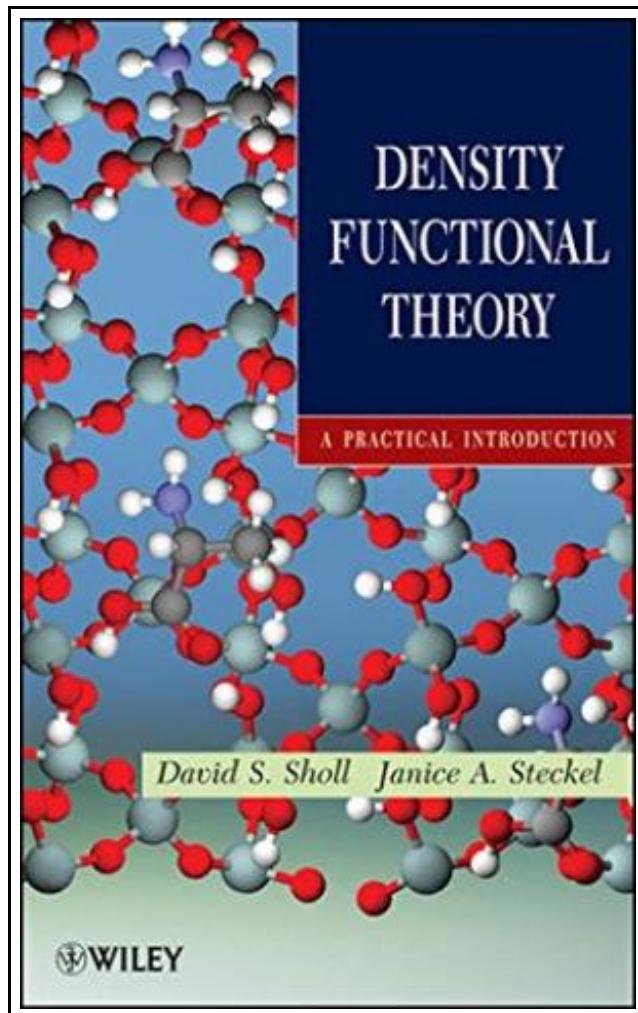


## Density Functional Theory: A Practical Introduction



Filesize: 1.63 MB

### Reviews

*Extremely helpful for all class of folks. I really could comprehend almost everything using this written e publication. You will not feel monotony at at any time of the time (that's what catalogs are for about in the event you check with me).*  
*(Prof. Melyna Dooley V)*

## DENSITY FUNCTIONAL THEORY: A PRACTICAL INTRODUCTION

[DOWNLOAD PDF](#)

Wiley-Interscience, 2009. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service! Summary: Chapter 1: What is Density Functional Theory?1.1 How To Approach This Book.1.2 Examples of DFT in Action.1.3 The Schrödinger Equation.1.4 Density Functional Theory - From Wavefunctions to Electron Density.1.5 The Exchange-Correlation Functional.1.6 The Quantum Chemistry Tourist.1.7 What Can't DFT Do?1.8 Density Functional Theory in Other Fields.1.9 How To Approach This Book (Revisited).Chapter 2: DFT Calculations for Simple Solids.2.1 Periodic Structures, Supercells, and Lattice Parameters.2.2 Face Centered Cubic Materials.2.3 Hexagonal Close Packed Materials.2.4 Crystal Structure Prediction.2.5 Phase Transformations. Chapter 3: Nuts and Bolts of DFT Calculations.3.1 Reciprocal Space and k-points.3.2 Energy Cutoffs.3.3 Numerical Optimization.3.4 DFT Total Energies - An Iterative Optimization Problem.3.5 Geometry Optimization. Chapter 4: DFT Calculations for Surfaces of Solids.4.1 Why Surfaces Are Important.4.2 Periodic Boundary Conditions and Slab Models.4.3 Choosing k-points for Surface Calculations.4.4 Classification of Surfaces by Miller Indices.4.5 Surface Relaxation.4.6 Calculation of Surface Energies.4.7 Symmetric and Asymmetric Slab Models.4.8 Surface Reconstruction.4.9 Adsorbates on Surfaces.4.10 Effects of Surface Coverage. Chapter 5: DFT Calculations of Vibrational Frequencies.5.1 Isolated Molecules.5.2 Vibrations of Collections of Atoms.5.3 Molecules on Surfaces.5.4 Zero Point Energies.5.5 Phonons and Delocalized Modes. Chapter 6: Calculating Rates of Chemical Processes Using Transition State Theory.6.1 A One-Dimensional Example.6.2 Multi-dimensional Transition State Theory.6.3 Finding Transition States.6.4 Finding the Right Transition State.6.5 Connecting Individual Rates to Overall Dynamics.6.6 Quantum Effects and Other Complications. Chapter 7: Equilibrium Phase Diagrams From Ab Initio Thermodynamics.7.1 Stability of Bulk Metal Oxides.7.2 Stability of Metal and Metal Oxide Surfaces.7.3 Multiple Chemical Potentials and Coupled Chemical Potentials. Chapter 8: Electronic Structure and Magnetic Properties.8.1 Electronic Density of States.8.2 Local DOS and Atomic Charges.8.3 Magnetism. Chapter 9: Ab Initio Molecular Dynamics.9.1 Classical Molecular Dynamics.9.2 Ab Initio Molecular Dynamics.9.3 Applications of Ab Initio Molecular Dynamics. Chapter 10: Accuracy and Methods Beyond "Standard" Calculations.10.1 How Accurate Are DFT Calculations?10.2 Choosing A...

