

Chapter 12

Review on Computational Materials Design and Its Applications

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ABSTRACT

In a normal study, if the structure or composition of a material is given, it is possible to study the properties and functions of the material. This is a direct challenge. As solution techniques have developed considerably, they have become quite sophisticated, both experimentally and computationally. The study area known as computational materials design uses computer modeling to find a solution to this "inverse problem." Using computer simulations, particularly those based on quantum theory, is a process known as computational materials design. The authors would like to introduce the current status and recent research on reactions at interfaces. The authors will explain the method of predicting the magnetism of a system called

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the dilute magnetic semiconductor, which has been attracting attention as the base material for semiconductor spintronics, based on a first-principles calculation. After a brief introduction to semiconductor spintronics, he will explain the method of handling the regularity peculiar to dilute magnetic semiconductors, using the band calculation method. New materials derived from carbon, such as carbon nanotubes, fullerenes, and grapheme, have been added to the traditional functional carbon materials such as diamond, graphite, and activated carbon. The tools used for materials informatics. With the aim of accelerating materials science research, data-driven materials research, that is, materials informatics research is becoming more active. One is the crystal structure prediction tool, CrySPY, and the other is the descriptor generation tool, LIDG, used for machine learning. as supercomputers, the knowledge and techniques required to master them are also changing, becoming more complex and sophisticated each year. The various techniques will be introduced in relation to the features of current computers in terms of single-CPU performance optimization and high-parallelism performance optimization.

INTRODUCTION

In a normal study, if the structure or composition of a material is given, it is possible to study the properties and functions of the material. This is a direct challenge. As solution techniques have developed considerably, they have become quite sophisticated, both experimentally and computationally. “Computational materials design “is a research field that solves this “inverse problem” using computer simulation. Computational materials design is a technique that uses computer simulations, especially those based on quantum theory, to elucidate the origin of, and the factors that govern the properties of, the material. Will introduce the design of magnetic materials for spintronics (Campbell & Olson, 2000; Olson, 1997; Olson, 2000; Saha & Olson, 2007). He will explain the method of predicting the magnetism of a system called the dilute magnetic semiconductor, which has been attracting attention as the base material for semiconductor spintronics, based on a first- principles calculation. After a brief introduction to semiconductor spintronics, he will explain the method of handling the regularity peculiar to dilute magnetic semiconductors, using the band calculation method. Next, he will introduce the method and results of calculating the magnetic interactions between the magnetic moments in a magnetic body and discuss the mechanism of the manifestation offer ferromagnetism in dilute magnetic semiconductors (Committee on Accelerating Technology Transition, 2004; Harlow, 2007; Jou et al., 2004; Lewis, n.d.; Vernerey et al., 2006). Finally, he will demonstrate how accurately the Curie temperature of dilute magnetic semiconductors can be predicted. This leads to the design of materials with more desirable functions and

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