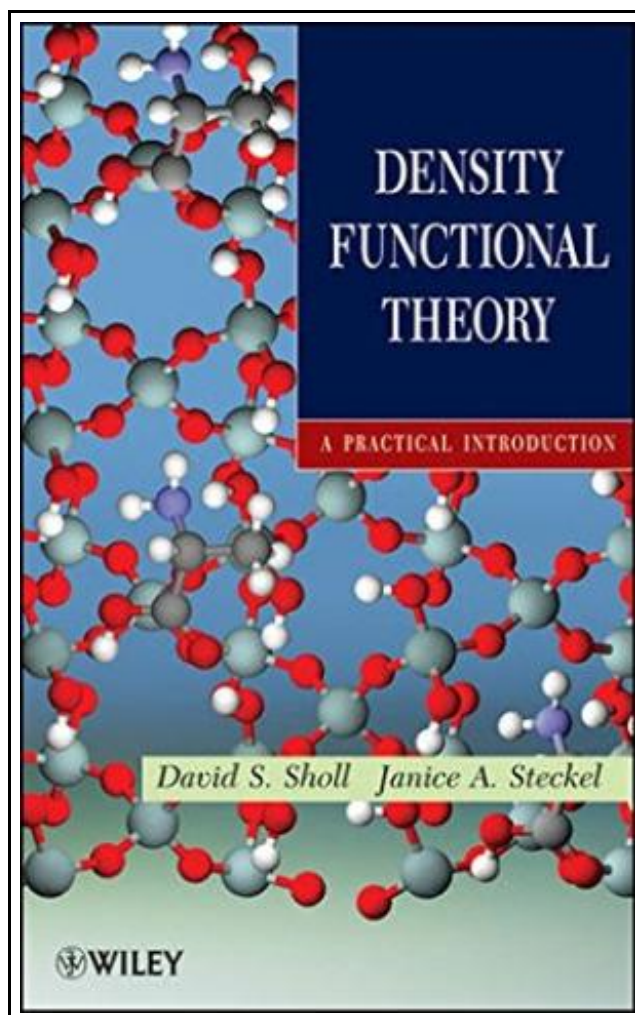


Density Functional Theory: A Practical Introduction



Filesize: 4.48 MB

Reviews

This created ebook is wonderful. I am quite late in start reading this one, but better then never. You may like the way the author compose this pdf.

(Frederic Lang)

DENSITY FUNCTIONAL THEORY: A PRACTICAL INTRODUCTION

DOWNLOAD



To read **Density Functional Theory: A Practical Introduction** eBook, please refer to the button under and download the ebook or have access to other information which might be related to DENSITY FUNCTIONAL THEORY: A PRACTICAL INTRODUCTION ebook.

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](#)

See Also



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

Follow the link beneath to read "Grandpa Spanielson's Chicken Pox Stories: Story #1: The Octopus (I Can Read Book 2)" file.

[Save Document »](#)



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

Follow the link beneath to read "The Web Collection Revealed, Premium Edition: Adobe Dreamweaver CS6, Flash CS6, and Photoshop CS6 (Stay Current with Adobe Creative Cloud)" file.

[Save Document »](#)



[PDF] Star Flights Bedtime Spaceship: Journey Through Space While Drifting Off to Sleep

Follow the link beneath to read "Star Flights Bedtime Spaceship: Journey Through Space While Drifting Off to Sleep" file.

[Save Document »](#)



[PDF] Maisy's Christmas Tree

Follow the link beneath to read "Maisy's Christmas Tree" file.

[Save Document »](#)



[PDF] JA] early childhood parenting :1-4 Genuine Special(Chinese Edition)

Follow the link beneath to read "JA] early childhood parenting :1-4 Genuine Special(Chinese Edition)" file.

[Save Document »](#)



[PDF] Edge] the collection stacks of children's literature: Chunhyang Qiuyun 1.2 --- Children's Literature 2004(Chinese Edition)

Follow the link beneath to read "Edge] the collection stacks of children's literature: Chunhyang Qiuyun 1.2 --- Children's Literature 2004(Chinese Edition)" file.

[Save Document »](#)