Table of Contents

1 Introduction 1

Part I Basic Description of Electrons and Photons in Crystals

2 The Essentials of Density Functional Theory and the Full-Potential Local-Orbital Approach
H. Eschrig 7
2.1 Density Functional Theory in a Nutshell 7
2.2 Full-Potential Local-Orbital Band Structure Scheme (FPLO) . . . 11
2.2.1 The Local Orbital Representation 12
2.2.2 Partitioning of Unity 14
2.2.3 Density and Potential Representation 14
2.2.4 Basis Optimization 15
2.2.5 Examples 15
2.2.6 Comparison of Results from FPLO and WIEN97 19

3 Methods for Band Structure Calculations in Solids
A. Ernst, M. Lüders 23
3.1 The Green's Function and the Many-Body Method 23
3.1.1 General Considerations 23
3.1.2 Quasi-Particles 29
3.1.3 Self-Energy 31
3.1.4 Kohn-Sham Approximation for the Self-Energy 34
3.2 Methods of Solving the Kohn-Sham Equation 39
3.3 GW Approximation 47

4 A Solid-State Theoretical Approach to the Optical Properties of Photonic Crystals
K. Busch, F. Hagmann, D. Hermann, S.F. Mingaleev, M. Schillinger . 55
4.1 Introduction 55
4.2 Photonic Bandstructure Computation 57
4.3 Defect Structures in Photonic Crystals 59
4.3.1 Maximally Localized Photonic Wannier Functions 60
4.3.2 Defect Structures via Wannier Functions 61

4.3.3 Localized Cavity Modes 62
4.3.4 Dispersion Relations of Waveguides 64
4.3.5 Photonic Crystal Circuits 66
4.4 Finite Photonic Crystals 68
4.5 Conclusions and Outlook 71

5 Simulation of Active and Nonlinear Photonic Nano-Materials in the Finite-Difference Time-Domain (FDTD) Framework
A. Klaedtke, J. Hamm, O. Hess 75
5.1 Introduction 75
5.2 Finite-Difference in Time-Domain 76
5.3 Uniaxial Perfectly Matching Layers (UPML) Boundary Conditions 80
5.4 Time-Domain Full Vectorial Maxwell-Bloch Equations 87
5.5 Computational Costs 90
5.6 Test Runs 92
5.7 Microdisk Laser Dynamics 95
5.8 Conclusion 98
Appendix A: Relations 99

6 Symmetry Properties of Electronic and Photonic Band Structures
W. Hergert, M. Däne, D. Ködderitzsch 103
6.1 Introduction 103
6.2 Group Theory Packages for Computer Algebra Systems 104
6.3 Basic Concepts in Group Theory 105
6.4 Representation Theory 106
6.4.1 Matrix Representations of Groups 106
6.4.2 Basis Functions of Irreducible Representations 109
6.5 Symmetry Properties of Schrödinger's Equation and Maxwell's Equations 110
6.6 Consequences of Lattice Periodicity 111
6.7 Electronic Band Structure 115
6.7.1 Compatibility Relations 116
6.7.2 Symmetry-Adapted Basis Functions 118
6.8 Discussion of Photonic Band Structures 120
6.8.1 Assignment of the IRs to the Photonic Band Structure . . . 120
6.9 Conclusions 123

Part II Simulation from Nanoscopic Systems to Macroscopic Materials

7 From the Cluster to the Liquid: Ab-Initio Calculations on Realistic Systems Based on First-Principles Molecular Dynamics
C. Massobrio, M. Celino, Y. Pouillon, I.M.L. Billas 129
7.1 Introduction 129
7.2 Theoretical Methods 133
7.2.1 First-Principles Molecular Dynamics 133
7.2.2 Details of Calculations 134
7.3 Selected Applications to Clusters and Disordered Systems 135
7.3.1 CuO_n Clusters 135
7.3.2 Si-Doped Heterofullerenes $C_{59}Si$ and $C_{58}Si_2$ 140
7.3.3 Disordered Network-Forming Materials: Liquid $SiSe_2$ 146
7.4 Concluding Remarks 154

