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Sommario/riassunto	This book provides a comprehensive guide to molecular simulations, focusing on their theoretical foundations and practical applications. Covering topics such as classical mechanics, quantum mechanics, statistical mechanics, probability theory, and computational techniques, it delves into the methodologies used for simulating molecular and atomic interactions. The text discusses numerical algorithms, force fields, simulation dynamics, and applications in areas like thermodynamics, structural properties, and transport coefficients. Intended for researchers, students, and professionals in chemistry, physics, and materials science, the book aims to bridge the gap between fundamental principles and advanced simulation practices through detailed explanations and practical examples.