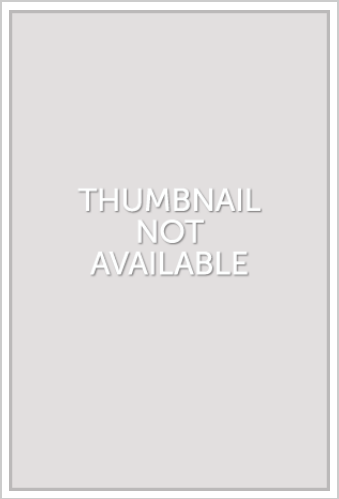

Computational Materials Science: An Introduction

By June Gunn Lee

CRC Press. Soft cover. Book Condition: New. International edition, Computational Materials Science: An Introduction covers the essentials of computational science and explains how computational tools and techniques work to help solve materials science problems. The book focuses on two levels of a materials system: the electronic structure level of nuclei and electrons and the atomistic/molecular level. It presents computational treatments of these system levels using molecular dynamics (MD) and first-principles methods, since they are most relevant in materials science and engineering. After a general overview of computational science, the text introduces MD methods based on classical mechanics and covers their implementation with run examples of XMD and LAMMPS. The author discusses first-principles methods based on quantum mechanics at an introductory level, using illustrations and analogies to assist students in understanding this difficult subject. The book then describes the density functional theory (DFT)-the first-principles method that can handle materials practically. It also reveals how each orbital of electron leads to particular properties of solids, such as total energy, band structure, and barrier energy. The final chapter implements the DFT into actual calculations with various run examples via the VASP program. Computational methods are contributing more than ever to the development of...

Reviews

This ebook is amazing. It can be rally interesting throgh looking at time. You may like how the author compose this ebook.
-- ***Nikko Bashirian***

The ideal book i actually read. It is one of the most awesome pdf i have study. I am just happy to tell you that this is basically the best book i have study in my own life and might be he finest ebook for actually.
-- ***Nettie Leuschke***