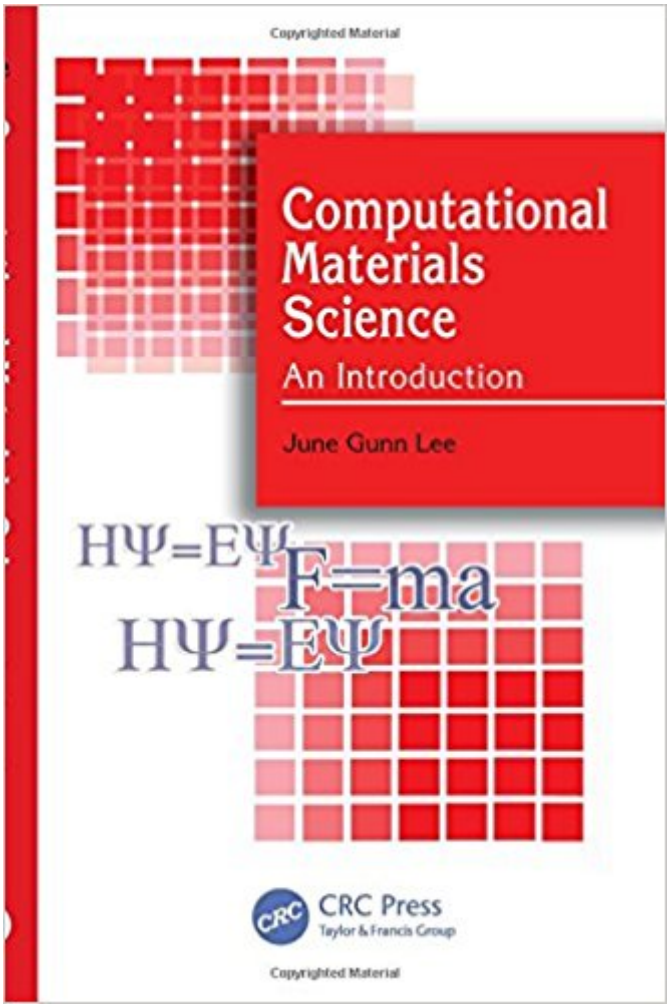
Computational Materials Science: An Introduction



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)â •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

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Customer Reviews

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. He has published roughly 70 papers on engineering ceramics and computational materials science. He earned a Ph.D. in materials science and engineering from the University of Utah.

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. XMD,LAMMPS,VASP) requires the user to know how to compile and run. The author doesn't give instructions on these codes, just input scripts, so you need to consult the manuals. I found this to be a problem with the last LAMMPS example in chapter 3, it seems the configuration file is not complete and only the experienced user can create it. Also, all the DFT calculations in chapter 7 are done with VASP, which is not available without acquiring a license from the group that manages it and from what I understand its only available for research groups and faculty.Update!!!Unfortunately I'm unable to perform any of the examples in chapter 7, since I don't have access to VASP. Upon a release of a second edition this chapter should be focused around an GNU licensed code such as Quantum-eEpresso etc.

The book in simple and practical. Has a lot of examples and although it is not among the best in

theoretical explanations, it is a very useful tool for people beginning in the field. I recommend the book.

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