8 Magnetism, Structure and Interactions at the Atomic Scale
V.S. Stepanyuk, W. Hergert 159
8.1 Introduction 159
8.2 Theoretical Methods 160
8.2.1 Calculation of Electronic Structure 160
8.2.2 Molecular Dynamics Simulations 161
8.3 Magnetic Properties of Nanostructures on Metallic Surfaces 163
8.3.1 Metamagnetic States of 3d Nanostructures on the Cu(001)Surface 164
8.3.2 Mixed Co-Cu Clusters on Cu(001) 166
8.3.3 Effect of Atomic Relaxations on Magnetic Properties of Adatoms and Small Clusters 166
8.4 Quantum Interference and Interatomic Interactions 169
8.5 Strain and Stress on the Mesoscale 171
8.5.1 The Concept of Mesoscopic Misfit 171
8.5.2 Strain and Adatom Motion on Mesoscopic Islands 172
8.5.3 Mesoscopic Relaxation in Homoepitaxial Growth 172

9 Molecular Dynamics Simulations in Biology, Chemistry and Physics
P. Entel, W.A. Adeagbo, M. Sugihara, G. Rollmann, A.T. Zayak, M. Kreth, K. Kadau 177
9.1 Molecular Dynamics as a Multidisciplinary Numerical Tool 177
9.2 Simulation of Biochemical Systems 180
9.2.1 Molecular Dynamics Simulation of Liquid Water 181
9.2.2 Simulation of β-Cyclodextrin-Binaphtyl and Water 187
9.2.3 Simulation of Bovine Rhodopsin 189

9.3 Simulation of Chemical Reactions in the Gas Phase 193
9.4 Simulation of Structural Transformations in Solids and Particles . 196
9.4.1 Simulation of the Phase Diagram of Fe-Ni and Ni-Mn-Ga Alloys 196
9.4.2 Simulation of the Structural Transformation in Fe-Ni Particles 198
9.4.3 Simulation of the Melting of Al Clusters 201

10 Computational Materials Science with Materials Studio®: Applications in Catalysis
M.E. Grillo, J.W. Andzelm, N. Govind, G. Fitzgerald, K.B. Stark 207
10.1 Introduction 208
10.2 Geometry Optimization in Delocalised Internal Coordinates 208
10.3 Transition State Searching 213
10.4 Transition State Confirmation Algorithm 214
10.5 Chemical Bonding and Elastic Properties of Corundum-Type Oxides: The Rhodium Oxide Case 217
10.6 Summary 220

11 Integration of Modelling at Various Length and Time Scales
S. McGrother, G. Goldbeck-Wood, Y.M. Lam 223
11.1 Introduction 223
11.2 Structure-Activity and Structure-Property Approaches 225
11.3 Atomistic and Mesoscale Simulations and Their Parameterisation 225
11.3.1 Atomistic Simulation 226
11.3.2 Mesoscale Methods 227
11.3.3 Applications of Mesoscale Modeling 229
11.4 Multiscale Modeling 230
11.4.1 From the Molecular to the Mesoscale 230
11.4.2 From Mesoscale to Finite Element Simulation 231
11.5 Conclusion 232

12 Simulation of the Material Behavior from the Engineering Point of View – Classical Approaches and New Trends
H. Altenbach 235
12.1 Introduction 235
12.2 Principles of Modelling 238
12.3 Phenomenological Models 240
12.4 Classical and Nonclassical Material Behavior Models 244
12.5 Analysis of Thin-Walled Structures 248

Part III Modern Methods of Scientific Computing

13 Parallel Implementation Strategies for Algorithms from Scientific Computing
T. Rauber, G. Rünger 261
13.1 Introduction 261
13.2 A Short Introduction to MPI 263
13.3 Modeling the Execution Time of MPI Operations 266
13.4 Example: Solving Systems of Linear Equations 267
13.4.1 Standard Iterative Methods 268
13.4.2 Sparse Iteration Matrices 269
13.4.3 Red-Black Ordering 272
13.5 Task and Data Parallel Execution 274
13.5.1 Overview of the Tlib Library 275
13.5.2 Example: Strassen Matrix Multiplication 278

14 Multi-Grid Methods – An Introduction
G. Wittum 283
14.1 Introduction 283
14.1.1 Historical Overview and Introduction to Multi-Grid Methods 283
14.1.2 Additive Multigrid 290
14.2 Convergence Theory 291
14.2.1 General Setting 291
14.2.2 The Smoothing Property 293
14.2.3 Approximation Property 295
14.3 Robustness 297
14.3.1 Robustness for Anisotropic Problems 297
14.3.2 Robustness for Convection-Diffusion Problems 302
14.4 Treatment of Systems of PDE 306
14.5 Adaptive Multigrid 307

Index 313