In the broad materials modeling community, density functional theory (DFT) is the byname for an assortment of techniques for quantitatively predicting the properties of atom collections—from isolated atoms and molecules to bulk solids and liquids—in which the electrons are treated quantum mechanically. At their heart, all such techniques are rooted in major theoretical developments of the mid-1960s by Pierre Hohenberg, Walter Kohn, and Lu Jeu Sham,1,2 who, broadly speaking, transformed the quantum problem of a system of interacting electrons to the comparatively simple problem of a system of noninteracting electrons subject to an effective potential that (in principle) faithfully captures the original system’s “many-body” attributes.

Some 45 years later, these arguably esoteric developments in theoretical physics have evolved into the aforementioned assortment of powerful, practical techniques for modeling materials, implemented in a wealth of highly sophisticated and efficient computer codes, both commercial and open-source. The unprecedented combination of high accuracy and computational efficiency has turned DFT into the method of choice for literally thousands of researchers around the world in a range of disciplines, including physics, chemistry, materials science, and several branches of engineering.

Given the numerous and diverse DFT practitioners, the value of having textbooks that synthesize and distill this broad subject is manifest. Indeed, there are several excellent monographs on DFT, from the venerable treatise by Robert Parr and Weitao Yang,2 to more recent volumes by Richard Martin3 and Jorge Kohanoff.4 However, most of these books emphasize theory, even in their discussions of techniques and applications. This isn’t a criticism; a solid understanding of the theoretical underpinnings of DFT and its applications is essential for a serious practitioner. However, none of these books provides an entry point to the subject—that is, a practical introduction for newcomers or outsiders needing a reading readiness of what DFT can and cannot do. Filling this lacuna is Density Functional Theory: A Practical Introduction by David S. Sholl and Janice A. Steckel.

Goals and General Approach

In their preface, Sholl and Steckel state that they “have aimed to find a balance between brevity and detail” to keep the book both accessible and useful to newcomers. The unprecedented combination of high accuracy and computational efficiency has turned DFT into the method of choice for literally thousands of researchers around the world in a range of disciplines, including physics, chemistry, materials science, and several branches of engineering.

The standard taxonomy for classifying different DFT approaches is to specify the type of basis functions used to express the Hamiltonian and wave functions. In this regard, the book focuses exclusively on the plane-wave method, one of the most widely used DFT approaches, particularly for spatially extended materials. For many of the applications presented, the type of basis functions used is entirely or largely irrelevant; thus, limiting the book’s scope to plane waves is not so severe a restriction. That said, the book is somewhat biased toward a subset of the full DFT community—albeit quite a large one.
The book is organized into 10 chapters, seven of which center on a specific type of DFT application. The remaining three—Chapters 1, 3, and 10 (the final chapter)—each explore different perspectives of the DFT method itself. Chapter 1 provides an overview of DFT and the book, including

- examples from the research literature showing DFT’s contribution to diverse fields,
- a brief introduction to the Hohenberg-Kohn-Sham theory that underlies all DFT methods,
- an overview of the broader quantum chemistry field and DFT’s place within it,

It’s at its best in Chapters 1, 3, and 10, where it addresses issues cutting across all DFT applications, from the overarching to the nitty-gritty.

- a discussion of what DFT can’t do, and
- advice to readers on how to approach the book.

Chapter 3 delves into the nuts and bolts of DFT calculations in general and the plane-wave method in particular. In addition to introducing fundamental concepts such as reciprocal space and pseudopotentials, this chapter addresses important computational issues, including $k$-point sampling, plane-wave cutoffs, optimization algorithms, self-consistency, and structural optimization. Throughout, the authors emphasize the importance of convergence testing for numerical approximations and give several illustrative examples.

The book ends with a chapter on DFT calculation accuracy. This is appropriate; after spending nine chapters largely discussing how much DFT can do, this final chapter reminds readers of the important obligation all researchers have of knowing their methods’ limitations and accuracy. The authors discuss both numerical accuracy and physical accuracy. The chapter also

- highlights the major categories of exchange-correlation functionals in use today,
- discusses the typical physical accuracy to be expected for various physical properties, and

Strengths and Weaknesses

Overall, this book has many positive attributes and will be of considerable use to its target audience; however, it also has its flaws. It’s at its best in Chapters 1, 3, and 10, where it addresses issues cutting across all DFT applications, from the overarching to the nitty-gritty. The seven applications chapters differ in their relative strengths and weaknesses.

Chapter 2, on predicting crystal structure, is quite good, offering novices a well-balanced, non-overwhelming starting point for hands-on DFT calculations. The two best applications chapters are Chapter 4, on surfaces, and Chapter 6, on chemical rates. They are well modulated and provide cogent explanations and fairly comprehensive coverage of their respective topics.

Three other applications chapters discuss calculations of more specialized properties. Chapter 4 gives a fairly comprehensive overview of DFT calculations for solid surfaces, carefully taking the readers through the computation of surface energies, structural relaxations and reconstructions, and molecular adsorption. Chapter 6 shows how DFT can be used in concert with transition state theory to predict rates of chemical processes. In addition, it discusses the nudged elastic band method for finding transition states and the kinetic Monte Carlo method for connecting individual rates to overall dynamics.

Finally, Chapter 7 presents the ab initio thermodynamics method for predicting equilibrium compositional phase diagrams. The last application chapter, Chapter 9, discusses the ab initio molecular dynamics (MD) method. Broadly speaking, ab initio MD is the same as classical MD, but with atomic forces calculated at each time step via DFT instead of a classical force field.
At the other extreme, Chapter 5, on vibrational properties, and Chapter 8, on electronic and magnetic structure, are by far the weakest. The techniques presented in Chapter 5 are at best inefficient, but also contain conceptual errors. Moreover, several important considerations in calculating vibrational modes are simply omitted. In Chapter 8, the emphasis on density of states to the near exclusion of other electronic-structure analysis techniques limits the usefulness of this chapter’s treatment of electronic structure. Also, given the dearth of practical information provided on spin-polarized calculations, it would have been better to simply omit any discussion of magnetic properties.

Perhaps the best feature of *Density Functional Theory: A Practical Introduction* is one that I’ve yet to mention: the exercises provided at the end of every chapter (except the first and last). As I often tell my students, “You can’t learn how to play basketball simply by reading about the rules and strategies or watching other people play; you have to go out and practice the skills.” The same holds for DFT. Sholl and Steckel emphasize this point and have chosen good, tractable end-of-chapter practice exercises. Some exercises give clear, well-defined problems, while others are more open-ended, leaving it to the reader to find a good solution. Given the wide availability of computing resources and good, well-documented (and sometimes free) plane-wave DFT codes, readers should find it easy and convenient to roll up their sleeves and dig in.

In pondering how to conclude this review, I thought about a patient seeking to assess his doctor’s advice by asking, “What would you do if this were happening to you?” The patient’s assumption is that doctors will settle for nothing but the best for themselves. Anticipating an analogous question in the minds of readers of this review, let me say that, after reading the review copy of *Density Functional Theory: A Practical Introduction* that CiSE provided, I went out and bought a second copy for my own research group. This book is not perfect, but it is good. And it is the only book at the right level for a DFT newcomer.

**References**


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