

Contents

Preface *xi*

| | | |
|----------|---|----------|
| 1 | Two-dimensional Transition Metal Dichalcogenides: A General Overview | 1 |
| | <i>Chi Sin Tang and Xinmao Yin</i> | |
| 1.1 | Introduction to 2D-TMDs | 1 |
| 1.2 | Crystal Structures of 2D-TMDs in Different Phases | 2 |
| 1.2.1 | Other Structural Phases | 3 |
| 1.2.2 | Phase Stability | 4 |
| 1.3 | Electronic Band Structures of 2D-TMDs | 7 |
| 1.3.1 | Electronic Band Structures of the 1H, 1T, and 1T' Phase | 8 |
| 1.3.2 | Indirect-to-Direct Bandgap Transition | 11 |
| 1.3.3 | Spin-Orbit Coupling and Its Effects and Optical Selection Rules | 13 |
| 1.4 | Excitons (Coulomb-Bound Electron-Hole Pairs) | 15 |
| 1.4.1 | Exciton Binding Energy | 16 |
| 1.4.2 | Excitons and Other Complex Quasiparticles | 18 |
| 1.4.3 | Resonant Excitons in 2D-TMDs | 19 |
| 1.5 | Experimental Studies and Characterization of 2D-TMDs | 20 |
| 1.5.1 | Synthesis of 2D-TMDs | 21 |
| 1.5.1.1 | Chemical Vapour Deposition | 21 |
| 1.5.1.2 | Molecular Beam Epitaxy | 22 |
| 1.5.2 | Optical Characterization | 23 |
| 1.5.2.1 | Photoluminescence | 23 |
| 1.5.2.2 | Spectroscopic Ellipsometry | 25 |
| 1.5.2.3 | Raman Characterization | 29 |
| 1.5.3 | Electronic Bandgap | 35 |
| 1.5.3.1 | Angle-Resolved Photoemission Spectroscopy | 35 |
| 1.5.3.2 | Scanning Tunneling Spectroscopy (STS) | 37 |
| 1.5.4 | Conclusions | 40 |
| | References | 40 |

| | | |
|----------|--|-----------|
| 2 | Synthesis and Phase Engineering of Low-Dimensional TMDs and Related Material Structures | 61 |
| | <i>Bijun Tang, Jiefu Yang, and Zheng Liu</i> | |
| 2.1 | Introduction | 61 |
| 2.2 | Structure of 2D TMDs | 62 |
| 2.3 | Synthesis of 2D TMDs | 64 |
| 2.3.1 | Top-Down Method | 65 |
| 2.3.2 | Bottom-Up Method | 66 |
| 2.4 | Phase Engineering of 2D TMDs | 66 |
| 2.4.1 | Direct Synthesis of TMDs with Targeted Phases | 68 |
| 2.4.1.1 | Precursor Selection | 68 |
| 2.4.1.2 | Catalyst | 70 |
| 2.4.1.3 | Temperature Control | 72 |
| 2.4.1.4 | Alloying | 74 |
| 2.4.2 | External Factor-Induced Phase Transformation | 79 |
| 2.4.2.1 | Ion Intercalation | 79 |
| 2.4.2.2 | Thermal Treatment | 81 |
| 2.5 | Conclusion | 82 |
| | References | 83 |
| | | |
| 3 | Thermoelectric Properties of Polymorphic 2D-TMDs | 87 |
| | <i>H. K. Ng, Yunshan Zhao, Dongzhi Chi, and Jing Wu</i> | |
| 3.1 | Introduction to 2D Thermoelectrics | 87 |
| 3.1.1 | Why 2D over 3D? | 88 |
| 3.1.2 | Why 2D Semiconductors? | 89 |
| 3.2 | Thermoelectric Transport | 89 |
| 3.2.1 | Boltzmann Transport Equation | 90 |
| 3.2.2 | Scattering Parameter for Different Mechanism | 92 |
| 3.2.2.1 | Ionized/Charged Impurity Scattering | 92 |
| 3.2.2.2 | Phonons Scattering | 93 |
| 3.2.2.3 | Carrier–Carrier Scattering | 94 |
| 3.2.2.4 | Surface Roughness Scattering | 95 |
| 3.3 | Experimental Characterization TE in 2D | 95 |
| 3.3.1 | Electrical Measurements | 95 |
| 3.3.1.1 | FET Measurements | 95 |
| 3.3.1.2 | Hall Measurements | 96 |
| 3.3.2 | Seebeck Measurement | 96 |
| 3.3.2.1 | ΔT Calibration | 97 |
| 3.3.2.2 | V_{TEP} Measurement | 97 |
| 3.3.3 | Thermal Conductivity | 98 |
| 3.3.3.1 | Raman Spectrometer | 99 |
| 3.3.3.2 | TDTR (FDTR) | 101 |
| 3.3.3.3 | Thermal Bridge Method (Electron Beam Heating Technique) | 102 |
| 3.3.3.4 | Other Thermal Property Measurement Methods | 104 |
| 3.4 | Manipulation of TE Properties in 2D | 106 |
| 3.4.1 | Tuning of Carrier Concentration | 107 |

