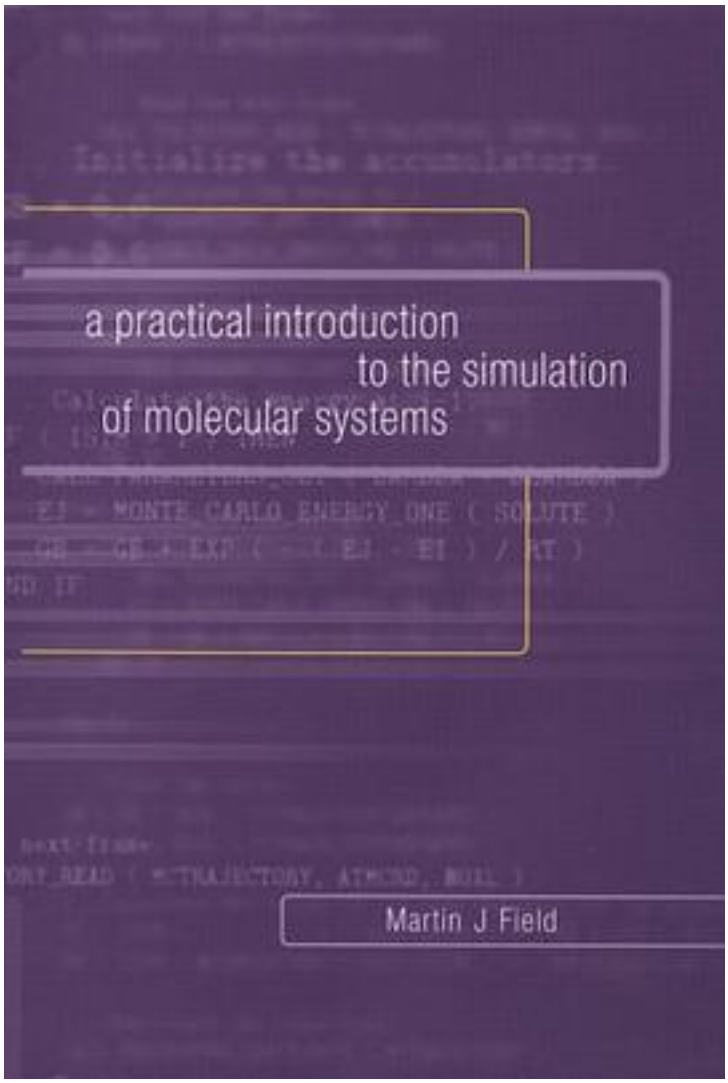
A Practical Introduction to the Simulation of Molecular Systems



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Molecular simulation is a powerful tool in materials science, physics, chemistry and biomolecular fields. This updated edition provides a pragmatic introduction to a wide range of techniques for the simulation of molecular systems at the atomic level. The first part concentrates on methods for calculating the potential energy of a molecular system, with new chapters on quantum chemical, molecular mechanical and hybrid potential techniques. The second part describes methods examining conformational, dynamical and thermodynamical properties of systems, covering techniques including geometry-optimization, normal-mode analysis, molecular dynamics, and Monte Carlo simulation. Using Python, the second edition includes numerous examples and program modules for each simulation technique, allowing the reader to perform the calculations and appreciate the inherent difficulties involved in each. This is a valuable resource for researchers and graduate students wanting to know how to use atomic-scale molecular simulations. Supplementary material, including the program library and technical information, available through www.cambridge.org/9780521852524.

作者介绍:

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标签

化学

数理

分子模拟

评论

我读到的第一本用 Python 解决领域专业问题的书，非常好。太喜欢了这本书里面描写的内容倒不是特别和我的研究相关，这本书主要是关于分子模拟的。但是这本书里面的代码，特别是Python代码的结构非常值得研究。也是配套的pDynamo库的说明书。上个链接 http://www.rm1.sparkle.pro.br/rm1-software/pdynamo，非常推荐。

只读了蒙卡一节，讲得太简单了吧……而且统计物理常用的梅氏蒙卡没讲到啊

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书评

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