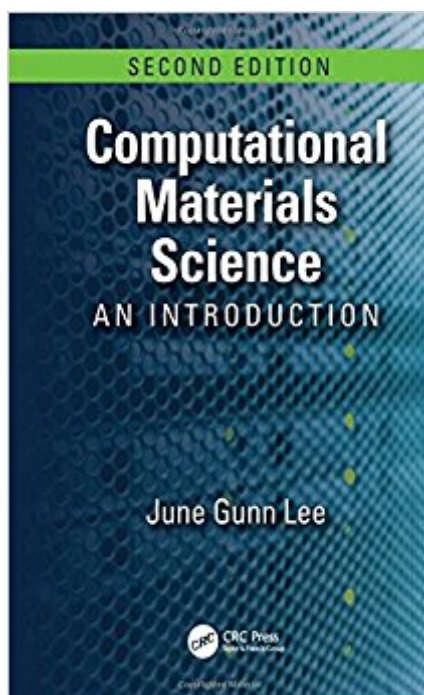


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Computational Materials Science: An Introduction, Second Edition



Synopsis

This book covers the essentials of Computational Science and gives tools and techniques to solve materials science problems using molecular dynamics (MD) and first-principles methods. The new edition expands upon the density functional theory (DFT) and how the original DFT has advanced to a more accurate level by GGA+U and hybrid-functional methods. It offers 14 new worked examples in the LAMMPS, Quantum Espresso, VASP and MedeA-VASP programs, including computation of stress-strain behavior of Si-CNT composite, mean-squared displacement (MSD) of ZrO₂-Y₂O₃, band structure and phonon spectra of silicon, and Mo-S battery system. It discusses methods once considered too expensive but that are now cost-effective. New examples also include various post-processed results using VESTA, VMD, VTST, and MedeA.

Book Information

Hardcover: 375 pages

Publisher: CRC Press; 2 edition (December 1, 2016)

Language: English

ISBN-10: 1498749739

ISBN-13: 978-1498749732

Product Dimensions: 6.2 x 0.7 x 9.2 inches

Shipping Weight: 13.6 ounces (View shipping rates and policies)

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