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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
