Kwansei Gakuin University
Report of Research Outcome

2025/03/14

To President

Department : Science and Technology
Position : Postdoctoral fellow
Name : Souren Adhikary

I report the outcome of the research as follows.

Name of the Fund/Program	□Sabbatical leave with grant □Sabbatical leave with no grant □KGU Joint Research □Individual Special Research ☒Postdoctoral fellow ※Please report by designated form as for "International Research Collaboration".
Research Theme	Theoretical studies on electronic and optical properties of two-dimensional materials
Research Site/Venue	Department of Nanotechnology for Sustainable Energy/Prof. Katsunori Wakabayashi's Lab
Research period	2024/04/01 ～ 2025/03/31 （ 12 months）

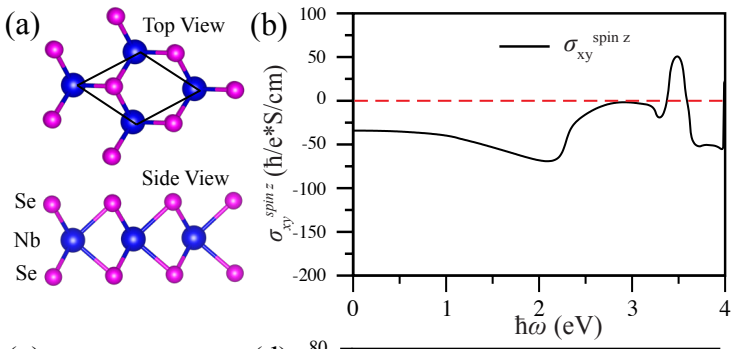
◆ **Summary of the research outcome** （approx. 2,500 words）

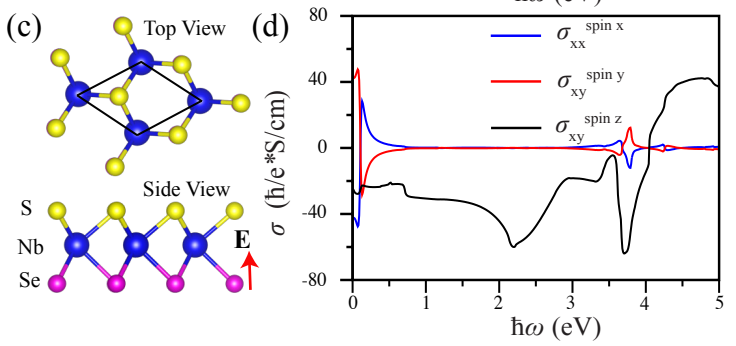
Please write down the outcomes in detail regarding the research theme above.

Introduction: Two-dimensional (2D) materials have emerged as a revolutionary platform for next-generation spintronic devices due to their unique electronic, optical, and spin-related properties. Materials like transition metal dichalcogenides (TMDs) with 2H phase have emerged as promising materials for spintronic applications due to their strong spin-orbit coupling (SOC), broken inversion symmetry, and valley-dependent spin dynamics, long spin lifetimes, and tunable band structures, making them ideal candidates for efficient spin transport and manipulation. One of the most energy-efficient approaches to controlling spin in TMDs is through light-driven spintronics. This process allows for ultrafast and non-dissipative spin manipulation, making it an ideal method for green energy source, low-power spintronic devices. Using first-principles calculations, we explore the effect of SOC in metallic $NbSe_2$ and NbSSe systems to generate pure spin current in presence of photons.

Project-1: Metallic $NbSe_2$ (see Fig. a) has been shown, both theoretically and experimentally, to possess an Ising-type SOC field. Due to this Ising-type SOC, spins in $NbSe_2$ align in the out-of-plane direction. This alignment leads to opposite spin splitting at the K and K` high-symmetric time-reversal points. Therefore, electrons at K and K` can be distinguished using the spin index. This opposite spin splitting results in a finite spin Berry curvature (SBC).

Now, if we apply an in-plane electric field, the finite SBC results in spin current in the transverse direction. Furthermore, we explore this finite SBC for spin current generation using light. We find that monolayer $NbSe_2$ exhibits high spin current conductivity at an incident photon energy of around 2-3 eV (see Fig. b).





Project-2: Monolayer Janus NbSSe (see Fig. c) exhibits both Ising- and Rashba-type SOC, due to the broken in-plane inversion symmetry and out-of-plane mirror symmetry, respectively. Similar to the $NbSe_2$, Ising-type SOC leads to out-of-plane spin alignment and opposite spin splitting at K and K`points in NbSSe. Whereas, Rashba-type SOC leads to spin-momentum locking, enabling spin splitting at the center of the Brillouin zone. Although, Ising-type and Rashba-type spin splitting occur in different energy scale. We calculate SBC and found a finite value for both out-of-plane (S_z)and in-plane (S_x and S_y) spin components. Consequently, we have computed the spin current conductivity for both out-of-plane and in-plane spin components and present the results in Fig. d. Spin currents due to S_x and S_y exhibit a peak at a photon energy of 0.1 eV, which corresponds to the energy where Rashba spin splitting occurs.

Publications:

(1) "Optically Generated Spin Current in Two-Dimensional Metallic 2H-MX_2 (M = Nb and Ta and X = S and Se): Role of Anisotropic Spin Splitting" **S. Adhikary** and K. Wakabayashi, *J. Phys. Chem. C*, **128**, 34, 14514-14521 (2024).

(2) "Spin current generation in two-dimensional Janus NbSSe using light: A first principle study" **S. Adhikary**, T. Kameda and K. Wakabayashi, *Communicated* (2025).

(3) "Light-Triggered Disordered-to-Ordered Phase Transition with Ultralong Giant Persistent Photoconductivity" K. Sakaushi, W. S. Lee, **S. Adhikary**, H. Un, Y. Matsushita, H. Sirringhaus, K. Wakabayashi, K. Tsukagoshi, and H. Nishihara, Will be published (2025).

(4) "Strain Effects on Electronic Properties Cobalt-Based Coordination Nanosheets" K. Nishigomi, Y. Yi, **S. Adhikary**, K. Tsukagoshi and K. Wakabayashi, *Under Review* (2025).

Conferences:

(1) 79th Annual Meeting (Sept. 2024), The Physical Society of Japan (Oral Presentation) (Hokkaido University)

(2) MNC 2024, Sponsored by The Japan Society of Applied Physics (Poster Presentation), (Kyoto, Nov. 2024)

(3) CREST, トポロジー領域 合同セミナー Kyoto Institute of Technology (Poster Presentation), (Kyoto Nov. 2024)

(4) The 72nd JSAP Spring Meeting 2025, (Tokyo University of Science, Noda Campus, March 2025) (Oral Presentation)

Deadline : Within two months after finishing the research period.

Sabbatical leave with grant: Submit this report to President with confirmation by the dean of school you belong to.

※Postdoctoral fellow is required to submit this report with confirmation by the dean of graduate school before the end of employment period.

Where to submit : Organization for Research and Development and Outreach (NUC)

◆We put this report on the web of KGU. If there is any problem about it because of difficulties on your research, please let us know.