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<<蛋白质计算机模拟>>

图书基本信息

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内容概要

This textbook covers a course of computer simulation of proteins for science major students, It consists of two knowledge blocks： Molecular Dynamics （MD） and Full Electron Structure Calculation of Proteins. We shall also discuss two main subjects: Knock-off Proteins and Protein-Lig and Interactions. However we shall not discuss the folding dynamics of proteins. These are discussed in "Cluster-Linux-Parallel Calculation System".

The Full Electron Structure Calculation of Proteins is one of the new features of this textbook. We assume the readers have the basic knowledge of computer languages, proteins and physics. Still, information on Unix , TCL and Phthon are included briefly in this textbook as a refreshing exercise. The keystone of this textbook is to elaborate the computer simulation of proteins. Therefore, merely reading this textbook is not enough. The students must practice all the problem examples on computers while studying. Otherwise, the students will not understand the topics discussed in this textbook.

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作者简介

周麟祥，物理学教授。
1939年12月生，原籍浙江嘉兴。
1960年毕业于厦门大学物理系。
1993-1997年任美国林肯大学客座教授。
曾在厦门大学任教。
目前在复旦大学物理系主要从事蛋白质分子动力学和全电子结构的计算机模拟研究工作。
帅建伟，物理学教授。
1968年6月生，原籍四川。
1995年毕业于厦门大学物理系。
1996-2007年在香港、日本、德国、美国任职。
2007年回国前，在美国加州大学Irvine分校工作。
现在厦门大学物理系任闽江学者特聘教授，从事生物系统计算机模拟的研究工作。

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