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研究課題名（和文）Spin-Valley Coupled Two Dimensional Magnetic Materials : Valley Polarization & Quantum Anomalous Hall Effect

研究課題名（英文）Two Dimensional Magnetic Material: Spintronics & Valleytronics Applications

研究代表者

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研究成果の概要（和文）：このプロジェクトの主な目的は、材料シミュレーションによって、スピントロニクスやバレートロニクスへの応用のための最も有望な候補材料を見つけ、スクリーニングすることであった。この観点から、室温で存在する可能性の高い新しい2次元磁性材料を設計する。(1)次世代スピントロニクスデバイスの候補となりうる強磁性遷移金属酸化物層Cr2O3を示した。(2)熱力学的に安定な2次元ブリスター構造における量子バレーホール効果の実現の可能性を示した。本研究では、外場なしでスピンフィルタリングとスピンバレーコントラストホール効果を実現する新しいアプローチを提供した。

研究成果の学術的意義や社会的意義
It is scientifically important in material science to find promising 2D materials that are likely to exist. This research was based on the computational approaches of materials simulation to find and screen the most promising candidate materials to expedite the materials characterization.

研究成果の概要（英文）：First work is related to spin conductance of electrons in magnetic tunnel junctions. This study reveals the effect of various electrode materials on spin transport that can help to develop 2D materials based efficient spintronics devices. In another work, we used first-principles calculations to search and design new 2D magnetic material. It is demonstrated that the ferromagnetic transition metal oxide layer of Cr2O3 layer can exist at room temperature which can be ideal for next-generation spintronics applications. Regarding the work on valleytronics, I investigated the possibility of realizing quantum valley Hall effects (QVHE) in blistered structures. The geometric distortion in blisters induces magnetic state in otherwise paramagnetic graphene. This spin degree of freedom gives rise to spin-filtered QVH states, and the valley conductivity is quantized. This study provides a pathway to realize the spin-filtered and valley contrasting QVH effects in the absence of external fields.

研究分野：Condensed matter physics

キーワード：Magnetic 2D material　DFT　Spintronics　Valleytronics　Spin-valley hall

１．研究開始当初の背景

Study on two-dimensional (2D) materials is receiving great research interest owing to their extraordinary physical properties. 2D materials have shown the most promising phenomena named “spintronics” and “valleytronics”. Recently, tremendous amount of research attention is focused on these phenomena.
Magnetic 2D materials are very important for spintronics applications like spin transistors. Practically, magnetic materials allow us to control charge as well as quantum spin state. But up to date, all 2D materials like graphene, MX2, Phosphorene etc. lack magnetism. Thus, to unravel the properties of novel 2D magnetic structures that can be used for spintronics applications is very important. On the other hand, 2D materials with broken inversion symmetry and strong spin-orbit coupling (SOC) show valleytronics phenomena. The utilization of valley degree of freedom, which is also called valley pseudospin, as the information carrier is the main context of valleytronics. Valley in 2D materials is degenerated but distinguishable which appears at corners of hexagonal Brillouin zone (±K points with index $\tau = \pm 1$) in the absence of inversion symmetry, due to the opposite Berry curvature. In the binging, the fundamentals of valley degeneracy and inter-valley coupling were investigated. Recently, several methods such as applying magnetic field, magnetic impurities, and magnetic substrates have been utilized to achieve Zeeman-type valley splitting.
Hence, new magnetic 2D structures that constitute a binary valley degree of freedom along with magnetism can be potential candidates for spintronics as well as valleytronics device applications.

２．研究の目的

2D materials have shown most promising phenomena named spintronics and valleytronics. Because of the several practical limitations of the existing 2D materials, this project aimed to find these phenomena in new “2D magnetic materials”. The key purposes of the project were: (1) prediction of a magnetic 2D material, and (2) understand rich physics of valleytronics in 2D layers.
The key scientific questions were: (i) how the existing 2D non-magnetic materials behave in the presence of magnetic layers, (ii) can we expect new 2D magnetic structures that are likely to exist at room temperature for applications of spintronics and valleytronics, (iii) how to overcome the difficulty of achieving valley polarization without external perturbation. The main theme of this project was the realization of new magnetic 2D materials, which would help to understand rich physics of valleytonics due to spin–orbit coupling (SOC) that is hard to explain by experimental techniques. Lastly the combination of valley pseudospin and magnetism is explored to tune these properties simultaneously and provide a practical and easy way to realize these phenomena in experimental world.

３．研究の方法

Ab Initio Calculations: In the present work, I used the efficiency of density functional theory to unravel the electronic and magnetic structures of promising candidates of new 2D materials.
Structure Prediction: I used new 2D structures by using efficient evolutionary algorithm that allowed us to find global structures minima and their alternative stable and meta stable allotropes.
Thermal and Mechanical Stability: By calculating the phonon dispersion curve, I investigated the dynamical stability. Molecular dynamics calculations were performed to check the thermal stability.
Electronic, Physical & Magnetic Properties: Standard DFT methodology both plane wave (PAW) and localized pseudo atomic orbitals ((PAOs)) tools were used to explore all physical properties.
Wannier Calculations: Tight-binding Hamiltonian was constructed with the help of maximally localized Wannier functions (MLWFs) to find berry curvatures and quantum hall conductivity.
Transport calculations: Spin transport properties at zero bias voltage of the device using magnetic 2D layers were investigated by using the non-equilibrium Green's function method.

