

Preface

With the development of science and technology, more and more complex materials such as porous materials, ion liquid, liquid crystals, thin films and colloids etc. are being developed in laboratories. However, it is difficult to prepare these advanced materials and use them on a large scale without some experience. Therefore, molecular thermodynamics, a method that laid emphasis on correlating and interpreting the thermodynamic properties of a variety of fluids in the past, has been recently employed to study the equilibrium properties of complex materials and establish thermodynamic models to analyse the evolution process of their components, microstructures and functions during the preparation process. In this volume, some important progress in this field, from fundamental aspects to practical applications, is reviewed.

In the first chapter of this volume, Prof. Jianzhong Wu presents the application of Density Functional theory (DFT) for the study of the structure and thermodynamic properties of both bulk and inhomogeneous fluids. This chapter presents a tutorial overview of the basic concepts of DFT for classical systems, the mathematical relations linking the microstructure and correlation functions to measurable thermodynamic quantities, and the connections of DFT with conventional liquid-state theories. While for pedagogy the discussion is limited to one-component simple fluids, similar ideas and concepts are directly applicable to mixtures and polymeric systems of practical concern. This chapter also covers a few theoretical approaches to formulate the thermodynamic functional. Some illustrative examples are given on applications of DFT to liquid structure, interfacial properties, and surface and colloidal forces. DFT provides a rigorous mathematic framework to describe the structure and thermodynamic properties of liquids from a molecular perspective.

In the second chapter of this volume, Prof. G. Sadowski describes the state of the art in modeling complex fluids, using analytical equations of state. Many applications demonstrate that these models can successfully be applied to describe and even to predict the phase behavior of a whole variety of substances, ranging from small gas molecules to organic solvents and polymeric systems.

Polymer blends or copolymers have multi-scale complex structures that can be used as templates to prepare various complex materials. In the third chapter of this

volume, Prof. Honglai Liu has developed theoretical methods based on equation of state, which can be used comprehensively to study the multi-scale structure of polymer systems, including phase diagrams, morphologies and their evolution of the micro-phase separation, densities and composition profiles in different domains and molecular configurations in the interfacial region.

Ionic liquids have been extensively evaluated as environmental-friendly or “green” solvents, catalysts and materials for a broad range of multifarious processes. They are becoming one of the important development aspects of the complex system, so chapter IV, written by Prof. Suojiang Zhang et al introduces ionic liquids and relative process design. They discuss the related research work on ionic liquids and process design, including the preparation and physical properties of ionic liquids, the application of molecular simulation in the development of applications and process design of ionic liquids, typical applications of ionic liquids and a brief overview of the toxicity of ionic liquids. The study of ionic liquids is just beginning and it is hoped that this chapter will help in the industrial applications of ionic liquids in the future.

Advanced materials are usually obtained by hydrothermal, microwave, and CVD processes. It is generally difficult to achieve the scale-up of advanced materials due to the lack of fundamental theory. The chemical engineering approach, based on thermodynamics, transfer theory and reaction engineering, has been proved to be effective for the scale-up of the product synthesis. In the final chapter of this volume, Prof. Xiaohua Lu and his co-authors present recent progress in this field and discuss how to use the thermodynamic method, combined with transport principles, molecular simulation and modern characterization, for synthesis and application of advanced materials on a large scale.

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