

Contents

About the Editors XV

List of Contributors XVII

Preface XXIII

Part I: Fundamentals 1

1 **Quantum Spin Hall Effect and Topological Insulators** 3

Frank Ortmann, Stephan Roche, and Sergio O. Valenzuela

References 9

2 **Hybridization of Topological Surface States and Emergent States** 11

Shuichi Murakami

2.1 Introduction 11

2.2 Topological Phases and Surface States 12

2.2.1 Topological Insulators and Z_2 Topological Numbers 12

2.2.2 Weyl Semimetals 13

2.2.3 Phase Transition between Topological Insulators and Weyl semimetals 15

2.3 Hybridization of Topological Surface States and Emergent States 19

2.3.1 Chirality of the Surface Dirac Cones 19

2.3.2 Thin Film 20

2.3.3 Interface between Two TIs 21

2.3.4 Superlattice 25

2.4 Summary 28

Acknowledgments 29

References 29

3	Topological Insulators in Two Dimensions	31
	<i>Steffen Wiedmann and Laurens W. Molenkamp</i>	
3.1	Introduction	31
3.2	2D TIs: Inverted HgTe/CdTe and Inverted InAs/GaSb Quantum Wells	33
3.2.1	HgTe/CdTe Quantum Wells	33
3.2.2	The System InAs/GaSb	35
3.3	Magneto-Transport Experiments in HgTe Quantum Wells	36
3.3.1	Sample Fabrication	36
3.3.2	Transition from <i>n</i> - to <i>p</i> -Conductance	37
3.3.3	Magnetic-Field-Induced Phase Transition	38
3.4	The QSH effect in HgTe Quantum Wells	40
3.4.1	Measurements of the Longitudinal Resistance	41
3.4.2	Transport in Helical Edge States	43
3.4.3	Nonlocal Measurements	44
3.4.4	Spin Polarization of the QSH Edge States	45
3.5	QSH Effect in a Magnetic Field	45
3.6	Probing QSH Edge States at a Local Scale	48
3.7	QSH Effect in InAs/GaSb Quantum Wells: Experiments	49
3.8	Conclusion and Outlook	51
	Acknowledgements	52
	References	52
4	Topological Insulators, Topological Dirac semimetals, Topological Crystalline Insulators, and Topological Kondo Insulators	55
	<i>M. Zahid Hasan, Su-Yang Xu, and Madhab Neupane</i>	
4.1	Introduction	55
4.2	Z_2 Topological Insulators	58
4.3	Topological Kondo Insulator Candidates	69
4.4	Topological Quantum Phase Transitions	74
4.5	Topological Dirac Semimetals	76
4.6	Topological Crystalline Insulators	84
4.7	Magnetic and Superconducting Doped Topological Insulators	89
	Acknowledgements	95
	References	96
	Part II: Materials and Structures	101
5	Ab Initio Calculations of Two-Dimensional Topological Insulators	103
	<i>Gustav Bihlmayer, Yu. M. Koroteev, T. V. Menshchikova, Evgeni V. Chulkov, and Stefan Blügel</i>	
5.1	Introduction	103
5.2	Early Examples of 2D TIs	104
5.2.1	Graphene and the Quantum Spin Hall Effect	104
5.2.2	HgTe: Band Inversion and Topology in a 2D TI	108

