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*