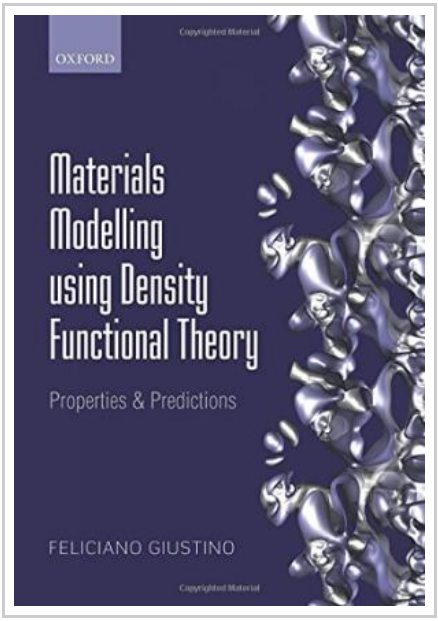

Materials Modelling Using Density Functional Theory: Properties and Predictions

By Associate Professor of Materials Modelling Feliciano Giustino

Oxford University Press, United Kingdom, 2014. Paperback. Book Condition: New. 244 x 170 mm. Language: English . Brand New Book. 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...

Reviews

Very useful to all of category of people. I actually have read through and that i am sure that i will likely to go through once more again in the foreseeable future. I realized this book from my i and dad advised this publication to find out.
-- ***Alta Kirlin***

This is the very best publication i have got read until now. It is definitely simplified but shocks within the fifty percent of the pdf. You may like how the article writer create this pdf.
-- ***Rosario Durgan***