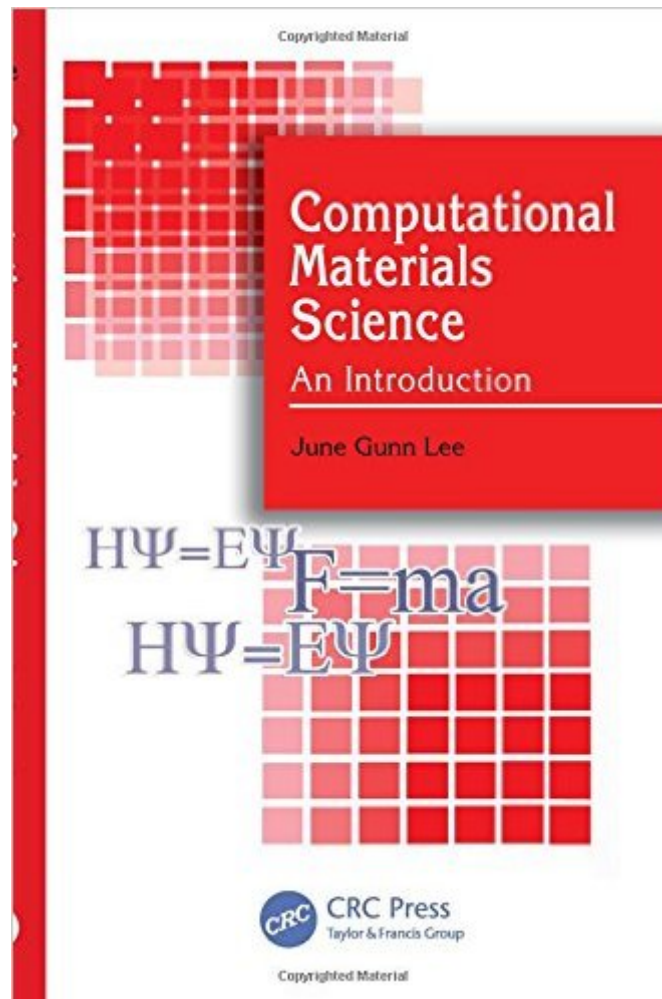


The book was found

Computational Materials Science: An Introduction



Synopsis

Computational Materials Science: An Introduction covers the essentials of computational science and explains how computational tools and techniques work to help solve materials science problems. The book focuses on two levels of a materials system: the electronic structure level of nuclei and electrons and the atomistic/molecular level. It presents computational treatments of these system levels using molecular dynamics (MD) and first-principles methods, since they are most relevant in materials science and engineering. After a general overview of computational science, the text introduces MD methods based on classical mechanics and covers their implementation with run examples of XMD and LAMMPS. The author discusses first-principles methods based on quantum mechanics at an introductory level, using illustrations and analogies to assist students in understanding this difficult subject. The book then describes the density functional theory (DFT) – the first-principles method that can handle materials practically. It also reveals how each orbital of electron leads to particular properties of solids, such as total energy, band structure, and barrier energy. The final chapter implements the DFT into actual calculations with various run examples via the VASP program. Computational methods are contributing more than ever to the development of advanced materials and new applications. For students and newcomers to computational science, this text shows how computational science can be used as a tool for solving materials problems. Further reading sections provide students with more advanced references.

Book Information

Hardcover: 302 pages

Publisher: CRC Press; 1 edition (September 27, 2011)

Language: English

ISBN-10: 1439836167

ISBN-13: 978-1439836163

Product Dimensions: 6.1 x 0.7 x 9.2 inches

Shipping Weight: 1.2 pounds (View shipping rates and policies)

Average Customer Review: 4.0 out of 5 stars – See all reviews (2 customer reviews)

Best Sellers Rank: #1,109,612 in Books (See Top 100 in Books) #104 in Books > Engineering & Transportation > Engineering > Materials & Material Science > Extraction & Processing #755 in Books > Science & Math > Chemistry > Physical & Theoretical #2979 in Books > Textbooks > Science & Mathematics > Chemistry

Customer Reviews

Just purchased this book. So far I'm impressed for the following reasons:1. Its compact, only 280 pages or so.2. The book is targeted towards the user (Materials Scientist and Engineer) rather than the programmer or code development.3. The above makes it extremely ideal for someone who is trying to use computational methods to perform research and science.4. The book does a good job at describing the basics and then in the following chapter gives a handful of examples.As of right now I strongly suggest this text to anyone (or course) who would like to get started with Computational Materials Science. The title is accurate for the contents inside (opposed to other texts which say they are intros but are not). I commend Dr. June Gunn Lee on this work and hope it is followed up with an advanced version which tackles complex simulations and data analysis.I haven't finished reading the text so I will return to update this review.Update!!!Just started the first-principles chapters. Let me say Dr. June Gunn Lee hits the nail right on the head. His simple but effective delivery of this topic is superb.I'm sure many physicist would feel he does injustice to the topic but they're not engineers and usually get caught up in the formalism. I'm always hesitant to pick up a text which claims to be an introduction to 1st principles but are impossible to follow. I really like this textbook. I think its simple yet effective and doesn't scare away the undergraduate/1st year graduate MSE student. I really hope there is an advanced text in the works.One thing to note is the reader needs to be fairly comfortable in Linux and Windows environments. This is because the Software used (e.g.

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

Computational Materials Science: An Introduction Introduction to Computational Materials Science: Fundamentals to Applications Computational Fluid Mechanics and Heat Transfer, Third Edition (Series in Computational and Physical Processes in Mechanics and Thermal Sciences) Computational Photochemistry, Volume 16 (Theoretical and Computational Chemistry) In Silico Medicinal Chemistry: Computational Methods to Support Drug Design (Theoretical and Computational Chemistry Series) Phillips' Science of Dental Materials, 11e (Anusavice Phillip's Science of Dental Materials) Phillips' Science of Dental Materials (Anusavice Phillip's Science of Dental Materials) Engineering Materials 2, Fourth Edition: An Introduction to Microstructures and Processing (International Series on Materials Science and Technology) A Primer on Scientific Programming with Python (Texts in Computational Science and Engineering) Understanding Molecular Simulation, Second Edition: From Algorithms to Applications (Computational Science) Scientific Computing with MATLAB and Octave (Texts in Computational Science and Engineering) Computational Science and Engineering Computational Partial Differential Equations Using MATLAB (Chapman & Hall/CRC Applied Mathematics & Nonlinear Science) A First Course in

Numerical Methods (Computational Science and Engineering) Algorithms in Bioinformatics: A Practical Introduction (Chapman & Hall/CRC Mathematical and Computational Biology) Introduction to Computational Biology: Maps, Sequences and Genomes (Chapman & Hall/CRC Interdisciplinary Statistics) A Computational Introduction to Digital Image Processing, Second Edition Ideals, Varieties, and Algorithms: An Introduction to Computational Algebraic Geometry and Commutative Algebra (Undergraduate Texts in Mathematics) Materials North American Edition w/Online Testing: Materials - North American Edition, Second Edition: engineering, science, processing and design Ceramics: Mechanical Properties, Failure Behaviour, Materials Selection (Springer Series in Materials Science)

[Dmca](#)