. Prior to that, he was a professor at the Department of Electronics, Peking University, China. His research is focused on energy transfer and harvesting in nanostructured materials.



Yong-Wei Zhang is principal scientist and deputy executive director at the Institute of High Performance Computing (IHPC), A*STAR, Singapore. He received his PhD from Northwestern Polytechnical University, China, after which he worked at several prestigious institutions, including Brown University, USA. His research is focused on using theory, modeling, and computation as tools to study the relationship between structures and properties of materials, mechanical-thermal coupling and mechanical-electronic coupling of 1D and 2D materials, mechanics in biology and bio-inspired materials, and design.



JENNY STANFORD
PUBLISHING

V634
ISBN 978-981-4774-64-2



9 789814 774642