

## Contents

### Preface *xi*

- 1 The 2D Semiconductor Library 1**  
*Zheng Zhang and Yue Zhang*
  - 1.1 Introduction 1
  - 1.2 Emerging 2DLMs for Future Electronics 3
    - 1.2.1 Classification 3
    - 1.2.2 Elemental 2DMLs 3
      - 1.2.2.1 IV A Group 3
      - 1.2.2.2 V group A 6
      - 1.2.2.3 III A Group 7
    - 1.2.3 Hexagonal Boron Nitride (h-BN) 8
    - 1.2.4 Transition Metal Dichalcogenides (TMDCs) 9
    - 1.2.5 Transition Metal Carbides (TMCs) 12
    - 1.2.6 Transition Metal Oxides (TMOs) 15
  - References 18
  
- 2 The 2D Semiconductor Synthesis and Performances 33**  
*Xiang Chen, Qijie Liang and Yue Zhang*
  - 2.1 Exfoliation 33
    - 2.1.1 Starting from Graphene 33
    - 2.1.2 Semiconducting 2D Materials 34
    - 2.1.3 Big Family of Exfoliated 2D Materials 34
    - 2.1.4 Mechanical Exfoliation of 2D Materials 34
    - 2.1.5 Liquid Exfoliation of 2D Materials 35
    - 2.1.6 Other Exfoliation Method of 2D Materials 37
  - 2.2 Chemical Vapor Deposition 38
    - 2.2.1 Overview of Chemical Vapor Deposition 38
    - 2.2.2 Atmospheric Pressure Chemical Vapor Deposition (APCVD) 40
      - 2.2.2.1 Synthesis of Single-Element Materials (Graphene) 40
      - 2.2.2.2 Synthesis of TMDCs Bielement Materials 42
      - 2.2.2.3 Synthesis of Multielement Materials 48

2.2.3	Low-Pressure Chemical Vapor Deposition (LPCVD)	48
2.2.3.1	Synthesis of Single-Element Materials (Graphene)	48
2.2.3.2	Synthesis of TMDCs Bielement Materials	49
2.2.3.3	Synthesis of Multielement Materials	51
2.2.4	Plasma-Enhanced Chemical Vapor Deposition	53
2.2.4.1	Overview	53
2.2.4.2	Synthesis of Graphene by PECVD	54
2.2.4.3	Synthesis of VG Nanosheets by PECVD	56
2.2.4.4	Synthesis of TMDCs by PECVD	56
2.2.5	MOCVD	57
2.2.5.1	Overview	57
2.2.5.2	Synthesis of III-V Group Semiconductor by MOCVD	59
2.2.5.3	Synthesis of TMDCs by MOCVD	60
	References	63

### **3 The VdW Heterostructure Controllable Fabrications** 69

*Zheng Zhang, Qingliang Liao and Yue Zhang*

3.1	Wet Transfer	69
3.1.1	Substrate Etching Techniques	69
3.1.2	Electrochemical Delamination Methods	72
3.1.3	Wedging Transfer Method	74
3.2	Controllable Selective Synthesis	76
3.2.1	Controllable Synthesis of 2D-2D Heterostructures	76
3.2.1.1	Vertical 2D-2D Heterostructures	76
3.2.1.2	Horizontal 2D-2D Heterostructures	79
3.2.1.3	One-Dimensional Heterostructures	80
3.2.2	Controllable Synthesis of 2D-1D Heterostructures	82
3.2.3	Controllable Synthesis of 2D-3D Heterostructures	85
3.3	Dry Transfer	86
3.3.1	Thermal-release Tape	86
3.3.2	Stamps	88
3.3.3	The Pick-up Methods	89
	References	93

### **4 The Mixed-dimensional VdW Heterostructures** 97

*Pei Lin, Baishan Liu and Zheng Zhang*

4.1	Categorization of Mixed-dimensional VdWHs	97
4.2	Strategies for Constructing Mixed-dimensional VdWHs	99
4.2.1	Transfer-assisted Assembly of Mixed-dimensional VdWHs	99
4.2.2	Direct Growth of Mixed-dimensional VdWHs	100
4.3	Electronic and Sensing Applications	101
4.3.1	Transistors and Spintronics	101
4.3.2	Chemical Sensors	102
4.4	Optoelectronic and Photonic Applications	104
4.4.1	2D-0D Hybridization	104

4.4.2	2D-1D Hybridization	105
4.4.3	2D-3D Hybridization	108
4.5	Energy Applications	111
4.5.1	Application in Photocatalytic Water Splitting	111
4.5.2	Application in Rechargeable Batteries	112
4.5.3	Application in Supercapacitors	114
4.6	Conclusions	115
	References	116
<b>5</b>	<b>The VdW Heterostructure Interface Physics</b>	<b>125</b>
	<i>Guangjie Zhang, Yang Ou, Peifeng Li and Qingliang Liao</i>	
5.1	Band Alignment and Charge Transfer in VdWHs	126
5.2	Magnetic Coupling in VdWHs	129
5.2.1	Applications in Valleytronics	132
5.2.2	Application in Spintronics	134
5.3	Moiré Pattern	134
5.3.1	Band Structure in Moiré Lattice	134
5.3.2	Flat Band-Introduced Superconductivity in Bilayer Graphene	135
5.3.3	Moiré Excitons	135
5.3.4	Moiré Lattice Topology	136
5.4	VdWHs for Protection	137
5.4.1	Introduction of Hexagonal Boron Nitride	137
5.4.2	Graphene Capsulated by h-BN	138
5.4.3	Transition Metal Dichalcogenides Capsulated by h-BN	140
5.4.4	Black Phosphorus Capsulated by h-BN	141
5.5	Characterization Techniques for VdWHs	142
5.5.1	Scanning Transmission Electron Microscopy for Characterization of Structural and Related Properties	142
5.5.2	Scanning Probe Microscopy for Characterization of Structural and Electrical Properties	144
5.5.3	Optical and Vibrational Spectroscopy for Characterization of Electron-, Exciton-, and Phonon-Related Properties	145
	References	147
<b>6</b>	<b>The VdW Heterostructure Multi-field Coupling Effects</b>	<b>157</b>
	<i>Junli Du, Baishan Liu and Zheng Zhang</i>	
6.1	Introduction	157
6.2	The Multifield Coupling Effect Characterization for 2D Van der Waals Structures	158
6.2.1	The Multifield Microscopy Techniques on 2D VdW Structures	158
6.2.1.1	The Electric-Field-Integrated STM-STS Technique	159
6.2.1.2	The Thermal-Field-Integrated STM-STS Technique	160
6.2.1.3	The Multifield-Integrated TEM Technique	161
6.2.1.4	The Optical-Field-Integrated KPFM Technique	162
6.2.2	The Multifield Optical Spectroscopy Techniques on 2D VdW Structures	163

