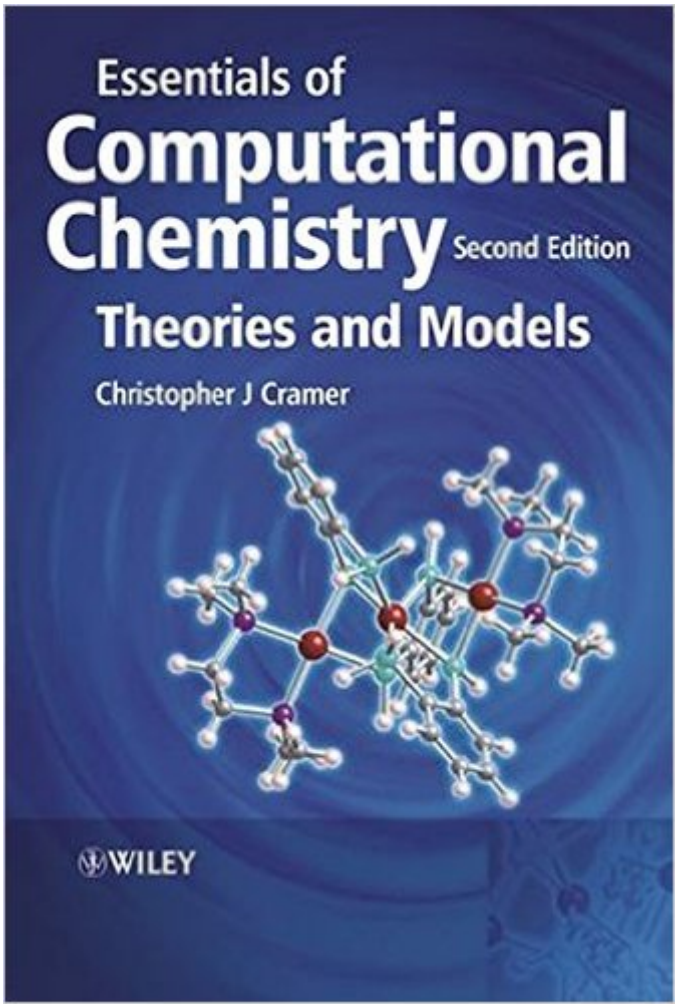
Essentials Of Computational Chemistry: Theories And Models



Synopsis

Essentials of Computational Chemistry provides a balanced introduction to this dynamic subject.Â Suitable for both experimentalists and theorists, a wide range of samples and applications are included drawn from all key areas.Â The book carefully leads the reader thorough the necessary equations providing information explanations and reasoning where necessary and firmly placing each equation in context.

Book Information

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Customer Reviews

This book is a follow-up to a previous release and is a great textbook for learning how to simulate atoms, molecules, and fluid mixtures using a variety of techniques. Its positive attributes includes the following:1. The author makes it a point to explain the various phrases, acronyms, and terms common in the field, but which may confuse the novice or outsider. For example, the first chapter explains the concept of a potential energy surface, how it can be obtained, and the information that can be gleaned from it. These are simple concepts to those experienced in atomistic modeling but can be mysterious to newcomers.2. The mathematics in the text are simple enough to be understood without the reader having to resort to proving things herself, but they are complete enough to understand how physical concepts are represented and solved. The equations are also set apart from the text such that they are easy to read.3. There are a lot of diagrammatic figures that explain what is going on; i.e. how atoms interact via certain empirical potentials. One can also tell that the figures were made specifically to teach a concept, and are not reproductions from a

publication.4. The text is appropriate for first-year graduate students in physics, engineering, and chemistry, and the book provides chapters dedicated to quantum mechanics and thermodynamics, the two topics science and engineering students have the most difficulty in.5. The case study at the end of each chapter are well laid out and do a good job of illustrating the concepts taught in that chapter.6. There are a lot of flowcharts that show the process by which a calculation is carried out. See for example the appendix on determining the point symmetry of a molecule.

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