Chemical Modeling. From Atoms to Liquids

Description: Chemical Modeling equips the reader with the knowledge to understand the behaviour of solids, gases and liquids in terms of the basic properties of their atoms, molecules, and polymer chains. In particular the interactions between these fundamental building blocks and the intermolecular and intramolecular potentials are examined. Carefully structured, the book starts by the discussion of classical, quantum and statistical mechanics which then leads on to a discussion of modeling techniques applied to solids, gases and liquids. The subject is brought to life through many real life examples and practical illustrations.

Features

* Classical mechanics and quantum mechanics are both introduced from a basic level
* Explains the relationships between microscopic and macroscopic quantities
* Gives an up–to–date treatment of a variety of chemical modeling techniques
* Avoids unnecessary mathematical rigour
* Carefully structured into ‘bite–sized’ chapters

Ideal for undergraduates of chemistry, chemical physics, physics, materials science and polymer science.

Contents:

Describing Macroscopic Systems.

Thermodynamics.

Résumé of Classical Mechanics.

Modeling Simple Solids (i).

Introduction to Quantum Mechanics.

Electric Multipoles, Polarizabilities and Intermolecular Forces.

Some Statistical Ideas.

Applications of the Boltzmann Distribution.

Modeling Simple Solids (ii).

Molecular Mechanics.

Molecular Dynamics and Monte Carlo Techniques.

The Ideal Monatomic Gas.

Quantum Gases.

Introduction to Statistical Thermodynamics.

Modeling Atoms.

Diatomics.

Quantum Modeling of Larger Systems.
Describing Electron Correlation.
The Band Theory of Solids.
Modeling Polymeric Materials.
Modeling Liquids.
Appendices.
Suggestions for Further Reading.
Index.

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