- 6.2.2.1 The TERS Technique Based on STM and Raman Spectroscopy 163
- 6.2.2.2 The S-SNOM Based on AFM 165
- 6.2.3 The Perspective of Multifield Integration Characterization for 2D VdW Structures 166
- 6.3 The Multifield Modulation for Electrical Properties of 2D Van der Waals Structures 167
  - 6.3.1 Strain-Engineered Electrical Properties of 2D VdW Structures 167
  - 6.3.2 Electric Field-Engineered Electrical Properties of 2D VdW Structures 169
  - 6.3.3 Thermal-Engineered Electrical Properties of VdW Structures 171
- 6.4 The Multifield Modulation for Optical Properties of 2D Van der Waals Structures 172
  - 6.4.1 Strain-Engineered Optical Properties of 2D VdW Structures 173
  - 6.4.2 Electric-Engineered Optical Properties of 2D VdW Structures 175
  - 6.4.3 Thermal-Engineered Optical Properties of VdW Structures 177
- References 178

## **7 VdW Heterostructure Electronics 187**

*Xiankun Zhang, Xiang Chen and Yue Zhang*

- 7.1 Van der Waals PN Junctions 188
- 7.2 Van der Waals Metal–Semiconductor Junctions 192
- 7.3 Field-effect Transistor 197
  - 7.3.1 Basic Structure 198
  - 7.3.2 Advantage Characteristics 199
  - 7.3.3 2D Dielectric Materials 199
- 7.4 Junction Field-Effect Transistor 201
  - 7.4.1 Current–Voltage Features 202
  - 7.4.2 Working Principle 203
  - 7.4.3 Device Structure 205
  - 7.4.4 Applications 205
- 7.5 Tunneling Field-Effect Transistor 208
  - 7.5.1 The History of TFET 208
  - 7.5.2 Mechanism of TFET 209
  - 7.5.3 Application of TFET 211
- 7.6 Van der Waals Integration 213
- References 216

## **8 VdW Heterostructure Optoelectronics 223**

*Qi Zhang, Zhuo Kang and Yue Zhang*

- 8.1 Photodetectors 223
  - 8.1.1 Photovoltaic Effect 228
  - 8.1.2 Photoconductive Effect 229
  - 8.1.3 Tunneling Effect 231
  - 8.1.4 Photo-Thermoelectric Effect 233
  - 8.1.5 Improvement Strategies 234
- 8.2 Light Emission 236

8.2.1	Light-Emitting Diodes	236
8.2.2	Lasering	242
8.2.3	Single Photon	244
8.3	Optical Modulators	245
8.3.1	All-Optical Modulators	245
8.3.2	Electro-Optic Modulators	246
8.3.3	Thermo-Optic Modulators	247
	References	248
<b>9</b>	<b>VdW Heterostructure Electrochemical Applications</b>	<b>261</b>
	<i>Xiankun Zhang and Zhuo Kang</i>	
9.1	Solar Energy	262
9.2	Van der Waals Heterostructure Application in Hydrogen Energy	267
9.2.1	Producing Hydrogen by Water Photolysis	268
9.2.2	Producing Hydrogen by Water Electrolysis	270
9.3	Battery	271
9.3.1	Lithium-ion Batteries, Sodium-ion Batteries, Potassium-ion Batteries	273
9.3.2	Supercapacitors	276
9.4	Catalyst	277
9.5	Biotechnology	282
9.5.1	Biosensors	283
9.5.2	Tissue Engineering	284
	References	286
<b>10</b>	<b>Perspective and Outlook</b>	<b>295</b>
	<i>Zheng Zhang and Yue Zhang</i>	
10.1	Overall Development Status of 2D Materials	295
10.1.1	Material Preparation: Scalability, Uniformity, and Reproducibility	297
10.1.2	Metrology	297
10.1.3	Construction of Heterostructure: Industry-Compatible Integration Process	299
10.2	Compatibility Between 2D Van der Waals Device Processing and Silicon Technology	301
10.2.1	Compatibility of 2D Van der Waals Device Integration with Traditional Silicon-Based Process	301
10.2.2	Differences Between 2D Van der Waals Devices and Traditional Silicon-Based Processes	303
10.2.3	2D Van der Waals Device Integration Beyond Silicon Technology	305
10.3	Promising Roadmap of Van der Waals Heterostructure Devices [Medium term: 5 years, Long term: 5–10 years]	307
10.4	Promising Roadmap of Optoelectronic Device	309
10.5	Conclusion and Prospect	310
	References	311
	<b>Index</b>	<b>317</b>