| | | |
|----------|---|------------|
| 3.4.2 | Strain Engineering | 107 |
| 3.4.3 | Band Engineering | 110 |
| 3.4.3.1 | Layer Thickness and Band Convergence | 110 |
| 3.4.4 | Phase Transition | 112 |
| 3.5 | Future Outlook and Perspective | 115 |
| | References | 117 |
| 4 | Emerging Electronic Properties of Polymorphic 2D-TMDs | 127 |
| | <i>Tong Yang, Zishen Wang, Jiaren Yuan, Jun Zhou, and Ming Yang</i> | |
| 4.1 | Electronic Structure and Optical Properties of 2D-TMDs | 127 |
| 4.1.1 | Electronic and Optical Properties of 1H-Phase 2D-TMDs | 127 |
| 4.1.2 | Electronic and Optical Properties of 1T-Phase 2D-TMDs | 131 |
| 4.2 | Polaron States of 2D-TMDs | 133 |
| 4.2.1 | Holstein Polarons in MoS ₂ | 133 |
| 4.2.1.1 | Experimental Characterizations of Holstein Polarons | 133 |
| 4.2.1.2 | Theoretical Simulations of the Spectral Functions | 136 |
| 4.2.2 | Asymmetric Intervalley Polaron Effects on Band Edges of 2D-TMDs | 137 |
| 4.2.3 | Polaron Effects on the Band Gap Size of 2D-TMDs | 139 |
| 4.3 | Valley Properties of 2D-TMDs | 143 |
| 4.3.1 | Circularly Polarized Light | 147 |
| 4.3.2 | External Field | 148 |
| 4.3.3 | Magnetic Metal Doping | 148 |
| 4.3.4 | Magnetic Substrate | 149 |
| 4.4 | Charge Density Waves of 2D-TMDs | 151 |
| 4.4.1 | Charge Density Waves in TMDs | 151 |
| 4.4.2 | Effects of CDW on Electronic Properties | 154 |
| 4.4.3 | Mechanisms in CDW Transitions | 155 |
| 4.4.4 | Manipulation of CDWs | 158 |
| 4.5 | Janus Structures of 2D-TMDs | 159 |
| 4.5.1 | Fabrication Approaches for Janus 2D TMDs | 159 |
| 4.5.2 | Emerging Properties of Janus 2D TMDs | 160 |
| 4.5.3 | Potential Applications of Janus 2D TMDs | 160 |
| 4.6 | Moiré Superlattices of 2D-TMDs | 161 |
| | References | 165 |
| 5 | Magnetism and Spin Structures of Polymorphic 2D TMDs | 181 |
| | <i>Meizhuang Liu, Zuxin Chen, Jingbo Li, Yuli Huang, Kuan Eng Johnson Goh, and Andrew T. S. Wee</i> | |
| 5.1 | Two-dimensional Ferromagnetism | 182 |
| 5.2 | Cr-based Magnetic Materials and Device Applications | 183 |
| 5.3 | Polymorphic 2D Cr-based Magnetic TMDs | 191 |
| 5.4 | Magnetism in 2D Vanadium, Ion, Manganese Chalcogenides | 200 |
| 5.5 | Conclusions and Outlook | 204 |
| | Acknowledgements | 204 |
| | References | 205 |

