

SECOND EDITION

Computational Materials Science

AN INTRODUCTION

June Gunn Lee



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Computational Materials Science An Introduction

June Gunn Lee



Computational Materials Science An Introduction:

Computational Materials Science June Gunn Lee, 2016-11-25 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

Computational Materials Science June Gunn Lee, 2011-09-27 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

Introduction to Computational Materials Science Richard LeSar, 2013-03-28 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

Introduction to Computational Materials Science [electronic Resource]. R. LeSar, 2013 [Computational Materials Engineering](#) Koenraad George Frans Janssens, Dierk Raabe, Ernest Kozeschnik, Mark A Miodownik, Britta Nestler, 2010-07-26 Computational Materials Engineering is an advanced introduction to the computer aided modeling of essential material properties and behavior including the physical thermal and chemical parameters as well as the mathematical tools used to perform simulations Its emphasis will be on crystalline materials which includes all metals The basis of Computational Materials Engineering allows scientists and engineers to create virtual simulations of material behavior and properties to better understand how a particular material works and performs and then use that knowledge to design improvements for particular material applications The text displays knowledge of software designers materials scientists and engineers and

those involved in materials applications like mechanical engineers civil engineers electrical engineers and chemical engineers Readers from students to practicing engineers to materials research scientists will find in this book a single source of the major elements that make up contemporary computer modeling of materials characteristics and behavior The reader will gain an understanding of the underlying statistical and analytical tools that are the basis for modeling complex material interactions including an understanding of computational thermodynamics and molecular kinetics as well as various modeling systems Finally the book will offer the reader a variety of algorithms to use in solving typical modeling problems so that the theory presented herein can be put to real world use Balanced coverage of fundamentals of materials modeling as well as more advanced aspects of modeling such as modeling at all scales from the atomic to the molecular to the macro material Concise yet rigorous mathematical coverage of such analytical tools as the Potts type Monte Carlo method cellular automata phase field dislocation dynamics and Finite Element Analysis in statistical and analytical modeling

Computational Materials Science Kaoru Ohno, Keivan Esfarjani, Yoshiyuki Kawazoe, 2018-04-14 This textbook introduces modern techniques based on computer simulation to study materials science It starts from first principles calculations enabling to calculate the physical and chemical properties by solving a many body Schroedinger equation with Coulomb forces For the exchange correlation term the local density approximation is usually applied After the introduction of the first principles treatment tight binding and classical potential methods are briefly introduced to indicate how one can increase the number of atoms in the system In the second half of the book Monte Carlo simulation is discussed in detail Problems and solutions are provided to facilitate understanding Readers will gain sufficient knowledge to begin theoretical studies in modern materials research This second edition includes a lot of recent theoretical techniques in materials research With the computers power now available it is possible to use these numerical techniques to study various physical and chemical properties of complex materials from first principles The new edition also covers empirical methods such as tight binding and molecular dynamics

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