Contents

About the Authors *xiii*
Acknowledgments *xv*

1 Introduction *1*
1.1 Background *1*
1.2 Types of 2D Materials *4*
1.3 Perspective of 2D Materials *6*
References *7*

2 Electronic Structure of 2D Semiconducting Atomic Crystals *9*
2.1 Theoretical Methods for Study of 2D Semiconductors *9*
2.1.1 Density Functional Theory *9*
2.1.2 Linear Scaling Three-Dimensional Fragment (LS3DF) Method *10*
2.1.3 GW Approximation *10*
2.1.4 Semiempirical Tight-Binding Method *10*
2.1.5 Nonequilibrium Green's Function Method *11*
2.2 Electronic Structure of 2D Semiconductors *11*
2.2.1 Graphyne Family Members *11*
2.2.2 Nitrogenated Holey Graphene *14*
2.2.3 Transition Metal Dichalcogenides *15*
2.3 Prediction of Novel Properties in 2D Moiré Heterostructures *19*
2.3.1 $MoS_2/MoSe_2$ Moiré Structure *19*
2.3.2 Graphene/Nitrogenated Holey Graphene Moiré Structure *26*
2.3.2.1 Atomic Structure: Ordered Stacking Versus Moiré Pattern *26*
2.3.2.2 Renormalized Fermi Velocity *31*
References *33*

3 Tuning the Electronic Properties of 2D Materials by Size Control, Strain Engineering, and Electric Field Modulation *35*
3.1 Size Control *35*
3.2 Strain Engineering *40*
3.3 Electric Field Modulation *48*
References *52*

4 Transport Properties of Two-Dimensional Materials: Theoretical Studies *55*
4.1 Symmetry-Dependent Spin Transport Properties of Graphene-like Nanoribbons *55*
4.1.1 Graphene Nanoribbons *55*
4.1.2 Graphyne Nanoribbon *57*
4.1.3 Silicene Nanoribbons *59*
4.2 Charge Transport Properties of Two-Dimensional Materials *61*
4.2.1 Phonon Scattering Mechanism in Transport Properties of Graphene *61*
4.2.2 Phonon Scattering Mechanism in Transport Properties of Transition Metal Dichalcogenides *63*
4.2.3 Anisotropic Transport Properties of 2D Group-VA Semiconductors *67*
4.3 Contacts Between 2D Semiconductors and Metal Electrodes *69*
4.3.1 Carrier Schottky Barriers at the Interfaces Between 2D Semiconductors and Metal Electrodes *69*
4.3.2 Partial Fermi Level Pinning and Tunability of Schottky Barrier at 2D Semiconductor–Metal Interfaces *70*
4.3.3 Role of Defects in Enhanced Fermi Level Pinning in 2D Semiconductor/Metal Contacts *72*
References *75*

5 Preparation and Properties of 2D Semiconductors *79*
5.1 Preparation Methods *79*
5.1.1 Mechanical Exfoliation *79*
5.1.2 Liquid-Phase Exfoliation *81*
5.1.3 Vapor-Phase Deposition Techniques *85*
5.2 Characterizations of 2D Semiconductors *90*
5.2.1 Surface Morphology (SEM, OM, and TEM) *90*
5.2.2 Thickness (Raman, AFM, and HRTEM) *92*
5.2.3 Phase Structure (HRTEM and STEM) *93*
5.2.4 Band Structure (Optical Absorption and Photoluminescence, ARPES) *94*
5.2.5 Chemical Composition and Chemical States (XPS and EDS) *94*
5.3 Electrochemical Properties of 2D Semiconductors *96*
References *97*

6 Properties of 2D Alloying and Doping *99*
6.1 Introduction *99*
6.2 Advantages of 2D Alloys *99*
6.2.1 Adjustable Bandgap *100*
6.2.2 Carrier-Type Modulation *103*
6.2.3 Phase Change *104*
6.2.4 Application of 2D Semiconductor Alloys in the Field of Magnetism *107*
6.2.5 Improve Device Performance *108*

6.3 Preparation Methods for 2D Alloys *110*
6.3.1 Chemical Vapor Transport (CVT) *110*
6.3.2 Physical Vapor Deposition (PVD) *111*
6.3.3 Chemical Vapor Deposition (CVD) *113*
6.4 Characterizations of 2D Alloys *114*
6.4.1 STEM *115*
6.4.2 Raman Spectroscopy *115*
6.4.3 Photoluminescence (PL) Spectrum *119*
6.5 Doping of 2D Semiconductors *119*
References *121*

7 Properties of 2D Heterostructures *123*
7.1 Conception and Categories of 2D Heterostructures *123*
7.2 Advantages and Application of 2D Heterostructures *125*
7.3 Preparation Methods for 2D Heterostructures *129*
7.3.1 Mechanical Transfer: Liquid Method and Dry Method *130*
7.3.2 Chemical Methods *131*
7.4 Characterizations of 2D Heterostructures *137*
References *139*

8 Application in (Opto) Electronics *143*
8.1 Field-Effect Transistors *143*
8.2 Infrared Photodetectors *145*
8.2.1 Figures of Merit *146*
8.2.2 Photodetection Mechanism *147*
8.2.2.1 Photothermoelectric Effect *147*
8.2.2.2 Bolometric Effect *147*
8.2.2.3 Photogating Effect *148*
8.2.2.4 Photovoltaic Effect *148*
8.2.2.5 Plasmonic Effect *148*
8.2.3 Typical 2D-Based Infrared Photodetectors *149*
8.2.3.1 Graphene Infrared Photodetectors *149*
8.3 2D Photodetectors with Sensitizers *151*
8.3.1 Graphene-based Hybrids Detectors *151*
8.3.2 TMD-Based Hybrid Detectors *152*
8.3.3 Plasmonic Sensitized Detectors *153*
8.4 New Infrared Photodetectors with Narrow Bandgap 2D Semiconductors *155*
8.5 Future Outlook *156*
8.5.1 Optoelectronic Memory of 2D Semiconductors *156*
8.5.2 Solar Cells *161*
References *162*

9 Perspective and Outlook *165*

Index *167*