| | | |
|----------|--|------------|
| 6 | Recent Progress of Mechanical Exfoliation and the Application in the Study of 2D Materials | 211 |
| | <i>Yunyun Dai, Xinyu Huang, Xu Han, Jiangang Guo, Xiangfan Xu, Lei Wang, Luqi Liu, Ningning Song, Yeliang Wang, and Yuan Huang</i> | |
| 6.1 | Introduction | 211 |
| 6.2 | Different Ways for Preparing 2D Materials | 213 |
| 6.2.1 | Chemical Vapor Deposition (CVD) | 213 |
| 6.2.2 | Mechanical Exfoliation (ME) | 213 |
| 6.3 | New Mechanical Exfoliation Methods | 214 |
| 6.3.1 | Oxygen Plasma Enhanced Exfoliation | 214 |
| 6.3.2 | Gold Film Enhanced Exfoliation | 218 |
| 6.4 | Application of Mechanical Exfoliation Method | 222 |
| 6.4.1 | Electrical Properties and Devices | 222 |
| 6.4.1.1 | Screening of Disorders | 223 |
| 6.4.1.2 | Electrical Contacts of 2D Materials | 225 |
| 6.4.2 | Optical Properties and Photonic Devices | 227 |
| 6.4.2.1 | Photodetectors | 227 |
| 6.4.2.2 | Optical Modulators | 228 |
| 6.4.2.3 | Single Photon Emitters | 228 |
| 6.4.3 | Moiré Superlattice and Devices | 230 |
| 6.4.3.1 | Graphene/h-BN Moiré Superlattice | 230 |
| 6.4.3.2 | Twisted Graphene Moiré Superlattice | 231 |
| 6.4.3.3 | Twisted TMD Moiré Superlattice | 231 |
| 6.4.4 | Magnetic Properties and Memory Devices | 232 |
| 6.4.4.1 | Ferromagnetism in 2D Materials | 235 |
| 6.4.4.2 | Antiferromagnetism in 2D Materials | 237 |
| 6.4.5 | Thermal Conduction | 240 |
| 6.4.6 | Superconductors | 244 |
| 6.4.6.1 | 2D Superconductors and Their Characteristics | 244 |
| 6.4.6.2 | Regulation Methods | 247 |
| 6.5 | Summary and Outlook | 249 |
| | Acknowledgments | 249 |
| | References | 250 |
| 7 | Applications of Polymorphic Two-Dimensional Transition Metal Dichalcogenides in Electronics and Optoelectronics | 267 |
| | <i>Yao Yao, Siyuan Li, Jiajia Zha, Zhuangchai Lai, Qiyuan He, Chaoliang Tan, and Hua Zhang</i> | |
| 7.1 | Field-Effect Transistors (FETs) | 268 |
| 7.1.1 | Homojunction-based FETs Formed by Phase Transition | 269 |
| 7.1.2 | Homojunction-based FETs Formed by Direct Synthesis | 270 |
| 7.2 | Memory and Neuromorphic Computing | 272 |
| 7.3 | Energy Harvesting | 275 |

| | | |
|----------|--|------------|
| 7.4 | Photodetectors | 277 |
| 7.5 | Solar Cells | 282 |
| 7.6 | Perspectives | 284 |
| | References | 285 |
| 8 | Polymorphic Two-dimensional Transition Metal Dichalcogenides: Modern Challenges and Opportunities | 293 |
| | <i>Chi Sin Tang, Xinmao Yin, and Andrew T. S. Wee</i> | |
| 8.1 | Summing up the Chapters | 293 |
| 8.2 | Projecting the Future: Challenges and Opportunities | 295 |
| 8.3 | Global Challenges and Threats | 296 |
| 8.3.1 | Clean and Renewable Energy Sources | 297 |
| 8.3.2 | Water Treatment and Access to Clean Water | 299 |
| 8.3.3 | Healthcare and Pandemic Intervention | 302 |
| 8.3.4 | Food Safety and Security | 305 |
| 8.3.4.1 | Agricultural Production, Sustainability, Productivity, and Protection | 306 |
| 8.3.4.2 | Roles of 2D-TMDs in Food Packaging and Preservation | 306 |
| 8.4 | Exponential Growth in Demands for Modern Computation | 307 |
| 8.4.1 | Deep Learning and Artificial Intelligence | 307 |
| 8.4.2 | Internet of Things and Data Overload | 308 |
| 8.5 | Conclusion | 312 |
| | References | 312 |
| | Index | 325 |

