

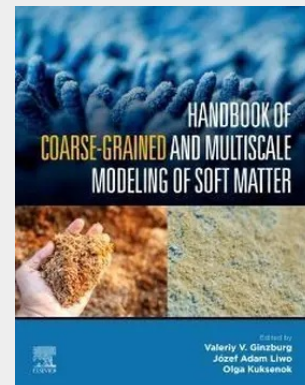
Handbook of Coarse-Grained and Multiscale Modeling of Soft Matter

From the Fundamentals to Scientific and Industrial Applications

Handbook of Coarse-Grained and Multiscale Modeling of Soft Matter: From the Fundamentals to Scientific and Industrial Applications provides a comprehensive overview of multiscale modeling of soft materials, with a special emphasis on the details of the coarse-graining process and the development of multiscale modeling workflows, going from chemical structure to mesoscale morphology to mechanical, physical, transport, electrical, and optical properties of final materials. Starting with general principles and the fundamentals of coarse-graining, the book then reviews particle-based modeling approaches (molecular dynamics and dissipative particle dynamics), field-based models, such as self-consistent field theory and density functional theory, and data-driven and AI-based models. Additional sections cover examples of various systems of interest (synthetic polymers, liquid crystals, surfactants, nanocomposites, and biopolymers), along with specific challenges and questions. Final sections cover specific case studies where modeling is used to help solve industrial problems in the fields of polymer recycling, personal care, energy, transportation, and others. Each chapter is written by a leading academic or industrial scientist working in the specific area.

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