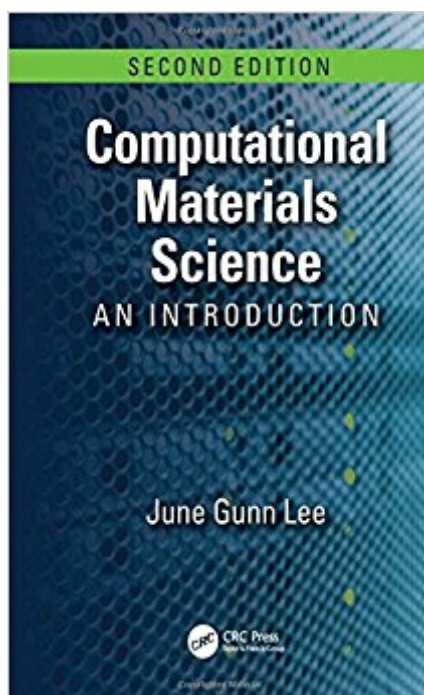


The book was found

# 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 ZrO<sub>2</sub>-Y<sub>2</sub>O<sub>3</sub>, 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)

Average Customer Review: Be the first to review this item

Best Sellers Rank: #318,478 in Books (See Top 100 in Books) #18 in [Books > Engineering & Transportation > Engineering > Materials & Material Science > Extraction & Processing](#) #72 in [Books > Science & Math > Physics > Solid-State Physics](#) #195 in [Books > Science & Math > Physics > Electromagnetism](#)

## Customer Reviews

"The delightful and pragmatic style of this book is irresistible. It intrigues the reader to start using the leading methods in computational materials science, to simulate interesting systems, and to become excited about the remarkable capabilities of today's computational methods." — Erich Wimmer, Materials Design, Inc., Angel Fire, New Mexico, USA "Books such as this allow my students — the new generation — to catch up with our fast progressing knowledge and technology. Definitely, this book has help me to teach density functional theory to my students and mentees. I will continually use this book for my class and research." — Al Rey Villagracia, De La Salle University, Manila, Philippines "This text takes you on a working

tour of the most important computational methods available to materials scientist today. You get to know the underlying theory with enough detail to manage understanding, and it projects you to the next stages of employing particular codes to solve problems and predict properties. Better than a Hitchhikers guide through the materials computational galaxy because it's intentionally a guide not a random one." Rene Corrales, University of Arizona, USA "The second edition of Computational Materials Science: An Introduction improves upon the first version of the textbook. It includes examples designed to be used with Open Source Computational Codes. This opens the book to many more students worldwide. I commend the author for this outstanding addition. The second edition continues the well written explanations present in the first. It covers the mechanics of calculations in enough detail so that the techniques are understood by the reader. The examples highlight important problems in condensed matter physics. They also go into detail where the calculations have problems. I find that this helps students to understand the limitations of the techniques. The author has really written an excellent textbook for computational materials science." Jeff Terry, Illinois Institute of Technology, USA "Simulation remains a discipline that is usually acquired in a research lab. This is particularly true in a chemistry department. How do the students then get knowledge of the simulation techniques? One response is a book like Computational Materials Science where theory is simply explained, and several exercises are shown. Moreover, materials are currently important in science, and simulation will play an increasingly important role. More and more publications are published where a simulation part needs to be inserted. However, most of the time, it has been carried out by non-expert persons! This book is certainly intended for them." Armand Soldera, University of Sherbrooke, Quebec, Canada "This is a book designed with a beginning practitioner in mind. It presents key insights in a format that is highly accessible. The author uses plenty of analogies and everyday examples and draw parallels with the subject matter. The presentation of the material is not overly burdened by equations and formulae. Even so, the author does a remarkable job of helping the reader make choices that are faced in practice." Sachin Shanbhag, Florida State University, USA "...a good text. It suites well for Engineering students." Oleg Rubel, McMaster University, Hamilton, Ontario, Canada

June Gunn Lee is an emeritus research fellow in the Computational Science Center at the Korea Institute of Science and Technology, where he has worked for 28 years. Currently, he is also lecturing at the University of Seoul. He has published about 70 papers on engineering ceramics and computational materials science. He received his M.S. and Ph.D. in Materials Science and

Engineering from the University of Utah, U.S.A.

[Download to continue reading...](#)

Computational Materials Science: An Introduction, Second Edition Freezing Colloids: Observations, Principles, Control, and Use: Applications in Materials Science, Life Science, Earth Science, Food Science, and Engineering (Engineering Materials and Processes) Introduction to Computational Materials Science Introduction to Computational Materials Science: Fundamentals to Applications Computational Materials Science: An Introduction Computational Fluid Mechanics and Heat Transfer, Third Edition (Series in Computational and Physical Processes in Mechanics and Thermal Sciences) Introduction to Computational Science: Modeling and Simulation for the Sciences, Second Edition Current Topics in Computational Molecular Biology (Computational Molecular Biology) Theoretical Neuroscience: Computational and Mathematical Modeling of Neural Systems (Computational Neuroscience Series) Simulating Enzyme Reactivity: Computational Methods in Enzyme Catalysis (Theoretical and Computational Chemistry Series) Computational Approaches to Protein Dynamics: From Quantum to Coarse-Grained Methods (Series in Computational Biophysics) The Power of Computational Thinking: Games, Magic and Puzzles to Help You Become a Computational Thinker Materials North American Edition w/Online Testing: Materials - North American Edition, Second Edition: engineering, science, processing and design Engineering Materials 3: Materials Failure Analysis: Case Studies and Design Implications (International Series on Materials Science and Technology) (v. 3) Introduction to Practical Peridynamics: Computational Solid Mechanics Without Stress and Strain (Frontier Research in Computation and Mechanics of Materials) Computational Materials Science: From Ab Initio to Monte Carlo Methods (Springer Series in Solid-State Sciences) A Computational Introduction to Digital Image Processing, Second Edition Understanding Molecular Simulation, Second Edition: From Algorithms to Applications (Computational Science Series, Vol 1) Engineering Materials 2, Fourth Edition: An Introduction to Microstructures and Processing (International Series on Materials Science and Technology) Engineering Materials 2: An Introduction to Microstructures, Processing and Design (International Series on Materials Science and Technology) (v. 2)

[Contact Us](#)

[DMCA](#)

[Privacy](#)

[FAQ & Help](#)