（様式６号）「課程博士用」

学 位 論 文 の 要 旨

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学位論文題目 First-principles study of electric field effects on graphene-based structures for battery and spintronic materials application

（グラフェン系物質における電界効果の第一原理計算：バッテリー材料およびスピントロニクス材料への応用）

Two-dimensional (2D) materials have garnered significant attention due to their exceptional properties and potential applications in future electronic devices. However, the extraction of graphene can result in imperfect graphene with defects and impurities that limit its performance, while its lack of a bandgap restricts its application in electronic devices. To overcome the issues, alternately, recent efforts have been carried out to explore ways to use the imperfect graphene in application. One approach involves deliberately introducing defects, such as vacancy defects and interlayer defects, forming heterostructures. Defected graphene has shown promise in increasing the capacity of lithium batteries, while for spintronics applications, combining graphene with materials possessing a larger spin-orbit coupling (SOC), i.e., transition metal dichalcogenides (TMD), is necessary. The purpose of this study is to investigate theoretically defected graphene-based structures and their application in battery and spintronics technologies, where an external electric field, commonly used in semiconductors, is utilized to maximize the capacity of lithium battery and spin generation manipulation for spintronics devices.

The dissertation consists of seven chapters. Chapter one explains the background and purpose of the study. Chapter two describes the methodologies of calculations. The method of density functional theory (DFT), which is performed by utilizing full-potential linearized augmented plane wave method within generalize gradient approximation including dispersion correction of van der Waals interaction are presented.

Chapter three focuses on the construction of defected-graphene and germanene to gain understanding of their electronic and structural properties. The investigation included calculating the formation energy of monovacancies in monolayer graphene and monolayer germanene and found that monovacancies in graphene exhibit highly stable with the formation energy of 7.6 eV, while those in germanene are less stable with 2.03 eV. The latter can be attributed to the unique low buckling characteristic of germanene. It was further conducted on multivacancy in germanene where the most stable multivacancy structures is consisted of even-numbered vacancies. The appropriate structures identified through this study will be used for further calculations.

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Chapter four provides an extended study of defected-bilayer graphene evaluating the intercalation of lithium in bilayer graphene, motivated by the need to develop more efficient energy storage systems. In contrast to graphite, which has a lower capacity for lithium storage, bilayer graphene has a higher theoretical capacity due to its larger surface area. The present analysis showed that an external electric field could significantly increase lithium stability in defected-bilayer graphene which led to increase of lithium intercalation to up to 12 atoms. This result shows a 140% increase of capacity of lithium compared to pristine bilayer graphene.

In chapter five, calculations were performed to examine how the electronic structure of graphene-MoS_2 is affected by stacking orientation, element substitution, and interlayer distance. The results indicate that the electronic structures are not significantly influenced by the stacking orientation, in contrast to how element substitution and interlayer distance successfully modify them. Bandgap opening is importantly emerged by forming the heterostructure via a symmetry breaking of carbon staking-sites on MoS_2. The findings are crucial for further research aimed at manipulating the electronic properties of graphene-MoS_2 heterostructure.

In Chapter six, the influence of an external electric field on bandgap opening and spin Hall conductivity in graphene-MoS_2 heterostructure was investigated. As a result, an increase in the electric field induced an out-of-plane polarization, primarily driven by the presence of MoS_2, resulting in insulator to metallic transformation of the heterostructure, which led to an increase in spin Hall conductivity up to 170 Ω^{-1} cm^{-1}. Our findings demonstrate the potential of spin generation in graphene-MoS_2 heterostructure through spin Hall conductivity, which can be tuned by an electric field. These results open up possibilities for the application of graphene-MoS_2 heterostructure in spintronics applications.

Chapter seven remarks conclusions and prospects of the study.