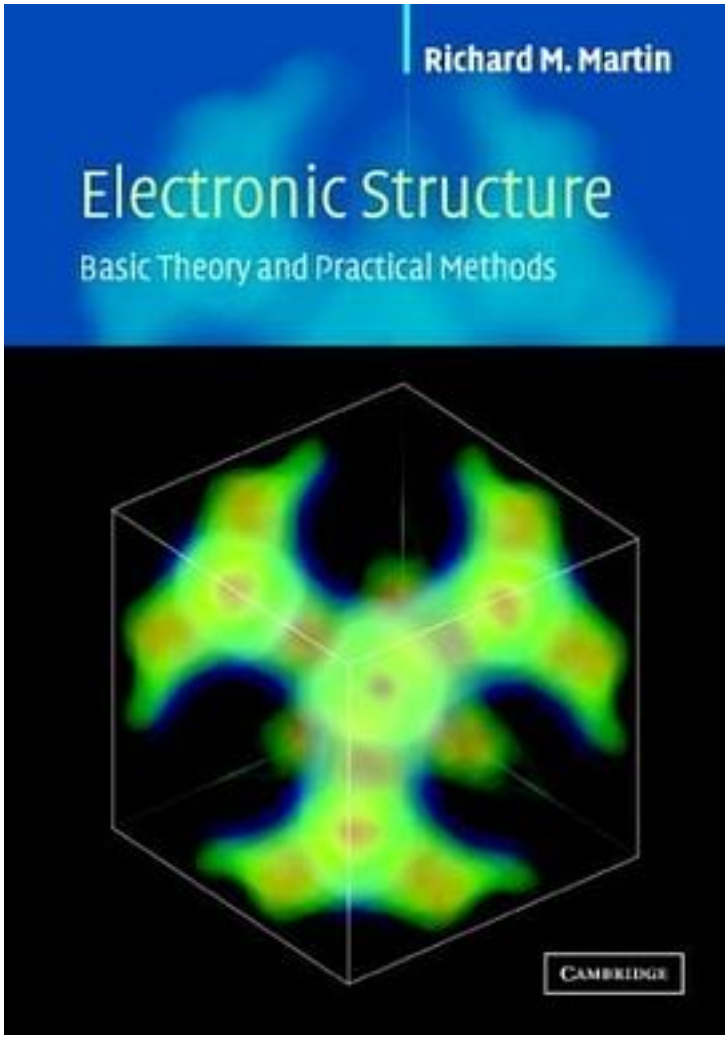
Electronic Structure



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The study of the electronic structure of materials is at a momentous stage, with the

emergence of new computational methods and theoretical approaches. This volume provides an introduction to the field and describes its conceptual framework, the capabilities of present methods, limitations, and challenges for the future. Many properties of materials can now be determined directly from the fundamental equations of quantum mechanics, bringing new insights into critical problems in physics, chemistry, and materials science.

作者介绍:

Richard Martin is Professor of Physics at the University of Illinois at Urbana-Champaign. He is a recipient of the Alexander von Humboldt Senior Scientist Award, and is a fellow of the American Physical Society (APS) and the American Association for the Advancement of Science. He has served on several editorial boards of the APS, including Physical Review and Physical Review Letters, and Reviews of Modern Physics where he was associate editor for condensed matter theory.

Appendix K. Useful relations and formulas
Appendix L. Numerical methods
Appendix M. Iterative methods in electronic structure
Appendix N. Code for empirical pseudopotential and tight-binding: schematic description
Appendix O. Units and conversion factors.
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标签

物理

电子结构

计算

第一性原理

量子

dft

DFT

理论化学

评论

DFT必读～～

怎么说呢？这本书说自己的特色是数学推导省略了，抓住了物理的精华。其实仔细读的

时候非常痛苦，为啥呢？数学上不清楚，你姑且认为它是成立的吧，但是很快作者又使用了这个公式并且说明哪里哪里是正确的，哪里我近似了，对于DFT这么多近似的书，其实非常费力。同时DFT本身也是十分博杂导致这本书基本上就是可以做手册不可做教科书。

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书评

从题目上来看， Richard
Martin老先生力求给出电子结构计算领域的全貌，这点在参考文献的体例，和推荐读物，以及附录里体现的尤其明显。
但是很明显，固体物理或者整个凝聚态领域是一个大杂烩，
旁支繁杂，却无甚中心思想。定量地理解材料物性是电子结构计算的主要...

是我们系做第一性原理计算的研究组几乎人手一本的书。我这个业余的也买了一本平装，还不错。准备仔细看的，但是发现以我的背景（材料专业，本科和研究生上过两次固体物理，后者用Ashcroft&Mermin做教材）要消化这本书上的预备知识比较困难。我的办法是只好乖乖退回A&M夯实基础...

对于做第一性原来的人来说，这本书作为入门还是不错地。
内容很广泛，但不够深入，基本上对目前的电子结构理论作了一个大的总结。
也很适合闲来无事随手翻阅。

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