Contents

Preface

I Introduction

A Quantum Mechanics of Materials

A1 Introduction to Density Functional Theory
R. Zeller

A2 Magnetism in Density Functional Theory
G. Bihlmayer

A3 The Optimized Effective Potential Method
S. Pittalis and S. Kurth

A4 Time Dependent Density Functional Theory
A. Schindlmayr

A5 The *GW* Approximation
Ch. Friedrich and A. Schindlmayr

A6 Linear Scaling Electronic Structure Methods
S. Goedecker

A7 Car-Parrinello Molecular Dynamics and Reaction Kinetics
K. Schroeder

A8 Density Functional Theory in Practice
S. Blügel

A9 Electron Correlations
E. Koch

A10 Modern Electron Correlation Methods in Quantum Chemistry
Th. Müller

A11 Quantum Monte Carlo Methods for Electronic Structure Problems
C. Filippi

A12 Building Model Hamiltonians for Strongly Correlated Materials
E. Pavarini

A13 Dynamical Mean Field Theory
A. Liebsch

A14 The Numerical Renormalization Group for Quantum Impurity Models
T.A. Costi

A15 The Density-Matrix Renormalization Group
U. Schollwöck

A16 Introduction to Quantum Computation and Quantum Information Theory
G. Arnold and M. Richter

B Statistical Physics and Soft Matter

B1 Statistical Mechanics
J.K.G. Dhont

B2 Monte Carlo Simulations
G.A. Vliegenthart

B3 Molecular Dynamics Simulations
R.G. Winkler

B4 Brownian Dynamics Simulations
G. Nägele

B5 Mesoscale Hydrodynamics Simulations
M. Ripoll

B6 Structure and Phase Behavior of Polymer Systems
M. Müller

B7 Dynamics of Glass Forming Polymers
D. Richter

B8 Phase Behavior of Colloidal Systems
C.N. Likos

B9 Coarse-Grained and Continuum Models of Membranes
G. Gompper and H. Noguchi

B10 Biological Nanomachines
A. Baumgärtner

B11 How to Fold Proteins on Computers?
U.H.E. Hansmann

B12 Dynamics of Glass Forming Systems
R. Zorn

B13 How to Simulate Granular Matter
D.E. Wolf

C Continuum Theory

C1 Interfacial Pattern Formation
K. Kassner

C2 Hydrodynamics
W. Zimmermann

C3 Phase-Field Simulations
B. Nestler

C4 Elasticity, Friction, and Fracture
R. Spatschek

D Computing and Numerics

D1 Optimization of Numerical Codes
S. Goedecker

D2 Parallel Computing
B. Mohr

D3 Numerical Linear Algebra
I. Gutheil

D4 Algorithms for Optimization
H. Lustfeld

D5 Multiscale and Multigrid Procedures
B. Steffen

E Index