



Density Functional Theory: A Practical Introduction

David Sholl, Janice A Steckel

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Demonstrates how anyone in math, science, and engineering can master DFT calculations

Density functional theory (DFT) is one of the most frequently used computational tools for studying and predicting the properties of isolated molecules, bulk solids, and material interfaces, including surfaces. Although the theoretical underpinnings of DFT are quite complicated, this book demonstrates that the basic concepts underlying the calculations are simple enough to be understood by anyone with a background in chemistry, physics, engineering, or mathematics. The authors show how the widespread availability of powerful DFT codes makes it possible for students and researchers to apply this important computational technique to a broad range of fundamental and applied problems.

Density Functional Theory: A Practical Introduction offers a concise, easy-to-follow introduction to the key concepts and practical applications of DFT, focusing on plane-wave DFT. The authors have many years of experience introducing DFT to students from a variety of backgrounds. The book therefore offers several features that have proven to be helpful in enabling students to master the subject, including:

- Problem sets in each chapter that give readers the opportunity to test their knowledge by performing their own calculations
- Worked examples that demonstrate how DFT calculations are used to solve real-world problems
- Further readings listed in each chapter enabling readers to investigate specific topics in greater depth

This text is written at a level suitable for individuals from a variety of scientific, mathematical, and engineering backgrounds. No previous experience working with DFT calculations is needed.

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