Preface

"Computational materials science" uses computing soft wares to investigate the effects of changes in material composition and structure on material properties or device performance. This course is a new interdisciplinary course of materials science and technology, which has gradually become an important professional course of materials science. Based on this course, students can also study the postgraduate courses such as "Materials calculation and design". These courses use computer softwares to perform two functions: one is to explain some microscopic mechanisms that are not easy to obtain in material experiments, and the other is to predict the properties of materials or devices. Computational materials science is not only the third research tool besides pure theoretical research and experimental research, but also the bridge between them. Computational materials science has even influenced the paradigm of materials research, starting with designing materials, then preparing and characterizing materials, and finally testing the properties of materials.

The calculation and design of materials science need the unity of knowledge and practice involved physics, chemistry, materials science and computer science. As we all know, the knowledge system based on modern physics and chemistry is large and wide, students are required to master material finite element analysis, molecular dynamics, first principles calculation and Monte Carlo simulation. At the same time, students also need to understand the application of computational materials in the fields of energy, electronics, chemical industry, metallurgy and pharmaceutical engineering. The "practice" is practical and requires students to select appropriate physical and mathematical models and related software and hardware for material modeling, simulation and analysis. Based on the fundamental principles of computational materials science, students engage in material development and design exploration. The first feature is common to the general emerging interdisciplinary

courses, and the second is common to many engineering courses. The two features of this course make it difficult to achieve the teaching purpose in a short period (32 hours) using traditional teaching methods and traditional teaching materials. This course covers almost all areas of materials science, and it is impossible to address all issues in one textbook. Therefore, it is necessary to use a case-based approach to teaching.

At present, the courses and teaching materials of computational materials science are mainly based on profound theoretical introduction with many papers and little hands-on practice. In the class, most students can only learn a few principles and formulas, it is hard for most students to build atomic model, to write input script, to use software, to analyze results and to identify errors in calculation. Another important aspect is that undergraduates don't know exactly what work can be done in computational materials science, while most postgraduates don't know how to choose an appropriate research topic by employing computational materials science and designing a research programs to study. Appropriate criteria for this course include the following factors: innovation, appropriate method and computing power. Computational materials science can be involved in almost any experimental field of materials science, but it does not mean omnipotent. This textbook is based on the process of students' practical operation, and can even be used for self-learning computational materials. Then students can calculate the composition, structure and performance of various materials, obtain specific results and discuss them, and reach the level of writing scientific paper as well as provide help for understanding and designing materials. In recent years, as the level of education in China continues to improve, more and more international students come to China to pursue undergraduate or postgraduate degree. An English professional textbook will help them understand the essence of this course as soon as possible and be able to operate it. For Chinese students, the cases in the textbook help them master the basic methods and operation steps of computational materials science as soon as possible, rather than being limited to complex theoretical study. It also helps students express and analyze the research

results in proper English, and helps them improve their international communication skills including thesis writing.

The main contents of this textbook include: a comprehensive introduction to the methods of atomic simulation, molecular dynamics, Monte Carlo calculation, first principles calculation and finite element calculation. Common calculation software such as GULP, LAMMPS, ATAT, VASP, CASTEP and ANSYS are used to investigate the mechanical, thermal, optical and electrical properties of the surfaces, interfaces and nanostructures of metals, semiconductors and insulators. This book will be used as the educational materials for undergraduate or postgraduate students who study "computational materials science" or "material calculation and design" courses.

Three teachers from the School of Materials Science and Engineering (SMSE) of Lanzhou University of Technology (LUT) compiled this book. Among them, professor Tang Fuling is responsible for the whole book, associate professor Li Junchen had compiled and reviewed chapters 1 to 5, and professor Lu Xuefeng had compiled and reviewed chapters 6 to 9. Three teachers from School of Bailie Mechanical Engineering, Lanzhou City University participated in the compilation of this book. They are associate professor Si Fengjuan (Chapters 1 and 9), engineer Hu Yuxia (Chapters 2 and 5) and assistant professor Shi Yanyan (Chapter 3). Liang Zefen, associate professor of School of Mechanical and Electrical Engineering of Lanzhou Institute of Technology (LIT), and Hu Wei, lecturer of School of Material Engineering of LIT, respectively wrote chapters 4 and 6, and Zhao Qingshan, lecturer of Lanzhou Petrochemical University of Vocational Technology, wrote Chapters 7 and 8. This book has been edited under the guidance of many colleagues and put forward valuable suggestions for revision. This book includes the models and processing methods online, nonprofit as education materials for undergraduate or postgraduate students. The postgraduate students Luo Yaqiao, Zhao Fenning, Wei Chengdong, Gao Qing, Zhao Xudong and some other students of the authors have performed the practical simulation of this textbook, wrote the text and drawn the charts. All

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