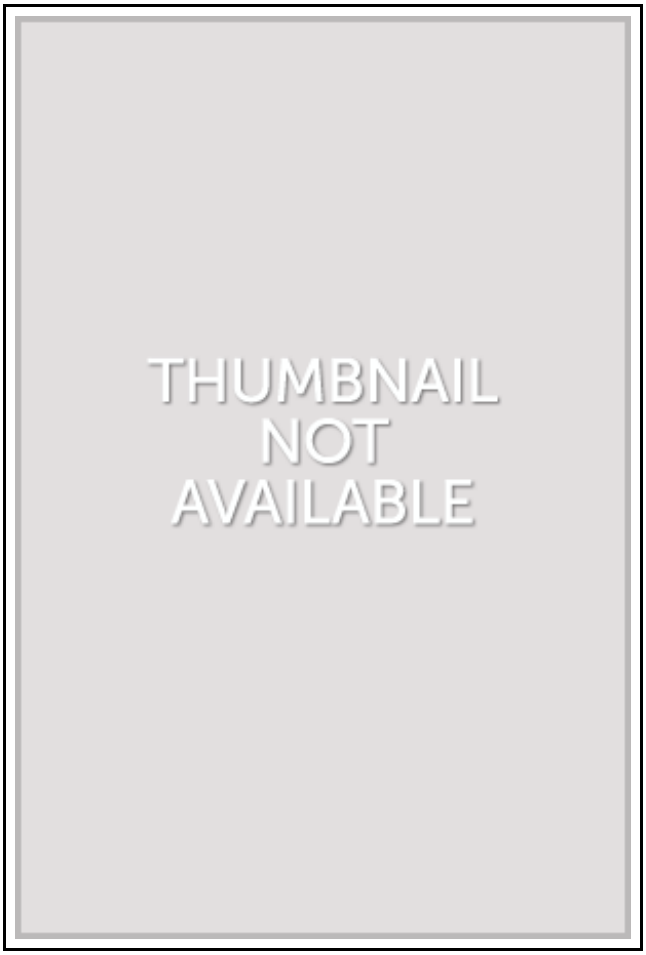
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Reviews

An extremely wonderful book with perfect and lucid explanations. This really is for those who statte that there had not been a worth reading. Your way of life span will be convert when you comprehensive reading this book.

(Effie Douglas)

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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 advanced materials and new applications. For students and newcomers to computational science, this text shows how computational science can be used as a tool for solving materials problems. 0.

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