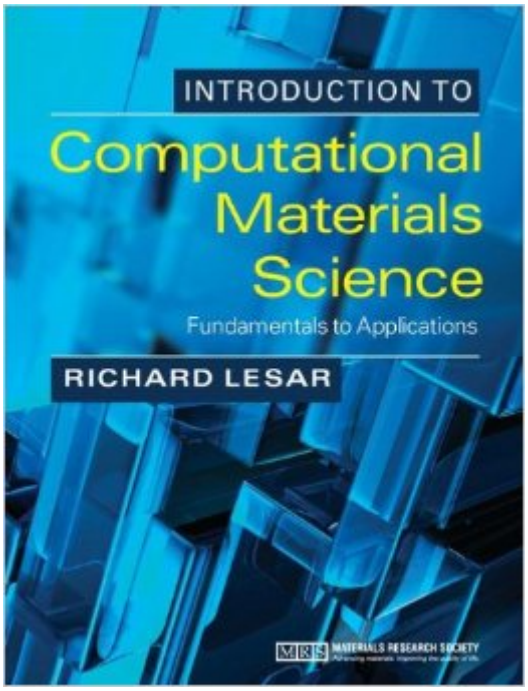
Introduction To Computational Materials Science: Fundamentals To Applications



Synopsis

Emphasising essential methods and universal principles, this textbook provides everything students need to understand the basics of simulating materials behavior. All the key topics are covered from electronic structure methods to microstructural evolution, appendices provide crucial background material, and a wealth of practical resources are available online to complete the teaching package. Modeling is examined at a broad range of scales, from the atomic to the mesoscale, providing students with a solid foundation for future study and research. Detailed, accessible explanations of the fundamental equations underpinning materials modelling are presented, including a full chapter summarising essential mathematical background. Extensive appendices, including essential background on classical and quantum mechanics, electrostatics, statistical thermodynamics and linear elasticity, provide the background necessary to fully engage with the fundamentals of computational modelling. Exercises, worked examples, computer codes and discussions of practical implementations methods are all provided online giving students the hands-on experience they need.

Book Information

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Customer Reviews

In the last 3-4 years a few Introduction to computational material science books have come out. Much of the earlier ones , although good, were more focused on specific length and time scales (i.e. either atomic, diffusive, continuum, etc.). This text attempts to be an intro style survey of the most relevant types of computational approaches in materials science and it does a great job at it. Dr.

Richard LeSar clearly and concisely covers the basics of electronic structure calculations, atomistics, and microstructure evolution using mesoscopic methods. I've reviewed "Computational Materials Science: An Introduction" by Dr. June Gune Lee which is an excellent book if your planning on using other codes/software to carry out your computational investigations (Also it only covers Molecular Dynamics and Density Functional Theory). This book differs in that it is targeted more towards understanding the techniques and being able to develop,implement, and code them on your own. For this reason I think this book is slightly more ideal for an undergraduate or 1st year graduate student who wants to learn about computational materials science.Pros:1. Well written and easy to read.2. Covers a good amount of topics.3. FANTASTIC Appendix.4. Available download resources are very nice.5. Good for someone who wants to establish a solid foundation in Comp.-MSECons:1. Could be less expensive (paperback edition?).2. Although the first edition; there a a decent amount of typos.

+ Good selection of topics to give an overall overview of the field and its potential for development of innovative engineering practices.- More problems should be added at the end of each chapters.

Excellent book congratulations to the author

Reference Book

Good.

Method: Theory and Applications (Wiley Series in Computational Mechanics) Computational Biomechanics for Medicine: New Approaches and New Applications Molecular Modeling at the Atomic Scale: Methods and Applications in Quantitative Biology (Series in Computational Biophysics) Fundamentals of Nursing: Human Health and Function (Craven, Fundamentals of Nursing: Human Health and Functionraven, Fundamentals of Nurs) Solid Lubrication Fundamentals and Applications (Materials Engineering) Dielectric Spectroscopy of Polymeric Materials: Fundamentals and Applications (ACS Professional Reference Book) Thermal Energy Storage Using Phase Change Materials: Fundamentals and Applications (SpringerBriefs in Applied Sciences and Technology) Magnetic Materials: Fundamentals and Applications A Primer on Scientific Programming with Python (Texts in Computational Science and Engineering) Scientific Computing with MATLAB and Octave (Texts in Computational Science and Engineering)