

Contents

Preface ix

1	An Introduction to Density Functional Theory (DFT) and Derivatives	1
1.1	The Problem of a N-electron System	1
1.2	The Thomas–Fermi Theory for Electron Density	3
1.3	The First Hohenberg–Kohn Theorem	3
1.4	The Second Hohenberg–Kohn Theorem	5
1.5	The Kohn–Sham Equations	5
1.6	The Local Density Approximation (LDA)	7
1.7	The Generalized Gradient Approximation (GGA)	8
1.8	The LDA+U Method	8
1.9	The Heyd–Scuseria–Ernzerhof Density Functional	9
1.9.1	Introduction to Tight-Binding Approximation	9
1.9.2	Matrix Elements of Tight-Binding Hamiltonian	10
1.9.3	Matrix Elements with the Help of Wannier Function	10
1.9.4	Example for a Graphene Model	10
1.10	Introduction to $k \cdot p$ Perturbation Theory	11
1.10.1	Solution for Non-degenerate Bands	11
1.10.2	Solution for Degenerate Bands	12
1.10.3	Explicit Hamiltonian of $k \cdot p$ Perturbation Theory	12
	References	13
2	New Physical Effects Based on Band Structure	17
2.1	Valley Physics	17
2.1.1	Spontaneous Valley Polarization	22
2.1.2	Valley Polarization by Foreign Atom Doping	31
2.1.3	Valley Polarization in van der Waals Heterostructures	37
2.2	Rashba Effects	43
	References	55

3	Ferromagnetic Order in Two- and One-Dimensional Materials	65
3.1	Intrinsic Ferromagnetic Order in 2D Materials	66
3.2	Intrinsic Ferromagnetic Order in 1D Molecular Nanowires	73
	References	75
4	Two-Dimensional Topological States	81
4.1	Topological Insulators	82
4.1.1	Graphene	82
4.1.2	HgTe/CdTe Quantum Wells	83
4.1.3	Z_2 Invariant and Spin Chern Number	84
4.1.4	Large Gap Quantum Spin Hall Insulators	86
4.2	Topological Crystalline Insulators	91
4.2.1	SnTe Thin Films	91
4.2.2	IV–VI Monolayers	93
4.2.3	Topological Phase Transition Between 2D TCI and TI	94
4.2.4	Dual Topological Insulator	96
4.2.5	TCI in 2D Ferromagnets	100
4.3	Quantum Anomalous Hall Effect	103
4.4	Antiferromagnetic Topological Insulators	107
4.5	Mixed Topological Semimetals	113
	References	118
5	Calculation of Excited-State Properties	123
5.1	Green's Function Many-Body Perturbation Theory	123
5.2	Excitonic Effects and Band Gap Renormalization in Two-Dimensional Materials	130
5.3	Electron–Phonon Effects on the Excited-state Properties	133
5.4	Nonlinear Optical Response	136
5.5	Optical Properties of van der Waals Heterostructures of Two-Dimensional Materials	137
	References	139
6	Charge Carrier Dynamics from Simulations	145
6.1	Time-Dependent Density Functional Theory and Nonadiabatic Molecular Dynamics	145
6.2	Applications of TDDFT and NAMD in Two-Dimensional Materials	148
	References	155
7	Simulations for Photocatalytic Materials	159
7.1	Photocatalysis and Photocatalytic Reactions	159
7.2	Photoresponsivity and Photocurrent from Simulations	164
7.3	Simulation for Localized Surface Plasmon Resonance	174
	References	182

8	Simulations for Electrochemical Reactions	195
8.1	Single-atom Catalysts	195
8.2	Stability of Catalyst	197
8.3	Electrochemical Reactions	199
8.3.1	Hydrogen Evolution Reaction (HER)	199
8.3.2	Oxygen Evolution Reaction (OER)	203
8.3.3	Oxygen Reduction Reaction (ORR)	204
8.3.4	Nitrogen Reduction Reaction (NRR)	204
8.3.5	Electrocatalytic Activity Evaluated from the First-principles Calculations	209
8.3.6	Simulations for Nitrogen Reduction Reaction	220
	References	232
	Index	239