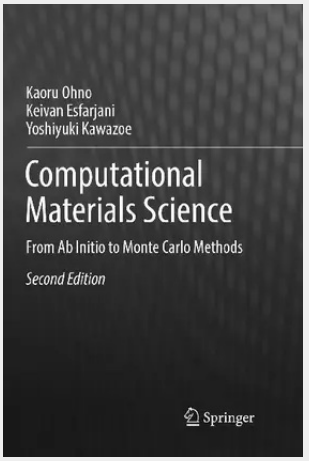
Ohno / Esfarjani / Kawazoe

Computational Materials Science

From Ab Initio to Monte Carlo Methods



This textbook introduces modern techniques based on computer simulation to study materials science. It starts from first principles calculations enabling to calculate the physical and chemical properties by solving a many-body Schroedinger equation with Coulomb forces. For the exchange-correlation term, the local density approximation is usually applied. After the introduction of the first principles treatment, tight-binding and classical potential methods are briefly introduced to indicate how one can increase the number of atoms in the system. In the second half of the book, Monte Carlo simulation is discussed in detail. Problems and solutions are provided to facilitate understanding. Readers will gain sufficient knowledge to begin theoretical studies in modern materials research.
This second edition includes a lot of recent theoretical techniques in materials research. With the computers power now available, it is possible to use these numerical techniques to study various physical and chemical properties of complex materials from first principles. The new edition also covers empirical methods, such as tight-binding and molecular dynamics.

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90,94 €
84,99 € (zzgl. MwSt.)

Lieferfrist: bis zu 10 Tage

Artikelnummer: 9783662585870
Medium: Buch
ISBN: 978-3-662-58587-0
Verlag: Springer
Erscheinungstermin: 01.02.2019
Sprache(n): Englisch
Auflage: 2. Auflage 2018
Produktform: Kartoniert
Gewicht: 663 g
Seiten: 427
Format (B x H): 155 x 235 mm

fachmedien.de
WISSEN. EINFACH. FINDEN.

23.11.2026 | 07:24 Uhr

Kundenservice Verlag Dr. Otto Schmidt KG
Neumannstraße 10, 40235 Düsseldorf | kundenservice@otto-schmidt.de | 0221-93738-997 (Inland)