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2.2.5 Dispersion Bonding2.3 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 Algorithms5.2.1 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 Variables6.5 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 Theory8.4 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