Research on the Application of Computational Materials Science in Undergraduate Teaching

ZHUANG Quan[a]; LI Dongyong[b]; LI Xiangyang[b]; MA Xinjun[c],*

[a] Lecturer. Nano Innovation Institute, College of Chemistry and Material Science, College of Mathematics and Physics, Inner Mongolia Minzu University, Tongliao, Inner Mongolia, China.
[b] Nano Innovation Institute, College of Chemistry and Material Science, College of Mathematics and Physics, Inner Mongolia Minzu University, Tongliao, Inner Mongolia, China.
[c] Professor. Nano Innovation Institute, College of Chemistry and Material Science, College of Mathematics and Physics, Inner Mongolia Minzu University, Tongliao, Inner Mongolia, China.
*Corresponding author.

Abstract

In this paper, by taking first-principles software as examples, we apply computational materials science to the teaching process of undergraduates majoring in physics, chemistry and materials. We pay attention to the connection between theoretical research and experimental models, makes the abstract principle intuitive and dynamic, and facilitates students' understanding of knowledge, a deep understanding of the structure of materials and the relationship between theoretical properties and macro properties, which can greatly enhance students' initiative and creativity in participating in teaching activities. To a great extent, this has played a role of computational simulation as a bridge between theoretical teaching and experimental teaching to continue to explore the complementary relationship between computational simulation, theoretical teaching and experimental teaching, build a teaching model for the application and design ability training of materials and chemistry talents.

Key words: Computational materials science; First-principles software; Teaching design

1. INTRODUCTION

At present, with the progress of human society and the deepening of scientific research, the performance requirements of materials are also continuously improving. The research scale is constantly decreasing, and the research of some functional materials even reaches the electronic level. The difficulty and cost of experiments are constantly increasing, and it is difficult to meet the needs of contemporary scientific research by relying on material research. Therefore, we should not only pay attention to the traditional theory and experimental teaching, but also pay attention to combining theory with practice, integrate with the scientific frontier, and analyze the micro mechanism related to material properties with the help of new methods and technologies.

In the current scientific research, the theoretical model and the research system used are relatively complex, and the theoretical calculation amount required is very large, and many problems cannot be solved only by the traditional analytical derivation method. For example, in addition to the results of molecular hydrogen ions (dihydrogen cations), the quantum many-body problem cannot be solved analytically, let alone in a closed form. Computational materials (computational materials science) have opened up a new road, and it is the fusion and intersection of disciplines, materials science, computer science, physics and chemistry and other multidisciplinary fusion and intersection of disciplines, using the computer's powerful computing ability to solve the scientific problem of complex system, and the rapid

development has become the essential material science research, and has become a widely concerned of emerging disciplines. Computational material science mainly includes two aspects: on the one hand, which combines the theoretical method and effective computer program to calculate and predict the other hand, through some numerical calculation methods or reasonable mathematical model to simulate the actual process and provide guidance and support for the experiment. The former makes the research and development of materials more prospective; and the latter helps to make the experimental results of specific material systems to general theory, so computational materials science builds a bridge between materials science theory and experimental research.

Computational materials science, as a new discipline closely combining theory and practice, is used in the traditional teaching of undergraduate majors in physics, chemistry and materials, such as, with solid state physics, material physics, material science, solid chemistry and physical chemistry and other theoretical courses. Demonstration experiments, autonomous experiments, the change law of the composition, crystal structure and properties of the simulated materials are on the basis of a certain theoretical level to visualize and concrete the theoretical knowledge learned, to deepen the students' understanding of the basic knowledge and stimulate students' enthusiasm and interest in learning and improve teaching quality and teaching efficiency, which make the teaching process to a higher and more comprehensive level of cognition. Taking Materials Studio (MS), Vienna ab initio simulation package (VASP), Vesta and other first-principles calculation software and visualization software based on density functional theory as examples, this paper applies computational materials science to the teaching process of undergraduates majoring in physics, chemistry and materials, pays attention to the connection between theoretical research and experimental models, makes the abstract principle intuitive and dynamic, and facilitates students' understanding of knowledge, a deep understanding of the structure of materials and the relationship between theoretical properties and macro properties, which can greatly enhance students' initiative and creativity in participating in teaching activities. To a great extent, this has played a role of computational simulation as a bridge between theoretical teaching and experimental teaching to continue to explore the complementary relationship between computational simulation, theoretical teaching and experimental teaching, build a teaching model for the application and design ability training of materials and chemistry talents.

