

## Materials Modelling Using Density Functional Theory: Properties and Predictions



Filesize: 8.85 MB

### ***Reviews***

*A must buy book if you need to adding benefit. It really is simplified but unexpected situations in the 50 percent of your book. Its been developed in an exceptionally straightforward way and it is merely soon after i finished reading through this pdf where in fact transformed me, modify the way i think.*  
**(Dalton Mertz)**

## MATERIALS MODELLING USING DENSITY FUNCTIONAL THEORY: PROPERTIES AND PREDICTIONS



Oxford University Press. Hardback. Book Condition: new. BRAND NEW, Materials Modelling Using Density Functional Theory: Properties and Predictions, Feliciano Giustino, This book is an introduction to the quantum theory of materials and first-principles computational materials modelling. It explains how to use density functional theory as a practical tool for calculating the properties of materials without using any empirical parameters. The structural, mechanical, optical, electrical, and magnetic properties of materials are described within a single unified conceptual framework, rooted in the Schrodinger equation of quantum mechanics, and powered by density functional theory. This book is intended for senior undergraduate and first-year graduate students in materials science, physics, chemistry, and engineering who are approaching for the first time the study of materials at the atomic scale. The inspiring principle of the book is borrowed from one of the slogans of the Perl programming language, 'Easy things should be easy and hard things should be possible'. Following this philosophy, emphasis is placed on the unifying concepts, and on the frequent use of simple heuristic arguments to build on one's own intuition. The presentation style is somewhat cross disciplinary; an attempt is made to seamlessly combine materials science, quantum mechanics, electrodynamics, and numerical analysis, without using a compartmentalized approach. Each chapter is accompanied by an extensive set of references to the original scientific literature and by exercises where all key steps and final results are indicated in order to facilitate learning. This book can be used either as a complement to the quantum theory of materials, or as a primer in modern techniques of computational materials modelling using density functional theory.



**[Read Materials Modelling Using Density Functional Theory: Properties and Predictions Online](#)**



**[Download PDF Materials Modelling Using Density Functional Theory: Properties and Predictions](#)**

## Relevant Kindle Books



### **Six Steps to Inclusive Preschool Curriculum: A UDL-Based Framework for Children's School Success**

Brookes Publishing Co. Paperback. Book Condition: new. BRAND NEW, Six Steps to Inclusive Preschool Curriculum: A UDL-Based Framework for Children's School Success, Eva M. Horn, Susan B. Palmer, Gretchen D. Butera, Joan A. Lieber, How...

[Download eBook »](#)



### **Perfect Numerical and Logical Test Results**

Cornerstone. Paperback. Book Condition: new. BRAND NEW, Perfect Numerical and Logical Test Results, Joanna Moutafi, Marianna Moutafi, Have you been asked to sit a numerical or logical reasoning test? -Do you need some help preparing...

[Download eBook »](#)



### **A Dog of Flanders: Unabridged; In Easy-to-Read Type (Dover Children's Thrift Classics)**

Dover Publications, 2011. Paperback. Book Condition: New. No Jacket. New paperback book copy of A Dog of Flanders by Ouida (Marie Louise de la Ramee). Unabridged in easy to read type. Dover Children's Thrift Classic....

[Download eBook »](#)



### **It's Just a Date: How to Get 'em, How to Read 'em, and How to Rock 'em**

HarperCollins Publishers. Paperback. Book Condition: new. BRAND NEW, It's Just a Date: How to Get 'em, How to Read 'em, and How to Rock 'em, Greg Behrendt, Amiira Ruotola-Behrendt, A fabulous new guide to dating...

[Download eBook »](#)



### **You Shouldn't Have to Say Goodbye: It's Hard Losing the Person You Love the Most**

Sourcebooks, Inc. Paperback / softback. Book Condition: new. BRAND NEW, You Shouldn't Have to Say Goodbye: It's Hard Losing the Person You Love the Most, Patricia Hermes, Thirteen-year-old Sarah Morrow doesn't think much of the...

[Download eBook »](#)