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Computer Simulation of Polymeric Materials

Applications of the OCTA System

- Is the first published sourcebook on the OCTA system
- Introduces many practical examples from researchers in both academia and industry
- Includes detailed processes and tips on simulation that readers can apply to their own research projects

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.

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