2. SOFTWARE INTRODUCTION

The first-principles calculation method based on density functional theory is the most important theoretical method to study the micro electronic structure. This method only needs to use the five basic variables of electronic static mass, electronic charge mass, speed of light, Boltzmann constant and Planck constant and the crystal structure model of the system. Starting from quantum mechanics, a series of physical and chemical properties such as electronic properties, mechanical properties, optical properties and magnetic properties can be calculated by numerically solving Schrodinger equation. In recent years, with the advent and continuous improvement of a series of crystal structure prediction software such as Calypso, USPEX, Magus, ELocR [1-5] and the first-principles calculation software of VASP, MS, Quantum-Espresso, abinit, WIEN2k [6-9], computational materials science has achieved unprecedented development. This paper mainly introduces MS software, VASP software and Vesta, which are widely used and easy to operate, and carries out the operation teaching of these three software in the teaching process of computational materials.

VASP, the full name of Vienna Ab-initio Simulation Package, is a software package for electronic structure calculation and quantum mechanics molecular dynamics simulation developed by G. kresse and his partners. Of the University of Vienna, it is one of the most popular commercial software in material simulation and computational material science research.

The full name of MS is Materials Studio, a new generation of material computing software launched by Accelrys company in the United States. It can not only perform a series of calculations required by chemistry, materials and other disciplines, but also has a powerful model building function and three-dimensional visualization function, and can be operated and operated on the PC.

Vesta is a three-dimensional visualization program, which can be used to display structural models and volume data, such as charging density and crystal models and can export high-resolution pictures or videos.

3. TEACHING DESIGN

3.1 Setting Knowledge Points
In specialized courses, they are related to physics, materials and chemistry, such as solid state physics, fundamentals of material physics, fundamentals of material science, solid state chemistry, material thermodynamics and dynamics, and physical chemistry, knowledge points, such as crystal structure, energy band structure, band gap, X-ray diffraction, phase diagram, etc. The physical and chemical properties, such as refractive index, reflectivity, and dielectric constant of materials will also be involved. After completing the explanation of knowledge points, such as phase diagram, crystal structure and electronic band structure, we then use MS software to carry out

modeling demonstration, and explain the calculation and analysis process of crystal energy band and other properties with VASP software, so as to give an intuitive and visual explanation for these basic knowledge, and connect the macro properties of materials with the micro mechanism, so that students will have an overall understanding and understanding of the knowledge system of material science.

3.2 Introduction to Density Functional Theory

Density functional theory (DFT) is a theory about multi-body correlation system, which is the modern theoretical basis of single electron approximation. In essence, the Schrodinger equation is solved by taking the electron density distribution function as the variable instead of the independent variable in the wave function, which makes it possible to solve the eigenvalues of the wave function of the complex system. At present, Density Functional Theory has been widely used in physics, chemistry and material related fields, especially to study the properties of molecules and condensed matter. At present, Density Functional Theory is widely used in computational simulation software to solve Schrodinger equation, which can calculate and study the structure and properties of materials. Combined with molecular dynamics, it has made significant progress in material design, synthesis and simulation calculation, and has become an important

foundation and core technology of computational materials science.

