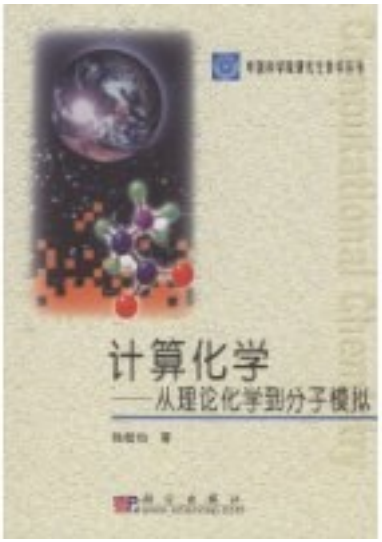
# 计算化学

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《计算化学:分子和量子力学理论及应用导论(原著第2版)(英文版)》内容简介：重要的概念（例如，分子力学，从头计算、半经验及密度泛函理论）都辅以其扼要的历史背景和顶尖科。学家的人物介绍。计算化学基础理论构架的阐述都配以清晰的计算实例。2003年第1版以来直到2009年底的学科重要进展，都已纳入本版中。增加了第1版未涉及的内容，例如，溶剂化效应，如何做CASSCF计算，过渡元素等。每章章末附有习题，用于测试读者的理解程度。至于较难的习题，其中有些没有直接明确解的，可到书末寻找答案。附有大量参考文献，可以帮助读者核查所有关键论点的基础，启发深入思考。使得《计算化学:分子和量子力学理论及应用导论(原著第2版)》不仅是教科书，还是一部极具参考价值的科学著作。

《计算化学:分子和量子力学理论及应用导论(原著第2版)》特别适合计算化学和理论化学专业的高年级本科生和研究生、科研院所和企业从事计算化学相关领域的专业人员，同时也可用于自学和指导用书。

作者介绍:

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## 评论

好不容易啃完这本书，数学推导看的一知半解的，不过大概也理解了整个计算过程是怎么样的。

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## 书评

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