[Read Density Functional Theory: A Practical Introduction Online](#)[Download PDF Density Functional Theory: A Practical Introduction](#)

## Other PDFs

---



### **Grandpa Spanielson's Chicken Pox Stories: Story #1: The Octopus (I Can Read Book 2)**

HarperCollins, 2005. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service! Summary: Foreword by Raph Koster. Introduction. I. EXECUTIVE

CONSIDERATIONS. 1. The Market. Do We Enter the Market? Basic Considerations. How...

[Download eBook »](#)

---



### **The Web Collection Revealed, Premium Edition: Adobe Dreamweaver CS6, Flash CS6, and Photoshop CS6 (Stay Current with Adobe Creative Cloud)**

Cengage Learning, 2012. Book Condition: New. Brand New, Unread Copy in Perfect Condition.

A+ Customer Service! Summary: You can now maximize and integrate the design and development power of Adobe Creative Suite 6 with WEB...

[Download eBook »](#)

---



### **Star Flights Bedtime Spaceship: Journey Through Space While Drifting Off to Sleep**

CreateSpace Independent Publishing Platform, 2013. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service! Summary: "Star Flights Bedtime Spaceship" is a charming and fun story with the purpose to help children...

[Download eBook »](#)

---



### **Maisy's Christmas Tree**

Candlewick, 2014. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service! Summary: The final scene of the gang caroling around the tree, complete with paper crowns from British Christmas crackers, is...

[Download eBook »](#)

---



### **JA] early childhood parenting :1-4 Genuine Special(Chinese Edition)**

paperback. Book Condition: New. Ship out in 2 business day, And Fast shipping, Free Tracking number will be provided after the shipment. Paperback. Pub Date :2006-01-01 Pages: 179 Publisher: the China Pictorial Our book is all...

[Download eBook »](#)



### **Untold Stories - The Diaries: Diaries Pt. 2**

BBC Audiobooks Ltd, 2005. Audio Cassette. Book Condition: New. . A new, unread, unused book in perfect condition with no missing or damaged pages. Shipped from UK. Orders will be dispatched within 48 hours of

[Save ePub »](#)



### **Meritocracy: A Love Story**

Haus Publishing, 2011. Paperback. Book Condition: New. A new, unread, unused book in perfect condition with no missing or damaged pages. Shipped from UK. Orders will be dispatched within 48 hours of receiving your order.

[Save ePub »](#)



### **The Story of Christopher Columbus (Paperback)**

DK Publishing, United States, 2001. Paperback. Book Condition: New. American.. 222 x 146 mm. Language: English . Brand New Book. Find out how explorer Christopher Columbus survived great danger on the high seas on his

[Save ePub »](#)



### **SY] young children idiom story [brand new genuine(Chinese Edition)**

paperback. Book Condition: New. Ship out in 2 business day, And Fast shipping, Free Tracking number will be provided after the shipment.Paperback. Pub Date :2003-05-01 Pages: 151 Publisher: Anhui Literature and Art Shop Books All

[Save ePub »](#)



### **Art appreciation (travel services and hotel management professional services and management expertise secondary vocational education teaching materials supporting national planning book)(Chinese Edition)**

paperback. Book Condition: New. Ship out in 2 business day, And Fast shipping, Free Tracking number will be provided after the shipment.Pages Number: 146 Publisher: Higher Education Pub. Date :2009-07-01 version 2. This book is

[Save ePub »](#)