学　位　論　文　内　容　の　要　旨

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学　位　論　文　題　名

Exploration of novel two dimensional materials by using first principle calculation and materials informatics approach

(マテリアルズ・インフォマティクスと第一原理計算を用いた新規二次元材料の探索)

Materials Informatics (MI) gains recently remarkable attention from both academic and industrial field with the goal of efficient material research. A traditional approach for material development is carried out in research laboratory with hidden failure experiment and its feedback by individual specialized researchers. This approach normally requires time and cost to develop practical materials due to its try-and-error process, but at the same time, this costly "error" process can be a great information for the next success.

The material design now is advanced with a development of computation equipment and methodology; some specified systems can be simulated by computation with sufficient accuracy, such as fluid dynamics and chemical dynamics. In the field of materials design, density functional theory (DFT) is one of the revolutionary simulation methods for novel materials modeling since it can provide various kind of information from its calculations, for example, band structure analysis for electronic device, bulk modulus estimation for structure materials, reaction path evaluation for catalysis, etc. Material predictions have been achieved by DFT calculations particularly against nanomaterials, such as nanoclusters, nanotubes and two dimensional materials. And some of them are successfully synthesized and applied into functional materials. Two dimensional materials are remarkable nanomaterials among those materials because of its unique properties with wide range application: from mechanical to medical usage. However, simulation has still disadvantage of its accuracy and implementation for real material design, therefore, it cannot be "the best" method for material design.

Consequently, simulations still rely on researchers experience in the process of designing the new model materials, even though this process can be replaced costly experimental process. MI is one covering tool for this empirical side in material design; predicting new materials from exist data by applying data science. This method has great potential to discover new materials since the all prediction process is conducted by stiff computation algorithm, consequently, all data is treated equally, unlike researchers' inspiration or experience. However, MI is developing method because of its novelty.

In this study, both computational (DFT) and MI method are implemented to discover novel two dimensional materials with the goal of establishment for MI approach.

In Chapter 1, the overview of MI is explained: from the history to its concept and outlook to the future research. The current progress in MI among both academic and industries are explained.

In Chapter 2, two dimensional materials, target materials of this research is introduced in the view of its history and remarkable properties.

In Chapter 3, the fundamentals of first principle calculation are introduced. The fundamental equations

and theories are explained.

In Chapter 4, the implementation of the calculation code is explained. In particular, GPAW code, a DFT calculation code applied in the studies, are explained from the point of view to feature functions, installation, and high throughput calculation.

In Chapter 5, the research result achieved by first principle calculation is introduced. Hexagonal boron nitride (h-BN) is commonly known substance with graphite-like layered materials. And two-dimensional boron phosphide (h-BP) is predicted its existence and semiconductive property by first principle calculation. Group XV atoms are common in these h-BN and h-BP two-dimensional materials, hence, boron with Group XV atoms (M: As, Sb and Bi) are investigated and evaluated by first principle calculations due to designing novel materials. As a result, those single layer boron based novel two-dimensional materials turned out to be energetically stable, and their electronic property suggests a potential application for semiconductor and catalyst. Band gap and binding energy in these single layer boron based two dimensional materials turned out to be proportionate to the Allen electronegativity. Additionally, the layered structures are investigated, and zigzag formation is proposed in B-Sb and B-Bi. And electronic structure turned out to differ from single layer materials.

In Chapter 6, the fundamentals of machine learning is introduced for the explanation for MI method within this research. The variation of machine learning method is explained in the views of ML implementation, and Naive Bayes, implemented algorithm in the study, is introduced.

In Chapter 7, the implementation of machine learning is explained. Scikit-learn, a machine learning module for machine learning in Python language program is introduced for MI implementation.

In Chapter 8, the combined research result with first principle calculations and MI is introduced. Novel two-dimensional magnets are explored by materials informatics approach and investigated by first principle calculations. 216 computational two-dimensional material data within an open database is collected and explored by machine learning. Gaussian naïve Bayes algorithm is applied to predict MoS_2 shaped (AB_2) and graphene shaped(AB) two-dimensional magnets with a high magnetic moment. As a result, novel 254 AB and AB_2 two dimensional materials are explored as candidates with high magnetic moments. By the evaluation of first principle calculations, 7 candidates are found to be energetically stable and have a high magnetic moment: $MnPd_2$, FeS, CrSe, CrS, MnTe, MnSe, and MnS.

In Chapter 9, the research achievements are summarized, and future research goal is described by the consideration from the obtained result from this research.