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Autore	Brazdova Veronika
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Altri autori (Persone)	BowlerDavid R
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Nota di contenuto	Atomistic Computer Simulations; Contents; Preface; References; Color Plates; Part One The World at the Atomic Scale; 1 Atoms, Molecules and Crystals; 1.1 Length- and Timescales; 1.2 Electrons in an Atom; 1.3 Local Environment of an Atom; 1.3.1 Electrons; 1.3.2 Local Arrangement of Atoms; 1.4 Most Favorable Arrangement of Atoms; 1.4.1 The Concept of Total Energy; 1.4.2 Beyond the Total Energy; 1.4.3 The Most Stable Configuration; References; 2 Bonding; 2.1 Electronic Ground State; 2.2 Types of Bonds; 2.2.1 Covalent Bonding; 2.2.2 Ionic Bonding; 2.2.3 Metallic Bonding; 2.2.4 Hydrogen Bonding

2.2.5 Dispersion Bonding; 2.3 Bond Breaking and Creation; 2.4 Distortion of Bonds; References; 3 Chemical Reactions; 3.1 Chemical Equations; 3.2 Reaction Mechanisms; 3.3 Energetics of Chemical Reactions; 3.4 Every (Valence) Electron Counts; 3.5 The Energy Zoo; References; 4 What Exactly is Calculated?; 4.1 What Can Be Calculated?; 4.2 What Actually Happens?; 4.3 Models and Simulation Cells; 4.4 Energies; 4.5 Terms; 4.6 Liquid Iron: An Example; References; Part Two Introducing Equations to Describe the System; 5 Total Energy Minimization; 5.1 The Essential Nature of Minimization; 5.2 Minimization Algorithms; 5.2.1 Steepest Descents; 5.2.2 Conjugate Gradients; 5.2.3 Quasi-Newton Methods; 5.2.4 Alternatives; 5.2.5 Exploring Landscapes; 5.2.6 Scaling and Computational Cost; 5.3 Optimize with Success; 5.3.1 Initial Configuration; 5.3.2 Initial Forces, Choice of Algorithm and Parameters; 5.3.3 Fixing Atoms; 5.3.4 Scaling with System Size; 5.4 Transition States; 5.5 Pseudokeywords; References; 6 Molecular Dynamics and Monte Carlo; 6.1 Equations of Motion; 6.2 Time and Timescales; 6.3 System Preparation and Equilibration; 6.4 Conserving Temperature, Pressure, Volume or Other Variables; 6.5 Free Energies; 6.6 Monte Carlo Approaches; 6.7 Pseudokeywords for an MD Simulation; References; Part Three Describing Interactions Between Atoms; 7 Calculating Energies and Forces; 7.1 Forcefields; 7.1.1 Reliability and Transferability; 7.2 Electrostatics; 7.3 Electronic and Atomic Motion; 7.3.1 The Born-Oppenheimer Approximation; 7.3.2 Approximating the Electronic Many-Body Problem; 7.4 Electronic Excitations; References; 8 Electronic Structure Methods; 8.1 Hartree-Fock; 8.2 Going Beyond Hartree-Fock; 8.3 Density Functional Theory; 8.4 Beyond DFT; 8.5 Basis Sets; 8.6 Semiempirical Methods; 8.7 Comparing Methods; References; 9 Density Functional Theory in Detail; 9.1 Independent Electrons; 9.2 Exchange-Correlation Functionals; 9.3 Representing the Electrons: Basis Sets; 9.3.1 Plane Waves; 9.3.2 Atomic-Like Orbitals; 9.4 Electron-Nuclear Interaction; 9.4.1 Pseudopotentials; 9.4.2 PAW; 9.4.3 Using All Electrons; 9.5 Solving the Electronic Ground State; 9.5.1 Charge Mixing and Electrostatics; 9.5.2 Metals and Occupancy; 9.6 Boundary Conditions and Reciprocal Space; 9.7 Difficult Problems; 9.8 Pseudokeywords

Sommario/riassunto

Many books explain the theory of atomistic computer simulations; this book teaches you how to run them. This introductory "how to" title enables readers to understand, plan, run, and analyze their own independent atomistic simulations, and decide which method to use and which questions to ask in their research project. It is written in a clear and precise language, focusing on a thorough understanding of the concepts behind the equations and how these are used in the simulations. As a result, readers will learn how to design the computational model and which parameters o

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Descrizione fisica	1 online resource (265 p.)
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Nota di contenuto	FROM 'SCIENCE IN THE MAKING' TO UNDERSTANDING THE NATURE OF SCIENCE An Overview for Science Educators; Copyright; Contents; Preface; Acknowledgments; 1 Introduction; 2 'Science in the Making' and Heuristic Principles in a Historical Context; 3 Students' and Teachers' Understanding of the Nature of Science; 4 How to Introduce the Nature of Science in the Classroom; 5 The Role of Heuristic Principles in Understanding the Nature of Science; 6 How the Views of Leon Cooper (Nobel Laureate) can Influence In-service Teachers' Understanding of the Nature of Science 7 Martin Perl's (Nobel Laureate) Perspective on the Nature of Science and Teaching Science 8 Conclusion: From 'Science in the Making' to Understanding the Nature of Science; References; Index
Sommario/riassunto	"The Nature of Science is highly topical among science teacher educators and researchers. Increasingly, it is a mandated topic in state curriculum documents. This book draws together recent research on Nature of Science studies within a historical and philosophical framework suitable for students and teacher educators. Traditional

science curricula and textbooks present science as a finished product. Taking a different approach, this book provides a glimpse of "science in the making" -- scientific practice imbued with arguments, controversies, and competition among rival theories and explanations" -- Provided by publisher.
