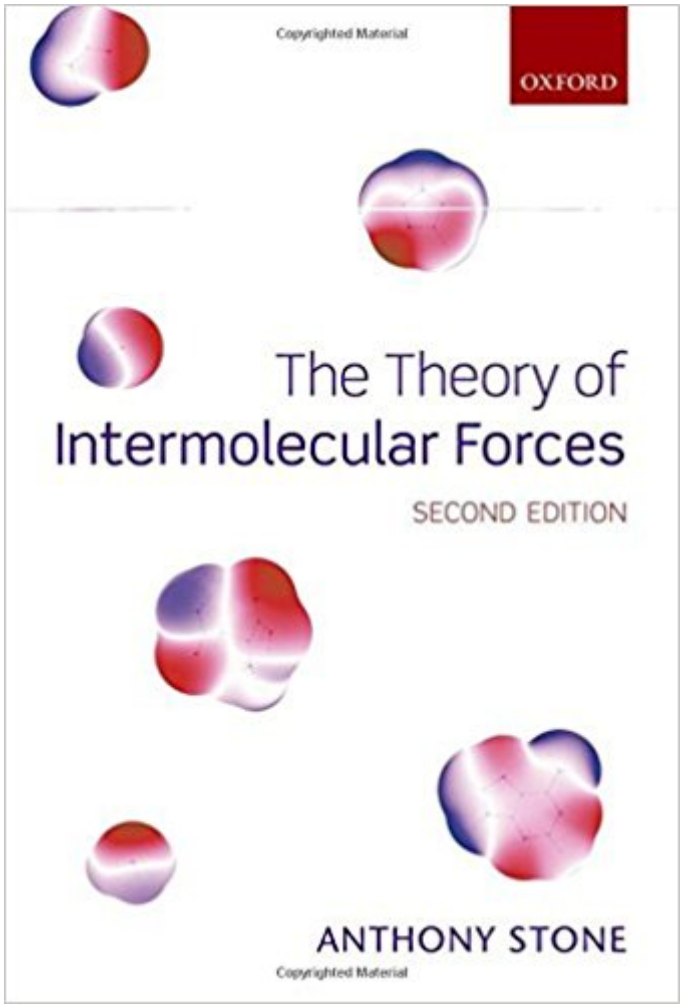
The Theory Of Intermolecular Forces, 2nd Edition



Synopsis

The theory of intermolecular forces has advanced very greatly in recent years. It has become possible to carry out accurate calculations of intermolecular forces for molecules of useful size, and to apply the results to important practical applications such as understanding protein structure and function, and predicting the structures of molecular crystals. The Theory of Intermolecular Forces sets out the mathematical techniques that are needed to describe and calculate intermolecular interactions and to handle the more elaborate mathematical models. It describes the methods that are used to calculate them, including recent developments in the use of density functional theory and symmetry-adapted perturbation theory. The use of higher-rank multipole moments to describe electrostatic interactions is explained in both Cartesian and spherical tensor formalism, and methods that avoid the multipole expansion are also discussed. Modern ab initio perturbation theory methods for the calculation of intermolecular interactions are discussed in detail, and methods for calculating properties of molecular clusters and condensed matter for comparison with experiment are surveyed.

Book Information

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Customer Reviews

"Professor Stone’s 1996 monograph The Theory of Intermolecular Forces is ’must’ reading for all researchers working in the area of intermolecular reactions. Since the time this monograph was first published, there have been major advances in both electronic structure theory and the development of force fields based on accurate electronic structure calculations on model systems. In the new edition Professor Stone has done an outstanding job at including information on recent

developments on both of these fronts. In addition, the new edition provides valuable new insights into issues such as the role of charge transfer and charge penetration in intermolecular interactions. As a result, it will prove to be especially valuable to researchers engaged in the development of accurate force fields for modeling chemical, biological, and materials systems as well as to those who are users of force field methods." --Kenneth D. Jordan, University of Pittsburgh"Anthony Stone has updated his book to take account of progress in theory and computation during the intervening 16 years. The new edition retains the clear pedagogical nature of the original work and replaces it as an essential and unique source of the theory underlying the details of molecular interactions." --Gabriel G. Balint-Kurti, University of Bristol"The first edition of this book, published in 1996, has become the standard text and reference in the field of intermolecular forces. The current edition mainly updates the text by describing research published in the intervening years. A comparison of the two editions shows how significant was the progress during this time period, as the text was enlarged by nearly 30%. Thus, with the present extension, the book will certainly be an even more useful reference than before." --Krzysztof Szalewicz, University of Delaware

Anthony Stone, Emeritus Professor, Theoretical Chemistry, University of CambridgeAnthony Stone, Emeritus Professor of Theoretical Chemistry, University of Cambridge, studied at the University of Cambridge, and after a short period in the United States took up a teaching and research position at Cambridge, where he has remained. He retired in 2006.

perfect

Everything about this book was great except the packaging. It arrived with all the corners of the hardcover bent. L

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