1. Record Nr. UNINA9910828121003321

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Titolo	Materials modelling using density functional theory : properties and predictions / / Feliciano Giustino
Pubbl/distr/stampa	Oxford, [England] ; ; New York, New York : , : Oxford University Press, , 2014 ©2014
ISBN	0-19-163943-5 0-19-163942-7
Descrizione fisica	1 online resource (303 p.)
Disciplina	620.11015118
Soggetti	Materials - Mathematical models
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	""2.5 Independent electrons approximation"""2.6 Exclusion principle""; ""2.7 Mean-field approximation""; ""2.8 Hartree--Fock equations""; ""2.9 Kohn--Sham equations""; ""3 Density functional theory""; ""3.1 Total energy of the electronic ground state""; ""3.2 Kohn--Sham equations""; ""3.3 The local density approximation""; ""3.4 Self-consistent calculations""; ""3.5 Remit of density functional theory and limitations""; ""4 Equilibrium structures of materials: fundamentals""; ""4.1 The adiabatic approximation""; ""4.2 Atomic forces"" ""4.3 Calculating atomic forces using classical electrostatics"""4.4 How to find the equilibrium configuration using calculated forces""; ""5 Equilibrium structures of materials: calculations vs. experiment""; ""5.1 Structure of molecules""; ""5.2 Structure of crystals""; ""5.3 Comparison of DFT structures with X-ray crystallography""; ""5.4 Structure of surfaces""; ""5.5 Comparison of DFT surface reconstructions with STM""; ""6 Elastic properties of materials""; ""6.1 Elastic deformations""; ""6.2 Intuitive notions of stress and strain using computer experiments"" ""6.3 General formalism for the elastic properties of solids"""6.4 Calculating elastic constants using the DFT total energy""; ""6.5 Examples of calculations of elastic constants""; ""6.6 The stress theorem""; ""6.7 DFT predictions for materials under extreme conditions""; ""7 Vibrations of molecules and solids""; ""7.1 Heuristic

notion of atomic vibrations""; ""7.2 Formal theory of vibrations for classical nuclei""; ""7.3 Calculations of vibrational eigenmodes and eigenfrequencies""; ""7.4 Vibrations of crystalline solids""; ""8 Phonons, vibrational spectroscopy and thermodynamics""
""8.1 Basics of Raman and neutron scattering spectroscopy"""""8.2 Going beyond the classical approximation for nuclei""; ""8.3 Vibrons and phonons""; ""8.4 Phonon density of states""; ""8.5 Phonon DOS and pressure--temperature phase diagrams""; ""9 Band structures and photoelectron spectroscopy""; ""9.1 Kohn--Sham energies and wavefunctions""; ""9.2 Calculation of band structures using DFT""; ""9.3 Basics of angle-resolved photoelectron spectroscopy""; ""9.4 Metals, insulators and semiconductors""; ""9.5 The band gap problem""; ""10 Dielectric function and optical spectra""
""10.1 The dielectric function of a model solid""

Sommario/riassunto

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