MOLECULAR INTERACTIONS

CONCEPTS AND METHODS

David A. Micha

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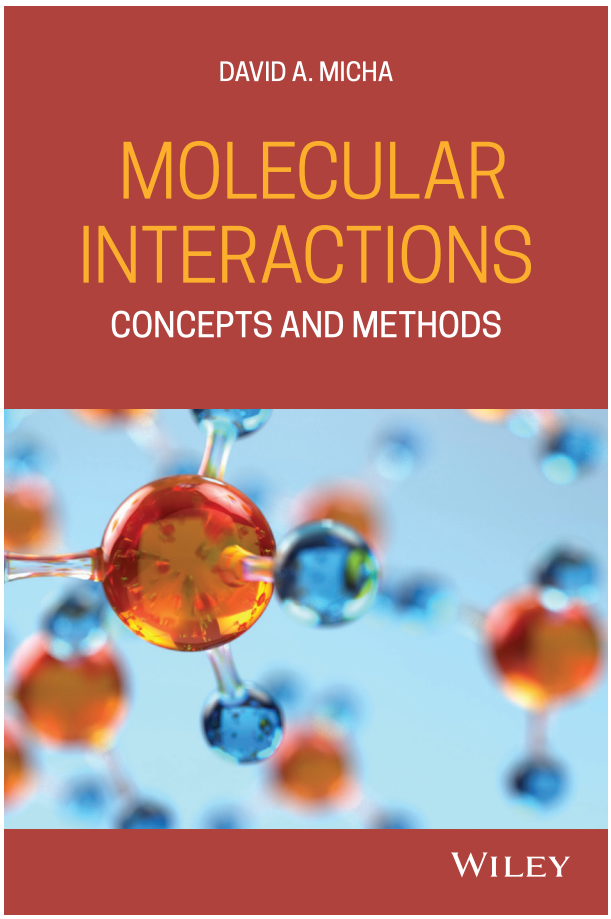

An up-to-date and comprehensive text that explores intermolecular forces

Molecular Interactions offers a comprehensive guide that examines the fundamental concepts and methods of intermolecular forces. The text provides a quantitative treatment based on molecular properties, introducing realistic models and theoretical tools needed to obtain physical properties. All chapters include an introduction to the qualitative aspects of molecular interactions and then explore the interactions treated in a quantitative fashion.

The author—a noted expert on the topic—examines the concepts and quantitative aspects of molecular interaction such as electrostatic, induction, and dispersion forces and shows how they extend to intermediate and short ranges for ground and excited states. The text includes a survey of model potential functions. It offers an exploration of recent developments in the field including electronically non-adiabatic interactions, correlated many-electron treatments, generalized density functional theory, decomposition, and embedding of molecular fragments for large systems. It also presents the most recent developments using artificial intelligence with network training for many-atom system. It includes molecular interactions between two many-atom systems, interactions in condensed matter, and interactions of molecules with surfaces.

This important text:

- Presents the concepts and methods of molecular interactions used in calculations
- Offers comprehensive descriptions starting from atomic structure
- Provides the theory and computational approaches needed for many-atom interactions
- Contains illustrative applications to many physical systems and worked examples

Written for students and researchers in chemical physics, materials sciences, molecular biology, pharmaceuticals, and medical sciences, *Molecular Interactions* offers an authoritative guide to the fundamentalconcepts and methods as well as information on the most recent innovations that have relevance for new materials, biological phenomena, and energy and fuels production.

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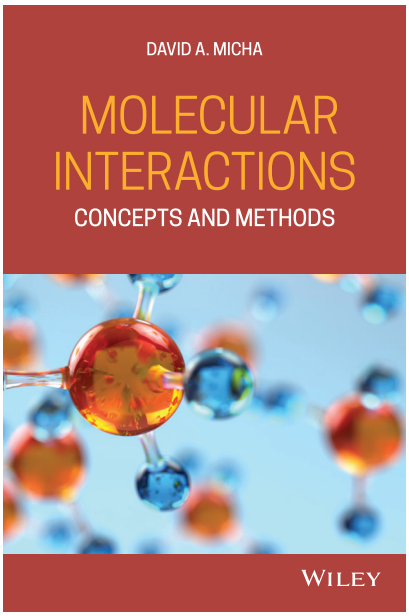

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David A. Micha, PhD, is a Professor of Chemistry and Physics at the University of Florida, presently Adjunct and Emeritus, with continuing research activity. His many research interests include molecular interactions and kinetics, and quantum molecular dynamics involving energy transfer, electron transfer, light emission, reactions in gas phase collisions, and also at solid surfaces. He is an author in over 220 research publications and co-editor of seven science books. His work has been recognized with awards from the Alfred P. Sloan Foundation and the Dreyfus Foundation, and with an Alexander von Humboldt Senior Scientist Award. Dr. Micha has been the organizer of several Pan-American Workshops and is a co-organizer of the "Sanibel Symposium on Theory and Computation for the Molecular and Materials Sciences" at the University of Florida.

FROM THE PREFACE

Intermolecular forces are essential in many applications of molecular and materials properties to technologies contributing to the needs of society. To illustrate the enormous impact of the subject, some of their subjects (and their applications) are storage of hydrogen in solids (fuel cells), storage and transport of ions in solids (batteries), synthesis of thermally stable and conducting surfaces (solar energy devices), delivery of compounds through biological cell membranes (pharmacology), catalysis and photocatalysis in electrochemical cells (sustainable fuel production), atmospheric reactions (environmental sciences), efficient fuel combustion (transportation and energy), and solvation and lubricants (machinery). Furthermore, as the quantitative tools of chemistry and physics in this book have become more useful and common in biology, pharmaceutics, and medicine, its contents should also be of interest in these new areas of applications.

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