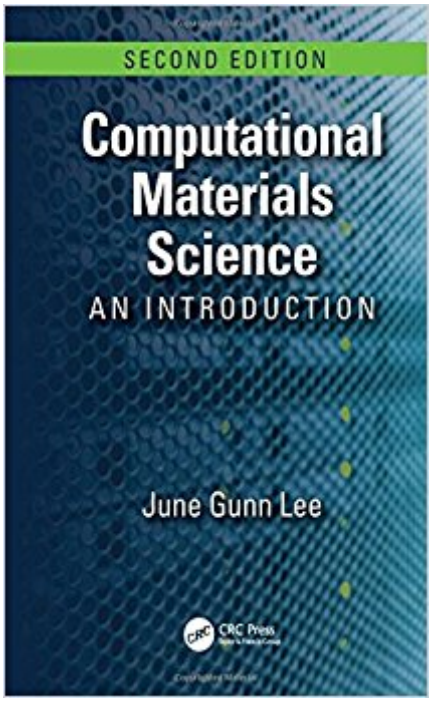
Computational Materials Science: An Introduction, Second Edition



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

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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 todayâ ™s computational methods." â • Erich Wimmer, Materials Design, Inc., Angel Fire, New Mexico, USA "Books such as this allow my students â “ 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. "â • Al Rey Villagracia, De La Salle University, Manila, Philippines "This text takes you on a â ˆworkingâ ™ 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 â ˆHitchhikers guide through the materials computational galaxyâ ™ because itâ ™s intentionally a guide not a random one." â • 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."â • 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 â ˆsimplyâ ™ 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."â • 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." â •Sachin Shanbhag, Florida State University, USA "....a good text. It suites well for Engineering students." â •Oleg Rubel, McMaster University, Hamilton, Ontario, Canada

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