# <<计算机化学与分子设计>>

## 图书基本信息

书名：<<计算机化学与分子设计>>

13位ISBN编号：9787040182965

10位ISBN编号：7040182963

出版时间：2009-3

出版时间：高等教育出版社

作者：范波涛 等著

页数：490

## 前言

In 1997, the Chinese scientists working in France organized an activity to support the western development of China. We arrived at Lanzhou University. I had the opportunity to meet Professors HU Zhide, JIA Zhongjian, ZHENG Rongliang, LIU Mancang, and other teaching staffs of the Chemistry Department. The scientific exchange between us reached to a common point in research and scientific domains. Based on this same point of view, we signed a series of cooperation agreements, which include their requirement to open a summer class in Computer Chemistry for graduated students. This proposal obtained the support of the Ministry of Education of China. Professors DOUCET J.P. and PANAYE A. of University Paris 7-Denis Diderot expressed also their concerns and supports. Next year, 1998, the summer class was opened, this course of speciality was officially inserted in the list of teaching plan. . Encouraged by this successful beginning, Professor HU Zhide and Professor LIU Mancang suggested me to publish my course in order to solve the problem that the students lack teaching materials. After the discussion with Professor ZHANG Ruisheng, by considering the fact that the time is too short, we thought that we can not publish a book covering a large scope of this domain. Therefore we can only publish a book with limited contents. Thanks to Lanzhou University, this teaching material was published in 1998. But because of the short time, it lacks a global plan. Moreover, the contents covered by this book are also limited, so we are not satisfactory for this version. I'm now Professor of University Paris 7, and lead a research group, the laboratory of "Molecular Simulation and Molecular Information", in ITODYS institute. At the same time, I'm also the Director of Institute of Chemoinformatics of Lanzhou University. I have almost 20 years of experience in research and teaching of computer chemistry and published more than 120 papers and reviews in this area. My teaching experience covers almost all aspects of this area. Therefore, I hope to write a book which gathers the contents of our research and teaching work, in order to provide a reference to all researchers and graduated students worked in this domain. Great thanks to High Education Press of China. Their heartily invitation gave me a good opportunity to realize my hopes. After receiving the invitation, I invited two colleagues who work long time in Chemoinformatics, to work together for writing this book. One is Professor ZHANG Ruisheng of Lanzhou University, another is Associate Professor YAO Jianhua of Shanghai Institute of Organic Chemistry. The modern computer chemistry covers a large scope of contents. It includes the traditional computational chemistry, molecular graph theory and applications, chemoinformatics, molecular modeling, molecular design (including drug design), molecular simulation, QSAR/QSPR, and so on. .. In this book, we cite and refer a lot of literatures reported by specialists. For example, in molecular modeling, personally I consider that the best book is "Molecular Modeling: Principles and Applications" , written by A. Leach. In some related chapters of our book, we cited some contents of this reference book. About the mathematical principle of artificial neural network, we referred the book "Des reseaux de neurones", EYROLLES, 1990, written by E. Davalo and P. Naim. Massart et al. developed RBFNN (Massart is a great specialist in this area). The important statements about the theory and applications were reported in their published papers. These papers are the basis of RBFNN. In our book, some of their remarkable works have been cited and referred. We cited also the works of our laboratory. These results are all the research works of my colleagues and PhD students, including Professor Doucet, Professor Panaye, Professor HU Zhide, Professor LIU Mancang, Dr. Barbault, Dr. Petitjean, Dr. Maldonado, Dr. CHEN Haifeng, Dr. YAO Xiaojun, Dr. XIA Hairong, Dr. LIU Huangxiang, Professor GAO Kun, and so on. I would like to mention specially Professor Doucet and Dr. Maldonado, because a very important part of their works has been cited in this book. I express here my sincere thanks to these colleagues and students. I thank also my family, my wife and children. Without their supports, encouragement and concerns, without a good environment of writing, I can not certainly finish the writing of this book. This work was supported in part by National Natural Science Foundation of China through Grants 20572120.

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## 内容概要

This book covers two parts: Computer Chemistry and Molecular Design. It presented several approaches employed in molecular design step by step. Molecular graph and presentation as the start point, it introduced several methods of Computer Chemistry concerned with molecular design: property recognition of chemical structure, artificial neural network and data analysis.

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## 书籍目录

## 章节摘录

插图：All the minimization methods described above fall under this general schema ofsuccessive line minimizations. In this section we consider a class of methods whosechoice of successive directions does not involve explicit computation of the func-tion's gradient. The methods introduced in the next section do require such gradi-ent calculations. It will be noted that we need not specify whether algorithm usesgradient information or not. That choice is up to us, and its optimization dependson our particular function. However, we can use or not use gradients in algorithmin the choice of directions, since in this latter role they can drastically reduce thetotal computational burden.But what if, in your application, calculation of the gradient is out of thequestion, you might first think of this simple method:Take the unit vectorsel, e2, eN as a set of directions. Using the above algorithm, move along thefirst direction to its minimum, then from there along the second direction to itsminimum, and so on, cycling through the whole set of directions as many times asnecessary, until the function stops decreasing.This dumb method is actually not too bad for many functions. Even moreinteresting is why it is bad, i.e. very inefficient, for some other functions. Considera function of two dimensions whose contour map （level lines） happens to definea long, narrow valley at some angle to the coordinates basis vectors. Then theonly way "down the length of the valley" going along the basis vectors at eachstage is by a series of many tiny steps. More generally, in N dimensions, if thefunction's second derivatives are much larger in magnitude in some directions thanin others, then many cycles through all N basis vectors will be required in orderto get anywhere.

## 编辑推荐

《Computer Chemistry and Molecular Design》介绍了：Encouraged by this successful beginning, Professor HU Zhide and Professor LIU Mancang suggested me to publish my course in order to solve the problem that the students lack teaching materials. After the discussion with Professor ZHANG Ruisheng, by considering the fact that the time is too short, we thought that we can not publish a book covering a large scope of this domain. Therefore we can only publish a book with limited contents.

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