



Molecular Thermodynamics of Complex Systems

(Structure and Bonding)

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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, - crostructures 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 tut- ial 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 - ids, 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.



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