４．研究成果

The first work was related to spin conductance of hot electrons in magnetic tunnel junctions (MTJs) using graphene sheet. Previous studies are only limited to symmetric junctions in which electrode materials on both sides of 2D layer are the same. The investigation includes graphene based symmetric (electrode = Ni) as well as non-symmetric (electrode = Ni and Co) junctions. This study reveals the effect of various electrode materials on spin transport property that can help to develop 2D materials based efficient spintronics devices.
In spintronics, a key challenge is the generation of 100% spin-polarized current at the Fermi level. A half-metal, i.e., a material which filters the current into a single spin channel, meets this demand. Nonetheless, previously reported 2D half-metallic materials failed to satisfy the key factors such as large spin gap, giant magnetic anisotropy energy, and high Curie temperature. Hence, searching for an intrinsic half-metal that accomplishes the above-mentioned features in monolayer remains a great challenge. In this study, I used first-principles calculations to search and design of new 2D magnetic layer. I demonstrated that the Cr_2O_3 ML is thermodynamically stable at room temperature. I also demonstrated that the Ising ferromagnetic transition metal oxide layer of Cr_2O_3 is an ideal candidate for next-generation spintronics applications.
Regarding the work on valleytronics, we investigated the possibility of realizing quantum valley Hall effects (QVHE) in 2D graphene blisters. The blister structures are composed of pentagonal and heptagonal rings of carbon atoms, which show a strong tendency toward out-of-plane deformation with increasing blister size. The geometric distortion induces exchange

splitting (magnetic state) in otherwise paramagnetic (no magnetism) graphene. Unlike the ribbon edges, these atomic-scale blisters are fully immersed within the graphene sheet and hence, its magnetic state is protected from contamination and reconstruction effects that could hamper experimental detection. This spin degree of freedom gives rise to spin-filtered QVH states, and the valley conductivity is quantized in two valleys. The study provides a pathway to realize the spin-filtered and valley contrasting QVH effects in the absence of external fields.

５．主な発表論文等

〔雑誌論文〕　計3件（うち査読付論文　3件／うち国際共著　2件／うちオープンアクセス　2件）

１．著者名 Farooq M. Umar、Hashmi Arqum、Ono Tomoya、Huang Li	４．巻 6
２．論文標題 Spin-valley Hall phenomena driven by Van Hove singularities in blistered graphene	５．発行年 2020年
３．雑誌名 npj Computational Materials	６．最初と最後の頁 197
掲載論文のDOI（デジタルオブジェクト識別子） 10.1038/s41524-020-00470-9	査読の有無 有
オープンアクセス オープンアクセスとしている（また、その予定である）	国際共著 該当する

１．著者名 Hashmi Arqum、Nakanishi Kenta、Farooq Muhammad Umar、Ono Tomoya	４．巻 4
２．論文標題 Ising ferromagnetism and robust half-metallicity in two-dimensional honeycomb-kagome Cr2O3 layer	５．発行年 2020年
３．雑誌名 npj 2D Materials and Applications	６．最初と最後の頁 39
掲載論文のDOI（デジタルオブジェクト識別子） 10.1038/s41699-020-00174-0	査読の有無 有
オープンアクセス オープンアクセスとしている（また、その予定である）	国際共著 該当する

１．著者名 Hashmi Arqum、Nakanishi Kenta、Ono Tomoya	４．巻 89
２．論文標題 Graphene-based Symmetric and Non-Symmetric Magnetoresistive Junctions	５．発行年 2020年
３．雑誌名 Journal of the Physical Society of Japan	６．最初と最後の頁 034708～034708
掲載論文のDOI（デジタルオブジェクト識別子） 10.7566/JPSJ.89.034708	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 －

〔学会発表〕　計2件（うち招待講演　0件／うち国際学会　1件）

１．発表者名 Arqum Hashmi
２．発表標題 Intrinsic ferromagnetic 2D honeycomb-kagome monolayer of Cr2O3
３．学会等名 The physical society of Japan
４．発表年 2019年

１．発表者名
Arqum Hashmi
２．発表標題
Robust Half-Metallicity and Perfect Spin Filtering in 2D oxide layer
３．学会等名
American Physical Society March Meeting 2020（国際学会）
４．発表年
2020年

〔図書〕　計0件

〔産業財産権〕

〔その他〕

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６．研究組織

	氏名 （ローマ字氏名） （研究者番号）	所属研究機関・部局・職 （機関番号）	備考

７．科研費を使用して開催した国際研究集会

〔国際研究集会〕　計0件

８．本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関