PREFACE

The ultimate objective of the profession of chemical engineering is the manufacture of chemicals and products that improve societal and economic conditions. Achieving this goal often requires that chemical engineers understand and exploit many physical, chemical, and biological phenomena. In recent years, chemical engineers have increasingly been involved in the design, synthesis, and manufacture of high-value-added products and chemicals. These technologies often demand that product properties and processing methods be controlled with precision. Similar issues arise in research aimed toward developing more efficient processing of petroleum products and developing catalysts for synthesis of alternative fuels. In some cases, product properties must be precisely controlled at the macroscopic level, and in other cases, the properties that we seek are on much smaller scales (nanometers to micrometers). One way to confront this challenge with both classes of systems is to learn how to manipulate system characteristics at the molecular and/or mesoscopic scales so that we obtain the desired properties. Learning how molecular constitution and mesoscopic characteristics influence the properties of a system of interacting components can only be addressed by synergistic experimental and theoretical research. The pertinent experimental and theoretical methods must be able to interrogate systems on a wide range of length and time scales. Chemical engineers are playing an important role in the development and application of a number of such experimental and theoretical tools. These research efforts are taking steps toward developing the knowledge base required to relate structures to properties for both synthetic and biological systems. This volume of *Advances in Chemical Engineering* focuses on theoretical and computational efforts at the frontiers of a number of different application areas that benefit from such research.

The bedrocks of the theoretical and computational methods that allow study of relationships between molecular and mesoscopic scale events and system properties are quantum and statistical mechanics. Thus, this volume comprises chapters that describe the development and application of quantum and statistical mechanical methods to various problems of technological relevance. The application areas include catalysis and reaction engineering, processing of materials for microelectronic applications, polymer science and engineering, fluid phase equilibrium, and combinatorial methods for materials discovery. The theoretical methods that are discussed in the various

chapters include electronic structure calculations, *ab initio* molecular dynamics simulations, Monte-Carlo simulation methods, field-theoretic methods, and various theories of the liquid state. The diversity of application areas represented in this volume reflects the fact that methods based on quantum and statistical mechanics now play an important role in research that is relevant to a variety of technologies. The diversity of methods discussed in this volume reflects the fact that for complex problems no single method can serve as a panacea. In other words, studying properties influenced by phenomena at different length and time scales requires a hierarchy of methods.

This collection of articles is not a comprehensive compendium of the interesting work being done to study complex systems using quantum and statistical mechanical methods. It is hoped, however, that this representative sampling of work being carried out by chemical engineers in this broad area will provide the beginning graduate student and the experienced practitioner with a sense of the current state of the art and the challenges that need to be confronted in the future. My personal opinion is that future volumes dedicated to this broad topic will witness a greater emphasis on nonequilibrium phenomena, the coupling of quantum and statistical mechanical approaches, and more applications focused on biomedical problems.

My fellow editors of *Advances in Chemical Engineering,* the staff at Academic Press, and I thank the authors for taking time out of their busy schedules to contribute to this volume. The effort involved in writing good review articles is a selfless service to the profession and is truly appreciated. A personal note of thanks is also extended to the authors for their patience during the review and production process.

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