Contents

Contributors *page* xi

Introduction 1

Part I **5**

1 **Graphene: Basic Properties** 7
- 1.1 Chemical Bonding and Ground-State Structure 7
- 1.2 Thermal (In)Stability of 2D Crystals 9
- 1.3 Electronic Structure of Single-Layer Graphene 11
- 1.4 Electronic Structure of Bilayer Graphene 17
- 1.5 Graphene as a Bridge between Condensed Matter and High-Energy Physics 20
- 1.6 References 21

2 **Electrical Transport in Graphene: Carrier Scattering by Impurities and Phonons** 25
- 2.1 Boltzmann Transport Theory 25
- 2.2 Charged Impurities 28
- 2.3 Resonant Scatterers 31
- 2.4 Corrugations of the Graphene Sheet 33
- 2.5 Phonons 34
- 2.6 References 36

3 **Optical Properties of Graphene** 38
- 3.1 Tunable Interband and Intraband Transitions in Electrically Gated Graphene 39
- 3.2 Landau Level Transitions in Graphene under a Magnetic Field 43
- 3.3 Plasmon Excitations in Graphene 44
- 3.4 Bilayer and Multilayer Graphene 46
- 3.5 References 48

4 **Graphene Mechanical Properties** 52
- 4.1 Introduction 52
- 4.2 Experiments 53

	4.3	Non-linear and Anisotropic Response of Graphene	57
	4.4	Experimental Validation	61
	4.5	Instabilities	63
	4.6	Defective Graphene	64
	4.7	Conclusion	68
	4.8	References	68
5	**Vibrations in Graphene**		71
	5.1	Structure and Vibrations of Monolayer Graphene	71
	5.2	Many-Layers Graphene and the Interlayer Vibrations in 2D Systems	74
	5.3	The Quantum Nature of Atomic Vibrations	77
	5.4	Phonon Coherence Length in Graphene	79
	5.5	Probing Phonons Near Defects and Edges/Grain Boundaries	79
	5.6	References	83
6	**Thermal Properties of Graphene: From Physics to Applications**		90
	6.1	Thermal Conductivity of Graphene and Few-Layer Graphene	90
	6.2	Isotope and Rotational Engineering of Thermal Properties of Graphene	93
	6.3	Graphene Applications in Thermal Management Technologies	96
	6.4	Conclusions	100
	6.5	References	101
7	**Graphene Plasmonics**		104
	7.1	Macroscopic Approach to Graphene Plasmonics	104
	7.2	Microscopic Approach	111
	7.3	Plasmon Damping	115
	7.4	Experimental Observation of Graphene Plasmons	117
	7.5	Applications	134
	7.6	References	136
8	**Electron Optics with Graphene p–n Junctions**		141
	8.1	Introduction	141
	8.2	Basic Electrical Properties of p–n Junctions	142
	8.3	Photon Analogies for Carriers in Graphene	148
	8.4	Future Directions	156
	8.5	References	157
9	**Graphene Electronics**		159
	9.1	Introduction	159
	9.2	Graphene RF Transistors and Circuits	160
	9.3	Graphene Nanostructures	166
	9.4	Bilayer Graphene Transistors	169

	9.5 Vertical Graphene Transistors	171
	9.6 Conclusion	174
	9.7 References	175
10	**Graphene: Optoelectronic Devices**	180
	10.1 Introduction	180
	10.2 Light to Current Conversion	181
	10.3 Photodetectors	184
	10.4 Light Modulators	187
	10.5 Ultra-Fast Lasers	189
	10.6 Thermal Radiation Sources	191
	10.7 Passive Optical Elements	192
	10.8 Transparent Conductive Electrodes	193
	10.9 References	194
11	**Graphene Spintronics**	197
	11.1 Introduction to Spintronics	197
	11.2 Advantages of Graphene for Spintronics	198
	11.3 How to Measure Spin Lifetimes in Graphene and 2D Materials	200
	11.4 New Spin Relaxation Mechanisms	206
	11.5 Proximity Effects and Spin Gating	212
	11.6 References	215
12	**Graphene–BN Heterostructures**	219
	12.1 Introduction	219
	12.2 Mechanical Assembly of Graphene–BN Heterostructures	220
	12.3 High-Performance Graphene	225
	12.4 Beyond Graphene	232
	12.5 References	233
13	**Controlled Growth of Graphene Crystals by Chemical Vapor Deposition: From Solid Metals to Liquid Metals**	238
	13.1 Introduction	238
	13.2 CVD Method for Graphene Growth	239
	13.3 Prospects	250
	13.4 References	251
Part II		**257**
14	**Electronic Properties and Strain Engineering in Semiconducting Transition Metal Dichalcogenides**	259
	14.1 Introduction	259
	14.2 Electronic Structure	260

