

MOLECULAR MODELING APPLICATIONS IN CRYSTALLIZATION

Crystallization is an important purification process used in a broad range of industries, including pharmaceuticals, foods, and bulk chemicals. In recent years, molecular modeling has emerged as a useful tool in the analysis and solution of problems associated with crystallization. Modeling allows more focused experimentation based on structural and energetic calculations, instead of intuition and trial and error.

This book is the first to offer a general introduction to molecular modeling techniques and their application in crystallization. After explaining the basic concepts of molecular modeling and crystallization, the book goes on to discuss how modeling techniques are used to solve a variety of practical problems related to crystal size, shape, internal structure, and properties.

With chapters written by leading experts and an emphasis on problem-solving, this book will appeal to scientists, engineers, and graduate students involved in research and the production of crystalline materials.

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Edited by
ALLAN S. MYERSON



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Preface

Crystallization from solution is an important separation and purification process used in a wide variety of industries. In addition to product purity, it is often necessary to control the external shape and size of the crystals and to produce the desired polymorph and/or optical isomer. In some applications it is necessary to inhibit the formation of crystals or control their size and shape by the use of an additive.

Molecular modeling or calculational chemistry are terms that are used to describe techniques that employ quantum mechanics and statistical mechanics in conjunction with computer simulation to study the chemical and physical properties of materials.

In recent years, molecular modeling has emerged as a useful tool in the solution of a number of the crystallization problems mentioned above. In particular, modeling allows more focused experimentation based on structural and energetic calculations instead of intuition and trial and error. The availability of commercial modeling packages has led to its widespread use in many industrial and academic laboratories. These packages often lead to investigators treating the modeling process as a “black box” without understanding the basic principles underlying the methods. The purpose of this book is to explain the basic concepts of molecular modeling and their application to problems in crystallization.

The first two chapters introduce basic molecular modeling concepts (Chapter 1) and the basics of crystals and crystallization (Chapter 2). These chapters are aimed at the nonspecialist who needs an introduction to the area. The remaining chapters deal with molecular modeling techniques for molecular crystals (Chapter 3), the role and selection of additives (Chapter 4), modeling techniques in ionic systems (Chapter 5), and chirality (Chapter 6).

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