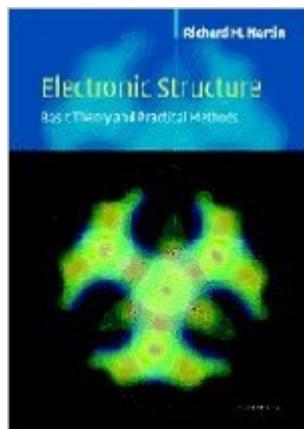


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Electronic Structure: Basic Theory And Practical Methods (Vol 1)



Synopsis

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.

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Customer Reviews

This book was recommended to me to help me in my research, and has turned out to be one of the best recommendations I have ever received. This is a great book; by far the best I have come across on the topic of computing the properties of condensed phase materials by quantum mechanical simulations. Here are the reasons why.1. The chapters are well laid out and one chapter flows neatly to the next.2. The math is kept to a minimum; the author makes a point of communicating important principles and ideas in concise sentences without resorting to derivations. This is ideal for engineers like me; who by training do not know that much math as compared to physicists who specialize in the solid state.3. Important ideas are clarified up front. Many texts will lead the reader through long and windy paths of proofs and logic before arriving at the conclusion; thereby losing their reader in the process. Not here; important points are stated clearly at the beginning and at the end of each section.4. Compare, contrast, and context. There are many ideas, models, approximations, and theorems that have been developed in the past century related to

electronic structure. Many of these are closely related to each other in their inspiration, derivation, practice, and/or applications. This book makes the connections between the different concepts. For a non-expert reading through the electronic structure literature, terms like APW, OPW, PAW, LAPW, LMTO, etc... can be quite confusing if not placed within an overriding context. This book provides that context.5. Good use of appendices. Electronic structure is a lot like politics; most practitioners in either field did not receive formal educations in the subject, but instead got into it under the apprenticeship of other people.

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