

<<计算物理学>>

图书基本信息

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## &lt;&lt;计算物理学&gt;&gt;

## 内容概要

This Second Edition has been fully updated. The wide range of topics covered in the First Edition has been extended with new chapters on finite element methods and lattice Boltzmann simulation. New sections have been added to the chapters on density functional theory, quantum molecular dynamics, Monte Carlo simulation and diagonalisation of one-dimensional quantum systems.

The book covers many different areas of physics research and different computational methodologies, with an emphasis on condensed matter physics and physical chemistry. It includes computational methods such as Monte Carlo and molecular dynamics, various electronic structure methodologies, methods for solving partial differential equations, and lattice gauge theory. Throughout the book, the relations between the methods used in different fields of physics are emphasised. Several new programs are described and these can be downloaded from [www.cambridge.org/9780521833462](http://www.cambridge.org/9780521833462)

The book requires a background in elementary programming, numerical analysis and field theory, as well as undergraduate knowledge of condensed matter theory and statistical physics. It will be of interest to graduate students and researchers in theoretical, computational and experimental physics. Jos THIJSEN is a lecturer at the Kavli Institute of Nanoscience at Delft University of Technology.

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## 章节摘录

版权页：插图：Now we can define the problems in a more abstract way. It is convenient to consider continuum problems. The candidate solutions ( for example the possible conformations ) form a phase space, and the merit function has some complicated shape on that space - it contains many valleys and mountains, which can be very steep. The solution we seek corresponds to the lowest valley in the landscape. Note that the landscape is high-dimensional. You may think, naively, that a standard numerical minimum finder can solve this problem for you. However, this is not the case as such an algorithm always needs a starting point, from which it finds the nearest local minimum, which is not necessarily the best you can find in the conformation space. The set of points which would go to one particular local minimum when fed into a steepest descent or other minimum-finder ( see Appendix A4 ) is called the basin of attraction of that minimum. Once we are in the basin of attraction of the global minimum we can easily find this global minimum; the problem is to find its basin of attraction.



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