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Nota di contenuto	Part I - BASICS OF CLASSICAL MECHANICS -- Chapter 1: Principles of classical dynamics -- Chapter 2: Foundations of Newtonian dynamics -- Chapter 3: Many-particle systems -- Chapter 4: Mechanical descriptors -- Chapter 5: Rigid body -- Chapter 6: Analytical Mechanics -- Part 2 - BASICS OF QUANTUM MECHANICS -- Chapter 7: Wave-particle duality of matter -- Chapter 8: Quantization of the energy -- Chapter 9: Quantization of the angular momentum -- Chapter 10: Postulates of quantum mechanics -- Part 3 - FIRST-PRINCIPLES MOLECULAR DYNAMICS -- Chapter 11: Dynamics of electrons and nuclei -- Chapter 12: Classical limit of the nuclear motion -- Part 4 - CLASSICAL MOLECULAR DYNAMICS -- Chapter 13: Classical molecular dynamics -- Chapter 14: Extended systems -- Part 5: TIME EVOLUTION OPERATORS -- Chapter 15: Integrating the

equations of motion.

Sommario/riassunto

This molecular dynamics textbook takes the reader from classical mechanics to quantum mechanics and vice versa, and from few-body systems to many-body systems. It is self-contained, comprehensive, and builds the theory of molecular dynamics from basic principles to applications, allowing the subject to be appreciated by readers from physics, chemistry, and biology backgrounds while maintaining mathematical rigor. The book is enhanced with illustrations, problems and solutions, and suggested reading, making it ideal for undergraduate and graduate courses or self-study. With coverage of recent developments, the book is essential reading for students who explore and characterize phenomena at the atomic level. It is a useful reference for researchers in physics and chemistry, and can act as an entry point for researchers in nanoscience, materials engineering, genetics, and related fields who are seeking a deeper understanding of nature.