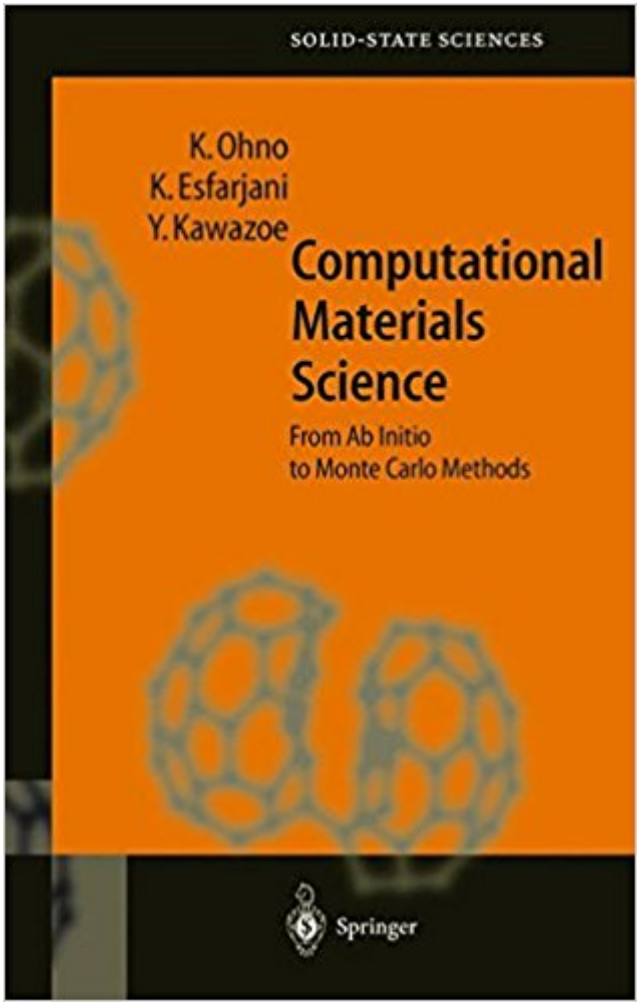
Computational Materials Science: From Ab Initio To Monte Carlo Methods (Springer Series In Solid-State Sciences)



Synopsis

Powerful computers now enable scientists to model the physical and chemical properties and behavior of complex materials using first principles. This book introduces dramatically new computational techniques in materials research, specifically for understanding molecular dynamics.

Book Information

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Customer Reviews

This book introduces modern techniques based on computer simulation to study materials science. It starts from first principles calculations that enable the physical and chemical properties to be revealed by solving a many-body Schroedinger equation with Coulomb forces. For the exchange-correlation term, the local density approximation is usually applied. After the introduction of the first principles treatment, tight-binding and classical potential methods are briefly introduced to indicate how one can increase the number of atoms in the system. In the second half of the book, Monte Carlo simulation is discussed in detail. Readers can gain sufficient knowledge to begin theoretical studies in modern materials research.

I read this book to learn more about my field of study; computational materials science. I found it thorough; it covered all the major aspects for modelling of condensed phases at the atomic scale: Monte Carlo, Moleculary Dynamics, statistical thermo, and ab initio methods.The strong point of this book compared to others on the same subject is that the amount of space devoted to the various

subjects closely corresponds to the amount of work done in those subjects. Therefore, a lot of space is spent on empirical and semi-empirical methods.Density functional theory, which is the workhorse of today's high-end simulations, gets shorted here. Only a couple of pages are spent on it. This contrasts strongly with other books on the same subject, like the books by Raabe, or Catlow, or Finnis, where DFT gets at least a whole chapter to itself.Likewise, there is not much on electronic structure. There are a fair number of examples in this book, but few are simple enough for the first-timer to follow. The examples tend to show of the abilities of simulations; and not the nuts and bolts of how to do them.As such, this book is great for an introductory course on computer simulations of materials; assuming the reader has a background in materials science. It is not a good book for a course on DFT, computational quantum mechanics, or solid state calculations.

With an exponentially growing computational power, more precise and exact treatments of problems of condensed matter physics become affordable, and the dark corners of material science become clearly understandable. At the same time, new methods are becoming developed, that allow for better treatments of various kinds of problems in this field.This book is a gem, written by three active frontiers on this subject and can be of great value to anyone doing computations in material science. An almost complete and up to date review of the methods used in this field with great lists of references for further studies.In addition to the workers in this field, I highly recommend this book to anyone who wants to know what happens in the Material Science today.

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