5.3	Thin Bi and Sb Films	112
5.3.1	Bilayers	112
5.3.2	Thicker Layers	115
5.3.3	Alloyed Layers	118
5.3.4	Supported Layers	119
5.4	Compounds	121
5.4.1	Binary Compounds of A_2B_3 Type	122
5.4.2	Ternary Compounds: $A'A_2B_4$ and $A'_2A_2B_4$ Types	124
5.5	Summary	125
	Acknowledgments	126
	References	126
6	Density Functional Theory Calculations of Topological Insulators	131
	<i>Hyungjun Lee, David Soriano, and Oleg V. Yazyev</i>	
6.1	Introduction	131
6.2	Methodology	132
6.2.1	Foundations of Density Functional Theory	132
6.2.2	Practical Aspects of DFT Calculations	136
6.2.3	Including Spin–Orbit Interactions	139
6.2.4	Calculating Z_2 Topological Invariants	143
6.3	Bismuth Chalcogenide Topological Insulators: A Case Study	144
6.3.1	Bulk Band Structures of Bi_2Se_3 and Bi_2Te_3	144
6.3.2	Topologically Protected States at the (111) Surface of Bismuth Chalcogenides	148
6.3.3	Nonstoichiometric and Functionalized Terminations of the Bi_2Se_3 (111) Surface	151
6.3.4	High-Index Surfaces of Bismuth Chalcogenides	155
6.4	Conclusions and Outlook	156
	References	157
7	Many-Body Effects in the Electronic Structure of Topological Insulators	161
	<i>Irene Aguilera, Ilya A. Nechaev, Christoph Friedrich, Stefan Blügel, and Evgenii V. Chulkov</i>	
7.1	Introduction	161
7.2	Theory	163
7.3	Computational Details	166
7.4	Calculations	167
7.4.1	Beyond the Perturbative One-Shot GW Approach	167
7.4.2	Analysis of the Band Inversion	169
7.4.3	Treatment of Spin–Orbit Coupling	170
7.4.4	Bulk Projected Band Structures	174
7.4.4.1	Bi_2Se_3	175
7.4.4.2	Bi_2Te_3	179
7.4.4.3	Sb_2Te_3	182

7.5	Summary	184
	Acknowledgments	187
	References	187
8	Surface Electronic Structure of Topological Insulators	191
	<i>Philip Hofmann</i>	
8.1	Introduction	191
8.2	Bulk Electronic Structure of Topological Insulators and Topological Crystalline Insulators	192
8.3	Bulk and Surface State Topology in TIs and TCIs	194
8.4	Surface Electronic Structure in Selected Cases	198
8.4.1	Bi Chalcogenite-Based Topological Insulators	198
8.4.2	The Group V Semimetals and Their Alloys	200
8.4.3	Other Topological Insulators	203
8.4.4	Topological Crystalline Insulators	203
8.5	Stability of the Topological Surface States	207
8.5.1	Stability with Respect to Scattering	207
8.5.2	Stability of the Surface States' Existence	208
	Acknowledgements	211
	References	211
9	Probing Topological Insulator Surface States by Scanning Tunneling Microscope	217
	<i>Hwansoo Suh</i>	
9.1	Introduction	217
9.2	Sample Preparation Methods	219
9.3	STM and STS on Topological Insulator	220
9.3.1	Topography and Defects	221
9.3.2	STS and Band Structure of Topological Insulators	223
9.3.3	Landau Quantization of Topological Surface States	225
9.4	Conductance Map Analysis of Topological Insulator	229
9.4.1	Magnetically Doped Topological Insulator	233
9.4.2	Superconductor, Topological Insulator, and Majorana Zero Mode	235
9.5	Conclusions	236
	References	237
10	Growth and Characterization of Topological Insulators	245
	<i>Johnpierre Paglione and Nicholas P. Butch</i>	
10.1	History of Bismuth-Based Material Synthesis	245
10.2	Synthesis and Characterization of Crystals and Films	246
10.3	Native Defects and Achieving Bulk Insulation	252
10.4	New Material Candidates and Future Directions	256
	References	260

