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Nota di bibliografia	Includes bibliographical references at the end of each chapters and index.
Nota di contenuto	Expected Target of Polymer Simulation -- Coarse-Grained Simulation -- Overview of OCTA -- COGNAC: Coarse-grained Molecular Dynamics Simulator -- SUSHI: Density Functional Theory Simulator -- PASTA & NAPLES: Rheology Simulator -- MUFFIN: Multi Phase Simulator -- KAPSEL: Colloidal Dispersion Simulator -- Melt Viscoelasticity -- Crystallization of Polymers -- Polymer Blends: Bulk Property -- Polymer Blends: Interfacial Strength -- Composites: Morphology -- Composites: Interfacial Strength -- Cross-linked Rubber -- Thermoplastic Elastomers -- Filler-filled Rubbers -- Structures of the Surface and Interface -- Glass Transition at the Surface and Interface -- Evaporation from Polymer Solution -- Crystallization in Thin Films of n-alkanes -- Improvement of Adhesive Properties utilizing Segregation of Oligomers and Investigation of Its Mechanism by SUSHI Simulation -- Adsorption of Polyelectrolytes -- Adsorbed Structures and Surface Forces -- Analysis of Relaxation Mechanism of Thread-like Micelle Solution -- Vesicle Formation -- Electrolyte Membranes -- Orientation

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Sommario/riassunto

This book is the first to introduce a mesoscale polymer simulation system called OCTA. With its name derived from "Open Computational Tool for Advanced material technology," OCTA is a unique software product, available without charge, that was developed in a project funded by Japanese government. OCTA contains a series of simulation programs focused on mesoscale simulation of the soft matter COGNAC, SUSHI, PASTA, NAPLES, MUFFIN, and KAPSEL. When mesoscale polymer simulation is performed, one may encounter many difficulties that this book will help to overcome. The book not only introduces the theoretical background and functions of each simulation engine, it also provides many examples of the practical applications of the OCTA system. Those examples include predicting mechanical properties of plastic and rubber, morphology formation of polymer blends and composites, the micelle structure of surfactants, and optical properties of polymer films. This volume is strongly recommended as a valuable resource for both academic and industrial researchers who work in polymer simulation.