14.3 From Density Functional Theory to Tight-Binding Approximation 264
14.4 Including Strain in the Tight-Binding Hamiltonian 268
14.5 Low-Energy Model of Strained Transition Metal Dichalcogenides 270
14.6 Strain Engineering in Transition Metal Dichalcogenides 272
14.7 References 276

15 Valley-Spin Physics in 2D Semiconducting Transition Metal Dichalcogenides 279
15.1 Introduction 279
15.2 Electronic Structure at the Band Edges 280
15.3 Valley-Spin Physics in Monolayers 283
15.4 Valley and Spin Physics in Bilayers 289
15.5 References 292

16 Electrical Transport in MoS_2: A Prototypical Semiconducting TMDC 295
16.1 Introduction 295
16.2 Ballistic Transport Simulations 297
16.3 Scattering Mechanisms 299
16.4 Point Defects 303
16.5 References 308

17 Optical Properties of TMD Heterostructures 310
17.1 Fundamentals of 2D TMD Heterostructures 310
17.2 Interlayer Exciton Properties 315
17.3 Valley Optoelectronic Properties of 2D Heterostructure 319
17.4 Outlook 325
17.5 References 326

18 TMDs – Optoelectronic Devices 329
18.1 Introduction 329
18.2 Light-Emitting Diodes and Lasers 330
18.3 Photovoltaic Devices 333
18.4 Photodetectors 336
18.5 Valley-Dependent Optoelectronic Devices 340
18.6 References 342

19 Synthesis of Transition Metal Dichalcogenides 344
19.1 Introduction 344
19.2 Mechanism of Growth 345
19.3 Sulfurization/Selenization of Transition Metal Oxides 345
19.4 Metal Organic Chemical Vapor Deposition 351
19.5 Physical Vapor Phase Transport 351
19.6 Summary and Outlook 354
19.7 References 354

20	**Defects in Two-Dimensional Materials**	359
	20.1 Introduction	359
	20.2 Point Defects	360
	20.3 Topological Defects: Dislocations and Grain Boundaries	363
	20.4 Dislocations in Bilayer Materials	370
	20.5 Other 1D Defects – Edges, Interfaces, and Nanowires	372
	20.6 Summary	375
	20.7 References	376
Part III		**379**
21	**Theoretical Overview of Black Phosphorus**	381
	21.1 Crystal and Electronic Band Structures	381
	21.2 Electronic Properties	389
	21.3 Optical Properties	392
	21.4 Thermal Properties	399
	21.5 Mechanical Properties – Elasticity	405
	21.6 Concluding Remarks	408
	21.7 References	408
22	**Anisotropic Properties of Black Phosphorus**	413
	22.1 Synthesis of Black Phosphorus	414
	22.2 Anisotropic Response of Black Phosphorus	416
	22.3 Conclusion	429
	22.4 References	429
23	**Optical Properties and Optoelectronic Applications of Black Phosphorus**	435
	23.1 Introduction	435
	23.2 Optical Properties	435
	23.3 Optoelectronic Devices	442
	23.4 Outlook and Remarks	450
	23.5 References	452
24	**Silicene, Germanene, and Stanene**	458
	24.1 Introduction	458
	24.2 The Advent of Silicene	458
	24.3 Epitaxial Silicene	459
	24.4 Electronic Structure of Silicene	462
	24.5 Functionalization of Silicene	463
	24.6 Multilayer Silicene	465
	24.7 Germanene and Stanene	467
	24.8 Summary	469
	24.9 References	469

25 Predictions of Single-Layer Honeycomb Structures from First Principles 472
25.1 Motivation and Methodology 472
25.2 Group IV Elements: Silicene, Germanene 474
25.3 Group III–V and II–VI Compounds 478
25.4 Group V Elements: Nitrogene and Antimonene 480
25.5 Transition Metal Oxides and Dichalcogenides 481
25.6 Conclusions 482
25.7 References 482

Index 485