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Approach; 8.3 Reactive Force-Field Approach; Chapter 9 Quantum Mechanical Simulation Methods; 9.1 Born-Oppenheimer Approximation and Pseudopotentials; 9.2 Hartree-Fock Method; 9.3 Density Functional Theory
9.4 Meaning of the Single-Electron Energies within DFT and HF9.5 Approximations for the Exchange-Correlation Functional EXC; 9.5.1 Local Density Approximation; 9.5.2 Generalized Gradient Approximation; 9.5.3 Hybrid Functionals; 9.6 Wave Function Representations; 9.6.1 Real-Space Representation; 9.6.2 Plane Wave Representation; 9.6.3 Local Basis Sets; 9.6.4 Combined Basis Sets; 9.7 Concepts Beyond HF and DFT; 9.7.1 Quasiparticle Shift and the GW Approximation; 9.7.2 Scissors Shift; 9.7.3 Excitonic Effects; 9.7.4 TDDFT; 9.7.5 Post-Hartree-Fock Methods; 9.7.5.1 Configuration Interaction (CI)
9.7.5.2 Coupled Cluster (CC)9.7.5.3 Møller-Plesset Perturbation Theory (MPn); Chapter 10 Multiscale Approaches; 10.1 Coarse-Grained Approaches; 10.2 QM/MM Approaches; Chapter 11 Chemical Reactions; 11.1 Transition State Theory; 11.2 Nudged Elastic Band Method; Part III Industrial Applications; Chapter 12 Introduction; Chapter 13 Microelectronic CMOS Technology; 13.1 Introduction; 13.2 Work Function Tunability in High-k Gate Stacks; 13.2.1 Concrete Problem and Goal; 13.2.2 Simulation Approach; 13.2.3 Modeling of the Bulk Materials; 13.2.4 Construction of the HKMG Stack Model
13.2.5 Calculation of the Band Alignment13.2.6 Simulation Results and Practical Impact; 13.3 Influence of Defect States in High-k Gate Stacks; 13.3.1 Concrete Problem and Goal; 13.3.2 Simulation Approach and Model System; 13.3.3 Calculation of the Charge Transition Level; 13.3.4 Simulation Results and Practical Impact; 13.4 Ultra-Low-k Materials in the Back-End-of-Line; 13.4.1 Concrete Problem and Goal; 13.4.2 Simulation Approach; 13.4.3 The Silylation Process: Preliminary Considerations; 13.4.4 Simulation Results and Practical Impact; Chapter 14 Modeling of Chemical Processes
14.1 Introduction

Sommario/riassunto

An overview of the latest computational materials science methods on an atomic scale. The authors present the physical and mathematical background in sufficient detail for this highly current and important topic, but without unnecessary complications. They focus on approaches with industrial relevance, covering real-life applications taken from concrete projects that range from tribology modeling to performance optimization of integrated circuits. Following an introduction to the fundamentals, the book describes the most relevant approaches, covering such classical simulation methods as simpl