3.3 Software Operation and Related Content Demonstration

Using the visualizer visualization core module in MS software, it is very convenient to build a variety of materials, surfaces, interfaces and other models, control these configurations with the mouse, and analyze the structure of related systems from multiple angles, which makes it easier for students to form intuitive concepts. The structural database in MS can be used for teaching demonstration. For example, the crystal structure of diamond and graphite needs to be used in the comparative teaching of the microstructure of diamond and graphite. The crystal structure file of diamond and graphite can be easily imported from the structures/ceramics database folder of MS software (as shown in Figure 1). It can be demonstrated for students in class from different crystal planes to show the structural differences between the two in an all-round and three-dimensional way. Then we can build the 5×5 supercell of graphite through the menu option build ->symmetry - > supercell, which can show its layered structure more clearly. This will give students a vivid, intuitive and dynamic concept, so that they can easily establish a spatial model in their mind and understand the knowledge points they learned.
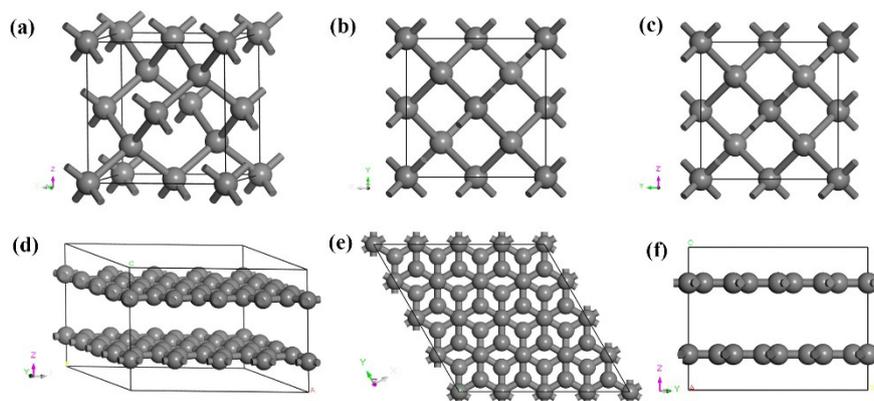
Figure 1
Erystal structure of diamond and graphite. (A-C) are the front view, top view and side view of the diamond respectively; (d-f) the front view, top view and side view of 5 ×5 supercell structure for graphite. The coordinate axis orientation of different schematic diagrams is marked in the lower left corner.

It can be found that each carbon atom is connected to at most four other carbon atoms through the demonstration of diamond primitive cell by the visualizer module, which can explain the covalent bond of carbon atoms and the sp^3 hybridization therein. The carbon atoms in graphite are stacked in two dimensions, and the carbon in each layer forms a hexagonal structure, forming sp^2 hybrid. After preparing the input files (INCAR, KPOINTS, POTCAR, etc.) for corresponding calculations and taking the primitive cell of diamond and graphite as POSCARs, through a series of calculations such as optimization and

self consistency calculations by VASP software, we can get the properties of electronic band structure, density of states, and electronic localization function (ELF), and visualize the ELF by Vesta software. It can give a deep analysis of bonding behavior in diamond and graphite, and deepen students' understanding of electronic structure and bonding behavior.

In addition, the crystal structure modeling is explained in an extended way, demonstrating the operation of using the materials project database to find and download the crystal structure, and using the lattice constants and

atomic occupation information provided in the literature to establish the crystal model.

In the teaching of X-ray diffraction, the reflex module in MS can be used to simulate the X-ray, neutron and electron diffraction patterns of powder crystal materials, which can be used to verify the experimental results and demonstrate the teaching.

3.4 Software Operation Practice

In addition to the explanation of theoretical courses, practical courses with certain hours will also be arranged to lead the students to operate the software. Since the operation of VASP software requires the Linux system platform, the students are divided into 5~6 groups to collectively carry out the practical operation exercises of MS, Vesta and VASP software in groups, so that they can discuss with each other within or between groups when they encounter problems. Finally, taking the group as a unit, the students' modeling operation results are counted, and the software calculation results on the server side are monitored in real time to get the feedback of the teaching effect in time.

4. CONCLUSION

For the course content with strong theory, the latest material calculation software is applied to traditional teaching, and the abstract and difficult concepts are intuitively displayed in the form of graphics with the help of software. The computing resources used in the computing simulation software can be computers in multimedia teaching and students' own laptops, and the remote server can be directly connected through the network. The application of calculation examples can cultivate students' initiative, consciousness and creativity in learning, improve their theoretical level and practical ability, increase their interest in physics, chemistry, materials and other related disciplines, which can deepen their understanding of scientific research.

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