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# BOOK REVIEW

**Modelling of Structure and Reactivity in Zeolites.** Edited by C. R. A. CATLOW. Harcourt Brace Jovanovich Ltd., London, 1992. viii + 260 pp. $97.00.

Recent advances in both theoretical techniques and computer hardware allow computational chemistry investigations to make substantial contributions to our understanding of zeolites. This book presents an overview of the various calculations and modeling techniques that have been applied in investigations of zeolites. In 10 chapters, 23 contributors discuss the present state-of-the-art in modeling zeolite structure and properties including cationic siting, Si/Al ratio, sorption, diffusion, and chemical activity using a variety of computational techniques, e.g., molecular dynamics simulations, Monte Carlo, semiempirical calculations, density functional, and ab initio methods. Computer graphics are also emphasized as an important tool in data analysis. Both successes and failures are discussed, as well as optimistic prospects for the future.

Suitable for either an experienced researcher or graduate student, the book brings together a number of scientists recognized as leaders in the theory and modeling of zeolites. As an overview, a large number of topics are covered in sufficient detail to define and explain the points of interest at the expense of sacrificing technical details. However, each chapter is accompanied by a lengthy list of references for the reader requiring greater depth. As explicitly stated by several authors, the ultimate goal of modeling zeolites is three fold: (i) to construct new structures with (ii) designed properties and (iii) to provide a procedure for their synthesis. The book addresses the challenges in each of these three categories. Both topological and lattice energy minimization techniques are shown to provide paths to constructing possibility new zeolite frameworks. The thermodynamic stability of the models is investigated through molecular dynamics simulation, where procedures are given for calculating structural and dynamical quantitites. Quantities such as structure factors, vibrational spectra, and transport coefficients may be directly compared to experimentally observed values. Example calculations are given for determining cation sites and the diffusion and adsorption sites of small molecules in zeolites. The chemical properties of zeolites are investigated through density functional methods and quantum mechanical studies. Professor Joachim Sauer provides a detailed review of the quantum chemical studies performed in the past decade as well as the more recent and accurate cluster models. The importance of both the model and the level of the calculation is stressed in the interpretation of the results from quantum-chemical investigations. The final chapter qualitatively addresses the synthesis of zeolites through a population balance analysis which treats zeolite crystallization as a reactive kinetic process.

Throughout the book the authors touch on the problem and inadequacy of many of the modeling techniques to properly account for the complex interactions typical of zeolites. The examples presented contribute to our understanding of zeolites but rarely provide more than a qualitative description of the structure and properties. Though the authors exhibit great expectations for future models of zeolites, it is clear that the level of sophistication required to attain the ultimate goal will not be achieved easily. For those interested in initiating modeling efforts into the study of zeolites, it should be pointed out that many of the examples and results discussed and presented in this book appear to have been obtained with commercial or proprietary software, much of which is tied to the Biosym Catalysis Consortium. Perhaps a bit premature for an overview, given the level of the results obtained to date, this is the first book to provide a comprehensive look at the various modeling methods applied in the study of zeolites. It is sure to become a standard reference for future publications.

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