Part III: Electronic Characterization and Transport Phenomena 265

11	Topological Insulator Nanostructures 267
	<i>Seung Sae Hong and Yi Cui</i>
11.1	Introduction 267
11.2	Topological Insulators: Experimental Progress and Challenges 268
11.3	Opportunities Enabled by Topological Insulator Nanostructures 270
11.4	Synthesis of Topological Insulator Nanostructures 271
11.4.1	Vapor-Phase Growth 271
11.4.2	Solution-Phase Growth 273
11.4.3	Exfoliation 273
11.4.4	Heterostructures 274
11.4.5	Doping and Alloying 275
11.5	Fermi Level Modulation and Bulk Carrier Control 276
11.6	Electronic Transport in Topological Insulator Nanostructures 279
11.6.1	Weak Antilocalization and Magnetic Topological Insulators 280
11.6.2	Shubnikov–de Haas Oscillations 280
11.6.3	Insulating Behavior at Ultrathin Limit 283
11.6.4	Aharonov–Bohm Effect and 1D Topological States 283
11.6.5	Superconducting Proximity Effect in TI Nanodevices 286
11.7	Applications and Future Perspective 286
11.8	Conclusion 288
	References 289
12	Topological Insulator Thin Films and Heterostructures: Epitaxial Growth, Transport, and Magnetism 295
	<i>Anthony Richardella, Abhinav Kandala, and Nitin Samarth</i>
12.1	Introduction 295
12.2	MBE Growth of Topological Insulators 297
12.2.1	HgTe 299
12.2.2	Bi and Sb Chalcogenides 300
12.2.2.1	Bi_2Se_3 303
12.2.2.2	Bi_2Te_3 303
12.2.2.3	Sb_2Te_3 304
12.2.2.4	$(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ 305
12.2.2.5	Film Growth, Quality, and Stability 305
12.3	Transport Studies of TI Thin Films 306
12.3.1	Shubnikov–de Haas Oscillations 308
12.3.2	Quantum Corrections to Diffusive Transport in 3D TI Films 309
12.3.3	Mesoscopic Transport in 3D TI Films 310
12.3.4	Hybridization Gaps in Ultrathin 3D TI Films 311
12.4	Topological Insulators Interfaced with Magnetism 313
12.4.1	Bulk Ferromagnetism 313

12.4.2	Ferromagnetic Insulator/Topological Insulator Heterostructures	315
12.5	Conclusions and Future Outlook	321
	Acknowledgments	321
	References	321
13	Weak Antilocalization Effect, Quantum Oscillation, and Superconducting Proximity Effect in 3D Topological Insulators	<i>Hongtao He and Jiannong Wang</i> 331
13.1	Introduction	331
13.2	Weak Antilocalization in TIs	331
13.3	Quantum Oscillations in TIs	340
13.4	Superconducting Proximity Effect in TIs	344
13.5	Perspective	353
	References	353
14	Quantum Anomalous Hall Effect	<i>Ke He, Yanyu Wang, and Qikun Xue</i> 357
14.1	Introduction to the Quantum Anomalous Hall Effect	357
14.1.1	The Hall Effect and Quantum Hall Effect	357
14.1.2	The Anomalous Hall Effect and Quantum Anomalous Hall Effect	359
14.2	Topological insulators and QAHE	360
14.3	Experimental Procedures for Realizing QAHE	362
14.3.1	Strategies for Experimental Observation of QAHE	362
14.3.2	Growth of Ultrathin TI Films by Molecular Beam Epitaxy	364
14.3.3	Band structure Engineering in $(Bi_{1-x}Sb_x)_2Te_3$ ternary alloys	366
14.3.4	Ferromagnetism in Magnetically Doped Topological Insulators	367
14.3.5	Electrical Gate Tuning of the AHE	370
14.4	Experimental Observation of QAHE	371
14.5	Conclusion and Outlook	374
	References	375
15	Interaction Effects on Transport in Majorana Nanowires	<i>Reinhold Egger, Alex Zazunov, and Alfredo Levy Yeyati</i> 377
15.1	Introduction	377
15.2	Transport through Majorana Nanowires: General Considerations	380
15.2.1	Model	380
15.2.2	Majorana–Meir–Wingreen Formula	381
15.2.3	Conductance for the Noninteracting $M = 2$ Case	382
15.3	Majorana Single-Charge Transistor	383
15.3.1	Charging Energy Contribution	383
15.3.2	Theoretical Approaches	384
15.3.3	Master Equation Approach	386

15.3.4	Coulomb Oscillations: Linear Conductance	388
15.3.5	From Resonant Andreev Reflection to Teleportation	389
15.3.6	Finite Bias Sidepeaks	389
15.3.7	Josephson Coupling to a Superconducting Lead	391
15.4	Topological Kondo Effect	392
15.4.1	Low-Energy Theory	393
15.4.2	Majorana Spin	394
15.4.3	Renormalization Group Analysis	394
15.4.4	Topological Kondo Fixed Point	395
15.4.5	Conductance Tensor	396
15.5	Conclusions and Outlook	397
	Acknowledgments	397
	References	398

Index 401

