



Thermodynamics and Statistical Mechanics of Macromolecular Systems

Michael Bachmann

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The structural mechanics of proteins that fold into functional shapes, polymers that aggregate and form clusters, and organic macromolecules that bind to inorganic matter can only be understood through statistical physics and thermodynamics. This book reviews the statistical mechanics concepts and tools necessary for the study of structure formation processes in macromolecular systems that are essentially influenced by finite-size and surface effects. Readers are introduced to molecular modeling approaches, advanced Monte Carlo simulation techniques, and systematic statistical analyses of numerical data. Applications to folding, aggregation, and substrate adsorption processes of polymers and proteins are discussed in great detail. Particular emphasis is placed on the reduction of complexity by coarse-grained modeling, which allows for the efficient, systematic investigation of structural phases and transitions. Providing insight into modern research at this interface between physics, chemistry, biology, and nanotechnology, this book is an excellent reference for graduate students and researchers.

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